The effect of parallelization on a tetrahedral mesh optimization method

D. Benitez, E. Rodríguez, J.M. Escobar, R. Montenegro

SIANI Research Institute

University of Las Palmas de Gran Canaria, SPAIN

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UNIVERSIDAD DE LAS PALMAS DE GRAN CANARIA

SIANI

Motivation

- Untangling and smoothing of tetrahedral meshes is an important step in the optimization of meshes in problems with moving boundaries because it provides simulations with elements of good quality
- Improving the speed of mesh generation helps users iterate problem setup faster
- There are currently no parallel mesh untangling algorithms in existence
- There are also no parallel simultaneous mesh untangling and smoothing techniques in the literature

Outline

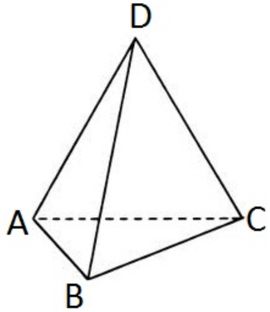
- **We propose a new parallel algorithm for simultaneous untangling and smoothing of tetrahedral meshes** (it is a tetrahedral mesh optimization method)
- **We also provide a detailed analysis of its parallelization on a many-core computer:**
  - **parallel scalability**
  - **load balancing**
  - **parallelism bottlenecks**
  - **influence of 3 graph coloring algorithms**

Summary

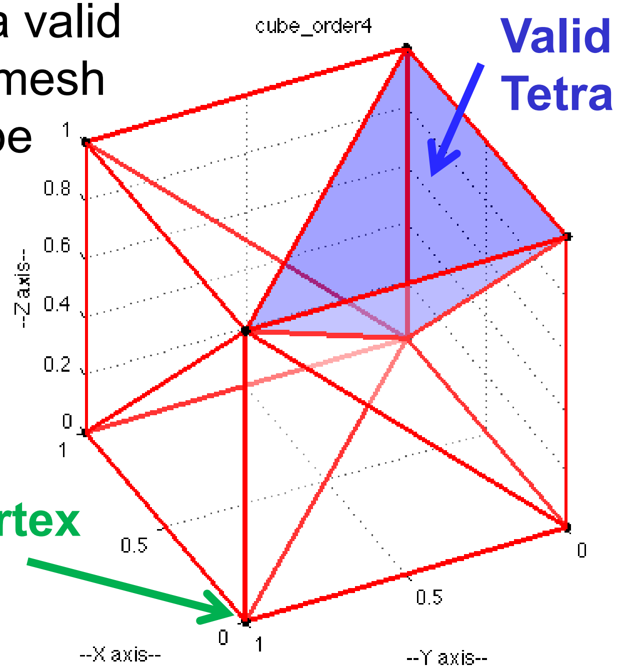
- Our mathematical approach to tetrahedral mesh optimization
- The novel parallel algorithm
- Experimental methodology
- Performance scalability
- Load balancing
- Parallelism bottlenecks
- Influence of coloring algorithms on parallel performance
- Conclusions and future work

Our mathematical approach to tetrahedral mesh optimization

Equilateral tetrahedron



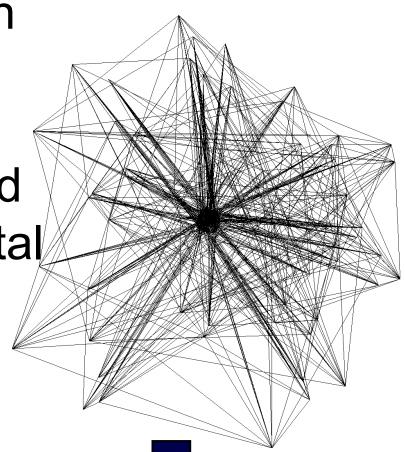
Example of a valid tetrahedral mesh for a cube



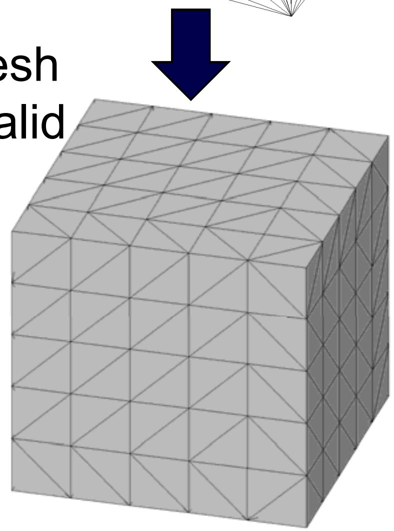
Valid Tetrahedron

A mesh vertex (node)

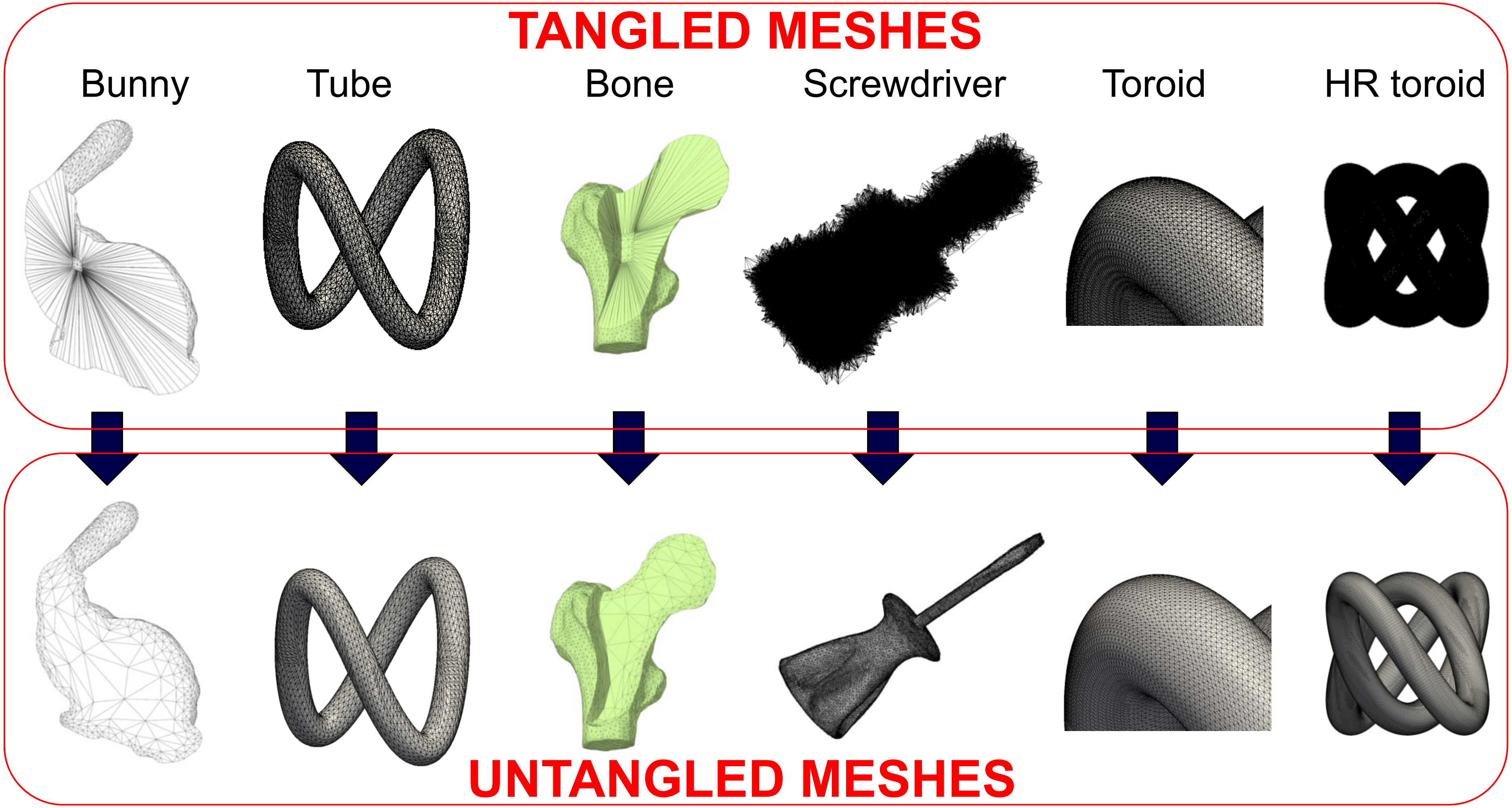
Tetrahedral mesh with non-valid tetrahedra (artificially tangled for our experimental tests)



