

# Fracture and Fragmentation of Simplicial Finite Element Meshes using Graphs

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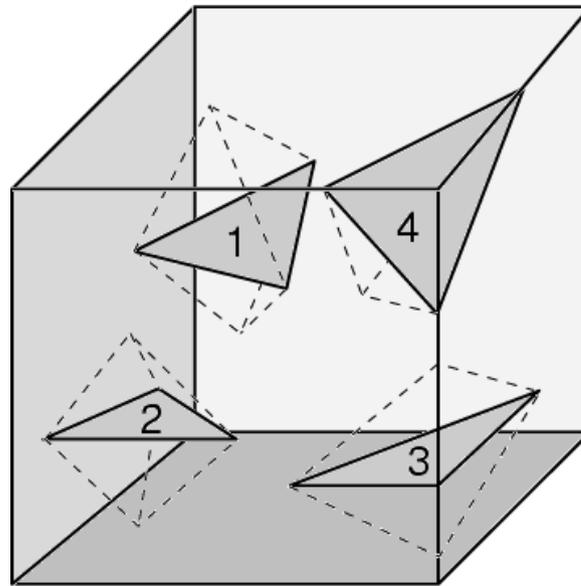
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CAT Workshop  
Santa Fe, NM, August 29, 2009

# Existing Fracture Algorithm

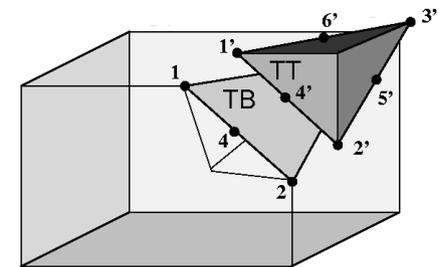
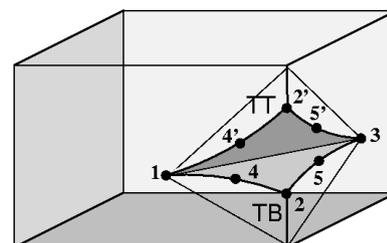
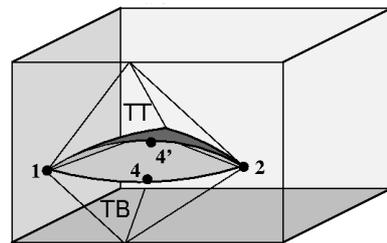
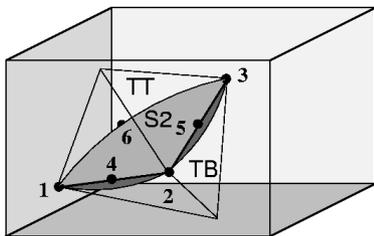
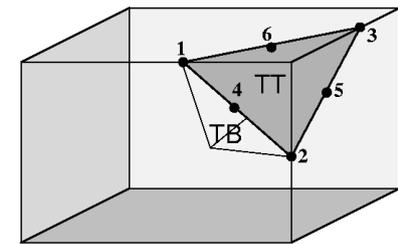
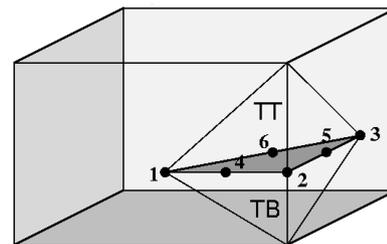
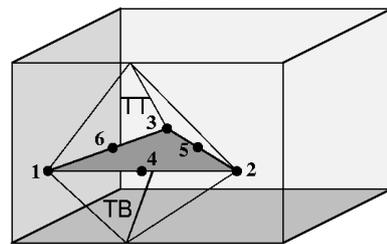
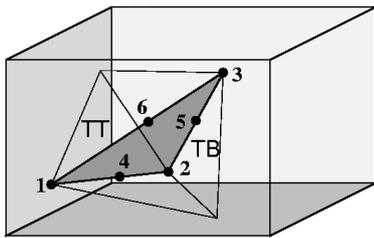
Implemented using a 4-way linked-list data structure.



Pandolfi and Ortiz (1999)

# Fragmentation Cases

Change of topology according to the number of boundary sides of the triangle to be duplicated:



0 sides

1 side

2 sides

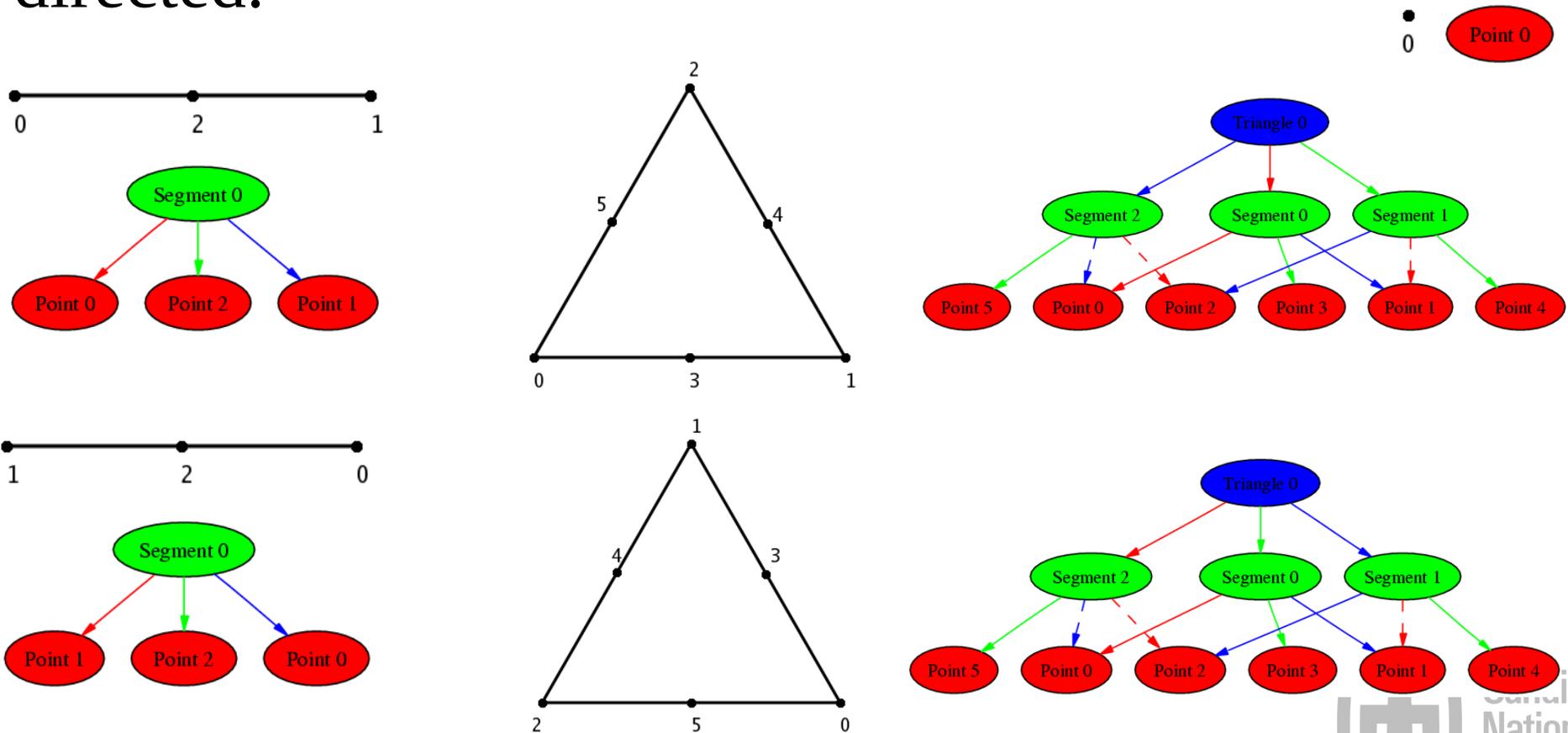
3 sides

# Motivation

- Parallel 3D fracture and fragmentation.
- Parallel 3D contact.
- Same topology representation for both.
- Reuse for 2D if possible.
- Better performance for large meshes.
- Independence of interpolation scheme.
- Correctness.

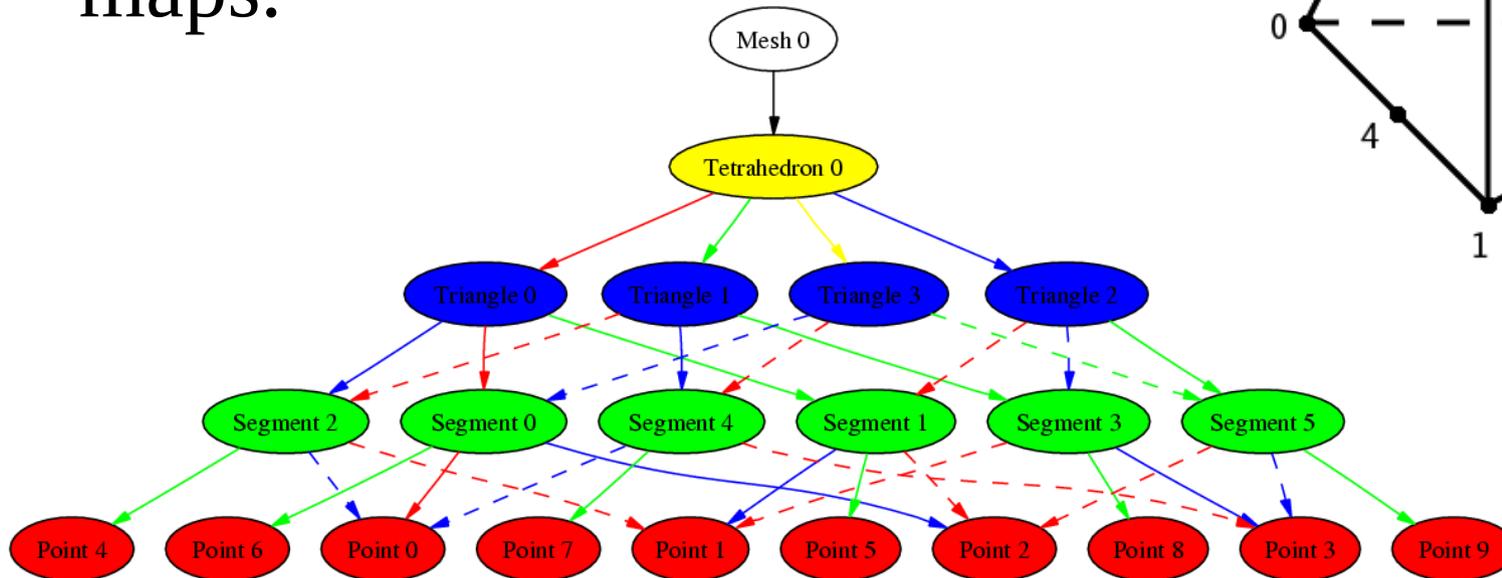
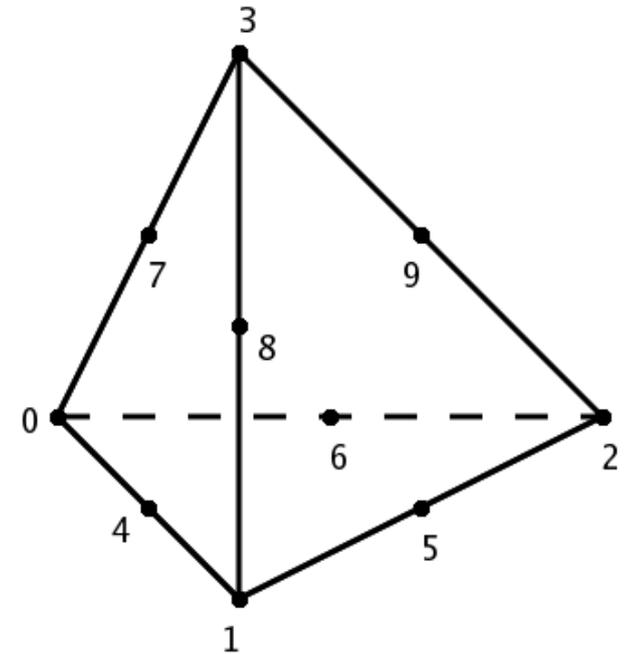
# Simplices as Graphs

Simplices are graphs vertices, and colored edges represent connectivity and orientation. Graphs are directed.



# FE Meshes as Graphs

- Building of graph is top-down.
- Vertices are shared.
- Original orientation kept by color maps.



# FE Meshes as Graphs

Simplex:

$$\sigma = [x_0, \dots, x_n]$$

Face operator:

$$d_i(\sigma) := [x_0, \dots, x_{i-1}, x_{i+1}, \dots, x_n]$$

Incidence number:

$$[\sigma^p, \sigma^{p-1}] := \begin{cases} 0 & \text{if } \sigma^p \cap \sigma^{p-1} = \emptyset \\ 1 & \text{if } \sigma^{p-1} = d_i(\sigma^p) \\ -1 & \text{if } \sigma^{p-1} = -d_i(\sigma^p) \end{cases}$$

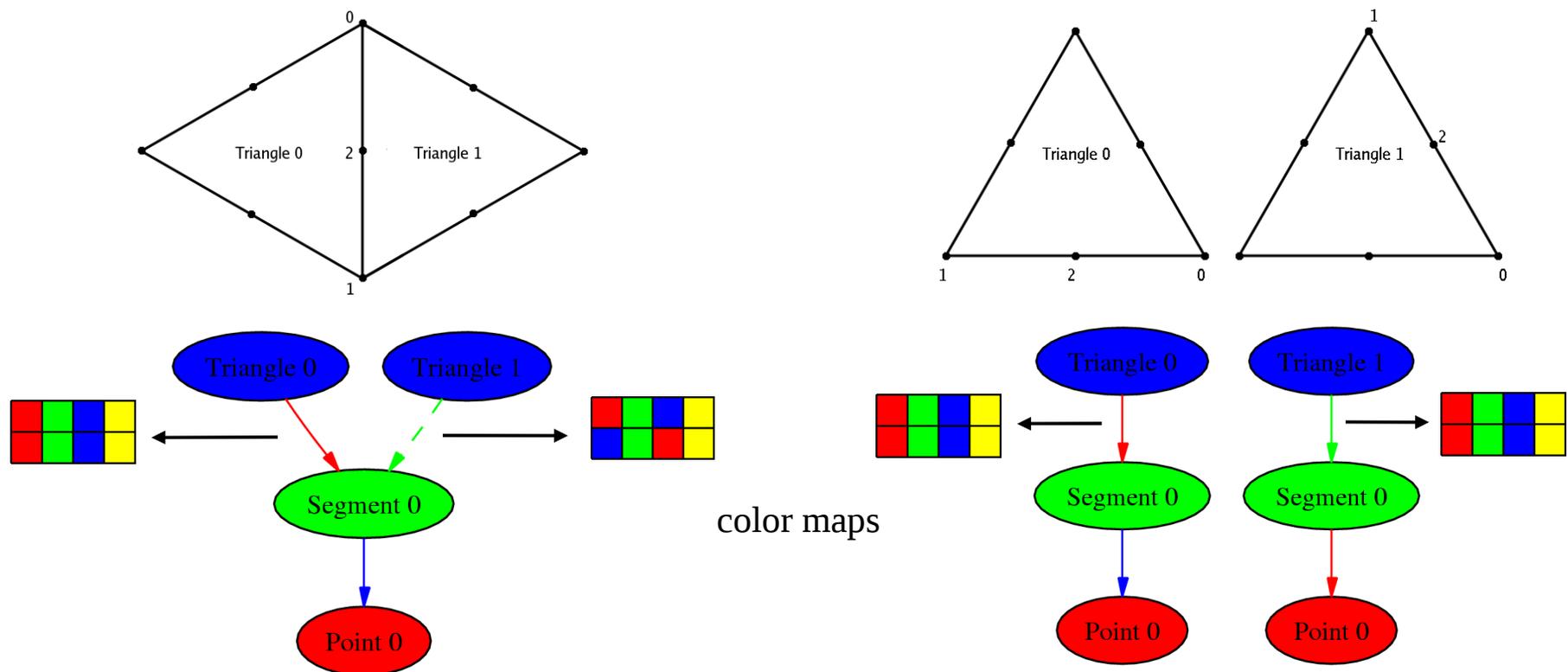
Graph:

$$V = \{v \mid v = f(\sigma) \in \mathbb{N}, \sigma \in K\}$$

$$E = \{e \mid e = (u, v), u = f(\sigma^p) \in V, v = f(\sigma^{p-1}) \in V, \sigma^p \in K, \sigma^{p-1} \in K, [\sigma^p, \sigma^{p-1}] \neq 0\}$$

