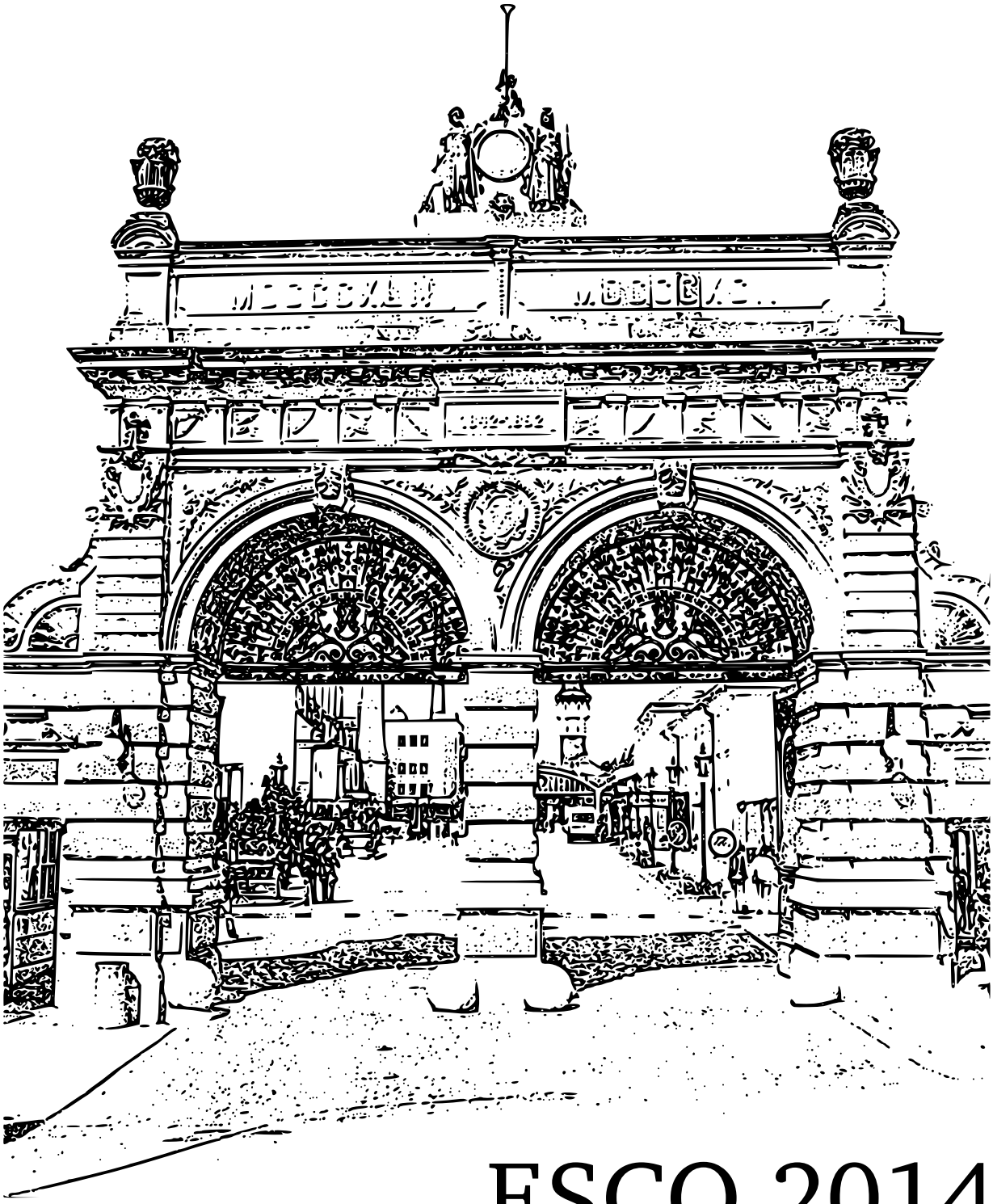

ESCO 2014

This is a joint publication of the University of Nevada (Reno, USA), University of West Bohemia (Pilsen, Czech Republic), Czech Technical University (Prague, Czech Republic), Institute of Thermomechanics (Prague, Czech Republic), and FEMhub Inc (Reno, USA).

ESCO 2014
4th European Seminar on Computing

Editors:	Pavel Solin (University of Nevada, Institute of Thermomechanics)
	Lukáš Koudela (University of West Bohemia)
Publisher:	University of West Bohemia
	Univerzitní 8, 306 14 Plzeň
	Czech Republic
Year:	2014

Contact Information

Mailing address:
ESCO 2014 Conference
FEMhub Inc.
5490 Twin Creeks Dr.
Reno, NV 89523
U.S.A.
E-mail: esco2014@femhub.com
Web page: http://esco2014.femhub.com/
Phone: 1-775-848-7892

ESCO 2014

4rd European Seminar on Computing, Pilsen, Czech Republic, June 15 - 20, 2014

Main Thematic Areas

Interdisciplinary computational projects, Multiphysics coupled problems, Higher-order computational methods, GPU computing, Cloud computing, Computing with Python and Octave, Open source projects.

Application Areas

Computational electromagnetics, Civil engineering, Nuclear engineering, Mechanical engineering, Nonlinear dynamics, Fluid dynamics, Climate and weather modeling, Computational ecology, Wave propagation, Acoustics, Geophysics, Geomechanics and rock mechanics, Hydrology, Subsurface modeling, Biomechanics, Bioinformatics, Computational chemistry, Stochastic differential equations, Uncertainty quantification, and others.

Scientific Committee

- Valmor de Almeida (Oak Ridge National Laboratory, Oak Ridge, USA)
- Zdenek Bittnar (Faculty of Civil Engineering, CTU Prague)
- Alain Bossavit (Laboratoire de Genie Electrique de Paris, France)
- John Butcher (Auckland University, New Zealand)
- Antonio DiCarlo (University Roma Tre, Rome, Italy)
- Ivo Dolezel (Czech Technical University, Prague, Czech Republic)
- Stefano Giani (University of Nottingham, UK)
- Mahdi Homayouni (Azad University, Isfahan, Iran)
- Pavel Karban (University of West Bohemia, Pilsen, Czech Republic)
- Darko Koracin (Desert Research Institute, Reno, USA)
- Dmitri Kuzmin (University of Erlangen-Nuremberg, Germany)
- Stephane Lanteri (INRIA, Sophia-Antipolis, France)
- Jichun Li (University of Nevada, Las Vegas, USA)
- Shengtai Li (Los Alamos National Laboratory, Los Alamos, USA)
- Alberto Paoluzzi (University Roma Tre, Rome, Italy)
- Francesca Rapetti (University of Nice, France)
- Sascha Schnepp (Technical University of Darmstadt, Germany)
- Stefan Turek (Technical University of Dortmund, Germany)

Organizing Committee

- Pavel Solin (University of Nevada, Reno & Institute of Thermomechanics, Prague)
- Pavel Karban (University of West Bohemia, Pilsen)
- Lukas Koudela (University of West Bohemia, Pilsen)
- Jaroslav Kruis (Czech Technical University, Prague)
- Pavel Kus (University of West Bohemia, Pilsen)
- Sascha Schnepp (ETH Zurich, Switzerland)

ESCO 2014 Sponsors

Table of Contents

I Abstracts of Keynote Lectures

Multiphysical Computations of Electrical Machines Using FEM 21
Oszkár Bíró

From Damage Model to Transport Properties in Concrete 22
Frédéric Dufour

Shape, Homology, Persistence, and Stability 23
Herbert Edelsbrunner

Reduced Order Modeling for Nonlinear Evolution Equations 24
Jean-Frédéric Gerbeau

Is 2.44 Trillion Unknowns the Largest Finite Element System That Can Be Solved Today? . . . 25
Ulrich Rüde

II List of Participants

Simulating Realistic Traffic Flow in a Smart City 29
Gabriel Aguilera-Venegas

Solution of the Heat Equation in Spheroidal Wave Functions 30
Rajai Alassar

Simulating Additive Manufacturing Processes With a 3D Free Surface Lattice Boltzmann Method 31
Regina Ammer

Fast MATLAB Assembly of FEM Matrices in 2D and 3D: Edge Elements 32
Immanuel Anjam

Energy Utilization for CO2 Capture in the Cement Industry 33
Udara Arachchige

On the Computation of Resonances in Exterior Helmholtz Problems with a Frequency-dependent Material Response. 34
Juan Carlos Araujo-Cabarcas

Improved Accuracy for Time-Splitting Methods for the Solution of Parabolic Equations 35
Andrés Arrarás

Benchmarks for an Implementation of Parareal in the C++ Domain Specific Embedded Language STELLA 36
Andrea Arteaga

Numerical Modeling of Crack Problem in Axisymmetric Geometry: The Case of Adhesive Lap Joints 37
Franck Assous

Harmonic Mappings Related to the M-fold Starlike Functions 38
Melike Aydogan

Buoyancy Driven Flows with SPH Method: Application to Real and Boussinesq Flows 39
Samiullah Baig

Melting and Solidification Using the SPH Method 40
Samiullah Baig

Groundwater Flow Parameter Identification Using Flow and Transport Models 41
Aleš Balvín

Parallel Multiphysics Simulations of Charged Particles in Microfluidic Flows 42
Dominik Bartuschat

Valorization of Petroleum Loads by Thermal Process 43
Nourredine Ben Tahar

Synthesis of Local Catalysts and There Application for Catalytic Processes 44
Nourredine Ben Tahar

Multi-time-step Domain Decomposition Algorithms for Evolution Problems 45
Michal Benes

The Impact of the Masonry Temperature During Restoration to the Thermal Stress of Historic Masonry 46
Pavel Beran

Semi-analytical Static Aeroelastic Analysis and Response of Flexible Subsonic Wings - Including 3D Aerodynamics 47
Marco Berci

Multiscale Simulation Using Lagrangian Particles 48
Xin Bian

Efficient Simulation of Time Dependent Thermal Fluid-Structure Interaction 49
Philipp Birken

Lattice Boltzmann Study of the Drag Correlation for Dilute and Moderately Dense Fluid-particle Systems 50
Simon Bogner

Approximate Riemann Solver for Shallow Water Equations in Horizontal Centrifugal Casting of Work Rolls 51
Jan Bohacek

Modeling of SiNx Thin Films Growth Process Using Kinetic Monte Carlo Method 52
Adil Bouhadiche

Dihedral Angle Sums of Nonobtuse Simplices 53
Jan Brandts

Density Functional Calculations for Small Molecules Using a Combined LCAO (Linear Combination of Atomic Orbitals) and Finite Element Basis Set 54
Moritz Braun

Modeling Water Flow in Fractured Porous Media Using Non-compatible Meshes of Different Dimension. 55
Jan Brezina

Comparison of Discontinuous Galerkin Time Integration Schemes for the Solution of Flow Problems With Deformable Domains 56
Ondřej Bublík

Application of Markov Chain Monte Carlo Method to Retrieve Initial Conditions 57
Zbigniew Bulinski

Comparison of Frequency Domain and Time Domain Model of a Distributed Power Supplying System With Active Power Filters 58
Dawid Bula

Immersed-boundary Lattice Boltzmann Method for Simulation of Incompressible Viscous Flows Around Moving Objects 59
Jun Cao

Conformance Criteria for Validation of Target Volume Surface Reconstructed From Delineation 60
Bartosz Chaber

A-phi Finite Element Method With Composite Grids for a Transient Eddy Current Problem . . 61
Tao Chen

Multi-level Decoupling of Coupled Free Flow With Porous Media Flow Systems 62
Prince Chidyagwai

A Random Set Approach Applied to the Definite Integration of Uncertain Functions Determined by a Low Number of Measurements 63
Jan Chleboun

Mortar FEs on Overlapping Meshes : Application to Magnetodynamics 64
Alexandra Christophe

On 0/1 Polytopes With Nonobtuse Triangulations. 65
Abdullah Cihangir

Numerical Analysis of Wave Propagation in Reissner-Mindlin Phononic Plates 66
Robert Cimrman

A Pendulum With a 2D-continuum Cord 67
Homero De La Fuente

A Fuzzy-Genetic Algorithm for Makespan Reduction in Job Shop Environments With Sequence-Dependent Setup Time and Re-entrant Work Flow 68
Negin Dehghanian

A New Predictive Solar Radiation Numerical Model 69
Felipe Díaz

Critical Angles of Approximation Methods of Boundary Integral Equations 70
Victor Didenko

A New, Very Efficient Initialization Mechanism for Analog Self-Organizing Neural Networks Implemented in the CMOS Technology 71
Rafał Długosz

A Novel Recursive Algorithm Used to Model the Hardware Programmable Neighborhood Mechanism of the Self-Organizing Neural Networks 72
Rafał Długosz

Anisotropic Hp-adaptive Discontinuous Galerkin Method for Numerical Solution of Partial Differential Equations 73
Vit Dolejsi

Optimization of Parallel Path Magnetic Technology Actuator 74
Jiří Doubek

Linear-Scaling Hartree-Fock Exchange and Hybrid XC Functionals With Plane-Wave Basis Set Accuracy 75
Jacek Dziedzic

Partition of Unity Methods for Approximation of Point Water Sources in Porous Media 76
Pavel Exner

Selection of Appropriate Risk-based Maintenance Strategy by Using Fuzzy Analytical Hierarchy Process 77
Mohammad Ferdousmakan

Mathematical Modeling of Coupled Conductive and Radiative Heat Transfer in Polymeric Foams 78
Pavel Ferkl

Modeling of Polaron States in Classical Molecular Chains at Finite Temperatures 79
Nadezhda Fialko

Fast Poisson Solver PoisFFT and Its Application to Turbulence Modelling 80
Vladimír Fuka

CFD Simulation of Interaction Between Fluid and Vibrating Profile 81
Petr Furmánek

Numerical Simulation of Flows Through Experimental Turbine Cascade 82
Jiří Fürst

A Portable Knowledge Based System for Car Breakdown Evaluation 83
José Luis Galán-García

A Genetic Algorithm and an Exact Algorithm for Classifying the Items of a Questionnaire Into Different Competences 84
José Luis Galán-García

A Posteriori Error Estimates for Nonconforming Approximation of Multiple Eigenvalues 85
Francesca Gardini

Space-time Finite Element Method for the Magma-rock Interaction Problem 86
Deepak Garg

Solving an Elliptic Eigenvalue Problem via Automated Multi-Level Substructuring and Hierarchical Matrices 87
Peter Gerds

High-Order/hp-Adaptive Multilevel Discontinuous Galerkin Methods 88
Stefano Giani

PoliMIce: A Open Simulation Framework for Three-dimensional Ice Accretion 89
Giulio Gori

Particle Simulations on NVIDIA GPUs 90
Nicolin Govender

Solving Systems of Differential Equations by Algebrizability of Vector Fields in $\Re^3$. 91
María Esther Grimaldo Reyna

Algebrizability of Planar Vector Fields 92
María Esther Grimaldo Reyna

A Posteriori Estimates for Interior Penalty Discontinuous Galerkin Eigenvalue/eigenfunction Approximations. 93
Luka Grubisic

Grid Convergence for Adaptive Simulations of Three-dimensional Normal Drop Impacts Onto Liquid Films 94
Paola Brambilla

Hardware Accelerated Neural Computing in Embedded Systems 95
Karol Gugała

Image Local Descriptor Matching Coprocessor for Embedded Systems 96
Karol Gugała

Large Scale Simulations of Rigid Fiber Suspensions 97
Katarina Gustavsson

On Approximation of Parametric Eigenvalue Problems 98
Harri Hakula

Numerical Simulation of Circumferentialy Averaged Flow in a Multistage Turbine 99
Jan Halama

Coupled Code System for Nuclear Reactor Fuel Loading Optimization 100
Milan Hanuš

FLLOP: A Novel Massively Parallel QP Solver 101
Václav Hapla

Molecular Dynamics Simulations in Engineering 102
Hans Hasse

Sensitivity Analysis of a FEM Model and Its Use in Material Identification 103
Jan Heczko

Development of a Fuzzy Logic Controller for Variable Quality Control Charts 104
Seyed Mahdi Homayouni

Automatic Differentiation for Matlab With ADiMat 105
Alexander Hück

Probabilistic Estimation of Material Parameters Based on a Set of Experimental Curves 106
Eliška Janouchová

The Hybridized Numerical Methods for PDEs 107
Youngmok Jeon

Fully Discrete $A - \phi$ Finite Element Method for Maxwell's Equations With Nonlinear Conductivity 108
Tong Kang

New Behaviour Emulation for Autonomous Self-learning Agent. 109
Igor Karoń

Numerical Computation of Flow Noise Around a Circular Cylinder Using LES 110
Karthik Karunakaran

Modeling the Propagation of Electromagnetic Waves in Human Retina: Numerical Analysis and Simulations 111
Maryam Khaksar Ghalati

To Problem of Dynamic Compression (Expansion) of Spherical Cavity in VIiscous Incompresible Liquid 112
Alexey Kiselev

Simulation of Plasmonic Nanostructures With the Nonlinear Quantum Hydrodynamic Model . 113
Ueli Koch

Heterogeneous Parallel Method for the Construction of Multi-dimensional Smoothing Splines 114
Igor Kohanovsky

Multisensor Data Fusion Using Neural Networks 115
Krzysztof Kolanowski

Scale Separation in Fast Hierarchical Solvers for Discontinuous Galerkin Methods 116
Lukas Korous

Numerical Simulation of the Fluid-Structure Interaction Between an Elastic Body and Compressible Flow by the Space-Time Discontinuous Galerkin Method 117
Adam Kosík

High-speed Rotation Induction Heating in Thermal Clamping Technology 118
Lukas Koudela

Coupled Thermo-hydro-mechanical Model for Concrete Structures 119
Tomáš Koudelka

Morphing Algorithm for Building Individualized 3D Skeleton Model From CT Data 120
Zuzanna Noemi Krawczyk

Algorithms for Coupled Non-linear Thermo-Mechanical Analysis of Building Structures 121
Tomas Krejci

The (3+1)- Dimensional Discontinuous Galerkin Trefftz Method 122
Fritz Kretzschmar

On Angle Conditions in the Finite Element Method 123
Michal Krizek

Complete Proposal and Optimization of Nonlinear Actuator Based on Higher-Order Finite Element Analysis and Evolutionary Algorithms 124
Petr Kropík

Discrete Element Model of Coagulation of Emulsions 125
Martin Kroupa

Coupling of Mechanical Damage With Moisture Transport 126
Jaroslav Kruis

Coupled Heat Transport and Darcian Water Flow in Freezing Soils 127
Lukáš Krupička

Probabilistic Modelling of Heterogeneous Materials Based on Image Analysis 128
Anna Kučerová

An Algorithm of Delaunay-like Surface Points Triangulation 129
Jan Kucwaj

Solving the Nonlinear Richards Equation Model with Adaptive Domain Decomposition 130
Michal Kuraz

Determination of the Optimum Pair of Values of Radii of a Full-Height Dielectric Sample of Annular Cross-Section in a Coaxial Resonant Cavity for Measurement of the Dielectric Constant 131
Roman Kushnin

Evaluation of miniMax Criterion in Constrained Design Domains 132
Matěj Lepš

Comparison of Adaptively Updated Surrogate Models for Reliability Analysis 133
Matěj Lepš

Analysis of the Impact of Interpolator's Order on the Accuracy of Electric Current Spectrum Estimation Method in the Presence of Noise 134
Michał Lewandowski

An Adjoint-based Numerical Method to Recover the Medium Properties From Seismic Data . . 135
Wenyuan Liao

An Uniform Approach to Bound Eigenvalues of Self-adjoint Differential Operators 136
Xuefeng Liu

Computing Morava K-theory Euler Characteristics for P-groups 137
Alexander Lomadze

Optimization of Parameters in SDFEM for Different Spaces of Parameters 138
Petr Lukas

A Computational Approach to Quantifying the Uncertainty in Prior Assumptions for Linear Inverse Problems 139
Aaron Luttman

Benchmarking and Quantifying Uncertainty in Surface Velocities Calculated From Photonic Doppler Velocimetry 140
Aaron Luttman

The Estimation of Parameters of Hydrological Model BILAN Using the SCDE for Monthly Simulation of Hydrological Balance 141
Petr Maca

Simulation of Multiple Particle Movement in Electromagnetic Field 142
František Mach

Time Series and Countable Banach Space Techniques 143
Ivo Marek

Dynamic Load Balancing in Lattice Boltzmann Solver MUSUBI With Complex Spacer Geometry in Electrodialysis 144
Kannan Masilamani

Solving Richards Equation With Adaptive Schwarz Type Domain Decomposition and Smoothed Prolongators 145
Petr Mayer

Solution of Inverse Problem for Segmented Capacitance Sensor 146
Petr Mayer

Optimization of Location-Routing Problem for Cross-Docks in Urban Waste Collection Network Considering Stochastic Supply and Demand 147
Sajjad Mazaheri

Flat-based Control of Variable Speed Wind Turbines 148
Abderrahmen Mechter

Metadomotic Optimization Using Genetic Algorithms 149
Salvador Merino

New BEM-based Library Aimed at HPC and Its Applications 150
Michal Merta

Numerical Modeling of Induction Heating of Low-Temperature Casting Metals 151
Kateřina Mizerová

Algebraic Flux Correction Schemes for High-Order B-Spline Based Finite Element Approximations 152
Matthias Möller

Trend and Fractality Assessment of Mexico's Stock Exchange 153
Javier Morales

Flow Behavior and Heat Transfer Model for a Mixture of Gas and Particles Inside Cyclone Separators. 154
Javier Morales

Neural Forecast Model of Electricity Demand With Up to One Day Lead Time 155
Omid Motlagh

Possibilities for Improvement in Calculations for 2D Coupled Problems in Electrical and Thermal Field 156
Lubomír Musálek

Stabilized Finite Element Methods for Stokes-Darcy Problems 157
Kamel Nafa

Numerical Study of Water Entry of 3D Rigid Wedge Under Free Fall 158
Vinod V. Nair

Numerical Modeling of Aluminium Foam on Two Scales 159
Jiří Němeček

Adaptive Mesh Refinement in Lattice Boltzmann Simulations 160
Philipp Neumann

HPC Optimization for Challenging Engineering Problems 161
Ales Nevaril

SAR Variation in a Human Head Due to Intrinsic Resonances 162
Denys Nikolayev

Modelling and Simulation of an Unshielded Stripline 163
Denys Nikolayev

A DG Implementation of a Novel Hybrid RANS/LES Technique With RANS Reconstruction . 164
Michele Nini

Modeling of Crosstalk Phenomenon for Electro-Magnetic Systems by Bilateral Coupling of PDAEs 165
Helia Niroomand Rad

Parameter Polyoptimization of PSS2A Power System Stabilizers Operating in a Multi-machine Power System Including the Uncertainty of Model Parameters 166
Adrian Nocoń

Breaking Periodicity in Simulation of Microstructured Materials 167
Jan Novák

Stochastic Finite Element Methods With Spectral Element Basis Functions 168
Saulo Pomponet Oliveira

Numerical Approximation of Fredholm Integral Equations by Orthogonal Wavelets 169
Saulo Pomponet Oliveira

Analysis of an Augmented Mixed Finite Element Method for the Stokes-Darcy Coupled Problem 170
Ricardo Oyarzua

Spread Spectrum Modulation Based on Strongly Nonlinear System With Chaotic Behaviour . . 171
David Pánek

A Computational Framework for Cochain Calculus 172
Alberto Paoluzzi

Probabilistic Assessment of Failure Risk of the Building Envelope Thermally Insulated From the Inside 173
Jan Pasek

Numerical Simulation of the Temperature Impacts on the Structural Integrity of the Stone Temples in Angkor, Cambodia 174
Jan Pasek

Compensation Based on Active Power Filters – the Cost Minimization 175
Marian Pasko

Parallel Profiling of Water Distribution Networks Using the Clément Formula 176
Guilherme Peretti Pezzi

Minimizing Control Error of the Basic PID Controller Using the Grey System's Theory 177
Janusz Pochmara

Behavior of Magnetorheological Fluid Under Alternating Magnetic Field 178
Petr Polcar

Flows in 3D Channel With Vibrating Walls 179
Petra Pořízková

Numerical Modelling of Viscous and Viscoelastic Fluids Flow for Generalized Newtonian and Oldroyd-B Fluids 180
Vladimír Prokop

Solution to Maxwell Equations in Axisymmetric Singular Domains 181
Irina Raichik

Comparisons Between a Local Multigrid Method and H-Adaptive Methods in Solid Mechanics 182
Isabelle Ramière

A Boundary Integral Approach to Compute Resonances in Open N-disk Systems 183
Francesca Rapetti

Thermofluiddynamical Numerical Simulations of Particle-laden Flows in (Bio) Chemical Fluidized Bed Reactors 184
Cornelia Rauh

Numerical Simulation of Under-expanded Jets of Dense Gases With an Adaptive Finite Volume Method 185
Barbara Re

Analytical Threeshold Voltage Model Considering Quantum Size Effects for Nanocrystalline Silicon Thin Film Transistors 186
Riad Remmouche

Sequentially Optimal Sensor Placement in Thermoelastic Models 187
Ilka Riedel

Multiscale Models of Liver Perfusion Based on Computational Homogenization 188
Eduard Rohan

A Bayesian Approach to Linear and Nonlinear Identification Problems 189
Bojana Rosic

Turning a Serial Forward Code Into a Parallel Inverse Code 190
Mohammad Ali Rostami

Mesh Generation Using Dynamic Sizing Functions 191
Florian Rudolf

Automatic Finite Volume Discretizations Through Symbolic Computations 192
Karl Rupp

3D Simulation of the Water Storage Process in the Feathers of Sandgrouses 193
Alexander Rüttgers

Parallel Simulator for Decentralized Trustworthy Computing System 194
Bartosz Sawicki

Multistep Time Integration Solver for Stiff Bioheat Equation 195
Bartosz Sawicki

A Periodic Basis System of the Smooth Interpolation Space 196
Karel Segeth

Adaptive Step-size Control in Obreshkov Predictor–Corrector Pairs 197
Pavla Sehnalová

Optimal Experimental Design With the EFCOSS Framework 198
Ralf Seidler

Comparison Between CFD and XFOIL Predictions for High Lift Low Reynolds Number Airfoils 199
Miguel Silvestre

BDDC for Mixed-Hybrid Formulation of Flow in Porous Media With Combined Mesh Dimensions 200
Jakub Šístek

High Performance Scientific Computing @cs.pub.ro 201
Emil Slusanschi

Analysis of Wind Induced Aramid Anchor Cable Using a Simplified Fluid-Structure Interaction Method 202
Robert Soltys

Modeling Transport Processes in Fractured Porous Media With Discontinuous Galerkin Method 203
Jan Stebel

Energy Transmission, Reactive Power and Stability of Nonlinear Systems 204
Milan Stork

Form Finding and Analysis of Inflatable Dams 205
Matthew Streeter

Modeling of Heat and Mass Transfer in Supercritical Geothermal Systems 206
Mario-Cesar Suarez-Arriaga

On Numerical Simulations of Fluid-Structure Interactions: Modelling of Gust Response 207
Petr Sváček

Training Algorithm for Stochastic Model of Biological Neural Network 208
Aleksandra Świetlicka

Modeling of Salt Crystallization in Historical Mortars 209
Jan Sýkora

Immune Optimal Design of 2-D and 3-D Structures 210
Miroslaw Szczepanik

Intelligent Optimization of Reinforced Structures 211
Miroslaw Szczepanik

Computational Challenges in Simulating ETMAs 212
Walerian Szyszkowski

Molecular Dynamics on 146 000 Cores 213
Nikola Tchipev

Pattern Recognition Using the Likelihood Function of Multiple Change-Points 214
Victor Tercero Gomez

A Local Discontinuous Galerkin Method for (Non) Isothermal Flow With Phase Transitons . . . 215
Lulu Tian

preCICE - a Library for Partitioned Fluid-Structure Interaction on Massively Parallel Systems 216
Benjamin Uekermann

Answering Reachability Queries on Streaming Graphs 217
Gulay Unel

SPH Simulation of 2D Driven Turbulence 218
Alireza Valizadeh

A Conceptual Design Approach to the Development of an Open-Rack Structure for Miniload AS/RS Based on Biomimetics 219
Mohammadreza Vasili

Turbulent Transition Modeling Through Mechanical Considerations 220
Rui Vizinho

Computational Modeling of Real Structures Made of Strain-hardening Cement Composites . . . 221
Jan Vorel

Comparison of Deterministic and Probabilistic Approaches to Identify the Dynamic Moving Load of a Reinforced Concrete Beam 222
Julien Waeytens

Some Algebra and Geometry Characteristics of Rational Space Curves of Type (1,1,d-2) 223
Haohao Wang

On the Use of Multiple Heterogeneous Devices to Speedup the Execution of a Computational Model of the Human Immune System 224
Rodrigo Weber dos Santos

Parallel and Adaptive Algorithms for Cardiac Electrophysiology Simulations 225
Rodrigo Weber dos Santos

A Flexible Material Database for Computational Science and Engineering 226
Josef Weinbub

High Order Space-Time Finite Element Schemes for Viscodynamic Wave Equations With Application to Stenosis Diagnosis 227
John Whiteman

Unsteady Optimal Control Problems Arising From Chemical Processes 228
Hamdullah Yücel

Multiscale Simulations of Copper Defects in High External Electric Fields 229
Vahur Zadin

Application of Multiphysics and Multiscale Simulations to Optimize Industrial Wood Drying Kilns 230
Vahur Zadin

Impact Force Reconstruction and Localization on Thin-walled Composite Structure 231
Robert Zemčík

Two Dimensional Integration Simulation of Indirect Drived Laser Fusion 232
Chuanlei Zhai

Wind Tunnel Blockage and Three-dimensional Effects in Wind Tunnel Testing of Ice Accretion Over Airfoils and Wings 233
Marta Zocca

Solution to Microstructural Fields Based on Schur Complement Method and Wang Tiles 234
Lukáš Zrůbek

P-Multigrid Technique for the Numerical Solution of Algebraic Systems Arising From the Discontinuous Galerkin Discretization of PDEs 235
Andrej Živčák

Part I

Abstracts of Keynote Lectures

Multiphysical Computations of Electrical Machines Using FEM

Oszkár Bíró
Graz University of Technology
biro@tugraz.at

Abstract

Coupled electromagnetic, mechanical, acoustic and thermal problems arising in electrical machines are simulated using computational techniques. The interaction between magnetic and structural mechanical systems is demonstrated by a finite element structural investigation of the end-winding deformations of a turbo-generator. The multiphysical treatment of acoustical problems is illustrated by weakly coupled electromagnetic, structural dynamic and acoustic simulations. Finally, a procedure based on computational fluid dynamics for acquiring the convective heat transfer coefficients is presented in order enable coupled electro-thermal finite element simulations. This work has been supported by the Christian Doppler Research Association (CDG) and by the ELIN Motoren Gmbh

References

1. B. WEILHARTER AND O. BÍRÓ AND H. LANG AND S. RAINER. Computation of the Noise Radiation of an Induction Machine Using 3D FEM/BEM. COMPEL 30 (2011) 1737-1750.
2. M.HETTEGGER AND O. BÍRÓ AND B. STREIBL AND H. NEUDORFER. Measurements and Simulations of the Heat Transfer on End Windings of an Induction Machine. COMPEL 30 (2011) 1727-1736.

From Damage Model to Transport Properties in Concrete

Frédéric Dufour, Mohamad Ezzedine El Dandachy, Matthieu Briffaut
Univ. Grenoble Alpes
frederic.dufour@3sr-grenoble.fr,
mohamad.ezzedineeldandachy@3sr-grenoble.fr,
matthieu.briffaut@3sr-grenoble.fr

Abstract

In engineering practice, the durability of concrete structures is usually dealt with crack opening. Furthermore, for confinement structures, the leakage rate under service loads must be assessed to estimate the structural performance. The advanced numerical modelling of cracking in reinforced concrete structures may be dealt with either by means of advanced discontinuous models (e.g., X-FEM) or using continuous constitutive models. The issue of this contribution is to propose two numerical modelling to get leakage rate through a concrete specimen and validate them against experimental results. In both methods, the first step is to model the cracking by means of the Mazars damage model regularised by the stress based nonlocal approach (Giry et al, 2011) which provides a very realistic damage field at failure. Then, the two approaches are distinct. A first possibility is to assess the crack path either using a topological search (Bottoni et al, 2014) or the global tracking algorithm (Dufour et al, 2012). Once the crack path is estimated, along the discretised crack surface, the opening can be computed by equivalence with a strong discontinuity approach (Dufour et al, 2008). These first three steps allow to assess crack properties as in discontinuous models with a rather good estimation against experimental results (Giry et al, 2014). The final step is to prescribe the Poiseuille's law along the crack surface to estimate the leakage rate. The second method is directly based on the damage field assuming a relation between damage and permeability as in Pijaudier-Cabot et al (2009). In this case, the permeability is obtained at any integration point and is used to compute the leakage rate point wise in the volume rather than along a surface as in the first method. Clearly the first method must be used only when a macrocrack is clearly developed. In opposite, the second approach can be used for any damage level. The validation of both approaches against experimental results is performed on the leakage rate perpendicular to the disk of a splitting test under loading.

References

1. C. Giry and F. Dufour and J. Mazars. Modified nonlocal damage model based on stress state influence. IJSS., 48 (25-26), 3431-3443 (2011).
2. M. Bottoni and F. Dufour and C. Giry. Topological search of the crack pattern from a continuum mechanical computation. Eng. Struct. (2014).
3. F. Dufour and G. Legrain and G. Pijaudier-Cabot and A. Huerta. Estimate of crack opening from a 2D continuum-based FE computation. IJNAMG (2013).
4. F. Dufour and G. Pijaudier-Cabot and M. Choinska and A. Huerta. Extraction of a crack opening from a continuous approach using regularized damage models. Comp. & Conc., 5 (4), 375-388 (2008).
5. C. Giry and C. Oliver-Leblond and F. Dufour and F. Ragueneau. Cracking analysis of reinforced concrete structures. EJECE (2014).
6. G. Pijaudier-Cabot and F. Dufour and M. Choinska. Permeability due to the increase of damage in concrete: from diffuse to localised damage distributions. JEM, Vol. 135, 9, p. 1022-1028 (2009).

Shape, Homology, Persistence, and Stability

Herbert Edelsbrunner
IST Austria
edels@ist.ac.at

Abstract

My personal journey to the fascinating world of geometric forms started 30 years ago with the invention of alpha shapes in the plane. It took about 10 years before we generalized the concept to higher dimensions, we produced working software with a graphics interface for the 3-dimensional case, and we added homology to the computations. Needless to say that this foreshadowed the inception of persistent homology, because it suggested the study of filtrations to capture the scale of a shape or data set. Importantly, this method has fast algorithms. The arguably most useful result on persistent homology is the stability of its diagrams under perturbations.

References

1. HERBERT EDELSBRUNNER. Shape, Homology, Persistence, and Stability. NA.

Reduced Order Modeling for Nonlinear Evolution Equations

Jean-Frédéric Gerbeau, Damiano Lombardi, Elisa Schenone
INRIA and UPMC Paris 6
jean-frederic.gerbeau@inria.fr, damiano.lombardi@inria.fr,
elisa.schenone@inria.fr

Abstract

The increasing power of computers allows to address more and more complex models for real-world applications. Nevertheless, the need to solve reduced order models still exist in many situations: real-time solution, rapid prototyping, PDE solvers for mobile devices, fast evaluation of cost functions for optimization problems, *etc*. Several methods exist to approximate the solutions of PDEs with a reduced number of degrees of freedom (Reduced Basis Methods, Proper Orthogonal Decomposition, , *etc*). But time-dependent problems dominated by transport or propagation phenomena remain a challenge for reduced-order modelling.

The purpose of this talk will be to introduce a new reduced-order modelling approach to solve nonlinear evolution partial differential equations. It is based on approximations of generalized Lax pairs. Contrary to other reduced-order methods, the basis on which the solution is searched for evolves in time according to a dynamics specific to the problem. It is therefore well-suited to solving problems with progressive front or wave propagation. Another difference with other reduced-order methods is that it is not based on an off-line / on-line strategy.

The method will be illustrated on various problems, including Korteweg-de Vries, Fisher-Kolmogorov and equations used in cardiac electrophysiology for the simulation of electrocardiograms.

References

1. J-F. GERBEAU AND D. LOMBARDI . Approximated Lax Pairs for the Reduced Order Integration of Nonlinear Evolution Equations". J. Comput Phys. 265 (2014) 246-269.

Is 2.44 Trillion Unknowns the Largest Finite Element System That Can Be Solved Today?

Ulrich Rüde
FAU Erlangen-Nürnberg
ulrich.ruede@fau.de

Abstract

Supercomputers have progressed beyond the Peta-Scale, i.e. they are capable to perform in excess of 10^{15} operations per second. However, these systems are massively parallel and have a heterogeneous architecture that presents many challenges for developing suitable algorithms and software. Only hierarchical algorithms with asymptotically optimal efficiency can exploit the potential of extreme scale computing. However, mathematically optimal algorithms are not necessarily fast. I will present parallel multigrid based solvers for FE problems with beyond a trillion unknowns that are designed to achieve "textbook efficiency". A trillion elements is e.g. enough to discretize the whole volume of planet with a global resolution of about 1 km. Since the compute times are around 1 minute for computing a single solution, these algorithms can still be used reasonably within an implicit time stepping procedure or a nonlinear iteration.

References

1. BJÖRN GMEINER AND TOBIAS GRADL AND FRANCISCO GASPAR AND ULRICH RÜDE . Optimization of the multigrid-convergence rate on semi-structured meshes by local Fourier analysis. Computers and Mathematics with Applications, 65(4) pp. 694-711, 2012.
2. BJÖRN GMEINER AND ULRICH RÜDE AND HOLGER STENGEL AND CHRISTIAN WALUGA AND BARBARA WOHLMUTH. Towards Textbook Efficiency for Parallel Multigrid. Submitted to: Numerical Mathematics Theory, Methods and Applications.

Part II

List of Participants

Simulating Realistic Traffic Flow in a Smart City

Jose Luis Galán-García, Gabriel Aguilera-Venegas, María Á. Galán-García, Pedro Rodríguez-Cielos
Dept. Applied Mathematics. University of Málaga
jlgalan@uma.es, gabri@ctima.uma.es, magalan@ctima.uma.es, prodriguez@uma.es

Abstract

Dijkstra's algorithm [1] is one of the most well known algorithm to solve the shortest path problem (SPP). When applied to real situations, although the shortest path can be computed with Dijkstra's algorithm, it is not always the chosen one. In traffic situations, for example, the driver may not know the shortest path to follow. Even more, although the driver knows the shortest one, he/she may prefer choosing another path.

There are different studies [2-4] where extensions of Dijkstra's algorithm are used when the lengths of edges are no fixed. These extended versions of Dijkstra's algorithm can be adapted in order to simulate real situations in traffic. However, another approach consists of considering fixed lengths on edges and introducing some variations simulating the drivers' behaviours.

In this work we present a modification on the Dijkstra's algorithm in order to simulate real situations in which the shortest path is not always chosen. As an example of application, we will extend the ATISMART model [5], introduced in FEMTEC 2013, where an accelerated-time simulation of car traffic in a smart city was described. In this previous work, all cars in the system used the Dijkstra's algorithm to choose the shortest path from their inputs to their exits.

In this talk, the extended model ATISMART$^+$ for traffic flow simulation in smart cities is presented. This model includes more realistic situations considering different drivers' behaviours.

As for the previous model, the implementation of ATISMART$^+$ is carried out using a Computer Algebra System (CAS), specifically MAXIMA, together with a graphic user interface, developed in JAVA.

References

1. E. W. DIJKSTRA. A note on two problems in connexion with graphs. Numerische Mathematik 1 (1959) 269-–271.
2. Y. DENGA AND Y. CHENB AND Y. ZHANGA AND S. MAHADEVANC. Fuzzy Dijkstra algorithm for shortest path problem under uncertain environment. Applied Soft Computing 12(3) (2012) 1231–1237.
3. WANG SHU-XI. The Improved Dijkstra's Shortest Path Algorithm and Its Application. Procedia Engineering 29 (2012) 1186-1190.
4. SATHI MUKHERJEE. Dijkstra's Algorithm for Solving the Shortest Path Problem on Networks Under Intuitionistic Fuzzy Environment. J Math Model Algor 11(4) (2012) 345–359.
5. J. L. GALÁN-GARCÍA AND G. AGUILERA-VENEGAS AND P. RODRÍGUEZ-CIELOS. An Accelerated-Time Simulation for Traffic Flow in a Smart City. J. Comput. and Appl. Math. (2013). http://dx.doi.org/10.1016/j.cam.2013.11.020.

Solution of the Heat Equation in Spheroidal Wave Functions

Rajai Alassar
King Fahd University of Petroleum & MInerals
alassar@kfupm.edu.sa

Abstract

The solution of the heat equation on a spheroidal geometry is presented using two methods. In the first, we implement the spheroidal wave functions as basis. Separating the heat equation in spheroidal coordinates results in two equations which are satisfied by the Angular Wave Functions and the Radial Wave Functions. These functions are also known as the spheroidal harmonics. This name originates from the fact that as the oblateness parameter vanishes, the angular functions, which apart from normalization and phase factors, are essentially the popular spherical harmonics. The second solution is numerical in which we expand the temperature in the angular direction in terms of Legendre functions and then solve the resulting set of differential equations in the radial direction using an implicit finite difference scheme. The two solutions are compared and verified against the limiting case of a sphere.

References

1. G. ARFKEN. Mathematical Methods for Physicists. 3rd ed. Orlando, FL: Academic Press, 1985.
2. P. MOON AND AND D.E. SPENCER. Field Theory for Engineers. Princeton, NJ: Van Nostrand, 1961..
3. P.M. MORSE AND AND H. FESHBACH. Methods of Theoretical Physics, Part I. New York: McGraw-Hill, 1953.
4. M. ABRAMOWITZ AND I. A. STEGUN. Handbook of Mathematical Functions. 9th ed. New York: Dover, 1970.

Simulating Additive Manufacturing Processes With a 3D Free Surface Lattice Boltzmann Method

Regina Ammer
Friedrich-Alexander University Erlangen-Nürnberg
regina.ammer@fau.de

Abstract

Additive manufacturing processes like electron beam melting (EBM) produce complex metallic structures layer by layer from metal powder. Especially EBM opens many new opportunities for aircraft manufacturers as well as for producers of medical implants. However, until now the parts cannot manufactured at sufficient speed to make them economically viable for any but specific very high value applications.

In order to speed up the build time and quality of EBM products a thorough understanding of the beam-powder interaction is gained by three-dimensional (3D) [1,2] numerical simulations. For the numerical discretization we use a multi-speed Lattice Boltzmann approach with a volume-of-fluid based free surface method. Our model regards hydrodynamic effects, like melt flow, capillarity and wetting, as well as thermal effects, like beam absorption, melting and solidification. In order to take account the high computational costs of 3D simulations the implementation is carefully parallelized [3] and optimized and the most relevant simulations are done on state-of-the-art supercomputers.

The numerical results were validated against real experimental data where size and surface structure of the melt pool as well as its lifespan and temperature are concerned. The good agreement of numerical and experimental results show the high potential of the LB approach to understand and explore complex processes like EBM. It also justifies the development of new strategies by numerical simulations to accelerate and improve the EBM building process. These enhanced manufacturing strategies will be presented and new modeling ideas how evaporation pressure can be included into the model will be shown.

References

1. C. KÖRNER AND E. ATTAR AND P. HEINL. Mesoscopic simulation of selective beam melting processes.. J. Mater. Process. Tech. 211 (2011) 978 .
2. R. AMMER AND M. MARKL AND U. LJUNGBLAD AND C. KÖRNER AND U. RÜDE. Simulating fast electron beam melting with a parallel thermal free surface lattice Boltzmann method.. Comput. Math. Appl 67 (2014) 318 - 330 .
3. M. MARKL AND R. AMMER AND U. LJUNGBLAD AND U. RÜDE AND C. KÖRNER. Electron Beam Absorption Algorithms for Electron Beam Melting Processes Simulated by a Three-Dimensional Thermal Free Surface Lattice Boltzmann Method in a Distributed and Parallel Environment.. Procedia Comput. Sci. 18 (2013) 2127 .

Fast MATLAB Assembly of FEM Matrices in 2D and 3D: Edge Elements

Immanuel Anjam
University of Jyväskylä, Finland
immanuel.anjam@jyu.fi

Jan Valdman
University of Ostrava, Czech Republic
jan.valdman@vsb.cz

Abstract

Based on ideas of the paper of T. Rahman and J. Valdman [1] we propose an effective and flexible way to assemble finite element stiffness and mass matrices in MATLAB for problems discretized by edge finite elements. Typical edge finite elements are Raviart-Thomas used in discretizations of H(div) spaces and Nedelec elements in discretizations of H(curl) spaces. The major loops in the code have been vectorized using the so called array operation in MATLAB, and no low level languages like the C or Fortran have been used for the purpose. The implementation is based on having the vectorization part separated, in other words hidden, from the original code thereby preserving its original structure, and its flexibility as a finite element code. The code is fast and scalable with respect to time.

References

1. T. RAHMAN AND J. VALDMAN. Fast MATLAB assembly of FEM matrices in 2D and 3D: nodal elements. Applied Mathematics and Computation 219(13): 7151-7158, 2013.

Energy Utilization for CO2 Capture in the Cement Industry

Udara Arachchige
Telemark University College, Porsgrunn, Norway
udaraspra@gmail.com

Abstract

The concentration of the atmospheric carbon dioxide (CO2) has risen with the impact of the industrial revolution. The atmospheric CO2 concentration is calculated as 380 ppmv approximately [1]. One of the main reason for global warming is a huge impact of usage of fossil fuel based power plants for energy generation. The cement industry flue gas is considered for this study. The flue gas data and other necessary information for model development are taken from the literatures. The flue gas capture model is developed in Aspen Plus simulation software. The CO2 capture model is previously has developed by the author and used for this study as well [2]. The same flue gas data are taken for the consideration [2]. The high energy penalty in the re-generation process is the main disadvantage with CO2 capture plant. The minimization of the amount of energy required in the stripper column is important. Therefore, heat integration plays a vital role in process optimization with carbon capture. The available excess heat in the cement manufacturing process is calculated. The amount of energy available in the process is around 18MW for developed base case. The dimensions of the required waste heat boiler are calculated. The main idea of the calculation is to evaluate the required surface area of the cooling tubes to exchange the available heat in the flue gas.

References

1. INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE (IPPC). Summary for policymakers. In: Climate Change 2007: The Physical Science Basis. Cambridge University Press, 2007..
2. ARACHCHIGE U.S.P.R. AND KAWAN D. AND TOKHEIM L.A. AND MELAAEN M.C. Impact of kiln thermal energy demand and false air on cement kiln flue gas CO2 capture. International journal of energy and environment, 5-1, 45-52, 2014..

On the Computation of Resonances in Exterior Helmholtz Problems with a Frequency-dependent Material Response.

Juan Carlos Araujo-Cabarcas, Christian Engström
Umeå University
juan.araujo@math.umu.se, christian.engstrom@math.umu.se

Abstract

Energy peaks are of fundamental importance in the study of wave propagation in open domains. The localization of these peaks is closely related to the scattering resonances [1].

In this talk, we approximate resonances by using a discontinuous Galerkin method together with a perfectly matched layer (PML) [2]. The problem corresponds to a highly non-normal operator with a large pseudospectrum, which on the discrete level cause spurious eigenvalues. High order curvilinear elements are therefore used to decrease the number of spurious eigenvalues.

The eigenvalue problem is in our setting linear if the material parameters are independent of the spectral parameter. However, the material response is generally frequency-dependent resulting in nonlinear spectral problems. We study cases with a rational dependence on the spectral parameter and the use of a PML layer then preserves the rational structure after discretization. We employ a linearization technique [3] and a Krylov subspace method to solve the resulting linearized eigenvalue problem.

References

1. M. Lenoir and M. Vullierme-Ledard and C. Hazard. Variational formulations for the determination of resonant states in scattering problems. SIAM J. Math. Anal., vol. 23, pp. 579–608, May 1992.
2. S. Kim and J. E. Pasciak. The computation of resonances in open systems using a perfectly matched layer. Math. Comput., vol. 78, no. 267, pp. 13751398, 2009.
3. Y. Su and Z. Bai. Solving rational eigenvalue problems via linearization. SIAM J. Matrix Anal. Appl., vol. 32, pp. 201–216, Mar. 2011.

Improved Accuracy for Time-Splitting Methods for the Solution of Parabolic Equations

Andrés Arrarás, Laura Portero
Departamento de Ingeniería Matemática e Informática, Universidad Pública de Navarra
andres.arraras@unavarra.es, laura.portero@unavarra.es

Abstract

We consider the numerical solution of parabolic equations of the form

$$u_t - Au = f,$$

supplemented with suitable initial and boundary conditions. Here, A is a second-order elliptic differential operator.

If $Au = \nabla \cdot (k\nabla u)$, with $k(\mathbf{x})$ uniformly positive, locally one-dimensional (LOD) methods (such as alternating direction and fractional step schemes) are well-known alternatives to classical implicit time-stepping procedures that lead to faster numerical algorithms. Nevertheless, such LOD methods often introduce a large splitting error that degrades the effectiveness of the resulting algorithms. In [1] and [2], the authors propose a modification of the right-hand side of certain LOD approaches which virtually eliminates this splitting error. The additional computational cost required by this procedure is less than ten per cent of the cost of the original LOD algorithm.

In this work, we extend the previous technique to more general parabolic problems involving an elliptic operator $Au = \nabla \cdot (K\nabla u)$, where $K(\mathbf{x})$ is a symmetric and positive definite full tensor. For that purpose, two different strategies are investigated. The first one is based on the use of alternating direction methods that explicitly handle the mixed derivative terms (cf. [3]). In the second approach, we study domain decomposition time-splitting techniques (cf. [4]), which can also be applied on non-Cartesian grids. Computational results illustrate the behaviour of the proposed algorithms.

References

1. T. ARBOGAST AND C.-S. HUANG AND S.-M. YANG. Improved accuracy for alternating-direction methods for parabolic equations based on regular and mixed finite elements. Math. Models Methods Appl. Sci. 17 (2007) 1279-1305.
2. J. DOUGLAS JR. AND S. KIM. Improved accuracy for locally one-dimensional methods for parabolic equations. Math. Models Methods Appl. Sci. 11 (2001) 1563-1579.
3. K.J. IN 'T HOUT AND B.D. WELFERT. Unconditional stability of second-order ADI schemes applied to multi-dimensional diffusion equations with mixed derivative terms. Appl. Numer. Math. 59 (2009) 677-692.
4. T.P. MATHEW AND P.L. POLYAKOV AND G. RUSSO AND J. WANG. Domain decomposition operator splittings for the solution of parabolic equations. SIAM J. Sci. Comput. 19 (1998) 912-932.

Benchmarks for an Implementation of Parareal in the C++ Domain Specific Embedded Language STELLA

Andrea Arteaga, Daniel Ruprecht, Rolf Krause
Università della Svizzera Italiana USI
andrea.arteaga@env.ethz.ch, daniel.ruprecht@usi.ch,
rolf.krause@usi.ch

Abstract

As modern supercomputers demand an ever growing degree of parallelism, concurrency becomes a critical property also of numerical methods. In recent years, time-parallel methods have become an interesting and more and more widely studied extension of classical, serial time marching schemes. Parareal, introduced in (Lions et al., 2001), is a popular method of this type. There exists a number of studies investigating its mathematical properties and performance for different kinds of applications, but very few works address and compare specifically its implementation on state-of-the-art hardware.

The talk will present first an implementation of Parareal in combination with a finite difference discretization in space for the advection-diffusion equation, using the C++ domain-specific embedded language (DSEL) STELLA (Gysi et al., 2014) for stencil evaluations. A number of benchmarks on the newly installed Cray XC30 "Piz Daint" at the Swiss National Supercomputing Centre are reported. The multi-functional backend of the stencil library allows to compare runtimes and speedup on different hardware: Spatial stencils can e.g. be executed either on multiple CPUs in a node using multi-threading or on the NVIDIA® Tesla® K20X GPU available at each node of "Piz Daint". The talk will discuss how the choice of hardware can affect Parareal's performance. It will also comment on the impact of e.g. direct communication between GPUs and the use of asynchronous communication strategies to overlap communication with computation. Furthermore, other important issues like energy consumption are addressed.

References

1. T. GYSI AND O. FUHRER AND C. OSUNA AND T. SCHULTHESS. STELLA: A DSEL library for performance portable implementation of stencil computations on structured grids. In preparation, 2014.
2. J.-L. LIONS AND Y. MADAY AND G. TURINICI. A "parareal" in time discretization of PDE's. Comptes Rendus de l'Académie des Sciences - Series I - Mathematics, 2001.

Numerical Modeling of Crack Problem in Axisymmetric Geometry: The Case of Adhesive Lap Joints

Franck Assous
Ariel University & Bar-Ilan University, Israel
franckassous@netscape.net

Michael Michaeli, Anatoly Golubchik
IMI, Ramat Hasharon 47100, Israel
michael.michaeli@gmail.com, anatoly.golubchik@gmail.com

Abstract

In this work, we propose a fast and accurate numerical method to compute stress fields near a crack tip. We consider the case of dissimilar materials, mainly when a crack is located at the interface between different materials, that is material with different elastic properties. As it is well known, the presence of cracks - as the presence of reentrant edge or corners on the boundary, called *singularities*, can create singular fields, i.e. unbounded fields in their neighborhood. This makes such problems difficult to solve accurately, and standard numerical methods need to be modified to handle such difficulties. Based on our previous work [1], we derive a new variational formulation, which provides the solution in terms of displacements field in the case of a crack existence, for an axisymmetric domain. We develop the implementation of our method in the case of stress fields calculations in tubular adhesive lap joints between circular tubes, where the thickness of the lap joint can be much smaller than the thickness of the circular tubes. Numerical examples will be shown to illustrate the efficiency of the approach. The case of a crack in a domain made of several different layers will also be considered.

References

1. F. ASSOUS AND M. MICHAELI AND A. GOLUBCHIK. Numerical Method for Stress fields Calculation in Dissimilar Material With Interface Crack. Appl. Numer. Maths 67 (2011) 187-203.

Harmonic Mappings Related to the M-fold Starlike Functions

Melike Aydogan
Işık University
melike.aydogan@isikun.edu.tr

Yasar Polatoglu
Istanbul Kultur University
y.polatoglu@iku.edu.tr

Yasemin Kahramaner
Istanbul Ticaret University
ykahramaner@iticu.edu.tr

Abstract

In the present paper we will give some properties of the subclass of harmonic mappings which is related to m-fold starlike functions in the open unit disc $\mathbb{D} = \{z||z| < 1\}$. Throughout this paper we restrict ourselves to the study of sense-preserving harmonic mappings. We also note that an elegant and complete treatment theory of the harmonic mapping is given in Duren's monograph [1]. The main aim of us to investigate some properties of the new class of us which represented as in the following form, $S^*H(m) = \left\{ f = h(z) + \overline{g(z)} | f \in SH(m), \frac{g'(z)}{h'(z)} \prec b_1 p(z), h(z) \in S^*(m), p(z) \in P^{(m)} \right\}\Big\}$. where $h(z) = z + \sum_{n=1}^{\infty} a_{mn+1} z^{mn+1}$, $g(z) = \sum_{n=0}^{\infty} b_{mn+1} z^{mn+1}$, $|b_1| < 1$.