Optimized tetrahedral mesh without non-valid tetrahedra

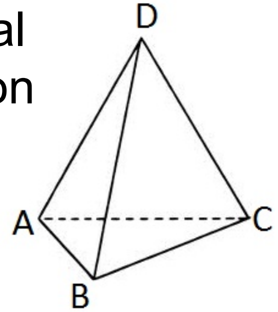


Our mathematical approach to tetrahedral mesh optimization



Our mathematical approach to tetrahedral mesh optimization

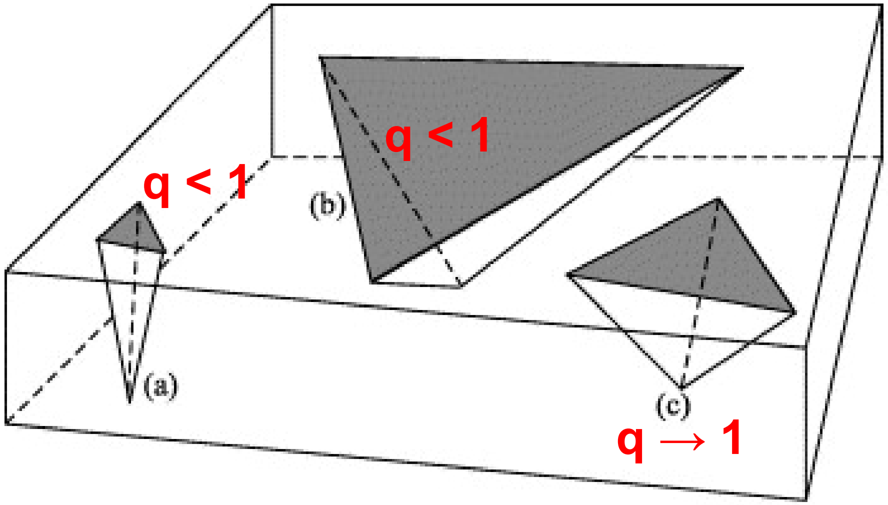
Equilateral tetrahedron



Its quality (q) specifies the degree to which regularity is achieved:

q=1: equilateral tetrahedron

q<1: non-equilateral tetrahedron



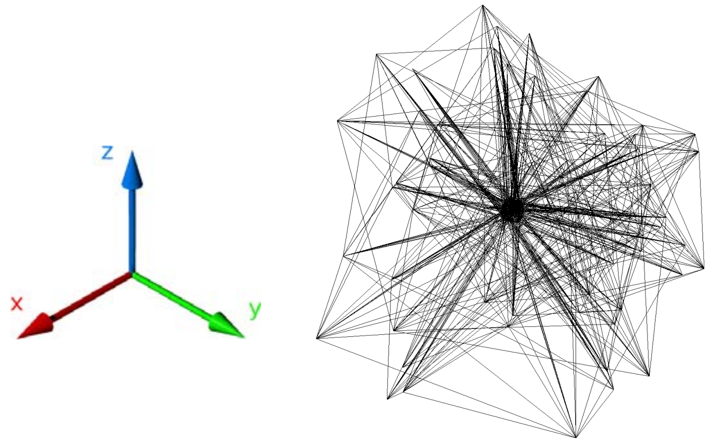
(a) A small triangle on the surface makes a tetrahedron too thin

(b) A large triangle on the surface makes a tetrahedron too flat

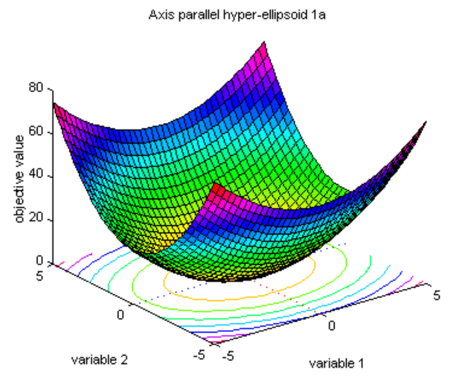
(c) An appropriately sized surface triangle makes a tetrahedron of desired shape

Our mathematical approach to tetrahedral mesh optimization

- **M : a tetrahedral mesh**
- $\boldsymbol{v}$ **: inner mesh node**
- $x_{\boldsymbol{v}}$ **: node position**
- $\mathbb{N}_{\boldsymbol{v}}$ **: the local submesh (set of tetrahedra connected to the node** $\boldsymbol{v}$**)**



- $K(x_{\boldsymbol{v}})$ **: objetive function that measures the quality of the local submesh**



Our mathematical approach to tetrahedral mesh optimization

- **Our untangling and smoothing technique finds the new position $x_{\boldsymbol{v}}$ that each inner mesh node $\boldsymbol{v}$ must hold, in such a way that $K(x_{\boldsymbol{v}})$ is optimized**
- **This process repeats several times for all the nodes of the mesh M**
- **Mathematical details:** J. M. Escobar , E. Rodrıguez , R. Montenegro , G. Montero , J. M. Gonzalez-Yuste (2003) Simultaneous untangling and smoothing of tetrahedral meshes. Computer Methods in Applied Mechanics and Engineering, 192: 2775-2787