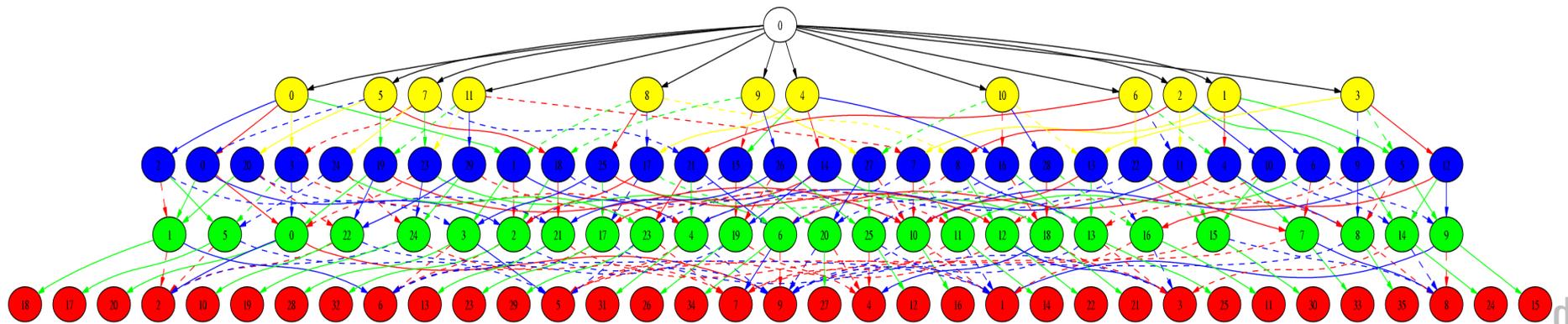
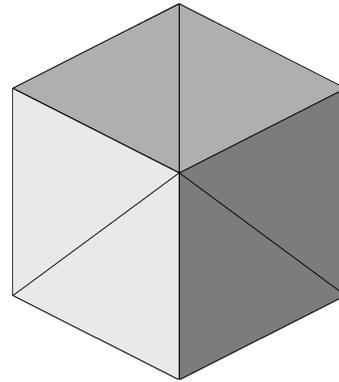
# Local Ordering as Color Maps

Triangle 0 sees point 0 as the blue point in segment 0. Triangle 1 sees it as red.



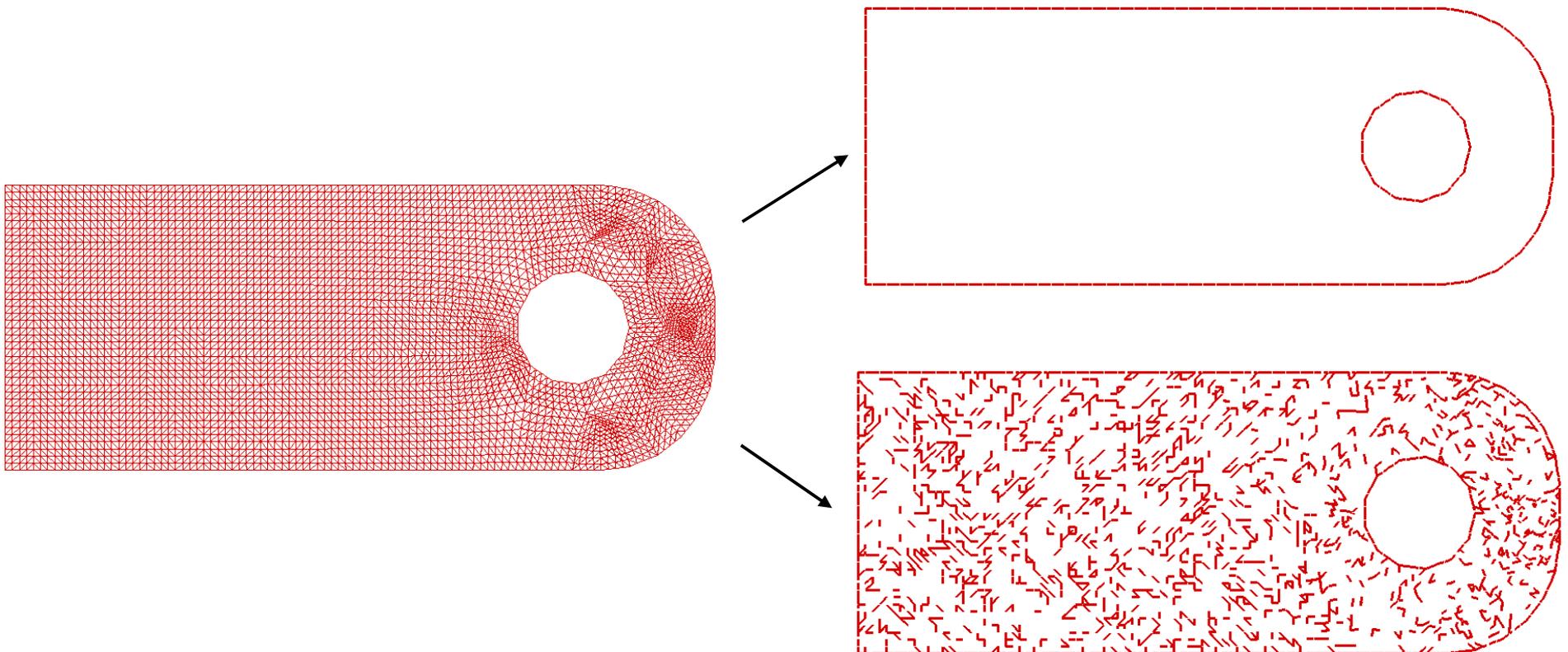
# Cube Mesh as Graph

Graphs are quite complex even for meshes with a few elements.



# Plate with Hole Mesh

Same graph representation works for 2D. Easy to extract useful features.



# Simplex Graph Properties

- Simplices are vertices.
- Edges represent connectivity.
- Directed graph.
- Built top-down.
- Edge color is local order of  $n$ -simplex wrt to  $(n+1)$ -simplex.
- An  $n$ -simplex may be shared by many  $(n+1)$ -simplices.



# Simplex Graph Properties (2)

- Edge color map modifies color of edge directly below if target vertex is shared.
- Color maps are linear maps akin to reflections and rotations, or single and double permutations.
- Graph depth represents the dimension of the mesh. Works for  $N$  dimensions.
- Connectivity array can always be recovered from graph.

# Graph Fracture Algorithm

- Mark open triangles, segments, and corner points.
- Build segment subgraphs.
- Clone open triangles.
- Split segment vertices.
- Build point subgraphs.
- Split point vertices.

# Graph Fracture Algorithm

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**Algorithm 1.** SPLIT( $G, U, n, i$ ) Split articulation points.

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**Require:**  $U \subset V_i, i \leq n - 1$

1. **for all**  $v \in U$  **do**
  2.   **if**  $i < n - 2$  **then**
  3.     SPLIT( $G, D^-(v), n, i + 1$ )
  4.   **else**
  5.     CLONE( $G, D^-(v), n$ )
  6.   **end if**
  7.    $G'' \leftarrow G'(v) \setminus v$  // Check whether  $v$  is an articulation point
  8.   **for all**  $j \in \{2, \dots, N(G'')\}$  **do**
  9.      $Y \leftarrow \{u \mid u \in G''_j, g(u) = i + 1\}$
  10.     $V' \leftarrow \{V', z\}$  // Split the vertex in the subgraph and graph
  11.    **for all**  $u \in Y$  **do**
  12.      $E' \leftarrow E' \setminus (u, v)$
  13.      $E' \leftarrow \{E', (u, z)\}$
  14.    **end for**
  15.   **end for**
  16. **end for**
- 

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**Algorithm 2.** CLONE( $G, U, n$ ) Duplicate fractured interface simplices.

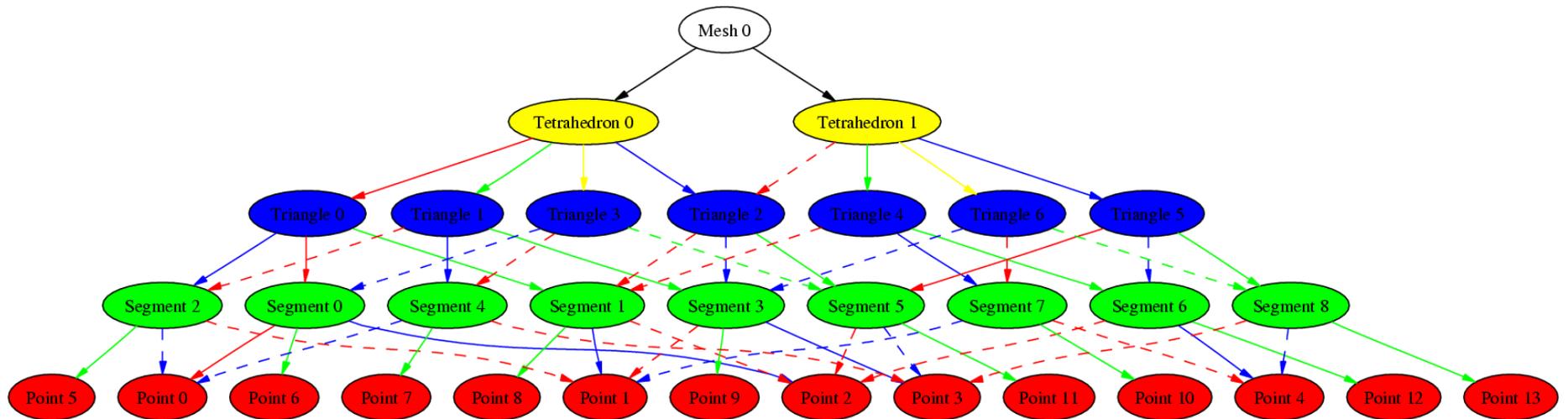
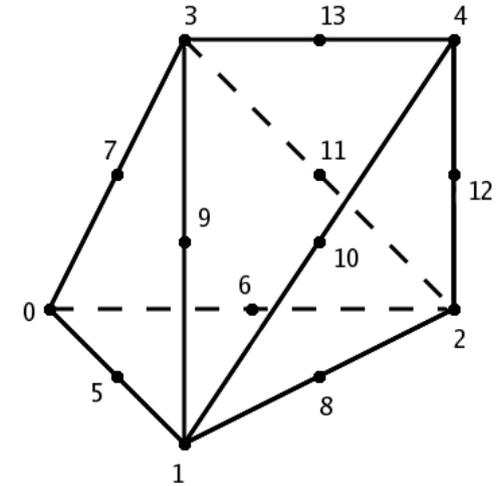
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**Require:**  $U \subset V_{I,n-1}$

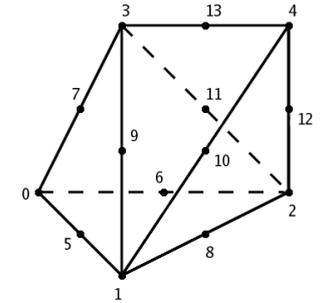
1. **for all**  $v \in U$  **do**
  2.   **if**  $v \in V_{F,n-1}$  **then**
  3.      $Y \leftarrow D^-(v)$  // Note that  $d^-(v) = 2$ , hence  $|Y| = 2$
  4.      $u_1 \leftarrow u \in Y$  s.t.  $[f^{-1}(u_1), f^{-1}(v)] = 1$
  5.      $u_2 \leftarrow u \in Y$  s.t.  $[f^{-1}(u_2), f^{-1}(v)] = -1$
  6.      $V \leftarrow \{V, w\}$
  7.      $E \leftarrow E \setminus (u_2, v)$
  8.      $E \leftarrow \{E, (u_2, w)\}$
  9.     **for all**  $z \in D^+(v)$  **do**
  10.       $E \leftarrow \{E, (w, z)\}$
  11.     **end for**
  12.   **end if**
  13. **end for**
-

# Two-Tetrahedra Mesh

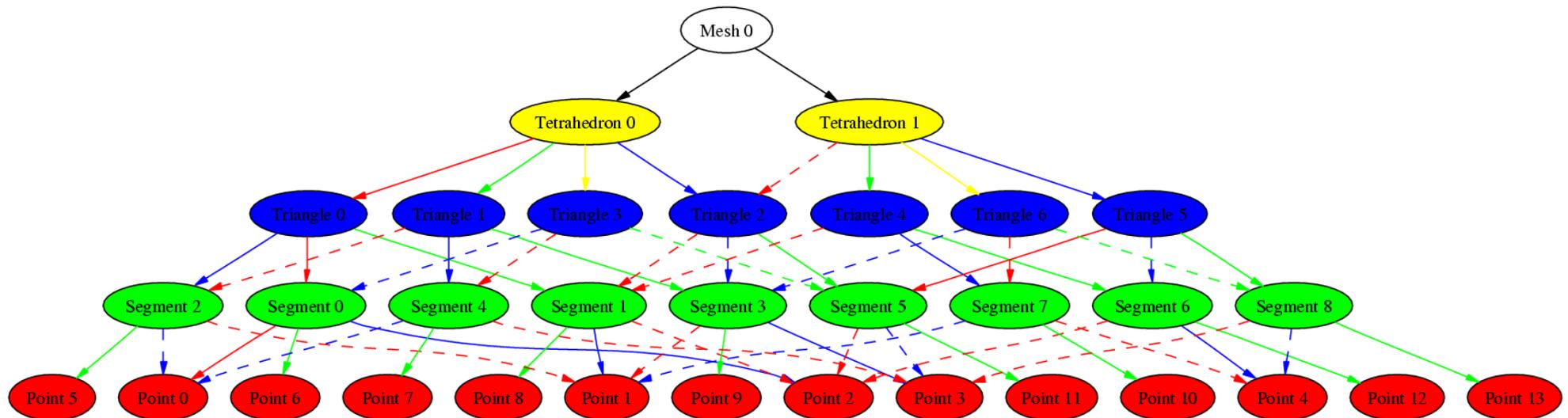
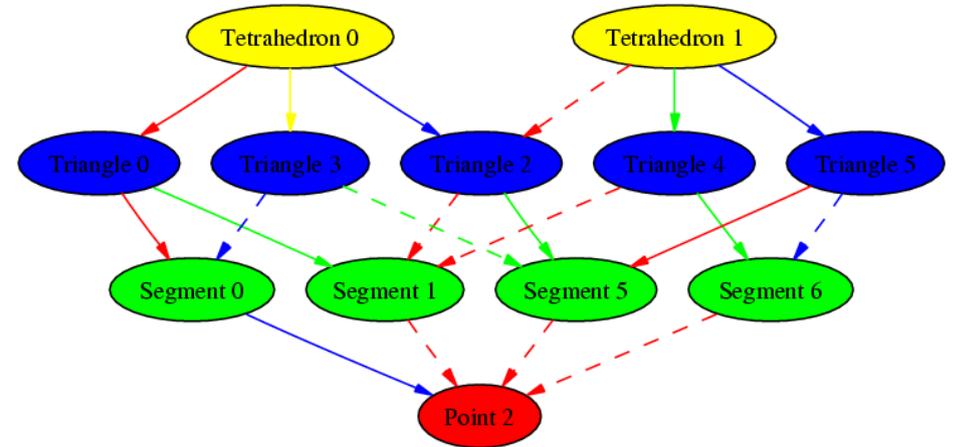
- Single shared triangle.
- Open simplices are triangle 2, segments 1,3,5 and points 1,2,3.