References

1. P. DUREN. Univalent Functions. Grundiehren der Mathematischen Wissenchafter. Vol. 259, Springer-Verlag, New York, (1983).
2. P. DUREN. Harmonic Mappings in the Plane. Cambridge Tracts in Mathematics. Vol. 156, Cambridge University Press, Cambridge UK, (2004).
3. S. FUKUI AND K. SAKAGUCHI. An extension of a theorem of S.Ruscheweyh. Bull. Fac. Ed. Wakayama Univ. Natur. Sci. No:29, (1980), 1-3.
4. A. W. GOODMAN. Univalent Functions. Vol. I and Vol. II, Mariner publishing Co. Inc. , Tampa Fl, (1983).
5. I. GRAHAM AND G. KOHR. Geometric function theory in one and higher dimensions. Pure and Applied Mathematics, A Dekker series Monographs and Textbooks, (2003).

Buoyancy Driven Flows with SPH Method: Application to Real and Boussinesq Flows

Samiullah Baig, Andreas Ludwig, Menghwai Wu
Montan university , A-8700 Leoben, Franz-Josef street 18,Austria, office@unileoben.ac.at
samiullah.baig@unileoben.ac.at, ludwig@unileoben.ac.at,
office@unileoben.ac.at

Abdellah Kharicha
Montan University , A-8700 Leoben, Franz-Josef street 18,Austria, office@unileoben.ac.at
abdellah.Kharicha@notes.unileoben.ac.at

Abstract

We present a study of simulation buoyancy driven flow using a particle method. The particle method used is Smooth Particle Hydrodynamics, which has matured into a unified numerical technique for a variety of flow problems. The method is mesh free, which makes its implementation much easier than mesh based methods. The nature of the numerical issues encountered in a mesh free method, such as SPH are different from FVM or FEM methods. We identify the numerical issues related to incompressible buoyancy driven flow. The test case is a 2D closed vessel filled with a fluid which exchanges heat with the fixed walls. There are two specific regimes we consider a Boussinesq approximation and a general one. The method developed for general regime can deal with density variations much larger than the variations encountered in Boussinesq flows. The implementation is in CUDA/C on GPU. The results for test cases are compared with FVM based solver FLUENT in terms of accuracy and speedup.

References

1. J.J. MONAGHAN. Simulating Free Surface Flows with SPH. J. Comput. Phys. 110 (1994) 399-406.
2. F. ARISTODEMO AND I. FEDERICO AND P. VELTRI AND A. PANIZZO . Two Phase SPH Modeling of Advective Diffusive Processes. Environmental Fluid Mechanics 10(2010)451-470.
3. K.SZEWC UNDEFINED AND J. POZORSKI AND A.TANIERE UNDEFINED. Modeling of Natural Convection with Smooth Particle Hydrodynamics Non-Boussinesq Regime. International Journal of Heat and Mass Transfer 54(2011)4807-4816.

Melting and Solidification Using the SPH Method

Abdellah Kharicha
Montan University , A-8700 Leoben, Franz-Josef street 18,Austria, office@unileoben.ac.at
abdellah.Kharicha@notes.unileoben.ac.at

Samiullah Baig, Andreas Ludwig, Menghwai Wu
Montan university , A-8700 Leoben, Franz-Josef street 18,Austria, office@unileoben.ac.at
samiullah.baig@unileoben.ac.at, ludwig@unileoben.ac.at,
office@unileoben.ac.at

Abstract

Particle methods have gained a reputation for simulating a wide variety of flows, both single phase and multiphase. The problem of using these mesh free methods for simulating solidification has not been addressed satisfactorily. The issues and complexities can be compounded in the presence of more than one phase and flow. We present a mathematical model and a CUDA based Smooth Particle Hydrodynamics(SPH) numerical scheme for the solidification of a fluid in a confined vessel, the fluid being driven by buoyancy due to temperature differences. The scheme uses the inherent features of the WCSPH i.e. the Weakly Compressible SPH to model the phase change from liquid to solid. The solidified part is modelled to deform according to laws of solid mechanics. This is done to simulate the effect of temperature variations on the deformation of the solidified part of the mold. The results are compared with experiments.

References

1. J.J. MONAGHAN. Simulating Free Surface Flows with SPH. J. Comput. Phys. 110 (1994) 399-406.
2. F. ARISTODEMO AND I. FEDERICO AND P. VELTRI AND A. PANIZZO. Two Phase SPH Modeling of Advective Diffusive Processes. Environmental Fluid Mechanics 10(2010)451-470.
3. K.SZEWC AND J. POZORSKI AND A.TANIERE. Modeling of Natural Convection with Smooth Particle Hydrodynamics Non-Boussinesq Regime. International Journal of Heat and Mass Transfer 54(2011)4807-4816.
4. B. SOLANTHALER AND J. SCHLAFLI AND R. PAJAROLA. A Unified Particle Model for Fluid-Solid Interaction. Computer Animation and Virtual Worlds 18(2007)69-82.

Groundwater Flow Parameter Identification Using Flow and Transport Models

Aleš Balvín
Technical University of Liberec & Czech University of Life Sciences Prague
ales.balvin@tul.cz

Milan Hokr
Technical University of Liberec
milan.hokr@tul.cz

Michal Kuráž
Czech University of Life Sciences Prague
kuraz@fzp.czu.cz

Abstract

The aim of this study is to evaluate different numerical flow and transport models in geological environment of particular locality (water supply tunnel, Berdichov, Czech Rep.).

We considered three model configurations with different dimensions and complexity: 1) two-dimensional models, 2) three-dimensional models with fracture and without real surface, 3) three-dimensional model with real surface geometry, fractures and natural borders. The flow models were calibrated to real measured flow rates and the transport models were fitted to residence time estimated from concentration of natural isotopes. We evaluate hydraulic conductivity and porosity and we compare it with real laboratory measurement.

Model concept and numerical scheme are based on combination of 2D discrete fractures and 3D equivalent continuum. The models were computed in the FLOW123D open source simulation code [1], which has been developed at the Technical university of Liberec. The flow equation is solved by the mixed-hybrid finite element method. The advective transport equation is solved by the finite volume method, with upwind weighting and explicit time steps and to compare with implicit discontinuous Galerkin method.

References

1. O. SEVERYN AND M. HOKR AND J. KRALOVCOVA AND J. KOPAL AND M. TAUCHMAN. Flow123D: Numerical Simulation Software for Flow and Solute Transport Problems in Combination of Fracture Network and Continuum. Technical report, Technical University of Liberec, Liberec, Czech Republic, 2008..
2. M. HOKR AND I. SKARYDOVA AND D. FRYDRYCH. Modelling of tunnel inflow with combination of discrete fractures and continuum. Comput. Vis. Sci. 15 (1) (2012), 21-28..

Parallel Multiphysics Simulations of Charged Particles in Microfluidic Flows

Dominik Bartuschat, Ulrich Rüde
Friedrich-Alexander University Erlangen-Nürnberg
dominik.bartuscaht@cs.fau.de, ulrich.ruede@fau.de

Abstract

Computer simulations incorporating and coupling multiple physical effects rapidly gain importance in science and engineering. However, the high computational complexity of such multiphysics simulations often requires the use of parallel supercomputers when realistic scenarios are studied.

We present parallel multiphysics simulations of charged particles in electrokinetic flows. These simulations couple three different physical effects: Rigid body dynamics of individual particles represented with full geometrical resolution, fluid flow modeled by a two-relaxation-time lattice Boltzmann algorithm [1], and electric potential represented by a finite volume discretization. For solving the partial differential equation that models the electric potential, a cell-centered multigrid algorithm has been implemented [2]. The LBM and the rigid body simulation are coupled by means of the momentum exchange method [3] with a four-way interaction developed in [4]. The fully parallelized algorithms are implemented in the WALBERLA software framework.

We describe the overall simulation algorithm and its components, together with different simulation setups. To show the physical correctness of our simulations, we present validations for various model parameters. Finally, we show the parallel scaling behavior of the algorithm on an advanced high performance computer.

References

1. I. GINZBURG AND F. VERHAEGHE AND D. D'HUMIERES. "Two-relaxation-time lattice Boltzmann scheme: About parametrization, velocity, pressure and mixed boundary conditions". Commun. Comput. Phys. 3 (2008), 427-478.
2. D. BARTUSCHAT AND D. RITTER AND U. RUEDE. "Parallel multigrid for electrokinetic simulation in particle-fluid flows". in "High Performance Computing and Simulation (HPCS). Madrid 2012", IEEE (2012), pp. 374-380.
3. D. YU AND R. MEI AND L.-S. LUO AND W. SHYY. "Viscous flow computations with the method of lattice Boltzmann equation". Prog. Aerosp. Sci. 39 (2003), 329-367.
4. J. GÖTZ AND K. IGLBERGER AND C. FEICHTINGER AND S. DONATH AND U. RÜDE. "Coupling multibody dynamics and computational fluid dynamics on 8192 processor cores". Parallel Comput. 36 (2010), 142-141.

Valorization of Petroleum Loads by Thermal Process

Nourredine Ben Tahar
M'hamed Bougara Universty
nbentahardz@yahoo.fr

Hadj Mimoun
M'hamed Bougara Universty
hmimon@yahoo.fr

Abstract

This research was performed in order to allow the study of the chemical composition influence of the coking process load on the efficiency and the quality of coke. For this reason, the coking of the following loads was realized: Atmospheric residue (RAT), vacuum Residue (RSV) and catalytic Residue of cracking (RCC). (The residues are obtained from an Algerian crude oil).As the oil residues are rich for their strongly polar composition, such as the asphaltene resins, and complex structures units (SCU), which has a role in the formation of coke, and as the dispersion of these latter improves the quality of coke, a study on the stability of aggregation was carried out by the addition of one stabilizer (oil Extract) in the coking process load. The Compounding (Extracted from /RCC oil) has been derived to the best efficiency of coke. The study consists of the influence, this is characterized by the analyses Infra-red (IR) and x-ray diffraction (XRD).

References

1. V. SIMANZHENKOV AND R. IDEM. Crud oil chemistry. CRC Press, 2003, pp 337-344.

Synthesis of Local Catalysts and There Application for Catalytic Processes

Nourredine Ben Tahar
M'Hamed Bougara University
nbentahardz@yahoo.fr

Abstract

Solid catalysts for petroleum refining and catalytic transformations have been developed starting from local Algerian materials, mainly "bentonite". These catalysts are used for the transformation of the heavy fractions and the residues of the oil by the catalytic processes leading to obtaining clean and environmentally friendly petrol (fuel) as well as petroleum fractions that are considered as important raw materials for petrochemical, pharmaceutical, and cosmetic industry. The preparation of modified catalysts using Algerian local bentonite enriched by oxides to give them a better performance for the validation of certain fractions of oil and condensate is described.

References

1. H. MIMOUN AND G. OTMANINE. lecturers at University. .
2. P. WUITHIER. Chemical Engineering. Paris 1972.
3. MICHEL GUISNET RAMO AND FERNANDO RIBEIRO. an Nanoworld The Zeolites Service of Catalysis. EDP Sciences, Paris 2006.
4. M. MILLAN. Pillared clays as catalysts for hydrocraking of heavy liquids fuels. Applied Catalysis 2005.
5. G. ROTHENBERG. Catalysis Concepts and Green Applications. Wiley-VCH Verlag GmbH & Co. in Weinheim, Germany 2008 .

Multi-time-step Domain Decomposition Algorithms for Evolution Problems

Michal Benes
Czech Technical University in Prague
benes@mat.fsv.cvut.cz

Abstract

We present the asynchronous multi-domain time integrators with a dual domain decomposition method for the initial boundary-value problems for parabolic equations. Time integration schemes, based on the generalized trapezoidal family of methods, are constructed for the parabolic equation and implemented into a variational finite element framework. For efficient parallel computing, we use the dual domain decomposition method with local Lagrange multipliers to ensure the continuity of the primary unknowns at the interface between subdomains. The α-method for time discretization and the multi-domain spatial decomposition enable us to use different types of integrators (explicit vs. implicit) and different time steps on different parts of a computational domain, and thus efficiently capture the underlying physics with less computational effort. The energy conservation of our asynchronous integration scheme is investigated using the Energy method. We illustrate the performance of proposed multi-domain time integrators by means of several examples.

References

1. THOMAS J. R. HUGHES. The Finite Element Method: Linear Static and Dynamic Finite Element Analysis. Dover Publications, 2000.

The Impact of the Masonry Temperature During Restoration to the Thermal Stress of Historic Masonry

Pavel Beran
Centre of Excellence Telč, Institute of Theoretical and Applied Mechanics of the Academy of Sciences of the Czech Republic, 19000 Praha 9, Prosecká 76, Czech Republic
beran@itam.cas.cz

Abstract

Historical buildings are usually created from ancient masonry. Durability of these historical buildings is based on durability of masonry which degrades by several reasons. During the typical degradation cumulative process the mortar is crumbled from the joints between stones. During restoration the empty edges of joints are usually filled by the new (repair) mortar. In general, the material characteristics of mortar and stone (brick) may be different in many aspects. The aim of restorer is application of compatible mortar [1]. The objective of this paper is to detect the dependence of thermal stress in historic heterogeneous masonry on the temperature during restoring. The dependence of values of thermal stress in masonry on temperature during renovation was obtained by means of 3-D finite element model. This model represents the block of ashlar masonry between exterior and interior. The south-western wall was selected because in this kind of wall is the highest thermal gradient during summer in Prague in Czech Republic. The numerical analysis is coupled problem and was divided into two steps. The first one is the transient heat transfer analysis [2] by which the impact of solar radiation and the changes of air temperatures during real climatic conditions in Prague were simulated. The temperature fields obtained from the heat transfer analysis are the loadings of the model during the computation of stress. The computation of stress is the second step of analysis. The masonry was modelled during stress analysis as the heterogeneous material. The stones and the mortar in joints have different values of coefficient of thermal expansion. The data of the reference year in Prague were used as the loading of the model. From whole reference year were selected two weeks. The results indicate that the temperature during renovation significantly affects the values of the thermal stress in masonry. The temperatures during renovation could be in climatic conditions in Prague, Czech Republic in interval 5 – 30 C. The higher stress values origin when during the renovation the temperatures are near the boundary values and the absolute value of stress is highest when the temperature during renovation is 30 C. Moreover, for the typical values of thermal expansion of stone and mortar the tensile stresses originate in stones in winter. The stone blocks are usually the most historically valuable parts of the masonry. Thus, the performance of renovation in hot summer is more dangerous for historically valuable stones than during the time when the temperatures are lower.

References

1. J. J. HUGHES AND J. VÁLEK. Mortars in Historic Buildings – Review of the Conservation. Technical and Scientific Literature, Historic Scotland, Edinburgh 2003..
2. H. HENS. Building Physics – Heat, Air and Moisture, . Ernst and Sohn Verlag fűr Architektur und technische Wissenschaften GmbH und Co. KG, Berlin, 2007.

Semi-analytical Static Aeroelastic Analysis and Response of Flexible Subsonic Wings - Including 3D Aerodynamics

Marco Berci
University of Leeds
M.Berci@leeds.ac.uk

Abstract

A semi-analytical model for the combined static aeroelastic analysis and response of flexible subsonic wings is presented. The proposed model accounts for the presence of wing ailerons, so that steady manoeuvres can also be analysed and control reversal investigated, especially for the case of swept wings. A Rayleigh beam with generic distribution of wing inertia and stiffness is employed for the structural model. Three degrees of fidelity are considered for the aerodynamic modelling, accounting for three-dimensional flow effects in different ways: tuned strip theory, modified strip theory and lifting line theory; standard strip theory is also presented for comparison and completeness. Results are obtained and critically discussed for all fluid-structure interaction models, with respect relevant aerodynamic and structural parameters. The formulated modified strip theory is shown to be an excellent compromise between the low computational cost of strip theory and the high accuracy of lifting line theory; thus, it is suggested as very effective tool for the multidisciplinary design and optimisation of flexible subsonic wings.

References

1. R.L. BISPLINGHOFF AND ET. AL.. Aeroelasticity. Addison-Wesley, 1996.
2. Y.C. FUNG. An Introduction to the Theory of Aeroelasticity. Dover, 1993.
3. G.W. PETTIT. Model to Evaluate the Aerodynamic Energy Requirements of Active Materials in Morphing Wings. MSc Thesis, Virginia Polytechnic Institute and State University, 2001.

Multiscale Simulation Using Lagrangian Particles

Xin Bian, Zhen Li, George Karniadakis
Brown University
xin_bian@brown.edu, ,

Abstract

Flow phenomena with multiple spatial and temporal scales are ubiquitous in biomedical and microfluidic applications. Concurrently coupling the multiscale phenomena is a reasonable choice: simulating efficiently the bulk flow with a continuum solver, where macroscopic behavior is sufficient and resolving accurately certain small regions with a mesoscopic or microscopic method, where thermal fluctuations are significant or molecular behavior is not known a priori. This strategy stems from the domain decomposition scheme based on the classical Schwartz alternating method. We have adopted and implemented three particle methods, namely, smoothed particle hydrodynamics (SPH), (smoothed) dissipative particle dynamics (SDPD), and molecular dynamics separately, together covering a large spectrum of spatial-temporal scales. A common feature of these methods is that they are all Lagrangian mesh-free methods, all of which are based on pairwise particle interactions derived from different potentials at different scales. To accomplish multiscale coupling via domain decomposition we formulate a Lagrangian coupling framework, which is based on a Lagrangian kernel using local information within a characteristic length.

References

1. D. A. FEDOSOV AND G. E. KARNIADAKIS.. Triple-decker: interfacing atomistic-mesoscopic-continuum flow regimes. J. Comput. Phys., 228:1157–1171, 2009.

Efficient Simulation of Time Dependent Thermal Fluid-Structure Interaction

Philipp Birken
Lunds University
philipp.birken@na.lu.se

Tobias Gleim, Detlef Kuhl, Andreas Meister
University of Kassel
tgleim@uni-kassel.de, kuhl@uni-kassel.de,
meister@mathematik.uni-kassel.de

Abstract

We consider thermal fluid structure interaction to model industrial gas quenching in steel forging, where hot steel is cooled using cold high pressured gas. This allows to define properties of the finished steel part locally at low cost and without environmental problems.

For the numerical simulation, a partitioned approach via a Dirichlet-Neumann coupling and a fixed point iteration is employed. In time, previously developed efficient time adaptive higher order time integration schemes are used [1]. The respective models are the compressible Navier-Stokes equations and the nonlinear heat equation, where the parameter functions are obtained from measurements on a specific steel. To validate the method, results are compared to inhouse experiments, where a heated plate is placed in the local wind tunnel and subsequently cooled by the crossflow.

Furthermore, the use of different vector extrapolation methods for convergence acceleration techniques of the fixed point iteration is analyzed [2]. In particular, Aitken relaxation and minimal polynomial extrapolation (MPE) are considered. Finally, we consider the use of extrapolation inside the time integration scheme to find a suitable initial guess for the nonlinear systems.

References

1. P. BIRKEN AND K. J. QUINT AND S. HARTMANN AND A. MEISTER. A Time- Adaptive Fluid-Structure Interaction Method for Thermal Coupling. Comp. Vis. in Science, Vol. 13(7), 331–340, 2011.
2. A. SIDI. A Review of two vector extrapolation methods of polynomial type with applications to large-scale problems. J. Comp. Phys., Vol. 3(3), 92– 101, 2012.

Lattice Boltzmann Study of the Drag Correlation for Dilute and Moderately Dense Fluid-particle Systems

Simon Bogner, Ulrich Rüde
Universität Erlangen-Nürnberg, Lehrstuhl für Systemsimulation, Cauerstraße 11, 91058 Erlangen
simon.bogner@fau.de, ruede@fau.de

Swati Mohanti
CSIR-Institute of Minerals and Materials Technology, Bhubaneswar-751013, India
swati.mohanty@gmail.com

Abstract

With the advent of high-speed computers, gas-solid systems have become accessible to direct numerical simulation. Particle-resolved computations help to improve understanding of the phase interaction as it appears for instance in fluidized bed reactors. In this talk a numerical study of the drag on monodisperse, spherical particles in flow is presented. We apply a lattice Boltzmann method based on a two relaxation time collision operator to obtain reliable predictions of the average per-particle drag force. From these predictions a closure relation of the drag dependency on the bed density and the particle Reynolds number is obtained. We have included bed densities ranging from 0.01 to 0.35 and Reynolds numbers up to 300. At low solid volume fraction, the obtained correlation is close to the widely-used Wen & Yu – correlation.

We also compare our results to previous numerical studies: There has been reported a discrepancy between results obtained using different numerical methods, namely the comprehensive lattice Boltzmann study of Beetstra et al. (2007) and the predictions based on an immersed boundary - pseudo-spectral Navier-Stokes approach by Tenneti et al. (2011). The present study excludes significant finite resolution effects, which have been suspected to cause the reported deviations, but does not coincide exactly with either of the previous studies. This indicates the need for yet more accurate simulation methods in the future.

References

1. R. Beetstra and M. A. van der Hoef and and J. A. M. Kuipers. Drag force of intermediate Reynolds number flow past mono- and bidisperse arrays of spheres. Fluid Mechanics and Transport Phenomena, 53(2):489-501, 2007.
2. S. Tenneti and R. Garg and and S. Subramaniam. Drag law for monodisperse gas- solid systems using particle-resolved direct numerical simulation of flow past fixed assemblies of spheres. International Journal of Multiphase Flow, 37:1072–1092, 2011.

Approximate Riemann Solver for Shallow Water Equations in Horizontal Centrifugal Casting of Work Rolls

Jan Bohacek, Abdellah Kharicha, Menghuai Wu, Andreas Ludwig
University of Leoben
jan.bohacek@unileoben.ac.at, abdellah.kharicha@unileoben.ac.at,
menghuai.wu@unileoben.ac.at, andreas.ludwig@unileoben.ac.at

Abstract

A complex flow of the liquid metal spreading and solidifying inside a horizontally rotating cylindrical mold was simplified by means of the 2D shallow water equations (SWE) leading to significant computational savings. The SWE were derived in the rotating frame of reference; therefore, fictitious forces (the centrifugal force and the Coriolis force) were applied. In addition, other forces such as the bed shear force, the force of gravity, the wind shear force and forces resulting from the variable liquid/solid interface were taken into account. An approximate Riemann solver was used to calculate wave speeds with corresponding wave strengths. The Godunov's explicit updating formulas were used along with the high resolution corrections to improve the order of accuracy. All momentum source terms were treated as a stationary wave and were well-balanced for steady states. An entropy fix was applied to avoid expansion shocks. In the liquid metal, the heat advection equation was a part of the Riemann solver, whereas the heat diffusion was solved separately after each flow time step. Inside the mold and the solidifying shell, the 3D heat diffusion was solved. The speed of the liquid/solid interface was determined by fulfilling the 1D Stefan condition. Convective and radiative heat losses from free surfaces were included in the model. The mold filling was realized by a 2D Gaussian mass source. A thermal resistance was considered in contact between the mold and the solidifying shell representing the refractory material. Numerical results for a specific mold and casting parameters are shown in the present paper.

References

1. R. J. LEVEQUE. Finite volume methods for hyperbolic systems. Cambridge University Press (2002) 429-431.
2. D. L. GEORGE. Augmented Riemann solvers for the shallow water equations over variable topography with steady states and inundation. J. Comput. Phys. 227 (2008) 3089-3113.
3. J. MURILLO AND P. GARCIA-NAVARRO. Wave Riemann description of friction terms in unsteady shallow flows: Aplication to water and mud/debris floods. J. Comput. Phys. 231 (2012) 1963-2001.
4. J. A. DANTZIG AND M. RAPPAZ. Solidification. Lausanne: EPFL Press (2009) 134.

Modeling of SiNx Thin Films Growth Process Using Kinetic Monte Carlo Method

Adil Bouhadiche, Hachemi Bouridah
Laboratoire d'Etude des Matériaux, Université de Jijel BP98 Ouled Aissa Jijel 18000, Algeria
a.bouhadiche@gmail.com, hachemi.bouridah@gmail.com

Abstract

Silicon nanocrystals have attracted a great deal of attention in the last few years, because these nanomaterials are expected to exhibit a quantum size effect and therefore have a potential for application to optoelectronics. In this context, the production of the light emission from silicon nanocrystals has been widely studied in SiNx thin films. However, the properties of these films are strongly controlled by their deposition parameters (temperature, total pressure, gas flow ratio. . .). Consequently, the simulation of the deposit phase is crucial to design the material with the desired properties. In this work, we use a simulation program based on the kinetic Monte Carlo (kMC) method able to describe the deposition process of SiNx thin films obtained by low-pressure chemical vapour deposition (LPCVD) technique with a mixture of disilane (Si2H6) and ammonia (NH3). Simulation results describe well the different stages of the SiNx deposition process. Keywords: Kinetic Monte Carlo; SiNx deposit phase; amorphous silicon cluster.

References

1. J. HUANG AND G. ORKOULAS AND P. D. CHRISTOFIDES. Porosity control in thin film solar cells. Chem. Eng. Sci. 94 (2013) 44–53.
2. P. TEMPLE-BOYER AND L. JALABERT AND E. COUDERC AND E. SCHEID AND P. FADEL AND B. ROUSSET. Properties of nitrogen doped silicon films deposited by low pressure chemical vapour deposition from disilane and ammonia. Thin Solid Films 414 (2002)13–17.
3. H. BOURIDAH AND H. HAOUES AND M. R. BEGHOUL AND F. MANSOUR AND R. REMMOUCHE AND P. TEMPLE-BOYER. Study of silicon nanocrystals formation in annealed amorphous in situ nitrogen doped silicon thin films obtained by low pressure chemical vapor deposition. Acta Phys. Pol. A 121 (2012)175–177.

Dihedral Angle Sums of Nonobtuse Simplices

Jan Brandts, Abdullah Cihangir
Korteweg-de Vries Institute for Mathematics, University of Amsterdam, Netherlands
J.H.Brandts@uva.nl, A.Cihangir@uva.nl

Abstract

Although the sum of the dihedral angles of a simplex was already studied in the fifties, not many applied mathematicians can even say what is the sum of the six dihedral angles of a tetrahedron. In this presentation, we first review known results in this context, then we specialize them to the subclass of nonobtuse simplices. Nonobtuse simplices are useful in the context of triangulating computational domains in the Finite Element Method but also in pure geometry they are well known.

As main application for relations between angles and angle sums we hope to contribute towards solving the open problem whether the longest edge bisection algorithm, as a means to refine tetrahedral finite element meshes, generates only a finite number of congruence classes, as in known to be the case for triangles. Other applications may arise in the context of the One Neighbor Conjecture for nonobtuse 0/1-simplices in the context of 0/1-polytopes.

References

1. J.H. BRANDTS AND A. CIHANGIR. Dihedral Angle Sums of Nonobtuse Simplices. To be submitted to Conference Proceedings.

Density Functional Calculations for Small Molecules Using a Combined LCAO (Linear Combination of Atomic Orbitals) and Finite Element Basis Set

Moritz Braun, Dietmar Kolb
University of South Africa
moritz.braun@gmail.com, dr-kolb@web.de

Abstract

Any method, such as the density functional approach or the Hartree-Fock method, that employs effective one-particle Schrödinger-like equations to calculate the properties of molecules and incorporates all electrons, faces the challenge, that the basis set must accommodate the behaviour of the molecular orbitals in three different regimes:
1. The region close to the nuclei, where the cusp should be properly taken care of,
2. The interstitial region, where the orbitals are slowly changing and, finally,
3. The asymptotic region, where the exponential decay depending on the orbital energy must be observed.

Currently the two dominating basis sets in state of the art molecular quantum chemistry calculations are Gaussians[1] and Slater orbitals[2]. The former are very expedient for calculations but cannot in principle exactly satisfy the requirements in the first and the third region. On the other hand Slater orbitals can be chosen to exactly satisfy the requirements in regions one and three, but are computationally more demanding than Gaussians.

In the present contribution results of density functional calculations using a basis set combined from numerically determined radial atomic orbitals and finite element functions on a suitable grid of intermediate resolution for a number of small molecules are presented.

References

1. R. Ditchfield and W. J. Hehre and J. A. Pople. Self Consistent Molecular Orbital Methods. IX. An Extended GaussianType Basis for Molecular Orbital Studies of Organic Molecules. The Journal of Chemical Physics 54 (1971) 724.
2. G. Te Velde and F. M. Bickelhaupt and E. J. Baerends et al. Chemistry with ADF. Journal of Computational Chemistry, 22(2001), No. 9, 931–967.

Modeling Water Flow in Fractured Porous Media Using Non-compatible Meshes of Different Dimension.

Jan Brezina
Technical University of Liberec
jan.brezina@tul.cz

Abstract

Deep final repositories for nuclear waste are planned in rocks with low permeability, namely in granite, in order to minimize transport of a possible leakage to the surface. A regional model of water flow and transport processes in the granite has to deal with presence of relatively tiny fracture zones of significantly higher hydraulic permeability. One possible approach is to treat these fracture zones as an independent domain of lower dimension and introduce a coupling with the surrounding matrix.

In our contribution, we consider simplified model consisting of a 2d matrix domain and of a fracture domain as a network of 1d lines. We shall consider both saturated and partially saturated water flow (Richards' equation). The coupling between domains follows dual-continuum approach where the flux q from the matrix domain to the fracture domain is given as

$$q = k_{21}\big(h_{2d} - h_{1d}\big)$$

with k_{21} proportional to the smaller of hydraulic conductivities K_{2d}, K_{1d} which in turn are functions of the pressure heads h_{2d}, h_{1d} respectively.

Matrix domain is discretized by a triangular mesh while the fracture domain is discretized by an arbitrary (non-compatible) mesh of 1d lines. Equations are discretized by mixed-hybrid method using zero order Raviart-Thomas finite elements. We present a general concept how to introduce coupling between domains into mixed-hybrid formulation on non-compatible meshes using particular projection operators. We provide two examples of such projections and demonstrate application of resulting two numerical couplings on several test cases.

Proposed numerical couplings admit straight extension to the 3d-2d case however implementation of an efficient algorithm for tracking intersections of 3d and 2d elements, which is of its own interest, has yet to be finished.

References

1. V. MARTIN AND J. JAFFRÉ AND J.E.ROBERTS UNDEFINED. Modeling fractures and barriers as interfaces for flow in porous media.. SIAM Journal on Scientific Computing, 26(5):1667, 2005..
2. J. BREZINA AND M. HOKR. Mixed-Hybrid formulation of multidimensional fracture flow.. In 7th International Conference, NMA 2010, Borovets, Bulgaria, August 20-24, 2010, pp 125-132, Springer..

Comparison of Discontinuous Galerkin Time Integration Schemes for the Solution of Flow Problems With Deformable Domains

Ondřej Bublík, Jan Vimmr, Alena Jonášová
University of West Bohemia
obublik@ntis.zcu.cz, jvimmr@ntis.zcu.cz, jonasova@ntis.zcu.cz

Abstract

In recent years, the discontinuous Galerkin (DG) finite element method has become more popular for the solution of the system of Navier-Stokes equations in time-dependent domains. The success of the DG method lies in the fact that it naturally achieves stability and enables arbitrary order of spatial accuracy. Both properties are particularly difficult to combine in the case of the finite element and the finite volume methods. Another advantage of the DG method is that with suitably chosen basis functions, the DG method in the ALE formulation automatically satisfies the geometric conservation law [1]. Compared to other common methods, the main disadvantage of the DG method is the large number of unknowns, which can considerably slow down the overall computation. Therefore, to overcome this major drawback, it is necessary to use an efficient time integration scheme. The main objective of our study is to compare the computational efficiency of selected explicit and implicit time integration schemes. To eliminate the time step restriction in the case of the explicit scheme, the method is improved using the local time stepping method. The motion of the mesh is described with the help of the blending function proposed in [2]. All numerical simulations are performed on the 2D test case in the form of the flapping NACA 0012 airfoil. The effectiveness of the explicit and implicit DG methods is evaluated in terms of CPU time that is necessary for the computation to achieve the preselected simulation time.

References

1. V. T. NGUYEN. An arbitrary Lagrangian–Eulerian discontinuous Galerkin method for simulations of flows over variable geometries. , Journal of Fluids and Structures Volume 26, Issue 2, (2010), 312–329.
2. P.-O. PERSSON AND J. BONET AND J. PERAIRE. Discontinuous Galerkin solution of the Navier–Stokes equations on deformable domains. Computer Methods in Applied Mechanics and Engineering Volume 198, Issues 17–20, (2009), 1585–1595.

Application of Markov Chain Monte Carlo Method to Retrieve Initial Conditions

Zbigniew Bulinski
Institute of Thermal Technology, Silesian University of Technology, Konarskiego 22, 44-100 Gliwice, Poland
zbigniew.bulinski@polsl.pl

Helcio R.B. Orlande
Department of Mechanical Engineering, COPPE, Federal University of Rio de Janeiro, UFRJ, Cid. Universitaria, Cx. Postal 68503 Rio de Janeiro, RJ, 21941-972, Brazil
helcio@mecanica.coppe.ufrj.br

Abstract

This paper presents application of the Markov Chain Monte Carlo method to reconstruct initial temperature field based on the measurements of time dependent temperature. Temperature recordings were carried out just in a few selected sampling points of a solid slab which was cooled down. Metropolis-Hastings algorithm was coupled with commercial computational fluid dynamics (CFD) software to sample the unknown distribution of unknown initial temperature field. In the direct problem conduction in the solid material and convection at the boundary was considered. Temperature values inside each computational cell at the beginning of cooling process were considered as a unknowns. Hence, the problem is highly dimensional and as influence of initial conditions diminish quickly, it is ill-conditioned as well. Influence of prior distribution and numer of sampling points were considered and reported in the work.

References

1. Z.P. BULINSKI AND A.J. NOWAK AND K. KASZA AND L. MATYSIAK. Retrieving of the initial moisture field in porous material based on temperature measurements during drying. Inverse Problems in Science and Engineering 20, Issue 5, 2012, 691-705.
2. D. CALVETTI AND E. SOMERSALO. A Gaussian hypermodel to recover blocky objects. Inverse Problems 23, 2007, 733-754.
3. D. CALVETTI AND E. SOMERSALO. Hypermodels in the Bayesian imaging framework. Inverse Problems 24, 2008, 034013.
4. J. KIPIO AND E. SOMERSALO. Statistical and computational inverse problems. Springer Verlag, New York 2004.

Comparison of Frequency Domain and Time Domain Model of a Distributed Power Supplying System With Active Power Filters

Dawid Bula, Michal Lewandowski
Silesian University of Technology
dawid.bula@polsl.pl, michal.lewandowski@polsl.pl

Abstract

The growing complexity of modern power systems and an increasing number of the non-linear loads, has been forcing the use of more advanced methods of computer modeling and simulation. Usually, one of the two main types of electric system models are used [3], [2]: a model described in the time domain and a model described in the frequency domain. The time domain model is based on the differential or difference equations, which are solved using the numerical algorithms [3]. This approach shows the dynamics of the modeled system, but requires significant computing power, and is often used in the analysis of individual system components or a system with a small number of elements [1]. In the case where the size of the analyzed system is significant, or a large number of simulations for a variety of system parameters is performed, the frequency domain model is preferred [4]. For a nonlinear power system, this model is usually based on spectral analysis and comes down to the description of the system as a series of linear models representing the steady-state of a system separately for each harmonic. Nonlinear sources and loads are then often modeled using the current injection method [3], [4]. The frequency domain approach reduces the required computational effort needed for solving the system's equations (algebraic equations are used instead of differential equations), which is particularly important in tasks such as optimization of size and location of active power filters (APF) [4], [5]. The main disadvantage of the presented frequency domain method is a significant simplification of the system's model, and the ability to simulate only the steady-state operation of the system. This work presents a comparison of the two models of the same distributed power system. Both types of system models (time domain and frequency domain model) are described along with their implementation. Simulation results for a considered power system containing APF are included, as well as a comparison of the obtained computational effort. The research allowed to draw conclusions about the reliability of the frequency model applied to the modeling of distributed power systems containing APF.

References

1. T. Adrikowski and D. Bula and M. Pasko. Simulation of active power filter with prediction control in MATLAB and OrCAD environments with using SLPS interface. Electrical Review (Przeglad Elektrotechniczny) 2011 R. 87 no 5, pp. 1-5.
2. J. Arrillaga and N.R Watson. Power system harmonics, second edition. Wiley, England, 2003.
3. J.C. Das. Power System Analysis, Short Circuit Load Flow and Harmonics. Marcel Dekker, Inc., New York, 2002.
4. D. Grabowski and M. Maciazek and M. Pasko. Sizing of active power filters using some optimization strategies. COMPEL vol. 32, no 4, 2013, pp. 1326-1336.
5. Wang Yan-Song and Shen Hua and Liu Xue-Min and Liu Jun and Guo Song-Bo. Optimal Allocation of the Active Filters Based on the Tabu Algorithm in Distribution Network. Proceedings of International Conference on Electrical and Control Engineering ICECE 2010, 2010, pp. 1418-1421.

Immersed-boundary Lattice Boltzmann Method for Simulation of Incompressible Viscous Flows Around Moving Objects

Xixiong Guo, Jun Cao
Ryerson University, Dept. of Mechanical and Industrial Engineering
xixiong.guo@ryerson.ca, jcao@ryerson.ca

Chengwen Zhong
Northwestern Polytechnical University
zhongcw@nwpu.edu.cn

Abstract

Relevant to a large number of industrial applications, moving boundary problems have been routinely simulated using different computational fluid dynamics approaches. As a novel strategy, this study is aimed at enhancing the variant immersed-boundary lattice Boltzmann method (IB-LBM) by more seamlessly connecting the feedback model with local mesh refinement techniques, so that an enlarged class of moving boundary problems, including the interactions between flowing fluids and moving objects of engineering interests, can be numerically investigated. Owing to the utilization of both explicit and implicit schemes in the present approach, the advantages resulting from this hybrid method, such as simple principle, easy implementation, and inherent satisfaction of no-slip boundary condition for solid surfaces, are fully exhibited. The local mesh refinement procedure employed in the present approach relies on the bubble function, which requests only the spatial interpolation but no temporal interpolation. Ranging from the flows around a single cylinder of both stationary and mobile natures to the flow around bi-cylinders in motion with respect to each other, a variety of test cases performed in this study has demonstrated the accuracy of the present IB-LBM approach when compared to the results obtained by using other numerical methods. Moreover, the IB-LBM is also employed to simulate a more challenging flow associated with a flapping wing as moving object, the analysis is fully provided on the influences of the Reynolds number, flapping amplitude, and phase difference between the translation and rotation motions on the aerodynamic performance in this case, and the usefulness and effectiveness of this new approach are further revealed.

References

1. J. WU AND C. SHU. Implicit velocity correction-based immersed boundary-lattice Boltzmann method and its applications. J. Comput. Phys. 228 (2009) 1963-1979.

Conformance Criteria for Validation of Target Volume Surface Reconstructed From Delineation

Jacek Starzyński, Robert Szmurło, Bartosz Chaber, Zuzanna Krawczyk
Warsaw University of Technology
jstar@ee.pw.edu.pl, robert.szmurlo@ee.pw.edu.pl,
chaberb@iem.pw.edu.pl, zuzanna.n.krawczyk@gmail.com

Anna Zawadzka
Maria Słodowska-Curie Institute of Oncology
a.zawadzka@zfm.coi.pl

Abstract

CT or MRI datasets with delineated regions of the interest (tumor volume and normal tissue) are crucial for planning radiotherapy treatment. Accurate delineation is tedious, time consuming and often leads to significant interobserver discrepancies [Villeirs et al.].

Delineated target volumes can be processed, using a surface reconstruction algorithms, to generate a 3D surface mesh. Although the quality of reconstructed surfaces can be very high in a technical sense, the medical conformance with the real volume can be very different.

This paper describes how different conformance criteria evaluate the generated surface mesh. The analysis of the efficiency of the criteria applied to real medical data is presented. Two data sets prepared by clinical oncologists are being used.The first one are radiotherapy planning datasets with delineation of various quality. The second set contains datasets for the same patient group, but the target volumes had been delineated with extra care and are used as the reference.

In the literature the works related to the topic of this paper [Villeirs et al., Kouwenhoven et al., Anke et al.] use conformity indexes to measure similarity of two (or more) volumes based on differences in 2D dimensions delineated by different oncologists. This paper presents results of comparison of various conformance indexes in application to the automatically reconstructed surface meshes and the accurate reference delineation.

References

1. Villeirs G. M. and Van Vaerenbergh K. Interobserver delineation variation using CT versus combined CT + MRI in intensity-modulated radiotherapy for prostate cancer. Strahlentherapie und Onkologie, Current Discussion, 2005, Vol. 181, pp. 423-430.
2. Kouwenhoven E. and Giezen M. and Struikmans H. Measuring the similarity of target volume delineations independent of the number of observers. Physics in Medicine and Biology, Vol. 54, 2009, pp. 2863-2873.
3. Anke M. Van Mourik and Paula H. M. Elkhuizen and Danny Minkema and Joop C. Duppen. Multiinstitutional study on target volume delineation variation in breast radiotherapy in the presence of guidelines. Radiotherapy and Oncology, Vol. 94, 2010, pp. 286-291.

A-phi Finite Element Method With Composite Grids for a Transient Eddy Current Problem

Tao Chen, Tong Kang
Department of Applied Mathematics, School of Science, Communication University of China
chentao@cuc.edu.cn, kangtong@cuc.edu.cn

Abstract

The $A - \phi$ finite element method with fine and coarse grids (composite grids) is presented to solve a transient eddy current problem. In this method, some local domains with which are concerned can be handled conveniently by using the fast adaptive composite grid method (FAC). An optimal error estimate of the corresponding approximation has been obtained. To solve the discrete $A - \phi$ system in the global domain efficiently, we design an iteration which combines FAC with classic steepest descent. We prove that this method converges with a bounded rate independent of the mesh sizes.

References

1. J. BRAMBLE AND J. PASCIAK AND J. WANG AND J. XU. Convergence estimates for multigrid algorithms without regularity assumptions. Math. Comp. 57 (1991) 23-45.
2. T. KANG AND K. I. KIM. Fully discrete potential-based finite element methods for a transient eddy current problem. Computing 85 (2009) 339-362.
3. K. I. KIM AND T. KANG. A potential-based finite element method of time-dependent Maxwell's equations. Int. J. Computer Math. 83 (2006) 107-122.
4. S. MCCORMICK AND J. THOMAS. The fast adaptive composite grid method (FAC) for elliptic boundary value problems. Maths. Comp. 46 (1986) 439-456.
5. J. XU. Two-grid discretization techniques for linear and nonlinear PDEs. SIAM J. Numer. Anal. 33 (1996) 1759-1777.

Multi-level Decoupling of Coupled Free Flow With Porous Media Flow Systems

Prince Chidyagwai
Loyola University Maryland
pchidyagwai@loyola.edu

Abstract

We present a multi-level decoupling technique for solving coupled systems of partial differential equations arising from the modeling of free flow coupled with porous media flow. The flow in the free flow region is governed by either the Stokes or Navier-Stokes equations and flow in the porous medium is described by Darcy's Law. The model is completed by interface conditions specifying the continuity of the normal component of velocity between the free flow region and the porous medium, a balance of forces and the Beavers-Joseph-Saffman law. Coupled Navier-Stokes/Stokes with Darcy models have applications in science and engineering, for example studying filtration systems in engineering systems and modeling blood flow in biology. We present a multi-numerics scheme based on continuous finite elements to approximate the flow in the free flow region and the Discontinuous Galerkin method to approximate the flow in the porous medium. The Discontinuous Galerkin method is well-suited to approximating the solution in the porous medium due to the discontinuous permeability that arises in modeling ground-water flow and the continuous finite element provides an adequate approximation of flow in the free-flow region. The fully coupled model is computationally expensive to solve over large domains. Multi-level methods offer computational efficiency by solving the fully coupled problem on a coarse mesh (thus computationally less expensive) and using the solution from the coarse mesh to decouple the model on a finer mesh. This method naturally decouples the problem into two systems; one for the free flow region and the other for the porous medium region. The information from the solution to the coupled problem on the coarse mesh provides boundary values for the interface for each decoupled system. We present numerical results to verify the theoretical convergence rate of the numerical solution from the decoupled scheme. Further, we compare the accuracy of the decoupled numerical scheme to the fully coupled scheme. Decoupling the problem into two relatively smaller systems allows for the use of numerical solvers that are optimized to solve the free flow and porous media flow problems. In addition the these smaller systems can be solved in parallel and thus further increasing the computational efficiency of the solver.

References

1. CHIDYAGWAI UNDEFINED AND PRINCE AND RIVIÈRE AND BÉATRICE UNDEFINED. A two-grid method for coupled free flow with porous media flow. Advances in Water Resources 34.9 (2011): 1113-1123..
2. MU UNDEFINED AND MO AND XU AND JINCHAO UNDEFINED. A two-grid method of a mixed Stokes-Darcy model for coupling fluid flow with porous media flow. SIAM journal on numerical analysis 45.5 (2007): 1801-1813.
3. CHIDYAGWAI UNDEFINED AND PRINCE AND RIVIÈRE AND BÉATRICE UNDEFINED. On the solution of the coupled Navier–Stokes and Darcy equations. Computer Methods in Applied Mechanics and Engineering 198.47 (2009): 3806-3820..
4. CHIDYAGWAI UNDEFINED AND PRINCE AND RIVIÈRE AND BÉATRICE UNDEFINED. Numerical modelling of coupled surface and subsurface flow systems. Advances in Water Resources 33.1 (2010): 92-105..

A Random Set Approach Applied to the Definite Integration of Uncertain Functions Determined by a Low Number of Measurements

Jan Chleboun
Faculty of Civil Engineering, Czech Technical University in Prague
chleboun@mat.fsv.cvut.cz

Abstract

A time-dependent quantity Q is measured at $p < 10$ time points t_i, $i = 1, \ldots, p$. A few measurements, say $m \approx 4$, are performed at each t_i. The number of measurements is too low to allow for satisfactory statistical analysis. The goal is to integrate Q over the time interval $[t_1, t_p]$.

The integral is approximated by a quadrature formula using the nodes t_i, $i = 1, \ldots, p$. Values $Q(t_i)$ are not known exactly; they are uncertain. Various intervals possibly covering $Q(t_i)$ are taken into consideration and evaluated on the basis of local probabilities originating from the measurements at t_i. Each combination of t_i-dependent weighted intervals that possibly cover $Q(t_i)$ leads to a weighted interval of possible values of the integral of Q over $[t_1, t_p]$. The latter weighted intervals form a set of focal elements known from the Dempster-Shafer evidence theory. As a consequence, belief (*Bel*) and plausibility (*Pl*) measures can be calculated for a sequence of tested intervals. The maximum of *Bel* and *Pl* indicates the interval that is subsequently declared the most trustworthy representative of the uncertain integral.

References

1. B. M. AYYUB AND G. J. KLIR. Uncertainty Modeling and Analysis in Engineering and the Sciences. Chapman & Hall/CRC, Taylor & Francis Group, Boca Raton, 2006.
2. A. BERNARDINI. What are the Random and Fuzzy Sets and How to Use them for Uncertainty Modelling in Engineering Systems?. In: I. Elishakoff (ed.): Whys and Hows in Uncertainty Modelling, Probability, Fuzziness and Anti-Optimization, Wien, New York, 1999.

Mortar FEs on Overlapping Meshes : Application to Magnetodynamics

Alexandra Christophe, Laurent Santandrea, Guillaume Krebs, Yann Le Bihan
Lab. de Genie Electrique de Paris, CNRS & Univ. Paris-Sud
alexandra.christophe@lgep.supelec.fr,
laurent.santandrea@lgep.supelec.fr,
guillaume.krebs@lgep.supelec.fr, yann.le-bihan@lgep.supelec.fr

Francesca Rapetti
Lab. Dieudonne, Dept. Math., Univ. de Nice
frapetti@unice.fr

Abstract

The finite element (FE) method is frequently used in magnetodynamics as well suited to treat problems with complex geometries while keeping a simplicity in the implementation. However, some modelisations, as in eddy current (EC) non destructive testing (NDT), present the particularity to have moving parts. A global remeshing can be necessary which causes expensive CPU time. Domain decomposition methods allowing to take into account the movement without having to remesh the whole computational domain. The mortar element method (MEM), a variational non-conforming domain decomposition approach [1] offers attractive advantages in terms of flexibility and accuracy. In its original version for non-overlapping subdomains, the information is transferred through the skeleton of the decomposition by means of a suitable L^2-projection of the field trace from the master to the slave subdomains. A MEM with overlapping subdomains has been proposed to coupled a global scalar potential defined everywhere in the considered domain and a local vector potential defined only in (possibly moving)conductors [2], and later applied to study electromagnetic brakes [3]. In this paper, a new FE-MEM able to deal with moving non-matching overlapping grids is introduced, in order to realize the bidirectional transfer of information between fixed parts and moving ones. With this variant, the field source can be in the moving part. Numerical examples are presented to support the theory (with both node and edge elements), going from problems with known solution, to state the optimality of the method, to EC-NDT applications, in order to underline the flexibility and efficiency of the proposed approach.

References

1. C. BERNARDI AND Y. MADAY AND A. PATERA. A new non-Conforming approach to domain decomposition: the mortar element method. Seminaire XI du College de France, Brezis & Lions eds., in Nonlinear PDEs and their applications, Pitman, pp. 13-51, 1994..
2. Y. MADAY AND F. RAPETTI AND B. I. WOHLMUTH. Mortar element coupling between global scalar and local vector potentials to solve eddy current problems. Numerical mathematics and advanced applications. Enumath 2001 proc., Brezzi F. et al. eds., Springer-Verlag Italy (Milan) pp. 847-865, 2003...
3. B. FLEMISH AND Y. MADAY AND F. RAPETTI AND B. I. WOHLMUTH. Scalar and vector potentials' coupling on nonmatching grids for the simulation of an electromagnetic brake.. COMPEL 24-3 (2005) 1061-1070.

On 0/1 Polytopes With Nonobtuse Triangulations.

Abdullah Cihangir
University of Amsterdam
a.cihangir@uva.nl

Abstract

Our interest in nonobtuse triangulations stems from the following two facts. First, Finite Element Methods are known to satisfy discrete maximum principles if the triangulation of the physical domain consists of nonobtuse simplices. Second, as a special case of the question what the minimal amount of simplices is with which the n-cube can be triangulated, considered triangulations of the n-cube using nonobtuse simplices only. Surprisingly, for each value of n, only two distinct nonobtuse triangulations were proved to exist.

In this presentation we consider nonobtuse triangulations of the more general class of 0/1-polytopes, i.e., convex hulls of vertices of the unit n-cube. We investigate which 0/1-polytopes allow nonobtuse triangulations, and if they do, how many distint ones there exist. We present some computational data generated using Matlab.

References

1. A. CIHANGIR. On 0/1 polytopes with nonobtuse triangulations.. To be submitted to the Conference Proceedings.

Numerical Analysis of Wave Propagation in Reissner-Mindlin Phononic Plates

Robert Cimrman
New Technologies - Research Centre, University of West Bohemia, Plzeň, Czech Republic
cimrman3@ntc.zcu.cz

Eduard Rohan
Department of Mechanics, University of West Bohemia, Plzeň, Czech Republic
rohan@kme.zcu.cz

Abstract

We study wave propagation in Reissner-Mindlin plates of a strongly heterogeneous material, where the heterogeneities repeat periodically. Such materials exhibit phononic bang gaps, i.e. frequency ranges where "mass density" coefficients are negative and no solution in form of waves exists. In bulk elasticity the band gaps can be determined directly from the frequency dependence of the mass tensor derived by means of homogenization theory. In plates, however, the mass tensor has two sub-blocks corresponding to the in-plane rotations and the deflections and it is unclear how negativity of each of the two blocks combines and relates to the bang gap presence. In this contribution we map this problem by performing numerical calculations for various frequency ranges on particular physical domains made of the homogenized Reissner-Mindlin plate materials.

References

1. E. ROHAN AND F. SEIFRT AND B. MIARA. Numerical simulation of acoustic band gaps in homogenized elastic composites. International Journal of Engineering Science 47 (2009) 573-594.
2. E. ROHAN AND B. MIARA. Band gaps and vibration of strongly heterogeneous Reissner-Mindlin elastic plates. Comptes Rendus Mathematique 349 (2011) 777-781.

A Pendulum With a 2D-continuum Cord

Homero De La Fuente , Javier Almaguer, Javier Morales
Universidad Autonoma de Nuevo Leon
Dante_Alighieri390@hotmail.com, almagerjavier@gmail.com,
tequilaydiamante@yahoo.com.mx

Abstract

This work analyses the trajectory in the plane of a pendulum with an uniform mass and attached to a cord of lenght "ℓ" and uniform mass distribution, the system have a fixed pivot point. The cord isn't a rigid body and can be deformed, that's why the whole system requires two continuum polar coordinates to be treated. Using the framework of Classical Field Theory, a nonlinear system of partial differential equations is obtained, which with adequate boundary conditions, it represents the studied system in this work. A finite-volume approximation based algorithm is used for the numerical simulation of this system. The main goal of this work, in a more general context, is to be use it as an example for the study and simulation of two dimensional systems with diverse boundary conditions and characterized with a continuum set of coordinates.

References

1. H. L. ARMSTRONG.. Effect of the mass of the cord on the period of a simple pendulum.. Am. J. Phys. 464, (1976) 564..
2. C. G. MONTGOMERY.. Pendulum on a massive cord.. Am. J. Phys. 46, (1978) 411..
3. S. DESCHAINE AND B. H. SUITS.. The hanging cord with a real tip mass.. Eur. J. Phys. 29 (2008) 1211-1222..
4. ROBERT A. NELSON AND M. G. OLSSON.. The pendulum-Rich physics from a simple system.. Am. J. Phys. 54 (1986), 112-121..
5. S. NAGULESWARAN.. A "Direct" solution for the free vibration of a hanging uniform cord with a particle tip mass.. Journal of Sound and Vibration, 191(3) (1996), 453-458..
6. L. P. POOK.. Understanding Pendulums: A Brief Introduction.. Springer, USA, 2011..
7. HERBERT GOLDSTEIN AND CHARLES P. POOLE JR. AND JOHN L. SAFKO. . Classical Mechanics.. Third edition, Addison Wesley, USA, 2001..
8. L. D. LANDAU AND E. M. LIFSHITZ.. The Classical Theory of Fields.. Fourth Edition: Volume 2 (Course of Theoretical Physics Series), Butterworth-Heinemann, New Delhi, 2000..
9. EITAN TADMOR.. A review of numerical methods for nonlinear partial differential equations.. Bulletin of American Mathematical Society, 49 (2012) 507-554..