The novel parallel algorithm

- **<u>Sequential</u> algorithm (SUS) for the simultaneous untangling and smoothing of a tetrahedral mesh M**

function OptimizeNode($x_{\boldsymbol{v}}$, $\mathbb{N}_{\boldsymbol{v}}$)
  Optimize objective function K($x_{\boldsymbol{v}}$)
end function
procedure SUS
  Q $\leftarrow$ 0
  k $\leftarrow$ 0
  while Q < λ **and** k < maxIter **do**
    for each vertex $\boldsymbol{v} \in M$ **do**
      $x'_{\boldsymbol{v}} \leftarrow$ OptimizeNode($x_{\boldsymbol{v}}$,N_v)
    end do
    Q $\leftarrow$ quality(M)
    k $\leftarrow$ k+1
  end do
end procedure

The novel parallel algorithm

- **<u>Sequential</u> algorithm (SUS) for the simultaneous untangling and smoothing of a tetrahedral mesh M**

```
function OptimizeNode(x_v, N_v)
  Optimize objective function K(x_v)
end function
procedure SUS
  Q ← 0
  k ← 0
  while Q < λ and k < maxIter do
    for each vertex v ∈ M do
      x'_v ← OptimizeNode(x_v, N_v)
    end do
    Q ← quality(M)
    k ← k+1
  end do
end procedure
```

INPUTS:

- *M* : tangled tetrahedral mesh,
- *maxIter* : maximum number of untangling and smoothing iterations
- N_v : set of tetrahedra connected to the free *node* v
- x_v :is the initial position of the free node
- x'_v : its position after optimization, which is implemented with procedure *OptimizeNode()*
- *Q* measures the lowest quality of a tetrahedron of *M*
- *quality()* : function that provides the minimum quality of mesh *M*

The novel parallel algorithm

- <u>Sequential</u> algorithm (SUS) for the simultaneous untangling and smoothing of a tetrahedral mesh M

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end function
procedure SUS
    Q $\leftarrow$ 0
    k $\leftarrow$ 0
    while Q < λ **and** k < maxIter **do**
        for each vertex $\boldsymbol{v} \in M$ **do**
            $x'_{\boldsymbol{v}} \leftarrow$ OptimizeNode($x_{\boldsymbol{v}}$,N_v)
        end do
        Q $\leftarrow$ quality(*M*)
        k $\leftarrow$ k+1
    end do
end procedure

OUTPUT:

•an untangled and smoothed mesh *M*, whose minimum quality must be larger than an user-specified threshold λ

The novel parallel algorithm

- **<u>Sequential</u> algorithm (SUS) for the simultaneous untangling and smoothing of a tetrahedral mesh M**

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        for each vertex $\boldsymbol{v} \in M$ **do**
            $x'_{\boldsymbol{v}} \leftarrow$ OptimizeNode($x_{\boldsymbol{v}}$,N_v)
        end do
        Q $\leftarrow$ quality(M)
        k $\leftarrow$ k+1
    end do
end procedure

This algorithm iterates sequentially over all the mesh vertices in some order, at each step adjusting the spatial coordinates x'_v ***of*** a free node $\boldsymbol{v}$

The novel parallel algorithm

- **<u>Sequential</u> algorithm (SUS) for the simultaneous untangling and smoothing of a tetrahedral mesh M**

```
function OptimizeNode(x_v, ℕ_v)
  Optimize objective function K(x_v)
end function
procedure SUS
  Q ← 0
  k ← 0
  while Q < λ and k < maxIter do
    for each vertex v ∈ M do
      x'_v ← OptimizeNode(x_v, N_v)
    end do
    Q ← quality(M)
    k ← k+1
  end do
end procedure
```

This process repeats several times for all the nodes of the mesh M

The novel parallel algorithm

- **<u>Parallel</u> algorithm (pSUS) for the simultaneous untangling and smoothing of a tetrahedral mesh *M***

function OptimizeNode(x_v, $\mathbb{N}_v$)
  Optimize objective function K(x_v)
end function
procedure Coloring(G=(V,E))
G is partitioned into independent sets I={I_1, I_2, …} using C_1, C_2 or C_3 coloring algorithm
end procedure

Its inputs *are the same* as described for sequential algorithm

procedure pSUS
  I $\leftarrow$ Coloring(G=(V,E))
  k $\leftarrow$ 0
  Q $\leftarrow$ 0
  while Q < λ **and** k < maxIter **do**
    for each independent set $I_i \in$ I **do**
      for each vertex $v \in I_i$ **in parallel do**
        $x'_v \leftarrow$ OptimizeNode(x_v,N_v)
      end do
    end do
    Q $\leftarrow$ quality(*M*)
    k $\leftarrow$ k+1
  end do
end procedure

The novel parallel algorithm

- **Parallel** algorithm (**pSUS**) for the simultaneous untangling and smoothing of a tetrahedral mesh *M*

```
function OptimizeNode(x_v, N_v)
   Optimize objective function K(x_v)
end function
procedure Coloring(G=(V,E))
G is partitioned into independent
sets I={I_1, I_2, …} using C_1, C_2 or C_3
coloring algorithm
end procedure
```

We implemented graph coloring with procedure Coloring(), which partitions the mesh in a disjoint sequence of independent sets: I_1, I_2, …

```
procedure pSUS
   I ← Coloring(G=(V,E))
   k ← 0
   Q ← 0
   while Q < λ and k < maxIter do
     for each independent set I_i ∈ I do
       for each vertex v ∈ I_i in parallel do
         x'_v ← OptimizeNode(x_v,N_v)
       end do
     end do
     Q ← quality(M)
     k ← k+1
   end do
end procedure
```

The novel parallel algorithm

- **<u>Parallel</u> algorithm (pSUS) for the simultaneous untangling and smoothing of a tetrahedral mesh *M***

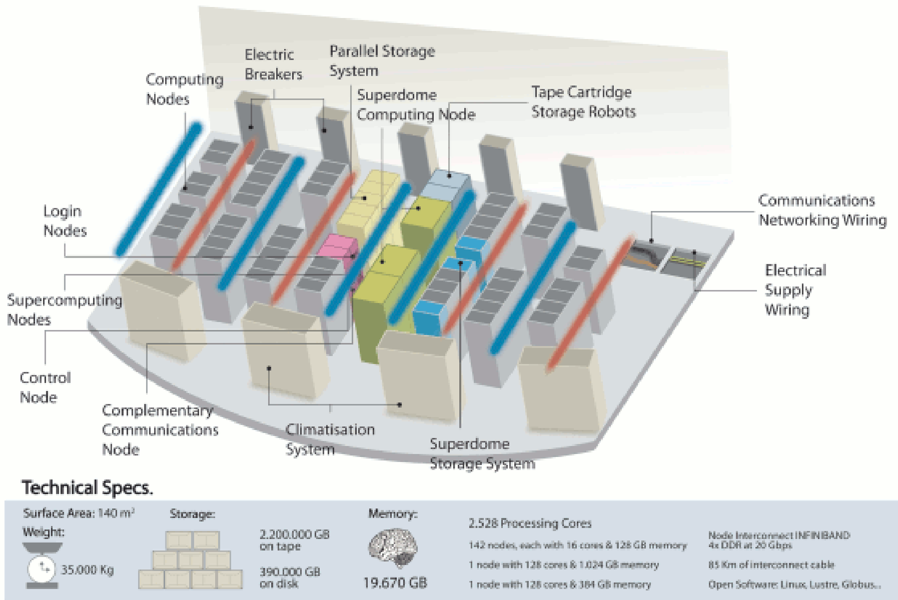
function OptimizeNode(x_v, $\mathbb{N}_v$)
  Optimize objective function K(x_v)
end function
procedure Coloring(G=(V,E))
G is partitioned into independent sets I={I_1, I_2, …} using C_1, C_2 or C_3 coloring algorithm
end procedure