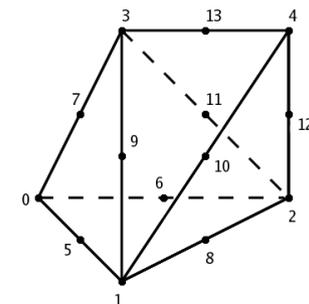


# Fracture Algorithm (1)



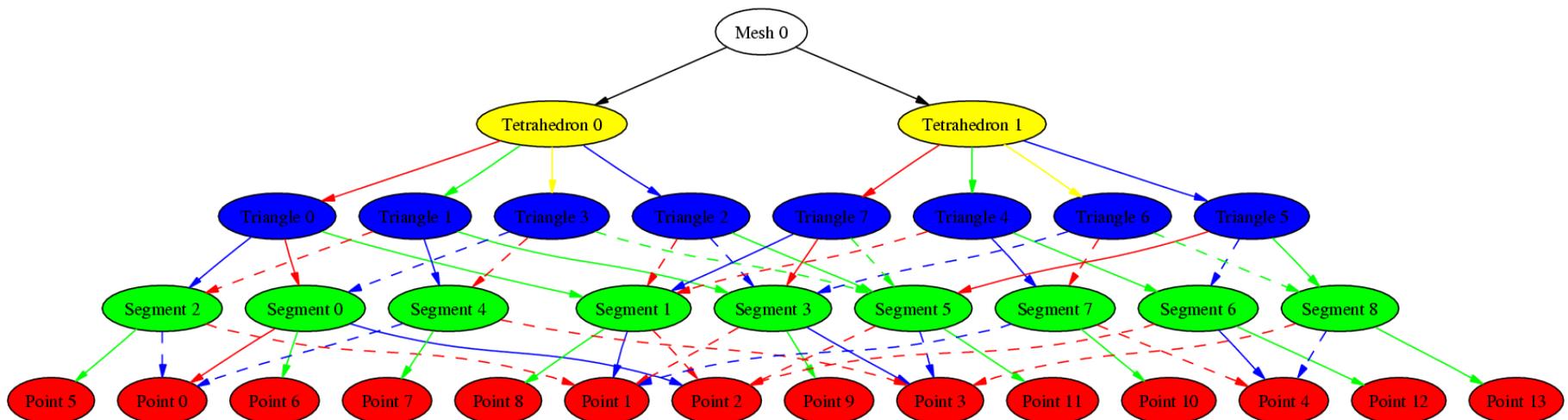
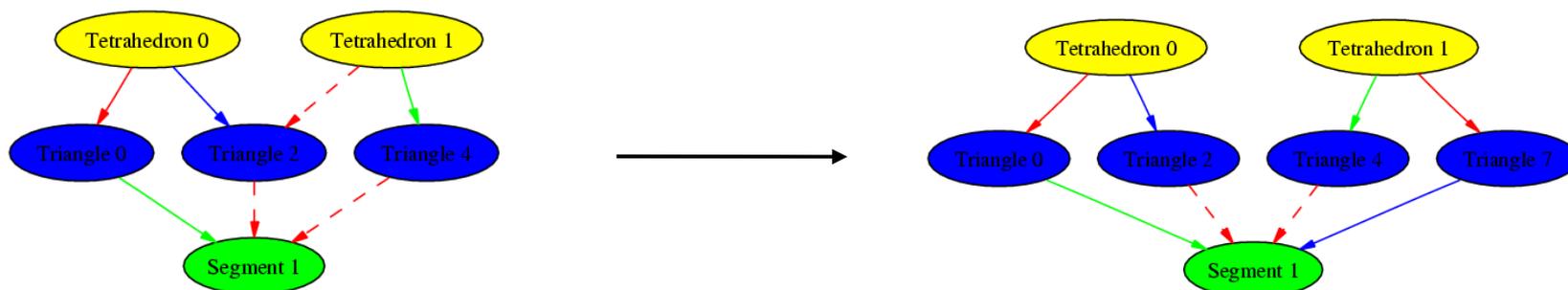
First selected open point is 2, so process open segments 1 and 5 attached to it.

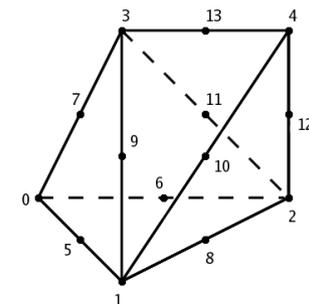




# Fracture Algorithm (2)

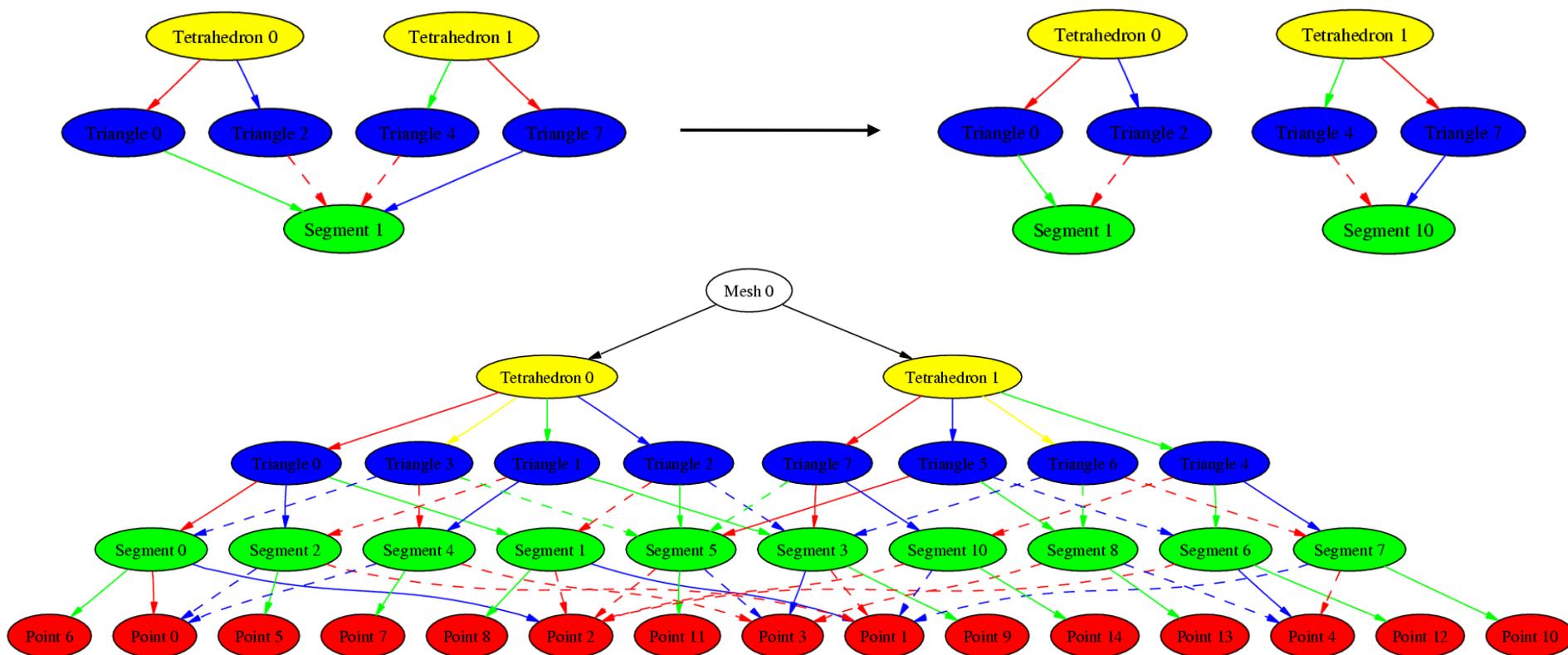
Extract subgraph for segment 1, which clones open triangle 2, creating triangle 7.

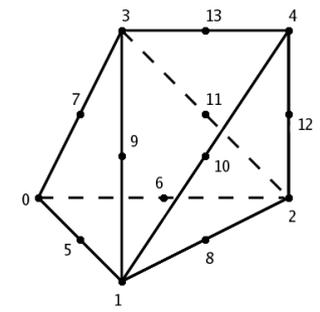




# Fracture Algorithm (3)

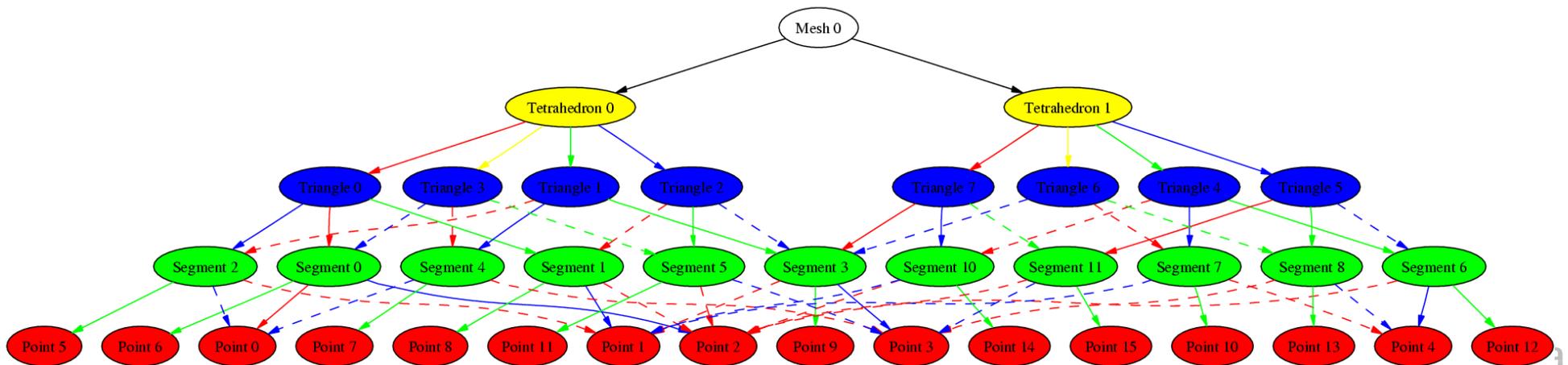
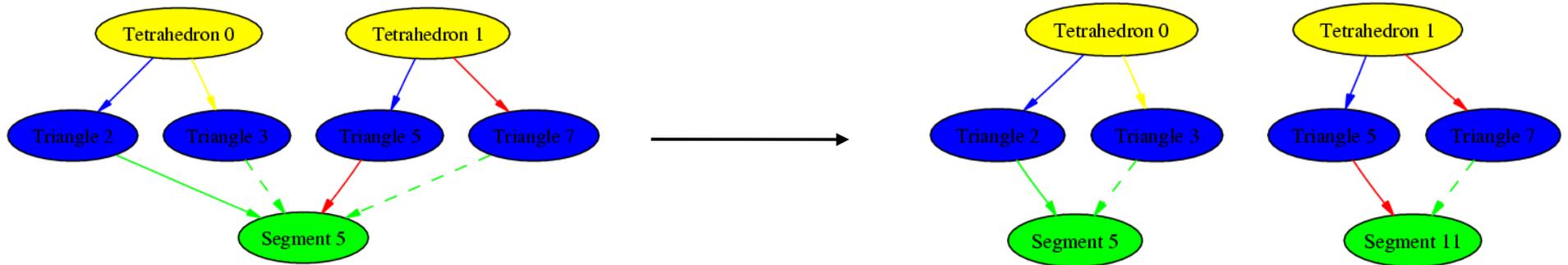
There are 2 branches in segment 1's subgraph, so the segment is split.

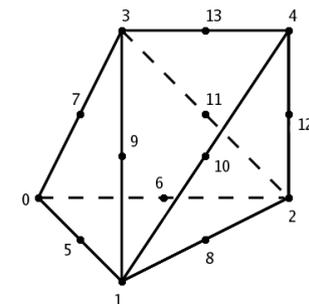




# Fracture Algorithm (4)

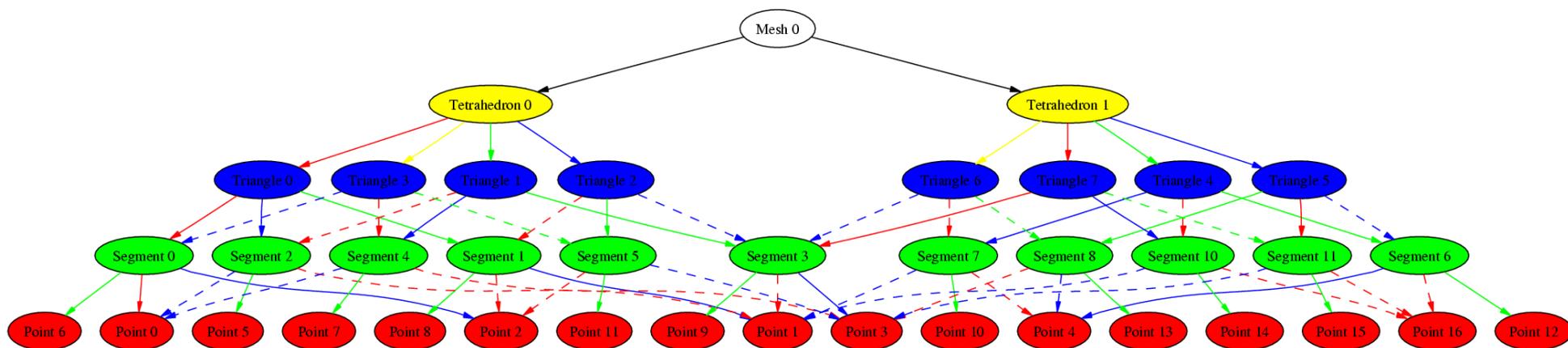
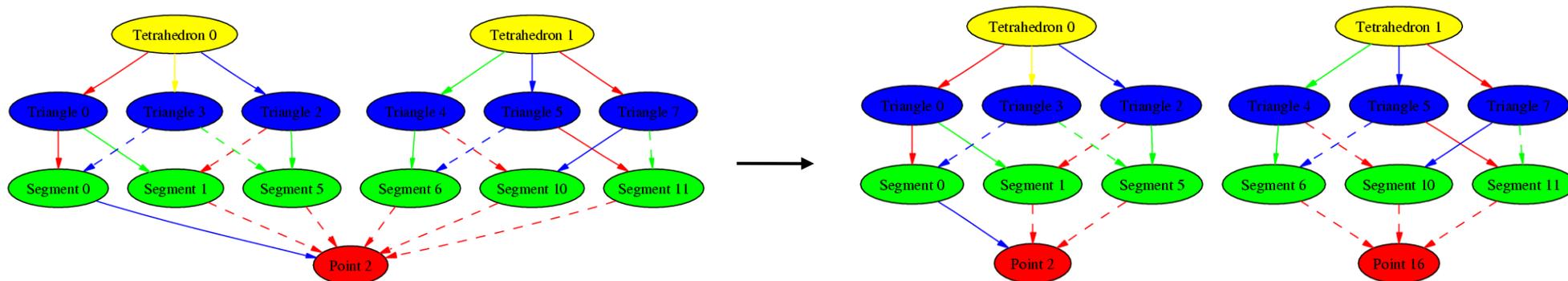
Next is segment 5, now attached to 0 open triangles.  
Its subgraph has 2 branches.