A Fuzzy-Genetic Algorithm for Makespan Reduction in Job Shop Environments With Sequence-Dependent Setup Time and Re-entrant Work Flow

Negin Dehghanian
Department of Industrial Engineering, Najafabad Branch, Islamic Azad University, Isfahan, Iran
nd.dehghanian@gmail.com

Seyed Mahdi Homayouni
Department of Industrial Engineering, Lenjan Branch, Islamic Azad University, Isfahan, Iran
homayouni.mahdi@gmail.com, homayouni@iauln.ac.ir

Abstract

Job shop scheduling problem (JSSP) is one of the important issues in the planning and operation of manufacturing systems (Gupta, 2002). In a job shop system with flexible machines, reducing setup time is an important factor for better performance (Ciavotta et al., 2013). Previously, researches have been performed about the sequence-dependent setup time (SDST)-JSSP; however, few researches has been reported on SDST-JSPP with re-entrant work flows (Sun, 2009). This is an NP-hard problem meaning that existing mathematical methods are not efficient for solving such problems, especially in large instances (Lin et al., 2010). Therefore, researchers have applied (meta)heuristic methods (e.g. genetic algorithm (GA)) to achieve near optimal solutions (Kargarfard and Kheirkhah, 2010). In this study, a GA has been developed to solve the SDST-JSSP with re-entrant work flows aiming to reduce makespan. Because this problem has a rough solution space, the GA may lead to the premature convergence. Thus, a fuzzy logic controller (FLC) is designed to improve the performance of the GA in solving the problem. In the fuzzy-genetic algorithm (FGA), the FLC makes changes in crossover and mutation rates of the GA to create a balance between exploration and exploitation of the GA throughout its various iterations of solving the problem. At last, using the sensitivity analysis, effects of parameters such as maintenance and delay times on the makespan are discussed. The results of research indicate that the application of FGAs leads to better solutions to such problems.

References

1. M. CIAVOTTA AND G. MINELLA AND R. RUIZ. Multi-Objective Sequence Dependent Setup Times Permutation Flowshop: A New Algorithm and A Comprehensive Study. Europ. J. Oper. Res. (2013) DOI: 10.1016/j.ejor.2012.12.031.
2. J.N.D. GUPTA. An Excursion in Scheduling Theory: An Overview of Scheduling Research in the Twentieth Century. Prod. Plan. & Cont. 13 (2002) 105–116..
3. M. KARGARFARD AND M. KHEIRKHAH. Using Genetic Algorithms and Priority Rules for Solving Project Scheduling Problem with Resource Constraints. International Conference on Project Management, Tehran, Iran..
4. T.L. LIN AND S.J. HORNG AND T.W. KAO AND Y.H. CHEN AND R.S. RUN AND R.J. CHEN AND J.L. LAI AND I. KUO. An Efficient Job-shop Scheduling Algorithm Based on Particle Swarm Optimization. Expert Sys. with Appl. 37 (2010) 2629-2636.
5. J.U. SUN. A Genetic Algorithm for a Re-entrant Job-Shop Scheduling Problem with Sequence-Dependent Setup Times. Eng. Opt. 41 (2009) 505-520.

A New Predictive Solar Radiation Numerical Model

Felipe Díaz, Gustavo Montero, José María Escobar, Eduardo Rodríguez, Rafael Montenegro
University of Las Palmas de Gran Canaria
felipe.diaz@ulpgc.es, gustavo@dma.ulpgc.es, jescobar@dsc.ulpgc.es,
erodriguez@dis.ulpgc.es, rafa@dma.ulpgc.es

Abstract

A predictive solar radiation numerical model is presented. Starting from the works of [1], a solar radiation numerical model is developed [2] considering the terrain surface through 2-D adaptive meshes of triangles [3] which are constructed using a refinement/derefinement procedure in accordance with the variations of terrain surface and albedo. The effect of shadows is considered in each time step. Solar radiation is first computed for clear-sky (CS) conditions and then, real-sky values are computed daily in terms of the CS index computed using all the observational data which are available for each day at several points of the studied zone. One of the most important problems of generating electrical energy from solar radiation is the lack of knowledge about the actual generating capacity of a facility due to the random nature of the primary energy source. One way for minimizing this problem is using short-term predictive possibilities offered by the existing meteorological forecasting models such as MM5, HIRLAM, etc. The model developed in this work allows the incorporation of data provided by weather prediction models in order to obtain values of radiation (irradiance and irradiation), likely in the short term. The process consists of evaluating the values of real-sky radiation from the calculated clear-sky ones, but computing the CS index values, for each time step, from a spatial interpolation of the values obtained by means of the weather forecasting model. This way we will get to know both, irradiance and irradiation values, anywhere on the domain including the influence of the topography and elevation considering the shadows. This fact is very useful since the existing forecasting models do not take into account the elevation map, nor the cast shadows. Adding the addecuate photovoltaic and/or solar thermal power models, the electrical power generation can be estimated with the accuracy of the weather forecasting model. This is a very interesting tool from the electrical engineering point of view since it allows to increase the penetration of solar energy in the power system without adding instability. The whole problem has been tested in Gran Canaria Island (Canary Islands - Spain).

References

1. M. Šúri and J. Hofierka. A New GIS-based Solar RadiationModel and its application to photovoltaic assessments. Transactions in GIS 8 (2) (2004), pp. 175–170.
2. F. Díaz and G. Montero and J.M. Escobar and E. Rodríguez and R. Montenegro. An Adaptive Solar Radiation Numerical Model. Journal of Computational and Applied Mathematics 236 (18) (2012), pp. 4611–4622.
3. G. Montero and J.M. Escobar and E. Rodríguez and R. Montenegro. Solar radiation and shadow modelling with adaptive triangular meshes. Solar Energy 83 (7) (2009), pp. 998–1012.

Critical Angles of Approximation Methods of Boundary Integral Equations

Victor Didenko, Anh My Vu
Universiti Brunei Darussalam
diviol@gmail.com, anhmy7284@gmail.com

Abstract

In theory of approximation methods for integral equations used for solving boundary value problems there is a well known effect that an approximation method may become unstable if the boundary contains corner points. In order to overcome these difficulties, various modifications of known algorithms have been proposed. Theoretical studies of such modified algorithms require a lot of effort and the results obtained are not always complete. The present work is aimed to study the behaviour of common approximation methods for two famous boundary integral equations–viz. for the Sherman-Laurichella and double layer potential equations considered on simple closed piecewise smooth contours. The stability of the methods depend on the invertibility of certain operators connected with the corner points of the boundary. As a rule, these operators have a complicated structure and their invertibility cannot be verified analytically. On the other hand, we propose a numerical approach which allows us to find the opening angles of the corner points which cause instability. For example, it is shown that in the interval $(\varepsilon, 2\pi - \varepsilon)$, $\varepsilon > \pi/10$, Galerkin and Nyström methods have only a few such critical angles. Therefore, in most cases the methods mentioned are stable and do not require any modification. Note that this work continues investigations of [1],[2],[3].

References

1. V. D. DIDENKO AND J. HELSING. Stability of the Nyström method for the Sherman-Lauricella equation. SIAM J. Numerical Analysis, 49 (2011) 1127-1148.
2. V. D. DIDENKO AND J. HELSING. Features of the Nyström Method for the Sherman-Lauricella Equation on Piecewise Smooth Contours. East Asian Journal on Applied Mathematics, 1 (2011) 403–414.
3. V. D. DIDENKO AND J. HELSING. Nyström method for the Muskhelishvili equation on piecewise smooth contours. SIAM J. Numerical Analysis, 51 (2013) 1757–1776.

A New, Very Efficient Initialization Mechanism for Analog Self-Organizing Neural Networks Implemented in the CMOS Technology

Rafał Długosz, Marta Kolasa, Tomasz Talaśka
University of Technology and Life Sciences, Faculty of Telecommunications, Computer Science and Electrical Engineering, Bydgoszcz, Poland
rafal.dlugosz@gmail.com, markol@utp.edu.pl,
tomasz.talaska@gmail.com

Abstract

Efficiency of training of Neural Networks (NN) depends on many parameters, such as proper polarization of neurons' weights. The initialization, which has to be done before starting the learning phase, is in particular important in Winners Take All (WTA) NNs, which belong to self-organizing learning algorithms proposed by T. Kohonen [1]. In networks of this type properly selected initial values of neurons' weights have influence on the number of the, so called, dead neurons and finally on the quantisation error of the network. Dead neurons usually occur in the situations in which initial values of the weights as well as training data cover different areas in the input data space.

In software implemented NNs any type of the initialization can be performed easily by single instructions only. Another situation exists in transistor level realizations of neural networks in which particular neurons operate in parallel. In such systems each neuron is a separate computation unit (CU) located in a given place of the chip. To perform the initialization in this case we have to provide the programming signals to each CU. This increases the complexity of the chip.

The paper presents a new CMOS implementation of the initialization mechanism based on Convex Combination Method algorithm. The proposed mechanism is part of the WTA NN implemented by the authors in the CMOS TSMC 180nm technology [2]. The concept is attractive in hardware implementation, as it does not require additional programming lines and additionally it takes into account the morphology of the input data set. In this approach to initialize the weights we use the the same mechanism, after some modifications, that is further used in the learning phase to adapt the weights.

(The "Development of Novel Ultra Low Power, Parallel Artificial Intelligence Circuits for the Application in Wireless Body Area Network Used in Medical Diagnostics" project is realized within the POMOST programme of Foundation for Polish Science, cofinanced from European Union, Regional Development Fund)

References

1. T. KOHONEN. Self-Organizing Maps. Springer Verlag, Berlin, 2001.
2. R. DŁUGOSZ AND T. TALAŚKA AND W. PEDRYCZ AND R. WOJTYNA. Realization of the Conscience Mechanism in CMOS Implementation of Winner-Takes- All Self-Organizing Neural Networks. IEEE Transactions on Neural Networks, Vol. 21, Iss.6, pp. 961–971, June 2010.

A Novel Recursive Algorithm Used to Model the Hardware Programmable Neighborhood Mechanism of the Self-Organizing Neural Networks

Marta Kolasa, Tomasz Talaśka, Rafał Długosz
University of Technology and Life Sciences, Faculty of Telecommunications, Computer Science and Electrical Engineering, Bydgoszcz, Poland
markol@utp.edu.pl, tomasz.talaska@gmail.com,
rafal.dlugosz@gmail.com

Abstract

The presented work is a part of a bigger project that aims at developing a new specialized chip based on Artificial Neural Networks (ANNs). The system offering an ultra low energy consumption and low chip area will find the application in health monitoring system based on Wireless Body Area Networks (WBAN) used in monitoring of various biomedical signals, such as ECG signals.

Looking from the hardware realization point of view, the most interesting learning algorithms are those that require simple arithmetic operations. One of such algorithms is Self-Organizing Map (SOM) [1, 2], in which only additions, subtractions, multiplications and abs() operations are required. In this case the overall chip can dissipate relatively low power and occupy small chip area, which are paramount features in WBAN [2].

One of the important steps of the overall project is to develop an advanced software model of the SOM (realized in C++) that will enable modeling various physical phenomena and constraints common in hardware design. One of the key building block of the SOM is the neighborhood mechanism (NM) that in the proposed hardware architecture will operate in an asynchronous fashion and additionally fully in parallel [2]. The investigations show that, depending on the learning data set, different SOM topologies are optimal, and therefore the NM has to be programmable [2]. To exactly model such a complex block we have proposed a new recursive algorithm. The algorithm is very simple and what is the main advantage here it operates almost in the same way like it will operate in hardware implemented SOM.

(The "Development of Novel Ultra Low Power, Parallel Artificial Intelligence Circuits for the Application in Wireless Body Area Network Used in Medical Diagnostics" project is realized within the POMOST programme of Foundation for Polish Science, cofinanced from European Union, Regional Development Fund)

References

1. C.R. Leite and D.L. Martin and G.R. Sizilio and K.E. Dos Santos and B.G. de Araujo and R.A. Valentim and A.D. Neto and J.D. de Melo and A.M. Guerreiro. Classification of cardiac arrhythmias using competitive networks. 2010 Annual International Conference of the IEEE Engineering in Medicine and Biology Society, EMBC'10, pp. 1386-1389.
2. R. Długosz and M. Kolasa and W. Pedrycz. A Parallel Programmable Asynchronous Neighborhood Mechanism for Kohonen SOM Implemented in CMOS Technology. IEEE Transactions on Neural Networks, 22 (12), 2011, pp. 2091–2104.

Anisotropic Hp-adaptive Discontinuous Galerkin Method for Numerical Solution of Partial Differential Equations

Vit Dolejsi
Charles University Prague
dolejsi@karlin.mff.cuni.cz

Abstract

We present a completely new hp-anisotropic mesh adaptation technique, which can be simply employed for the numerical solution of partial differential equations with the aid of a discontinuous Galerkin finite element method. This method is based on piecewise polynomial but discontinuous approximation and it simply deals with anisotropic (thin and long) elements and with different polynomial approximation degrees on different elements. The presented algorithm generates quite general anisotropic triangular grids and the corresponding polynomial approximation degrees. The idea is to construct a hp-anisotropic mesh such that

i) the interpolation error of the (unknown) exact solution $u : \Omega \to R$ in the $L^q(\Omega)$-norm, $q \in [1, \infty]$ is under the given tolerance,
ii) the number of degree of freedom is minimal.

Under the assumption that the exact solution is sufficiently regular, we derive an "optimal" triangle with the barycentre at each $x \in \Omega$. Moreover, we set an "optimal polynomial approximation degree" at x. Furthermore, we give an argumentation that this approach works also for non-smooth functions. Finally, using a minimization of a functional, we define optimal triangulation of Ω and set the optimal approximation polynomial degree distribution over Ω. This approach is supported by a set of numerical experiments, which demonstrate the efficiency of this anisotropic strategy in comparison with an hp-isotropic method and a h-anisotropic one.

References

1. V. DOLEJSI. Anisotropic hp-adaptive method based on interpolation error estimates in the L^q-norm. Appl. Numer. Math. (submitted).

Optimization of Parallel Path Magnetic Technology Actuator

Jiří Doubek, Libor Straka, Zdeněk Novák
Czech Technical University in Prague
doubejir@fel.cvut.cz, strakli1@fel.cvut.cz, novakzd5@fel.cvut.cz

Lubomír Musálek
Institute of Thermomechanics AS CR
musalek@it.cas.cz

Abstract

The paper deals with modeling and optimization of Parallel Path Magnetic Technology actuator. The aim is to set optimized input parameters based on a real arrangement of the actuator. Actuators based on the Parallel Path Magnetic Technology (PPMT) use advanced control of magnetic fluxes in their parts and magnetic forces acting between them. The technology uses two or more permanent magnets placed in the magnetic circuit in parallel position, and an appropriate number of field coils. The mentioned arrangement consists of two long ferromagnetic bars that are separated by two permanent magnets oriented in the same way and fixed to them. Two other shorter side bars made of ferromagnetic material are placed along the magnets. They are, however, free and can move. Each of the long bars carries a field coil that is connected to a source of current. Their connection is antiparallel. The magnetic fluxes in the system are controlled by generally time varying external currents in the coils. The movement of one shorter side bar of the PPMT actuator is controlled by a mechanical spring. The process of optimization will be represented by a proper method. Since there are many input parameters acting on the final behavior of the given system, the task stands for a multi-objective optimization problem. So-called posteriori methods, such as Non-dominated Sorting Genetic Algorithm-II (NSGA-II) or method based on simulated annealing approach, seem to be applicable. The paper is focused on the optimization processes but it describes the arrangement of the system, its mathematical model, and the most important results too.

References

1. G. A. Robertson and T. R. Tyler and P. J. Piper. Lightweight High Efficiency Electric Motors for Space Applications. [patent]. USA. M11-0777. Granted on 5. 12. 2011.
2. L. Musálek and J. Doubek and J. Kyncl and Z. Novák and L. Straka. Static and Dynamic Characteristics of PPMT Electromagnet. In: IC-SPETO. Gliwice - Ustroń, 2013. ISBN 978-83-85940-35-7.
3. M. Kuczmann and A. Iványi. The Finite Element Method in Magnetics. Akademiai Kiadó, Budapest, 2008.

Linear-Scaling Hartree-Fock Exchange and Hybrid XC Functionals With Plane-Wave Basis Set Accuracy

Jacek Dziedzic
University of Southampton & Gdansk University of Technology
J.Dziedzic@soton.ac.uk

Chris-Kriton Skylaris
University of Southampton
C.Skylaris@soton.ac.uk

Abstract

Local and semilocal functionals used in density functional theory (DFT) calculations have long been known to underestimate band gaps and to incorrectly describe the energetics of small molecules, among other deficiencies [1]. The hybrid functional approach, where Hartree-Fock exchange is included into the exchange-correlation functional offers a more accurate description of geometries and of several properties, such as bond energies and band gaps, particularly for metal oxides [2].

We present a resolution-of-identity-based approach [3] for evaluating the Hartree-Fock exchange energy with a computational cost that scales linearly with the number of atoms. We discuss the conditions that need to be satisfied to ensure the proposed technique is stable and accurate. We describe the implementation of this approach in the linear-scaling DFT code ONETEP [4], which can perform such calculations with near-complete basis set accuracy.

We validate the method against energies, forces and equilibrium bondlengths [2], computed with conventional, cubic-scaling DFT codes, demonstrating excellent agreement, even with approaches using an all-electron description and Gaussian basis sets. We show qualitative agreement between B3LYP calculations performed with our technique and the predictions [5] of DFT+U for the binding of O2 and CO to a simplified model of myoglobin.

We conclude with a description of a hybrid (MPI+OpenMP) parallelisation strategy for the proposed implementation, which offers excellent scaling up to hundreds of CPU cores. Benchmarks for larger systems, demonstrating the linear-scaling of the computational time with the size of the system and strong scaling will also be presented.

References

1. M. Marsman and J. Paier and A. Stroppa and G. Kresse. Hybrid functionals applied to extended systems. J. Phys. Cond. Matt. 20, 064201 (2008).
2. V. N. Staroverov and G. E. Scuseria and J. Tao and J. P. Perdew. Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. J. Chem. Phys. 23, 12129 (2003).
3. J. Dziedzic and Q. Hill and C.-K. Skylaris. Linear-scaling calculation of Hartree-Fock exchange energy with Non-orthogonal Generalised Wannier Functions. J. Chem. Phys. 139 214103 (2013).
4. C.-K. Skylaris and P. D. Haynes and A. A. Mostofi and M. C. Payne. Introducing ONETEP: Linear-scaling density functional simulations on parallel computers. J. Chem. Phys. 122, 084119 (2005).
5. D. J. Cole and D. D. O'Regan and M.C. Payne. Ligand Discrimination in Myoglobin from Linear-Scaling DFT+U. J. Phys. Chem. Lett. 3, 1448 (2012).

Partition of Unity Methods for Approximation of Point Water Sources in Porous Media

Pavel Exner
Technical University of Liberec
pavel.exner@tul.cz

Abstract

People often consider in their models of flow in porous media very large areas which can contain various phenomenons of very small scale compared with the size of the areas. These can be some disruptions of the porous media, e.g. cracks and wells, or material inhomogeneities which cause large gradients in pressure head and velocity or even their discontinuities.

Using the standard FEM (Finite Element Method) we are unable to properly approximate the quantities in the vicinity of these disturbances, unless we introduce cells of the same scale in the mesh. This leads to very fine meshes which highly increase computational costs. We use XFEM method to overcome this problem and demonstrate it on a steady quasi-three-dimensional model of multi-aquifer system containing hydro-geological wells which cause singularities in solution. We follow the work [2] of R. Gracie and J. R. Craig who have already used the XFEM on a similar model.

We consider steady flow in a system of aquifers (2D layers of given thickness) which are separated by impermeable layers. The distribution of pressure head in each aquifer is described by Poisson equation. The communication between aquifers is possible only through wells which can be seen as 1D problems. The transfer between wells and aquifers can be treated in two ways – as a balance over the boundary of the wells or as flow sources in the area of aquifer. We compared both approaches.

In the theoretical part of our work we derived the weak formulation of the problem and we proved the existence and the uniqueness of the weak solution according to Lax-Milgram lemma.

We implemented both the XFEM (eXtended Finite Element Method) and h-adaptive FEM with linear finite elements. Measured XFEM convergence rate $O(h^{1.7})$ and FEM convergence rate $O(h^{0.4})$ are in good agreement with results of R. Gracie and J. R. Craig.

Next, we used the SGFEM method (Stable Generalized FEM, introduced by U. Banerjee and I. Babuška in [3]) to solve the model. This method improves numerical properties of the linear system. We did also time profiling, observed number of degrees according to size of enriched area and investigated numerical properties to show the benefits and disadvantages of XFEM and SGFEM methods.

Our work is now aimed at using XFEM/SGFEM in mixed method to approximate both pressure head and velocity.

References

1. P. EXNER. Partition of Unity Methods for Approximation of Point Water Sources in Porous Media. Master's thesis, Technical University of Liberec, 2013, web: http://bacula.nti.tul.cz/ pavel.exner/.
2. R. GRACIE AND J. R. CRAIG. Modelling Well Leakage in Multilayer Aquifer Systems Using the Extended Finite Element Method. Finite elements in Analysis and Design, Elsevier B.V., 46:504-513, 2010.
3. I. BABUŠKA AND U. BANERJEE. Stable Generalized Finite Element Method (SGFEM). Mathematics Faculty Scholarship, Paper 139, 2011, web: http//surface.syr.edu/mat/139.

Selection of Appropriate Risk-based Maintenance Strategy by Using Fuzzy Analytical Hierarchy Process

Mohammad Ferdousmakan
Department of Industrial Engineering, Islamic Azad University, Najafabad Branch, Isfahan, Iran
ferdousmakan.m@gmail.com

Mohammadreza Vasili, Mehdi Vasili
Department of Industrial Engineering, Islamic Azad University, Lejan Branch, Isfahan, Iran
vasili@iauln.ac.ir, m.vasili@iauln.ac.ir

Tang S.H., Ng Thai Lim
Department of Mechanical & Manufacturing Engineering, Faculty of Engineering, Universiti Putra Malaysia, Selangor, Malaysia
saihong@upm.edu.my, ng.thai.lim@gmail.com

Abstract

Today, continued pressure on industries for reducing costs and improving customer satisfaction has resulted in increasingly detailed examinations of maintenance practices (Mechefske and Wang, 2003). Due to high investments for purchase, construction and commissioning of industrial machines, a proper maintenance schedule is more demanding. With the proliferation of new and complex equipment maintenance strategies, the selection of an optimal strategy has become more difficult. For this purpose, and in order to increase the availability and reliability levels of production facilities, the limitation of risk per equipment should also be taken into account. The selection of maintenance strategies is a typical multi criteria decision making (MCDM) problem (Wang et al., 2007). In this study, an integrated model of risk management and fuzzy analytical hierarchy process (fuzzy AHP) is proposed to select the optimal maintenance strategy. The risk priority matrix is made for five different risk levels, including vital, undesirable, tolerable, acceptable, and desire.With Fuzzy AHP technique, four possible alternatives are analyzed: emergency maintenance (EM), preventive maintenance (PM), condition based maintenance (CBM), and total productivity maintenance (TPM). In order to characterize each of the above-mentioned maintenance strategies, four criteria including reliability, maintainability, availability, and cost (Komal et al., 2010) are considered. The proposed method is used for selecting the best maintenance strategy for an important Iranian petrochemical plant.

References

1. C. K. MECHEFSKE AND Z. WANG. Using fuzzy linguistics to select optimum maintenance and condition monitoring strategies. Mechanical Systems and Signal Processing, vol. 17, pp. 305-316, 2003.
2. L. WANG AND J. CHU AND J. WU. Selection of optimum maintenance strategies based on a fuzzy analytic hierarchy process. International Journal of Production Economics, vol. 107, pp. 151-163, 2007.
3. K. KOMAL AND S. P. SHARMA AND D. KUMAR. RAM analysis of repairable industrial systems utilizing uncertain data. Applied Soft Computing, vol. 10, pp. 1208-1221, 2010.

Mathematical Modeling of Coupled Conductive and Radiative Heat Transfer in Polymeric Foams

Pavel Ferkl, Richard Pokorny, Juraj Kosek
Department of Chemical Engineering, Institute of Chemical Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic
pavel.ferkl@vscht.cz, richard.pokorny@vscht.cz, juraj.kosek@vscht.cz

Abstract

Good heat insulation significantly reduces the costs associated with heating and air conditioning of buildings. Heat insulators are commonly produced from highly porous materials. Between the most utilized materials are rigid polymeric foams, usually based on polystyrene or polyurethane. Even though these materials are on the market for a long time, there is still large room for the improvement of the heat insulating properties of mass-produced polymeric foams.

Good heat insulator must provide sufficient resistance to both the conduction and the radiation. Heat conduction can be reduced by increasing the foam porosity, by the choice of the blowing agent or by the significant reduction of cell size (Coquard and Baillis, 2009). Heat radiation is strongly influenced by the foam porosity, the cell diameter, the fraction of polymer in struts, the wall thickness and the radiation absorption coefficient of polymer (Ferkl et al, 2013).

To investigate the quantitative influence of all these parameters we developed the mathematical model of coupled heat transfer by conduction and radiation inside spatially three-dimensional multiphase medium. The physical model leads to a set of partial differential equations, which are numerically solved by the finite volume method. Due to the large number of gas cells, the foam must be discretized using non-equidistant meshes with high aspect ratios. For the solution of the large sparse system of linear equations we tested algebraic multigrid method and several open source band solvers. When the foam contains many thousands of gas cells, the resulting system matrix often becomes very ill-conditioned, and thus the extended or quadruple precision of floating point numbers must be used.

Based on the extremely low conductivity of the inorganic aerogels, many researchers are investigating the production of polymeric nanofoams with the expectation that they will have better mechanical properties and retain the great insulating properties of aerogels. The results of our model show that the low conductivity of the polymeric nanofoam is not guaranteed for any polymer but can be ensured by the selection of the polymer with high absorption coefficient.

Acknowledgement: Support from EC FP7 project MODENA (NMP4-SL-2013-604271) and specific university research (MSMT No 20/2014) is acknowledged.

References

1. R. COQUARD AND D. BAILLIS. Numerical investigation of conductive heat transfer in high-porosity foams.. Acta Mater. 57 (2009), 5466-5479.
2. P. FERKL AND R. POKORNY AND M. BOBAK AND J. KOSEK. Heat transfer in one-dimensional micro- and nanocellular foams. Chem. Eng. Sci. 97 (2013) 50-58.

Modeling of Polaron States in Classical Molecular Chains at Finite Temperatures

Victor Lakhno, Nadezhda Fialko
Institute of Mathematical Problems of Biology, Russian Academy of Sciences, Pushchino
lak@impb.psn.ru, fialka@impb.psn.ru

Abstract

The possibility of applying biological macromolecules, especially DNA, in nanobioelectronics currently attracts attention of researchers. For example, DNA can be used when designing electronic microarrays and as a molecular wire. Therefore, the study of the conducting properties of polynucleotide chains is of great interest [1,2].

There are two possible mechanisms for the charge mobility in homogeneous DNA, polaron and band. At present, there is a conception that the current carriers in DNA are polarons. In the vast majority of modern papers polaron states in molecular chains are calculated for zero temperature. And it is assumed that polaron properties do not change significantly if the temperature is non-zero, but much smaller than the characteristic energy equal to the depth of the polaron level. However, the results of our computational experiments on the charge transfer along classical chains lead us to suggestion that in a infinitely long chain the polaron is destroyed, no matter how small the temperature is.

We studied the model based on the semiclassical Holstein Hamiltonian for a discrete sites chain [3,4]. In the case of DNA, the site is a complementary base pair. The excess charge is introduced in the chain. Taking into account the temperature fluctuations, the classical subsystem of equations becomes the Langevin-type equations [5]. In computing terms, the problem reduces to finding the set of trajectories of the system – the charge dynamics from different initial conditions and with different values of the random force, which modeling thermostat, and then to calculate the average time-dependencies over the simulations. It is shown that at high temperatures the polaron states are destroyed, and temperature of the "polaron destruction" depends on the parameters of the chain, e.g. on the coupling constant of quantum subsystem with a classical one. It is also shown that this temperature depends on the chain length. The longer the chain, the smaller the temperature of destruction is, and in the limit of infinite chains it tends to zero. Qualitative explanation of the results is obtained on the basis of statistical properties of the system.

This work is supported by RFBR, grants 13-07-00256, 14-07-00894.

References

1. A. OFFENHAUSSER AND R. RINALDI (EDS.). Nanobioelectronics – for Electronics, Biology, and Medicine. New York Springer (2009) 337 p.
2. V.D. LAKHNO. DNA Nanobioelectronics. Int. J. Quant. Chem. 108 n.11 (2008) 1970–1981.
3. T. HOLSTEIN. Studies of Polaron Motion. Ann. Phys. 8 n. 3 (1959) 325–389 .
4. V.D. LAKHNO AND N.S. FIALKO. Solvation Effects on Hole Mobility in the Poly G/Poly C Duplex. Russian J. Phys. Chem. A 86 n. 5 (2012) 832-836 .
5. P.S. LOMDAHL AND W.C. KERR. Do Davydov Solitons Exist at 300 K?. Phys. Rev. Lett. 55 n. 11 (1985) 1235-1238.

Fast Poisson Solver PoisFFT and Its Application to Turbulence Modelling

Vladimír Fuka , Josef Brechler
Department of Meteorology and Environment Protection, Faculty of Mathematics and Physics,
Charles University in Prague
vladimir.fuka@mff.cuni.cz, josef.brechler@mff.cuni.cz

Abstract

The parallel fast Poisson solver PoisFFT is described in this contribution. It will be released as open-source under the GPL licence soon. Its aim is to provide simple access to routines solving a Poisson equation on a uniform Cartesian grid with different boundary conditions to programs, that do not want to depend on large multi-purpose frameworks. It should therefore replace calls to obsolete libraries like FISHPACK[1]. The possible boundary conditions include homogeneous Dirichlet, homogeneous Neumann and periodic boundary conditions.

The library solves the Poisson equation using the Fast Fourier Transformations and uses FFTW[2] library as a backend and can use its OpenMP and pthreads parallelization. For MPI parallelization it depends on the PFFT[3] library, that also depends on FFTW. Performance and scaling tests are performed. PoisFFT is written in Fortran 2008, and C and C++ interfaces are provided.

The usage of the solver is showed on the Large Eddy Simulation model for turbulent atmospheric flows called CLMM (Charles University Large-Eddy Microscale Model)[4] and it is demonstrated, that the Poisson equation solution is fast enough in order not to be a bottleneck of the computation.

References

1. P. SWARZTRAUBER AND R. SWEET. Efficient FORTRAN Subprograms for the Solution of Elliptic Partial Differential Equations. NCAR Technical Note NCAR/TN-109+IA (1975).
2. M. FRIGO AND S. G. JOHNSON. The Design and Implementation of FFTW3. Proceedings of the IEEE 93 (2) (2005), 216–231.
3. M. PIPPIG. PFFT - An Extension of FFTW to Massively Parallel Architectures. SIAM J. Sci. Comput., 35(3) (2013), C213-C236.
4. V. FUKA AND J. BRECHLER. Large Eddy Simulation of the Stable Boundary Layer. Finite Volumes for Complex Applications VI Problems & Perspectives Springer Proceedings in Mathematics Volume 4 (2011), 485-493.

CFD Simulation of Interaction Between Fluid and Vibrating Profile

Petr Furmánek, Karel Kozel
Czech Technical University in Prague, Faculty of Mechanical Engineering, Department of Technical Mathematics
petr.furmanek@fs.cvut.cz, karel.kozel@fs.cvut.cz

Abstract

Aero-elastic effects (e.g. buffeting of flutter) which can occur in flows around profiles and wings have usually a significant influence on both the flow-field and the solid body. Possibilities how to simulate them numerically with the use of commercial CFD codes are still very limited and such problems are often solved by a problem-tailored software solvers. The aim of this work is to compare two different approaches to this problem. Both of them are based on the finite volume method. The first one is simulation with an in-house solver using the so called Modified Causon's scheme (derived from TVD form of the classical predictor-corrector MacCormack scheme), which is extended in order to simulate unsteady flows with the use of the ALE method. The second one is simulation with open-source solver package OpenFOAM. OpenFOAM incorporates many solvers suited to various CFD problems. For unsteady fluid-structure interaction the so called pimpleDyMFoam solver is used. This solver uses the PIMPLE algorithm, allows for various discretization schemes and also employs ALE method for computation on moving meshes. A flow over NACA 0012 profile is simulated, while the profile itself is moving with two degrees of freedom (oscillations around an elastic axis and motion in direction of vertical axis). The motion itself is induced by the flowing air and described by system of two ordinary 2nd order differential equations. More inlet velocities, initial deviation angles and shifts in vertical direction are considered. Stiffness is modelled both as linear and non-linear. Obtained results are compared with NASTRAN analysis and results of in-house code by Radek Honzátko from Department of Technical Mathematics (Faculty of Mechanical Engineering, CTU in Prague). Critical velocities for unstable oscillations are in the same interval for all simulated cases.

References

1. J. Čečrdle and J. Maleček. Verification FEM Model of an Aircraft Construction with Two and Three Degrees of Freedom. Technical report R-3418/02, Aeronautical Research and Test Establishment, Prague, Letňany, (in Czech) (2002).
2. P. Sváček. Numerical Modelling of Aeroelastic Behaviour of an Airfoil in Viscous Incompressible Flow. Applied Mathematics and Computation. vol. 217, no. 11, p. 5078-5086. ISSN 0096-3003, (2011)..
3. P. Sváček and M. Feistauer and J. Horáček. Numerical Simulation of Flow Induced Airfoil Vibrations with Large Amplitudes. Journal of Fluids and Structures, Volume 23, Issue 3, April 2007, Pages 391-411, ISSN 0889-9746, http://dx.doi.org/10.1016/j.jfluidstructs.2006.10.005. (http://www.sciencedirect.com/science/article/pii/S0889974606001253).

Numerical Simulation of Flows Through Experimental Turbine Cascade

Jiří Fürst, Petr Louda
Czech Technical University in Prague
Jiri.Furst@fs.cvut.cz, Petr.Louda@fs.cvut.cz

Petr Straka
Aerospace Research and Test Establishment
straka@vzlu.cz

Abstract

The article deals with the numerical simulation of transonic flows through 2D model of experimental turbine cascade mounted in the test section of the wind tunnel. The main goal was to investigate the differences between infinite model of cascade with periodical boundary conditions and a model corresponding to real experimental setup wit limited number of blades and including the effects of wind tunnel walls. The flow model is based on the Favre-averaged Navier-Stokes equations describing the motion of an ideal compressible gas. The effects of turbulence are modeled with the help of several variants of k-ω turbulence models including the transitional versions. The numerical solution was calculated using in-house software based on the finite volume method for structured multi-block or unstructured hybrid meshes. The results show that the flow is influenced by wind tunnel walls especially in the outermost channels.

References

1. D. ŠIMURDA AND J. FÜRST AND M. LUXA. 3D Flow Past Transonic Turbine Cascade SE 1050 - Experiment and Numerical Simulations. Journal of Thermal Science, 22 (2013), 311-319.
2. J. FÜRST. A weighted least square scheme for compressible flows. pp. 625 – 632. Fürst, J. : A weighted least square schemeJ. Flow Turbulence and Combustion, Vol 76, No 4., pp 331-342, (2006).
3. P. STRAKA AND J. PŘÍHODA. Application of the algebraic bypass-transition model for internal and external flows. Proc. Conf. Experimental Fluid Mechanics, TU Liberec, pp.636–641, Liberec, (2010)..

A Portable Knowledge Based System for Car Breakdown Evaluation

Eugenio Roanes-Lozano
Algebra Dept., Universidad Complutense de Madrid, Spain
eroanes@mat.ucm.es

José Luis Galán-García, Gabriel Aguilera-Venegas
Applied Mathematics Dept., Universidad de Málaga, Spain
jlgalan@uma.es, gabri@ctima.uma.es

Abstract

This work arises from a real fact: an aunt of one of the authors kept on driving to the next gas station (to ask for advice) when the "oil pressure" dashboard light of her car went on. As a consequence of this decision, the engine was ruined. The importance of this dashboard light wasn't correctly evaluated!

Modern cars have many dashboard lights and not all drivers recognize or know the importance of all of them. Applications for smartphones, that help in recognizing the icons are now available (http://dashboardsymbols.com/the-symbols/). Red symbols usually indicate a safety issue or a serious problem, meanwhile yellow symbols use to indicate a not so urgent problem. Green and blue symbols usually provide information about the systems connected. But not all the "red icons" require of the same action (for instance, to "stop the car immediately" is not always required, although can be the best option sometimes).

We had previously developed knowledge based systems (KBS), whose underlying logic was Boolean or many-valued modal, for managing medical appropriateness criteria [1] and for the early detection of illnesses [2-4], using techniques borrowed from computer algebra (Gröbner bases).

Now smart devices have become popular and have an outstanding computing power. For example, the Computer Algebra System *Maxima* has been ported to the *Android* O.S. (available at https://sites.google.com/site/maximaonandroid). Consequently, the conditions for developing a useful portable application that evaluated the situation and recommended the best action to be carried out in case a dashboard light went on, exist. So, we have designed and developed such a KBS. It concludes explanations such as "power steering breakdown" and recommendations such as "refill the power steering reservoir" AND "drive carefully" AND "take the car to be repaired a.s.a.p.".

References

1. L. M. Laita and E. Roanes–Lozano and V. Maojo and E. Roanes–Macías and L. de Ledesma and L. Laita. An Expert System for Managing Medical Appropriateness Criteria based on Computer Algebra Techniques.. Computers and Mathematics with Applications 42/12 (2001) 1505–1522.
2. C. Pérez Carretero and L. M. Laita and E. Roanes–Lozano and L. Lázaro and J. González Cajal and L. Laita. A Logic and Computer Algebra-Based Expert System for Diagnosis of Anorexia.. Math. Comp. Simul. 58/3 (2002) 183–202.
3. C. Rodríguez–Solano and L. M. Laita and E. Roanes–Lozano and L. López Corral and L. Laita. A Computational System for Diagnosis of Depressive Situations.. Exp. Syst. Appl. 31 (2006) 47-55.
4. J. Piury and L. M. Laita and E. Roanes–Lozano and A. Hernando and F. J. Piury–Alonso and J. M. Gómez–Argüelles and L. Laita. A Gröbner bases-based rule based expert system for fibromyalgia diagnosis.. RACSAM 106/2 (2012) 443–456.

A Genetic Algorithm and an Exact Algorithm for Classifying the Items of a Questionnaire Into Different Competences

José Luis Galán-García, Salvador Merino, Javier Martínez, Miguel de Aguilera
Applied Mathematics Dept., Universidad de Málaga, Spain
jlgalan@uma.es, smerino@uma.es, javim@ctima.uma.es,
deaguilera@uma.es

Abstract

A Likert scale is a psychometric response scale primarily used in questionnaires to obtain participant's preferences or degree of agreement with a statement or set of statements [1]. Respondents are asked to indicate their level of agreement with a given statement by way of an ordinal scale. The most commonly used is a 5-point scale ranging from "Strongly Disagree" on one end to "Strongly Agree" on the other with "Neither Agree nor Disagree" in the middle.

Normally, when a company wants to check the capabilities and skills of their employees (or when looking for new employees), a huge Likert scale questionnaire is asked to be filled up. With such a questionnaire, different competences are evaluated and therefore, the result of a questionnaire will provide important information about capabilities and skills of the respondents for each competence.

As an example, we will describe, for a real questionnaire of 170 Likert items (questions) and 23 competences, how to classify each question with the corresponding competence. That is, to find out, for each Likert item, which competence is evaluated. We will present how to face and solve the problem using two different techniques:

1. **A genetic algorithm**, adapting characteristics of genetic algorithms such as selection, genetic engineering, crossover, mutation and cloning to our classification problem. One of the main advantages of this method is that it can even be used when there are less equations (filled questionnaires) than unknowns (items) and this technique can leads to find the required solution.
2. **An exact method**, by solving a quadratic system of n equations and n unknowns, converting it to a linear system which provides the solution in a easy way. This technique required the use of a Computer Algebra System (specifically, we used DERIVE) for exact computations. One of the main advantages of this technique is that if there are enough equations, this exact method will lead to the solution faster than the numerical approach.

After this example, we will set the basics to solve this competence-assignment problem for a generalized version of similar questionnaires with n Likert items for evaluating m competences using both techniques.

Finally, we will describe also other advantages and disadvantages of both techniques in addition of the ones described above.

References

1. WWW. WIKIPEDIA. Likert Scale. http://en.wikipedia.org/wiki/Likert_Scale.

A Posteriori Error Estimates for Nonconforming Approximation of Multiple Eigenvalues

Daniele Boffi, Francesca Gardini
Dipartimento di Matematica, Università degli Studi di Pavia, Italy
daniele.boffi@unipv.it, francesca.gardini@unipv.it

Ricardo G. Durán
Department of Mathematics, University of Buenos Aires, Argentina
rduran@dm.uba.ar

Lucia Gastaldi
Dipartimento di Ingegneria Civile, Architettura, Territorio, Ambiente e di Matematica, Università degli Studi di Brescia, Italy
lucia.gastaldi@ing.unibs.it

Abstract

We consider the approximation of the Laplace eigenproblem by nonconforming Crouzeix-Raviart finite elements. In the recent paper [1] a posteriori error estimators for the eigenfunctions and the eigenvalues were introduced, showing that the error estimator is equivalent to the energy norm of the eigenfunction error up to higher order terms. Moreover, the authors proved that the error estimator provides an upper bound for the error in the approximation of the first eigenvalue up to higher order terms as well. Here we present a new a posteriori error analysis paying particular care to the approximation of multiple eigenvalues. The analysis is based on a technique introduced by Knyazev and Osborn [2] for obtaining a priori error estimates of multiple eigenvalues of self-adjoint compact operators. Eventually, we report the results of some preliminary numerical tests of an adaptive procedure based on the error estimator.

References

1. E. Dari and R.G. Durán and C. Padra. A Posteriori Error Estimates for Non Conforming Approximation of Eigenvalue Problems. Appl. Numer. Math. 62 (2012) 580-591.
2. A.V. Knyazev and J.E. Osborn. New A Priori FEM Error Estimates for Eigenvalues. SIAM J. Numer. Anal. 43 (2006) 2647-2667.

Space-time Finite Element Method for the Magma-rock Interaction Problem

Deepak Garg, Antonella Longo, Paolo Papale
National Institute of Geophysics and Volcanology
deepak.garg@pi.ingv.it, longo@pi.ingv.it, papale@pi.ingv.it

Abstract

We present a decoupled solution approach for fluid-solid interaction problem. The aim is to develop a space-time Galerkin least square finite element method for magma-rock interaction problem. Magma is treated as a multi component, multiphase, compressible-incompressible fluid and rock is treated as an elastic material subject to time-dependent boundary conditions imposed by the motion of the interface and of the free Earth surface. The fluid and structure problems are solved independently and the coupling at the interface is done by considering the equilibrium conditions as boundary conditions. The discretised coupled solution from Navier Stokes equations for fluid flows, the elastodynamics equation for structure motion and the equation for mesh movement, is obtained by block iterative coupling method. The work will be useful to understand the link between surface data observed and deep magma dynamics in volcanic environment.

References

1. ANTONELLA LONGO AND MICHELE BARSANTI AND ANDREA CASSIOLI AND PAOLO PAPALE . A fi
nite element Galerkin/Least-squares method for computation of multicomponent compressible-incompressible flows. Computers & Fluids 67 (2012) 57–71.
2. T. E. TEZDUYAR AND S. SATHE AND R. KEEDY AND K. STEIN. Space-time fi
nite element techniques for computation of fluid-structure interactions. Comput. Methods Appl. Mech. Engrg. 195 (2006) 2002-2027.
3. J. J. W. VAN DER VEGT AND H. VAN DER VEN. Space-time discontinuous galerkin fi
nite element method with dynamic grid motion for inviscid compressible flows. Journal of Computational Physics 182 (2002) 546-585.

Solving an Elliptic Eigenvalue Problem via Automated Multi-Level Substructuring and Hierarchical Matrices

Peter Gerds, Lars Grasedyck
Institut für Geometrie und Praktische Mathematik, RWTH Aachen University
gerds@igpm.rwth-aachen.de, lgr@igpm.rwth-aachen.de

Abstract

To solve an elliptic eigenvalue problem we combine the automated multi-level substructuring (short AMLS) method with the concept of hierarchical matrices (short $\mathcal{H}$-matrices). AMLS is a substructuring method which projects the discretized eigenvalue problem onto a small subspace. A reduced eigenvalue problem has to be computed which delivers approximate solutions of the original problem.

Whereas the AMLS method is very effective in the two-dimensional case, the AMLS method is getting very expensive in the three-dimensional case, due to the fact that it computes the reduced eigenvalue problem via dense matrix operations.

Here, hierarchical matrices can help. $\mathcal{H}$-matrices are a data-sparse approximation of dense matrices which e.g. result from the discretisation of the inverse of elliptic partial differential operators. The big advantage of $\mathcal{H}$-matrices is that they allow matrix algebra in almost linear complexity.

In this talk we present how the AMLS method is combined with $\mathcal{H}$-matrices and how the reduced eigenvalue problem is computed by the fast $\mathcal{H}$-matrix algebra. Beside the discretisation error two additional errors occur, the projection error of the AMLS method and the error caused by the $\mathcal{H}$-matrix approximation. These errors, and the computational costs of the method as well, are controlled by several parameters. In this talk we benchmark the new method against a classical approach in various examples. Furhtermore, we discuss the computational complexity and show that we can compute the reduced eigenvalue problem in the three-dimensional case in almost linear complexity.

References

1. J. K. Bennighof and R. B. Lehoucq. An Automated Multilevel Substructuring Method for Eigenspace Computation in Linear Elastodynamics. SIAM J. Sci. Comput. 25 (2004) 2084-2106.
2. S. Börm and L. Grasedyck and W. Hackbusch. Introduction to Hierarchical Matrices with Applications. Engineering Analysis with Boundary Elements, 27 (2003) 405-422.
3. Chao Yang and Weiguo Gao and Zhaojun Bai and Xiaoye S. Li and Lie-Quan Lee and Parry Husbands and Esmond Ng. An Algebraic Substructuring Method for Large-Scale Eigenvalue Calculation. SIAM J. Sci. Comput. 27 (2005) 873-892.
4. Weiguo Gao and Xiaoye S. Li and Chao Yang and Zhaojun Bai. An Implementation and Evaluation of the AMLS Method for Sparse Eigenvalue Problems. ACM Trans. Math. Software 34 (2008) Art. 20, 28.

High-Order/hp-Adaptive Multilevel Discontinuous Galerkin Methods

Stefano Giani
Durham University
stefanogiani79@gmail.com

Paola Antonietti
MOX, Milan
paola.antonietti@polimi.it

Paul Houston
Univesity of Nottingham
Paul.Houston@nottingham.ac.uk

Abstract

We present a discontinuous Galerkin (DG) multilevel method with hp-adaptivity. The main advantage of this multilevel method is that the number of dimensions of the finite element space is independent on the presence of complicated or tiny features in the domain. In other words, even on a very complicated domain, an approximation of the solution can be computed with only a fistful of degrees of freedom. This is possible because two meshes are used: a fine mesh is used to describe the geometry of the domain with all its features, but the problem is actually solved on a coarse mesh that is, in general, too coarse to describe all the geometrical features of the domain. Unlikely other multilevel methods, this method does not perturb the problem, in the sense that the problem solved on the coarse mesh is always a discretization of the continuous problem, no matter how coarse the mesh is. The method itself is a hp-adaptive DG extension of composite finite elements (CFEs), introduced by S. Sauter a few years ago. Standard CFE methods are based on standard continuous Galerkin elements, which means that there are restrictions on the kind of boundary conditions that can be used. These limitations disappear by extending the method to DG elements.

The hp-adaptivity algorithm that we present for this multilevel method is completely automatic and capable of exploiting both local polynomial-degree-variation (p-refinement) and local mesh subdivision (h-refinement), thereby offering greater flexibility and efficiency than numerical techniques which only incorporate h-refinement or p-refinement alone.

This research has been funded by the EPSRC.

References

1. W. HACKBUSCH AND S.A. SAUTER. Composite finite elements for the approximation of PDEs on domains with complicated micro-structures. Numer. Math., 75:447–472, 1997.
2. P. ANTONIETTI AND S. GIANI AND P. HOUSTON. hp-Version Composite Discontinuous Galerkin Methods for Elliptic Problems on Complicated Domains. SISC, accepted.
3. S. GIANI AND P. HOUSTON. hp-Adaptive Composite Discontinuous Galerkin Methods for Elliptic Problems on Complicated Domains. Numerical Methods for Partial Differential Equations, submitted.
4. S. GIANI AND P. HOUSTON. Goal–Oriented Adaptive Composite Discontinuous Galerkin Methods for Incompressible Flows. Journal of Computational and Applied Mathematics, submitted.

PoliMIce: A Open Simulation Framework for Three-dimensional Ice Accretion

Mattia Garabelli, Giulio Gori, Marta Zocca, Giuseppe Quaranta, Alberto Guardone
Politecnico di Milano
mattia.garabelli@mail.polimi.it, giulio.gori@mail.polimi.it,
marta.zocca@mail.polimi.it, giuseppe.quaranta@mail.polimi.it,
alberto.guardone@polimi.it

Abstract

An open simulation framework is developed to perform two- and three-dimensional simulations of ice accretion over solid bodies in a wet air flow [1]. The PoliMIce (Politecnico di Milano Ice accretion software) library provides an unified framework allowing different aerodynamic and ice accretion software to communicate. The built-in ice accretion engine includes state-of-the-art ice formation models [2,3] and it implements a fully three-dimensional representation of the two-phase flow over the solid body to account for both rime and glaze ice formation. Numerical simulations are presented using the CFD open-source software OpenFOAM regarding in-flight ice accretion over two-dimensional airfoils and three-dimensional straight- and swept-wings. Simulation results compare fairly well with available experiments on ice accretion.

References

1. R. W. GENT AND N. P. DART AND J. T. CANSDALE. Aircraft icing. Phil. Trans R Soc Lond A, 2000.
2. T. G. MYERS AND D. W. HAMMOND. Ice and water film growth from incoming supercooled droplets. International Journal of Heat and Mass Transfer, 1999.
3. T. G. MYERS. Extension to the Messinger Model for Aircraft Icing. AIAA Journal, 2001.

Particle Simulations on NVIDIA GPUs

Nicolin Govender
University of Pretoria, CSIR South Africa
govender.nicolin@gmail.com

Abstract

Driven by the demand for real-time 3D graphics with prices kept low due to high selling volumes from the consumer gaming market, the programmable Graphic Processor Unit (GPU) has evolved into a multi-threaded processor which offers cluster type performance at a fraction of the cost [1]. The parallel nature of the GPU allows a large number of simple independent processes to be executed in parallel (SIMD) resulting in speed ups of a few hundred times for suitable applications over CPU implementations. One such application that is suited to parallel implementation is that of particle transport using discrete methods such as Monte Carlo (MC), Discrete Element Modeling (DEM) and Molecular Dynamics (MD).In this paper we focus on DEM [2]. DEM simulations are useful in a number of engineering disciplines with applications in mining, agriculture, pharmaceuticals and various other fields [3,4]. The computational cost of discrete methods limits the number of particles that can be simulated in a reasonable time frame without the use of a dedicated cluster. Industrial simulations typically requires millions of particles, which on current hardware is not computationally feasible. Thus continuum methods such as CFD are used even though they are approximate they yield solutions much faster. In this paper we will use GPU based code BLAZE-DEM developed by Govender et.al [5] to simulate a ball mill [6] containing millions of particles using a 12GB Nvidia K6000 graphics card. We will also discuss our GPU implementation and analyze the performance.

References

1. NVIDIA CUDA . cuda 5.5 toolkit. http://www.nvidia.com/cuda (2013).
2. P.A. CUNDALL AND O.D.L. STRACK.. A discrete numerical model for gran- ular assemblies. Geotechnique (1979), 29:47–65.
3. P. CLEARY. The filling of dragline buckets. Math. Eng. Ind. 29 (1998) 1–24.
4. W. KETTERHAGEN AND ET.AL UNDEFINED. Predicting the flow mode from hoppers using the discrete element method. Powder Technology 195 (2009) 1–10.
5. N GOVENDER AND ET.AL UNDEFINED. GPU based discrete element rigid body transport. 6th International Conference on Discrete Element Methods and related techniques, Mustoe G (ed.), Colorado School of Mines, 2013; 421-425..
6. B. MISHRA AND R. RAJAMANI. Simulation of charge motion in ball mills. part 1: experimental verifications. Int. J. Mineral Process 40 (1994) 171–186.

Solving Systems of Differential Equations by Algebrizability of Vector Fields in $\Re^3$.

María Esther Grimaldo Reyna, F. J . Almaguer-Martínez, R. Soto-Villalobos, M. V. I. Soto-Rocha
Universidad Autónoma de Nuevo León
megr_maac@yahoo.com.mx, almagerjavier@gmail.com,
robsotov@gmail.com, est_2@hotmail.com

Abstract

In this work a innovative technique to find the solution for systems of autonomous ordinary differential equations in $\Re^3$. is presented. Given an autonomous system of ordinary differential equations, the goal is to consider if the vector field f associated with the system is or not algebrizable. If f is algebrizable then is possible to find an algebra A, in which the system of differential equations can be rewritten in terms of a variable in that algebra. Later the solution of the system in the algebra A and the solution of the given original system are found.

References

1. L. V. AHLFORS. Complex Analysis. McGraw-Hill International Book Company, 1979.
2. E LÓPEZ GONZÁLEZ. Differential Equations over Algebras. Advances and Applications in Mathematical Sciences,8 Issue,2 (2011) 2189-214.
3. LORCH E. The Theory of Analytic Functions in Normed Abelian Vector Rings. Transactions of the American Mathematical Society, Vol. 54, No. 3 (1943), pp. 414-425.
4. PIERCE R. Associative Algebras. Springer-Verlag, New York, Heidelberg Berlin (1982).

Algebrizability of Planar Vector Fields

M.E Grimaldo Reyna, M.A Alcorta García
Universidad Autónoma de Nuevo León
megr_maac@yahoo.com.mx, maaracelia@gmail.com

M.E Frías-Armenta
Universidad De Sonora
martineduardofrias@gmail.com

E. López González
Universidad de Ciudad Juárez
elgonzal@uacj.mx

Abstract

Consider a planar vector field f. We give a method to determine the existence of an algebra with respect to the which f is Lorch-differentiable, when the algebra exists, it is found. We show for any Lorch-differentiable vector field, that their products by the constants of the algebra are their infinitesimal Lie symmetries. We give conditions under the which there exists a function $\alpha(x, y)$, called algebrizante factor, such that the product of αf is a Lorch-differentiable vector field. Inverse integrating factors are found for these vector fields.

References

1. J. WARD. From Generalized Cauchy-Riemann Equations to Linear Algebra. Proc. of the Amer. Math. Soc.Vol 4,(1953) 456-461.
2. E. LÓPEZ- GONZÁLEZ. Differential Equations over Algebras. Advances and Applications in Mathematical Sciences,8 Issue,2 (2012)189-214.
3. I. A. GARCÍA AND M. A. GRAU. A survey on the inverse integrating factor. Preprint arxiv:0903.0941v1 [math.DS] .

A Posteriori Estimates for Interior Penalty Discontinuous Galerkin Eigenvalue/eigenfunction Approximations.

Luka Grubisic
University of Zagreb
luka@math.hr

Abstract

We analyze the interior penalty Galerkin methods in the framework of operator theory. To this end we develop resolvent estimates in the limit of the large penalty parameter and present approximation estimates for both eigenfunctions as well as eigenvalues. This approach allows us to treat eigenfunction approximation error estimates in the associated discontinuous Galerkin norm and give geometric criteria for balancing the errors caused by leaving the variational domain of the operator as well as those made when truncating the approximation.

This is a joint work with S. Giani, H. Hakula and J. Ovall.

This work is submitted for the minysimposium Advances in Numerical Methods for Eigenvalue Problems and Applications (Stefano Giani, University of Durham))

References

1. L. GRUBISIC. Relative convergence estimates for the spectral asymptotic in the Large Coupling Limit. Integral Equations and Operator Theory, Volume 65, Number 1, 2009, Pages 51-81..