This parallel algorithm optimize in parallel the nodes of each independent set

procedure pSUS
  I ← Coloring(G=(V,E))
  k ← 0
  Q ← 0
  while Q < λ **and** k < maxIter **do**
    for each independent set $I_i \in$ I **do**
      for each vertex $v \in I_i$ **in parallel do**
        x'_v ← OptimizeNode(x_v,N_v)
      end do
    end do
    Q ← quality(*M*)
    k ← k+1
  end do
end procedure

Experimental methodology

- **Finis Terrae supercomputer (www.cesga.es), the third largest supercomputer in Spain**

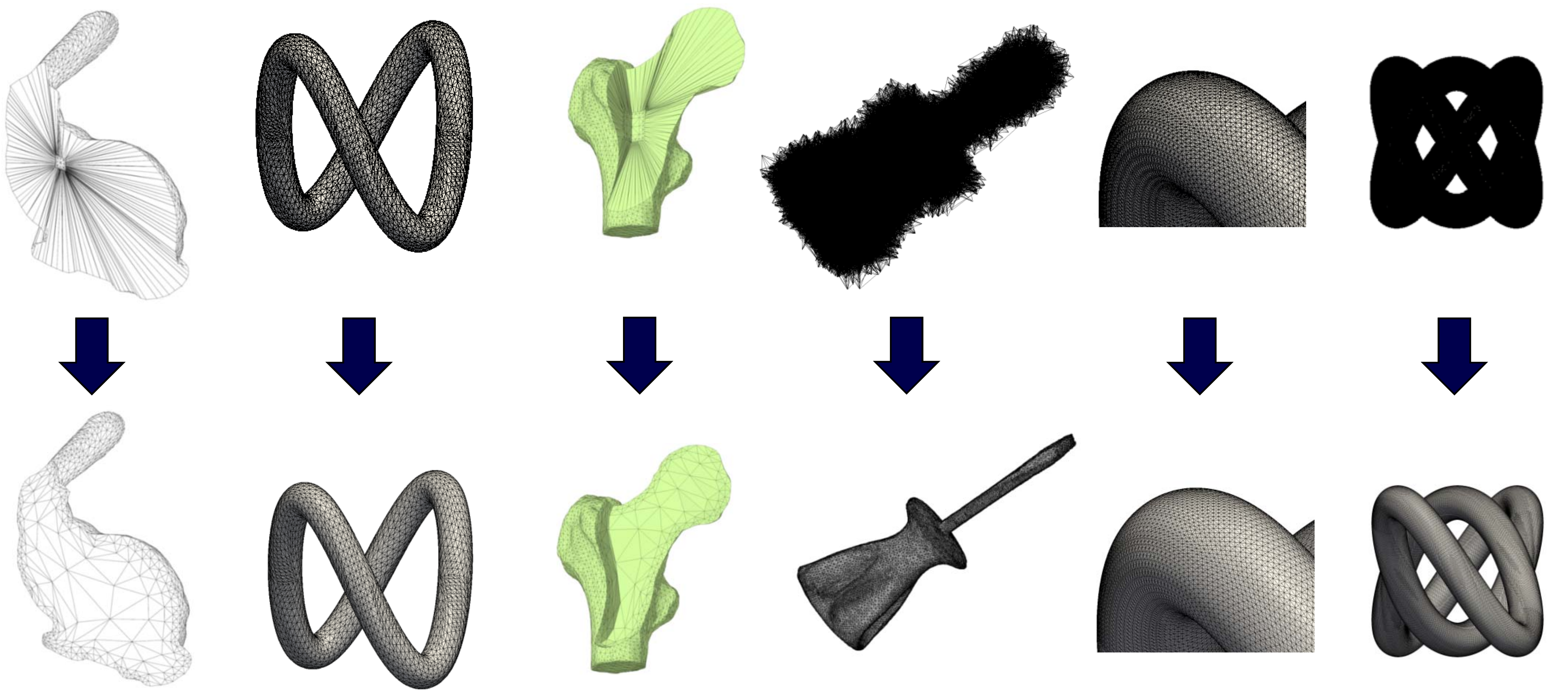


- **1 many-core node HP Integrity Superdome, with 128 cores Itanium Montvale and 1.024 GB (NUMA): shared memory architecture**

Experimental methodology

- **Six different tangled benchmark meshes**

“m=6358”	“m=9176”	“m=11525”	“m=39617”	“m=201530”	“m=520128”
Bunny	Tube	Bone	Screwdriver	Toroid	HR toroid



Experimental methodology

- **Description of the tangled benchmark meshes. The quality of non-valid tetrahedra is considered zero. So, the minimum quality is zero for all meshes**

Name	Number of vertices (m)	Number of tetrahedra	Average mesh quality	Number of inverted tetrahedra	Maximum vertex degree	Object
“m=6358”	6358	26446	0.2618	2215	26	Bunny
“m=9176”	9176	35920	0.1707	13706	26	Tube
“m=11525”	11525	47824	0.2660	1924	26	Bone
“m=39617”	39617	168834	0.1302	83417	26	Screwdriver
“m=201530”	201530	840800	0.2409	322255	26	Toroid
“m=520128”	520128	2201104	0.0657	1147390	26	HR toroid

Experimental methodology

- Intel C++ compiler 11.1 with “O2” flag
- Linux system kernel “2.6.16.53-0.8-smp”.
- The source code of the parallel version included OpenMP directives, which were disabled when the sequential version was compiled
- Both software versions were profiled with PAPI API, which uses performance counter hardware of Itanium 2 processors
- Hardware binding: processor and memory

Experimental methodology

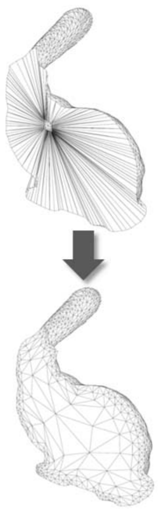
- For each benchmark mesh we run the parallel version multiple times using a given maximum number of active threads between 1 and 128
- Each run is divided into two phases
  - The first of them completely untangles a mesh. This phase loops over all mesh vertices repetitively
  - The second phase smoothes the mesh until successive iterations increases the minimum mesh quality less than 5%