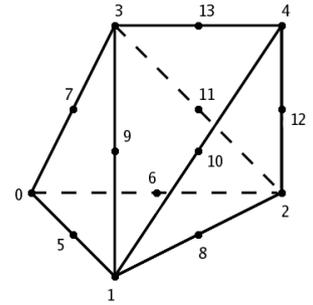


# Fracture Algorithm (5)

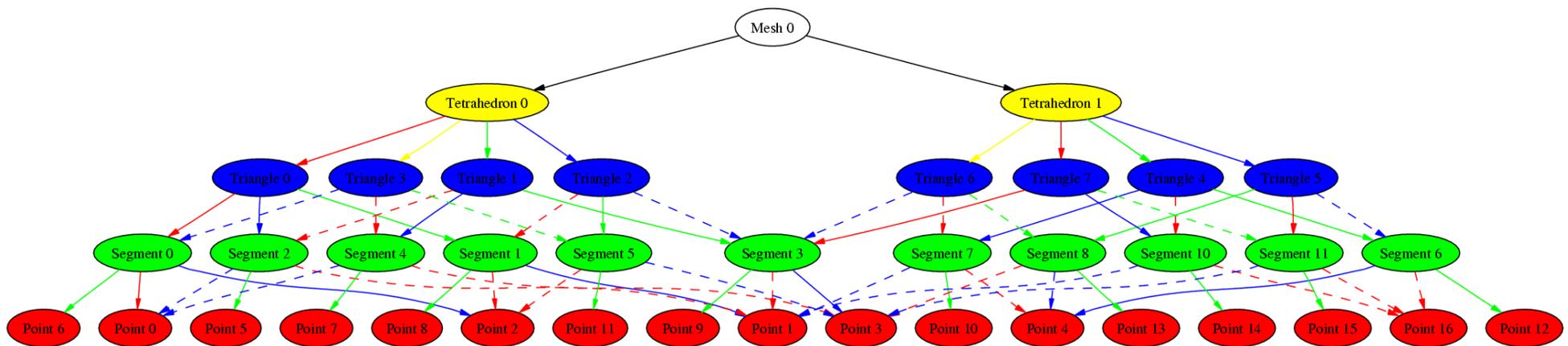
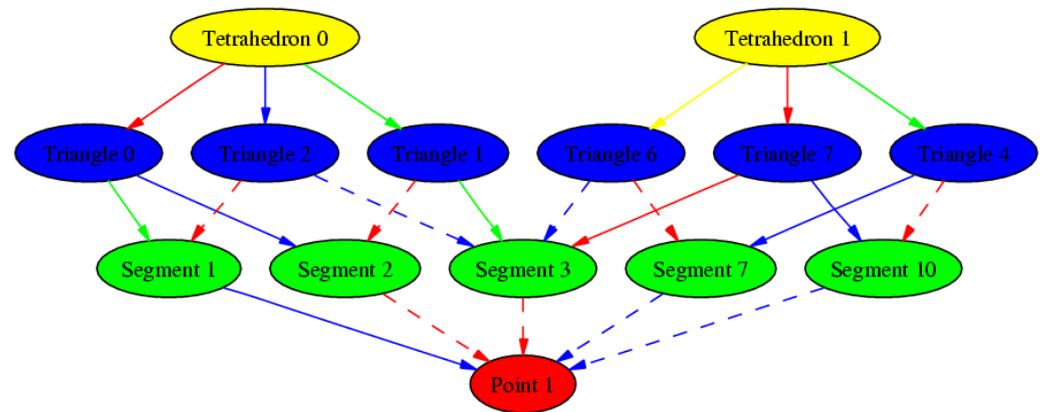
Both open segments for point 2 were split, its subgraph has 2 branches now.



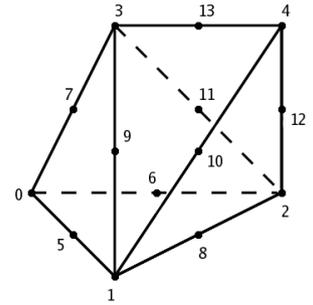
# Fracture Algorithm (6)



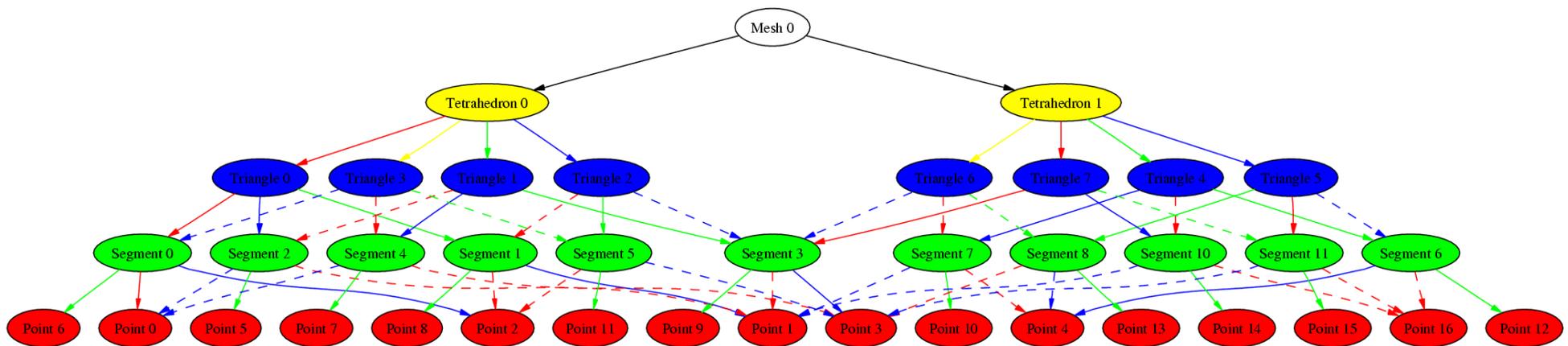
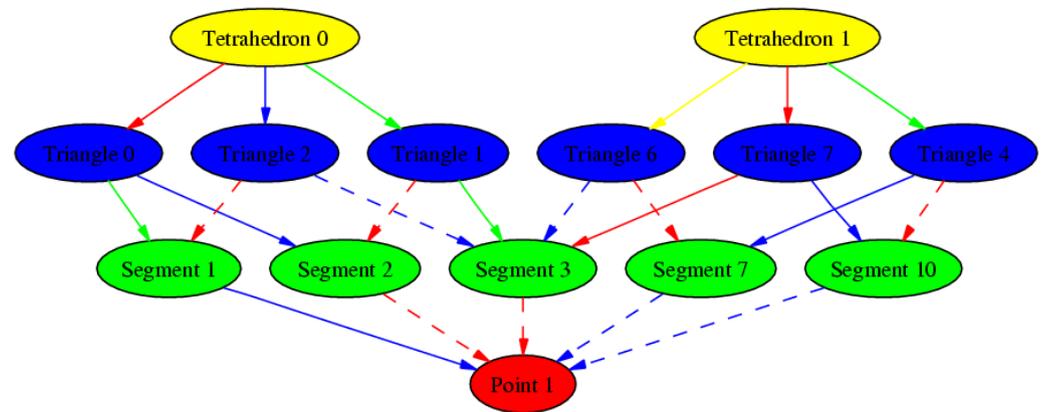
Next is point 1, with segment 3 the only remaining open segment.



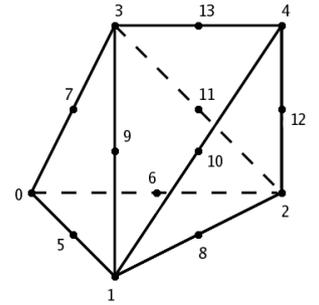
# Fracture Algorithm (6)



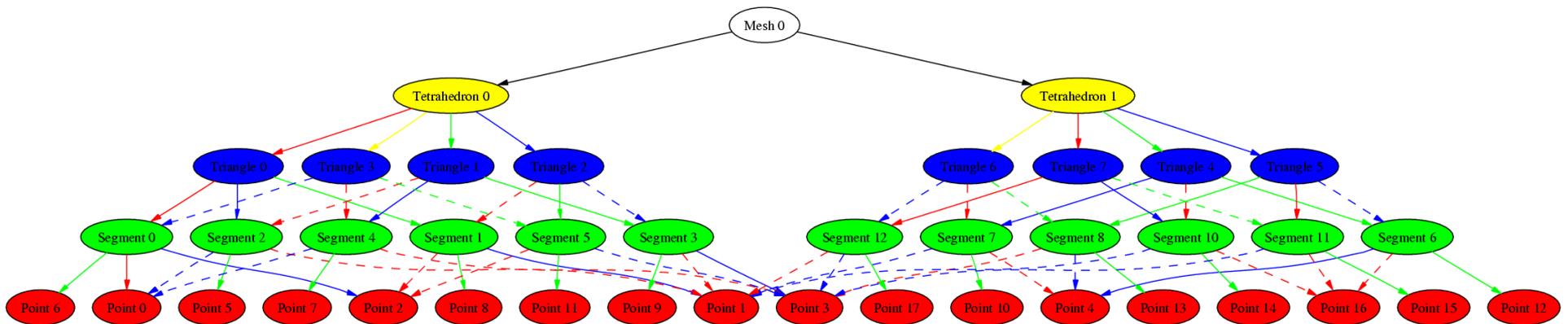
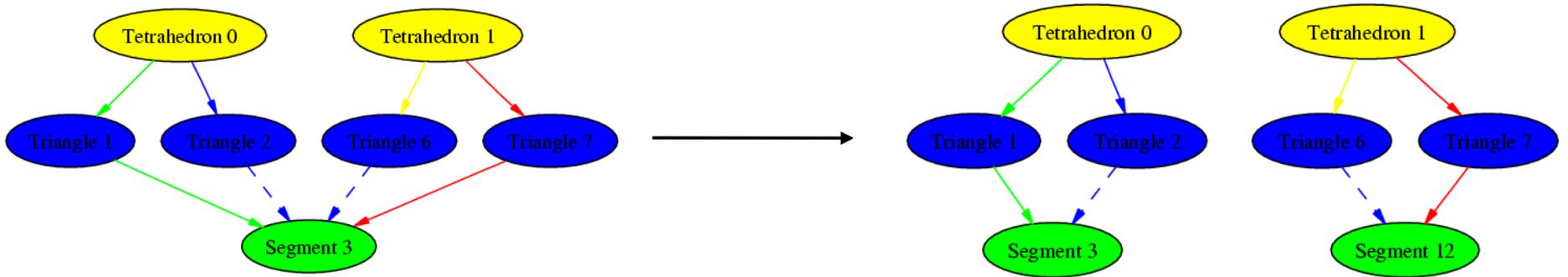
Next is point 1, with segment 3 the only remaining open segment.



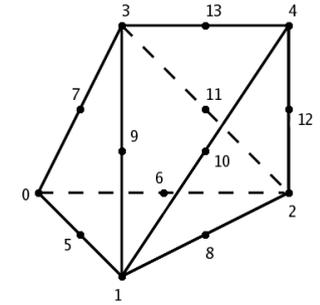
# Fracture Algorithm (7)



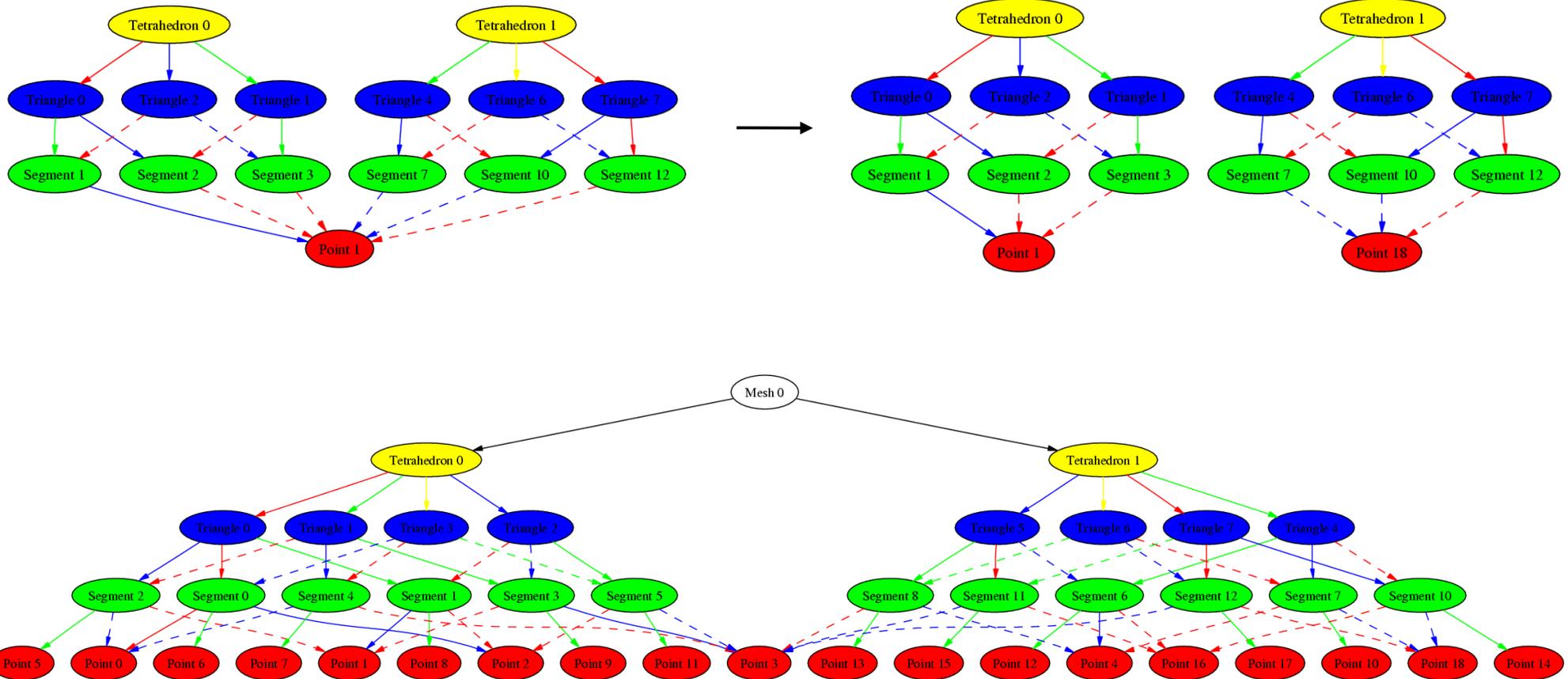
Segment 3 is split.

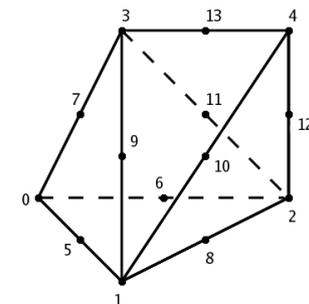


# Fracture Algorithm (8)



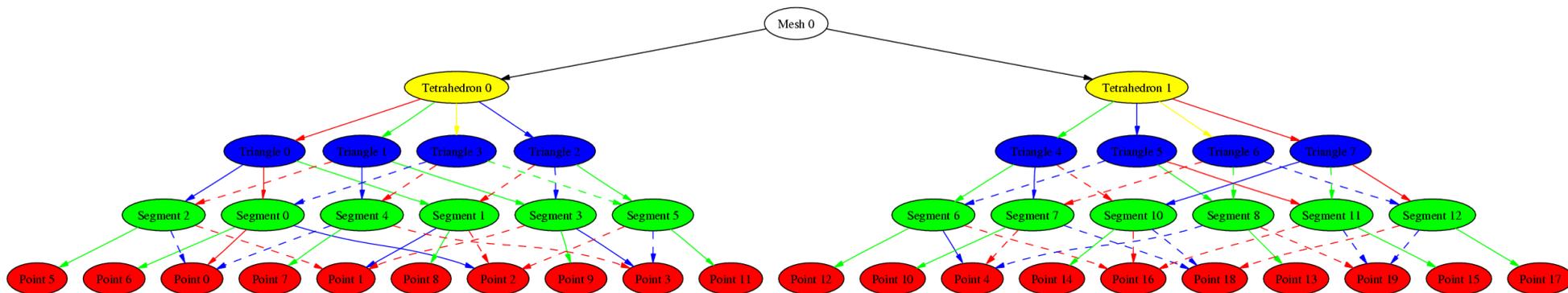
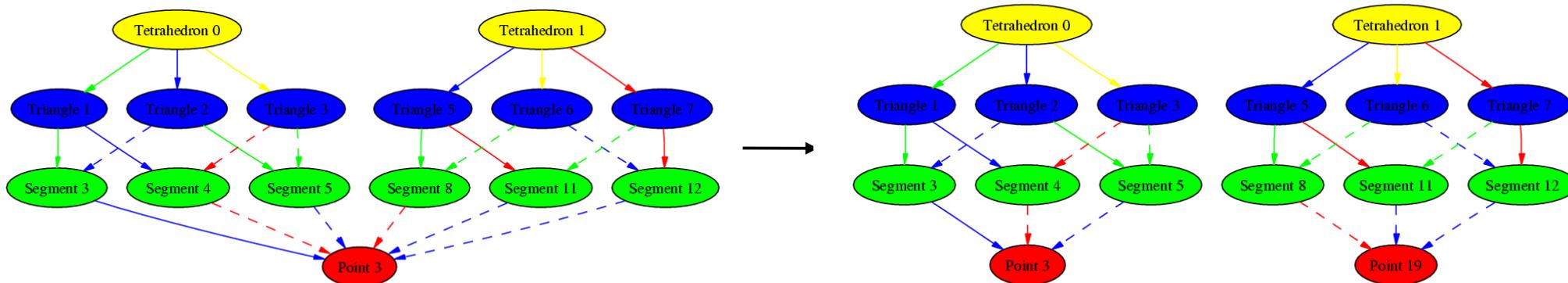
Point 1 is split.