Grid Convergence for Adaptive Simulations of Three-dimensional Normal Drop Impacts Onto Liquid Films

Paola Brambilla
Politecnico di Milano
paola.brambilla@mail.polimi.it

Giulio Romanelli
Lucerne University of Applied Sciences and Arts
giulio.romanelli@gmail.com

Abstract

Normal liquid drop impact on a liquid film [1,2] is studied numerically using a modified OpenFOAM solver in three-spatial dimensions, in which dynamic grid refinement is modified to accurately describe the initial conditions before impact [3]. Numerical simulations are found to accurately predict the evolution of the splashing lamella. A new procedure for assessing grid convergence is introduced, which is based on the definition of a hierarchical set of bounding boxes in which the total liquid volume is computed to assess global as well as local grid convergence.

References

1. RIEBER AND M. & FROHN AND A. 1999. A numerical study on the mechanism of splashing. Int. J. of Heat and Fluid Flow 20, 455–461, 1999.
2. COSSALI AND G. E. AND MARENGO AND M. AND COGHE AND A. AND ZHADANOV AND S. . The role of time in single drop splash on thin film. .. Experiments in Fluids 36, 888–900, 2004.
3. HIRT AND C. W. AND NICHOLS AND B. D. . Volume of fluid (VOF) method for the dynamics of free boundaries. J. of Computational Physics 39, 201–225, 1981..

Hardware Accelerated Neural Computing in Embedded Systems

Karol Gugała, Aleksandra Świetlicka, Andrzej Rybarczyk
Poznan University of Technology, Faculty of Computing, Chair of Computer Engineering
karol.gugala@put.poznan.pl, aleksandra.swietlicka@put.poznan.pl,
andrzej.rybarczyk@put.poznan.pl

Abstract

Nowadays embedded systems based computing solutions are getting on popularity in various areas - from mobile communication devices to complex control systems. Evolution of those systems allows to build more complex and intelligent solutions, such as using neural networks for data processing.

Recently, Extensible Processing Platform (EPP) solutions merging ARM based SoC and FPGA platform [1] [2] are getting more popular. This approach enables to create dedicated coprocessor and use it as computation accelerator in complex systems [3].

On the other hand there are various many-core processors available on the market which can be used as accelerators [4]. Greatest advantage of this approach is less power consumption than EPP based ones.

In this paper we focus on comparison on efficiency of implementation of neural networks based computing in embedded systems with use of EPP platforms and many-core CPU's. Main aspects we are focusing on are: power consumptions, processing speed and implementation cost.

References

1. XILINX INC.. Zynq-7000 All Programmable SoC First Generation Architecture. online resource www.xilinx.com [accessed 8-12-2013].
2. ALTERA INC.. User-Customizable ARM-Based SoC. online resource www.altera.com [accessed 8-12-2013].
3. A. RYBARCZYK AND M. SZULC. The concept of a microcontroller with neural-matrix coprocessor for control systems that exploits reconfigurable FPGAs. Robot Motion and Control, 2002. RoMoCo '02. Proceedings of the Third International Workshop on., pp: 123-1.
4. ADAPTEVA INC.. Epiphany-III 16 core 65nm Microprocessor. online resource http://www.adapteva.com/epiphanyiii/ [accessed 8-12-2013].

Image Local Descriptor Matching Coprocessor for Embedded Systems

Rafał Kapela
Poznan University of Technology, Faculty of Computing, Chair of Computer Engineering,
INSIGHT, Dublin City University, Dublin, Ireland
rafal.kapela@put.poznan.pl

Karol Gugała, Paweł Śniatała, Mateusz Majchrzycki
Poznan University of Technology, Faculty of Computing, Chair of Computer Engineering
karol.gugala@put.poznan.pl, pawel.sniatala@put.poznan.pl,
mateusz.majchrzycki@put.poznan.pl

Abstract

Embedded systems, found in leading consumer markets, often require compute-intensive applications, which are part of the implemented solutions. Video processing is one of such area, where computational demands are still increasing. The use of hardware accelerators, implemented in reprogrammable logic such as field-programmable gate arrays (FPGA), lets achieve processing speedups of orders of magnitude versus their counterpart CPU-based software approaches. The paper proposes extensible processing platform (EPP) based system, which consists of ARM embedded processor running Linux operating system and graphics co-processor implemented in FPGA.

The possible application of the proposed structure is illustrated by implementation of the Binary Robust Independent Elementary Features (BRIEF) [1] algorithm. ARM dual core processor that hosts Linux operating system is responsible for receiving, synchronizing and processing video frames or images intended for future description. For description of image/frame a BRIEF algorithm is applied. The main advantages of BRIEF are that it produces a binary output that can be compared based on the Hamming distance and it is the quickest from the all family of local image descriptors. FPGA-based co-processor accelerates the core of the descriptors matching system – nearest neighbours (NN) algorithm. Since BRIEF gives us a descriptors in binary form it is very convenient to use Hamming distance for calculations thus reducing the overall complexity of the matching algorithm. Since calculations of NNs for a single descriptor does not involve the knowledge about results for other descriptors from the query this calculations can be easily parallelized making the overall time performance of the system much more efficient. The hardware KNN coprocessor is designed to work in two modes. In both of them FIFO queues are used to exchange data between the hardware core and main unit. In the first stage IP core takes input data and saves them in internal memory. In the second stage the query descriptors are passed to the core where each of them is compared with the original ones in order to produce a vector of nearest neighbour indexes.

Proposed system can be robust base for further development of a mobile intelligent tracking and control systems.

References

1. Calonder Michael and Lepetit Vincent and Strecha Christoph and Fua Pascal. BRIEF: Binary Robust Independent Elementary Features. Lecture Notes in Computer Science, pp. 778-792, 2010.

Large Scale Simulations of Rigid Fiber Suspensions

Katarina Gustavsson
Royal Institute of Technology, KTH
katg@kth.se

Abstract

Fiber dynamics is of fundamental importance for understanding many flows arising in physics, biology and engineering. One typical example is paper-pulp, where the micro-structure of the suspension is made up of slender fibers in a fluid.

Here we present a numerical method designed to simulate, on a particle level, the dynamics of slender, rigid fibers immersed in an incompressible fluid. We consider microscopic, but non-Brownian fibers sedimenting due to gravity at very low Reynolds number, i.e. Stokes flow.

The key point in the development of the method is that Stokes equations can be reformulated as boundary integral equations acting on the surface of the immersed fibers. The great advantage with such a formulation is the reduction of dimensionality. Instead of solving a three-dimensional PDE for the motion of the fibers and the fluid velocity in the whole domain of interest, a system of two-dimensional boundary integral equations can be solved solely over the surface of the immersed fibers. Since the fibers are slender we can reduce the dimensionality of the problem even further by using a slender body approximation. This results in a model consisting of a system of coupled, one-dimensional integral equations acting on the fiber centerlines, [1, 2]. The model takes into account the hydrodynamic interactions between the fluid and the fibers and relates the forces exerted on the fibers to their velocities. It also captures the local interaction of the fiber with itself (as mediated by the fluid), as well as with all other fibers in the system.

Calculations of the hydrodynamic interactions are very time consuming due to their long-range nature. Each fiber interacts with all other fibers in the system leading to a computational effort of $O(M^2)$, where M is the total number of fibers. These interactions present a great challenge even to modern computers and fast summation algorithms e.g. the fast multipole method or a fast Ewald summation method are called for.

We present results from simulations showing some characteristic features of a sedimenting fiber suspension. E.g. a fiber suspension with an initial homogeneous and random distribution of fibers will form large scale inhomogeneities in the fiber distribution during sedimentation. Elongated fiber-dense streamers will form, surrounded by regions of clear fluid. This is all in agreement with what has been presented both in experiments and numerical simulations [3, 4].

References

1. G. K. BATCHELOR. Slender-body theory for particles of arbitrary cross-section in Stokes flow. J. Fluid Mech. 44 (1970) 419-440.
2. R. E. JOHNSON. An improved slender-body theory for Stokes flow. J. Fluid Mech. 99 (1980) 411-431.
3. A.-K. TORNBERG AND K. GUSTAVSSON. A numerical method for simulations of rigid fiber suspensions. J. Comput. Phys. 215 (2005) 172-196.
4. K. GUSTAVSSON AND A.-K. TORNBERG. Gravity induced sedimentation of slender fibers. Phys. Fluids 21 (2009) .

On Approximation of Parametric Eigenvalue Problems

Harri Hakula
Aalto University
Harri.Hakula@aalto.fi

Abstract

In this talk, the focus is on stochastic or parametric eigenvalue problems. In recent years there has been significant progress in the numerical solution of stochastic PDEs using different SFEM strategies. However, the eigenvalue problem remains a challenge.

In modern stochastic FEM it is assumed that random variables are introduced as series (spectral) expansions into the equations. So, for the model problem with a random coefficient $a(x, \omega)$: For a.e. $\omega \in \Gamma$, $x \in D$,

$$\nabla \cdot (a(x, \omega) \nabla u(x, \omega)) = \lambda(\omega) u(x, \omega),$$

where D and Γ refer to deterministic and stochastic dimensions, respectively, it is immediately clear that the randomness is on both sides of the equation. This implies that the standard methods cannot be used as such.

We illustrate with numerical examples the features of inverse power iteration based methods and collocation based methods that represent the state-of-the-art at the moment. In particular we concentrate on a new variant of hybrid Galerkin formulation where the basis functions are in tensor form, but collocation is used to adjust the eigenvalue information.

References

1. C. V. VERHOOSEL AND M. A. GUTIERREZ AND S. J. HULSHOFF. Iterative solution of the random eigenvalue problem with application to spectral stochastic finite element systems. nt. J. Numer. Meth. Engng., 68:2006:401–424.
2. ROMAN ANDREEV AND CHRISTOPH SCHWAB. Sparse Tensor Approximation of Parametric Eigenvalue Problems. in Numerical Analysis of Multiscale Problems, Springer 2012.

Numerical Simulation of Circumferentialy Averaged Flow in a Multistage Turbine

Jaroslav Fořt, Jiří Fürst, Jan Halama, Jiří Holman, Jan Karel, Vladimír Prokop, David Trdlička
CTU Prague
Jaroslav.Fort@fs.cvut.cz, Jiri.Furst@fs.cvut.cz,
Jan.Halama@fs.cvut.cz, Jiri.Holman@fs.cvut.cz,
Jan.Karel@fs.cvut.cz, Vladimir.Prokop@fs.cvut.cz,
David.Trdlicka@fs.cvut.cz

Abstract

Presented flow model is based on the solution of circuferentialy averaged Euler equation for the three-dimensional flow in a turbine. The computational domain is the real meridional cut of a turbine, i.e. the axial and the radial dimensions of the turbine are kept. The blockage due to the variable thickness of blades is taken into account. The shape of the blades (flow turning) is included in the form of prescribed flow angle. This flow model is coupled with a model which adds losses and flow deviation. The solution domain is discretized by a structured grid. Numerical solution is based on the iterative coupling of flow solver with the loss model. The flow solver uses a finite volume method with AUSM type flux. First tests show, that such solver is able to predict well flow angles and a radial distribution of flow. Such information is usefull for turbine designers, since it is possible to obtain reasonable amount of information about flow field in a multistage configuration during relatively short time, compared to fully three-dimensional simulation.

References

1. SIMON. J.F. AND LÉONARD O.. A Throughflow Analysis Tool Based on the Navier-Stokes Equations. Proc. of the 6th European Turbomachinery Conference (ETC'2005), Lille, France, 2005.
2. AUNGIER R.H.. Turbine Aerodynamics: Axial-Flow and Radial-Inflow Turbine Design and Analysis. ASME Press, 2006.
3. ZHU J. AND SJOLANDER S.A.. Improved Profile Loss and Deviation Correlations for Axial-Turbine Blade Rows. Proceedings of ASME Turbo Expo 2005, paper GT2005-69077.

Coupled Code System for Nuclear Reactor Fuel Loading Optimization

Jiří Egermaier, Milan Hanuš, Hana Kopincová, Roman Kužel, Zbyněk Vastl
University of West Bohemia
jirieggy@kma.zcu.cz, mhanus@kma.zcu.cz, kopincov@kma.zcu.cz,
rkuzel@kma.zcu.cz, zvastl@kma.zcu.cz

Abstract

Fuel loading optimization is an important part of nuclear reactor operation. To efficiently perform this task, nuclear engineers need to be supported by sophisticated software tools. In this contribution, we will present such a code system that is currently being developed as a joint project of the University of West Bohemia in Pilsen and the Czech Technical University in Prague.

The code combines state of the art combinatorial optimization methods with neutronic and thermal-hydraulic calculations in a modular way, using the standard Python language to facilitate the data transfers between modules. In order to increase the flexibility of the code and taking into account the size and complexity of modern reactor cores, the neutronics module must efficiently handle difficult-to-converge generalized eigenvalue problems on large, possibly highly anisotropic unstructured meshes. The use of novel solution methods is therefore required, such as those based on smoothed algebraic multigrid with aggressive coarsening which will be presented in the talk. Parallelization and GPU implementation of various parts of the code will also be discussed as these lead to significant increase of the speed of solution, critical for the repeated optimization searches.

References

1. N. BELL AND M. GARLAND. Cusp: Generic Parallel Algorithms for Sparse Matrix and Graph Computations. http://cusplibrary.github.com.
2. D. G. CACUCI (ED.). Handbook of Nuclear Engineering. Springer (2010).
3. OECD NEA. Neutronics/Thermal-hydraulics Coupling in LWR Technology: State-of-the-art Report. 2004.
4. A. LOGG AND K.-A. MARDAL AND G. N. WELLS ET AL.. Automated Solution of Differential Equations by the Finite Element Method. Springer (2012).
5. A. SCHIJVER. Combinatorial Optimization: Polyhedra and Efficiency. Springer (2003).
6. P. VANĚK AND J. MANDEL AND M. BREZINA. Algebraic Multigrid by Smoothed Aggregation for Second and Fourth Order Elliptic Problems. Computing 56 (1996) 179–196.

FLLOP: A Novel Massively Parallel QP Solver

Václav Hapla, David Horák, Alexandros Markopoulos, Lubomír Říha
IT4Innovations, VSB - Technical University of Ostrava
vaclav.hapla@vsb.cz, david.horak@vsb.cz,
alexandros.markopoulos@vsb.cz, lubomir.riha@vsb.cz

Abstract

Discretization of most engineering problems, described by partial differential equations, leads to large sparse linear systems of equations. However, problems expressible as elliptic variational inequalities, such as those describing the equilibrium of elastic bodies in mutual contact, are more naturally discretized to quadratic programming problems (QP). They can be thought of as a generalization of linear systems of equations being subject to equality and inequality constraints and take the form find $x = \arg\min_x \frac{1}{2}x^T Ax - b^T x$ s.t. $B_E x = c_E,\ B_I x \leq c_I,\ l \leq x \leq u$.

We present here our novel package FLLOP for quadratic programming and FETI domain decomposition, built on top of PETSc (similarly to TAO and SLEPc packages). Currently tested applications include mainly engineering problems of structure mechanics: linear elasticity, contact problems, elasto-plasticity, and shape optimization.

FLLOP API is designed to be easy-to-use but at the same time efficient and HPC-centric. One of the principal design decisions is decoupling of concepts of QP problems, QP transforms and QP solvers. A QP transform is a mapping deriving from the given original QP a new QP which is simpler or has some better properties. It is of course required that the solution of the original QP can be computed from the solution of the derived one. QP transforms often allow use of efficient solvers that are not compatible with the original QP. However, they are themselves solver-neutral. The typical workflow when solving a QP with FLLOP is as follows: (1) specification of the QP by the user, (2) an automatic or user-specified series of QP transforms, (3) an automatic or manual choice of a suitable solver, (4) solution of the most derived QPs by the chosen solver, (5) a series of reconstructions to get a solution of the original QP. The algebraic part of the FETI DDM method is a special QP transform.

References

1. V. HAPLA AND D. HORAK. A Comparison of FETI Natural Coarse Space Projector Implementation Strategies. Proceedings of PARENG2013 (2013) Paper 6, DOI 10.4203/ccp.101.6.
2. V. HAPLA AND D. HORAK AND M. MERTA. Use of direct solvers in TFETI massively parallel implementation. Proceedings of PARA 2012, LNCS 7782 (2013) 192-205, DOI 10.1007/978-3-642-36803-5_14.
3. D. HORAK AND V. HAPLA. TFETI coarse problem massively parallel implementation. ECCOMAS 2012 e-Book Full Papers (2012) 8260-8267, ISBN 978-395035370-9.
4. V. HAPLA AND D. HORAK. TFETI coarse space projectors parallelization strategies. Proceedings of PPAM 201, LNCS 7203 (2012) 152-162, DOI 10.1007/978-3-642-31464-3_16.
5. T. KOZUBEK AND V. VONDRAK AND M. MENSIK AND D. HORAK AND Z. DOSTAL AND V. HAPLA AND P. KABELIKOVA AND M. CERMAK. Total FETI domain decomposition method and its massively parallel implementation. Advances in Engineering Software 60–61 (2013) 14-22, DOI 10.1016/j.advengsoft.2013.04.001.
6. Z. DOSTAL. Optimal Quadratic Programming Algorithms: With Applications to Variational Inequalities. Springer Optimization and Its Applications, Book 23 (2009).
7. Z. DOSTAL AND T. KOZUBEK. An optimal algorithm and superrelaxation for minimization of a quadratic function subject to separable convex constraints with applications. Mathematical Programming 135 1-2 (2013) 195-220.

Molecular Dynamics Simulations in Engineering

Hans Hasse
University of Kaiserslautern
hans.hasse@mv.uni-kl.de

Abstract

Molecular dynamics (MD) simulations have long been recognized as valuable in physics, chemistry and biochemistry, but now also become increasingly important in different fields of engineering. At the heart of MD simulations is the description of the interaction of particles on the atomistic scale (usually single atoms of groups of a few atoms) by classical force fields. The attractiveness of the method is largely due to the fact that no further assumptions are used. Based on the force fields also complex scenarios can be simulated, the results are completely predictive, and should only depend on the choice of the force field. Major challenges arise from the limitations in number of particles and, more importantly, in the time span that can be covered. The present world record in system size for MD simulations is over $4 \cdot 10^{12}$ particles [1], corresponding to cubic box of a few micrometers length filled with a liquid, and, hence, an object that could almost be seen with the naked eye. Highly scalable MD codes, optimized for massively parallel execution on supercomputing architectures are available as free software [2].

After briefly discussing the development force fields, examples for applications of MD simulations in engineering are presented. They illustrate the benefits that can be drawn from MD simulations in that field but also the challenges, which include software and hardware issues as well as issues of modeling and simulation methods.

References

1. W. Eckhardt and A. Heinecke and R. Bader and M. Brehm and N. Hammer and H. Huber and H.-G. Kleinhenz and J. Vrabec and H. Hasse and M. Horsch and M. Bernreuther and C. Glass and C. Niethammer and A. Bode and H.-J. Bungartz. 591 TFLOPS Multi-Trillion Particles Simulation on SuperMUC. Supercomputing - Proceedings of the XXVIII. International Supercomputing Conference (ISC), Heidelberg, 2013; pp. 1–12.
2. LS1 Mardyn. http://www.ls1-mardyn.de/. Website, 2014.

Sensitivity Analysis of a FEM Model and Its Use in Material Identification

Jan Heczko
Department of Mechanics, Faculty of Applied Sciences, University of West Bohemia in Pilsen, Univerzitní 22, 306 14 Plzeň, Czech Republic
jheczko@kme.zcu.cz

Radek Kottner
European Centre of Excellence, NTIS - New Technologies for Information Society, Faculty of Applied Sciences, University of West Bohemia in Pilsen, Univerzitní 22, 306 14 Plzeň, Czech Republic
kottner@kme.zcu.cz

Abstract

The increasing interest in polymeric and biological materials is reflected in raising complexity of material models which describe effects such as nonlinear static response or history- and time-dependent behavior. Precise and reliable identification of such models and their use in design requires various types of experiments and appropriate computational methods. An inherent part of these methods is sensitivity analysis, either as a part of gradient-based optimization methods or to evaluate robustness and stability of design.

In this contribution we present an approach to sensitivity analysis of FEM-discretized model of a compressive test of rubber. Cylindrical specimen is used in the test and nonhomogeneous deformation arises due to friction between the specimen and the surfaces of the testing machine. Nonhomogeneity of deformation is the reason for using FEM. This uniaxial compression test is often used for material characterization (e.g. in [2, 3]), therefore the output of this work is of great practical importance. Sensitivity with respect to material parameters of a history-dependent nonlinear material model is derived using the direct differentiation method [1] and it is used in identification of material parameters and compared to finite differences.

References

1. M. KLEIBER AND H. ANTÚNEZ AND T. D. HIEN AND P. KOWALCZYK. Parameter Sensitivity in Nonlinear Mechanics: Theory and Finite Element Computations. John Wiley & Sons Ltd. 1997.
2. A. POŽIVILOVÁ. Constitutive modelling of hyperelastic materials using the logarithmic description. PhD thesis, Czech Technical University. 2002.
3. J. HECZKO AND R. KOTTNER AND T. KROUPA. Identification of Parameters of a Nonlinear Material Model Considering the Effects of Viscoelasticity and Damage. CMC: Computers, Materials & Continua, Vol. 33, No. 3, pp. 257-273. 2013.

Development of a Fuzzy Logic Controller for Variable Quality Control Charts

Seyed Mahdi Homayouni
Department of Industrial Engineering, Lenjan Branch, Islamic Azad University, Isfahan, Iran
homayouni.mahdi@gmail.com

Sai Hong Tang
Department of Mechanical & Manufacturing Engineering, Faculty of Engineering, Universiti Putra Malaysia, Selangor, Malaysia
saihong@upm.edu.my

Abstract

Quality control charts are used to depict the characteristics of quality of a product (Gulbay and Kahraman, 2007). Statistical quality control (SQC) techniques can help to predict the manufacturing process trend. Hence, one can reduce the amount of defective products, using these techniques (Montgomery, 2009). Applying the statistical quality control tools, especially when using the attributes face with many constraints. For example, a product can only be categorized into ”conforming” or ”nonconforming” for attributes and ”under control” or ”out of control” for variables. However, a product can also be placed somewhere between these two major categories (Aladdini et al., 2009). Some major problems with implementing SQC techniques includes the lack of flexibility of existing laws to monitor the production process, and needing to use human knowledge to assess the current state of the process. to overcome these problem some methods using fuzzy numbers and combine them with existing statistical control charts have been applied (Faraz and Shapiro, 2010; and Tong and Wang, 2012). People often express attributes or characteristics of a phenomenon (e.g. products), in words (known as linguistic variables). For example, a product can be beautiful, somewhat beautiful, or not beautiful (ugly). According to literature, none of the researches have applied fuzzy logic controllers for monitoring and quality control of products. In this paper, a general fuzzy logic controller is designed for controlling the variable quality characteristics. Moreover, fuzzy rules are designed for interpreting the quality control charts. Results of such control system is compared to those from the traditional statistical control charts.

References

1. A. ALAEDDINI AND M. GHAZANFARI AND M.A. NAYERI. A hybrid fuzzy-statistical clustering approach for estimating the time of changes in fixed and variable sampling control charts. Information Sciences, 179(11), 1769-1784, 2009..
2. A. FARAZ AND A. F. SHAPIRO. An application of fuzzy random variables to control charts. Fuzzy Sets and Systems, 161(20), 2684-2694, 2010..
3. M. GÜLBAY AND C. KAHRAMAN. An alternative approach to fuzzy control charts: Direct fuzzy approach. Information Sciences, 177(6), 1463-1480, 2007..
4. D.C. MONTGOMERY. Introduction to statistical quality control. , 6th ed. John Wiley and Sons Inc., USA, 2009..
5. X. TONG AND Z. WANG. . Fuzzy acceptance sampling plans for inspection of geospatial data with ambiguity in quality characteristics. Computers & Geosciences, 48(0), 256-266, 2012..

Automatic Differentiation for Matlab With ADiMat

Alexander Hück, Christian Bischof, Johannes Willkomm
TU Darmstadt
alexander.hueck@sc.tu-darmstadt.de,
christian.bischof@sc.tu-darmstadt.de,
johannes.willkomm@sc.tu-darmstadt.de

Abstract

The ADiMat software is a tool that offers *Automatic Differentiation* of any Matlab function using a hybrid approach combining source transformation and operator overloading. We give a brief overview of ADiMat and its functionality and recent performance improvements.

References

1. CHRISTIAN BISCHOF AND H. MARTIN BÜCKER AND BRUNO LANG AND A. RASCH AND ANDRE VEHRESCHILD. "Combining Source Transformation and Operator Overloading Techniques to Compute Derivatives for MATLAB Programs. IEEE Computer Society. Proceedings of the Second IEEE International Workshop on Source Code Analysis and Manipulation (SCAM 2002) 65-72.
2. JOHANNES WILLKOMM AND CHRISTIAN BISCHOF AND H. MARTIN BÜCKER. The New User Interface of ADiMat and How to Use it with DAE Solvers in Matlab and Octave. ICCE 2011 conference (2011).
3. FORTH UNDEFINED AND SHAUN A. An Efficient Overloaded Implementation of Forward Mode Automatic Differentiation in MATLAB. ACM Transactions on Mathematical Software (TOMS) (2006).
4. RALL UNDEFINED AND LOUIS B AND CORLISS AND GEORGE F. An Introduction to Automatic Differentiation. Computational Differentiation: Techniques, Applications, and Tools (1996) 1-17.

Probabilistic Estimation of Material Parameters Based on a Set of Experimental Curves

Eliška Janouchová, Anna Kučerová, Jan Sýkora
Faculty of Civil Engineering, Czech Technical University in Prague
eliska.janouchova@fsv.cvut.cz, anicka@cml.fsv.cvut.cz,
jan.sykora.1@fsv.cvut.cz

Abstract

Advances in meta-modelling and increasing computational capacity of modern computers permitted many researches to focus on parameter identification in probabilistic setting. Bayesian approach to parameter identification has several appealing advantages comparing to traditional data fitting, e.g. identification problem is well-posed, results provide probabilistic description of the actual knowledge about the parameters and not just a single value etc. However, the practical application of Bayesian inference to real experimental data opens many non-trivial problems concerning namely formulation of the a priori probability density functions or the likelihood functions. One has to pay attention to properly quantify and especially not to underestimate all the relevant uncertainties. Also the interpretation of experimental observations and their credibility needs to be done very carefully. In this contribution we present a comparison of different formulations of likelihood function for a set of experimentally measured curves and its impact on the resulting posterior distributions.

References

1. A. GELMAN AND J. B. CARLIN AND H. S. STERN AND D. B. RUBIN. Bayesian data analysis. 2nd ed. Boca Raton, FL: Chapman and Hall/CRC 2004.
2. W. M. BOLSTAD. Understanding Computational Bayesian Statistics. Hoboken, NJ: Wiley 2010.

The Hybridized Numerical Methods for PDEs

Youngmok Jeon
Ajou University
yjeon@ajou.ac.kr

Abstract

We introduce the hybridized methods for partial differential equations. The method consists of two procedures; (1) construction of local solution on each cell of a triangulation by assuming trace data of the solution on each cell boundary (2) patching them by using flux continuity on intercell boundaries. Hence, the global stiffness system contains only the skeleton data of the solution as unknown. Therefore, the major advantages of this approach are reduction of degrees of freedom by embedded static condensation property and the local flux conservation.

We introduce two different numerical approaches; one based on discontinuous Galerkin methods and the other on finite difference methods. For the discontinuous Galerkin type methods there have been many different approaches developed for the last 5-6 years. The major differences on those existing methods basically depend on what kind of local problem solvers are used. One may use the LDG method, penalty methods or the Bauman-Oden type nonsymmetric solver. In this talk we also introduce a FD type approach for the hybridized equation.

References

1. Y. JEON AND E.-J. PARK. New locally conservative finite element methods on a rectangular mesh. Numer. Math. 123 (2013) 97-119.

Fully Discrete $A - \phi$ Finite Element Method for Maxwell's Equations With Nonlinear Conductivity

Tong Kang, Chen Tao
Communication University of China
kangtong@cuc.edu.cn, chentao@cuc.edu.cn

Abstract

This paper is devoted to the study of a fully discrete $A - \phi$ finite element scheme to solve nonlinear Maxwell's equations based on backward Euler discretization in time and nodal finite elements in space. The nonlinearity is due to a field-dependent conductivity with the power-law form $|E|^{\alpha-1}$, $0 < \alpha < 1$. The system under study is hyperbolic and due to the nonlinear conductivity it lacks strong estimates of the second time derivative. We design a nonlinear time-discrete scheme for approximation in suitable function spaces. We show the well-posedness of the problem, prove convergence of our semidiscrete scheme based on boundedness of the second derivative in the dual space and derive the error estimate. Convergence of the nonlinear term is based on the Minty-Browder technique. We also discuss the error estimate for the fully discretized problem and support the theoretical result by some numerical experiments.

References

1. S. DURAND AND M. SLODICKA. Fully discrete finite element method for Maxwell's equations with nonlinear conductivity. IMA J. Numer. Anal. 31 (2011) 1713-1733.
2. T. KANG AND K. I. KIM. Fully discrete potential-based finite element methods for a transient eddy current problem. Computing, 85(2009) 339-362.

New Behaviour Emulation for Autonomous Self-learning Agent.

Igor Karoń, Andrzej Rybarczyk
Poznan University of Technology
igor.karon@doctorate.put.poznan.pl, andrzej.rybarczyk@put.poznan.pl

Abstract

Autonomous agents are widely invested field of research[1,2,4] but for truly autonomous behavior abilities like: autodiagnostic with self-repaire, self-lerning[4,5], accumulation of knowledge[5] new behaviours emulation is needed. Till now work focused on self-learning were focused mainly on new shapes recognition[4], Neural Network for control purpose learning and behaviour maping. Thus this work will focus on new behaviours emulation with simplified shape recognition.

Full work is simulation based which provides wider posibilities of algorithm testing for different robot shapes and abilities. For this work robot is represented as simple physical point with okreslonymi physical strength to move some objects, speed and maneuver abilities.Sensors used for image recognition are area based sensors where robot have posibilities to recognize object shape and color.

Behaviour emulation was based on FuzzyLogic module and Spiking Neuron Networks. Fuzzy Module was critical-rule base for new rules and Spiking Neuron Network generation and modification. Where behaviors have been base on both modules. Full description of presented system with carried experiments will be described in full paper.

References

1. JOSEPH MODAYIL AND BENJAMIN KUIPERS. Where do actions come from? Autonomous robot learning of objects and actions. Department of Computer Sciences The University of Texas at Austin.
2. J. M. HERRMANN AND K. PAWELZIK AND T. GEISEL. Self-Localization of Autonomous Robots by Hidden Representations. Autonomous Robots 7, 31–40 (1999).
3. KLAUS HOLTZ. Autosophy Networks yield self-learning Robot Vision. WESCON/'93. Conference Record.
4. S. F. DESOUKY AND H. M. SCHWARTZ. A Novel Hybrid Learning Technique Applied to a Self-Learning Multi-Robot System. Proceedings of the 2009 IEEE International Conference on Systems, Man, and Cybernetics.
5. S. K. JAYAWEERA AND Y. LI AND M. BKASSINY AND CH. CHRISTODOULOU AND K. A. AVERY. Radiobots: The Autonomous, Self-learning Future Cognitive Radios . 2011 International Symposium on Intelligent Signal Processing and Communication Systems (ISPACS) December 7-9, 2011.

Numerical Computation of Flow Noise Around a Circular Cylinder Using LES

Karthik Karunakaran, Bhattacharyya S K, Vengadesan S
Indian Institute of Technology Madras
karthikkaero@gmail.com, skbh@iitm.ac.in, vengades@iitm.ac.in

Abstract

In this paper, numerical simulations are conducted to obtain the flow noise around a 2D circular cylinder at a Reynolds number of 84,770. We use the Large eddy simulations (LES) coupled with the Ffowcs-Williams and Hawking's (FW-H) acoustic analogy to capture the flow induced noise. The obtained sound pressure time history is converted to sound pressure spectrum using the Welch's method. The effect of correlation length has also been investigated. The numerically obtained value of overall sound pressure level (OASPL) and the sound pressure spectrum are compared well with the measured data. The paper presents the procedure for the acoustic analogy method and its implementation in the software, and shows how flow induced noise generated by the turbulent boundary layer over a stationary surface can be computed numerically.

Keywords: Acoustics, CFD, Circular Cylinder, Flow Noise, Fluid-Structure Interaction, LES

References

1. W. F. KING AND E. PFIZENMAIER. An Experimental Study of Sound Generated by Flows Around Cylinders of Different Cross-Section. Journal of Sound and Vibration. 328 (2009) 318–337.
2. P. D. WELCH. The Use of Fast Fourier Transform for the Estimation of Power Spectra: A Method Based on Time Averaging Over Short, Modified Periodograms. IEEE Transactions on Audio Electroacoustics. AU-15 (1967) 70–73.
3. J. C. HARDIN AND S. L. LAMKIN. Aeroacoustic Computation of Cylinder Wake Flow. AIAA Journal. 22(1) (1984) 51-57.

Modeling the Propagation of Electromagnetic Waves in Human Retina: Numerical Analysis and Simulations

Adérito Araújo, Sílvia Barbeiro, Maryam Khaksar Ghalati
CMUC, Department of Mathematics, University of Coimbra
alma@mat.uc.pt, silvia@mat.uc.pt, maryam@mat.uc.pt

Abstract

The human retina is a complex structure that is responsible for the sense of vision. There are a number of eye-related pathologies that can be identified by analyzing the retinal layers in detail. Optical Coherence Tomography, OCT, is a relatively recent imaging technique that allows high-resolution imaging of the retina. It relies in certain optical characteristics of light to provide information of the eye fundus, facilitating the diagnosis of some eye pathologies. In order to better understand the information carried in an OCT, we must model in detail the behavior of the electromagnetic wave as it travels through the sample. Several different models have been developed to describe the interactions of the field with biological structures. Simulating the complexity of the retina, in particular the variation of the size and shape of each structure, distance between them and the respective refractive indexes, requires a rigorous approach that can be achieved by solving Maxwell's equations.

In this work we discuss the numerical discretization of the time-dependent Maxwell's equations. We have chosen to use the nodal discontinuous Galerkin (DG) method [1] for the integration in space due to the fact that it is a high-order accurate method that can easily handle complex geometries. Moreover, local refinement strategies can be incorporated due to the ability of the method to deal with irregular meshes with hanging nodes and local spaces of different orders. We focus on deriving convergent estimates of fully discrete schemes. To illustrate the theoretical results we present some numerical examples

References

1. J. HESTHAVEN AND T. WARBURTON. Nodal Discontinuous Galerkin Methods: Algorithms, Analysis, and Applications. Springer, 2008.

To Problem of Dynamic Compression (Expansion) of Spherical Cavity in VIiscous Incompresible Liquid

Alexey Kiselev
Mechanics and Mathematics Faculty of Moscow Lomonosov State University
akis2006@yandex.ru

Abstract

Exact solution of one-dimensional dynamic problem of compression (expansion) of spherical layer in incompressible viscous liquid are obtained, assuming that, at the initial instant of time, motion of liquid be missing, and on external and internal surfaces of layer act pressures, which depend on time. In case, when external boundary of layer recede to infinity, and pressure there be constant, and pressure in cavity (bubble) be missing (Zababaxin problem [1]), show that under arbitrary initial radius of bubble its filling of liquid always happen for finite time. If initial radius of bubble strive to zero, then time of its collapse strive to finite value, which depend only from ratio of dynamic viscosity of liquid to pressure on infinity. Velocity of filling of small bubble strives to zero. Obtained exact solution can be used to test calculation programmers and to estimate the effectiveness of numerical methods.

References

1. E.I. ZABABAXIN. Filling of Bubbles in Vscous Lquid. J. of Appl. Math. and Mech. 24 (1960) 1129-1131.

Simulation of Plasmonic Nanostructures With the Nonlinear Quantum Hydrodynamic Model

Ueli Koch
Institute of Electromagnetic Fields (IEF), ETH Zürich
uelikoch@ethz.ch

Abstract

Modern fabrication techniques allow the production of plasmonic nanostructures with separation distances on an atomic scale (¡ 2nm) [1]. In such devices, the purely classical Drude model is no longer valid and leads to unphysically strong field enhancement. In recent simulations [1, 2], a nonlocal correction is added to account for the nonlocality of free electrons in a metal. Nevertheless, this model is still linear and restricts electron movement to the metal. The nonlinear quantum hydrodynamic model [3, 4] is capable to compute electron densities leaking out of the metal and quantum effects by adding additional potentials. This work presents how the hydrodynamic model is coupled to Maxwell's equations to compute the performance of plasmonic devices in active or passive state. The problem is highly nonlinear which is why we apply perturbation theory. We solve for the nonlinear stationary solution using a fixed-point iteration method with Anderson acceleration. The dynamics are finally computed by solving the linear perturbations of our stationary solution.

References

1. C. Ciracì and R. T. Hill and J. J. Mock and Y. Urzhumov and A. I. Fernández-Domínguez and S. A. Maier and et al.. Probing the Ultimate Limits of Plasmonic Enhancement. Science, vol. 337, pp. 1072-1074, 2012.
2. Q. Huang and F. Bao and and S. He. Nonlocal effects in a hybrid plasmonic waveguide for nanoscale confinement. Optics Express, vol. 21, pp. 1430-1439, 2013.
3. J. E. Sipe and V. C. Y. So and M. Fukui and and G. I. Stegeman. Analysis of second-harmonic generation at metal surfaces. Physical Review B, vol. 21, pp. 4389-4402, 1980.
4. N. Crouseilles and P. A. Hervieux and and G. Manfredi. Quantum hydrodynamic model for the nonlinear electron dynamics in thin metal films. Physical Review B, vol. 78, p. 155412, 2008.

Heterogeneous Parallel Method for the Construction of Multi-dimensional Smoothing Splines

Vladimir Gorbunov
Ulyanovsk State University, Ulyanovsk, Russia
vkgorbunov@mail.ru

Igor Kohanovsky
ELI Beamlines, Institute of Physics, Czech Academy of Sciences, Czech Republic
igor.kohanovsky@gmail.com

Abstract

A problem of reconstruction of multivariate dependency under incomplete data set arises in many areas of research. Often there is a finite set of experimental measurements $\{\tilde{u}_i\}_{i=1}^m$ and we may treat an unknown function $\varphi(x)$ as an element of Reproducing Kernel Hilbert space $H(R^n)$. Consider the following data model

$$(f_i, \varphi) = u_i\,, \qquad \tilde{u}_i\ = u_i + \epsilon_i \qquad 1 \le i \le\ m, \tag{1}$$

where f_i — linearly independent linear continuous functionals, $\{u_i\}$ — "exact value of measurement", and $\{\epsilon_i\}$ — random value uniformly distributed in $[-\delta_i, \delta_i]$. Hence we have a system of constraints

$$|(f_i, \varphi) - \tilde{u}_i| \le \delta_i\,, \qquad 1 \le i \le\ m\,. \tag{2}$$

Problem of reconstruction of the function φ satisfying with (2) is underdetermined. To resolve it we introduce a penalty functional J

$$(J, \varphi) = \|\varphi - \varphi_0\|_H^2\,, \tag{3}$$

and find a function φ in the Hilbert space H to minimize J subject to (2) (where φ_0 is a trial function, and $\|\cdot\|_H$ denotes the H norm). Solution of this problem is a generalized spline of Atteia-Laurent [1], following to the work [2] we name it as a "smoothing normal spline".

In this work we present a GPU accelerated method of the constructing normal smoothing spline based on parallel version of the quadratic programming algorithm. Simplified version of the method can be applied for solving interpolating problem within particle-in-cell simulation framework. Results of numerical experiments are presented.

References

1. P.-J. LAURENT. Approximation et optimization. Paris, 1972.
2. GORBUNOV V.K. A Method of Normal Spline Collocation. Computational Mathematics and Mathematical Physics. 1989. V.29. N2. PP.212-224.

Multisensor Data Fusion Using Neural Networks

Krzysztof Kolanowski
Poznan University of Technology
Faculty of Computing
Chair of Computer Engineering
krzysztof.kolanowski@put.poznan.pl

Abstract

Navigation at the present time is common and found in many applications military and civilian. Use the navigation providing high accuracy makes it necessary to use different sensors and combines their readings.

This paper presents a solution that combines data received from five sensors using Artificial Neural Networks. Training data for Neural Network was generated by data fusion from samples collected during the flight of Quadcopter using Kalman Filter.

Integration readings from many different sensors helps to minimize errors of navigation and weaknesses of individual sensors.

The precise location in space plays an important role in many fields such as robotics, navigation, human motion analysis and human-machine interface.

To verify the functioning of proposed system performed series of tests. Used ten sets of samples from which three were used to learn the Elman Neural Network and the other for verification. Performed simulations using Matlab proved the proper functioning of the presented solution. Solutions were compared using the the different quantities of neurons and different learn methods.

References

1. F. CARON AND E. DUFLOS AND D. POMORSKI AND P. VANHEEGHE. GPS/IMU data fusion using multisensor Kalman filtering. Information Fusion 7 (2006) pp. 221-230.
2. B. BARSHAN AND H. F. DURRANT-WHYTE. Inertial navigation systems for mobile robots. vol. 11, pp. 328–342, June 1995..
3. L. OJEDA AND J. BORENSTEIN. Flexnav: fuzzy logic expert rule-based position estimation for mobile robots on rugged terrain. in Proc. IEEE International Conference on Robotics and Automation ICRA '02, vol. 1, pp. 317–322, May 11–15, 2002.
4. D. H. TITTERTON AND J. L. WESTON. Strapdown inertial navigation technology. The Institution of Electrical Engineers, 2004.
5. S. BEAUREGARD. Omnidirectional pedestrian navigation for first responders. in Proc. 4th Workshop on Positioning, Navigation and Communication WPNC '07, pp. 33–36, Mar. 22–22, 2007.
6. H. J. LUINGE AND P. H. VELTINK. Inclination measurement of human movement using a 3-d accelerometer with autocalibration. vol. 12, pp. 112–121, Mar. 2004.
7. H. ZHOU AND H. HU. Human motion tracking for rehabilitation–a survey. Biomedical Signal Processing and Control, vol. 3, no. 1, pp. 118, 2008..

Scale Separation in Fast Hierarchical Solvers for Discontinuous Galerkin Methods

Dmitri Kuzmin, Vadym Aizinger
Universität Erlangen-Nürnberg
kuzmin@am.uni-erlangen.de, aizinger@math.fau.de

Lukas Korous
University of West Bohemia
korous@rice.zcu.cz

Abstract

We present a method for solution of linear systems resulting from discontinuous Galerkin (DG) approximations. The two-level algorithm is based on a hierarchical scale separation (HSS) such that the linear system is solved globally only for the cell mean values which represent the coarse scales of the DG solution. The system matrix of this coarse scale problem is exactly the same as in the cell-centered finite volume method. The higher order components of the solution (fine scales) are computed as corrections by solving small local problems. This technique is particularly efficient for DG schemes that employ hierarchical bases and leads to an unconditionally stable method for stationary and time-dependent hyperbolic and parabolic problems. Unlike p-multigrid schemes, only two levels are used for DG approximations of any order. The proposed method is conceptually simple and easy to implement. It compared favorably to p-multigrid in our numerical experiments. Numerical tests confirm the accuracy and robustness of the proposed algorithm.

References

1. D. KUZMIN. D. Kuzmin, A vertex-based hierarchical slope limiter for p-adaptive discontinuous Galerkin methods. Ergebnisberichte Angew. Math. 389, TU Dortmund, 2009. To appear in J. Comput. Appl. Math..

Numerical Simulation of the Fluid-Structure Interaction Between an Elastic Body and Compressible Flow by the Space-Time Discontinuous Galerkin Method

Adam Kosík, Miloslav Feistauer, Martin Hadrava
Charles University in Prague, Faculty of Mathematics and Physics
adam.kosik@atlas.cz, feist@karlin.mff.cuni.cz, martin@hadrava.eu

Jaromír Horáček
Institute of Thermomechanics, Academy of Sciences of the Czech Republic
jaromirh@it.cas.cz

Abstract

We are concerned with the numerical simulation of the interaction of compressible viscous fluid flow and an elastic structure in 2D. We discretize the equations representing the physical problem by the discontinuous Galerkin finite element method (DGM). We describe the discretization by the DGM of both the fluid flow problem in a time-dependent domain and the dynamic linear elasticity equation. The time dependence of the computational domain of the fluid flow is taken into account with the aid of the Arbitrary Lagrangian-Eulerian method (ALE), see, e.g., [2]. The construction of the ALE mapping is made by employing the static linear elasticity equation. We show that the DGM is applicable to the discretization of all the three problems involved (fluid flow, elastic material deformation and mesh movement), both in space and in time. Special attention is paid to the solution of the coupled fluid-structure interaction problem. Coupling of these two problems is realized via certain transient conditions, which are required to be satisfied. These conditions are met through several inner iterations. At each time level both the elastic body deformation and the fluid flow problem are solved several times. The presented method can be applied to solve a selection of problems of biomechanics, aerodynamics and aviation. We especially focus on the application of the developed method to the airflow in vocal folds. We present a numerical experiment of a flow through a 2D channel past a cylinder with an elastic beam. The model problem is inspired by the benchmark described in the paper of Hron and Turek, see [1]. The results of our experiments are compared with the existing literature.

References

1. J. HRON AND S. TUREK. A monolithic FEM solver for an ALE formulation of fluid-structure interaction with configuration for numerical benchmarking. Proceedings of the European Conference on Computational Fluid Dynamics, Egmond aan Zee, The Netherlands, September 5–8, 2006.
2. T. NOMURA AND T. J. R. HUGHES. An arbitrary Lagrangian-Eulerian finite element method for interaction of flow and a rigid body. Comput. Methods Appl. Mech. Engrg., **95**, 1992, 115–138.

High-speed Rotation Induction Heating in Thermal Clamping Technology

Lukas Koudela, Vaclav Kotlan
University of West Bohemia
koudela@kte.zcu.cz, vkotlan@kte.zcu.cz

Abstract

Hard-coupled model of high-speed rotation heating of a ferromagnetic clamping head is presented. The mathematical model is described by three coupled partial differential equations (for the distribution of electromagnetic field, temperature field and field of thermoelastic displacements) whose coefficients are temperature dependent functions. The system is solved numerically and the solution is performed by a fully adaptive higher-order finite element method developed by the hp-FEM group and used by the Agros2D application.

The results from different software are compared together and are verified by the experimental measurement because the methodology is illustrated by a concrete example which was built and measured. The results are evaluated and discussed.

References

1. V. RUDNEV AND D. LOVELESS AND R. COOK AND M. BLACK. Handbook of Induction Heating. CRC Press, Boca Raton, USA, 2002.
2. J. P. HOLMAN. Heat Transfer. McGraw Hill, New York, 2002.
3. B. BOLEY AND J. WIENER. Theory of Thermal Stresses. Wiley, New York, USA, 1960.
4. P. SOLIN ET AL. Hermes - Higher-Order Modular Finite Element System. http://hpfem.org.
5. P. KARBAN ET AL. Agros2D - Multiplatform C++ application for the solution of PDEs. http://agros2d.org.
6. P. KARBNA AND F. MACH AND P. KUS AND D. PANEK AND I. DOLEZEL. Numerical solution of coupled problems using code Agros2D. Computing 10.1007/s00607-013-0294-4.

Coupled Thermo-hydro-mechanical Model for Concrete Structures

Tomáš Koudelka, Jaroslav Kruis, Jiří Maděra
Department of Mechanics, Faculty of Civil Engineering of Czech Technical University in Prague
koudelka@cml.fsv.cvut.cz, jk@cml.fsv.cvut.cz, madera@fsv.cvut.cz

Abstract

Demands on thermal protection of buildings raised rapidly in last decades and this led to replacement of traditional building materials with more progressive ones. Actually, one of the popular material for building construction represents autoclaved aerated concrete (AAC) which exhibits good thermal and mechanical properties, low weight and good price. However, there also some limiting factors and drawbacks which should be taken into account in course of design process. One of them is connected volumetric changes due to change of moisture content which can lead to crack evolution in block of AAC itself as well as in connected materials such as plasters [1].

The paper presents coupled thermo-hydro-mechanical model for such concrete. Heat and moisture transfer are modelled by Kunzel and Kiessel's model [2] which takes into account water vapour, water transport and temperature effects. The mechanical model takes into account the shrinkage effect in dependence on the actual volumetric moisture content and crack propagation described by isotropic damage model.

References

1. M. JERMAN AND M. KEPPERT AND J. VÝBORNÝ AND R. ČERNÝ. "Hygric, thermal and durability properties of autoclaved aerated concrete". Construction and Building Materials, 41 (2013), 352-359.
2. H. M. KUNZEL AND K. KIESSL. "Calculation of heat and moisture transfer in exposed building components". Int. J. Heat Mass Tran. 40 (1997), 159-67.

Morphing Algorithm for Building Individualized 3D Skeleton Model From CT Data

Jacek Starzyński, Robert Szmurło, Zuzanna Noemi Krawczyk, Bartosz Chaber
Warsaw University of Technology
jstar@iem.pw.edu.pl, robert.szmurlo@ee.pw.edu.pl,
zuzanna.n.krawczyk@gmail.com, chaberb@iem.pw.edu.pl

Abstract

Digital 3D individualized model of the patient skeleton can be used for advanced orthopaedic operation planning and for patient positioning in radiotherapy. Creation of such model is time consuming operation, which requires a lot of prior experience and anatomical knowledge.

The paper proposes a new approach for effective extraction of smooth, regular 3D triangular surface mesh representing separated bones of the patient skeleton allowing to simulate joints movements and applied on them stress.

The idea of the algorithm is to fit a template 3D surface model of skeleton to the 3D voxel model created from patient CT scans. The procedure consist of two main stages. In the first stage the CT scans are being preprocessed (contrast adjustment, artifacts removal etc.) and then a rough three dimensional segmented voxel model is created. The voxel model contains only information if a voxel belongs to the bone structure or not (it does not distinguish specific bones nor connections between adjacent structures). Thus, for this phase automatic segmentation algorithms can be used.

In the second phase the bones are distinguished. The approach is based on the morphing of the template surface skeleton model to fit the segmented voxel model of bone structure. The goal function is defined with help of a non-conformity index. The non-conformity index can be defined as the ratio of the CT data bones structure voxels not matched by the template model. During morphing algorithm only anatomically motivated features like length, thickness and type of shape of the bone (elongated or oval) are taken into consideration.

A variety of bones morphing algorithms with the use of manually applied landmarks [Grassi et al.] or with automated procedure [Sigal et al.] were described in literature but according to the authors knowlage neither of them is using non-conformity index as its minimization criterion. Other methods for classification of anatomical structures in existing meshes performed in spectral domain also exist [Chowriappa et al.] In the paper we would like to focus on separation of bones and classification based on the morphing approach.

References

1. Grassi L. and Hraiech N. and Schileo E. and Ansaloni M. and Rochette M. and Viceconti M.. Evaluation of the generality and accuracy of a new mesh morphing procedure for the human femur.. Medical Engineering and Physics, Vol.33, 2011, pp. 112-120.
2. Sigal I. A. and Hardisty M. R. and Whyne C. M.. Mesh-morphing algorithms for specimen-specific finite element modeling.. Journal of Biomechanics, Vol. 41, 2008, pp. 1381-1389.
3. Chowriappa A. and Salunke S. and Mokin M. and Kan P. and Scott P.D.. 3D Vascular Decomposition and Classification for Computer-Aided Detection.. IEEE Transactions on Biomedical Engineering, Vol. 60, No 12, 2013.

Algorithms for Coupled Non-linear Thermo-Mechanical Analysis of Building Structures

Tomas Krejci, Tomas Koudelka, Jaroslav Kruis
Czech Technical University in Prague
krejci@cml.fsv.cvut.cz, koudelka@cml.fsv.cvut.cz,
jk@cml.fsv.cvut.cz

Abstract

The paper deals with a numerical model describing non-linear coupled thermo-mechanical behavior of building structures and materials. The spatial discretization of such problems by the finite element method leads to a system of non-symmetric and non-linear algebraic equations. The time discretization is based on the v-form of the generalized trapezoidal method and the Newton-Raphson method is used at each time step. Two possible algorithms of numerical solution are presented. There are the staggered form and the fully coupled form. In the staggered algorithm, the first part for transport processes is performed, where the temperature field is computed, then nodal values of temperature changes are transferred into the second mechanical part as a non-mechanical loading. Subsequently, nodal displacements and strains and stresses are performed in the mechanical part. In this algorithm, the time integration could be performed in a different way with different length of time steps because both transport and mechanical parts run separately. As for the fully coupled algorithm, the coupled thermo-mechanical problem is derived together. The stiffness-conductivity matrix and capacity matrix of the problem are assembled in the same time and all of the unknowns, displacements and actual temperatures, are solved together at each time step. Then the actual strains and stresses are completed. The advantages and disadvantages and differences of both algorithm are illustrated by the numerical simulation of behavior of Charles bridge in Prague, where the non-linear heat transfer and a mechanical damage model are used.

References

1. J. KRUIS AND T. KOUDELKA AND T. KREJCI. Efficient computer implementation of coupled hydro-thermo-mechanical analysis. Mathematics and Computers in Simulation (2010) 1578-1588.
2. J. KRUIS AND T. KOUDELKA AND T. KREJCI. Multi-physics analyses of selected civil engineering concrete structures. Communications in Computational Physics, 12(3) (2012) 885-918.

The (3+1)- Dimensional Discontinuous Galerkin Trefftz Method

Fritz Kretzschmar
Graduate School CE (TU-Darmstadt)
kretzschmar@gsc.tu-darmstadt.de

Abstract

In this work present the extension of the recently developed (1+1)-dimensional Discontinuous Galerkin Trefftz Finite Element Method [1, 2] to (3+1)-dimensions. The method employs space–time Trefftz basis functions [3] that exactly solve the underlying PDE system. One suitable choice of such basis functions are plane waves expressed as space-time polynomials of arbitrarily high order p. An application of Trefftz bases can exhibit spectral convergence under p enrichment in the whole space–time domain of interest Ω. Therefore, high order time integration is an inherent property of the method that clearly sets it apart from methods which employ high order approximations in space only.

To date we have completed our investigation of (1+1)-dimensional electromagnetic wave propagation problems and are now extending the research to (3+1)-dimensions. In the (3+1)-dimensional space-time setting Maxwell's equations form the underlying PDE system. With both the material parameters and the differentiations cast into operator form $\boldsymbol{\eta}_\epsilon$, $\boldsymbol{\eta}_\mu$ and $\mathbf{D} = (\partial_t \cdot, \nabla \times \cdot)$ the PDE system reads,

$$\mathbf{D} \cdot \boldsymbol{\eta}_\epsilon \cdot \mathbf{F} = \mathbf{J} \quad \text{and} \quad \mathbf{D} \cdot \boldsymbol{\eta}_\mu \cdot \mathbf{F} = 0. \tag{1}$$

Here the electric field $\mathbf{E} = (E_x, E_y, E_z)^{\mathbf{T}}$ and the magnetic field $\mathbf{H} = (H_x, H_y, H_z)^{\mathbf{T}}$ have been combined into a 6-dimensional field vector $\mathbf{F} = (\mathbf{E}, \mathbf{H})^{\mathbf{T}}$.