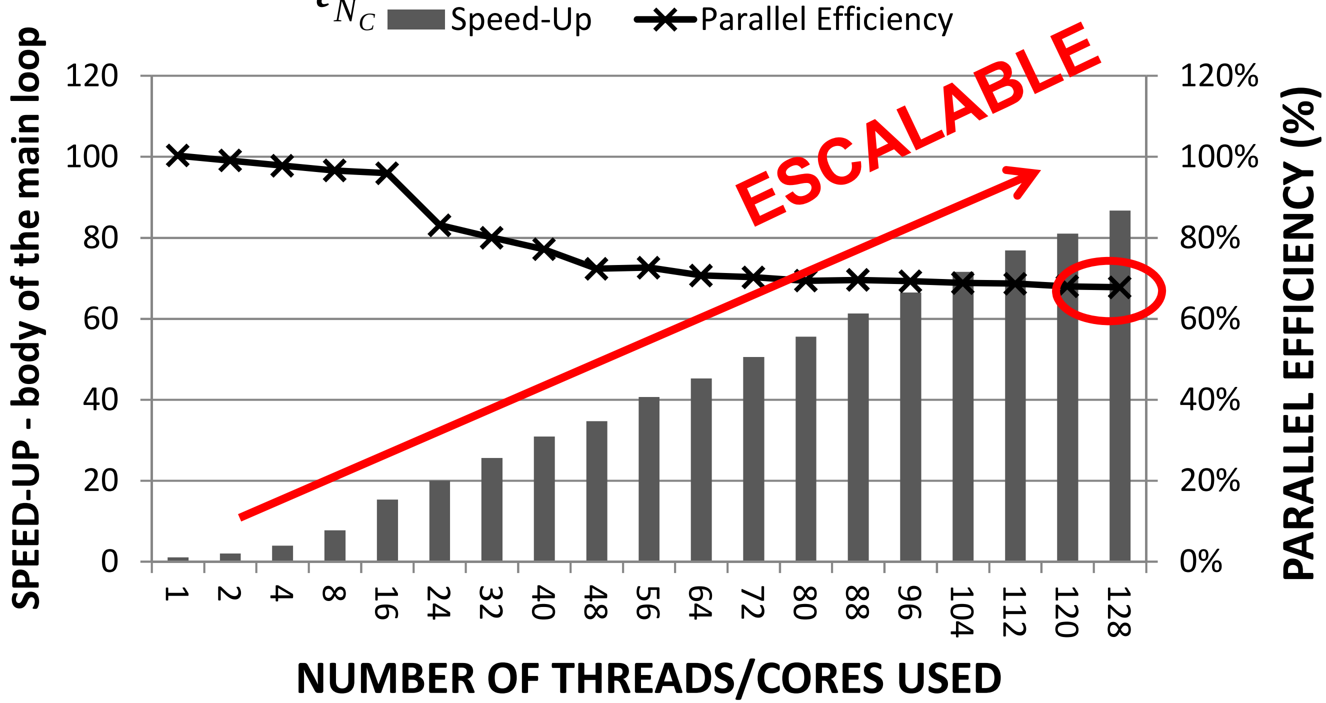
Performance scalability

- True speed-up and parallel efficiency of the body of the main loop

$$\underbrace{\text{the body of the main loop}}_{x'_v \leftarrow \text{OptimizeNode}(x_v, \text{N}_v)}$$

$$Speed-Up = \frac{t_S}{t_{N_C}} \qquad ParallelEfficiency = 100\% \times \frac{S_{N_C}}{N_C}$$

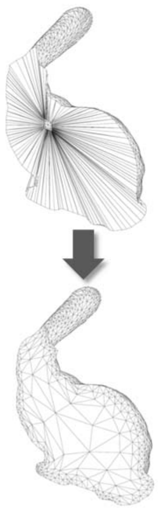




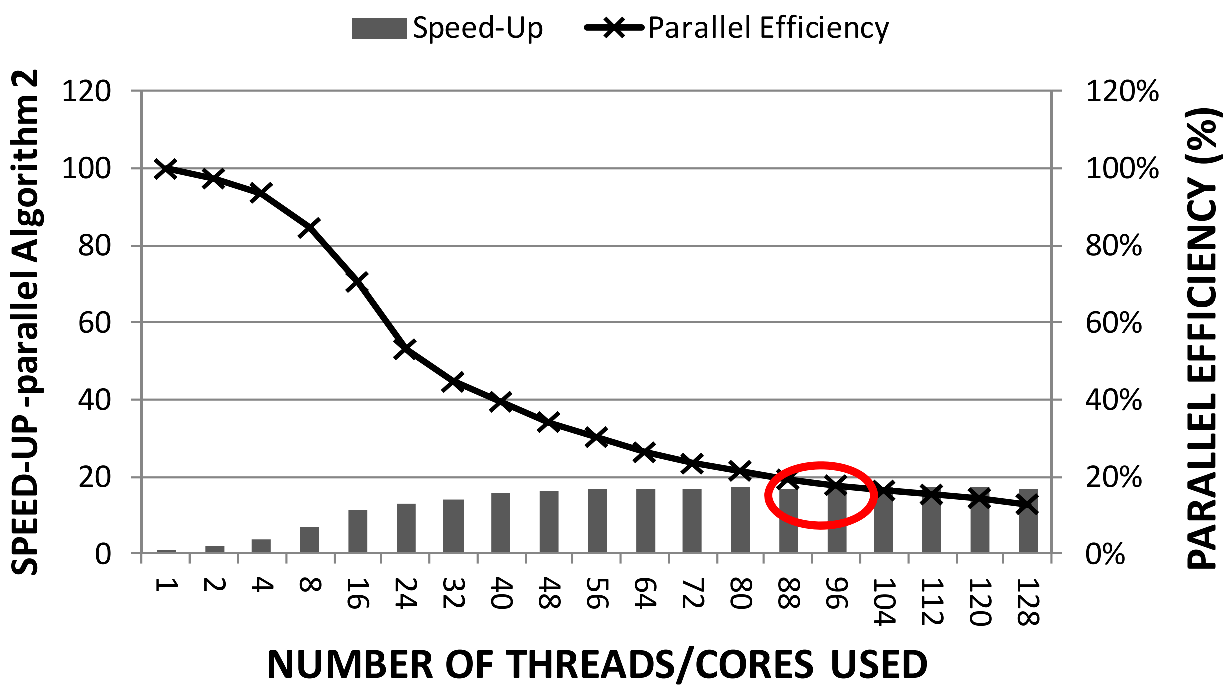
Performance scalability

- **True speed-up and parallel efficiency of the body of the complete parallel Algorithm**