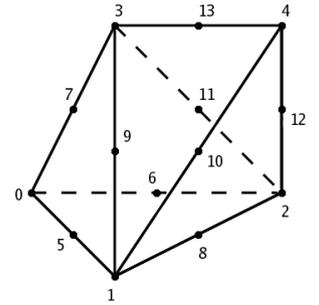


# Fracture Algorithm (9)

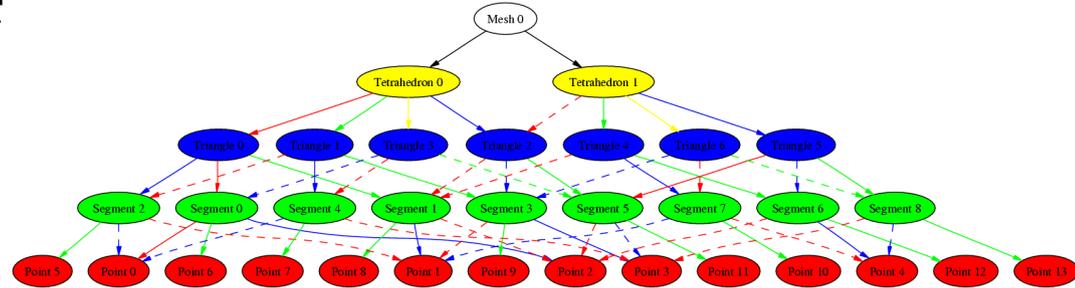
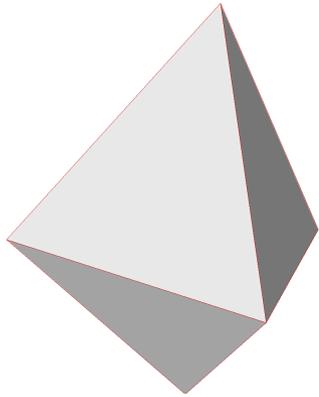
Finally point 3, with 0 open segments, is split, obtaining 2 separate tetrahedra.



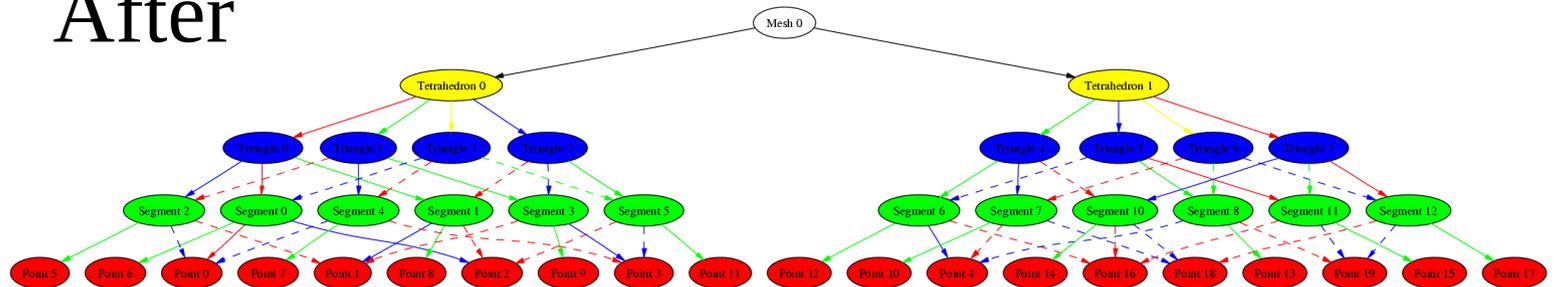
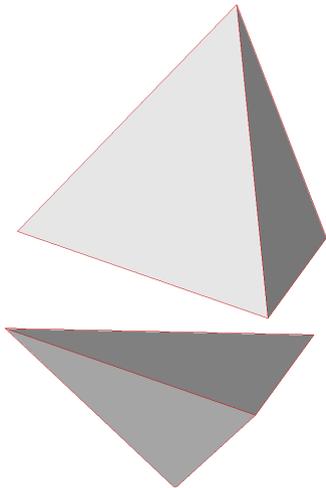
# Two-Tet Mesh and Graphs



Before

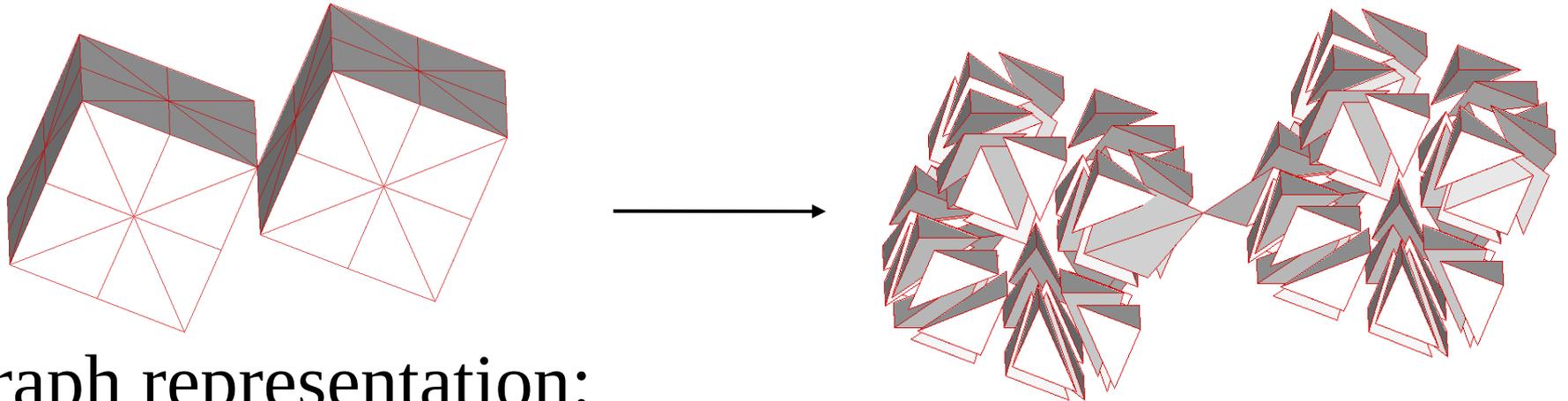


After

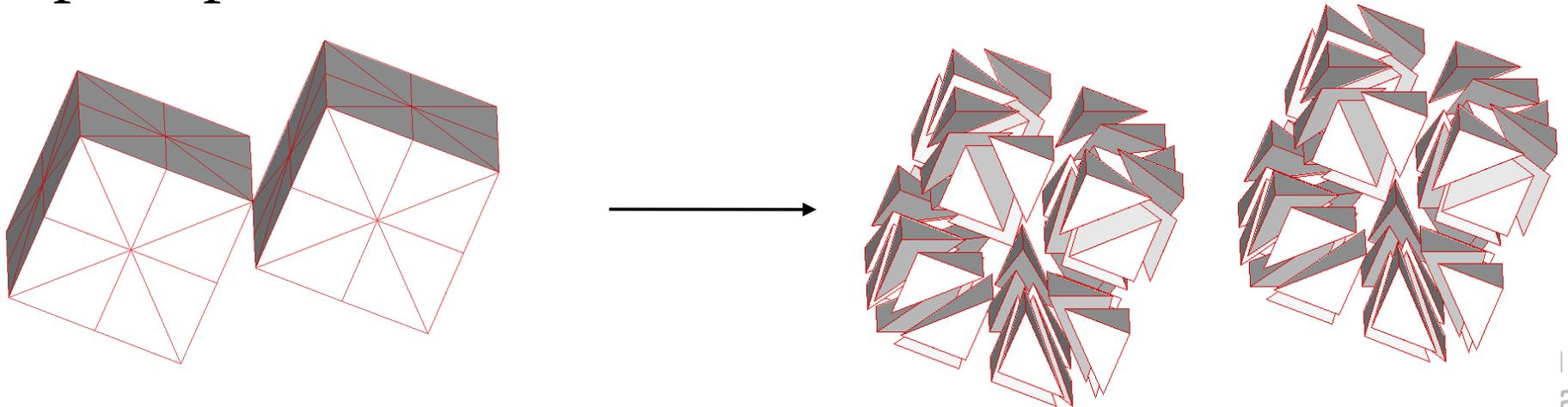


# Correctness – Point Cubes

Two cubes joined by a point. Fracture all internal triangles. Current algorithm:

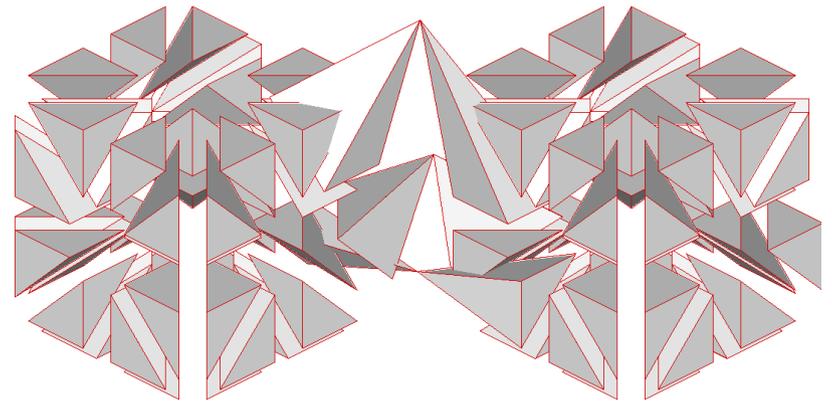
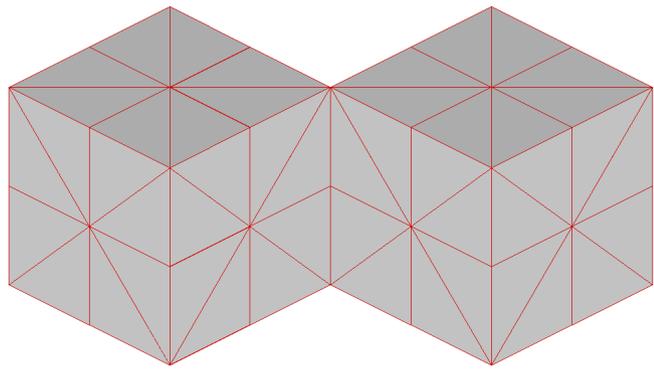


Graph representation:

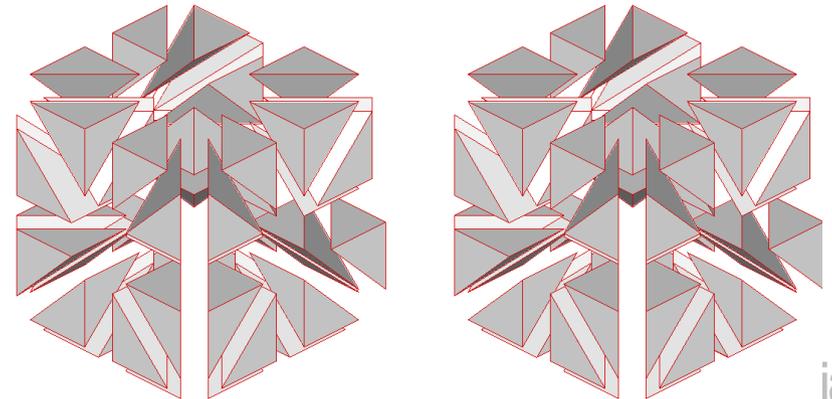
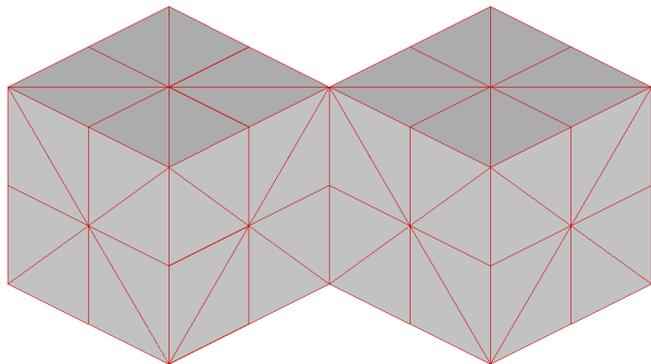


# Correctness – Edge Cubes

Two cubes joined by an edge. Fracture all internal triangles. Current algorithm:



Graph representation:



# Graph Fracture Properties

- Subgraphs greatly simplify fracture.
- Operations on subgraphs are mirrored on parent graph.
- Localized operations confined to subgraphs, essential for parallelization.
- Time complexity of initialization linear with number of elements.
- Time complexity of fracture linear with number of open simplices.

# Graph Fracture Properties (2)

- Non-manifold cases handled correctly.
- Significant reuse of code.
- Marking of open simplices is top-down.
- Building of subgraphs is bottom-up.
- Fracture is top-down.
- Works for both 2D and 3D.
- Recursive with each level in the graph.

# C++ Boost Graph Library

- Free peer-reviewed portable C++ source library.
- Works well with the C++ Standard Library.
- Generic, STL-like interface for manipulating and traversing graphs.
- Hides details of the graph data structure implementation.

# Performance Evaluation

- Reference fracture implementation is the one used in the ARES FE code.
- Tested 20 3D meshes of various sizes and geometries.
- Initialization time plotted as a function of the mesh size.
- Fracture time plotted as a function of triangles to fracture.

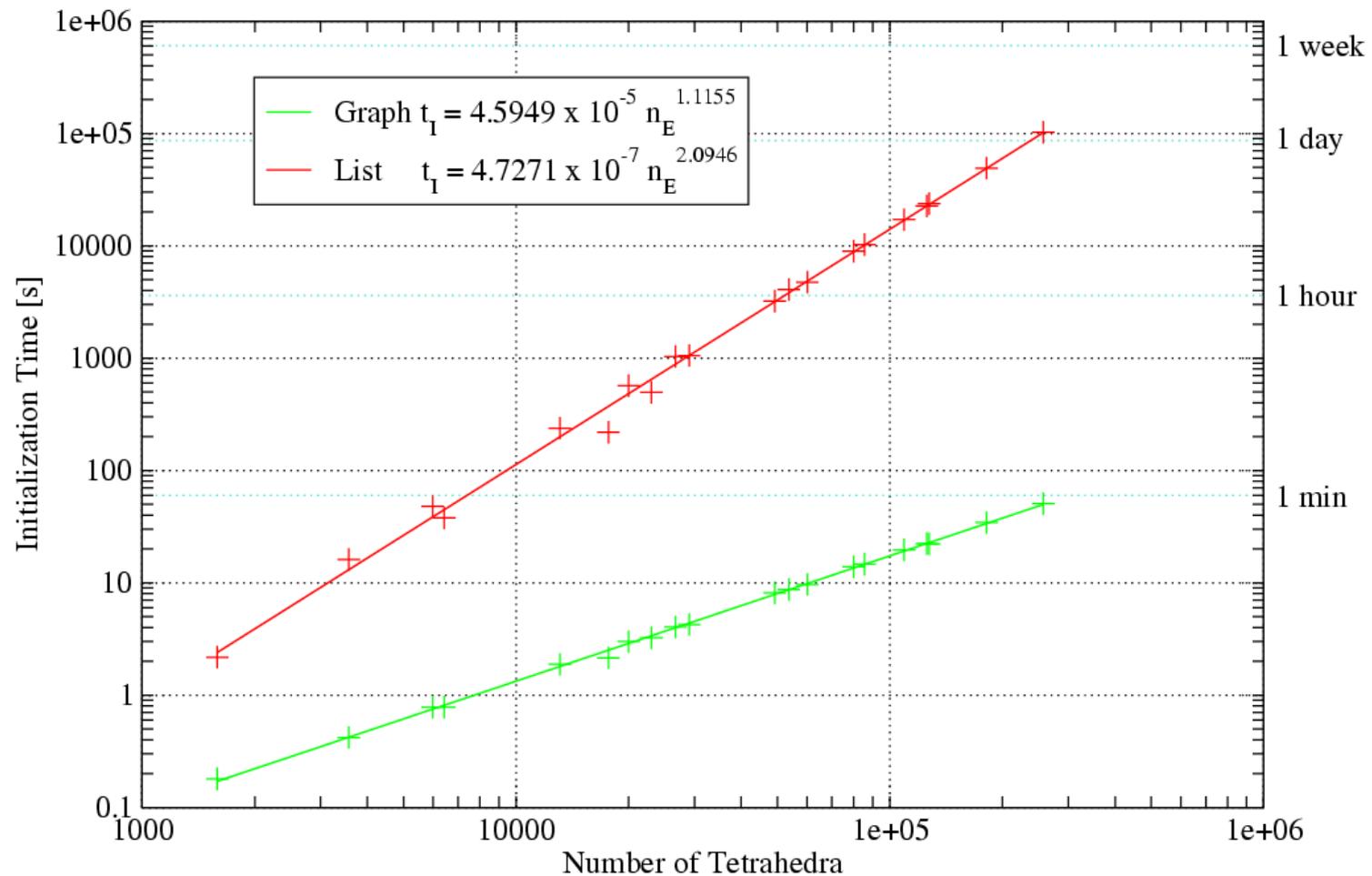
# Performance Evaluation (2)

- Improvements in C++ Boost library result in immediate performance gain.
- First implementation.
- Some performance tuning.
- No thorough profiling and extensive performance tuning yet.
- Tests performed using GCC on an Intel Xeon 1.5 GHz machine.