Transport polynomials

$$\mathbf{F}_i^p = \begin{pmatrix} \mathbf{E}_i \\ Z^{-1}\mathbf{H}_i \end{pmatrix} \cdot (\mathbf{n}_i \cdot \mathbf{r} - \mathrm{v}\, t)^p \,, \tag{2}$$

form a set of Trefftz basis functions. Here $\mathrm{v} = \sqrt{\epsilon\mu}^{-1}$ is the local speed of light and $Z^{-1} = \sqrt{\mu/\epsilon}$ the intrinsic impedance whereas p denotes the order of the polynomial.

In theory, infinitely many Transport polynomials are needed to represent the solution exactly; numerically, a finite set is used. The number of directions of the basis functions and, to a lesser extent, the directions $\mathbf{n}_i$ themselves therefore become a new adaptation parameter in addition to the usual h and p adaptation parameters. Our numerical results demonstrate the spectral convergence of the method; consequently, small sets of basis functions can result in a very high accuracy.

References

1. W. REED AND T. HILL. Triangular mesh methods for the neutron transport equation. Los Alamos Scientific Laboratory Report, 1973.
2. F. KRETZSCHMAR AND S. SCHNEPP AND I. TSUKERMAN AND T. WEILAND. Discontinuous Galerkin Methods with Trefftz Approximations. Accepted at JCAM, 2013 (Preprint in arXiv:1302.6459).
3. E. TREFFTZ. A counterpart to Ritz's Method. 2nd Int. Congress of Applied Mechanics, Zurich, 1926.

On Angle Conditions in the Finite Element Method

Michal Krizek
Institute of Mathematics, Academy of Sciences of the Czech Republic
krizek@cesnet.cz

Abstract

Angle conditions play an important role in the analysis of the finite element method. They enable us to derive the optimal interpolation order and prove convergence of this method, to derive various a posteriori error estimates, to perform regular mesh refinements, etc. Many other useful geometric angle conditions on the shape of elements have appeared in the literature. In this presentation we shall give a survey of various generalizations of the minimum and maximum angle conditions in the finite element method and present some of their applications.

References

1. J. BRANDTS AND A. HANNUKAINEN AND S. KOROTOV AND M. KRIZEK. On Angle Conditions in the Finite Element Method. SEMA Journal, Spanish Society for Applied Mathematics, 56 (2011) 81–95.

Complete Proposal and Optimization of Nonlinear Actuator Based on Higher-Order Finite Element Analysis and Evolutionary Algorithms

Petr Kropík, Lenka Šroubová, Roman Hamar
University of West Bohemia
pkropik@kte.zcu.cz, lsroubov@kte.zcu.cz, hamar@kte.zcu.cz

Abstract

The goal of the paper is to optimize an electromagnetic actuator with nonlinear structural parts (magnetic core, steel shell). The actuator with the limited geometrical dimensions must exhibit as high force acting on its movable element (plunger) as possible. Its static characteristic must be sufficiently flat in order to avoid too hard a collision of the plunger with the front end of the shell.

The analysis of the electromagnetic field of the actuator is carried out numerically by the FEM application Agros2D [1] fully controlled by a number of in-house scripts.

The in-house scripts used for generation of the actuator geometry and control of the optimization process have been implemented in the Python language as well as the used optimization package inspyred [2]. To solve the presented task, the multiobjective optimization has been used, for example the constrained Non-dominated Sorting Genetic Algorithm-II with elitism [3], Pareto Archived Evolution Strategy [4] etc. The convergence and solution accuracy is compared with the previously obtained results [5][6]. The methodology is illustrated with several examples whose results are discussed and explained in the graphical form.

References

1. P. KARBAN ET AL. Agros2D. [online]. http://agros2d.org.
2. GROUP OF AUTHORS. inspyred: Bio-inspired algorithms in python. [online]. http://inspyred.github.com.
3. K. DEB AND A. PRATAP AND S. AGARWAL AND T.A. MEYARIVAN. Fast and elitist multiobjective genetic algorithm: NSGA-II. IEEE Transactions On Evolutionary Computation 6(2), 2002.
4. P. DI BARBA. Multiobjective Shape Design in Electricity and Magnetism. Lecture Notes in Electrical Engineering 47, Springer, 2009.
5. P. KROPÍK AND L. ŠROUBOVÁ AND R. HAMAR. Optimization of an ActuatorWith Non-Linear Materials Using Evolutionary Algorithms and Higher-Order Finite Element Modeling. FEMTEC 2013, Las Vegas, U.S.A. 2013.
6. P. KROPÍK AND L. ŠROUBOVÁ AND R. HAMAR. Higher-Order Finite Element Modeling and Optimization of Actuator with Non-Linear Materials. COMPUTING, 2013, 95 (1), 487-499, 2013.

Discrete Element Model of Coagulation of Emulsions

Martin Kroupa, Michal Vonka, Juraj Kosek
ICT Prague, Department of Chemical Engineering, Technicka 5, 166 28 Prague 6
Martin.Kroupa@vscht.cz, Michal.Vonka@vscht.cz, Juraj.Kosek@vscht.cz

Abstract

Colloid systems are everywhere around us and are a part of our everyday lives. The understanding of colloids is developing fast in the last decades, but there are still many areas of the colloid science, which are not fully understood yet. One of the most important areas among them is the stability of colloids and the related problem of coagulation. It is a serious issue that has huge economic consequences in the manufacturing of many dispersions. Therefore, it is important to understand the conditions, which lead to coagulation, and to operate the processes in the way that prevents it.

Mathematical modeling is a useful tool for improving the understanding of colloid processes. The colloids are influenced by the phenomena occurring on a wide range of time and spatial scales, which require the employment of the meso-scale methods, such as the Discrete Element Method (DEM) used in this work. DEM is a grid-less method, which describes each particle by its size, position, velocity and rotation rate. DEM formulation of the problem results in the set of ordinary differential equations, which are solved numerically using multi-step integration methods. The main advantage of DEM is a very accurate incorporation of diverse force and torque interactions between particles. Our model is able to simulate behavior of the concentrated dispersion systems subjected to shear. The model describes coagulation of elastic, adhesive particles immersed in water. Therefore it captures the influence of several parameters of the colloid systems, such as the Hamaker constant, the surface potential, or the elastic properties of particles, etc.

For the dispersions of solid or liquid particles in water, we have shown that their behavior is strongly dependent on and sensitive to the physical and flow parameters of the systems. Using DEM, we performed parametric studies of the particulate system subjected to shear. The simulations were carried out with a large number of primary particles ($N \sim 5000$) and repeated calculations were made to obtain statistical characteristics of the system. We determined the conditions and combinations of parameters, which do not lead to coagulation or wall attachment of the particles, and therefore are safe for the operation of the system. It was found that the behavior of the system is strongly dependent on the particle volume fraction and that the more concentrated systems are more likely to coagulate. The results of this work help in the better understanding of the emulsion systems and improve the qualitative insight into the process of coagulation.

References

1. J. S. MARSHALL. Discrete-Element Modeling of Particulate Aerosol Flows. Journal of Computational Physics 2009, 228, 1541–1561.
2. A. ZACCONE AND D. GENTILI AND H. WU AND M. MORBIDELLI. Shear-induced reaction-limited aggregation kinetics of Brownian particles at arbitrary concentrations. Journal of Chemical Physics 2010, 132, 134903.

Coupling of Mechanical Damage With Moisture Transport

Jaroslav Kruis
Czech Technical University in Prague
jk@cml.fsv.cvut.cz

Abstract

Moisture transport in porous materials is relatively well described and formulated and several models suitable for particular materials are known. The moisture transport is usually accompanied with heat transport. For example, Künzel model [1] which describes coupled heat and moisture transport in porous materials is very popular in civil engineering.

Behaviour of quasi-brittle materials, such as concrete or rocks, can be described by damage theory. In this contribution, the isotropic damage model based on a single damage parameter is taken into account. The damage parameter is equal to zero for virgin material and is equal to one for fully destroyed material.

In the case of damaged porous material, water vapour permeability and liquid conduction coefficient should be changed with respect to the damage. The increase of the damage parameter means smaller part of solid phase and greater part of voids or cracks. There are two limit cases. For small values (close to zero) of damage parameter microcracks are assumed while for large values of damage parameter (close to one) discrete cracks are assumed and their width can be determined from the traction-separation law. Small values of the damage parameter is connected with higher diffusion while the higher damage parameter leads to the increase of moisture convection usually based on the Hagen-Poiseuille law. Between these two limit cases, logarithmic interpolation is used.

The coupling of damage mechanics with transport processes will be shown on an example of heat and moisture transport in porous material which is damaged by a mechanical load.

References

1. H. KÜNZEL. Simultaneous Heat and Moisture Transport in Building Materials. Fraunhofer IRB Verlag Stuttgart 1995.

Coupled Heat Transport and Darcian Water Flow in Freezing Soils

Lukáš Krupička
Czech Technical University in Prague,
lukas.krupicka@fsv.cvut.cz

Michal Beneš, Radek Štefan
Czech Technical University in Prague
benes@mat.fsv.cvut.cz, radek.stefan@fsv.cvut.cz

Abstract

This contribution deals with a model of coupled heat transport and the Darcian water flow in unsaturated porous media accounting for conditions of freezing and thawing. In the first part of this contribution, we describe a derivation of the model, which is based on basic conservation equations, e.g. mass conservation equation and energy conservation equation. The complete model consists of two nonlinear partial differential equations with unknown total pressure head u and temperature ϑ and prescribed boundary and initial conditions

$$\frac{\partial \theta_M(z,u,\vartheta)}{\partial t} = \nabla \cdot (k(z,u,\vartheta)\nabla\left(u + \psi(z,u,\vartheta)\right)),$$

$$C_p(z,u,\vartheta)\frac{\partial \vartheta}{\partial t} + L_f \rho_i \frac{\partial \theta_i(z,u,\vartheta)}{\partial t} = \nabla \cdot (\lambda(z,u,\vartheta)\nabla\vartheta) + c_p^{\ell}\,\rho_\ell\, k(z,u,\vartheta)\nabla(u+\psi(z,u,\vartheta)) \cdot \nabla\vartheta.$$

Numerical procedure is based on a semi-implicit time discretization, which leads to a system of coupled nonlinear stationary equations. The next part of this contribution deals with the existence of a weak solution to the discretized problem. We also present some ilustrative numerical examples. The spacial discretization is carried out by the FE-method and it is implemented in Matlab.

References

1. M. Dall'Amico and S. Endrizzi and S. Gruber and R. Rigon. A robust and energy-conserving model of freezing variably-saturated soil. The Cryosphere **2** (2011), 469–484.
2. M.L. Deangelis and E.F. Wood. A detailed model to simulate heat and moisture transport in a frozen soil. Hydrology, Water Resources and Ecology in Headwaters, IAHS Publ. no. 248, 1998.
3. L. Evans. *Partial Differential Equations*. American Mathematical Society, Providence, 1998.
4. S. Fučík and A. Kufner. *Nonlinear Differential Equations*. Elsevier, Oxford, 1980.
5. T. Gallouët and A. Monier. On the regularity of solutions to elliptic equations. Rendiconti di Matematica, Serie VII, Volume 19, Roma (1999), 471–488.
6. K. Hansson and J. Šimùnek and M. Mizoguchi. Water flow and heat transport in frozen soil: numerical solution and freeze-thaw applications. Vadose Zone Journal **3** (2004), 693–704.
7. R.W. Lewis and B.A. Schrefler. *The Finite Element Method in the Static and Dynamic Deformation and Consolidation of Porous Media*. John Wiley & Sons, Ltd. Baffins Lane, Chichester, 1998.
8. J. Nečas. *Introduction to the Theory of Nonlinear Elliptic Equations*. Teubner-Texte zur Mathematik, Leipzig, 1983.
9. J. Nečas. *Direct Methods in Theory of Elliptic Equations*. Springer, Heidelberg, 2012.

Probabilistic Modelling of Heterogeneous Materials Based on Image Analysis

Anna Kučerová, Jan Sýkora, Jan Zeman
Czech Technical University in Prague, Faculty of Civil Engineering
anicka@cml.fsv.cvut.cz, jan.sykora.1@fsv.cvut.cz,
zemanj@cml.fsv.cvut.cz

Abstract

Macroscopically heterogeneous materials, characterized mostly by comparable heterogeneity length-scale and structural sizes, can no longer be modelled by deterministic approach. It is convenient to introduce a probabilistic model with uncertain material properties described by random fields, see [1]. Nevertheless, introduction of random fields brings higher demands on quality of input data, especially on shape of covariance kernel representing the spatial correlation of random properties, see [2,3]. The present contribution is devoted to the construction of random fields based on an image analysis utilizing statistical descriptors, which were developed to describe the different morphology structure of multi-phase random material [4]. The whole concept is demonstrated on a simple numerical example of heat conduction where interesting phenomena can be clearly understood.

References

1. R. J. ADLER AND J. E. TAYLOR. Random Fields and Geometry. Springer, 2007.
2. C. SOIZE. Non-Gaussian positive-definite matrix-valued random fields for elliptic stochastic partial differential operators. Computer Methods in Applied Mechanics and Engineering, 195, 26-64, 2006.
3. C. SOIZE. Tensor-valued random fields for meso-scale stochastic model of anisotropic elastic microstructure and probabilistic analysis of representative volume element size. Probabilistic Engineering Mechanics, 23, 307-323, 2008.
4. S. TORQUATO. Random heterogenous materials. Springer-Verlag, New York, 2002.

An Algorithm of Delaunay-like Surface Points Triangulation

Jan Kucwaj
Department of Physics, Mathematics and Informatics, Cracow University of Technology, ul. Warszawska 24, 31-155 Cracow, Poland,
e-mail: jkucwaj@pk.edu.pl

Abstract

The purpose of the paper is to generalize the Delaunay [2] triangulation onto surfaces. A formal definition and appropriate algorithm are presented. Starting from plane domain Delaunay triangulation definition a theoretical approach is evaluated which is a background for further considerations. It is proved that in case of plane surface the introduced Delaunay triangulation of surfaces is identical with classical Delaunay triangulation of plane domain. The main idea of the algorithm is a coupling of the Delaunay property and the the advancing front technique [3]. The proposed algorithm is implemented and numerical results are shown. For the sake of the implementation it is assumed that points are given on the multiconnected surface with finite number of internal loops. The proposed algorithm can be applied to Computer Graphics The proposed algorithm can be applied to Computer Graphics as well to the discretization of boundary value problems for differential equations by finite element method, finite difference method or meshless methods.

References

1. P.B. DELAUNAY.. Sur la Sphere Vide . Bulletin de l'Academie des Sciences de l'URSS, Classe de Sciences Mathematiques et Naturelles, 793-800, 1934..
2. J. KUCWAJ. Delaunay Triangulation of Surfaces. Zeitschrift für Angewandte Mathematik und Mechanik , 76, S. 3, 249-250, 1996..
3. J. KUCWAJ. Glossary of grid generation, in "Handbook of grid generation". Edited by J.F. Thpmpson, B.K. Soni, N.P. Weatherwill, Boca Raton London New York Washington, D.C.", Appendix A-17 & Appendix B-29, 1999.
4. S.H. LO. Delaunay triangulation of non-convex planar domains. Int. J. Num. Meth. Engng, 28, 2695-2707, 1989..
5. S.H. LO. Finite element mesh generation and adaptive meshing, Progress in Structural Engineering and Materials. Int. J. Num. Meth. Engng, 4, 381-399, 2002. .

Solving the Nonlinear Richards Equation Model with Adaptive Domain Decomposition

Michal Kuraz
Czech University of Life Sciences Prague, Faculty of Environmental Sciences, Department of Water Resources and Environmental Modeling, Czech Republic
kuraz@fzp.czu.cz

Pavel Kus
Faculty of Electrical Engineering, University of West Bohemia, Pilsen, Czech Republic
pkus@rice.zcu.cz

Abstract

Richards equation is a governing mathematical model for a porous media flow that has a wide range of applications in civil and environmental engineering. The time derivate term is a derivative of mass (volume) function, and thus its improper discretization yields errors in mass balance. The mass balance consistency is crucial in any hydrological balance and contaminant transportation evaluations.

Due to the non-linearities involved both in spatial and temporal derivative terms an efficient and accurate numerical time integration algorithm should handle the selection of an adaptive time step. This problem has been already studied by (Tocci et al., 1997) for pressure head form of the Richards' equation, where it was shown how a differential algebraic equation implementation of the method of lines can provide effective and accurate numerical solution. The results were extended for the mixed form by (Miller et al., 2006). Another technique reflecting the curvature of the mass function was proposed by (Kuraz et al., 2010).

This paper aims to evaluate several time integration techniques in order to select a robust and economical method that will be futher implemented into Agros2D project (citace), where the Richards equation problem is currently in a process of implementation.

References

1. M.D. TOCCI AND C. T. KELLEY AND C. T. MILLER. Accurate and Economical Solution of the Pressure Head Form of the Richards Equation by the Method of Lines. Advances in Water Resources, 20, 1997, 1-14.
2. C. T. MILLER AND C. ABHISHEK AND M. W. FARTHING. A spatially and temporally adaptive solution of Richards' equation. Advances in Water Resources, 29, 2006, 525-545.
3. M. KURÁŽ AND P. MAYER AND M LEPŠ AND D. TRPKOŠOVÁ. An adaptive time discretization of the classical and the dual porosity model of Richards' equation. Journal of Computational and Applied Mathematics, 233, 12, 2010, 3167-3177.

Determination of the Optimum Pair of Values of Radii of a Full-Height Dielectric Sample of Annular Cross-Section in a Coaxial Resonant Cavity for Measurement of the Dielectric Constant

Roman Kushnin, Semenjako Janis
Riga Technical University
Romans.Kusnins@rtu.lv, semenako@inbox.lv

Abstract

The goal of this work is to find the optimum pair of values of radii of a full-height cylindrical sample of annular cross-section in a coaxial resonant cavity. A pair of values of radii of the sample is considered to be the optimum if the value of the measurement uncertainty corresponding to this pair is smaller than for other pairs of values for the specified value of the dielectric constant of the sample. A similar problem was considered in [1], where the optimal value of a circular cylindrical post in a cylindrical resonant cavity was found by using the well-known Monte Carlo method. In this work we also use the Monte Carlo method. The probability distributions for the model input quantities are assigned according to the principle of maximum entropy. Uncertainties taken into account in this work are the ones that are associated with measurement of the inner and outer radii of the sample, the outer radius of the cavity and the resonant frequency. Another similar problem was considered in [2], where the optimum value of the radius of a circular dielectric post in a rectangular waveguide was found for certain value of the dielectric constant of the post and for different measurement types.

The main drawback of the analysis is a large amount of the computation time it requires, because the Monte Carlo method requires a very large number of iterations in order for estimation of the measurement uncertainty to be reliable and because in each of these iterations the inverse scattering problem needs to be solved that, in turn, is very time consuming task.

In our case, the direct scattering problem is solved by dividing the geometry of the problem into separate homogenous regions in each of which the fields are expressed in terms of series of solutions of the Helmholtz equation with unknown variables. Then a transcendental equation is obtained by successively eliminating each of the unknown constants from a set of equations obtained by enforcing boundary conditions at the interfaces between regions with different values of the dielectric constant and the walls of the cavity, and using mutual orthogonality of cylindrical terms belonging to different regions.

For the sake of comparison, the results obtained for the case of the cylindrical resonant cavity for the same values of the dielectric constant of the sample are also presented.

References

1. E. PAEZ AND M. A. AZPURUA AND C. TREMOLA AND R. C. CALLAROTTI. Uncertainty Minimization in Permittivity Measurements in Shielded Dielectric Resonators. Progress In Electromagnetics Research M, Vol. 26, 127-141, 2012.
2. R. KUSHNIN AND J. SEMENJAKO. Determination of the Optimal Value of the Radius of a Circular Cylindrical Post in a Rectangular Waveguide for Measurement of the Dielectric Permittivity. PIERS Proceedings, 52 - 57, August 12-15, Stockholm, 2013.

Evaluation of miniMax Criterion in Constrained Design Domains

Eva Myšáková, Matěj Lepš
Czech Technical University in Prague, Faculty of Civil Engineering
eva.mysakova@fsv.cvut.cz, leps@cml.fsv.cvut.cz

Abstract

Space-filling criterion miniMax (mM) of a given design of experiments corresponds to the Largest Empty Sphere problem (LES) [Dickerson and Eppstein, 1995]. The objective is to find the largest (hyper)-sphere that includes no design point and whose center lies in the solved design domain. The value of the miniMax criterion is then equal to the radius of this largest sphere. Position of the largest sphere serves for detection of unexplored areas inside the domain. The smaller the miniMax value, the better the design. The evaluation of this criterion represents a complex problem. The exact value can be found using Voronoi diagram [Okabe et al., 2000]. The difficulties associated with finding of intersections of Voronoi edges with faces of the domain can be effectively solved by mirroring of the design points [Pronzato and Müller, 2012]. Unfortunately the time and computational demands of computation of the Voronoi diagram grow rapidly with dimensions. Since engineering praxis often faces constrained multidimensional problems the method for evaluation of the criterion in such domains is needed. The good estimate of the value can be found using algorithm of evolution strategy [Lee et al., 2004]. This contribution then presents comparison of already known approaches and new methods proposed by authors.

References

1. M. Dickerson and D. Eppstein. Algorithms for proximity problems in higher dimensions. Comput. Geom. 5 (1995) 277-291.
2. A. Okabe and B. Boots and K. Sugihara and S. N.Chiu. Spatial tessellations: concepts and applications of Voronoi diagrams. Wiley series in probability and statistics: Applied probability and statistics. Wiley. (2000).
3. L. Pronzato and W. G. Müller. Design of computer experiments: space filling and beyond. Statistics and Computing, 22-3 (2012) 681-701.
4. J.-S. Lee and T.-S. Cho and J. Lee and M.-K. Jang and T.-K. Jang and D. Nam and C. H. Park. A stochastic search approach for the multidimensional largest empty sphere problem. 2004.

Comparison of Adaptively Updated Surrogate Models for Reliability Analysis

Adéla Pospíšilová, Matěj Lepš
Czech Technical University in Prague, Faculty of Civil Engineering
adela.pospisilova@fsv.cvut.cz, leps@cml.fsv.cvut.cz

Abstract

Meta-models (or surrogate models, formerly response surfaces) are getting popular in engineering designs. They are used to simulate the behaviour of structures with less computational demands than the original model (e.g. finite element models). It is still necessary to evaluate this expensive original model few times in some specified points called Design of Experiments (DoE) [Sacks et al., 1989]. The first DoE is usually just space-filling to cover up the whole design space and the meta-model built with an initial DoE is therefore not very accurate everywhere. Recently, a new updating procedure of a general surrogate model has been proposed in [Myšáková et al., 2013]. New points are added to the meta-model to improve accuracy at important regions based on a result of multi-objective optimization. There are two criteria: first, a new support point should be in the vicinity of the limit state function. Second, to bring the maximum new information, the point should be far from other points, which is performed by appropriate distance metric. The final Pareto-front is clustered and the best points are added to DoE to train updated meta-model. In this contribution, various meta-models [Jin et al., 2001] are reviewed for their suitability for the proposed updating procedure. Their comparison is then conducted on a simple reliability-based optimization task.

References

1. R. Jin and W. Chen and T. W. Simpson . Comparative studies of metamodelling techniques under multiple modelling criteria. Structural and multidisciplinary optimization, 23 (2001) 1-13.
2. E. Myšáková and A. Pospíšilová and M. Lepš. Multiobjective adaptive updating of surrogate models. In Proc. 19th Int. Conf. Engineering Mechanics (2013), Inst. of Thermomechanics, Academy of Sciences of the Czech Rep., Prague.
3. J. Sacks and W. Welch and T. Mitchell and H. Wynn. Design and analysis of computer experiments. Statistical Science, (1989), 4(4):409-435.

Analysis of the Impact of Interpolator's Order on the Accuracy of Electric Current Spectrum Estimation Method in the Presence of Noise

Michał Lewandowski, Janusz Walczak
Silesian University of Technology
michal.lewandowski@polsl.pl, janusz.walczak@polsl.pl

Abstract

In modern methods of analysis and simulation of electrical power supply networks, it is often necessary to determine the frequency model of the network using a time domain measurement data [1], [3]. For example, for the non-linear loads described using the current injection model, it is necessary to determine the frequency spectrum of the current and the phasor (module and phase) of the first harmonic of the voltage [4]. Frequency spectrum estimation method presented in [4] is characterized by its high accuracy in comparison with a similar methods such as WIFTA or TDQS [6], while maintaining a relatively small demand for computing power in comparison with higher order Prony's methods [2]. Quality of the spectrum estimation method presented in [4] depends on two main factors: accuracy of the base frequency estimation and the accuracy of the interpolation. For the estimation of the base frequency a first order Prony's estimator is used, which properties are explained, among others, in [5]. To perform the signal interpolation, the method uses a fourth order Newton's interpolator. However, it is not shown in [4] how the order of interpolator affects the accuracy of the method. It is also not shown how the Newton's interpolator behaves in the presence of noise in the analyzed signal. This publication describes the results of the accuracy analysis of the spectrum estimation method presented in [4] for the case when it is applied using different interpolator orders, and the analyzed signal contains additive white Gaussian noise of various levels. The accuracy of the interpolation depends on both: the type and the order of the interpolator and the parameters of the interpolated signal. Conducted research shows how the accuracy of the interpolation algorithm used in [4] depends on the order of the interpolator at different signal to noise ratios and allows to determine the optimal interpolator order in terms of accuracy and required computing power. The presented results may provide a valuable guidelines for the implementation of the method on a microprocessor system with limited resources.

References

1. ARRILLAGA J. AND WATSON N.R.. Power System Harmonics, Second Edition. Wiley, England, 2003.
2. CHANG G. W. AND CHEN CH.I. An Accurate Time-Domain Procedure for Harmonics and Interharmonics Detection. ", IEEE Transactions on Power Delivery, Vol. 25, NO. 3, July 2010, pp. 1787-1795.
3. GRABOWSKI D. AND LEWANDOWSKI M. AND PIWOWAR A.. Verification of Nonlinear Element Models - the Case of a Six-Pulse Rectifier. Electrical Review, 89 (9), Warsaw, 2013, pp. 23-29.
4. LEWANDOWSKI M. AND WALCZAK J.. Current Spectrum Estimation Using Prony's Estimator and Coherent Resampling. COMPEL: The International Journal for Computation and Mathematics in Electrical and Electronic Engineering (accepted for publication on 28 August 2013).
5. ŁOBOS T. AND REZMER J.. Real-Time Determination of Power System Frequency. IEEE Transactions on Instrumentation and Measurement, vol. 46, no. 4, 1997, pp. 877-881.
6. ZHOU F. AND HUANG Z.Y. AND ZHAO C.Y. AND CHEN D.Y. Time Domain Quasi-Synchronous Sampling Algorithm for Harmonic Analysis. IEEE Proc. 14-th Conference on Harmonics and Quality of Power, 2010, pp. 1-5.

An Adjoint-based Numerical Method to Recover the Medium Properties From Seismic Data

Wenyuan Liao
University of Calgary
wliao@ucalgary.ca

Abstract

In this work we propose an adjoint-based computational method to solve the PDE-constrained optimization problem. The objective of this work is to numerically estimate the model parameters which appear as coefficients in the underlying elastic wave equation. First the problem is mathematically formulated as a PDE-constrained inverse problem in which the objective functional is defined as the misfit between observational data on part of the boundary and computed model output. The parameters to be recovered are the Lame parameters which describe the elasticity of the medium and are of great interest to geophysicists for the purpose of hydrocarbon exploration. In general these parameters are spatially varying coefficients, hence the discrete version of the inverse problem is computationally extensive due to the large size of the parameters. To resolve this issue, an alternative direction method has been proposed to solve the large scale minimization problem, in which the two parameters are updated alternatively, hence during each iteration, two half-sized inverse problems are solved. The gradient of the objective functional with respect to the model parameters are obtained by solving the adjoint PDEs, while the computed gradient is validated by automatic differentiation. Three different versions of the Conjugate Gradient method: the Fletcher-Reeves method, the Polak-Ribiere method, and the positive Polak-Ribiere method will be tested and compared using numerical examples arising from crosswell seismic models to demonstrate the accuracy, efficiency and effectiveness of the new method.

References

1. J. VIRIEUX AND S. OPERTO. An overview of full-waveform inversion in exploration geophysics. Geophysics, 74(2009), WCC1-WCC26.
2. A. TARANTOLA. Linearized inversion of seismic-refelection data. Geophysical Prospecting, 32(1984), 998-1015..

An Uniform Approach to Bound Eigenvalues of Self-adjoint Differential Operators

Xuefeng Liu
Waseda University
xfliu.math@gmail.com

Abstract

In this talk, I would like to introduce an uniform approach that gives explicit lower and upper bounds for self-adjoint elliptic differential operators by using finite element methods. Such approach is an extension of the result of [1]. As the application of this approach to concrete problems, we show how to bound eigenvalues of the Laplace operator, the Bi-harmonic operators on 1D, 2D and 3D spaces. Moreover, by further applying Lehmann-Goeriesch's theorem, high-precision eigenvalue bounds are possible.

References

1. XUEFENG LIU AND SHIN'ICHI OISHI. Verified eigenvalue evaluation for Laplacian over polygonal domain of arbitrary shape. SIAM J. Numer. Anal., 51(3), 1634-1654.

Computing Morava K-theory Euler Characteristics for P-groups

Alexander Lomadze
Tbilisi State University
aleksloma@yahoo.com

Abstract

This report serves the computational algebra topics. I am going to present a program, by using GAP system, which computes the Morava K-theory Euler characteristics for p-groups, i.e., rank of $K(s)^*(BG)$, as a $K(s)^*(pt) = F_p[v_s, v_s^{-1}]$- module, where BG is the classifying spave of the group G and $|v_s| = 2(1 - p^s)$.

Another theoretical way for such computation is a recursive formula by Hopkins at all, see M. Hopkins, N. Kuhn, and D. Ravenel : *Generalized group characters and complex oriented cohomology theories* , J. Amer. Math. Soc., **13, 3**(2000), 553-594.

References

1. M. BAKURADZE V. VERSHININ. MORAVA K-THEORY RINGS FOR THE DIHEDRAL, SEMIDIHEDRAL AND GENERALIZED QUATERNION GROUPS IN CHERN CLASSES. PROCEEDINGS OF THE AMERICAN MATHEMATICAL SOCIETY Volume 134, Number 12, December 2006,.

Optimization of Parameters in SDFEM for Different Spaces of Parameters

Petr Lukas
Charles University in Prague, Faculty of Mathematics and Physics, Sokolovska 83, 186 75 Praha 8
lukas@karlin.mff.cuni.cz

Abstract

The talk is devoted to the numerical solution of the scalar convection–diffusion equation. We present new results of an adaptive technique in finite element method based on minimizing a functional called error indicator $I_h : W_h \to \mathbb{R}$. The simplest form of such an indicator is

$$I_h(w_h) = \sum_{K \in \mathcal{T}_h, \overline{K} \cap \partial\Omega = \emptyset} h_K^2 \ \| - \varepsilon \Delta w_h + \boldsymbol{b} \cdot \nabla w_h + c w_h - f \|_{0,K}^2 \qquad \forall w_h \in W_h, \tag{1}$$

where we have used the notation from the article of V. John, P. Knobloch, S. B. Savescu. It is possible to enrich this indicator by other terms, which favour less smeared solution to diffuse one. One example of such a term is $\|\phi(|\boldsymbol{b}^\perp \cdot \nabla w_h|)\|_{0,1,K}$, where ϕ is a function like square root. The suitability of added terms depends on the problem we solve.

The parameter we are changing in the optimization process is currently the parameter τ from SUPG (SDFEM) method. We use more different finite element spaces (space of piecewise constant functions, piecewise linear continuous functions, and piecewise linear discontinuous functions) for the parameter τ. The talk is based on the article of V. John, P. Knobloch, S. B. Savescu.

References

1. V. JOHN AND P. KNOBLOCH AND S. B. SAVESCU. A posteriori optimization of parameters in stabilized methods for convection-diffusion problems - Part I. Comput. Methods Appl. Mech. Engrg. (2011), Volume 200, Issues 41–44, 1 October 2011, Pages 2916–2929.

A Computational Approach to Quantifying the Uncertainty in Prior Assumptions for Linear Inverse Problems

Aaron Luttman, Marylesa Howard, Michael Fowler
National Security Technologies, LLC
luttmaab@nv.doe.gov, howardmm@nv.doe.gov, fowlermj@nv.doe.gov

Abstract

A natural approach to quantifying uncertainty in solutions to linear inverse problems is to formulate the problem within a Bayesian framework and develop a Markov chain Monte Carlo (MCMC) scheme for sampling from the posterior density. This formulation requires a likelihood to penalize deviations of the solution from the modeled data and, for ill-posed inverse problems, a prior density that acts as a Bayesian form of regularization. The variation in the posterior density then gives a direct measure of uncertainty in the solution only if the prior distribution is accurate. If the chosen prior is not appropriate, then the variation in the posterior fails to capture the systematic errors caused by this bias. In this work we present a computational method for placing a hyperprior on the prior distribution assumption in order to quantify the bias errors associated with imperfect priors. We present the quasi-Bayesian formulation, an MCMC sampling scheme for computing the solution and a technique for quantifying the bias error as well as the random error. The method is demonstrated on applications in image analysis, including deconvolution problems and Abel inversion.

References

1. M. HOWARD AND A. LUTTMAN AND M. FOWLER. Sampling-based Uncertainty Quantification in Deconvolution of X-ray Radiographs. J. Comput. Appl. Math. (to appear).
2. J. BARDSLEY. MCMC-based Image Reconstruction with Uncertainty Quantification. SIAM J. Sci. Comput. Vol. 34 (2012), A1316-A1332 .

Benchmarking and Quantifying Uncertainty in Surface Velocities Calculated From Photonic Doppler Velocimetry

Eric Machorro, Aaron Luttman, Marylesa Howard, Rand Kelly
National Security Technologies, LLC
machorea@nv.doe.gov, luttmaab@nv.doe.gov, howardmm@nv.doe.gov,
kellyrp@nv.doe.gov

Abstract

Photonic Doppler velocimetry (PDV) is a heterodyne interferometric diagnostic used to calculate velocities of surfaces moving up to 50 km/s. Laser light is shone through a probe onto the moving surface, and the light reflected back is mixed with the original light, producing a signal on a digital oscilloscope. The velocity of the surface can be computed from the instantaneous frequency of the scope signal, but there are competing models for how the calculation should be performed. Given its ability to capture such high speeds, there are few other diagnostics that can be used to benchmark the different velocity calculations. In this work we present results comparing ultra high-speed video results to PDV calculations in experiments where a projectile is shot from a two-stage gas gun and impacts a steel plate. We show that there are significant differences in the velocity estimates from the competing analysis techniques, but that, in general, the PDV results compare well with the high-speed video results.

References

1. J. BLAIR AND E. MACHORRO AND A. LUTTMAN. Estimating the bias of local polynomial approximation methods using the Peano kernel. Contemp. Math., Vol. 586 (2013), 033134.
2. J. BLAIR. Filtering Error Estimates and Order of Accuracy via the Peano Kernel Theorem. Computer Standards and Interfaces, Vol. 33 (2011), 22-127.

The Estimation of Parameters of Hydrological Model BILAN Using the SCDE for Monthly Simulation of Hydrological Balance

Petr Maca, Martin Hanel, Pavel Pech
Faculty of Environmental Sciences CULS Prague
maca@fzp.czu.cz, hanel@fzp.czu.cz, pech@fzp.czu.cz

Adam Vizina, Stanislav Horacek, Ladislav Kasparek
T. G. Masaryk Water Research Institute, p.r.i.
adam-vizina@vuv.cz, stanislav-horacek@vuv.cz,
ladislav-kasparek@vuv.cz

Abstract

The non-linear parsimonious hydrological water balance model BILAN was extended using the global evolutionary optimisation algorithm. The newly developed SCDE algorithm – the Shuffled Complex Differential Evolution algoritm, was applied for the parameter estimation of BILAN model. The SCDE transforms the original algorithm of differential evolution with binomial crossover of Storn and Price (1997) into the distributed version using the periodic shuffling mechanism combined with the full migration. The three versions of SCDE, which differ according to SCDE mutation operators, were compared together with the BILAN's original local optimisation scheme based on the binary search. The simulation of monthly water balance was computed for the set of 234 watersheds in the Czech Republic. During the evaluation of identified hydrological models all BILAN models with parameters estimated using the SCDE versions outperformed BILAN models with parameters estimated using the current local optimisation scheme according to the selected performance metrics.

References

1. R. STORN AND K. PRICE . Differential evolution - A simple and efficient heuristic for global optimization over continuous spaces. JOURNAL OF GLOBAL OPTIMIZATION. 11, (1997) 341-359.

Simulation of Multiple Particle Movement in Electromagnetic Field

František Mach, Pavel Karban, Jan Kacerovský, Pavel Kůs, Ivo Doležel
University of West Bohemia
fmach@kte.zcu.cz, pkarban@kte.zcu.cz, jankac@kte.zcu.cz,
pkus@kte.zcu.cz, idolezel@kte.zcu.cz

Abstract

We present a multi-particle tracing algorithm, which will be used for problems where movement of charged particle is determined by field-particle interaction (charged particle interaction with electric and magnetic field) and particle-particle interaction. Presented algorithm also respect particle interaction with solid bodies in the system.

Algorithm is used for design of device for high-quality separation of triboelectrically charged plastic particles (triboelectric separator). The main principle of this separator is based on the Coulomb force acting on freely falling charged dielectric particles. Distribution of electric field in the system is solved numerically by a fully adaptive higher-order finite element method and the movement of particles in the device is determined by a Runge-Kutta-Fehlberg algorithm.

References

1. F. Mach and L. Adam and J. Kacerovský and P. Karban and I. Doležel. Evolutionary algorithm-based multi-criteria optimization of triboelectrostatic separator. Journal of Computational and Applied Mathematics, vol. 270, 134–142, 2014.
2. P. Karban and F. Mach and P. Kůs and D. Pánek and I. Doležel. Numerical solution of coupled problems using code Agros2D. Computing, vol. 95, 381-408, 2013.

Time Series and Countable Banach Space Techniques

Ivo Marek
Czech Technical University
marekivo@mat.fsv.cvut.cz

Abstract

A new approach to analyzing time series is proposed. The novelty consists in applying a concept of countable Banach (Hilbert) space techniques in place of the standard Banach/Hilbert space techniques. Such treatment allows one to consider time series under more general hypotheses than it has been done so far. We show the new approach by treating classical problems such as problem of invertibility also in presence of nonlinearities as well as open the door to solving some new ones allowed by the new techniques.

References

1. J. ANDEL . Statistical Analysis of Time Series. (1976)SNTL, Praha.
2. W. FELLER. An Introduction to Probability Theory and Its Applications. Wiley New York, London, Sydney, Toronto 1971 .
3. I.M. GELFAND AND N. YA. VILENKIN. Generalized Functions Vol. 4: Some Applications of Harmonic Analysis. Well equipped Hilbert Spaces. (In Russian) State Publishing House of Physics and Mathematics Literature, Moscow 1961.

Dynamic Load Balancing in Lattice Boltzmann Solver MUSUBI With Complex Spacer Geometry in Electrodialysis

Kannan Masilamani
Siemens AG, Corporate Technology, CT RTC ENC ENT-DE and Simulation Techniques and Scientific Computing, University of Siegen
kannan.masilamani@uni-siegen.de

Kartik Jain, Harald Klimach, Sabine Roller
Simulation Techniques and Scientific Computing, University of Siegen
kartik.jain@uni-siegen.de, harald.klimach@uni-siegen.de, sabine.roller@uni-siegen.de

Abstract

Electrodialysis is an energy efficient seawater desalination technique. It uses selective ion exchange membranes to remove salt ions from sea water under the influence of an applied external electrical field. In the electrodialysis module, a complex structure referred to as spacer is used in the channels to keep the membranes apart. This spacer influences the transport of salt ions and mixture in the flow channel. To tune this process, a large scale numerical simulation tool coupling several physical phenomena is developed and deployed on High Performance Computing (HPC) systems.

The Multi-species Lattice Boltzmann Method (LBM) [1] is chosen to simulate the transport of ions and mixture in the flow channel due to its advantages in incorporating complex geometries and its high scalability on HPC. This method is implemented in the open-sourced Lattice Boltzmann solver MUSUBI [2] which is part of the highly scalable simulation framework APES [3]. In APES framework, a nearly perfect load balancing is obtained by the deployed Space-Filling Curve (SFC) partitioning for simple domain setups. But in the flow channel with accurate boundary conditions for the Multi-Species LBM load imbalances arise by the complex setup. The SFC Partitioning Algorithm (SPartA) [4] is deployed to account for the varying costs associated with the additional boundary conditions. To ensure optimal load balancing, this algorithm is applied dynamically, enabling the adaptation to changing computational load. In this work, a performance analysis is done for the method on the Cray XE6 system Hermit at the HLRS. The influence of the dynamic load balancing in the specific application of seawater desalination for the Multi-Species LBM will be presented in detail.

References

1. J. Zudrop and S. Roller and P. Asinari. A lattice Boltzmann scheme for liquid mixtures – Part I. Model and analysis. Physical Review E (2013) (Under review) .
2. M. Hasert and K. Masilamani and S. Zimny and H. Klimach and J. Qi and J. Bernsdorf and S. Roller. Complex Fluid Simulations with the Parallel Tree-based Lattice Boltzmann Solver Musubi. J. Comput. Sci. (2013), http://dx.doi.org/10.1016/j.jocs.2013.11.001.
3. S. Roller et al. An adaptable simulation framework based on a linearized octree. In High performance computing on vector systems 2011, Editors: M. Resch, X. Wang, W. Bez, E. Focht, H. Kobayachi, and S. Roller, Springer.
4. D. Harlacher and H. Klimach and C. Siebert and F. Wolf and S. Roller. Dynamic Load Balancing for Unstructured Meshes on Space-Filling Curves. 26th IEEE IPDPS Workshop and PhD Forum (2012) 1655-1663.

Solving Richards Equation With Adaptive Schwarz Type Domain Decomposition and Smoothed Prolongators

Michal Kuraz
Czech University of Life Sciences
michal.kuraz@fsv.cvut.cz

Petr Mayer
Czech Technical University
pmayer@mat.fsv.cvut.cz

Abstract

Modeling of the transport processes in a vadose zone is an important role for predicting the reactions of soil biotopes to anthropogenic activity, e.g. modeling the contaminant transport, effect of soil water regime to changes in soil structure and composition, etc. The water flow is governed by Richards equation, the constitutive laws are typically supplied by van Genuchten's model, that could be understood as a pore size distribution function. Certain material with dominantly uniform pore sizes (e.g. coarse-grained material) could exhibit ranges of the constitutive function values within several orders of magnitude, possibly beyond the computer real numbers length. And thus the numerical approximation of Richards equation often requires solving the systems of equations that cannot be solved on a computer arithmetic. An appropriate decomposition of the domain into subdomains that cover only a limited range of the constitutive function values, and that will adaptively change reflecting the time progress of the model, will enable an effective and reliable solution of this problem. This paper is focused to improving the performance of the domain decomposition algorithm by applying different forms of a smoothed prolongator on subdomains' solution.

References

1. MICHAL KURAZ AND PETR MAYER AND VOJTECH HAVLICEK AND PAVEL PECH. Domain decomposition adaptivity for the Richards equation model. Computing (2013).

Solution of Inverse Problem for Segmented Capacitance Sensor

Petr Mayer
Czech Technical University
pmayer@mat.fsv.cvut.cz

Pavel Kůs
University of West Bohemia
pkus@rice.zcu.cz

Jakub Lev
Czech University of Life Sciences
jlev@tf.czu.cz

Abstract

The segmented capacitance sensor is a compromise between a simple capacitance throughput sensor (Kumhala et al., 2009) and electrical capacitance tomography (ECT) sensors. The idea of this sensor has already been described in several papers (Kumhala et al., 2012; Lev et al., 2013). It is composed of two plates between which a measured material can flow. The bottom plate is undivided while the upper plate is divided into eight segments in order to obtain several measurements. This is a fundamental difference from ECT sensors, which usually produce much more output signals. It is thus necessary to use different approach towards solution of the inverse problem. In the presented work we restricted ourselves to finding a curve which describes distribution of the material over the width of the conveyor belt. In the first step, an approximate curve is found from a library of precalculated responses with the smallest difference to the measured response. In the second step, attempts are made to fine-tune the curve by calculating responses to slightly modified curves. This brings a necessity of repeated calculations of electrostatic field distribution, which have to be performed in real-time. Individual calculations thus have to be very fast, but also precise to ensure high resolution of the reconstruction. Calculations are, however, very similar, since only a small portion of the computational domain is changed due to adding or removing small pieces of the material. Only few local stiffness matrices have to be recalculated each time, changing only few rows and columns of the global stiffness matrix. Many different approaches may be used to exploit this similarity by recalculating and reusing as much as possible. Several of them including modified LU decomposition and performing several iterations of suitable iterative solvers will be compared.

References

1. F. KUMHÁLA AND J. LEV AND M. WOHLMUTHOVÁ AND V. PROŠEK. First tests with segmented capacitive throughput sensor . Scientia Agriculturae Bohemica, 2012, vol 43, no 1, pp 22-27.
2. J. LEV AND P. MAYER AND M. WOHLMUTHOVÁ AND V. PROŠEK. The mathematical model of experimental sensor for material distribution detecting on the conveyor. Computing, 2013, vol 95, no Suppl 1, pp 521-536.
3. F. KUMHÁLA AND V. PROŠEK AND J. BLAHOVEC. Capacitive Throughput Sensor for Sugar Beets and Potatoes. Biosystems Engineering, 2009, vol 102, no 1, pp 36 - 43.

Optimization of Location-Routing Problem for Cross-Docks in Urban Waste Collection Network Considering Stochastic Supply and Demand

Sajjad Mazaheri
Department of Industrial Engineering, Najafabad Branch, Islamic Azad University, Isfahan, Iran
mazaheri_s2@yahoo.com

Seyed Mahdi Homayouni
Department of Industrial Engineering, Lenjan Branch, Islamic Azad University, Isfahan, Iran
homayouni.mahdi@gmail.com, homayouni@iauln.ac.ir

Abstract

Logistics network design is one of the most important strategic decisions in supply chain management. In general, network design decisions include determining the number, location, and capacity of facilities and the quantity of the flow between them (Pishvaee et al., 2010). In supply chain network, the "reverse" flow moves from customers through collection sites to reclamation facilities and is formed by used products. On the other hand, the "forward" flow moves from reclamation facilities directly to new products at points of sale (Santibanez-Gonzalez et al. 2013). The configuration of the reverse logistics network is a complex problem (Alumur et al., 2012). Most of this problems determine the optimal sites and capacity of collection centers, inspection centers, remanufacturing facilities, and recycling plants. This paper proposes a modeling framework for reverse logistics network design problems for: 1) find optimal location of cross docks with respect to the fixed stations and waste recycling companies and 2) vehicle routing to/from these cross docks. Decreasing construction cost of collection centers (opening and closing facility) and increasing flexibility in collection and distribution waste product, cross-dock system instead of distribution centers with stochastic supply and demand. Cross-docking is a logistics strategy in which freight is unloaded from inbound vehicles and it is (almost) directly loaded into outbound vehicles, with little or no storage in between (Van Belle et al., 2012). In this paper, many different waste types (such as types of paper, metal, plastic and etc.) are collected into waste collection centers and for separation and inspection are transported to the cross docks. After quality inspection, they are divided into recoverable products and scrapped products. Recoverable products are carried to the recycling companies and scrapped products are sent to the disposal centers. This problem is formulated as a mathematical model. Then, a metaheuristic algorithm is designed to find near optimal solutions of the large instances.

References

1. M.S PISHVAEE AND K. KIANFAR AND B. KARIMI. Reverse logistics network design using simulated annealing. Int. J. Adv. Manuf. Tech. 47 (2010) 269-281.
2. D.R. SANTIBANEZ-GONZALEZ AND A. DIABAT. Solving a reverse supply chain design problem by improved Benders decomposition schemes. Comp. & Ind. Eng. 66 (2013) 889–898.
3. S.A. AL UMUR AND S. NICKEL AND F. SALDANHA-DA-GAMA AND V. VERTER. Multi-period reverse logistics network design. Europ. J. Oper. Res. 220 (2012) 67-78.
4. J. VAN BELLE AND P. VALCKENAERS AND D. CATTRYSSE. Cross-docking: State of the art. Omega, 40 (2012) 827-846.

Flat-based Control of Variable Speed Wind Turbines

Abderrahmen Mechter, Karim Kemih
L2EI laboratory, Jijel University, Algeria
a.mechter@hotmail.com, k.kemih@gmail.com

Malek Ghanes
ECS-ENSEA, France
malek.ghanes@ensea.fr

Abstract

In this paper, we present a Flat nonlinear control method that allows the synthesis of a control law for a Variable Speed Wind Energy Conversion System (VSWECS) based on a Doubly Fed Induction Generator (DFIG). The used approach consists on calculating a control law basing on the flatness properties of the system in order to to optimize the produced electrical power of the DFIG for low wind speed. The results of simulation show feasibility of the proposed approach.

This work was supported by the CMEP- TASSILI project under Grant 14MDU920.

References

1. A. MECHTAR AND K. KEMIH AND A. KALFAT AND M. GHANES. Power Control for High Speed Wind by Using the Backstepping Strategy. 2nd International Symposium on Computer, Communication, Control and Automation 2013, Singapore.
2. M. FLIESS AND J. LEVINE AND P. MARTIN AND P. ROUCHON. A Lie Bäcklund approach to equivalence and flatness of nonlinear systems. IEEE Transactions on Automatic Control, 44(1999) 922-937.

Metadomotic Optimization Using Genetic Algorithms

Salvador Merino, Javier Martinez, Francisco Guzman
University of Malaga
smerino@uma.es, jmartinezd@uma.es, f_guzman@uma.es

Abstract

New technologies applied in domotic allow us to extract plenty of data about the usual behavior of occupants in any installation. Discipline that works with these data for the pursuit of new knowledge is called Metadomotic.

To achieve this learning and relationships between different data, we make use of the tools provided by artificial intelligence. Today the use of these techniques in solving problems is fully extended. Among the best known we will focus on the application of genetic algorithms, technical halfway between biology and mathematics, to try to resolve the issues raised in this paper.

This article proposes the classification of domotic parameters to optimize an objective function. In a nutshell we will try two possible applications:

1. The minimization of energy consumption through the classification of the parameters of use and consumption coefficients, inherent to each user and device

2. The maximization of industrial production through the influence of environment parameters

Once established several basic suboptimal solutions, they will be combined randomly, through the crossover, mutation and cloning, to try to find the optimal.

References

1. N. ANSARI AND E. HOU. Computational Intelligence for Optimization. Kuwer Academic Publishers, 1997..
2. D.E. GOLDBERG AND J.H. HOLLAND. Special Issue on Genetic Algorithms. Machine learning. Kluwer Academic Publishers, 1988.
3. S. MERINO AND J.L. GALAN AND J. MARTINEZ AND M. AGUILERA. Classifying the items of a Likert based questionnaire in different competences. ACA 2012.
4. Z. MICHALEWICZ AND M. SCHOENAUER. Evolutionary algorithms for constrained parameter optimization problems. Evolutionary Computation, 4:1–32, 1996.

New BEM-based Library Aimed at HPC and Its Applications

Michal Merta, Jan Zapletal
VSB-Technical University of Ostrava
michal.merta@vsb.cz, jan.zapletal@vsb.cz

Abstract

In the talk we present a newly developed library of parallel solvers based on the boundary element method (BEM). The BEM reduces the problem to the boundary of the computational domain, thus it is suitable for the discretization of exterior problems, e.g., sound scattering problems modelled by the Helmholtz and wave equations. Moreover, since the volume of the domain does not need to be discretized, BEM is also well suited for shape optimization problems, where one has to keep the computational mesh shape regular throughout the optimization process. In the first part of the talk we give a short overview of the library, including results of performance and scalability benchmarks. In the second part we present the application of the library for solving time-dependent wave equation or shape optimization problems.

References

1. S. SAUTER AND C. SCHWAB. Boundary Element Methods. Springer, 2010.
2. S. RJASANOW AND O. STEINBACH. The Fast Solution of Boundary Integral Equations. Springer, 2007.
3. S. SAUTER AND A. VEIT. A Galerkin method for retarded boundary integral equations with smooth and compactly supported temporal basis functions. Numer. Math. 123 (2013) 145-176.

Numerical Modeling of Induction Heating of Low-Temperature Casting Metals

Kateřina Mizerová, Jana Kuthanová, Pavel Karban, Pavel Kůs, František Mach
University of West Bohemia
katmiz@students.zcu.cz, janakuth@students.zcu.cz,
karban@kte.zcu.cz, pkus@rice.zcu.cz, fmach@rice.zcu.cz

Abstract

Induction heating of various metals is a well-known method of metal processing, which has been used for decades. In this work we address induction heating of Field's metal, which has very low temperature of melting (62 °C). It is the lowest melting temperature among non-toxic alloys. This metal represents a eutectic alloy of indium (51 %), bismuth (32.5 %) and tin (16.5 %). The main objective of this work is to construct experimental equipment for induction melting of Field's metal and to compare the measured results with a numerical model designed in Agros2D. Another solved issue which needs to be addressed is determination of material properties of the employed charge since specialized literature provides practically no information about this topic. Therefore the parameters were determined in this work, both experimentally or by calculation. The heat conductivity λ has been determined using the Wiedemann-Franz-Lorenz law, the specific heat c_{p} by using the Neumann–Kopp rule and density ρ has been measured. For the specific thermal capacity has been also estimated its dependence on temperature by using parametric analysis. Further this work deals with measurement of induction inside and outside the assembled induction furnace and determination of dependence of the melting temperature on heating time.

References

1. L. CHANG AND K.A. SHAIKH AND L. SHIFENG. Development of a Latchable Microvalve Employing a Low-Melting-Temperature Metal Alloy. Journal of electromechanical systems (2008), vol. 17, no. 5, pp. 1195-1203.
2. Z.H. HAN AND B. YANG AND J. CUMINGS. Synthesis of low-melting-point metallic nanoparticles with an ultrasonic nanoemulsion method. Ultrasonics (2010), vol. 51, no. 4, pp. 458-488.

Algebraic Flux Correction Schemes for High-Order B-Spline Based Finite Element Approximations

Matthias Möller
Delft Institute of Applied Mathematics, Delft University of Technology
m.moller@tudelft.nl

Abstract

In this paper we generalize the concept of algebraic flux correction (AFC) schemes which were developed for (multi-)linear Lagrange finite elements [2] and have been extended to quadratic [3] and non-conforming bilinear [6] elements to higher-order approximations making use of B-splines. B-spline based finite elements feature some amenable properties such as: partition of unity, compact support and strict positivity over the interior of their support. It is the latter property which makes them a favorable candidate for the generalization of AFC-schemes to higher order approximations.

The AFC methodology constitutes a generic framework for the design of positivity-preserving high-resolution schemes for convection-dominated transport problems [4, 5]. It is based on a set of algebraic criteria that are enforced a posteriori on the standard Galerkin finite element method. The main algorithmic steps of AFC-schemes are reviewed and extended to B-splines of arbitrary order.