procedure pSUS
…
while Q < λ **and** k < maxIter **do**
for each independent set $I_i \in I$ **do**
for each vertex $v \in I_i$ **in parallel do**
$x'_v \leftarrow \text{OptimizeNode}(x_v, N_v)$



m=6358



Performance scalability

- **Best runtime for the complete parallel algorithm (procedure pSUS)**

Name of tetrahedral mesh	Serial runtime (seconds)	Best parallel runtime (seconds)	Best number of cores	Best Speed-Up	Best parallel efficiency	Best coloring algorithm	Number of colors	Number of iterations (U&S)	Minimum mesh quality	Average mesh quality
m=6358	17.33	1.49	72	11.7X	16.2%	C_1	29	25	0.1319	0.6564
m=9176	37.25	1.17	88	31.9X	36.3%	C_3	29	26	0.2580	0.6823
m=11525	33.69	1.13	120	29.7X	24.8%	C_3	10	38	0.1109	0.6474
m=39617	87.40	1.59	128	54.9X	42.9%	C_1	31	11	0.1698	0.7329
m=201530	2505.37	81.28	128	30.8X	24.1%	C_2	21	143	0.2275	0.6687
m=520128	2259.72	41.86	120	54.0X	45.0%	C_3	34	36	0.2233	0.6750

Performance scalability

- **Performance model for our parallel algorithm based on Amdahl's law**

t_S	Sequential time
$t_{N_C}^{P}$	Parallel time without overhead
$t_{N_C} = t_{Nc}^{P} + t_{Nc}^{O}$	Parallel time with overhead

Speed-up

$$S_{N_C} = \frac{t_S}{t_{Nc}^{P} + t_{Nc}^{O}}$$

$$t = \frac{N_I}{IPC \times f}$$ CPU time

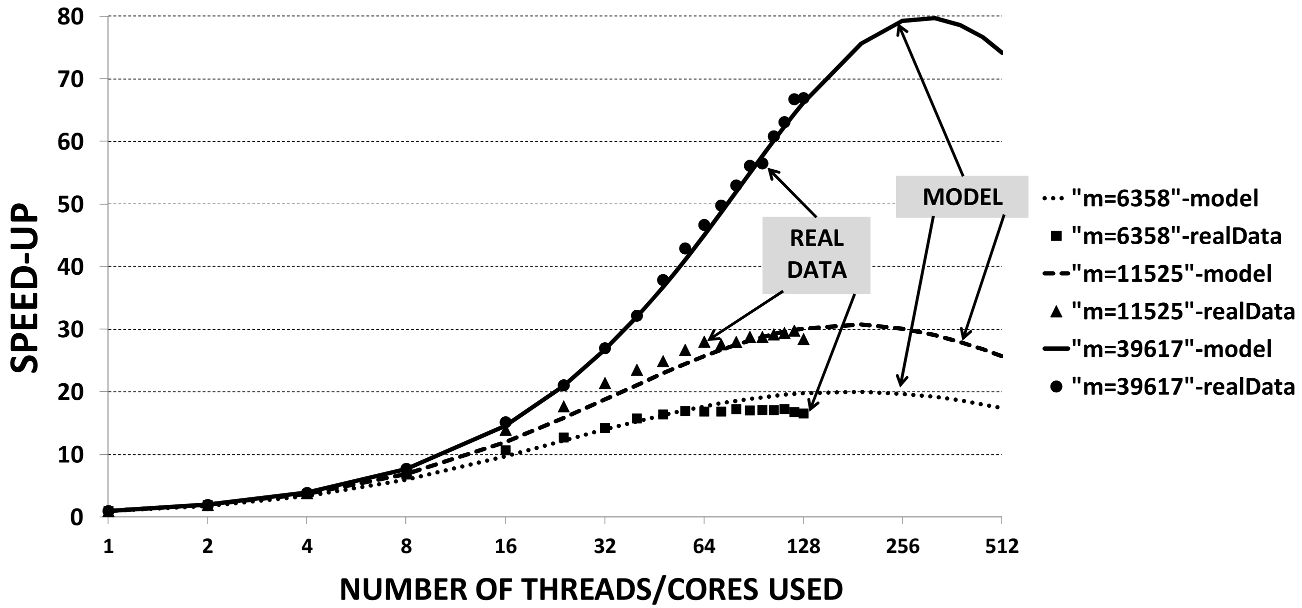
Performance scalability

- **Performance model for our parallel algorithm based on Amdahl's law**

$$S_{N_C} = \frac{t_S}{t_{Nc}^P + t_{Nc}^O} = \frac{\frac{t_S}{t_{Nc}^P}}{1 + \frac{t_{Nc}^O}{t_{Nc}^P}} = \frac{\frac{t_S}{t_{Nc}^P}}{1 + \theta_{N_C}}$$

$$t_{N_C}^P \approx \frac{t_S}{N_C}$$

$$\theta_{N_C} = \frac{t_{Nc}^O}{t_{Nc}^P} \underset{f=cons}{=} \frac{IPC_{Nc}^P \times N_I^O}{IPC_{Nc}^O \times N_I^P}$$

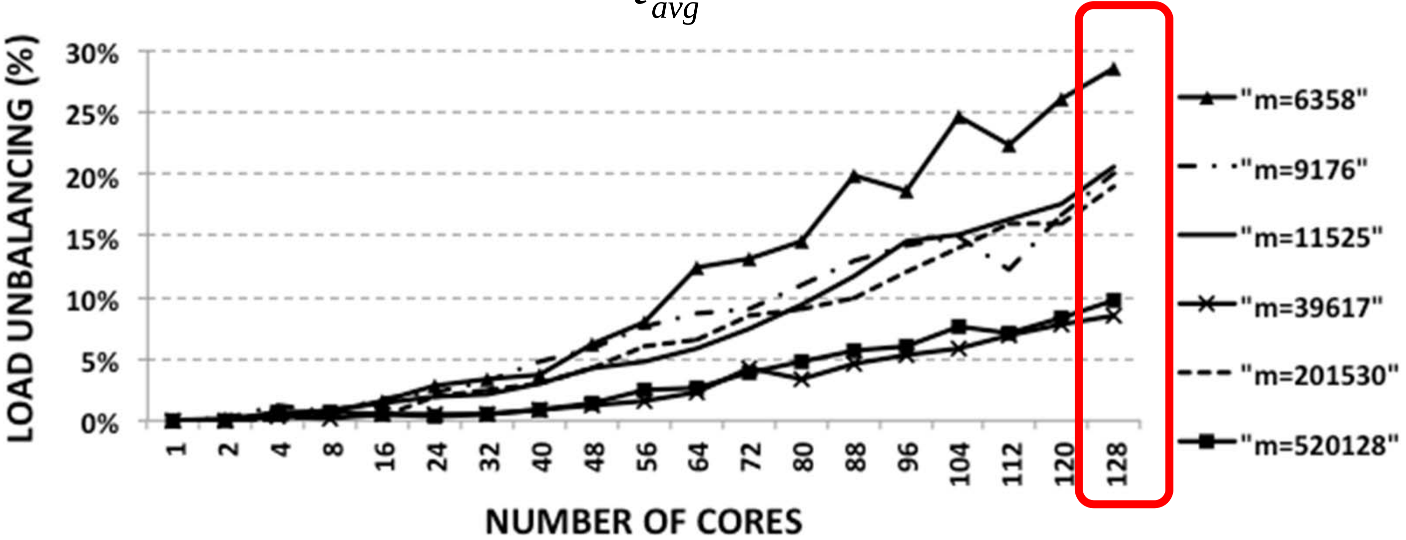


Conclusion: parallel efficiency deteriorate as the number of threads increases because they tend to be dominated by the thread scheduling overhead