# Initialization Time

## Time Complexity of Initialization

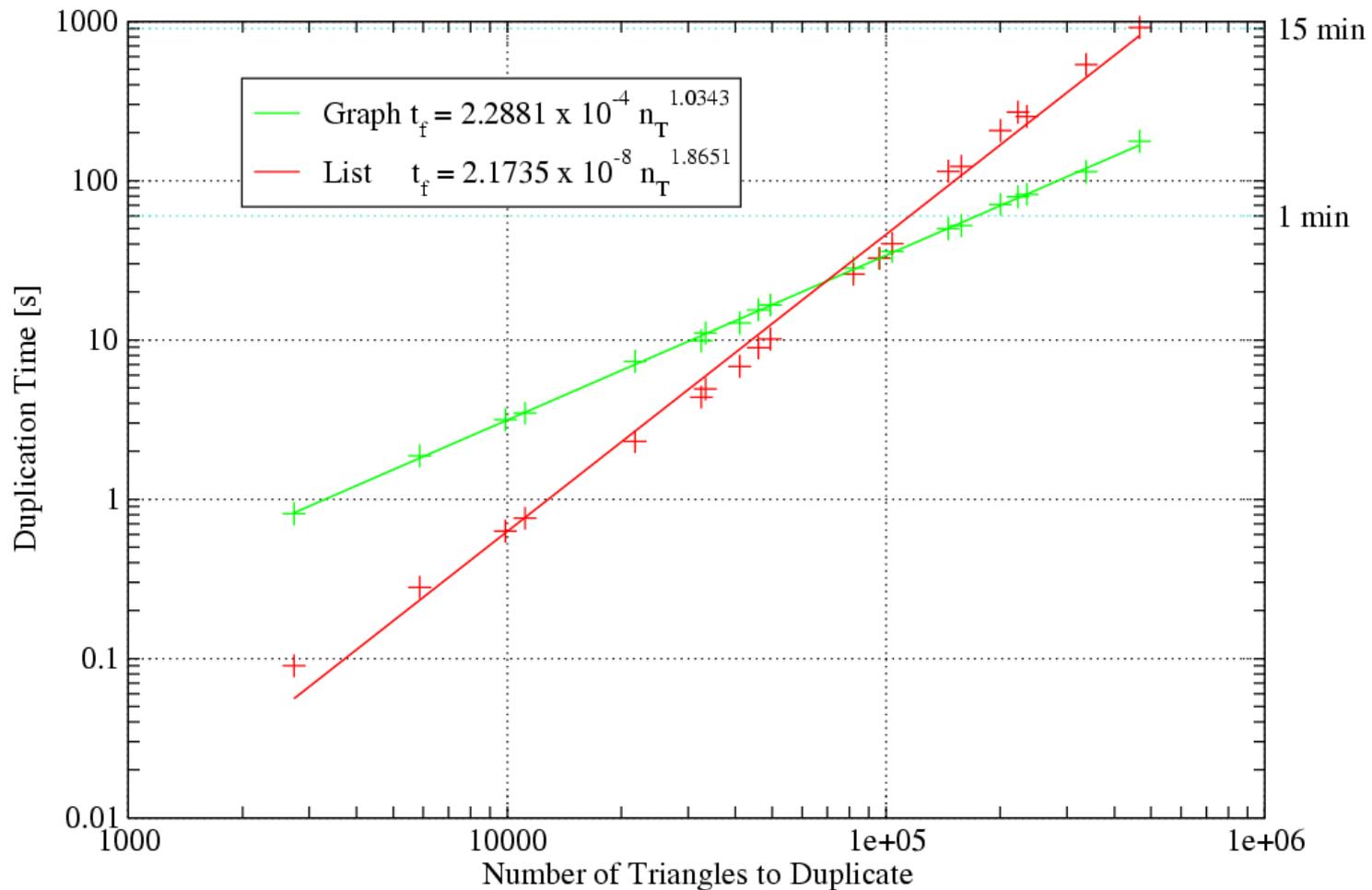
Comparison of 20 meshes



# Fracture Time

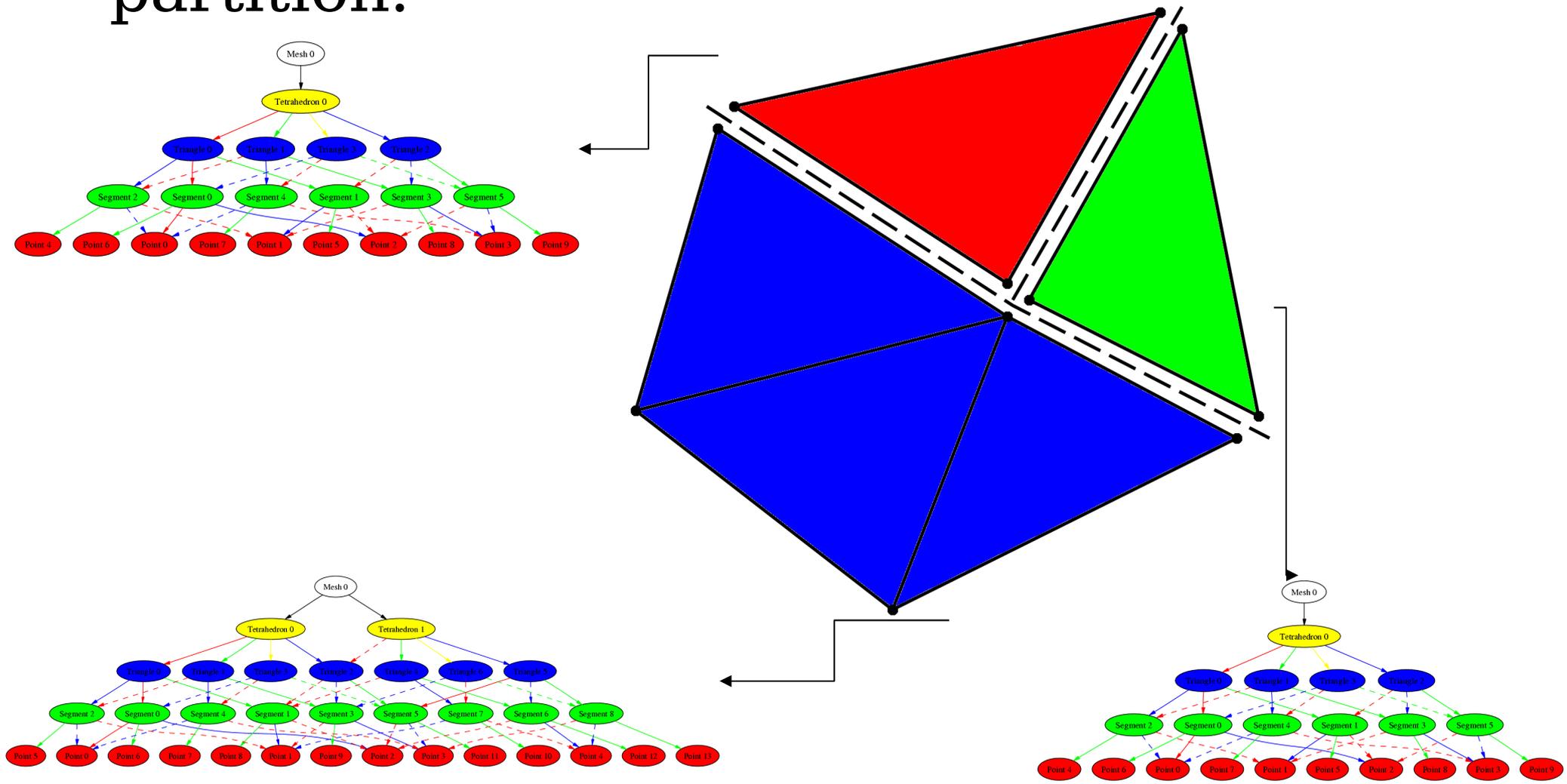
## Time Complexity of Fracture Algorithm

Comparison of 20 meshes



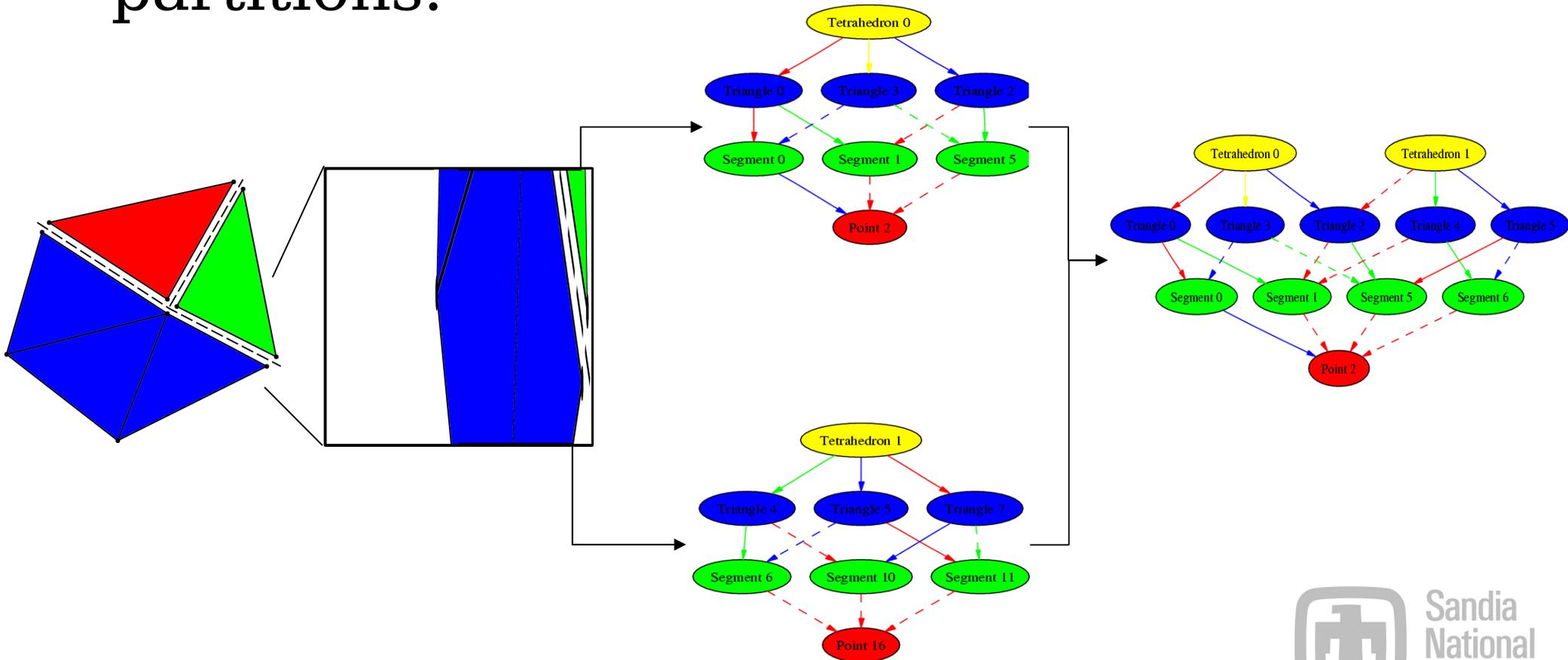
# 3D Graph Parallel Fracture

Partition mesh and create graph for each partition.



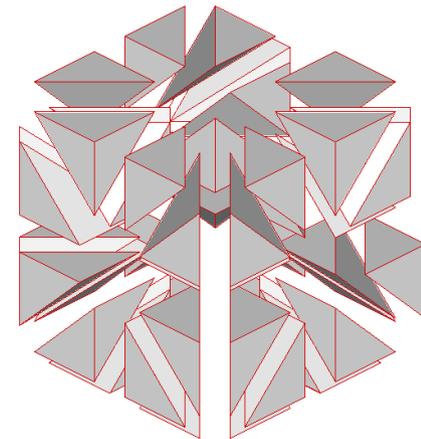
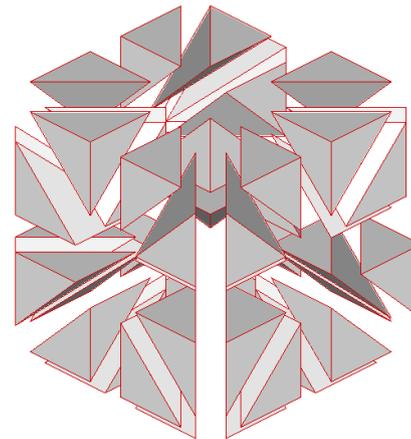
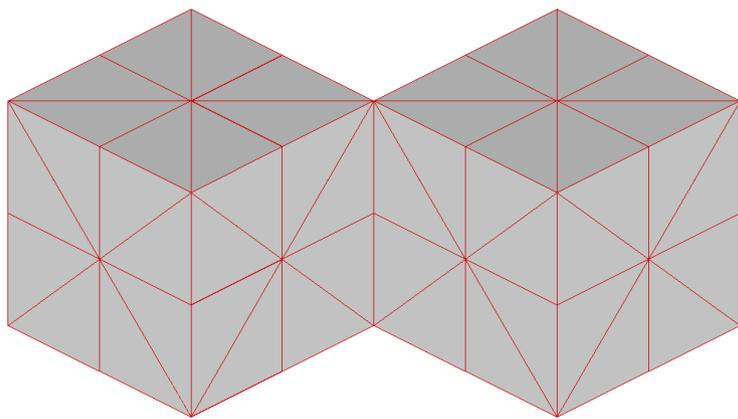
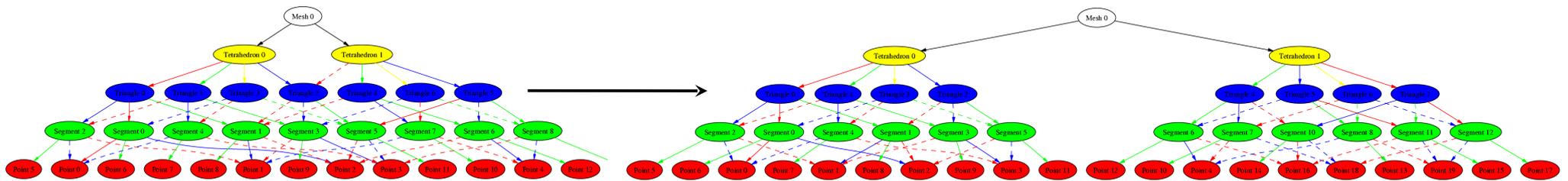
# 3D Graph Parallel Fracture

- On each fracture step mark open simplices.
- Partition-boundary points are missing parts of their subgraphs. Supplement from remote partitions.