In contrast to classical C^0 finite elements, it is possible to recover global C^{p-1} approximations from a p-th order B-spline basis which makes this approach particularly interesting in the framework of isogeometric analysis initiated in [1]. On the other hand, continuity can be reduced locally by increasing the multiplicity of entries in the underlying knot vector to improve the resolution of steep gradients. This special feature is embedded into the algebraic flux limiting process. The applicability of the suggested method is demonstrated for a set of representative test problems.

References

1. T.J.R. HUGHES AND J. COTTRELL AND Y. BAZILEVS. Isogeometric analysis CAD finite elements NURBS exact geometry and mesh refinement. Comput. Method Appl. M. 194 (2005) 4135-4195.
2. D. KUZMIN AND S. TUREK. Flux correction tools for finite elements. J. Comp. Phys. 175 (2002) 525-558.
3. D. KUZMIN. On the design of algebraic flux correction schemes for quadratic finite elements. J. Comput. Appl. Math. 218 (2008) 79-87.
4. D. KUZMIN. Algebraic flux correction I. Scalar conservation laws. Chapter 6 in: D. Kuzmin, R. Löhner, S. Turek: Flux-Corrected Transport, Springer, 2nd edition, 2012, 145-192.
5. D. KUZMIN AND M. MÖLLER AND M. GURRIS. Algebraic flux correction II. Compressible flow problems. Chapter 7 in: D. Kuzmin, R. Löhner, S. Turek: Flux-Corrected Transport, Springer, 2nd edition, 2012, 193-238.
6. M. MÖLLER. Algebraic flux correction for nonconforming finite element discretizations of scalar transport problems. Computing 95 (2013) 425-448.

Trend and Fractality Assessment of Mexico's Stock Exchange

Javier Morales, Francisco Javier Almaguer, Victor Tercero, Homero de la Fuente
UNIVERSIDAD AUTÓNOMA DE NUEVO LEÓN
tequilaydiamante@yahoo.com.mx, almagerjavier@gmail.com,
victor.tercero@gmail.com, dante_alighieri390@hotmail.com

Francisco Gerardo Benavides
INSTITUTO TECNOLÓGICO DE NUEVO LEÓN
fgbenavid@gmail.com

Abstract

The total value of domestic market capitalization of the Mexican Stock Exchange was calculated at 520 billion of dollars by the end of November 2013. To manage this system, and make optimum capital investments, its behavior needs to be predicted. However, randomness within the stock indices makes forecasting a difficult task. To address this issue, trends and fractality are studied using GNU R over the opening and closing prices, as well as the volume of transactions of the price and quotes index over the past 15 years. Exponential smoothing, R S analysis, and the Hurst exponent were used in this research. As a result, it was found that closing and opening prices differences seems to behave according to the power law. In this work, a discrete stochastic process such as the Weierstrass random walk is suggested to reduce the forecasting error.

References

1. BLACK UNDEFINED AND FISCHER AND SCHOLES AND MAYRON UNDEFINED. The pricing of options and cororate liabilities. Journal of Political Economy, 1973, Vol.81.
2. LALOUX UNDEFINED AND L. UNDEFINED AND POTTERS UNDEFINED AND M. AND ET AL.. Are financial crashes predictable?. Europhys. Lett, Vol. 45, 1 5, 1999.

Flow Behavior and Heat Transfer Model for a Mixture of Gas and Particles Inside Cyclone Separators.

Javier Morales, Oscar Zapata, Francisco Javier Almaguer, Victor Tercero
UNIVERSIDAD AUTÓNOMA DE NUEVO LEÓN
tequilaydiamante@yahoo.com.mx, oscar2582@yahoo.com.mx,
almagerjavier@gmail.com, victor.tercero@gmail.com

Marco Antonio Merino Rodarte, Antonino Pérez Hernández
CIMAV
mmerinorodarte@gmail.com, antonino.perez@cimav.edu.mx

Victor M Castaño Meneses
UNIVERSIDAD NACIONAL AUTÓNOMA DE MEXICO
meneses@servidor.unam.mx

Abstract

Cyclone separators have been widely used for separating dispersed particles into gases. In this work, cyclone is used as a heat transfer system between hot fluid and cold particles. Temperature for the air and particles were determined experimentally. The flow behavior of hot air and particles at room temperature inside a cyclone is modelled by the use of commercial package based on Computational Fluid Dynamics (CFD). The effect of particle size, velocity and temperature was investigated. The results between the flow behavior and that predicted by the model were compared. The simulation results confirmed the applicability of CFD models as a tool to study the critical variables on cyclone separators.

References

1. CRISTÓBAL CORTÉS AND ANTONIA GIL. Modeling the gas and particle flow inside cyclone separators. Progress in Energy and Combustion Science.
2. GUJUN WAN AND GUOGONG SUN AND XIAOHU XUE AND MINGXIAN SHI. Solid concentration simulation of different size particles in a cyclon separator powder technology . Podwer Technology 183 (2008) 94 104.

Neural Forecast Model of Electricity Demand With Up to One Day Lead Time

Omid Motlagh , George Grozev
CSIRO Ecosystem Sciences, 37 Graham Road, Highett, Victoria 3190, Australia
motlagh7@gmail.com, fixme@fixme.com

Tang Sai Hong
Department of Mechanical and Manufacturing Engineering, Faculty of Engineering, Universiti Putra Malaysia, 43400 Serdang UPM, Selangor, Malaysia
fixme@fixme.com

Sayed Mahdi Homayouni
Department of Industrial Engineering, Lenjan Branch, Islamic Azad University, Zarinshahr, Esfahan 84741, Iran
fixme@fixme.com

Abstract

Electricity demand forecasting is significant in management of supply-demand, service quality, and system protection. This article introduces a forecast model of electricity demand using relatively small database of historical observations. Fuzzy cognitive map is used to draw knowledge of correlations among intraday load levels in a number of selected days in past which serve as platform for future forecasts. In this model, while half-hourly intraday readings are assigned to the network nodes, synchronous differential Hebbian technique is used to train the network's adjacency matrix. The adjacency model is then used for demand projection with MAPE of 5.87

References

1. O. MOTLAGH AND S. H. TANG AND M. N. MASLAN AND FAIRUL AZNI JAFAR AND A. MASLITA AZIZ. A novel graph computation technique for multi-dimensional curve fitting. Connection Science, (2013) 25:2-3, 129-138.

Possibilities for Improvement in Calculations for 2D Coupled Problems in Electrical and Thermal Field

Jan Kyncl, Jiří Doubek
Department of Electrical Power Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague
kyncl@fel.cvut.cz, xdoubek@fel.cvut.cz

Lubomír Musálek
Institute of Thermomechanics, Academy of of Sciences of Czech Republic
musallub@it.cas.cz

Abstract

This paper describes the possibility of getting better result using Agros2D model in a particular case of lyophilization proces with coupled electrostatic and thermal field. The model is represented by a defrozing book at low pressure. The elektrostatic and thermal fields properties are assumed as functions of the local tempetrature. The most important change occured at 266 K which is the temperature of sublimation. At this temperature, the product of density and specific heat capacity is modeled as a proper Gaussian distribution function. The integral of this product corresponds to the heat of sublimation. The influence of the standard deviation parameter of the distribution and the division of the domain have been studied.

References

1. KASPER UNDEFINED AND JULIA CHRISTINA AND FRIESS UNDEFINED AND WOLFGANG UNDEFINED. The freezing step in lyophilization: Physico-chemical fundamentals, freezing methods and consequences on process performance and quality attributes of biopharmaceuticals.. European Journal of Pharmaceutics and Biopharmaceutics 78.2 (2011): 248-263.
2. TAO UNDEFINED AND ZHI UNDEFINED AND ET AL. Numerical simulation of conjugate heat and mass transfer process within cylindrical porous media with cylindrical dielectric cores in microwave freeze-drying.. International journal of heat and mass transfer 48.3 (2005): 561-572.
3. SADIKOGLU UNDEFINED AND H. UNDEFINED AND LIAPIS UNDEFINED AND A. I. AND CROSSER. UNDEFINED AND O. K. Optimal control of the primary and secondary drying stages of bulk solution freeze drying in trays. Technology 16.3-5 (1998): 399-431.
4. STOER UNDEFINED AND JOSEF UNDEFINED AND BULIRSCH UNDEFINED AND ROLAND UNDEFINED. Introduction to numerical analysis. Vol. 2. New York: Springer. 1993.

Stabilized Finite Element Methods for Stokes-Darcy Problems

Kamel Nafa
Department of Mathematics and Statistics, Sultan Qaboos University, Oman
nkamel@squ.edu.om

Abstract

Equal order mixed finite element methods are not stable for solving Stokes and Darcy systems. As a remedy to this instability, symmetric stabilization techniques such as subgrid, local projection and Bochev-Dohrmann methods were proposed and analyzed in Badia and Codina(2009), Becker and Braack(2001), Nafa andWathen(2009), and Bochev and Dorhmann (2006) . In this work we consider a coupled Stokes-Darcy problem where in one part of the domain the fluid motion is described by Stokes equations and for the other part the fluid is in a porous medium and described by Darcy law and the conservation of mass. Velocity and pressure on these two parts are mutually coupled by interface conditions derived by Saffman(1971). Such systems can be discretized by heterogeneous finite elements as analyzed by Layton et al. (2003). In more recent works, unified approaches become more popular. For instance, discontinuous Galerkin methods were analyzed by Girault and Riviere (2009), mixed methods by Karper et al. (2009), and stabilized methods by Braack and Nafa (2013). Here, we take the same variational formulation of the coupled problem as in Karper et al. (2009), but we discretize by standard equal-order finite elements and use symmetric stabilization techniques to stabilize the pressure together with the grad-div term to control the natural velocity norm on the Darcy subdomain. However, to obtain optimal error estimates we have to choose two different stabilization parameters for the two subdomains. The merit of the proposed approach consists in observing that the velocity is,in general,not continuous at the interface so we can use a single mesh for the two sets of equations.

References

1. S. BADIA AND R. CODINA . Unified stabilized finite element formulations for the Stokes and the Darcy problems. SIAM J. Numer. Anal. 47 (2009) 1971-2000..

Numerical Study of Water Entry of 3D Rigid Wedge Under Free Fall

Vinod V. Nair, S. K. Bhattacharyya
Department of Ocean Engineering, Indian Institute of Technology Madras, India
vinodnair.ae@gmail.com, skbh@iitm.ac.in

Abstract

The numerical study of water entry of a three dimensional (3D) rigid wedge under free fall is carried out, by finite volume discretization and volume of fluid (VOF) scheme to keep track of the free surface, by using a commercial solver. The different hydrodynamic parameters of the rigid wedge when it strikes the liquid surface under the action of gravity are investigated in the present study. The main parameters monitored are: displacement, velocity and acceleration as the wedge penetrates the water surface and rebounds; the pressure on the wedge, the wetted surface and the net hydrodynamic forces; all as functions of time. The simulations were conducted at different impact (or touch-down) velocities. The CFD parameters (for e.g. mesh, solver etc.) used in the simulations are discussed. The CFD results are compared with experimental results available in the literature with very good accuracy.

Keywords: Water Entry, CFD, 3D, Wedge, Slamming, Fluid-Structure Interaction.

References

1. T. VON KARMAN. The impact of seaplane during landing. NACA TN 321, October (1929).
2. H. WAGNER. Phenomena associated with impacts and sliding on liquid surfaces. Zeitschrift für Angewandte Mathematik und Mechanik. (1932).
3. E. YETTOU AND A. DESROCHERS AND AND Y. CHAMPOUX. Experimental Study on the Water Impact of a Symmetrical Wedge. Fluid Dynamics Research. 38 (2006) 47–66..

Numerical Modeling of Aluminium Foam on Two Scales

Jiří Němeček, František Denk
Czech Technical University in Prague
jiri.nemecek@fsv.cvut.cz, frantisek.denk@fsv.cvut.cz

Petr Zlámal
Institute of Theoretical and Applied Mechanics, AS CR
zlamal@itam.cas.cz)

Abstract

Metal foams are advanced engineered materials that excel in mechanical properties and very low density (Banhart, 2001; Miyoshi, 1998). Metal foams are hierarchical materials consisting of heterogeneous solid phase and air voids. The paper deals with highly porous aluminium foam known under the brand name Alporas. The overall porosity of the foam reaches 91

Both analytical (Mori-Tanaka, self-consistent) and numerical (FFT-based) elastic homogenizations have been successfully applied to the first composite level. Distinct phase material constants of the phases at the first level have been obtained from nanoindentation and used in homogenization schemes to predict overall level properties (Němeček et al., 2013b).

Unlike the first level, neither analytical nor continuum-based numerical homogenizations are applicable for the second (structural) level of the foam due to extreme material porosity. Therefore, two-dimensional finite element model have been constructed based on the real microstructure . A simple beam model based on Voronoi tessellation (with straight beams and constant equivalent cross sections) have been found efficient for predicting elastic properties whereas plastic properties were not captured well. The real structural shape was better described with two-dimensional finite element model. However, discretization of very thin walls have lead to a large increase in computational complexity. The approaches are compared in the paper for both predictive capabilities (elastic and plastic parameters) and computational costs.

References

1. J. BANHART. Manufacture, characterisation and application of cellular metals and metal foams. Progress in Materials Science, 46(6) (2001), 559-632.
2. T. MIYOSHI AND M. ITOH AND S. AKIYAMA AND A. KITAHARA. Aluminum Foam, 'Alporas': The Production Process, Properties and Applications. MRS Proceedings, 521(0), (1998).
3. J. NĚMEČEK AND VLASTIMIL KRÁLÍK AND JAROSLAV VONDŘEJC. Micromechanical analysis of heterogeneous structural materials. Cement and Concrete Composites, 36(0) (2013a) 85 - 92.
4. J. NĚMEČEK AND VLASTIMIL KRÁLÍK AND JAROSLAV VONDŘEJC. A two-scale micromechanical model for aluminium foam based on results from nanoindentation. Computers and Structures 128 (2013b) 136–145.

Adaptive Mesh Refinement in Lattice Boltzmann Simulations

Philipp Neumann, Hans-Joachim Bungartz
Department of Informatics, Technische Universität München
neumanph@in.tum.de, bungartz@in.tum.de

Abstract

Lattice Boltzmann methods provide a simple, yet powerful approach to simulate fluid flows on both micro- and macroscale. Static adaptivity [1,2] has been incorporated into the Lattice Boltzmann framework in the past. However, only little efforts have been made to extend the method by dynamic adaptivity, i.e. adaptive mesh refinement.

In this contribution, we present a methodology to (adaptive) mesh refinement in volumetric Lattice Boltzmann fluid simulations [3]. We review the underlying adaptive Lattice Boltzmann algorithm and discuss the extension to dynamic coarsening and refinement. The method is implemented in the software Peano [4] and validated in two- and three-dimensional channel flow scenarios. We particularly focus on the simulation of moving particles in nanopores.

Besides, we use the same methodology to solve the shallow water equations via Lattice Boltzmann [5,6] on dynamically changing grids. We consider breaking dam simulations where refinement is triggered depending on the gradient of the water level. Our results indicate very good agreement with pure fine grid solutions.

References

1. O. FILIPPOVA AND D. HÄNEL. Grid Refinement for Lattice-BGK Models. J. Comput. Phys. 147: 219–228, 1998.
2. H. CHEN. Volumetric formulation of the lattice Boltzmann method for fluid dynamics: Basic concept. Phys. Rev. E 58(3): 3955–3963, 1998.
3. P. NEUMANN AND T. NECKEL. A Dynamic Mesh Refinement Technique for Lattice Boltzmann Simulations on Octree-Like Grids. Computational Mechanics 51(2): 237–253, 2013.
4. T. WEINZIERL ET AL.. The Peano Framework. http://www.peano-framework.org, accessed: 2013-12-12.
5. J. G. ZHOU. Lattice Boltzmann Methods for Shallow Water Flows. Springer, 2004.
6. M. GEVELER AND D. RIBBROCK AND D. GÖDDEKE AND S. TUREK. Lattice-Boltzmann Simulation of the Shallow-Water Equations with Fluid-Structure Interaction on Multi- and Manycore Processors. Facing the Multicore-Challenge (Lecture Notes in Computer Science 6310), 92–104, Springer, 2011.

HPC Optimization for Challenging Engineering Problems

Petr Konas
SVS FEM, s.r.o. Skrochova 42, 615 00 Brno
pkonas@svsfem.cz

Slavek Licehammer
CERIT-SC, Masaryk University, Sumavska 15, 602 00 Brno
glory@ics.muni.cz

Ales Nevaril
AdMaS, Brno University of Technology, Veveri 95, 602 00 Brno
nevaril.a@admas.eu

Abstract

Paper is focused on optimization of network topology and individual configuration for real engineering problems with extreme requirements according to HW and computing performance. All realized tasks were accomplished on ANSYS products. GPU accelerators together with standard and non-standard HPC technology were used in tested environment for evaluation of general achievement for different categories of tested problems. National infrastructure Metacentrum provided by CESNET z.s.p.o was compared with specialized frame of SGI UV2000 and national supercomputing center IT4I. The biggest real engineering problems were computed in reasonable time. Process of assembling extremely time consuming and data challenging tasks is discussed. Optimization and modification of individual tasks for appropriate HPC solution is discussed and general recommendations were formed. Effective scaling and determination of usable count of computing cores for individual task's categories was realized.

References

1. P. KONAS AND J. BUCHAR AND L. SEVERA. Study of correlation between the fractal dimension of wood anatomy structure and impact energy. European Journal of Mechanics - A/Solids 28 (3) (2009) 545-550.
2. J. FEIT AND L. HEJTMANEK AND M. PROCHAZKA AND S. LICEHAMER AND L. MATYSKA. Hypertext Atlases of Pathology. 1st Ed. Heidelberg: Springer (2012) ISSN 0945-6317.
3. P. KONAS. Finite element modeling of wood structure. Programs and Algorithms of Numerical Mathematics 14 (2008) ISBN 978-80-8582355-4.

SAR Variation in a Human Head Due to Intrinsic Resonances

Denys Nikolayev
University of West Bohemia
d@deniq.com

Abstract

A human head tissue can support high-Q electromagnetic radio-frequency resonances given special radiation situations. This study evaluates necessary radiation conditions for electromagnetic resonance excitation in a 2D human head boundary representation phantom. We used finite element method to find eigenfrequencies and to compute electromagnetic field distributions. Radiation conditions were evaluated using the maximization of specific absorption rate due to randomly positioned multiple point sources that model a random array of infinite dipoles.

References

1. H. KRITIKOS AND H. SCHWAN. Formation of Hot Spots in Multilayer Spheres. IEEE Trans. Biomed. Eng. 23 (1976).
2. D. NIKOLAYEV. Radio Frequency Resonances inside a Human Head. Comput. Probl. Electr. Eng. 3(1) (2013).

Modelling and Simulation of an Unshielded Stripline

Denys Nikolayev, Pavel Karban
Department of Theory of Electrical Engineering, University of West Bohemia
nikolaye@kte.zcu.cz, karban@kte.zcu.cz

Zdeněk Kubík, Jiří Skála
Department of Applied Electronics and Telecommunications, University of West Bohemia
zdekubik@kae.zcu.cz, skalaj@kae.zcu.cz

Abstract

Unshielded stripline antenna is an essential instrument of electromagnetic compatibility studies. It is used primarily for generating uniform TEM field to test electromagnetic immunity. Defining the geometry of a stripline antenna could be a challenging task for a specified frequency range. It is due to various limiting factors; among them is the impedance of a stripline. Various approximation formulas used at present are adequate only if the ground plane is much larger than stripline and in proximity to it, which is not the case of a stripline antenna for EMC tests. This study demonstrates two approaches—2D static and 3D time harmonic—to the finite element simulation of a stripline in order to predict its impedance. The results demonstrate good agreement between two approaches. The developed 2D FEM model is a rigorous way for defining the optimal geometry of a stripline.

References

1. Z. KUBÍK AND D. NIKOLAYEV AND P. KARBAN AND J. SKÁLA AND M. HROMÁDKA. Optimization of electrical properties of parallel plate antenna for EMC testing. J. Comput. Appl. Math. (2014) DOI: 10.1016/j.cam.2013.12.054.
2. M. CRAWFORD. Generation of standard EM fields using TEM transmission cells. IEEE Trans. Electromagn. Compat., EMC-16(4) (1974) 189–195.
3. W. BITTINGER. Properties of open strip lines for EMC measurements. IEEE Intern. Symp. on Electromagn. Compat. (1993) 120–125.

A DG Implementation of a Novel Hybrid RANS/LES Technique With RANS Reconstruction

Antonella Abbà, Michele Nini
Politecnico di Milano
antonella.abba@polimi.it, michele.nini@polimi.it

Massimo Germano
Duke University
mg234@duke.edu

Marco Restelli
Max Planck Institute
marre@rzg.mpg.de

Abstract

A new hybrid RANS/LES technique, based on the hybrid filter proposed by Germano [1], has been studied. The novelty herein introduced is represented by the reconstruction of Reynolds stress tensor. As consequence, no explicit RANS model is needed. The LES modelling has been obtained using a dynamic-anisotropic model [2]. Nevertheless, it is worth noting that the technique is absolutely independent from the choice of the LES model.
Numerical formulation uses a variational approach with a Discontinous Galerkin (DG) space discretization and an explicit time integration. In fact, due to the high accuracy, parallelizability and the possibility of obtain a filter projecting the solution on different polynomial basis functions, DG method represents a very suitable tool for LES computing. Simulations have been performed using the open-source library FEMilaro [3].
The flow herein considered is a channel flow at low Mach number. In this preliminary work, for sake of simplicity, a constant value of RANS/LES blending factor has been considered.
First results show a good agreement with DNS data, confirming that the technique herein proposed can represent a promising approach to the numerical simulation of turbulent flows.

References

1. M. GERMANO. Properties of the hybrid RANS/LES filter. Theoretical and Computational Fluid Dynamics 17 (2004) 225–331.
2. A.ABBÀ AND A.C.CERCIGNANI AND L. VALDETTARO. Analysis of subgrid scale models. Computers & Mathematics with Applications Volume 46, Issue 4, August 2003 521–535.
3. M. RESTELLI AND C. DE FALCO. FEMilaro, Local Hybridizable Discontinuous Galerkin toolkit. http://code.google.com/p/ldgh/.

Modeling of Crosstalk Phenomenon for Electro-Magnetic Systems by Bilateral Coupling of PDAEs

Helia Niroomand Rad, Andreas Steinbrehcer
Technische Universität Berlin
nirooman@math.tu-berlin.de, steinbrecher@math.tu-berlin.de

Abstract

In this talk, we propose a new modeling approach in order to describe the *crosstalk* phenomenon in electro-magnetic systems. In particular, we are interested in modeling crosstalk in electrical circuits wherein electrical components such as inductors, capacitors, and resistors are sitting comparatively in short distances.

In our model, the crosstalk phenomenon is built by *bilateral coupling* of two phenomena: The *electro-magnetic induction* and the *dynamical behavior of electrical circuits*. We first introduce each phenomenon, and model them respectively by *partial differential equations* (PDEs) and *differential-algebraic equations* (DAEs). Then, we bring these two model equations together via suitable bilateral coupling relations. So far, often only the *unilateral coupling* has been investigated in literature, [3].

The induction is described fundamentally by a set of *Maxwell's equations* [1, 2], while the dynamical behavior is characterized via the *modified nodal analysis* (MNA) formalism, [4, 5]. Consequently, the PDEs derived by Maxwell's equations as well as the DAEs obtained by the MNA formalism lead to two subsystems of model equations which can be exploited to model the crosstalk phenomenon in bilateral coupling. Considering these two sets of equations as input-output systems, the bilateral coupling connects the output of one subsystem to the input of the other subsystem via coupling relations and inversely via re-coupling relations. These relations, which are in principle physical constitutive relations, are introduced in our model by suitable operator structures.

At the end, by the proposed bilateral coupling of two subsystems, derived from Maxwell's equations and the MNA formalism, we yield a system of *partial differential-algebraic equations* (PDAEs) describing the crosstalk phenomenon in electrical circuits.

References

1. A. Bartel and S. Baumanns and S. Schöps. Structural analysis of electrical circuits including magnetoquasistatic devices. Appl. Numer. Math., 61(12): 1257–1270, 2011.
2. P. G. Huray. Maxwell's Equations. Wiley-IEEE Press, New Jersey, 2011.
3. L. Jansen. A semi-explicit formulation of a coupled electromagnetic field/circuit problem. J. Comput. Appl. Math., 2013.
4. A. Steinbrecher and T. Stykel. Model order reduction of nonlinear circuit equations. Int. J. Circ. Theor. Appl., 41:1226–1247, 2013.
5. J. Vlach and K. Singhal. Computer Methods for Circuit Analysis and Design. Van Nostrand Reinhold, New York,1994.

[1] This work has been supported by European Research Council through Advanced Grant *MODSIMCONMP*.

Parameter Polyoptimization of PSS2A Power System Stabilizers Operating in a Multi-machine Power System Including the Uncertainty of Model Parameters

Paszek Stefan, Nocoń Adrian
Silesian University of Technology, Institute of Electrical Engineering and Computer Science
stefan.paszek@polsl.pl, adrian.nocon@polsl.pl

Abstract

In the paper there is presented the analysis of the parameter optimization results of the PSSA power system stabilizers when taking into account the uncertainty of the power system mathematical model parameters. The multi-criteria optimization is used for parameter optimization of the power system stabilizers. The paper presents a method for determining compromise sets - parameter values of PSS2A stabilizers operating in a multi-machine power system - when optimizing different multidimensional criteria. A genetic algorithm with tournament selection and a hybrid algorithm were used for the optimization. The system stabilizer parameter polyoptimization allows damping electromechanical swings efficiently without significant worsening the regulation waveforms of the terminal voltages of generating units in the analyzed power system. The analysis of the influence of the power system model parameter uncertainty on the quality of the results obtained is also performed.

References

1. KROPIK P. AND SROUBOVA L. AND HAMAR R.. Multi-objective optimization of actuator geometry based on genetic algorithm. XXXVI International Conference IC-SPETO, Ustroń, Poland, May 2013, pp. 71-72.
2. NANDAR C. S. A.. Robust PI control of smart controllable load for frequency stabilization of microgrid power system. Elsevier - Renewable Energy 56 (2013), pp. 16-23.
3. NOCOŃ A. AND PASZEK S.. Analysis of power system stabilizer Pareto optimization when taking into account the uncertainty of power system mathematical model parameters. Archives of Electrical Engineering 2011, Vol. 60(4), pp. 385-398.
4. NOCOŃ A. AND PASZEK S.. Synthesis of generator voltage regulator when applying polyoptimisation. Bulletin of the Polish Academy of Sciences – Technical Sciences, Volume 55, Issue 1, March 2007, pp. 43-48.
5. PASZEK S.. Use of Pareto optimization for tuning power system stabilizers. Bulletin of the Polish Academy of Science 2012 Vol. 60, No. 1, pp. 125-131.
6. ZHANG P. X. AND CAO Y. J. AND CHENG S. J.. Coordination of multiple PSSs using multi-objective genetic algorithm. Proceedings of the 5th Word Congress on Intelligent Control and Automation, 2004, pp. 5040-5044.

Breaking Periodicity in Simulation of Microstructured Materials

Jan Novák
Brno University of Technology
novakj@cml.fsv.cvut.cz

Martin Doškář, Martin Horák
Czech Technical University in Prague
martindoskar@gmail.com, nitramkaroh@seznam.cz

Abstract

The sustainable environmental tendencies lead to a highly optimized design of majority of consumer products. In Materials Engineering, this is mirrored by a race towards miniaturization, top product performance, and optimal energy consumption. A potential solution to these contradicting requirements is brought by custom designed composite materials, which finds the use of virtual laboratories that link the knowledge of characteristic physical processes taking place at the level of constituents with macro-scale behaviour. To contribute this goal, the generalization of a popular periodic unit cell approach to modelling of heterogeneous materials is presented. It rests on the idea of stochastic Wang tilings [1] to represent random material microstructures or fine scale local field patterns that can be used as the microstructure-informed enrichment functions in Generalized Finite Element environments. Preliminary result are outlined and discussed.

References

1. J. Novák and A. Kučerová and J. Zeman. Compressing random microstructures via stochastic wang tilings. hysical Review E 86 (4) (2012) 040104.

Stochastic Finite Element Methods With Spectral Element Basis Functions

Saulo Pomponet Oliveira, Stela Angelozi
Universidade Federal do Parana
saulopo@ufpr.br, stela_angelozi@yahoo.com.br

Juarez dos Santos Azevedo
Universidade Federal do Recôncavo da Bahia
juarezsa@gmail.com

Abstract

We study the numerical solution of transient partial differential equations with random coefficients. In particular, we are interested in the linear transport and the acoustic wave equations in heterogeneous media. The heterogeneity is represented by random fields that are approximated by a truncated Karhunen-Loève expansion. This expansion represents a second-order random field in terms of uncorrelated random variables and eigenfunctions of a homogeneous Fredholm integral equation of the second kind involving the covariance function of the random field. Some typical strategies are the use of the Cholesky factorization of the matrix defined by the covariance function evaluated at the grid points and the solution of the Fredholm integral equation by the Galerkin method with piecewise-constant basis functions (Phoon et al, 2004). We employ the spectral element method with Gauss-Lobatto-Legendre collocation points to discretize both the dependent variable and the Fredholm integral equation (Oliveira and Azevedo, 2014).

References

1. S. P. OLIVEIRA AND J. S. AZEVEDO. Spectral element approximation of Fredholm integral eigenvalue problems. J. Comput. Appl. Math. 257 (2014) 46-56.
2. K.K. PHOON AND H.W. HUANG AND S.T. QUEK. Comparison between Karhunen-Loeve and wavelet expansions for simulation of Gaussian processes. Comput. Struct. 82 (2004) 985-991.

Numerical Approximation of Fredholm Integral Equations by Orthogonal Wavelets

Saulo Pomponet Oliveira, Felipe Wisniewski
Universidade Federal do Parana
saulopo@ufpr.br, felipewisniewski@yahoo.com.br

Juarez dos Santos Azevedo
Universidade Federal do Recôncavo da Bahia
juarezsa@gmail.com

Abstract

In this work we shall investigate the numerical approximation of Fredholm integral equations of second kind by the Galerkin method with orthogonal wavelets. This method is particularly attractive for homogeneous equations, since the orthogonality of the basis functions leads to a standard (rather than a generalized) eigenvalue problem. This method has been thoroughly studied for the one-dimensional Haar basis (see, e.g., Phoon et al, 2002). When the kernel is smooth, one can achieve a higher convergent rate by using more regular bases, but in general it is not trivial to construct a wavelet basis in a bounded domain, even for compactly supportted orthogonal wavelets. In analogy with Liang et al (2001) but using a Gauss-type quadrature, we consider the family of wavelets on the interval proposed by Cohen,Daubechies and Vial (1993). We describe the derivation of the two-dimensional shape functions from the one-dimensional case and present preliminary numerical results illustrating the computation of eigenvalues for smooth and non-smooth covariance kernels.

References

1. A. COHEN AND I. DAUBECHIES AND AND P. VIAL. Wavelets in the Interval and Fast Wavelet Transforms. Appl. Comput. Harmon. Anal. 1 (1993) 54-81.
2. X.-Z. LIANG AND M.-C. LIU AND AND X.-J. CHE. Solving second kind integral equations by Galerkin methods with continuous orthogonal wavelets. J. Comput. Appl. Math. 136 (2001) 149-161.
3. K. K. PHOON AND S. P. HUANG AND S. T. QUEK. Implementation of Karhunen-Loève expansion for simulation using a wavelet-Galerkin scheme. Prob. Eng. Mech. 17 (2002) 293-303.

Analysis of an Augmented Mixed Finite Element Method for the Stokes-Darcy Coupled Problem

Ricardo Oyarzua
Universidad del Bio-Bio
royarzua@ubiobio.cl

Abstract

In this work we analyze an augmented mixed finite element method for the coupling of fluid flow with porous media flow. Flows are governed by the Stokes and Darcy equations, respectively, and the corresponding transmission conditions are given by mass conservation, balance of normal forces, and the Beavers-Joseph-Saffman law. We consider a semi-augmented mixed formulation, augmented in the Stokes domain and dual-mixed in the Darcy region, where the main unknowns are given by the stress, the vorticity and the velocity in the fluid, together with the velocity and the pressure in the porous medium. The approach, which extends recent results on the a priori and a posteriori error analysis of a fully-mixed formulation for the Stokes-Darcy model, is based on the introduction of the Galerkin least-squares type terms arising from the constitutive and equilibrium equations of the Stokes equation, and from the relations defining the free fluid pressure in terms of the stress tensor and the vorticity in terms of the free fluid velocity. All these terms are multiplied by stabilization parameters that can be chosen so that the resulting continuous formulation becomes well posed. We then apply the Fredholm and Babuška-Brezzi theories to derive sufficient conditions for the unique solvability of the resulting continuous and discrete formulations. Next, we derive a reliable and efficient residual-based a posteriori error estimator for the augmented mixed finite element scheme. The proof of reliability makes use of the global inf-sup condition, Helmholtz decomposition, and local approximation properties of the Clément interpolant and Raviart-Thomas operator. On the other hand, inverse inequalities, the localization technique based on element-bubble and edge-bubble functions, and known results from previous works, are the main tools to prove the efficiency of the estimator. This work is based on joint work with Jessika Camaño (Universidad Católica de la Santísima Concepción), Gabriel N. Gatica (Universidad de Concepción y CI^{2}MA-UDEC) and Pablo Venegas (University of Maryland).

References

1. G.N. GATICA AND R. OYARZÚA AND F.-J. SAYAS. Analysis of fully-mixed finite element methods for the Stokes-Darcy coupled problem. Mathematics of Computation, vol. 80,276 (2011), 1911-1948.
2. G.N. GATICA AND R. OYARZÚA AND F.-J. SAYAS. A residual-based a posteriori error estimator for a fully-mixed formulation of the Stokes-Darcy coupled problem. Computer Methods in Applied Mechanics and Engineering, vol. 200 (2011), 21-22, 1877-1891.
3. A. MÁRQUEZ AND S. MEDDAHI AND AND F.-J. SAYAS. Strong coupling of finite element methods for the Stokes-Darcy problem. http://axiv.org/abs/1203.4717.

Spread Spectrum Modulation Based on Strongly Nonlinear System With Chaotic Behaviour

David Pánek
University of West Bohemia
panek50@kte.zcu.cz

Abstract

Strongly nonlinear systems with chaotic behaviour bring new possibilities of proposing new communication schemes. The key features of chaotic behaviour i.e. longtime unpredictability and strong sensitivity on initial conditions allow encrypt transmitted information or even hide the whole communication process. The design of new chaos-based communication scheme consist of several steps. The first one is proposing of system with appropriate type of nonlinearity that exhibits chaotic behaviour. The behovoiur must be sufficiently irregular and it must be possible to modify this behaviour for working in required frequency range. The following step is design of transmitter and reciever based on this system and finding of the way how to synchronize these systems. The last step is ensuring of robustness of the whole system. The paper deals with the new communication scheme based on so called dissipation normal form. Usage of dissipation normal form allows systematic design of nonlinear systems of higher order which with specific chaotic behaviour that can work in continous or discrete time.

References

1. P. STAVROULAKIS. Chaos Application in Telecommunications . Taylor & Francis, New York, 2006.

A Computational Framework for Cochain Calculus

Alberto Paoluzzi, Antonio Di Carlo
University Roma Tre, Rome, Italy
apaoluzzi@me.com, adicarlo@mac.com

Vadim Shapiro
University of Wisconsin, Madison, USA
vshapiro@engr.wisc.edu

Abstract

This talk focusses on the design of the LAR-CC geometric library we are developing to support cochain calculus. Basically, k-cochains are discrete densities of quantities contained in the k-cells of a cell complex (such as a FE mesh), k being the dimension. The LAR (Linear Algebraic Representation) scheme [1] is a simple, general and effective representation of (co)chain complexes [2], based on a CSR (Compressed Sparse Row) representation [3] for characteristic matrices of linear spaces of (co)chains. LAR supports all topological incidence structures, is dimension-independent and not restricted to regular, i.e., dimensionally uniform complexes. It allows for fast validity checks of the topology of geometric models, possibly generated from 3D scanner data or extracted from 3D images, using only elementary linear algebra, namely, sparse matrix-vector multiplication.

We mean to cover also the integrated development environment (IDE) enabling documentation and multilanguage development of LAR. It hinges on a literate programming tool, that embeds the code into the documentation instead than vice versa. A design goal of the LAR-CC framework is to facilitate communicating the *whys* of software planning decisions, more than the mere tricky details of low-level coding. Using multiple programming languages is allowed and even encouraged. The `larcc` IDE integrates a few programming, documentation and version control tools, including LaTeX, *Nuweb*, *Pandoc*, and *Git*.

References

1. A. DiCarlo and V. Shapiro and and A. Paoluzzi. Linear Algebraic Representation for Topological Structures. Computer-Aided Design, 46, 1 , January 2014, pp. 269-274 .
2. DiCarlo and A. and Milicchio and F. and Paoluzzi and A. and and Shapiro V.. Discrete physics using metrized chains. 2009 SIAM/ACM Joint Conference on Geometric and Physical Modeling (New York, NY, USA, 2009), SPM '09, Acm, pp. 135–145.
3. A. Bulu
cc and J.R. Gilbert. Parallel Sparse Matrix-Matrix Multiplication and Indexing: Implementation and Experiments. SIAM J. Sci. Comput. 34 (2012) 170–191.

Probabilistic Assessment of Failure Risk of the Building Envelope Thermally Insulated From the Inside

Petr Kesl, Jan Pasek
University of West Bohemia
pkesl@kme.zcu.cz, pasek@kme.zcu.cz

Abstract

The building envelope insulated from the internal side is considered as risk structure. Internal thermal insulation causes increased stress of the exterior walls as well as load-bearing system of the building due to cyclic temperature changes in the external environment. The paper deals with the evaluation of the probability of the failure risk of such structural solution, depending on the variable boundary conditions (rigidity of the structure, strength of materials, values of temperature load).

References

1. J. PASEK. Impact of Internal Thermal Insulation Systems on Static Behaviour of Exterior Walls. Advanced Materials Research, 649 (2013), 11-14, ISSN: 1022-6680 .

Numerical Simulation of the Temperature Impacts on the Structural Integrity of the Stone Temples in Angkor, Cambodia

Jan Pasek
University of West Bohemia
pasek@kme.zcu.cz

Hansley Pravin Gaya
Dlubal Software
hansleygaya@gmail.com

Abstract

Medieval sandstone temples of Angkor were built between 9th and 14th century. Since their inception to the present have been loaded by numerous cycles of temperature changes that cause partially irreversible cyclic infinitesimal movements of the joints between the stone blocks. As a result of the process of contraction and expansion of stone structures is their total disintegration. The paper analyzes the process of disintegration of stone temples on the basis of numerical simulations of their static behaviour.

References

1. J. PASEK AND H.P. GAYA. Numerical simulations of the static behavior of stone temples in Angkor, Cambodia. WTA CZ, No 3/9 (2011), 16-21, ISSN 1213-7308.

Compensation Based on Active Power Filters – the Cost Minimization

Marcin Maciazek, Dariusz Grabowski, Marian Pasko, Michał Lewandowski
Silesian University of Technology
marcin.maciazek@polsl.pl, dariusz.grabowski@polsl.pl,
marian.pasko@polsl.pl, michal.lewandowski@polsl.pl

Abstract

There are more and more electrical and electronic devices available in the market which require high quality power supply. On the other hand, these devices are also the cause of power quality deterioration because of their nonlinear behaviour which influences the supplying power system. Moreover, dynamical changes of nonlinear loads during their normal operation make elimination of interferences impossible using simple compensators. Nowadays, active power filters (APF) [1], [2] are the only solution which is able to improve power quality in contemporary power systems with dispersed generation and dynamical changes of supplying current and voltage distortions. Many publications on optimization of APF sizing and allocation can be found in literature worldwide. However, the proposed solutions are based first of all on minimization of filter RMS currents or THD coefficients without direct application of economic criterion [3], [4], [5]. High costs of APFs result in need of optimization carried out from the economical point of view, which has been presented in the paper and could lead to wider application of APFs in the future. The paper shows that minimization of APF sizes is not enough to obtain the cheapest possible solution. In this sense the proposed approach can be treated as value added to the field. Two cases have been considered – active power filters with a classical control algorithm, which operates locally and aims at obtaining sinusoidal shape of waveforms in the point of installation, and active power filters with a modified control algorithm, which aims at reduction of waveform distortions in all nodes of an analysed power system [6]. Goal functions and optimization problems for both cases have been defined and simulation results have been presented.

References

1. H. AKAGI. Modern active filters and traditional passive filters. Bulletin of the Polish Academy of Sciences. Technical Sciences, vol. 54, no. 3, pp. 255–269, 2006..
2. M. MACIAZEK. Power theories applications to control active compensators. ", in Power Theories for Improved Power Quality, Power Systems Series, pp. 49–116, 2012..
3. A. MORADIFAR AND H.R. SOLEYMANPOUR. A Fuzzy Based Solution for Allocation and Sizing of Multiple Active Power Filters. Journal of Power Electronics, vol. 12, no. 5, pp. 830–841, 2012.
4. R. KEYPOUR AND H. SEIFI AND AND A. YAZDIAN-VARJANI. Genetic based algorithm for active power filter allocation and sizing. Electric Power Systems Research, vol. 71, no. 1, pp. 41–49, 2004..
5. Y.-Y. HONG AND Y.-K. CHANG. Determination of locations and sizes for active power line conditioners to reduce harmonics in power systems. IEEE Trans. on Power Delivery, vol. 11, no. 3, pp. 1610–1617, 1996..
6. D. GRABOWSKI AND M. MACIAZEK AND AND M. PASKO. Sizing of active power filters using some optimization strategies. The International Journal for Computation and Mathematics in Electrical and Electronic Engineering COMPEL, vol. 32, no. 4, pp. 1326–1336, 2013..

Parallel Profiling of Water Distribution Networks Using the Clément Formula

Guilherme Peretti Pezzi
University of Torino
peretti@di.unito.it

Evelyne Vaissié, Yann Viala
Société du Canal de Provence
Evelyne.VAISSIE@canal-de-provence.com,
Yann.Viala@canal-de-provence.com

Denis Caromel
caromel@unice.fr
Université de Nice Sophia Antipolis

Philippe Gourbesville
Polytech'Nice-Sophia
philippe.gourbesville@unice.fr

Abstract

Optimization of water distribution is a crucial issue which has been targeted by many modelling tools. Useful models, implemented several decades ago, need to be updated and implemented in more powerful computing environments. This paper presents the distributed and redesigned version of a legacy hydraulic simulation software written in Fortran (IRMA) that has been used for over 30 years by the Société du Canal de Provence in order to design and to maintain water distribution networks. IRMA was developed aiming mainly the treatment of irrigation networks – by using the Clément demand model and is now used to manage more than 6.000 km of piped networks. The growing complexity and size of networks requested to redesign the code by using modern tools and language (Java) and also to run distributed simulations by using the ProActive Parallel Suite.

References

1. A GRADIENT ALGORITHM FOR THE ANALYSIS OF PIPE NETWORKS. E. Todini and S. Pilati. Research Studies Press Ltd., 1988, pp. 1–20.
2. R. CLEMENT. Calcul des debits dans les reseaux d'irrigation fonctionnant a la demande. La Houille Blanche, vol. 5. Societe Hydrotechnique de France, 1966, pp. 553–576..
3. L. BADUEL AND F. BAUDE AND D. CAROMEL AND A. CONTES AND F. HUET AND M. MOREL AND AND R. QUILICI. Grid Computing: Software Environments and Tools. Springer-Verlag, January 2006, ch. Programming, Deploying, Compos- ing, for the Grid..
4. S. EISENSTAT AND M. C. GURSKY AND M. H. SCHULTZ AND AND A. H. SHERMAN. Yale sparse matrix package, ii. the nonsymmetric codes. Department of Computer Science, Yale University, Tech. Rep., 1977..
5. G. PERETTI PEZZI AND E. VAISSIE AND Y. VIALA AND B. GRAWITZ AND F. BONNADIER AND AND P. GOURBESVILLE. High Performance and Grid Computing Based Hydraulic Simulations Using the Clement Formule. Computing and Control for the Water Industry 2011, Exeter.

Minimizing Control Error of the Basic PID Controller Using the Grey System's Theory

Janusz Pochmara
Poznan University of Technology, Chair of Computer Engineering Poznan, Poland
janusz.pochmara@put.poznan.pl

Wojciech Grygiel
graduate of Poznan University of Technology
wojciech.grygiel25@gmail.com

Abstract

The Grey System's Theory allows for analyzing the behavior of complex systems that are not fully described by any model because of either insufficient information or there is no know mechanism that can describe the behavior. As the theory requires only small amount of data to predict future values of the system's output with high accuracy, it is possible to improve the basic PID controlled system without drastically rising the amount of calculations needed to perform the control. The improvement discussed in this paper includes changing the feedback loop to incorporate the Grey System's Theory calculation unit as well as the possible settings for the unit and their influence on the controlled system.

References

1. J. DENG. Introduction to Grey System Theory. The Journal of Grey System 1, pp. 1-24, October 1989.
2. S. LIU AND Y. LIN. Grey Information: Theory and Practical Applications. Springer, ISBN 1-85233-995-0, London 2006.
3. K. J. ASTROM AND T. HAGGLUND. PID Controllers: Theory, Design, and Tuning. Instrument Society of America, ISBN 1-55617-516-7, 1995.

Behavior of Magnetorheological Fluid Under Alternating Magnetic Field

Petr Polcar
University of West Bohemia in Pilsen
polcarp@kte.zcu.cz

Abstract

Several technical applications using exceptional physical properties of magnetorheological liquids are designed nowadays [1, 2]. Although direct current is commonly used to power these devices, the use of alternating current is demanded. To properly simulate and design such devices, the knowledge of the description of the behavior of commonly used magnetorheological liquids under the influence of the external alternating magnetic field is required. Certain time delay of viscosity to magnetic field change is known and observed [3, 4]. Theoretical background of this problem is summarized and experimentally verified by the use of a high speed camera on the fluid under different frequencies of alternating magnetic field commonly used in technical applications. Based on experimental results, description of the verified time-delays is stated.

Acknowledgement

The financial support of University of West Bohemia research project SGS-2012-039 is gratefully acknowledged.

References

1. P. POLCAR. , Construction and Experimental Verification of Magnetorheological Brake. Communications – Scientific Letters of the University of Zilina, 2(a), (2013) pp. 23-27.
2. J.D. CARLSON AND D.M. CATANZARITE AND K.A.ST. CLAIR. Commercial magneto-rheological fluid devices. International Journal of Modern Physics B (1996), 10 (23-24), pp. 2857-2865.
3. S. ODENBACH. Magnetoviscous effects in ferrofluids. Berlin: Springer (2002), 151 p., Lecture notes in physics. Monographs. ISBN 3-540-43068-7; ISSN 0940-7677.
4. I. MAZŮREK AND J. ROUPEC AND M. KLAPKA AND Z. STRECKER. Load and rheometric unit for the test of magnetorheological fluid. Meccanica (2013), 48 (3), pp. 631-641.

Flows in 3D Channel With Vibrating Walls

Petra Pořízková
Czech Technical University in Prague, Karlovo náměstí 13, 121 35, Prague 2, CZ
puncocha@marian.fsik.cvut.cz

Karel Kozel, Jaromír Horáček
Institute of Thermomechanics Academy of Sciences, Dolejškova 5, Prague 8, CZ
Karel.Kozel@fs.cvut.cz, jaromirh@it.cas.cz

Abstract

This study deals with numerical solution of 3D unsteady flow of compressible viscous fluid in the channel for low inlet airflow velocity. Mathematical models of flow is based on system of Navier-Stokes equations for laminar flow. The unsteadiness of the flow is caused by a prescribed periodic motion of a part of the channel wall with large amplitudes, nearly closing the channel during oscillations. The numerical solution is implemented using the finite volume method (FVM) and the predictor-corrector MacCormack scheme with Jameson artificial viscosity using a grid of quadrilateral cells. The unsteady grid of quadrilateral cells is considered in the form of conservation laws using Arbitrary Lagrangian-Eulerian method. The numerical results, acquired from a developed program, are presented for inlet velocity $\hat{u}_\infty = 4.12\mathrm{ms}^{-1}$ and Reynolds number $\mathrm{Re}_\infty = 4 \times 10^3$ and the wall motion frequency 100 Hz. Goal of this work is to describe mathematical model of flow in the channel which involves attributes of real flow as is "Coandă phenomenon", vortex convection and diffusion, jet flapping etc.

References

1. P. PUNČOCHÁŘOVÁ - POŘÍZKOVÁ AND J. HORÁČEK AND K. KOZEL AND J. FÜRST. Numerical simulation of unsteady compressible low Mach number flow in a channel. Engineering mechanics, **17**(2), 83-97, 2010.
2. P. POŘÍZKOVÁ AND K. KOZEL AND J. HORÁČEK. Simulation of Unsteady Compressible Flow in a Channel with Vibrating Walls - Influence of the Frequency. In: Computers and Fluids. 2011, vol. 46, no. 1, p. 404-410. ISSN 0045-7930.
3. P. PUNČOCHÁŘOVÁ - POŘÍZKOVÁ AND J. FÜRST AND J. HORÁČEK AND K. KOZEL. Numerical Solutions of Unsteady Flows with Low Inlet Mach Numbers. In: Mathematics and Computers in Simulation. 2010, vol. 80, no. 8, p. 1795-1805. ISSN 0378-4754.

Numerical Modelling of Viscous and Viscoelastic Fluids Flow for Generalized Newtonian and Oldroyd-B Fluids

Radka Keslerová, Karel Kozel, Vladimír Prokop
Czech Technical University in Prague
radka.keslerova@fs.cvut.cz, Karel.Kozel@fs.cvut.cz,
Vladimir.Prokop@fs.cvut.cz

Abstract

The aim of this paper is to describe and discuss the results of numerical simulation of steady flows of viscous and viscoelastic fluids. The mathematical models are Newtonian and Oldroyd-B models. Both models can be generalized by cross model in shear thinning meaning. Numerical tests are performed on three dimensional geometry, a branched channel with one entrance and two output parts. Numerical solution of the described models is based on cell-centered finite volume method using explicit Runge-Kutta time integration. In this case the artificial compressibility method can be applied.

References

1. P. LOUDA AND K. KOZEL AND J. PŘÍHODA AND L. BENEŠ AND T. KOPÁČEK. Numerical Solution of Incompressible Flow through Branched Channels. Journal of Computers & Fluids, 46 (2011) 318-324.
2. T. BODNÁR AND A. SEQUEIRA. Numerical Study of the significance of the non-Newtonian Nature of Blood in Steady Flow through Stenosed Vessel. Advances in Mathematical Fluid Mechanics (2010), 83-104.
3. R. KESLEROVÁ AND K. KOZEL. Numerical Modelling of Incompressible Flows for Newtonian and non-Newtonian Fluids. Mathematics and Computers in Simulation 80 (2010) 1783-1794.

Solution to Maxwell Equations in Axisymmetric Singular Domains

Franck Assous
Ariel University, Israel
franckassous@netscape.net

Irina Raichik
Bar-Ilan Universtity, Israel
irina.raichik@gmail.com

Abstract

We propose a new approach to solve the Maxwell equations in an axisymmetric *singular* 3D domain Ω, generated by the rotation of a *singular* polygon ω around one of its sides. This domain is *singular* in the sense that it contains reentrant corner or edges. We first consider the equations written in a (r, θ, z) geometry. Then, using a Fourier transform in θ, we reduce the 3D Maxwell equations to a series of 2D Maxwell equations, depending on the Fourier variable k. Hence, we will compute the solution to the 3D Maxwell equations by solving a certain number of 2D problems, depending on k.
Let us denote $(\mathbf{E_k}, \mathbf{B_k})$ the electromagnetic field solution for each mode k. Following [1] and [2], one can prove that this solution can be decomposed into a regular and a singular part. The regular part belongs to a space of regularity H^1, in which one can easily compute a numerical solution with a standard finite element method. The difficulty comes from the singular part that belongs to a finite-dimensional subspace, the dimension of which being related to the number of reentrant corners and edges of the 2D domain ω. We will propose a new method based on a decomposition of the computational domain into subdomains, and will derive an ad hoc variational formulation, in which the interface conditions are imposed with a method deduced from a Nitsche approach.
We will first consider the particular case $k = 0$ that corresponds to the two dimensional axisymmetric case. We will show how to compute $\mathbf{x_0^s}$, the singular part of the electric field solution $\mathbf{E_0}$, and then will derive the time-dependent variational formulation to compute the regular part of the solution. A similar approach can be used to compute $\mathbf{B_0}$. In a second part, we will generalize this approach to the $k \neq 0$ mode, which is not a straightforward extension at all. Following [2], this will require first to derive the system of equations solved by the singular parts for each k. Then to derive and solve the time-dependent variational formulation depending on k, for each mode. Finally to reconstruct the approximate 3D solution electromagnetic fields from each mode k. Some theoretical problems will appear, as the choice of number of Fourier modes to actually well reconstruct the full 3D solution, that is, the question of the convergence of the numerical Fourier series.

References

1. F. ASSOUS AND P. CIARLET AND S. LABRUNIE AND J. SEGRÉ. Numerical solution to the time-dependent Maxwell equations in axisymmetric singular domains:The Singular Complement Method. *J. Comput. Phys.*, 191, 147-176 (2003).
2. P. CIARLET AND S. LABRUNIE. Numerical Solution of Maxwell's equations in axisymmetric domains with the Fourier SIngular Complement Method. *Diff. Eqs & Appl.*, **3-1**, 113–155 (2011).

Comparisons Between a Local Multigrid Method and H-Adaptive Methods in Solid Mechanics

Isabelle Ramière, Hao Liu
CEA Cadarache, DEN, DEC, SESC, LSC
isabelle.ramiere@cea.fr, hao.liu@cea.fr

Lauréline Barbié, Frédéric Lebon
LMA Aix-Marseille Univ. CNRS Centrale Marseille
barbie@lma.cnrs-mrs.fr, lebon@lma.cnrs-mrs.fr

Abstract

Adaptive mesh refinement methods are currently commonly used when dealing with problems including local singularities (entrant corners, heterogeneities of coefficients, discontinuous boundary conditions, cracks,...). Two main approaches can be distinguished : adaptive methods (h-, p-, r-adaptive methods as well as their combinations : typically hp- or hr-adaptive methods) and local multigrid methods (typically LDC, FAC or FIC methods). From an initial coarse mesh, adaptive methods work on elements size, nodes relocation or degree of basis functions to design an optimal refined mesh. On the other hand, local multigrid methods also focus on elements size but through the addition of local structured meshes having finer and finer discretization steps. To the best of our knowledge local multigrid and h-adaptive methods, that both locally reduce the mesh step, have never been deeply compared especially in the context of structural mechanics where only a few recent studies have focused on local multigrid methods.
We propose here to compare in a solids mechanics framework the two h-adaptive strategies [2], namely the remeshing (conforming mesh) and the hierarchical (non-conforming mesh) strategy, to the Local Defect Correction multigrid method [3, 1] in terms of memory space and computation time. The Zienkiewicz and Zhu a posteriori error estimator is used to automatically detect the elements to be refined as well as to define the density function required for the h-adaptive methods. The test cases under study derive from nuclear engineering simulations of the mechanical pellet-cladding interaction [1]. This interaction implies local singularities due to discontinuous contacts which lead to very localised stress concentrations. Complete accurate 3-D simulations of this phenomena is still a challenging problem. For industrial modelling reasons, the finite element discretization has to be done with quadrangular linear elements. This constraint may penalize the performances of the remeshing h-adaptive method, which is the most performed adaptive method nowadays.