Load balancing

- **Load unbalancing when meshes with different number of vertices (m) and up to 128 Itanium2 cores are used. C_3 coloring algorithm and dynamic OpenMP thread scheduling are used**

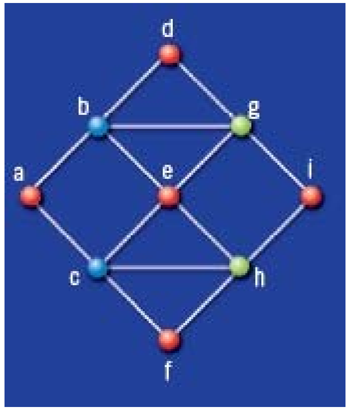
$$L_{N_C} = 100\,\% \times \frac{t_{\max} - t_{\min}}{t_{avg}} \qquad t_{max} > t_{avg} > t_{min} > 0$$



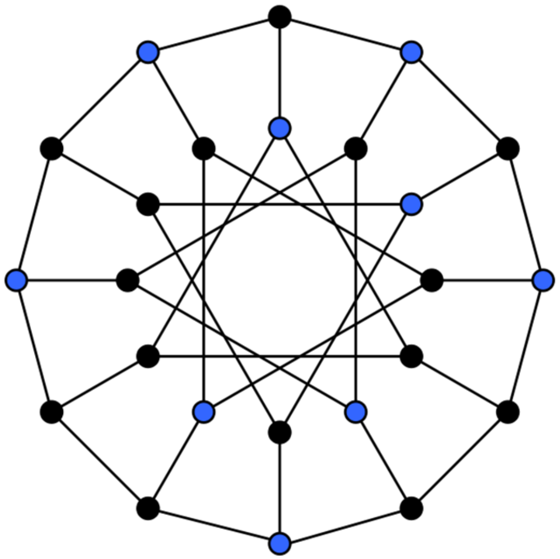
Parallelism bottlenecks

- During runtime of the main mesh optimization procedure, stall cycles of each parallel thread are in the range from 29%(1 core) to 58%(128 cores)
- These computation bottlenecks are located in:
  - double-precision floating-point units: from 70%(1c) to 27%(128c) of stall cycles
  - data loads: from 16%(1c) to 55%(128c)
    - cache memories: main source of data load stall cycles
    - NUMA (Non-Uniform Memory Access) memory: less than 1% of data load stall cycles
  - branch instructions: from 5%(1c) to 14%(128c)
  - “no-operation” instructions (40%): caused by the long instruction format and compiler inefficiency

Influence of coloring algorithms on parallel performance



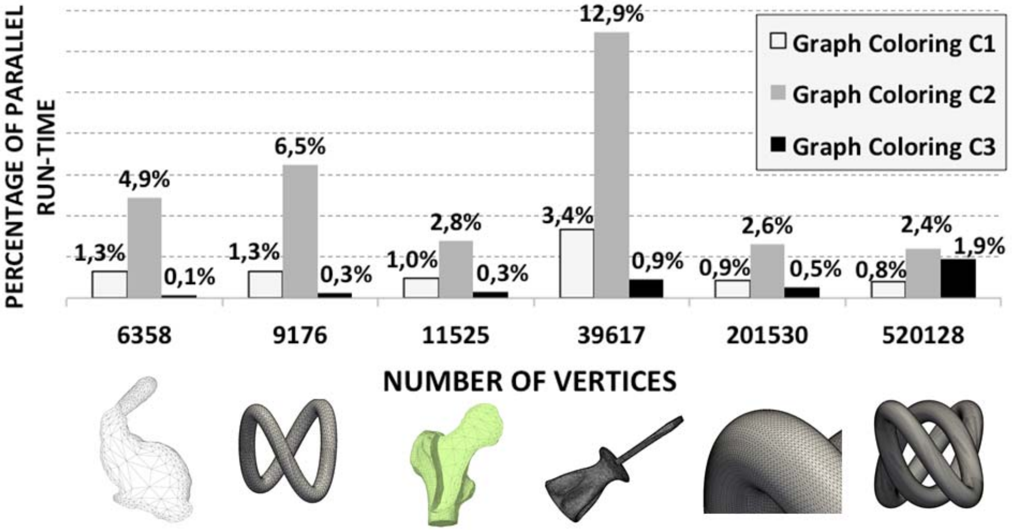
Distance-1 coloring : adjacent nodes do not have the same color



An independent set of a graph is a set of not adjacent vertices

Influence of coloring algorithms on parallel performance

- Percentage of total parallel runtime that is required by the three graph coloring algorithms C_1, C_2, and C_3 when the six benchmark meshes are untangled and smoothed and 128 Itanium2 processors are used