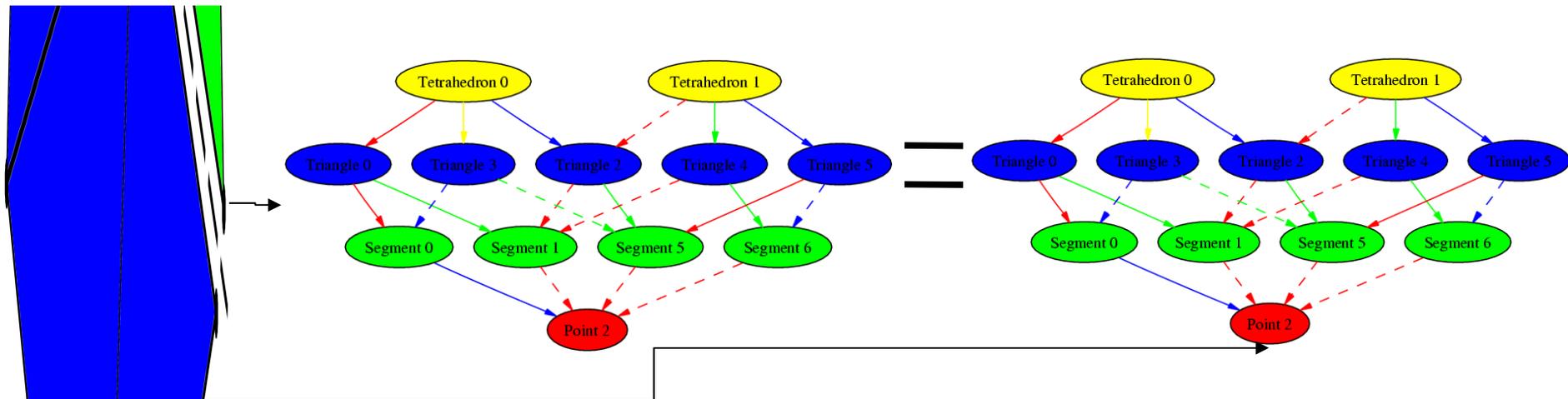
# 3D Graph Parallel Fracture

Apply serial fracture algorithm to each partition.



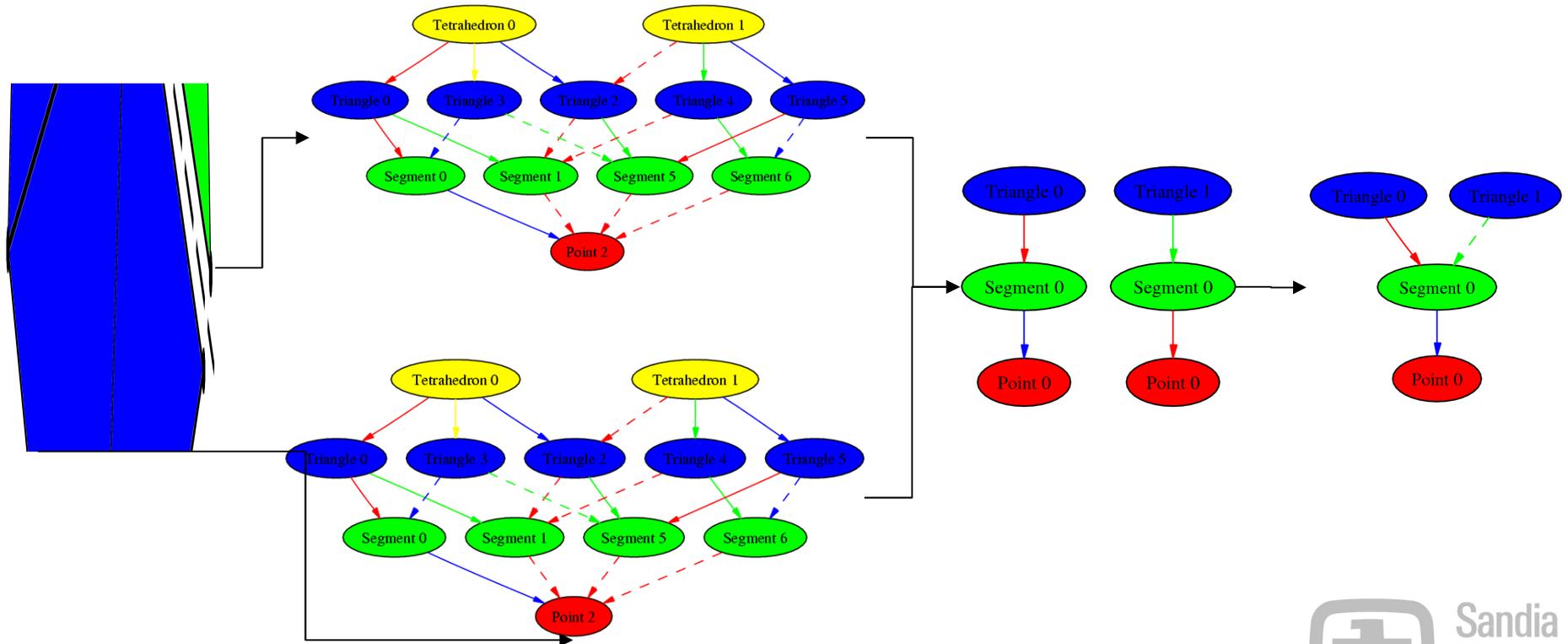
# 3D Graph Parallel Fracture

Subgraphs for partition-boundary points are in a consistent state across partition boundaries after serial fracture on each partition.



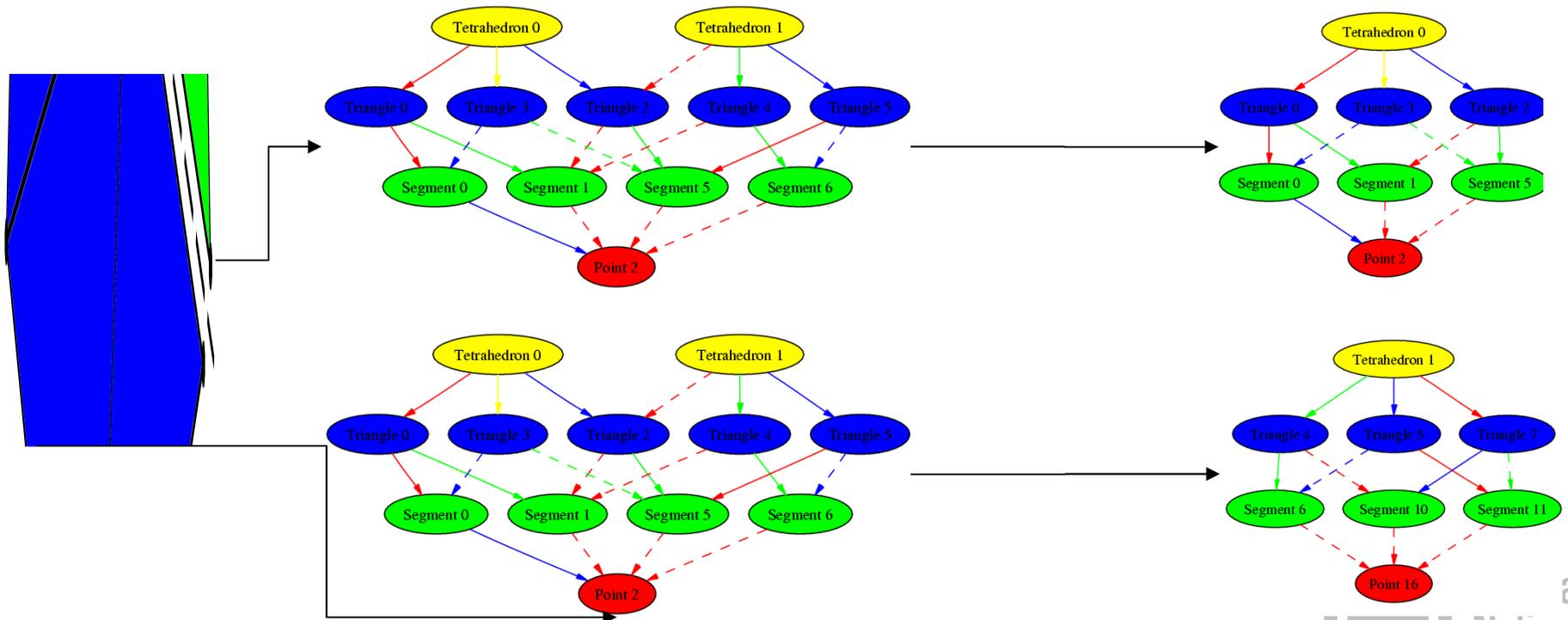
# 3D Graph Parallel Fracture

Exchange information between partition-boundary point subgraphs to identify and match newly created simplices across partition boundaries.



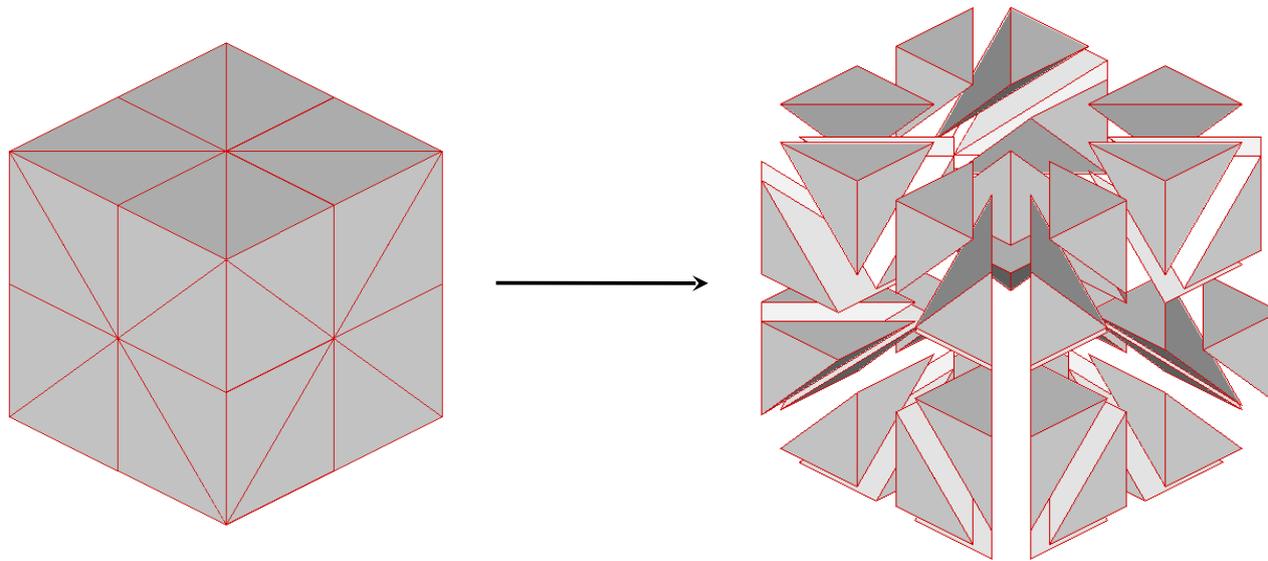
# 3D Graph Parallel Fracture

- Update boundary communicator.
- Discard the remote part of the graph for each partition and proceed with mechanics until next fracture step.



# Testing

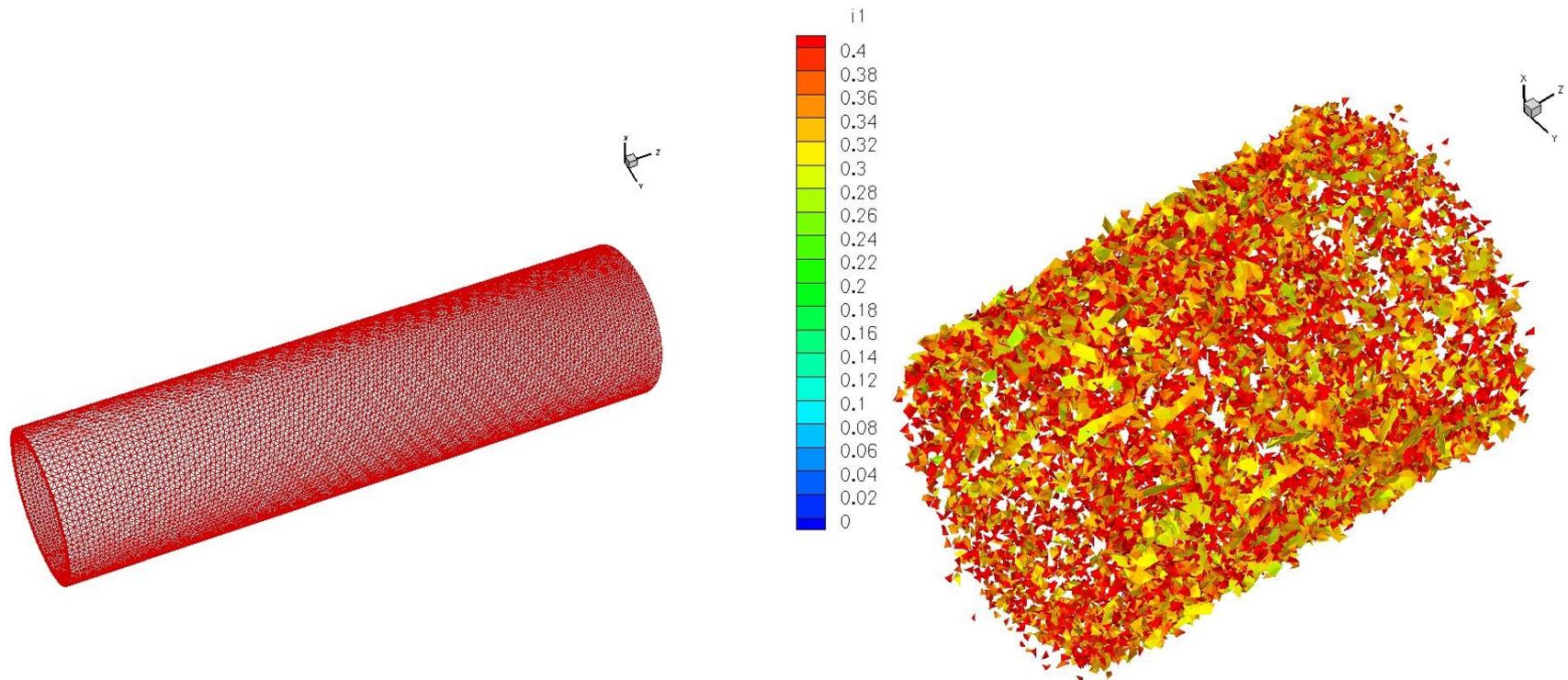
- Test on simple meshes yield the same results as serial fragmentation.
- The number of partitions is incremented until the partition algorithm (METIS) produces partitions with zero elements.