References

1. L. Barbié and I. Ramière and F. Lebon. Strategies around the local defect correction multi-level refinement method for three-dimensional linear elastic problems. Computers and Structures, volume 130, pp. 73-90, 2014.
2. W. Ehlers and M. Ammann and S. Diebels. h-Adaptive FE methods applied to single- and multiphase problems. International Journal of Numererical Methods in Engineering, volume 54, pp. 219-239, 2002.
3. W. Hackbusch. Local Defect Correction Method and Domain Decomposition Techniques. Springer- Verlag, Defect Correction Methods, Computing Supplementum, volume 5, pp. 89-113, 1984.

A Boundary Integral Approach to Compute Resonances in Open N-disk Systems

Gilles Lebeau, Laurent Michel, Francesca Rapetti
Lab. Dieudonne, Dept. Math., Univ. de Nice
lebeau@unice.fr, lmichel@unice.fr, frapetti@unice.fr

Abstract

Nowadays it is possible to extract resonances in open systems experimentally, even if they have a reasonable overlap, for example by using the method of harmonic inversion. We would like to investigate the resonances of open n-disk systems numerically, by a boundary integral (BI) method. According to the BI method, wave functions in the domain surrounding the system are expressed in terms of line integrals of the wave function and of its normal derivative along the system's boundary; resonances are obtained as roots of Fredholm determinants. The BI method is already used to compute stationary states of a quantum particle in nano-devices and quantum billiards (see [3] and references therein for applications and [2] for an introduction to theory). In this work, we study the BI approach, its numerical implementation and application for open n-disk systems. A comparison with experimental calculations [1] is hopefully provided.

References

1. S. BARKHOFEN AND J.J. METZGER AND R. FLEISCHMANN AND U. KUHL AND H.-J. STOCKMANN. Experimental Observation of a Fundamental Length Scale of Waves in Random Media. Physical Review Letters 111 (2013) 183-902.
2. G. LEBEAU. Propagation des ondes dans les dièdres. Mémoires de la SMF 60 (1995) 1-124.
3. H.E.TURECI AND H.G.L. SCHWEFEL. An efficient Fredholm method for the calculation of highly excited states of billiards. J. Phys. A: Math. Theor. 40 (2007) 13869-13882.

Thermofluiddynamical Numerical Simulations of Particle-laden Flows in (Bio) Chemical Fluidized Bed Reactors

Cornelia Rauh
Institute of Food Biotechnology and Food Process Engineering; TU Berlin
cornelia.rauh@tu-berlin.de

Naveed Iqbal
Institute of Fluid Mechanics; Friedrich-Alexander University Erlangen-Nuremberg
naveed.iqbal@lstm.uni-erlangen.de

Abstract

There are two basic approaches to model particle-laden flows: namely Eulerian-Eulerian (two-fluid models) and Eulerian-Lagrangian. In this work the later approach is used that is also known as CFD-DEM (CFD: Computational Fluid Dynamics; DEM: Discrete Element method) approach. The fluid phase is modelled using a continuum approach considering the transient, compressible and turbulent nature of the flow and particles are modelled with the Lagrangian approach. In the current study, the particle tracking as well as particle-particle interactions are taken into account. This model is capable of simulating flows with a wide range of particulate void fractions. Momentum exchange between the phases is modelled by combining the well-known Ergun's equation and Wen and Yu relation. These relations are used by several researchers [1, 2]. Collision forces between particles are calculated using a soft sphere model (spring, slider and dashpot model). The framework of OpenFOAM an open source CFD simulation code is used. In the current study, the simulation of a fluidized bed along with heat exchange between the phases is developed. The coupled mass, momentum and energy balance equations are used to calculate the flow behavior, thermal transport within the phases, the viscous dissipation and heat exchange due to radiation between the solid and fluid phase. Heat exchange due to radiation is modelled using P1-radiation model. The dimensions of the simulation domain are similar to Link et al. (2005) but with different particle properties. The temperature of air entering through a jet is 400K to see the effects of heat transfer to the particles. The particles have an initial temperature of 300K. The particles behavior, fluidization, bubble formation and temperature distribution of the particles are investigated in detail. Due to bubble formation during the fluidization process, the particles encounter different residence time that results in non-uniform temperature distribution. The particles residing for longer time like on the top of bubble have higher temperature. The results show a good qualitative agreement with the literature. The quantitative comparison is planned in near future.

References

1. Y. TSUJI AND T. KAWAGUCHI AND T. TANAKA. Discrete particle simulation of two-dimensional fluidized bed. Powder Technology, 77 (1993) 79-87.
2. J.M. LINK AND L.A. CUYPERS AND N.G. DEEN AND J.A.M. KUIPERS. Flow regimes in a spout-fluid bed: A combined experimental and simulation study. Chemical Engineering Science 60 (2005) 3425-3442.

Numerical Simulation of Under-expanded Jets of Dense Gases With an Adaptive Finite Volume Method

Barbara Re, Alberto Guardone
Politecnico di Milano
barbara.re@polimi.it, alberto.guardone@polimi.it

Cécile Dobrzynski
IMB, Institut Polytechnique de Bordeaux
cecile.dobrzynski@math.u-bordeaux1.fr

Abstract

Dense gas flows in the vicinity of the liquid-vapour saturation curve are investigated numerically using an adaptive-grid finite volume schemes. In particular, the shock configuration resulting from an under-expanded jet at the exit of a gas dynamic nozzle is studied for diverse stagnation conditions. The chosen approach requires no interpolation between the grids since the solution on the new adapted grid is automatically obtained in a conservative fashion by including additional numerical fluxes accounting for the mesh alteration. Numerical simulations expose a strong dependence of the size of the Mach disk and of its distance from the nozzle exit on the flow conditions.

References

1. J. HARINCK AND A. GUARDONE AND AND P. COLONNA. The influence of molecular complexity on expanding flows of ideal and dense gases,. Phys. Fluids, vol. 21, no. 8.
2. M. S. CRAMER AND R. N. FRY. Nozzle flows of dense gases. Phys. Fluids A 5, 1246 (1993).
3. A. GUARDONE AND M. PARSANI AND L. VIGEVANO. Numerical simulations of under-expanded nozzle flows of dense gases. Proceedings of the AIMETA Congress 2007.

Analytical Threeshold Voltage Model Considering Quantum Size Effects for Nanocrystalline Silicon Thin Film Transistors

Riad Remmouche, Rachid Fates, Hachemi Bouridah
LEM laboratory, Electronics Department, Jijel University
remmouche@yahoo.com, rachid.fates@yahoo.fr,
hachemi.bouridah@gmail.com

Abstract

The production of polycrystalline (either with micro or nano dimensions) silicon (poly-Si) thin films have been under development since a few years ago. The research interest in this field envisages the devices improvement for micro and optoelectronic applications. The active-matrix liquid-crystal displays (AMLCDs) commercial success has stimulated considerable research on thin-film transistors (TFTs). Nanocrystalline silicon (nc-Si) is a compromise solution between amorphous silicon (a-Si) and poly-Si. It is a good alternative to a-Si since it offers higher carriers mobility, and its application in TFTs is recent. The nanostructural properties of nc-Si films are important issues for these device applications. The consideration of nc-Si structure for circuit design and simulation, is thus vital to a rational description of the electrical and the electronic behavior of the device. Several authors have made considerable studies concerning the threeshold voltage and the different voltage relationships for poly-Si TFTs. However, few researchers have focused on the study of the nc-Si TFTs electrical characteristics. In the present study, we propose an analytical model allowing the calculation of nanocrystalline silicon thin film transistors threeshold voltage by considering a spherical shape of silicon nanocrystallites forming the channel. Results show that, according to the quantum effects on dielectric constant and band gap, the threeshold voltage values are strongly related to the silicon crystallites structure in terms of size and geometry. The confrontation of our results with existing research data shows a good agreement between the threeshold voltage shapes. and an interesting difference in the surface potential variation related to the morphology specificity considered in our theoretical approach.

References

1. W. W UA AND R. Y AO AND X. Z HENG AND . A new analytical threshold voltage model for the doped polysilicon thin-film transistors. Solid-State Electronics 53 (2009) 607–612.

Sequentially Optimal Sensor Placement in Thermoelastic Models

Ilka Riedel, Roland Herzog
TU Chemnitz
ilka.riedel@mathematik.tu-chemnitz.de,
roland.herzog@mathematik.tu-chemnitz.de

Abstract

We consider optimal sensor placement problems in thermoelastic solid body models. More precisely, our goal is to place temperature sensors in a near-optimal way, such that their measurements allow an accurate prediction of the thermally induced deformation at a particular point of interest. The latter is our quantity of interest.

By exploiting the particular structure of thermoelastic models, we present a linear estimator which first reconstructs the temperature field from tempeature measurements and afterward computes the displacement field and from there the quantity of interest. For the temperature state reconstruction we use model order reduction techniques such as Proper Orthogonal Decomposition and Balanced Truncation.

In order to optimize the quality of the estimator with respect to the sensor positions, we minimize a function of the eigenvalues of the estimators covariance matrix. To make the problem tractable and to take restrictions on the sensor locations into account in an easy manner, we allow the sensors only to lie in a predetermined finite (possibly large) set of potential locations. Moreover, we use a sequential (greedy) algorithm for the placement of one sensor at a time.

Numerical results are presented for the estimation of the tool center point displacement of a machine tool under thermal loading.

References

1. R. HERZOG AND I. RIEDEL. Sequentially Optimal Sensor Placement in Thermoelastic Models. Preprint, submitted to Optimization and Engineering.

Multiscale Models of Liver Perfusion Based on Computational Homogenization

Eduard Rohan, Vladimír Lukeš, Robert Cimrman
University of West Bohemia
rohan@kme.zcu.cz, vlukes@kme.zcu.cz, cimrman@ntc.zcu.cz

Abstract

Modeling of the liver perfusion belongs to very important and challenging problems of the biomechanics due to the large complexity of the blood vessels which form a hierarchical structure. Several scales of the vessel network can be distinguished which comprise three major systems: the hepatic and portal veins, and the portal arteries. In this paper we focus on modelling flow in the lowest level of the perfusion system which is generated by the liver lobules. These filtration units form quasi-periodic structures which can be handled using the homogenization technique.

Recently we developed homogenized models of poroelastic fluid saturated media which are suitable for describing such highly heterogeneous structures. Under normal physiological conditions, the deformation of the tissue can be disregarded for simulations of the flow. However, to simulate flow obstructions, or effects of resections, the deformation must be taken into account. Assuming a heterogeneous meso-structure at the lobular level is described using the Biot type continuum with large contrasts in the permeability, upscaling procedure leads to a macroscopic two-phase visco-poroelastic model with the fading memory properties. In a case of large deformation, the same homogenization schemes are used for linearized incremental formulations with updating micro-, or meso-structures using the two-scale solutions computed at previous time levels. There is an alternative to handle nonlinear response of the porous media in situations, where the permeability and other effective coefficients are modified by the deformation, although the linear kinematics is still valid. As an option, a homogenized model with dimensional reduction of the double porosity media organized in layers can be used; it allows for decomposition of a 3D volume into a system of coupled periodic layers which are described using 2D continua with effective permeabilities computed for 3D representative microstructures. This treatment allows to capture branching structures of the precapillaries. Numerical simulations for all the above mentioned models were obtained using the finite element method implemented in the SfePy (http://sfepy.org) software which is developed by our group.

References

1. E. ROHAN. Modelling large deformation induced microflow in soft biological tissues. Theor. and Comp. Fluid Dynamics, 20 (2006) 251-276.
2. E. ROHAN AND R. CIMRMAN. Two-scale modelling of tissue perfusion problem using homogenization of dual prous media. Int. Jour. for Multiscale Comput. Engrg. 8 (2010) 81-102.
3. E. ROHAN AND S. NAILI AND R. CIMRMAN AND T. LEMAIRE. Multiscale modelling of a fluid saturated medium with dual porosity: relevance to the compact bone. J. Mech. Phys. Solids 60 (2012) 857-881.

A Bayesian Approach to Linear and Nonlinear Identification Problems

Bojana Rosic, Hermann Matthies
Technische Universitaet Braunschweig
bojana.rosic@tu-bs.de, wire@tu-bs.de

Anna Kucerova, Jan Sykora
Technical University Prague
anicka@cml.fsv.cvut.cz, jan.sykora.1@fsv.cvut.cz

Abstract

Driven by the needs of applications in industry, the theory of inverse problems has become highly important. The state or parameter estimation from given observations of a mechanical system is generally an ill-posed inverse problem. The solution often does not exist, it is not unique and it is highly sensitive on the data perturbations. To resolve this issue, the deterministic identification procedures use different kinds of regularisation techniques which as a final result deliver a point estimate of the solution. However, the deterministic algorithms fully ignore the presence of uncertainty in a solution and its possible non-uniqueness. On the other hand, the inverse problem seen in a probabilistic Bayesian point of view does not encounter these difficulities. Namely, the parameter/state is modelled as random variable such that the process of obtaining more information through experiments in a Bayesian setting becomes well-posed. In this work we use the functional approximation of uncertainty and develop a purely deterministic procedure for the updating process not only for linear but also for nonlinear problems—linear and nonlinear spectral based Bayesian identification [1]. This is then contrasted to a fully Bayesian update based on Markov chain Monte Carlo sampling on a few numerical examples.

References

1. B. Rosic and A. Kucerova and J. Sykora and O. Pajonk and A. Litvinenko and H. G. Matthies. Parameter identification in a probabilistic setting. Eng. Structures, 50 (2013) 179-196.

Turning a Serial Forward Code Into a Parallel Inverse Code

Mohammad Ali Rostami
Department of Mathematics and Computer Science, Friedrich Schiller University Jena, Jena
a.rostami@uni-jena.de

Abstract

Advanced mathematical models to describe and analyze complicated phenomena of interest have led to a tremendous increase of the understanding in various disciplines, including physical, engineering, financial, and life sciences. There is also a long tradition in transforming these mathematical models into computer models to be efficiently executed on state-of-the-art computer architectures. These substantial advances were only possible by bringing together profound knowledge and sophisticated techniques from applied mathematics, computer science, and the corresponding application disciplines.

Often, the design and implementation of these forward models require substantial human effort that is justified by the scientific findings resulting from using these models to better understand the given application problem at hand. It is not uncommon to use these forward models over and over again while varying certain input parameters of interest. However, these computer models are increasingly used as the starting point for further, more advanced investigations that go far beyond executing the forward model multiple times with different input parameters. The design of these forward models should therefore consider the requirements of an inverse framework as well. Unfortunately, today, most forward models are designed without taking into account that they will be used to solve inverse problems.

Here, we focus on the interplay between parallel computing and automatic differentiation when designing a forward model considering a geothermal model [1]. To the best of our knowledge, there is no previous work dealing with this topic. Somehow related are approaches that try to reduce the computational complexity of a forward model that is used in an optimization framework. An example in the context of a geoscientific application is the approach in [2] that introduces a simplification of forward models in magnetotellurics to enable evolutionary optimization algorithms in three space dimensions. However, the reduction of the computational complexity is not our focus. The new contribution of our work [3] is to demonstrate the mutual dependencies between parallel computing used in various different ways for a forward model and automatic differentiation.

References

1. V. RATH AND A. WOLF AND AND H. M. BÜCKER. Joint three-dimensional inversion of coupled groundwater flow and heat transfer based on automatic differ- entiation: Sensitivity calculation, verification, and synthetic examples. Geophysical Journal International, vol. 167, no. 1, pp. 453–466, 2006.
2. B. ALEXANDER AND S. THIEL AND AND J. PEACOCK. Application of evolutionary methods to 3D geoscience modelling. n Proceedings of the Fourteenth International Conference on Genetic and Evolutionary Computation Conference, ser. GECCO '12. New York, NY, USA: ACM, 2012, pp. 1039–1046.
3. H. MARTIN BÜCKER AND M. ALI ROSTAMI AND AND RALF SEIDLER. Turning a Serial Forward Code into a Parallel Inverse Code: A Case Study from Geothermal Engineering. In Proceedings of the International Conference on Computers, Automatic Control, Signal Processing and Systems Science, 2014, pp. 22-25.

Mesh Generation Using Dynamic Sizing Functions

Florian Rudolf, Yannick Wimmer, Josef Weinbub, Karl Rupp, Siegfried Selberherr
Institute for Microelectronics, Technische Universität Wien
rudolf@iue.tuwien.ac.at, wimmer@iue.tuwien.ac.at,
weinbub@iue.tuwien.ac.at, rupp@iue.tuwien.ac.at,
selberherr@iue.tuwien.ac.at

Abstract

Assuming elements have a proper shape, the mesh element size is the primary parameter for adjusting the quality of the solution of most numerical simulation problems [1]. Smaller elements usually indicate a better resolution but also result in a higher number of elements, affecting the runtime performance of the simulation. Therefore, a good balance between the numerical quality and the runtime performance has to be found. In many simulation scenarios, a-priori information, like boundary conditions or non-uniform material properties, is available which can be used to optimize the mesh regarding the element size. Typically, the desired element size can be specified by global sizes for all elements of a (possibly partitioned) mesh or by scalar fields. While global sizes lack flexibility, scalar fields are difficult to treat due to their non-trivial impact, in particular, when using multiple scalar fields simultaneously. Additionally, some software libraries, like Triangle, support a callback mechanism for externally providing element size criteria in order to steer the mesh generation process. However, this option typically requires recompilation with specific compilation flags and the actual implementation of the element size function. We cope with this problem by extending our meshing software ViennaMesh [2] with a dynamic framework for defining the size of mesh elements with an XML-based configuration. The framework automatically manages the computation of the local element sizes and provides interfaces to mesh generation backends, like Triangle, Tetgen, CGAL, or Netgen. Arbitrary element size functions can be composed from scalar fields, arithmetic operations, and geometric predicates such as the local feature size [3]. We demonstrate the practicability of our approach by presenting a typical mesh generation workflow for microelectronic devices which require heterogeneous element sizes due to very thin layers and non-uniform material properties in the interior of the mesh. The resulting meshes are processed with the spherical harmonics simulator ViennaSHE [4], allowing to evaluate the mesh quality via, for instance, the convergence behavior.

References

1. S. CHENG ET AL. Delaunay Mesh Generation. CRC Press, 2013.
2. F. RUDOLF ET AL. ViennaMesh. http://viennamesh.sourceforge.net/.
3. J. RUPPERT. A Delaunay Refinement Algorithm for Quality 2-Dimensional Mesh Generation. J. Alg., 18(3), 1995.
4. K. RUPP ET AL. On the Feasibility of Spherical Harmonics Expansions of the Boltzmann Transport Equation for Three-Dimensional Device Geometries. In Proc. of IEEE IEDM, 2011.

Automatic Finite Volume Discretizations Through Symbolic Computations

Karl Rupp, Florian Rudolf, Josef Weinbub, Ansgar Jüngel, Tibor Grasser
TU Wien
rupp@iue.tuwien.ac.at, rudolf@iue.tuwien.ac.at,
weinbub@iue.tuwien.ac.at, juengel@asc.tuwien.ac.at,
grasser@iue.tuwien.ac.at

Abstract

The finite volume method is a popular method for the solution of systems of partial differential equations whenever local conservation properties are desired. However, engineering software usually does not reflect the underlying continuous mathematical formulation internally, but instead implements the discrete system directly, sacrificing a higher-level representation. As a consequence, the discretization code needs to be altered whenever the mathematical formulation changes. For modeling purposes, however, it is often desirable to only modify the mathematical formulation and let the software deal with the derivation of the discrete equations. In the context of computational fluid dynamics, OpenFOAM [1] has successfully demonstrated that such a goal can in principle be achieved.

We present results obtained from coupling the symbolic computation library ViennaMath [2] to a finite volume code to solve systems of PDEs on structured and unstructured grids in one, two, and three dimensions. As an example, a fully automatic Scharfetter-Gummel-like stabilization [3] of a finite volume method for a drift-diffusion system in the context of semiconductor device simulation is discussed. Nonlinear couplings are automatically handled through Picard iterations or a globalized Newton-Raphson scheme. Moreover, we demonstrate that the mathematical formulation can be easily changed to include additional details in the mathematical model. No recompilation of the source code is required, hence our approach is also suitable for graphical user interfaces as well as scripting languages such as Python, which are frequent requirements for engineering purposes.

References

1. OpenFOAM Foundation. OpenFOAM. http://www.openfoam.com/.
2. K. Rupp et al.. ViennaMath. http://viennamath.sourceforge.net/.
3. D. L. Scharfetter and H. K. Gummel. Large-Signal Analysis of a Silicon Read Diode Oscillator. IEEE Trans. El. Dev., 16:64-77, 1969.

3D Simulation of the Water Storage Process in the Feathers of Sandgrouses

Alexander Rüttgers, Michael Griebel
Institute for Numerical Simulation, University of Bonn, Germany
ruettgers@ins.uni-bonn.de, griebel@ins.uni-bonn.de

Heiko Schmied, Dieter Wittmann
Institute of Crop Science and Resource Conservation, University of Bonn, Germany
schmied@uni-bonn.de, wittmann@uni-bonn.de

Abstract

Sandgrouses (lat. Pteroclididae) [1] are a family of birds that mainly lives in dry areas of Africa and Asia. Due to large distances between the watering holes and the sandgrouses' nests, the adult birds have to transport water in their breast feathers over long distances to water their young. Although the enormous water storage capacity of the sandgrouses' feathers is reported in literature (cf. Cade and MacLean [2]), the process of water absorption is a matter of ongoing research.

Basing on recent results on the functional morphology of the sandgrouses' feathers by Schmied [3], we build a computer model to perform three-dimensional flow simulations of the storage process. For this purpose, we use our two-phase flow solver NaSt3DGPF [4,5] developed at the Institute for Numerical Simulation. The two fluid phases in NaSt3DGPF are distinguished with the levelset technique and surface tension is modeled with the Continuum Surface Force (CSF) method. The flow solver is parallelized on CPU with MPI and on GPU with Nvidia's CUDA architecture.

Using NaSt3DGPF we simulate the evolution of a water droplet in the feather structure of a sandgrouse. As the smallest structures of the feathers have a size in order of micrometers, surface tension effects are dominant on this length scale. Surface tension in the simulations is modeled explicitly which strongly increases the computing time. We therefore perform massively parallel computations to obtain results within reasonable time.

In this talk, we discuss the results of our water storage simulations. We do not only present the results in the sandgrouses' feather structure but also show results for a modified and further simplified geometry on the same length scale. To allow a better comparison, we analyze qualitative data such as the droplet's barycenter position, its rise velocity and give a measurement for the droplet's deformation over time.

References

1. E. DE JUANA. Family Pteroclidae (Sandgrouse). in Handbook of the Birds of the World 4 (1997) 30-57 .
2. T. CADE AND G. MACLEAN. Transport of water by adult sandgrouse to their young. The Condor 69 (1967) 323-343.
3. H. SCHMIED. Die wasserspeichernden Federn der Flughühner (Pteroclididae) - Funktionsmorphologie, Benetzungseigenschaften & technischer Nachbau. PhD Thesis, University of Bonn, 2014.
4. R. CROCE AND M. GRIEBEL AND M. SCHWEITZER. Numerical simulation of bubble and droplet deformation by a level set approach with surface tension in three dimension. Int. J. Num. Meth. Fluids 62(9) (2010) 963-993.
5. P. ZASPEL AND M. GRIEBEL. Solving incompressible two-phase flows on multi-GPU clusters. Comput. & Fluids 80 (2013) 356-364.

Parallel Simulator for Decentralized Trustworthy Computing System

Michal Zochniak, Bartosz Sawicki
Warsaw University of Technology
zochniam@iem.pw.edu.pl, bartosz.sawicki@ee.pw.edu.pl

Abstract

Simulations are widely used to recreate real word processes in the computational reality. Complex phenomena from physics, chemistry, medicine and many other domains can be studies using artificial models. Todays distributed computers systems can easily achieve complexity similar to real word objects. This problem has special importance for decentralized, heterogeneous networks of peer-to-peer nodes, where number of players reach millions. Behavior of such network is definitely indeterministic, and only simulators allow to understand its basis.

In previous works authors proposed peer-to-peer computing system focused on controlled reliability of results. There are many popular simulators for grid networks such as Simgrid or CloudSim, but none of them is focused on trust modeling. We created a simulator, which for given input parameters - number of nodes, nodes quality, number of jobs - would be able to estimate performance of the grid over time. The simulator is able to predict how would the hypothetical computing system behave, if jobs scheduling and trust management were implemented with presented methods and algorithms.

The simulator is based on discrete event concept. It's parallel implementation is in C++ using OpenMP API. It depends only on the OpenMP and standard C++ library, so can be compiled on any system supporting these (including Windows with Microsoft Visual C++ and Linux with GCC).

References

1. Sulistio and Anthony and C. Shin Yeo and and Rajkumar Buyya. Simulation of Parallel and Distributed Systems: A Taxonomy and Survey of Tools.. 2005-04. http://www. chinagrid. net (2002): 1-19..
2. Casanova and Henri and Arnaud Legrand and and Martin Quinson. Simgrid: A generic framework for large-scale distributed experiments.. Computer Modeling and Simulation, 2008. UKSIM 2008. Tenth International Conference on. IEEE, 2008.
3. Rodrigo N. Calheiros and Rajiv Ranjan and Anton Beloglazov and Cesar A. F. De Rose and Rajkumar Buyya. CloudSim: a toolkit for modeling and simulation of cloud computing environments and evaluation of resource provisioning algorithms. oftware - Practice and Experience, 2011, no 41, pp. 23-50.
4. Michał Zochniak and Bartosz Sawicki. Reliable peer-to-peer computing system. Przeglad Elektrotechniczny, 2014, (accepted for publication).

Multistep Time Integration Solver for Stiff Bioheat Equation

Bartosz Sawicki
Warsaw University of Technology
bartosz.sawicki@ee.pw.edu.pl

Abstract

For the first time, temperature distribution inside the living body was described by Harry. H. Pennes in 1948. Since that time bioheat equation (also known as a Pennes equation) is widely used in medicine and biotechnical science. From the mathematical point of view the equation could be seen as a extended diffusion problem:

$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u) - E(u)u + f, \tag{1}$$

where D is diffusion coefficient, $E(u)$ nonlinear perfusion function and f is volume heat source.

Solving of diffusion equation is quite a common task, which has been intensively investigated for many years. New challenges are coming with modern technologies which introduce specific parameters into the problem. One of such examples is Magnetic Fluid Hyperthemia, where ratio between D and f is so high that the equation has to be considered as a very stiff. In previous author works it was shown, that choosing wrong time integration solver has tremendous impact on the transient state solution.

The implicit multistep time integration scheme is a suggested method for stiff problems. Although it is more memory consuming than one-step methods (such as Runge-Kutta family), but has an advantage of incorporating knowledge of solution history. The Backward Differentiation Formula (BDF) is one of popular examples of multistep algorithms. Some authors reported that I could be less efficient than one-step methods, but it is the case specific observation.

The aim of this paper is to design multistep solver for stiff diffusion equation and to verify usefulness of BDF algorithm is such case. Comparison with one-step RungeKutta adaptive solver, as well as with simple Euler integration schemes will be presented.

References

1. BARTOSZ SAWICKI AND ARKADIUSZ MIASKOWSKI. Nonlinear Higher-order Transient Solver for Magnetic Fluid Hyperthermia. Journal of Comp. and Appl. Mathematics, (under review).
2. P. SOLIN AND L. KOROUS. Adaptive higher-order finite element methods for tran- sient PDEs problems based on embedded higher-order implicit Runge-Kutta methods. Journal of Computational Physics, vol. 231, pp. 1635-1649, 2012.
3. P. BIRKEN AND ET AL.. Efficient Time Integration for Discontinuous Galerkin Methods for the Unsteady 3D Navier-Stokes Equations. European Congress on Computational Methods and Applied Sciences and Engineering (ECCOMAS 2012), number Eccomas., 2012..

A Periodic Basis System of the Smooth Interpolation Space

Karel Segeth
Institute of Mathematics, Academy of Sciences, Prague
segeth@math.cas.cz

Abstract

The contribution is devoted to the problem of smooth interpolation of data in 1D. In addition to the exact interpolation of data at nodes, we are also concerned with the smoothness of the interpolating curve and its derivatives.

The interpolating curve is defined as the solution of a variational problem with constraints. The system of functions $\exp(ikx)$, k being an integer, is taken for the basis of the space where we measure the smoothness of the result. It also generates the functions used for the interpolation itself. Choosing different norms when measuring the smoothness, we arrive at different interpolating functions.

We discuss the proper choice of different norms for this way of approximation and present the results of several 1D numerical examples that show the advantages and drawbacks of smooth interpolation.

References

1. A. TALMI AND G. GILAT. Method for Smooth Approximation of Data. J. Comput. Phys. 23 (1977) 93-123.
2. K. SEGETH. Some Computational Aspects of Smooth Approximation. Computing 95 (2013) Suppl 1: S695-S708.

Adaptive Step-size Control in Obreshkov Predictor–Corrector Pairs

John Butcher
University of Auckland, Department of Mathematics, 38 Princes Street, 1142 Auckland, New Zealand
butcher@math.auckland.ac.nz

Pavla Sehnalová
Brno University of Technology, Faculty of Mechanical Engineering, Technická 2, 616 69 Brno, Czech Republic
sehnalova@fme.vutbr.cz

Abstract

In a previous paper [1], two-step predictor-corrector pairs, each based on two derivative formulae, were introduced. By using suitable Obreshkov quadratures [5], it is possible to obtain a fourth order two-step predictor and a one-step corrector. The methods were formulated using a Nordsieck representation [4] using the ideas developed by C. W. Gear [2]. This approach made local error estimation and variable stepsize possible and convenient.

The present paper aims to improve the behaviour of these method pairs by introducing a more sophisticated stepsize controller, based on PI control theory [3]. Additional improvements under consideration include the scale-and-modify technique and variable order based on a Lagrange multiplier optimisation approach.

This paper also focuses on stability regions of the method.

References

1. J. C. BUTCHER AND P. SEHNALOVÁ. Predictor–corrector Obreshkov pairs. Computing 95 (2013) 355-371.
2. W. C. GEAR. Numerical initial value problems in ordinary differential equations. Prentice-Hall Inc., Englewood Cliffs, N.J. (1971).
3. K. GUSTAFSSON AND M. LUNDH AND G. SÖDERLIND. A PI stepsize control for the numerical solution of ordinary differential equations. BIT 28 (1988) 270-287.
4. A. NORDSIECK. On numerical integration of ordinary differential equations. Math. Comp. 16(77) (1962) 22-49.
5. N. OBRESHKOV. Sochineniya. Tom 2. Bulgar. Akad. Nauk (1981).

Optimal Experimental Design With the EFCOSS Framework

Ralf Seidler, H. Martin Bücker
Friedrich Schiller University Jena
ralf.seidler@uni-jena.de, martin.buecker@uni-jena.de

Abstract

The most challenging problems arising in physics and other sciences can be tackeled by the use of specialized simulation software. This simulation is mostly based on some initial parameter sets, that describe the behavior of the system. To improve the simulation towards real world, one goal is to find exact values of these parameters. A technique on doing so, is to measure some values on the real world system. However, based on the description of the simulation, these measurements are most likely to introduce uncertainty. The advanced numerical technique optimal experimental design (OED) gives answeres to the question of how to minimize this uncertainty. We show the advantages of using the Environment For Combining Optimization and Simulation Software (EFCOSS) framework for solving such OED problems with the help optimization packages by using automatic differentiation of the simulation code.

References

1. "A. RASCH AND H. M. BÜCKER". "EFCOSS: An interactive environment facilitating optimal experimental design". "ACM Transactions on Mathematical Software 37.2 (2010) 13:1-13:37".
2. "A. C. ATKINSON AND A. N. DONEV". "Optimum Experimental Designs". "Oxford Science Publications (1992) Clarendon Press".
3. "L. B. RALL". "Automatic Differentiation: Tecniques and Applications". "Lecture Notes in Computer Science vol. 120 (1981) Springer".

Comparison Between CFD and XFOIL Predictions for High Lift Low Reynolds Number Airfoils

João Morgado, Miguel Silvestre
Dep. of Aerospace Sciences, University of Beira Interior
jmorgado@ubi.pt, mars@ubi.pt

Rui Vizinho, José Páscoa
Dep. of Electromechanical Engineering, University of Beira Interior
ruivizinhodeoliveira@sapo.pt, pascoa@ubi.pt

Abstract

Computational Fluid Dynamics is becoming increasingly popular in the design and optimization of devices that depend on aerodynamics. For fixed and rotary wings applications, the airfoil lift over drag coefficient is what most determines the device's performance such that selecting a suitable computational tool is crucial for the design engineer. In the case of airfoils operating at low Reynolds numbers (60,000;Re;500,000), an accurate prediction of the transition position along the chord is essential to correctly simulate their performance characteristics. It has been shown[1] that XFOIL code has this capability and is widely used for airfoil design and optimization. But, it is unclear if recent transition turbulence models can produce better airfoil performance predictions. In order to access the accuracy of the different methods available for airfoil analysis, several airfoils were analyzed and the results were compared with experimental data. The high-lift low-Reynolds numbers airfoils were analyzed using a conventional turbulence model, a new $\kappa-\kappa l-\omega$[2] model and XFOIL[3]code. The $\kappa-\kappa l-\omega$ is a phenomenological model which accounts for natural and bypass transition. The model available at openliterature was improved and implemented in OpenFoam. The XFOIL code was developed by Mark Drela and it couples high-order panels methods with fully coupled viscous/inviscid interaction. The flow conditions were replicated on the simulations and results were compared with the available experimental data presented in Ref.[4].

References

1. M. DRELA. Low Reynolds-Number Airfoil Design for the M.I.T. Daedalus Prototype: A Case Study. Journal of Aircraft, Vol. 25, No. 8 (1988) 724–732.
2. R. VIZINHO AND J. PÁSCOA AND M. SILVESTRE. High AltitudeTransitional Flow Computation for a Propulsion System Nacelle of MAAT Airship. SAE Int. J. Aerosp. Vol. 6, no. 2 (2013).
3. M. DRELA. XFOIL - An Analysis and Design System for Low Reynolds Number Airfoils. Low Reynolds Number Aerodynamics, T.J. Mueller, ed., Berlin: Springer-Velag, 1989, pp. 1–12.
4. M. S. SELIG AND J. GUGLIELMO. High Lift Low Reynolds Number Airfoil Design. J. Aircraft, vol. 34, no. 1(1997), pp. 72–79.

BDDC for Mixed-Hybrid Formulation of Flow in Porous Media With Combined Mesh Dimensions

Jakub Šístek
Institute of Mathematics of AS CR, Czech Republic
Czech Technical University in Prague, Czech Republic
sistek@math.cas.cz

Jan Březina
Technical University of Liberec, Czech Republic
jan.brezina@tul.cz

Bedřich Sousedík
University of Maryland, College Park, USA
sousedik@umd.edu

Abstract

The flow of water in granite rock, which represents e.g. one of the suitable sites for nuclear waste deposit, is conducted by a complex system of fractures with various topology and sizes. In the presented approach, the fractures are assumed to contain debris and they are modeled as porous media with specific permeabilities. The discretization is performed using the mixed-hybrid finite element method (FEM) with the lowest order Raviart-Thomas (RT0) elements. The resulting meshes are unstructured, and they combine different spatial dimensions (line elements in 1D, triangles in 2D, and tetrahedrons in 3D) to model the effect of fractures. The matrices of the arising systems of linear equations have a saddle-point structure.

We adapt the Balancing Domain Decomposition by Constraints (BDDC) [1,2] method to this type of problems. A new scaling operator in the BDDC method suitable for the studied problems is also proposed. The mixed-hybrid formulation allows to modify the saddle-point matrix to a symmetric and positive definite Schur complement with respect to interface Lagrange multipliers. The reduced system is solved by the preconditioned conjugate gradient (PCG) method, and the BDDC method is used as the preconditioner.

We describe our parallel implementation of the method and study its performance on several benchmark and real world problems. The extensions have been incorporated into our open-source solver library *BDDCML*, which has been combined with the *Flow123d* package for subsurface flow simulations. Numerical experiments confirm efficiency and scalability of the developed approach on up to 1024 computer cores.

References

1. X. Tu. A BDDC algorithm for flow in porous media with a hybrid finite element discretization. Electronic Transactions on Numerical Analysis **26** (2007).
2. J. Šístek and J. Březina and B. Sousedík. BDDC for mixed-hybrid formulation of flow in porous media with combined mesh dimensions. Submitted.

High Performance Scientific Computing @cs.pub.ro

Emil Slusanschi
University Politehnica of Bucharest
emil.slusanschi@cs.pub.ro

Abstract

In this talk we will give an overview of the High Performance Scientific Computing activities that are currently taking place at the Computer Science and Engineering of the University Politehnica of Bucharest, Romania. In particular, we will present applications from the areas of: meteorology, aerospace, astrophysics, image processing and seismology.

References

1. V. CHIHAIA AND E. SLUSANSCHI AND A. HERISANU AND P. PALADE AND N. TAPUS. High Performance Computing Infrastructure for materials Science. Revue Roumaine de Chimie, Academia Romana, Vol 55(11-12), pp. 1009-1015, 2010. nr. 11-12, ISSN 0035-3930, 2010..
2. E.SLUSANSCHI AND D. GUDU AND A. MIREA. Scalability Study of Two Weather Prediction Models. CSCS '13 Proceedings of the 2013 19th International Conference on Control Systems and Computer Science, pp. 129-136..
3. A. C. SIMA AND E. SLUSANSCHI. Optimizing Parallel CFD Simulations of 2D Compressible Flows. SYNASC 2012, 26-29 Septembrie 2012, Timisoara, Romania..
4. V.L. SPIRIDON AND E. SLUSANSCHI.. N-Body Simulations With GADGET-2. SYNASC 2013, 25-26 Septembrie 2013, Timisoara, Romania.pp 526-533..

Analysis of Wind Induced Aramid Anchor Cable Using a Simplified Fluid-Structure Interaction Method

Robert Soltys, Michal Tomko, Stanislav Kmet
Technical University of Kosice
robert.soltys@tuke.sk, michal.tomko@tuke.sk, stanislav.kmet@tuke.sk

Abstract

Wind-induced vibrations of aramid anchor cable using simplified fluid-structure interaction method are introduced. An incompressible fluid flow with Navier-Stokes equations has been applied for computation representing surrounded air environment. The accuracy of aerodynamic characteristics have been tested for applied type of plane fluid flow model. A number of parallel plane fluid models have been created along the anchor cable. Position of planes has been normal to the cable axis. Analysed cable has been modeled using line type elements similarly containing a number of slave elements supplying the cable section specially for providing interaction between created fluid and structural models. As turbulent flow has affected the translation of the supplying cable section an Arbitrary Lagrangian Eulerian approach has been considered. Spatial turbulent wind field has been applied for exciting dynamical behavior of the aramid cable. Based on previously measured and evaluated wind records the statistical and spectral characteristics were assigned for considered cable situation. Obtained wind characteristics were used for creating turbulent wind field consisted of longitudinal and lateral velocity components. Spatially correlated velocity components were considered as an inflow condition in created plane fluid flow models. Cable nodes displacement and trajectory character has been observing. Different response has been involved comparing to the cable loaded by distributed loading computed using Newton formulas. Using simplified fluid-structure interaction more realistic response has been obtained which has included aeroelastic effects not extracting vortex-induced excitations.

References

1. M. BREUER. A challenging test case for large eddy simulation: high Reynolds number circular cylinder flow. International Journal of Heat and Fluid Flow 21 (2000) 648-654.
2. A. VASALLO AND A. LORENZANA AND C.E. LAVIN. Coupling between structural and fluid dynamic problems applied to vortex shedding in a 90 m steel chimney. Journal of Wind Engineering and Industrial Aerodynamics 100 (2012) 30-37.
3. M. SHINOZUKA AND C.M. JAN. Digital simulation of random processes and its applications. Journal of Sound and Vibration 25(1) (1972) 111-128.
4. M. TOMKO AND S. KMET AND R. SOLTYS. Vibrations of an aramid anchor cable subjected to turbulent wind. Adv Eng Softw.
5. G. DEODATIS. Simulation of ergodic multivariate stochastic processes. J Eng Mech ASCE 122 (1996) 778-787.
6. J.D. HOLMES. Wind loading of structures. Spon Press, London - New York (2001).
7. G. SOLARI AND G. PICCARDO. Probabilistic 3-D turbulence modelling for gust buffeting of structures. Probabilistic Engineering Mechanics 16 (2001) 73-86.
8. L. CARASSALE AND G. PICCARDO. Non-linear discrete models for the stochastic analysis of cables in turbulent wind. Int J Non-linear Mech 45 (2010) 219-231.
9. S. KMET. Non-linear rheology of tension structural element under single and variable loading history Part I: Theoretical derivations. Structural Engineering and Mechanics 18(5) (2004) 565-589.

Modeling Transport Processes in Fractured Porous Media With Discontinuous Galerkin Method

Jan Březina, Jan Stebel
Technical University of Liberec
jan.brezina@tul.cz, jan.stebel@tul.cz

Abstract

Transport of substances and heat transfer in continuum can be described by a general advection-diffusion equation. We aim to develop a robust numerical method for modeling these processes in a fractured rock massif. The method will have to treat the following aspects of the model:

- *Complex geometry.* The rock matter, such as granite, contains system of thin layers (called fractures) that should be described by elements of lower dimension.
- *Heterogeneity.* The real material contains zones with hydraulic conductivity and dispersion tensor differing by orders of magnitude.
- *Advection/diffusion dominance.* At various scales, the problem can have character of first order hyperbolic or second order elliptic PDE.

In the talk the mathematical model for advection-diffusion equation in a domain with fractures will be presented and its well-posedness will be established. Further, we will describe the weighted interior penalty discontinuous Galerkin method [1] adopted to the system of domains with different dimensions and its performance will be demonstrated by example computations done with help of the computational code Flow123d [2].

The research has been supported by the Technology Agency of the Czech Republic under the project no. TA01021331.

References

1. A. Ern and A.F. Stephansen and P. Zunino. A discontinuous Galerkin method with weighted averages for advection–diffusion equations with locally small and anisotropic diffusivity. IMA Journal of Numerical Analysis, 29(2):235–256, 2009.
2. J. Březina and J. Stebel and J. Hnídek. Flow123d — simulator of underground water flow and transport in fractured porous media. Retrieved on 15 December 2013 from https://dev.nti.tul.cz/trac/flow123d.

Energy Transmission, Reactive Power and Stability of Nonlinear Systems

Daniel Mayer, Josef Hrusak
University of West Bohemia
mayer@kte.zcu.cz, hrusak@kae.zcu.cz

Milan Stork
University of West Bohemia/RICE
stork@kae.zcu.cz

Abstract

Voltage and current harmonics produced by nonlinear loads increase power losses and, therefore, have a negative impact on electric utility distribution systems and components. While the exact relationship between harmonics and losses is very complex and difficult to generalize, the well established concept of power factor does provide some measure of the relationship, and it is useful when comparing the relative impacts of nonlinear loads, providing that harmonics are incorporated into the power factor definition. While some harmonics are caused by system nonlinearities such as transformer saturation, most harmonics are produced by power electronic loads such as adjustable-speed drives and diode bridge rectifiers. In this paper the reactive power and stability of transmission line and system for nonsinusoidal situations, where nonlinear circuit voltages and currents contain harmonics are studied and simulated. The results may have an importance for control algorithms which enables better stability and reactive power suppression.

References

1. "R. M. MILASI AND A. F. LYNCH AND W. L. YUN". "Adaptive Control of a Voltage Source Converter for Power Factor Correction". "IEEE Transaction on Power Electronics, Vol. 28, No. 10, October 2013, pp. 4767 - 4779".
2. "D. MAYER AND J. HRUSAK & M. STORK". "On state-space energy based generalization of Brayton–Moser topological approach to electrical network decomposition". "Springer, Computing, Volume 95, Issue 1 Supplement, May 2013, pp 723-749".
3. "T. KAUR AND S. KAKRAN". "Transient Stability Improvement of Long Transmission Line System by Using SVC". "International Journal of Advanced Research in Electrical, Electronics and Instrumentation Engineering, Vol. 1, Issue 4, October 2012, pp.218-227".

Form Finding and Analysis of Inflatable Dams

Matthew Streeter, Landolf Rhode-Barbarigos, Sigrid Adriaenssens
Princeton University
mjs10@princeton.edu, landolf@gmail.com, sadriaen@princeton.edu

Abstract

Inflatable dams are flexible membrane structures inflated by air and/or water. Due to their ease of construction, rapid deployability and low cost, these systems have great potential for hazard mitigation applications in the context of global warming. However, designing inflatable dams is a challenging task as the dam's initial equilibrium shape has to be determined by either experimental or numerical form-finding methods. Furthermore, the dam's shape and the applied loading due to the air/water are coupled as changes in the form of the structure induce also changes in the loading. In this paper, a form finding and analysis technique for the cross-sectional analysis of an inflatable dam is proposed. Using this technique, the structural behavior of an inflatable dam is analyzed under different conditions of up and downstream water depth and internal pressure. The results show good agreement with existing studies in literature. The presented method provides thus an alternative computational tool for the design of inflatable dams.

References

1. H. B. HARRISON. The analysis and behavior of inflatable membrane dams under static loading. "Proceeding of the Institution of Civil Engineers, 48 (1970) 661-676".
2. ABDULLAH ALI NASSER ALHAMATI. Behavior of inflatable dams under hydrostatic conditions. "Suranaree J. Sci. Technology (2005) 12(1) 1-18".

Modeling of Heat and Mass Transfer in Supercritical Geothermal Systems

Mario-Cesar Suarez-Arriaga
Faculty of Sciences Michoacan University
mcsa50@gmail.com

Abstract

The energy of the Earth's interior is called geothermal heat. The temperature gradient between the core of the Earth (5000 degrees C) and the surface (15 C) comes from the continuous flow of its natural heat. This gradient covers a wide range of geothermal energy sources, which are found at different vertical intervals at specific temperatures. These resources range from very shallow depths of several hundred meters (102 m, [50, 100] C), then go through intermediate depths (103 m, [200, 370] C), up to the great deep (104 m, [400, 800] C), reaching the immense temperatures of the melted magmatic rocks. The fluids in deep systems can reach supercritical thermodynamic conditions with temperatures above 374 C and pressures above 220 bar. These fluids have a higher density; containing more volumetric enthalpy and energy, can provide twenty times more power per cubic meter than normal geothermal fluids currently used. Geothermal heat is a natural, renewable and reliable source of energy with environmental and cost advantages over other energy sources. Using geothermal energy makes unnecessary spending, using or burning fossil or nuclear combustibles, nor is it necessary to transport, store, taking care or separate the waste, neither to confine them to avoid toxic damage that could impact or affect the environment. Specific technology can be used to drill wells into the reservoir, bring its hot fluids to the surface, take the underground heat and transform it into electricity. This natural heat may also be used directly in several applications besides electricity generation. The transmission of heat from the geothermal system or porous reservoir towards the field's surface is essentially conductive and convective. The reservoir fluid contains several components whose dynamics are affected by petrophysical heterogeneity in different ways. In this paper the general partial differential equations of the simultaneous transport of heat and multicomponent fluid in porous rocks are introduced and numerically solved using the finite volume method. The solutions of some problems are presented to illustrate this technique.

References

1. J. BUNDSCHUH AND M.C. SUÁREZ. Introduction to the numerical modeling of groundwater and geothermal systems: Fundamentals of mass, energy and solute transport in porolastic rocks . 525 pp., ISBN: 978-0415401678. CRC Press, Taylor & Francis, 2010..

On Numerical Simulations of Fluid-Structure Interactions: Modelling of Gust Response

Petr Sváček
Czech Technical University in Prague, Faculty of Mechanical Eng.
petr.svacek@fs.cvut.cz

Abstract

This paper shall be interested in numerical simulations of mutual interactions of fluid flow with an airfoil. The main attention shall be paid to numerical simulations of the aeroelastic response of the airfoil to the sudden gust. Particularly, we shall address the finite element approximations of a flexibly supported airfoil subjected to a (two-dimensional) incompressible viscous flow. A sudden short change of flow condition will be considered. The structure vibration is be described by the equations of motions (system of nonlinear ordinary differential equations). The incompressible viscous flow is governed either by Navier-Stokes equations or, for the turbulent flow, by Reynolds averaged Navier-Stokes equations coupled with the $k-\omega$ turbulence model. The motion of the computational domain is treated with the aid of the arbitrary Lagrangian-Eulerian method.

The fully stabilized finite element method is used for the numerical approximation. The solution of the discrete linearized problem shall be performed by the multigrid method. The efficiency of the multigrid method depends on the applied smoother and the choice of the finite element couple. In the computations, either Vanka-type or Braess–Sarazin-type of smoothers are being used. For the very high Reynolds number the convergence rate of the multigrid method depends on the local anisotropic mesh refinement, the applied suitable stabilization, etc. Here, the convergence of the multigrid method shall be studied. The numerical results of the finite element method is presented.

References

1. P. SVACEK AND M. FEISTAUER. Application of a Stabilized FEM to Problems of Aeroelasticity. Numerical Mathematics and Advanced Application, 796–805, Berlin, 2004. Springer..
2. M. BERCI AND S. MASCETTI AND A. INCOGNITO AND P. H. GASKELL AND V. V. TOROPOV. Gust response of a typical section via CFD and analytical solutions. In: J. C. F. Pereira, A. Sequeira (Eds.), ECCOMAS CFD 2010, V. European Conference on Computational Fluid Dynamics, 2010.

Training Algorithm for Stochastic Model of Biological Neural Network

Aleksandra Świetlicka, Karol Gugała, Andrzej Rybarczyk
Poznan University of Technology
aleksandra.swietlicka@put.poznan.pl, karol.gugala@put.poznan.pl,
andrzej.rybarczyk@put.poznan.pl

Abstract

An important aspect of designing biological models of neuron or neural network is to consider their further applications. To do so it is necessary to introduce training algorithms into these models. In models of a single neuron it is commonly done with use of descent gradient method [2], while it is not enough while considering a biological neural network.

We are considering a stochastic version of biological neural network model, based on Markov kinetic schemes [1] which is derived from the classic Hodgkin-Huxley model presented in [3]. This model assumes dendritic structure of the neuron allowing to consider potential of the membrane to be different in each point of it.

To perform training of this kind of biological neural network we used method of descent gradient combined with method of Lagrange multipliers. Parameters of the model are considered as the weights of the neural network and each point of the considered structure has individual set of these weights. The use of Lagrange multipliers has an effect in set of nonlinear equations to be solved for each point of the structure and for each step of time.

Trained biological neural network is supposed to solve problems usually solved with artificial neural networks. In this paper, as a simple example, we are presenting its ability to adjust to given waveform of potential obtained with classic approach presented by Hodgkin and Huxley in [3] of dendritic structure of the neuron.

References

1. A. Destexhe and Z. F. Mainen and T. J. Sejnowski . Synthesis of Models for Excitable Membranes, Synaptic Transmission and Neuromodulation Using a Common Kinetic Formalism. Journal of Computational Neuroscience, no. 1, pp. 195-230, 1994.
2. K. Doya and A. I. Selverston and P. F. Rowat. A Hodgkin–Huxley Type Neuron Model That Learns Slow Non-Spike Oscillations. Proceeding of: Advances in Neural Information Processing Systems 6, 7th NIPS Conference, Denver, Colorado, USA, pp. 566-573, 1993.
3. A. L. Hodgkin and A. F. Huxley. A Quantitative Description of Membrane Current and Its Application to Conduction and Excitation in Nerve. Journal of Physiology, no. 117, pp. 500-544, 1952.

Modeling of Salt Crystallization in Historical Mortars

Stanislav Šulc, Jan Sýkora
CTU in Prague, Faculty of Civil Eng., Dept. of Mechanics, Thákurova 7, Prague, Czech Republic
stanislav.sulc@fsv.cvut.cz, jan.sykora.1@fsv.cvut.cz

Abstract

The aim of presented paper is modeling of degradation processes in historical mortars exposed to salt transport. Internal damage caused by crystallization in pores is one of the most important factors limiting the service life of historical structures. Coupling the transport processes with the mechanical part will allow us to address the impact of salt crystallization on the durability, strength and stiffness of mortars. This should be accomplished with the help of a complex thermo-hygro-mechanical model representing one of the prime objectives of this work. The proposed formulation is based on the extension of the classical poroelasticity models with the damage mechanics. The general framework of the proposed model was primarily inspired by the work published in [1, 2, 3, 4]. An example of two-dimensional salt transport is presented to support the theoretical derivations.

References

1. G. Castellazzi and C. Colla and S. de Miranda and G. Formica and E. Gabrielli and L. Molari and and F. Ubertini. A coupled multiphase model for hygrothermal analysis of masonry structures and prediction of stress induced by salt crystallization. Construction and Building Materials, 41, 717-731, 2013..
2. O. Coussy and P. Monteiro. Unsaturated poroelasticity for crystallization in pores. Computers and Geotechnics, 34, 279-290, 2007.
3. M. Koniorczyk and D. Gawin. Modelling of salt crystallization in building materials with microstructure – Poromechanical approach. Construction and Building Materials, 36, 860-873, 2012.
4. G. W. Scherer. Crystallization in pores. Cement and Concrete Research, 29, 1347-1358, 1999.

Immune Optimal Design of 2-D and 3-D Structures

Arkadiusz Poteralski, Miroslaw Szczepanik
Silesian University of Technology
arkadiusz.poteralski@polsl.pl, miroslaw.szczepanik@polsl.pl

Tadeusz Burczynski
Cracow University of Technology
tburczyn@pk.edu.pl

Abstract

The paper deals with an application of the artificial immune system (AIS) to the optimization of shape, topology and material properties of 2-D and 3-D structures. Structures considered in this work are analyzed by the finite element method (FEM). Optimization criteria that are taken into account concern minimize mass and/or compliance. Optimal properties of structures can be provided by using the computer aided optimization techniques. For example, an appropriate strength of structures can be established by changing their shape, topology and material properties. The choice of optimal shape and topology are the key elements defining the effectiveness of structures, and thus finding them is the problem of great practical interest. Using this approach shape, topology and material optimization is performed simultaneously. The important feature of this approach is the strong probability of finding the global optimal solutions received by the implementation of the immune algorithm. The described approach is free from limitations connected with classic gradient optimization methods. Coupling the finite element method and the immune algorithm gives an effective and efficient alternative optimization tool, which enables solving a large class of the optimization problems of mechanical structures. The main feature of the first proposed optimization method is the immune distribution of the material in the construction changing its material properties or by changing its thickness (for 2-D). This process leads to the elimination of the part of material from the construction and as a result the new shape and the topology of the construction emerges. Using interpolation surfaces (hyper surface) reduces the number of the design variables and shortens the time of the computation. The artificial immune systems (AIS) are developed on the basis of a mechanism discovered in biological immune systems and take only a few elements from the biological immune systems. The most frequently used are the mutation of the B cells, proliferation, memory cells, and recognition by using the B and T cells. The presented approach is based on the Wierzchon algorithm, but the mutation operator is changed. The Gaussian mutation is used instead of the nonuniform mutation in the presented approach. An effective tools of immune optimization of the 2-D and 3-D structures will be presented [1]. The numerical examples confirm the efficiency of the proposed optimization method and demonstrate that the method based on immune computation is an effective technique for solving computer aided optimal design problems.