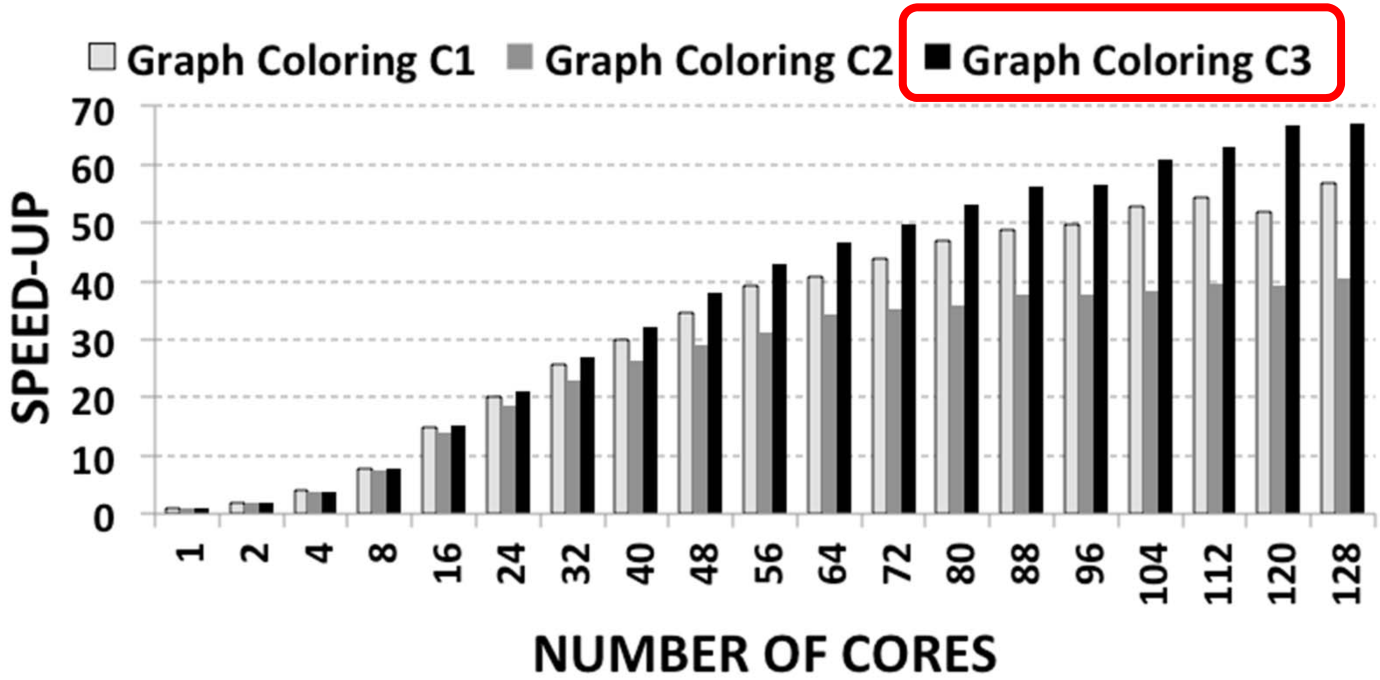


- This means that the computational load required by our parallel algorithm is much heavier than required by graph coloring algorithms.

Influence of coloring algorithms on parallel performance

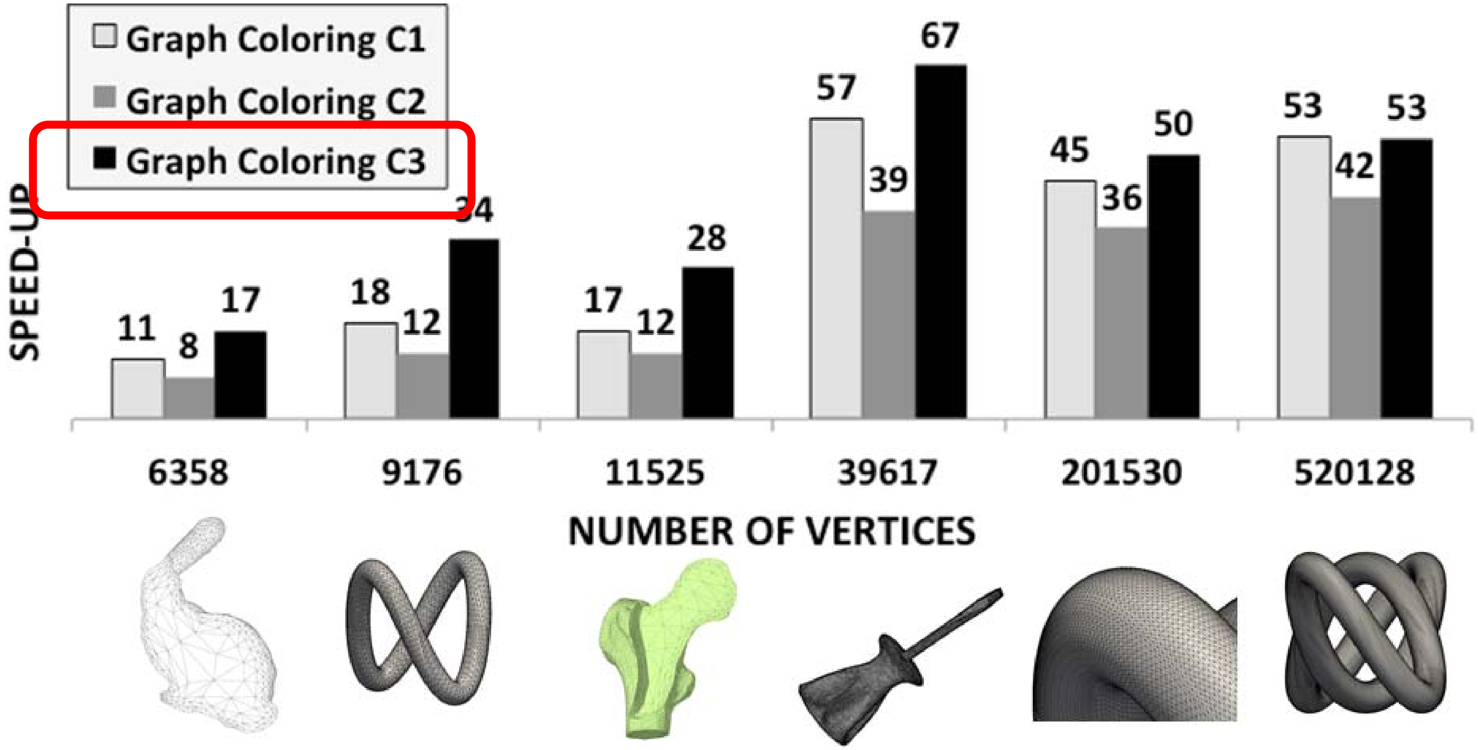
- **Speed-up achieved by the complete parallel algorithm (pSUS) depends on the mesh coloring algorithm**

m=39617



Influence of coloring algorithms on parallel performance

- **Speed-up achieved by the complete parallel algorithm (pSUS) for all six benchmark meshes when three graph coloring algorithms (C_1, C_2, and C_3) are used and all 128 shared-memory Itanium2 processors are active**



Conclusions

- **We demonstrate that this algorithm is highly scalable when run on a high-performance shared-memory many-core computer with up to 128 Itanium 2 processors.**
- **It is due to the graph coloring algorithm that is used to identify independent sets of vertices without computational dependency**

Conclusions

- We have analyzed the causes of its parallel deterioration on a 128-core shared-memory high performance computer using six benchmark meshes.
- It is mainly due to loop-scheduling overhead of the OpenMP programming methodology.
- The graph coloring algorithm has low impact on the total execution time. However, the total execution time of our parallel algorithm depends on the selected coloring algorithm.

Future work

- Our parallel algorithm is CPU bound and its demonstrated scalability potential for many-core architectures encourages us to extend our work to achieve higher performance improvements from massively parallel GPUs.
- The main problem will be to reduce the negative impact of global memory random accesses when the non-consecutive mesh vertices are optimized by the same streaming multiprocessor.