References

1. A. Poteralski and M. Szczepanik and J. Ptaszny and W. Kuś and T. Burczyński. Hybrid artificial immune system in identification of room acoustic properties. Inverse Problems in Science and Engineering, Publisher: Taylor & Francis 2013.

Intelligent Optimization of Reinforced Structures

Miroslaw Szczepanik, Arkadiusz Poteralski
Silesian University of Technology
miroslaw.szczepanik@polsl.pl, arkadiusz.poteralski@polsl.pl

Tadeusz Burczynski
Cracow University of Technology
tburczyn@pk.edu.pl

Abstract

Reinforced structures are often used in practice because they are resistant, stiff and stable. A typical area of application of such structures is an aircraft industry where light, stiff and highly resistant structures are required. Many aircraft elements are made as thin panels reinforced by stiffeners. Reinforced structures are frequently subjected to dynamic loads and it is important to get an information about their transient dynamic response. If the response is not satisfactory, it must be improved in order to satisfy proper requirements. These improvements can be achieved, for instance, by the optimization process. Optimal choice of number of stiffeners, their properties and locations in a structure decides about the effectiveness of the reinforcement. In the paper the reinforced structures are subjected to static and dynamic loads and analyzed by the FEM and also by coupled BEM and FEM. By means of coupled method the plates are modeled by the dual reciprocity BEM and the stiffeners by the FEM. Matrix equations of motion for the plate and stiffeners are coupled using conditions of compatibility of displacements and equilibrium of tractions along the common interfaces. The aim of optimization is to find the optimal locations of stiffeners in order to maximize stiffness of the structure or to minimize structure stresses. Strength of structures with an arbitrary geometry, material properties and boundary conditions can be obtained by carrying out laboratory tests but they are usually very expensive and time consuming. In order to reduce costs and time, computer simulations are performed instead of experimental investigations. As a result, static or dynamic quantities of interest like displacements, velocities, accelerations, forces, stresses, i.e. can be determined. The most versatile methods of analysis of structures subjected to arbitrary static and time dependent boundary conditions are the finite element method (FEM) and the boundary element method (BEM). The coupling of these methods is very desirable in order to exploit their advantages. Optimal properties of statically or dynamically loaded structures can be searched using the computer aided optimization tools. In the present paper, FEM or coupling FEM and BEM with swarm method in optimization of statically or dynamically loaded reinforced structures is presented. The additional comparisons of the effectiveness of particle swarm optimizer (PSO) with the effectiveness of the evolutionary algorithms (EA) and the artificial immune systems (AIS) are presented [1].

References

1. M. SZCZEPANIK AND A. POTERALSKI AND J. PTASZNY AND T. BURCZYŃSKI. Hybrid Particle Swarm Optimizer and Its Application in Identification of Room Acoustic Properties. Swarm and Evolutionary Computation - International Symposia, SIDE 2012 and EC 2012, Held in Conjunction with ICAISC 2012, Zakopane, Poland, April 29-May 3, 2012. Proceedings. Lecture Notes in Computer Science 7269 Springer 2012, ISBN 978-3-642-29352-8.

Computational Challenges in Simulating ETMAs

Walerian Szyszkowski, Darrel Hill
University of Saskatchewan
walerian.szyszkowski@usask.ca, was675@mail.usask.ca

Abstract

Electro-thermal micro-actuators (ETMA) are typically easier to control and have higher displacement/force outputs than other micro-actuators [1]. However, any analytical predictions and numerical simulations of their behavior are rather challenging, mainly because one has to consider simultaneously three different coupled physical environments i.e. electrical, thermal, and mechanical. The second factor is a relatively wide range of operating temperatures resulting in substantial variations of several parameters characterizing the material and each of the environments involved [2]. Consequently, so far analytical predictions of the operational characteristics of such devices have not been sufficiently accurate, and in practice new designs/modifications of ETMA still rely heavily on costly, time consuming, and numerous experimental testing. The cascaded ETMA made of nickel alloy and manufactured by using laser micro-fabrication technology is considered. For this device the coupling between the electrical and thermal fields have been found especially strong, and mainly via the temperature effects on the electrical resistivity and surface convection coefficients. Additionally, the first coefficient is influenced by a possible microstructure changes in the nickel, while the second coefficient is geometry and scale dependent. It is worthwhile to mention that, due to small dimensions of the actuators, any experimental measurement of these coefficients is far less accurate than the other parameters involved. A finite elements (FE) procedure is proposed that handles effectively the coupling between the electrical, thermal and mechanical fields in the ETMA by adjusting all the temperature sensitive material and model characteristics accordingly to the available measurement of the current, displacement and force in the actuator. The procedure is iterative and parametric, in which the corrections to parameters defining the characteristics are determined by comparing the ETMA's measured and the FE simulated performances. The issues of accuracy, convergence, numerical efficiency, and the importance of couplings between particular fields will be discussed in detail at the presentation. For example, it will be demonstrated that for reasonably good results only the measurements pertaining to the electrical and mechanical fields are needed, while cumbersome, unreliable, or just impossible measurements pertaining to the heat transfer and temperatures can be avoided. Once the temperature dependent characteristics for a particular type of ETMA were established, the numerical procedure can be used to simulate and optimize the micro-actuators of different geometrical configurations or to design the ETMA having particular voltage-force-displacement properties.

References

1. [1] T. MOULTON AND G.K. ANANTHASURESH. Micromechanical devices with embedded electro-thermal-compliant actuation. Sensors and Actuators A, Vol. 90, , pp. 38-48. (2001).
2. [2] C.P. HSU AND W.C. TAI AND W. HSU. Design and Analysis of an Electro-Thermally Driven Long-Stretch Micro Drive with Cascaded Structure. Proceedings of IMECE2002, (2002).

Molecular Dynamics on 146 000 Cores

Nikola Tchipev, Wolfgang Eckhardt, Philipp Neumann, Hans-Joachim Bungartz
TU München
tchipev@in.tum.de, eckhardw@in.tum.de, neumanph@in.tum.de,
bungartz@in.tum.de

Abstract

Molecular Dynamics has turned out to provide an accurate simulation method to investigate non-equilibrium, non-linear processes such as nucleation[1]. However, a huge number of molecules and thus sophisticated exploitation of parallelism on all levels–vectorisation, shared and distributed memory parallelism–is necessary to study the underlying physical phenomena.

We present the software *ls1 mardyn* which allows for large scale simulation of molecular systems. The software has shown to scale on recent HPC systems on up to 146 000 cores [2]. We discuss vectorisation as well as shared and distributed memory parallelisation concepts. We further present results on recent developments with respect to simulations on the MIC architecture.

References

1. M. Horsch and J. Vrabec and M. Bernreuther and S. Grottel and G. Reina and A. Wix and K. Schaber and H. Hasse. Homogeneous nucleation in supersaturated vapors of methane, ethane, and carbon dioxide predicted by brute force molecular dynamics. The Journal of Chemical Physics, 128(16):164510, 2008.
2. W. Eckhardt and A. Heinecke and R. Bader and M. Brehm and N. Hammer and H. Huber and H.-G. Kleinhenz and J. Vrabec and H. Hasse and M. Horsch and M. Bernreuther and C. Glass and C. Niethammer and A. Bode and H.-J. Bungartz. 591 TFLOPS Multi-Trillion Particles Simulation on SuperMUC. International Supercomputing Conference (ISC) Proceedings, 2013.

Pattern Recognition Using the Likelihood Function of Multiple Change-Points

Alvaro Cordero Franco, Jorge Garza Venegas, Victor Tercero Gomez, Fernando Camacho Vallejo, Javier Almaguer Martinez
Universidad Autonoma de Nuevo Leon
alvaro.corderofr@uanl.edu.mx, jag.venegas@gmail.com,
victor.tercerogm@uanl.edu.mx, jose.camachovl@uanl.edu.mx,
almagerjavier@gmail.com

Abstract

When monitoring systems over time like traffic flow, economy, manufacturing, fraud detection, hydrology, etc., the ability to detect structural changes and their initial time of occurrence provides key insights that might lead to a deeper understanding of causal relationships and better management. Most statistical developments in the field of change-point analysis has focused on a single change-point, while the study of multiple change-points in time series has been left behind to some extent due to the computational complexity of the analysis. In this research, using the likelihood function of multiple change-points, tests and estimators for multiple change-points in the mean of independent normal observations are presented. In addition, exact complexity of the procedure is calculated, and two heuristics, evolutionary and greedy algorithms, are proposed to facilitate the search for optimal solutions. Performance is measured in terms of estimation bias, standard error, and solving times. Both heuristics showed similar results. Nevertheless, the greedy one gave smaller solving times and the evolutionary had smaller biases. To facilitate implementation, a meta-routine is suggested to assist modeling and pattern recognition. Application is illustrated using real life observations from manufacture and economy. Analysts in many fields aiming to perform retrospective analysis of systems where patterns need to be indentified might find this methodology useful.

References

1. HINKLEY UNDEFINED AND D. V. . Inference about the change-point in a sequence of random variables. Biometrika. 57 (2011) 1-17. doi:10.1093/biomet/57.1.1.
2. ALY UNDEFINED AND E.-E. A. AND ABD-RABOU UNDEFINED AND A.-E. S. AND & AL-KANDARI AND N. M.. Tests for multiple change points under ordered alternatives. Metrika. 57 (2003) 209–221..
3. EASTERLING UNDEFINED AND D. R. AND & PETERSON AND T. C.. A new method for detecting undocumented discontinuities in climatological time series. International journal of climatology, 15 (1995), 369–377.
4. FU UNDEFINED AND Y.-X. UNDEFINED AND & CURNOW AND R. N.. Maximum likelihood estimation of multiple change points. Biometrika. 77 (1990) 563-573. doi:10.1093/biomet/77.3.563.
5. JANN UNDEFINED AND A. UNDEFINED. Multiple change-point detection with a genetic algorithm. Soft Computing-A Fusion of Foundations, Methodologies and Applications. 4(2000), 68–75..
6. TERCERO-GÓMEZ UNDEFINED AND V. G. AND CARMEN TEMBLADOR-PÉREZ AND M. UNDEFINED AND BERUVIDES UNDEFINED AND M. UNDEFINED AND & HERNÁNDEZ-LUNA AND A. UNDEFINED. Nonparametric Estimator for the Time of a Step Change in the Trend of Random Walk Models with Drift. Quality and Reliability Engineering International. 29 (2013) 23-51.

A Local Discontinuous Galerkin Method for (Non) Isothermal Flow With Phase Transitons

Lulu Tian, J.G.M. Kuerten, Jaap Van der Vegt
University of Twente
l.tian@utwente.nl, J.G.M.Kuerten@tue.nl,
j.j.w.vandervegt@utwente.nl

Yan Xu
University of science and technology of China
yxu@ustc.edu.cn

Abstract

In this presentation, we will discuss a local discontinuous Galerkin (LDG) scheme for a (non) isothermal flow model. The (non) isothermal Navier-Stokes-Korteweg system is used to model the dynamics of a compressible fluid exhibiting phase transitions between a liquid and a vapor phase when capillarity effects close to phase boundaries are taken into account. Standard numerical discretizations are known to violate discrete versions of inherent energy inequalities, thus leading to spurious dynamics of computed solutions. A conservative LDG method using discontinuous finite element spaces is proposed with a time-implicit Runge-Kutta integration. To capture the dynamic interface between the two phases accurately, control the capillarity effects and save computations, local refinement is applied. Computational experiments are provided to demonstrate the solvability and convergence of the LDG scheme. The methods are of arbitrary order of accuracy and free of numerical artifacts.

References

1. A.PROHL AND M.BRAACK . Stable discretization of a diffuse interface model for liquid-vapor flows with surface tension. ESAIM: Mathematical Modelling and Numerical Analysis, 47 (2013) 401-420.
2. A. PECENKO AND L. G. M. VAN DEURZEN AND J. G. M. KUERTEN AND C. W. M. VAN DER GELD. Non-isothermal two-phase flow with a diffuse-interface model. International Journal of Multiphase Flow, 37 (2011) 149-165.

preCICE - a Library for Partitioned Fluid-Structure Interaction on Massively Parallel Systems

Benjamin Uekermann, Bernhard Gatzhammer
Technische Universität München
uekerman@in.tum.de, gatzhamm@in.tum.de

Miriam Mehl
Universität Stuttgart
miriam.mehl@ipvs.uni-stuttgart.de

Abstract

The simulation of multi-physics applications, such as fluid-structure interaction, demands a high software flexibility in order to cover very different applications while keeping a decent time-to-solution. Partitioned black-box coupling of existing single-physics solvers with minimal altering of the codes is therefore a natural desire. For this purpose, we are developing the coupling library preCICE. We successfully coupled various in-house and commercial solvers with preCICE and have shown the desired flexibility.

The next development step should lead preCICE towards massively parallel systems, since those are a basic requirement of multi-physics applications. The simulation of blood flow in the human cardiovascular system, for example, benefits only from an elastic wall model, if the boundary layers of the flow are accurately resolved, leading to computational demanding simulations. In this talk, we want to discuss different aspects that are of importance to this development, including parallel coupling algorithms and efficient communication schemes.

References

1. B. GATZHAMMER. Efficient and Flexible Partitioned Simulation of Fluid-Structure Interactions. PhD Thesis. Technische Universität München, Institut für Informatk, 2014.
2. M. MEHL AND B. UEKERMANN AND H. BIJL AND D. BLOM AND B. GATZHAMMER AND A. VAN ZUIJLEN. Parallel Coupling Numerics for Partitioned Fluid-Structure Interaction Simulations. Submitted to SIAM SISC, 2013.

Answering Reachability Queries on Streaming Graphs

Gulay Unel
Isik University
gulay.unel@isikun.edu.tr

Abstract

Graph reachability is a fundamental problem in many applications, such as reasoning in lightweight formalisms, geographic navigation, XML/RDF/OWL query processing, etc. Many real world scenarios involve huge graphs and require fast algorithms to test for reachability between nodes. The problem becomes even more challenging when the graph is rapidly changing and received as a real-time stream of nodes and arcs. In this paper, we review current graph reachability algorithms and focus on how they can be adapted to the streaming setting. We also outline a new algorithm for answering reachability queries on huge, rapidly changing graphs.

References

1. H. WANG AND H. HE AND J. YANG AND P. S. YU AND J. XU YU. Dual Labeling: Answering Graph Reachability Queries in Constant Time. Proceedings of the 22nd International Conference on Data Engineering.

SPH Simulation of 2D Driven Turbulence

Alireza Valizadeh, Joe Monaghan
School of Mathematical Sciences, Monash University
alireza.valizadeh@monash.edu, joe.monaghan@monash.edu

Abstract

In this paper we extend our previous study of turbulence in two dimensions using SPH. The crucial role of the solid no-slip boundaries as sources of vorticity filaments, which significantly affects the flow evolution, has been revealed in laboratory experiments and numerical flow simulations. Keeping this in mind, we use mechanical stirrers moving on specified trajectories as the source of time-dependent forcing to generate turbulence. In addition, the ability of the SPH method in simulating the periodic and no-slip boundaries in turbulence driven by either stochastic forces or physical stirrers is studied. The key question of this study is: what are the minimal properties of a stirring trajectory that will produce turbulence with properties that are close to those of isotropic homogeneous turbulence?

References

1. VALIZADEH AND A. AND MONAGHAN AND J. J.. Smoothed particle hydrodynamics simulations of turbulence in fixed and rotating boxes in two dimensions with no-slip boundaries. Physics of Fluids, 24:035107(1–18), 2012..
2. VAN HEIJST AND G. J. F. AND CLERCX AND H. J. H. AND MOLENAAR AND D. AND . The effects of solid boundaries on confined two-dimensional turbulence. J. Fluid Mech. (2006), vol. 554, pp. 411–431.

A Conceptual Design Approach to the Development of an Open-Rack Structure for Miniload AS/RS Based on Biomimetics

Mohammadreza Vasili, Mehdi Vasili
Department of Industrial Engineering, Islamic Azad University, Lejan Branch, Isfahan, Iran
vasili@iauln.ac.ir, m.vasili@iauln.ac.ir

Sai Hong Tang
Department of Mechanical & Manufacturing Engineering, Faculty of Engineering, Universiti Putra Malaysia, Selangor, Malaysia
saihong@upm.edu.my

Abstract

Automated Storage and Retrieval Systems (AS/RSs) are frequently used in numerous manufacturing, warehousing and distribution centers around the world (Vasili et al., 2012). They offer the advantage of cost-effective utilization of time, space and equipment (Manzini et al., 2006). Therefore, in order to keep the system operating efficiently, the AS/RSs have to be designed in such a way that they can provide quick response for the storage and retrieval operations of products (Hu et al., 2010). This paper outlines some conceptual design principles to the development of an open-rack structure for miniload AS/RS. It suggests and then presents a procedure of biomimetics starting from a natural sorting algorithm to a new AS/RS rack configuration, which provides a higher performance for the system. For the conceptual development of proposed rack configuration, two idea generation methods are used. First, under the analogy method (Pugh, 1991), a physical system and a natural sorting algorithm (abacus and Bead-Sort algorithm, respectively) act as a stimulus for generating ideas and solutions. Bead–Sort algorithm shows positive integers by a set of beads (Arulanandham et al., 2002). Then, in order to apply the proposed ideas in a conventional AS/RS, the combination method is used. Using this method, the requirements for formation of the proposed ideas are extracted from existing AS/RSs and combined together to make up the final design concepts. Based on some defined criteria, the design concepts are evaluated and a desirable concept is selected in order to efficiently achieve the proposed specifications.

References

1. J.J. Arulanandham and C.S. Calude and M.J. Dinneen. Bead–Sort: A Natural Sorting Algorithm. EATCS Bull, 76 (2002), 153–162.
2. Y.-H. Hu and Z.D. Zhu and W.-J. Hsu. Load shuffling algorithms for split-platform AS/RS. Robotics and Computer-Integrated Manufacturing, 26(6), 677-685. 2010.
3. R. Manzini and M. Gamberi and A. Regattieri. Design and control of an AS/RS. The International Journal of Advanced Manufacturing Technology, 28(7), 766-774. 2006.
4. S. Pugh. Total design: integrated methods for successful product engineering. Wokingham, UK: Addison-Wesley, 1991.
5. M.R. Vasili and S.H. Tang and M. Vasili. Automated Storage and Retrieval Systems: A Review on Travel Time Models and Control Policies. In R. Manzini (Ed.), Warehousing in the Global Supply Chain: Advanced Models, Tools and Applications for Storage Systems. (pp. 159-210): Springer-Verlag international publisher, 2012.

Turbulent Transition Modeling Through Mechanical Considerations

Rui Vizinho, José Páscoa
Dep. of Electromechanical Engineering, University of Beira Interior
ruivizinhodeoliveira@sapo.pt, pascoa@ubi.pt

Miguel Silvestre
Dep. of Aerospace Sciences, University of Beira Interior
mars@ubi.pt

Abstract

Turbulent transition model development has recently became a very active research area. There are mainly two types of transition models. The empirical correlated transition models such as the one developed by Langtry in [1]. The second type is the phenomenological transition models. Most of these models simulate the physics of laminar kinetic energy first developed by Mayle and Schulz in [2]. One example of this type of transition closure is the k-kl-w transition model developed by Walters and Cokljat in [3]. The proposed new transition model approach takes into consideration the mechanical effects of mean flow shear on turbulence. As such it can be considered as a phenomenological transition model type. This is the case since there is an attempt to simulate a physical process of transition to turbulence. The mean distribution of turbulence Reynolds shear stresses such as $\overline{u'v'}$, equals to zero in isotropic turbulent conditions. However, as shown in the book of Kundu et al. [4] and others, under mean flow shear turbulence develops a trend of negative values for $\overline{u'v'}$. Also, in the book of Tennekes and Lumley [5], it is stated that turbulent vortices tend to orient themselves according to the imposed mean flow shear. In the present work this was related to a deformation trend of the turbulent vortices due to shear. The proposed mechanical approach was used to create the Vizinho transition model in [6]. This model was implemented in the open-source software OpenFOAM. The transition model behavior, characteristics, validation and comparisons are performed under various turbulence conditions and geometries. These include ERCOFTAC flat-plate test cases and 3D geometries.

Keywords: OpenFoam, transition model, mechanical, turbulence.

References

1. R. B. LANGTRY. A correlation-based transition model using local variables for unstructured parallelized cfd codes. Ph.D. thesis, Universität Stuttgart, Holzgartenstr. 16, 70174 Stuttgart (2006).
2. R. E. MAYLE AND A. SCHULZ. Heat transfer committee and turbomachinery committee best paper of 1996 award: The path to predicting bypass transition. J. Turbomachinery, 119 (3) (1997).
3. D. K. WALTERS AND D. COKLJAT. A three-equation eddy-viscosity model for reynolds-averaged navier-stokes simulations of transitional flow. J. Fluids Engineering 130 (12) (2008).
4. P. K. KUNDU AND I. M. COHEN AND D. R. DOWLING. Chapter 12 - turbulence, in: Fluid Mechanics. fifth Edition, Academic Press, Boston, (2012) 541-620.
5. H. TENNEKES AND J. L. LUMLEY. A First Course in Turbulence. M.I.T. Press, 1972.
6. R. VIZINHO AND J. PÁSCOA AND M. SILVESTRE. A mechanical approach to turbulence transition modeling. Universidade da Beira Interior (UBI), 2013, (Pre-Print).

Computational Modeling of Real Structures Made of Strain-hardening Cement Composites

Jan Vorel
CTU in Prague, Faculty of Civil Engineering
jan.vorel@fsv.cvut.cz

William Peter Boshoff
Stellenbosch University, Department of Civil Engineering
bboshoff@sun.ac.za

Abstract

Concrete has been used for many centuries as a safe and durable building material. Two of the main advantages of concrete are its high compressive strength and that it can be cast on the construction site into a variety of shapes and sizes. The most prominent disadvantages of concrete and other cementitious materials are their brittle failure behavior in tension and the low tensile strength. The low tensile strength is usually compensated for with steel reinforcement, but wide cracks leading to the corrosion of the steel reinforcement still occur during the normal use of concrete (Otieno et al.). These cracks lead to durability problems and cause structural degradation to occur more rapidly. Fiber Reinforced cement-based composites is a large group of composites with variety of properties. The reason for adding fibers is to overcome the brittleness of the concrete by improving the post-cracking behavior and enhancing ductility. The paper deals with the group of Strain Hardening Cement based Composite (SHCC) that exhibits excellent mechanical behavior showing tensile strain hardening and multiple fine cracks. It has been shown to reach a tensile strain capacity of more than 4

References

1. M. Otieno and M. Alexander and H.-D. Beushausen. Corrosion in cracked and uncracked concrete - influence of crack width, concrete quality and crack reopening. Magazine of Concrete Research 62 (6) (2010) 393–404.
2. V. Li and S. Wang. Tensile strain-hardening behavior of PVA-ECC. ACI Materials Journal 98 (6) (2001) 483–492.
3. W. Boshoff and G. van Zijl. Time-dependant response of ECC: Characterisation of creep and rate dependence. Cement and Concrete Research 37 (2007) 725–734.

Comparison of Deterministic and Probabilistic Approaches to Identify the Dynamic Moving Load of a Reinforced Concrete Beam

Julien Waeytens
University Paris-Est, IFSTTAR
julien.waeytens@ifsttar.fr

Bojana Rosic
TU Braunschweig
bojana.rosic@tu-braunschweig.de

Abstract

The dynamic loading applied to civil engineering structures is not well-known in general. Herein, we focus on the identification of dynamic moving loads, due to road traffic, applied to reinforced concrete beam included in bridges and viaducts. This information is useful for the structure monitoring. To determine the moving load, two inverse modeling techniques are proposed and compared. The first inverse modeling technique is deterministic and based on the optimal control theory. To get the control parameters, *i.e.* dynamic moving load, we minimize a data misfit functional using a gradient-like algorithm. The problem being not well-posed, Tikhonov regularization terms are considered in the cost functional. To reduce the computation time, the functional gradient is obtained using the adjoint state. This technique has been employed in *[Waeytens 2014]* to update the material parameters of a reinforced concrete beam. The second inverse modeling technique is probabilistic and based on Bayesian inference *[Rosic 2013]*. In this setting the control parameter is modelled as a (may be high-dimensional) random variable, where the randomness reflects the uncertainty about the knowledge of the true values. In this manner the prior belief about the model is introduced before seeing the data. After the observation is made, the prior distribution is updated through Bayes rule in a pure deterministic, algebraic manner via minimum variance estimator *[Rosic 2012]*. This approach has shown to be effective and reliable in comparison to most methods which take the form of integrals over the posterior and compute them by sampling, e.g. Markov chain Monte Carlo (MCMC).

In both strategies, the strain is measured at several points of the beam on the observation time interval $[0, T]$. The measurement are simulated numerically solving the 2D elastodynamics forward problem and are corrupted using white noise. The dynamic moving load is parametrized using four parameters: the loading velocity c_F (m/s), the loading amplitude F (N/m2), the loading length l_F (m) and the loading time t_F (s).

References

1. J. Waeytens and V. le Corvec and P. Leveque and D. Siegert and F. Bourquin. Elastodynamics model updating for the monitoring of reinforced concrete beam : methodology and numerical implementation. Applied Mechanics and Materials, 513-517 (2014) 3401-3406.
2. B. Rosić and A. Kučerová and J. Sýkora and O. Pajonk and A. Litvinenko and H. G. Matthies. Parameter identification in a probabilistic setting. Engineering Structures, 50 (2013) 179-196.
3. B. Rosić and A. Litvinenko and O. Pajonk and H. G. Matthies. Sampling Free Bayesian Update of Polynomial Chaos Representations. Journal of Computational Physics, 231 (17) (2012) 5761-5787.

Some Algebra and Geometry Characteristics of Rational Space Curves of Type (1,1,d-2)

Haohao Wang
Southeast Missouri State University
hwang@semo.edu

Abstract

The Rees algebra of an ideal $I \subset R$ defined as the graded algebra (with the elements of R having degree 0 and the elements of I having degree 1)

$$\text{Rees}(I) = R \oplus I \oplus I^2 \oplus ...$$

is a classical algebraic structure which has been studied for decades by the Commutative Algebra community. One motivation for this study is that it is related to a classical problem in elimination theory: the implicitization problem.

Rational curves and surfaces are widely used in Computer Aided Design, since it is easy to describe the points on these curves and surfaces by means of their parameter values. However, it is not convenient to use the parametric representations to describe the set of points that are common to two different parametrically defined curves or surfaces. Thus there is a need to go back and forth between a parametric and an implicit description of a curve or surface. This is, in essence, the implicitization problem: to develop efficient algorithms to generate implicit equations for a curve or surface for which one knows a parametric representation.

In this paper, we specialize the setting to rational space curves of type $(1, 1, d-2)$ in projective 3-space. We do not prove any new theorems about the structure of Rees algebras; rather our primary goal is to provide an algorithmic approach and to give elementary constructions for the minimal generators for the Rees algebra associated to these curves based solely on their μ-basis. Our approach is to study separately the cases when the rational curve is either singular or non-singular. If the rational space curve is singular, then we study separately the cases when the degree of the curve is either even or odd. The generators of the Rees algebra are all expressed entirely in terms of the three elements of the μ-basis. Our algorithm shows that the very complicated description of the generators of the Rees algebra can be simplified considerably in the case of rational space curves of type $(1, 1, d-2)$. The second goal of this paper is to illustrate the geometry behind the generators via a case study of rational quartic space curves. We will construct the implicit equations of the curve and the defining equations for the Rees algebra in a simple manner from the elements of the μ-basis.

References

1. D. Cox and J. W. Hoffman and H. Wang and undefined undefined. Syzygies and the Rees algebra. J. Pure Appl. Algebra, 212 (2008), 1787–1796..
2. N. Song and R. Goldman. μ-bases for polynomial system in one variable. Comput. Aided Geom. Design, 26 (2009), 217–230..
3. H. Wang and X. Jia and and R. Goldman. Axial moving planes and singularities of rational space curves. Comput. Aided Geom. Design, 26 (2009), 300–316..

On the Use of Multiple Heterogeneous Devices to Speedup the Execution of a Computational Model of the Human Immune System

Tiago M do Nascimento, João Marcos de Oliveira, Rodrigo Weber dos Santos, Marcelo Lobosco
Federal University of Juiz de Fora, Brazil
tiago.nascimento@uab.ufjf.br, jmarcosdo@gmail.com,
rodrigo.weber@ufjf.edu.br, marcelo.lobosco@ice.ufjf.br

Abstract

Parallelism is becoming ubiquitous: CPUs are composed of multiple cores, GPUs are composed by hundreds or even thousands of them, and APUs (Accelerated Processing Units)[1] are available using both technologies in a single chip. Despite the availability of such huge number of cores, sometimes they are not entirely explored by parallel programs due to their heterogeneous nature, which makes hard to use them simultaneously. In this scenario, OpenCL [2] offers an framework to develop parallel programs that allows simultaneous use of multiple heterogeneous devices to speedup the execution of a parallel code. However, it is the programmer's responsibility to implements his/her own load balancing strategy, since each device (APU, CPU, GPU) can have distinct characteristics, so the same task can have distinct execution time depending on the target device chosen. This work presents preliminary results of the execution on an APU of a parallel computational implementation of a mathematical model that describes some of the Human Immune System (HIS) cells and molecules [3]. A set of PDEs is used to describe the dynamics of such cells and molecules on a three dimensional section of tissue. This tissue is discretized into multiple points, and at each time step the same set of equations are computed for each point, using for this purpose distinct data. The number of points and time steps used in the simulation, as well as the type and amount of computation that must be performed for each point determine the total computation time. Results of particular interest for biologist demands a large amount of points or time steps with huge computational requirements, justifying the use of accelerators such as those available on APUs. OpenCL has been used to implement the parallel version of the code that executed simultaneously on all CPU and GPU cores available for use: 4 CPUs cores and 384 GPUs cores. In order to deal with the heterogeneity of the APU architecture, a load balancing strategy was implemented. The use of all devices available speedup the code up to 27 times when compared to the parallel version that executes using only the CPU cores and 10parallel version that uses only the GPU cores.

References

1. A. Branover and D. Foley and M. Steinman. AMD Fusion APU: LLANO. IEEE Micro, pp. 28- 37, March-April 2012.
2. A. Munshi et al. OpenCL Programming Guide. Addison-Wesley, 2012.
3. P. Rocha et al. A Three-Dimensional Computational Model of the Innate Immune System. Lecture Notes in Computer Science, v. 7333, pp. 691-706, 2012.

Parallel and Adaptive Algorithms for Cardiac Electrophysiology Simulations

Rafael Sachetto Oliveira
Federal University of Sao Joao del-Rei, Brazil
rsachetto@gmail.com

Rodrigo Weber dos Santos, Marcelo Lobosco, Johnny Moreira Gomes
Federal University of Juiz de Fora, Brazil
rodrigo.weber@ufjf.edu.br, mlobosco@gmail.com, johnnysn@gmail.com

Wagner Meira Junior, Denise Burgarelli
Federal University of Minas Gerais, Brazil
meira@dcc.ufmg.br, burgarelli@ufmg.br

Abstract

Computational models have become valuable tools for the study of the electrical behavior of the heart. However, the high complexity of the biophysical processes translates into expensive computational models. In this work we propose, implement and combine strategies using parallel computing and graphical processing unit (GPU), adaptive meshes in space and time adaptive methods in order to reduce the execution time of cardiac electrophysiology simulations. We compared different GPU implementations (OpenGL, NVIDIA CUDA and OpenCL) to a CPU multicore implementation that uses OpenMP. The OpenGL approach showed to be the fastest with a speedup of 446 for the solution of the nonlinear system of ordinary differential equations (ODEs) associated to the solution of the cardiac model, whereas CUDA was the fastest for the numerical solution of the parabolic partial differential equation with a speedup of 8. The use of the Autonomous Leaves Graph (ALG) adaptive mesh also proved attractive as the electrical wavefront that propagates corresponds only to a small fraction of the cardiac tissue. The use of uniform meshes leads to a high computational cost, as it requires a large number of mesh points. In this sense, the tests reported in this work show that the two-dimensional heart tissue model simulations were accelerated up to 80 times by using the ALG. Furthermore, we developed a parallel version of the Euler method with adaptive time step, using both multi-core or GPUs. Finally, we combine the developed parallel methods with the adaptive meshe techniques. The combination of these techniques allowed to achieve acceleration rates much higher than those found in recent work, reaching over 1,700 fold acceleration using only a machine equipped with 8 processors and a single GPU.

References

1. B. G. BARROS AND R. S. OLIVEIRA AND M. LOBOSCO AND R.W. DOS SANTOS AND W. MEIRA JR. Simulations of Complex and Microscopic Models of Cardiac Electrophysiology Powered by Multi-GPU Platforms. Computational and Mathematical Methods in Medicine, v. 2012, p. 1-13, 2012.
2. R. S. OLIVEIRA AND B. M. ROCHA AND D. BURGARELLI AND W. MEIRA JR AND R. W. DOS SANTOS. A parallel accelerated adaptive mesh algorithm for the solution of electrical models of the heart. International J. of High Performance Systems Architecture, v. 4, p. 89-100, 2012.

A Flexible Material Database for Computational Science and Engineering

Josef Weinbub, Karl Rupp, Florian Rudolf
Institute for Microelectronics, Technische Universität Wien
weinbub@iue.tuwien.ac.at, rupp@iue.tuwien.ac.at,
rudolf@iue.tuwien.ac.at

Abstract

Simulation tools in the area of computational science and engineering usually require access to a plethora of material parameters for modeling physical phenomena. Academic software projects typically focus on a single approach for providing this capability. For instance, an extensible markup language (XML)-based input file is used, containing all relevant material parameters, such as the permittivity for silicon [1]. These parameters are then imported and accessed via XML libraries, like pugixml [2]. Although this approach is effective, it confines the application to use a single specific material database backend. For small simulation projects, this is hardly an issue. However, the larger the project and the higher the required usability, the more it becomes important to support different – typically file-based – material databases and to reuse historically-grown material database files. We tackle these challenges by using a flexible material database mechanism. Flexibility refers to decoupling a simulation tool from the actual material database kernel, such as XML. In particular, we strive for exchangeability and expandability via a variable database mechanism, based on a dynamic class hierarchy. We ensure proper handling of physical units via incorporating unit checks, which are especially important for robust numerical simulations [3]. Also, we investigate interfacing with Python, becoming increasingly important in the computational science and engineering community due to its support for rapid-prototyping. The developed methods are utilized in the free open source library ViennaMaterials [4]. We show the applicability of our approach based on a finite volume-based simulation tool due to its popular use in the area of semiconductor device simulation. The flexibility of switching database backends is shown, thus decoupling the simulation tool from a specific approach, such as XML. Based on the depicted examples, we show the advantage of applying our flexible material database over relying on a single specific backend.

References

1. M. Gayer and G. Iannaccone. A Software Platform for Nanoscale Device Simulation and Visualization. In Proc. of ACTEA, 2009.
2. A. Kapoulkine. pugixml. http://pugixml.org/.
3. B. Stroustrup. Software Development for Infrastructure. Computer 45(1), 2012.
4. J. Weinbub et al.. ViennaMaterials. https://github.com/viennamaterials/.

High Order Space-Time Finite Element Schemes for Viscodynamic Wave Equations With Application to Stenosis Diagnosis

John Whiteman
BICOM, Brunel university, UK
john.whiteman@brunel.ac.uk

Abstract

In 2001 Werder et al. (hp-discontinuous Galerkin time stepping for parabolic problems. Comp. Meth. Appl. Mech Eng, 90) proposed a temporally discontinuous Galerkin scheme for treating parabolic problems. In that approach block systems arose due to the coupling of the spacial systems through inner products of the temporal basis functions. If polynomials of degree r are used in time, and the spacial finite element space has dimension D, the block system has dimension (r+1)D and is usually regarded as being too large for practical applications when r¿1. Werder et al. found that these matrices are diagonalizable, and hence the time-coupled computations within a time step can be decoupled. Using continuous Galerkin methods in space, we apply the DG-in-time method for the first time to second order wave equations in the context of elastodynamics with Maxwell-Zener visco-elasticity. Numerical results are presented which demonstrate the favourable effect on error and computational work of the moderately high-order temporal and spacio-temporal approximations. Finally an application using shear waves to produce a model for identifying stenosis in human coronary arteries is presented.

References

1. C KRUSE AND M MAISCHAK AND S SHAW AND J R WHITEMAN AND S E GREENWALD AND M BIRCH AND M P BREWIN AND H T BANKS AND Z P KENZAND S HU. High order space-time finite element schemesfor acoustic and viscodynamic wave equations with decoupling.. To Appear in Int Journal of Numerical Methods in Engineering, 2014.
2. H T BANKS AND S HU AND Z KENZ AND C KRUSE AND S SHAW AND J R WHITEMAN AND M BREWIN AND S GREENWALD AND AND M BIRCH. Model validation for a non-invasive artial stenosis detection problem.. Math Biosciences and Engineering 11,(2014) 427-448..

Unsteady Optimal Control Problems Arising From Chemical Processes

Hamdullah Yücel, Martin Stoll, Peter Benner
Max Planck Institute for Dynamics of Complex Technical Systems
yuecel@mpi-magdeburg.mpg.de, stollm@mpi-magdeburg.mpg.de,
benner@mpi-magdeburg.mpg.de

Abstract

This talk will focus on the numerical solution of unsteady optimal control problems governed by a system of convection diffusion partial differential equations (PDEs) with nonlinear reaction terms arising from chemical processes. Such problems are strongly coupled as inaccuracies in one unknown directly affect all other unknowns. Prediction of these unknowns is very important for the safe and economical operation of biochemical and chemical engineering processes. Further, the solutions of these PDEs can exhibit layers on small regions where the solution has large gradients, when convection dominates diffusion. To avoid spurious oscillations emerging from the layers, we use adaptive mesh refinement. The symmetric interior penalty Galerkin (SIPG) method with upwinding for the convection term is used for space discretization, whereas backward Euler is used for time discretization. Residual-based error estimators are used for the state, the adjoint and the control variables. The arising saddle point system is solved using a suitable preconditioner. Numerical examples are presented for convection dominated problems to illustrate the effectiveness of the adaptivity.

References

1. W. BARTHEL AND C. JOHN AND F. TRÖLTZSCH. Optimal boundary control of a system of reaction diffusion equations. ZAMM, Z. Angew. Math. Mech. 90 (2010) 966-982.
2. J. W. PEARSON AND M. STOLL. Fast iterative solution of reaction-diffusion control problems arising from chemical processes. SISC, Vol. 35 (2013) 987-1009.
3. H. YÜCEL AND M. STOLL AND P. BENNER. A Discontinous Galerkin Method for Optimal Control Problems Governed by a System of Convection-Diffusion PDEs with Nonlinear Reaction Terms. MPI Magdeburg Preprint MPIMD/13-10 (2013).

Multiscale Simulations of Copper Defects in High External Electric Fields

Mihkel Veske, Simon Vigonski, Alvo Aabloo, Vahur Zadin
Intelligent Materials and Systems Lab, Institute of Technology, Tartu University, Nooruse 1, 50411 Tartu, Estonia
mihkel.veske@ut.ee, simon.vigonski@ut.ee, alvo.aabloo@ut.ee, vahur.zadin@ut.ee

Flyura Djurabekova, Kai Nordlund
Division of Materials Physics, Department of Physics and Helsinki Institute of Physics, P.O.Box 43 (Pietari Kalmink. 2)0001,4 University of Helsinki
flyura.djurabekova@helsinki.fi, kai.nordlund@helsinki.fi

Abstract

Conducting materials placed in the external electric fields are subject to normal directional force that can lead to material and surface damage and plastic deformations, if material defects acting as stress concentrators are present. To understand the material failure initialization mechanisms and to design new and stronger materials, detailed knowledge of the internal structure of the material is needed. Using molecular dynamics we are limited to very short time length scales – respectively from pico to nanoseconds and from few to tens of nanometers. Continuum mechanics methods however, while being accurate at large scale become inaccurate in the range of few nm [1,2], when the surface stress effects become significant. To overcome these limitations, we use multiscale modeling of material bulk and surface. Instead of using level-set based method as in [1], we use solid mechanics based model to simulate nanoscale defects in Copper single crystal. We use fully coupled bulk-surface model and the finite element method to simulate anisotropic elastic behavior of material. In the model, the surface of the material is simulated as thin elastic layer on the surface mesh of the sample. Since the number of degrees of freedoms arising from the surface mesh, compared the bulk is small, leading to small additional computational cost. Accurate representation of the material surface is obtained using the elastic parameters from molecular dynamics simulations [3]. We apply the model in multiphysics setup and simulate the material behavior under high external electric field. We simulate series of nanoscale bulk and surface defects to investigate their effect to the stress distribution and to identify the strongest and weakest nanostructures. This kind of geometrical sensitivity analysis points out family of possible material defects acting as stress concentrators and identifies defects suitable for future studies with more accurate methods.

References

1. J. YVONNET AND H.L. QUANG AND Q.-C. HE. An XFEM/level set approach to modelling surface/interface effects and to computing the size-dependent effective properties of nanocomposites. Comput. Mech. 42 (2008) 119–131.
2. A.S. POHJONEN AND S. PARVIAINEN AND T. MURANAKA AND F. DJURABEKOVA. Dislocation nucleation on a near surface void leading to surface protrusion growth under an external electric field. J. Appl. Phys. 114 (2013) 033519.
3. V.B. SHENOY. Atomistic calculations of elastic properties of metallic fcc crystal surfaces. Phys. Rev. B. 71 (2005) 094104.

Application of Multiphysics and Multiscale Simulations to Optimize Industrial Wood Drying Kilns

Vahur Zadin, Heiki Kasemägi, Mihkel Veske, Simon Vigonski, Alvo Aabloo
Intelligent Materials and Systems Lab, Institute of Technology, Tartu University, Nooruse 1, 50411 Tartu, Estonia
vahur.zadin@ut.ee, heiki.kasemagi@ut.ee, mihkel.veske@ut.ee, simon.vigonski@ut.ee, alvo.aabloo@ut.ee

Abstract

Timber industry and export is important part of Estonian economy. Small or starting companies require affordable industrial scale equipment for wood drying and processing and often start by utilizing pre-existing infrastructure. To make wood drying equipment available under such conditions, custom design of the kiln is usually required. In this study we present finite element simulations based methodology to simulate and optimize industrial wood drying process and the design of custom made kilns. In current work, we apply multiscale-multiphysics modeling to simulate the drying process in the kiln. The complete model of the drying process is strongly nonlinear as the drying dynamics depends heavily from moisture and heat balance in the circulate air. To handle the dense packing of the processed materials, either very detailed geometrical model and fine mesh (leading to unreasonably large computational costs) or homogenization of the material is needed. In current approach, the model involves a homogenization procedure leading to the effective simulation of the moisture and heat balance and application of porous media flow of drying air in the processed material. The air flow in the kiln is simulated using Navier-Stokes equations, the model is finished by incorporating heat transport in solid and gas phase and moisture dynamics in wood and air. The moisture balance between processed material and air are coupled according to [1] and the moisture balance in the air is simulated according to [2,3]. In current work, we successfully managed at to adopt multiphysics-multiscale simulations to optimize industrial design and optimization of industrial wood drying kilns. We achieved the cost minimization of the kiln design while estimating necessary ventilating power and ensuring homogeneous drying of the processed material.

References

1. L. Chrusciel and E. Mougel and A. Zoulalian and T. Meunier. Characterisation of water transfer in a low temperature convective wood drier: influence of the operating parameters on the mass transfer coefficient. Holz Als Roh- Werkst. 57 (1999) 439–445.
2. H.-J. Steeman and M. Van Belleghem and A. Janssens and M. De Paepe. Coupled simulation of heat and moisture transport in air and porous materials for the assessment of moisture related damage. Build. Environ. 44 (2009) 2176–2184.
3. M. Van Belleghem and H.-J. Steeman and M. Steeman and A. Janssens and M. De Paepe. Sensitivity analysis of CFD coupled non-isothermal heat and moisture modelling. Build. Environ. 45 (2010) 2485–2496.

Impact Force Reconstruction and Localization on Thin-walled Composite Structure

Zemčík Robert, Bartošek Jan, Kroupa Tomáš, Klepáček Jan
University of West Bohemia
zemcik@kme.zcu.cz, bartose4@kme.zcu.cz, kroupa@kme.zcu.cz,
klepacek@kme.zcu.cz

Abstract

Impact reconstruction is performed on an airfoil segment made of laminated composite with attached piezoelectric transducers. The segment is made from glass textile using RTM (Resin Transfer Molding) technology. The reconstruction is based on deconvolution method and transfer functions. The structure is excited using impact hammer in pre-defined locations while the force is measured using embedded force sensor. The response is measured using piezoelectric patch transducers. The measured signals are used for the assessment of so-called transfer functions in form of a matrix since all measured data is represented as discrete vectors. During a random impact, the measured responses together with the transfer functions are used to calculate the force for each possible impact location. Then, the real impact location is found by minimizing the error between the measured and recalculated responses for impacts in all locations. The accuracy of several methods, namely the pseudo-inversion, least squares, quadratic programming and Tikhonov regularization, for the solution of the inverse problem is tested.

References

1. MARTIN M.T. AND DOYLE J.F.. Impact force identification from wave propagation responses. International Journal of Impact Engineering 18 (1996) 65–77.
2. DOYLE J.F.. A wavelet deconvolution method for impact force identification. Experimental Mechanics 37 (1997) 403–408.
3. SEYDEL R. AND CHANG F.-K.. Impact identification of stiffened composite panels: I. System development. Smart Materials and Structures 10 (2001) 354–369.
4. JACQUELIN E. AND BENNANI A. AND HAMELIN P.. Force reconstruction: analysis and regularization of a deconvolution problem. Journal of Sound and Vibration 265 (2003) 81–107.
5. GUNAWAN F.E. AND HOMMA H. AND KANTO Y.. Two-step B-splines regularization method for solving an ill-posed problem of impact-force reconstruction. Journal of Sound and Vibration 297 (2006) 200–214.
6. KUDU T. AND DAS S. AND MARTIN AND S.A. AND JATA K.V.. Locating point of impact in anisotropic fiber reinforced composite plates. Ultrasonics 48 (2008) 193–201.
7. ZHANG B. AND ZHANG J. AND WU Z. AND DU S.. A load reconstruction model for advanced grid-stiffened composite plates. Composite Structures 82 (2008) 600–608.
8. HU N. AND FUKUNAGA H. AND MATSUMOTO S. AND YAN B. AND PENG X.H.. An efficient approach for identifying impact force using embedded piezoelectric sensors. International Journal of Impact Engineering 34 (2007) 1287–1271.
9. ATOBE S. AND KUNO S. AND HU N. AND FUKUNAGA H.. Identification of Impact Force on Stiffened Composite Panels. Transactions of Space Technology Japan 7 (2009) 1–5.
10. SEKINE H. AND ATOBE S.. Identification of locations and force histories of multiple point impacts on composite isogrid-stiffened panels. Composite Structures 89 (2009) 1–7.
11. HANSEN P.C.. Regularization Tools. Numerical Algorithms 46 (2007) 189–194.

Two Dimensional Integration Simulation of Indirect Drived Laser Fusion

Chuanlei Zhai, Heng Yong, Shuanggui Li, Peng Song, Jin Qi, Juan Cheng, Rong Yang, Wenbing Pei, Peijun Gu
Institute of applied physics and computational mathematics
zhaichuanlei@iapcm.ac.cn, yongheng@iapcm.ac.cn,
lishuanggui@iapcm.ac.cn, songpeng@iapcm.ac.cn, qijin@iapcm.ac.cn,
chengjuan@iapcm.ac.cn, yangrong@iapcm.ac.cn,
peiwenbing@iapcm.ac.cn, gupeijun@iapcm.ac.cn

Abstract

The physics process in indirect-drived laser fusion are complicated. Numerical simulation become one important means of the research of laser fusion.

Based on the adaptive structured-mesh parallel software infrastructure (JASMIN), a 2D multi physics integration simulation code is developed to study the physical process and design targets for inertial confinement fusion, which is named by the LARED-Integration code. The LARED Integration code solves a large set of coupled, nonlinear equations that determine the temporal evolution of many spatial quantities as they are influenced by different physical processes.

Here, I shall present the numerical method for radiation hydrodynamics in the LARED-Integration code. Some simulation result of laser fusion will also be given to show the performance.

References

1. W.B. PEI. Scientific computing for laser fusion. physics in china, 38, 2009.

Wind Tunnel Blockage and Three-dimensional Effects in Wind Tunnel Testing of Ice Accretion Over Airfoils and Wings

Marta Zocca, Giulio Gori, Alberto Guardone
Politecnico di Milano
marta.zocca@mail.polimi.it, giulio.gori@mail.polimi.it,
alberto.guardone@polimi.it

Abstract

Wind tunnel testing of ice accretion [1] is simulated numerically to investigate the effects of tunnel blockage on two-dimensional airfoil testing and of the wall-wing interference at the wing tips in three-dimensional wing testing. The open source OpenFOAM (www.openfoam.org) software is used to compute the flow-field and the trajectory of water droplets. The PoliMIce software is used to solve the multi-phase flow around the body surface and to determine the thickness of the iced layer. Similarly to dry testing, wind tunnel blockage is found to produce a variation of the actual angle of attack of the airfoil with respect to the free-stream. However, due to the modification of the airfoil shape in time resulting from ice accretion, the blockage correction angle is a function of time. The wall-wing interference at the wing tips results in the occurrence of a shadow region where water droplets do not impinge. In the rime ice regime, the shadow region is therefore free of ice. In the glaze ice regime instead, the liquid film over the wing moves towards the end-wall and ice is observed in the shadow region. Simulation results compare fairly well with available experiments on ice accretion [2].

References

1. R. W. GENT AND N. P. DART AND J. T. CANSDALE. Aircraft icing. Phil. Trans R Soc Lond A, 2000 .
2. T. GILARDONI AND S. DE BETTIN AND M. SBORDONE. Swirl Anti-Ice System Full Scale Icing Wind Tunnel Test. Alenia Aermacchi S.p.A., 2008..

Solution to Microstructural Fields Based on Schur Complement Method and Wang Tiles

Lukáš Zrůbek, Jaroslav Kruis, Jan Novák
Department of Mechanics, Faculty of Civil Engineering, Czech Technical University in Prague
lukas.zrubek@fsv.cvut.cz, jk@cml.cvut.cz, novakj@cml.fsv.cvut.cz

Abstract

Analysis of micro-scale quantities (e.g. stresses, strains or displacements) in materials with heterogeneous microstructure is an essential step towards better understand of characteristic physical processes taking place at coarse scales. To this goal we present an approach based on Wang tilings [1] and the Schur Complement method [2].

Wang tilings are in principle affine to the game of domino, but instead of two-sided pieces Wang tiles are rendered by squares with piecewise edge information along the entire perimeter. The tiles are gathered in sets. The tiles of a single set involve a complete morphological information of the synthesized quantity [3]. Equally to the game of domino, tiles are placed side by side in a stochastic manner [4] such that it results in a tiled portion of plane without gaps, so called valid tiling. Since the microstructural fields are nonlocal tensors or vectors, the nearest neighbours of each tile in the tiling must be taken into account in order to keep their continuity across the edges. To that end a large number of micro-scale problems have to be solved [5].

With the fact that all tiles of a single set may be discretized by identical finite element mesh with a regular distribution of nodes, the solution to all admissible sub-scale problems (small tilings) can be obtained by the Schur complement method [6]. In particular, the internal unknowns are eliminated to obtain the Schur complements at first. After that each micro-scale problem can be defined only by means of tile interfaces and the appropriate system of equations is reduced by assembling only the Schur complements. The interior field values are simply obtained by the backward substitution at points where required. Moreover, as all solutions are independent, the problem is ideal for processor farming.

References

1. H. WANG. Proving theorems by pattern recognition - II. Bell Systems Technical Journal, 1-41, ISSN 0005-8580, 1961.
2. O. MEDEK AND J. KRUIS AND P. TVRDÍK AND Z. BITTNAR. Static Load Balancing Applied to Schur Complement Method. Computers and Structures, vol. 85, n. 9. pp. 489-498, doi:10.1016/j.compstruc.2006.08.025, 2007.
3. J. NOVÁK AND A. KUČEROVÁ AND J. ZEMAN. Compressing Random Microstructures via Stochastic Wang Tilings. Physical Review E, http://arxiv.org/abs/1206.0933, 2012.
4. M.F. COHEN AND J. SHADE AND S. HILLER AND O. DEUSSEN. Wang tiles for image and texture generation. ACM Transactions on Graphics, Citeseer, 287-294, ISSN 0730-0301, 2003.
5. L. ZRŮBEK AND A. KUČEROVÁ AND J. NOVÁK. Complex microstructural enrichment functions based on extended Wang tile sets. Proceedings of the Nano & Macro Mechanics 2012, 263-270, ISBN 978-80-01-05097-2, 2012.
6. J. KRUIS. Domain Decomposition Methods on Parallel Computers. Progress in Engineering Computational Technology, 299-322, ISBN 1-874672-22-9 hardback, 2004.

P-Multigrid Technique for the Numerical Solution of Algebraic Systems Arising From the Discontinuous Galerkin Discretization of PDEs

Andrej Živčák, Vít Dolejší
Charles University Prague, Faculty of Mathematics and Physics, Sokolovská 83, 186 75, Prague, Czech Republic
andrej.zivcak@gmail.com, dolejsi@karlin.mff.cuni.cz

Abstract

We deal with the discontinuous Galerkin (DG) method applied to the numerical solution of partial differential equations, namely to computational fluid dynamics problems. However, the presented approach can applied to various problems of scientific computing.

The DG method is based on piecewise polynomial but discontinuous approximation, which allows us to simply construct hierarchical basis functions locally for each element. The DG discretization leads to the necessity to solve large (non-)linear algebraic systems. Among the most efficient techniques for the numerical solution of algebraic systems belong the so-called *multigrid methods*.

Multigrid methods are based on coarser representations of the discretized problem. It can be used for solving linear as well as nonlinear problems. Very well known and widely used h-multigrid is based on geometrical hierarchy of computational meshes.

However, for the DG discretization, more suitable approach is the so-called p-multigrid, where a hierarchy of discretization spaces with respect to polynomial approximation degree p is considered.

Projection operators, which carry out the restriction and prolongation, depend on choice of basis functions. Due to the locality of basis function in the DG method we get local projection operators. Their form is very simple in the case of orthonormal basis functions and therefore an effortless implementation can be used.

We describe the application of the p-multigrid to the numerical solution of linear algebraic systems arising from the DG discretization. The restriction and prolongation operators are derived and several solution strategies are discussed. Moreover, a comparison of the efficiency of the p-multigrid technique with iterative solvers is presented. We also mention some weakness of our algorithm and give some outline of a possible use of a non-linear multigrid.

References

1. V. DOLEJŠÍ AND M. HOLÍK AND J. HOZMAN. Efficient solution strategy for the semi-implicit discontinuous Galerkin discretization of the Navier-Stokes equations. J. Comput. Phys. 230(11): 4176–4200, 2011.
2. V. DOLEJŠÍ. A design of residual error estimates for a high order BDF-DGFE method applied to compressible flows. Int. J. Numer. Meth. Fluids, 73(6): 523–559, 2013.
3. K. J. FIDKOWSKI AND T. A. OLIVER AND J. LU AND D. L. DARMOFAL. p-Multigrid Solution of High-order Discontinuous Galerkin Discretizations of the Compressible Navier-Stokes Equations. J. Comput. Phys. 207(1):92–113, 2005.