Cube example  
2 to 14 partitions

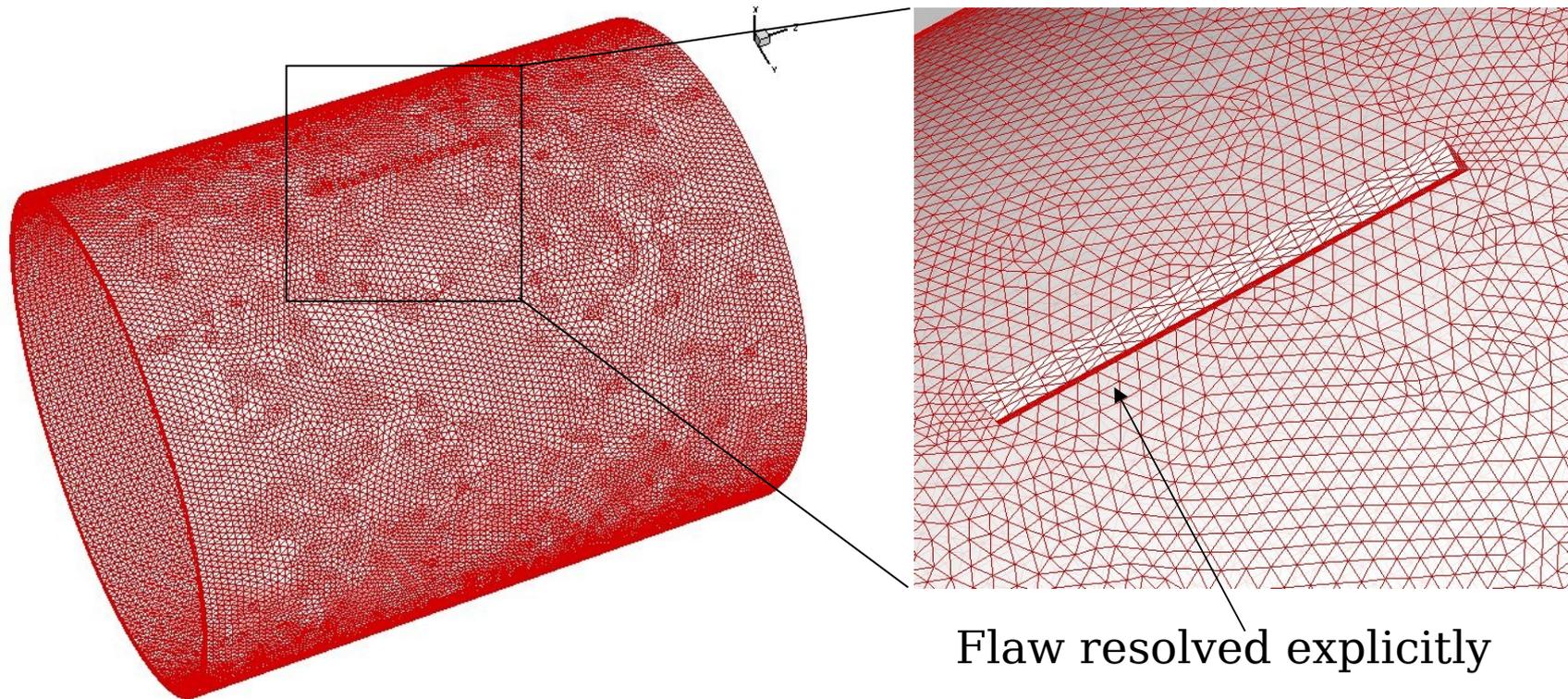
# Testing

- Test on simple meshes yield the same results as serial fragmentation.



Tube example  
2 to 8 partitions

# Coarse FE Mesh - Serial



Flaw resolved explicitly

Material model: Porous plasticity informed by QC

Interface model: Strain localization element

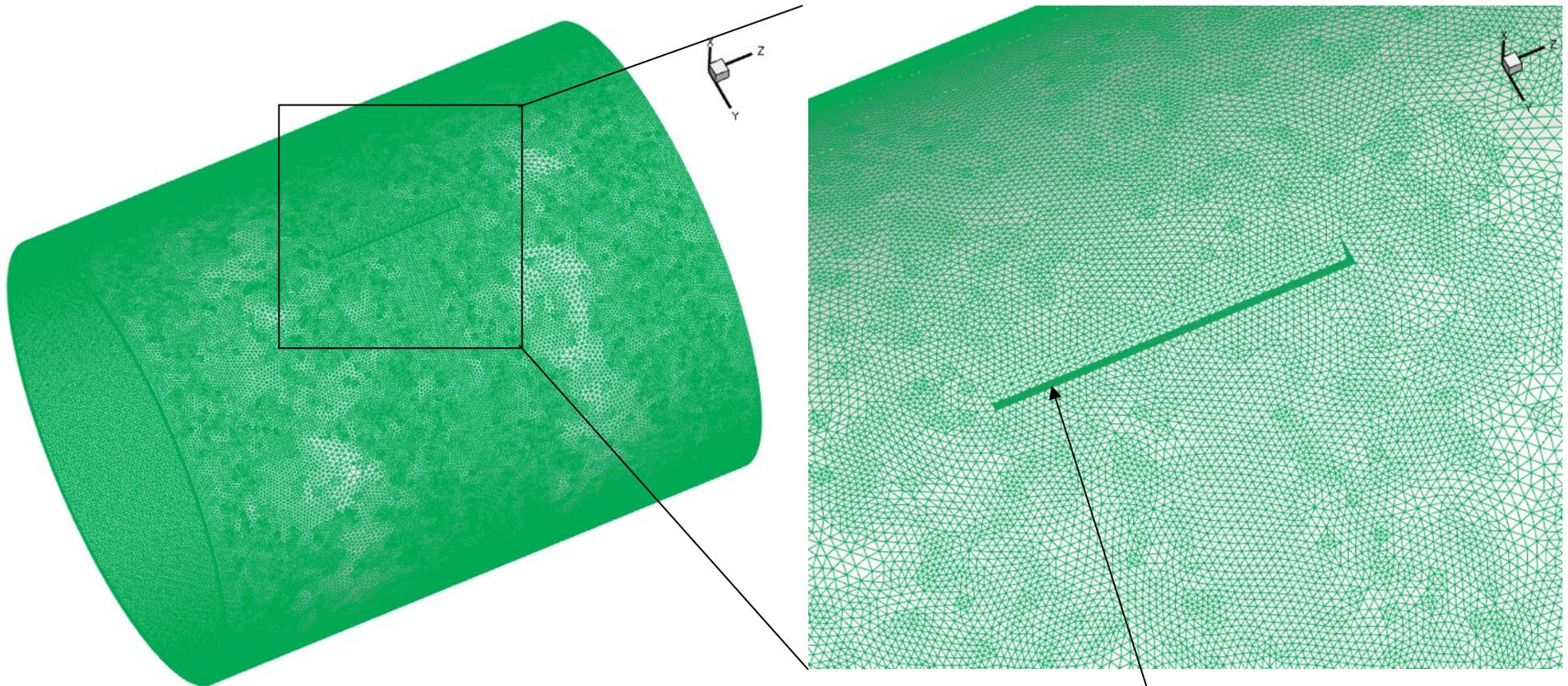
Failure criterion: critical plastic strain  $\sim 0.12$

Mesh: 39150 elements, 78850 nodes

Machine: Single-processor Linux PC,  $\sim 1$  week run time



# Fine FE Mesh - Parallel



Flaw resolved explicitly

Material model: Porous plasticity informed by QC

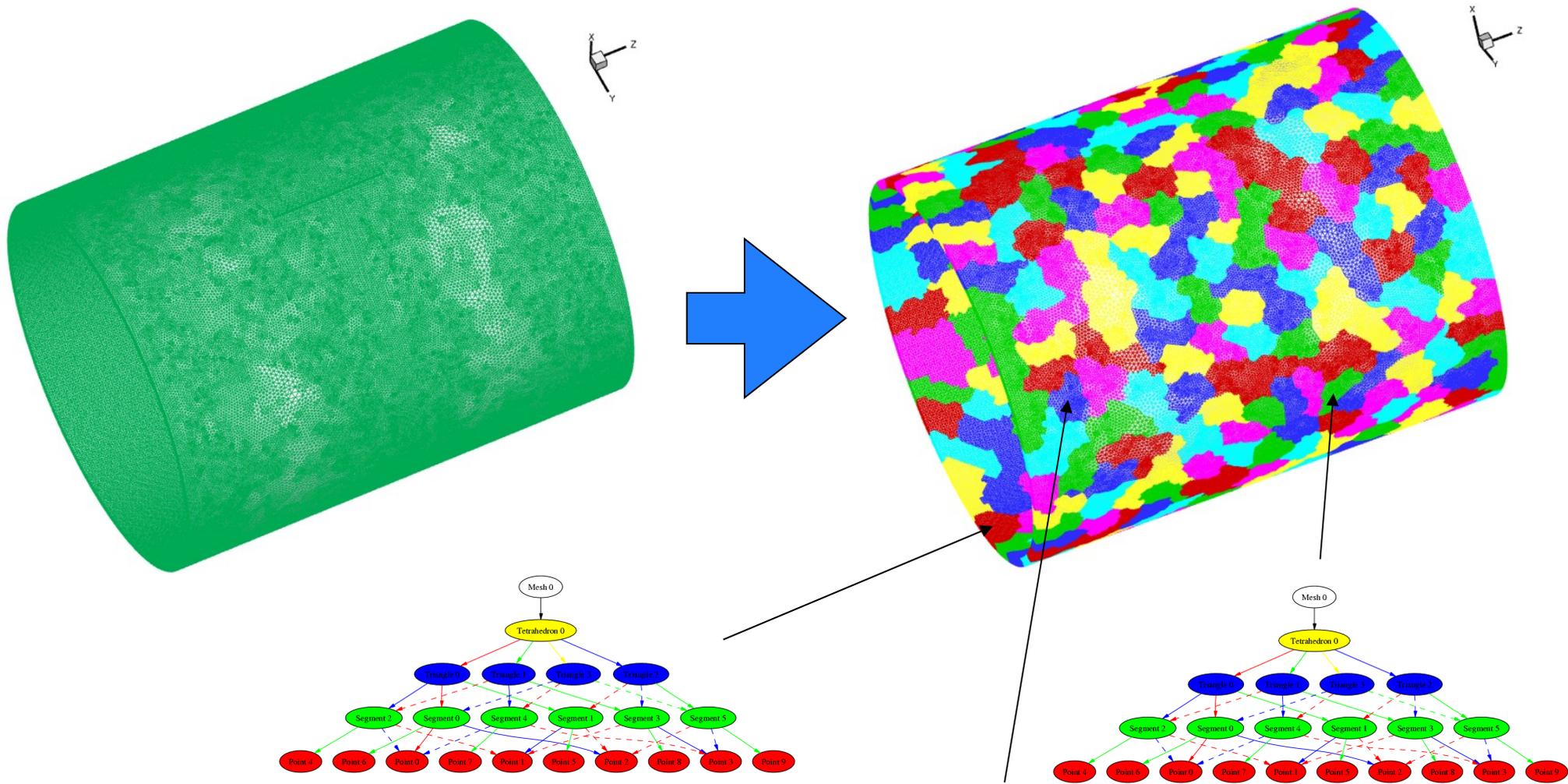
Interface model: Strain localization element

Failure criterion: critical plastic strain  $\sim 0.12$

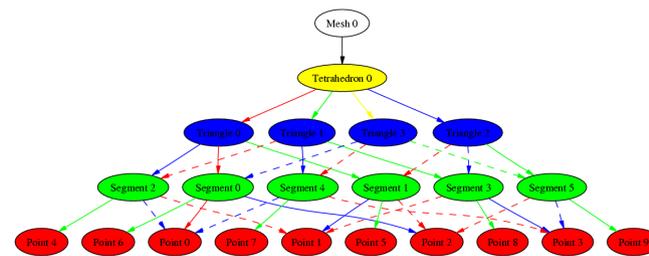
Mesh: 220945 elements, 399998 nodes

Machine: LLNL ALC, 400 processors, 8 hours run time

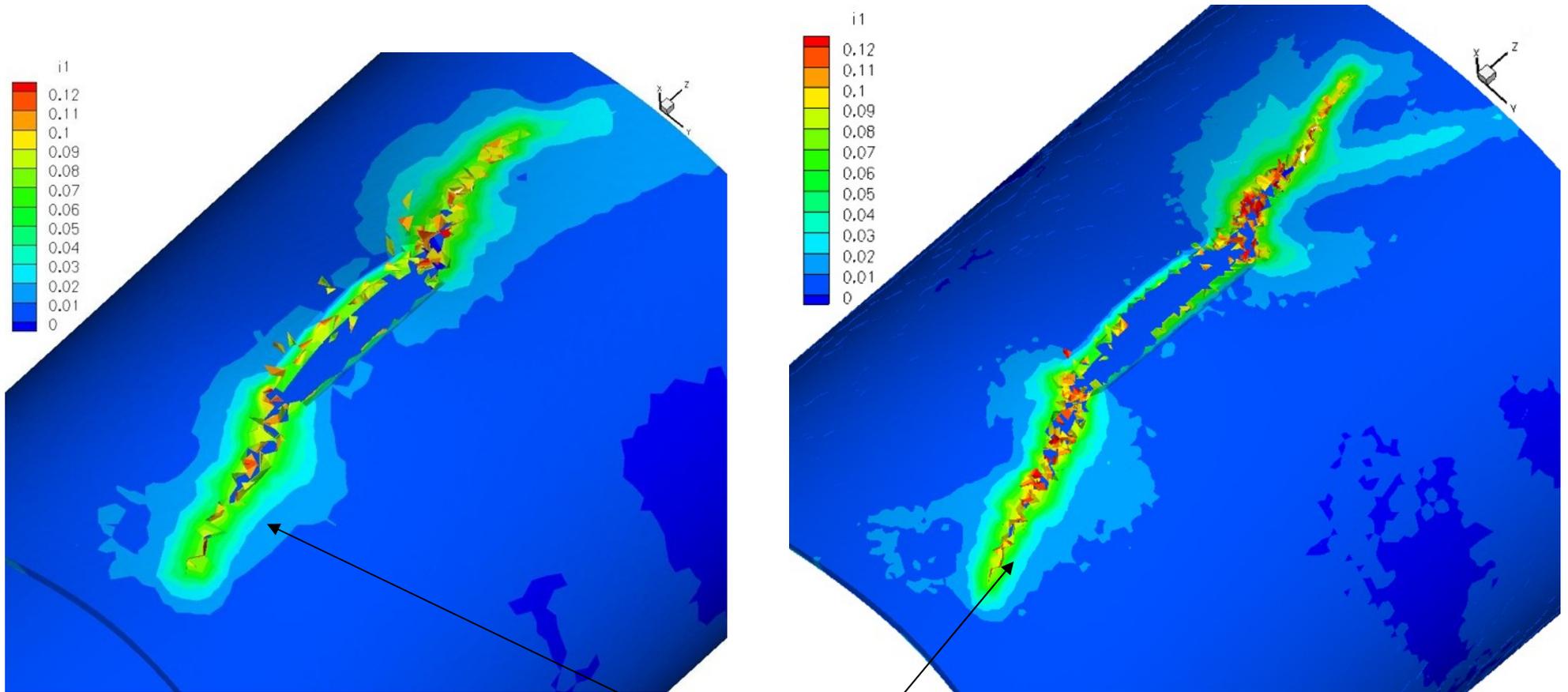
# 3D Graph Parallel Fracture



Partition mesh and create graph for each partition.



# Results: Coarse, Fine Meshes



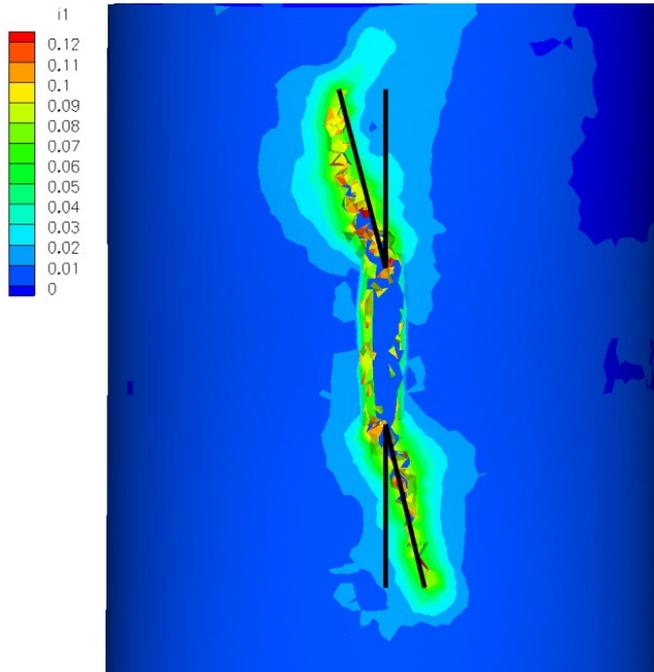
Coarse Mesh - Serial

Kinked cracks

Fine Mesh - Parallel

Configuration at  $75 \mu\text{s}$   
with initial torsion

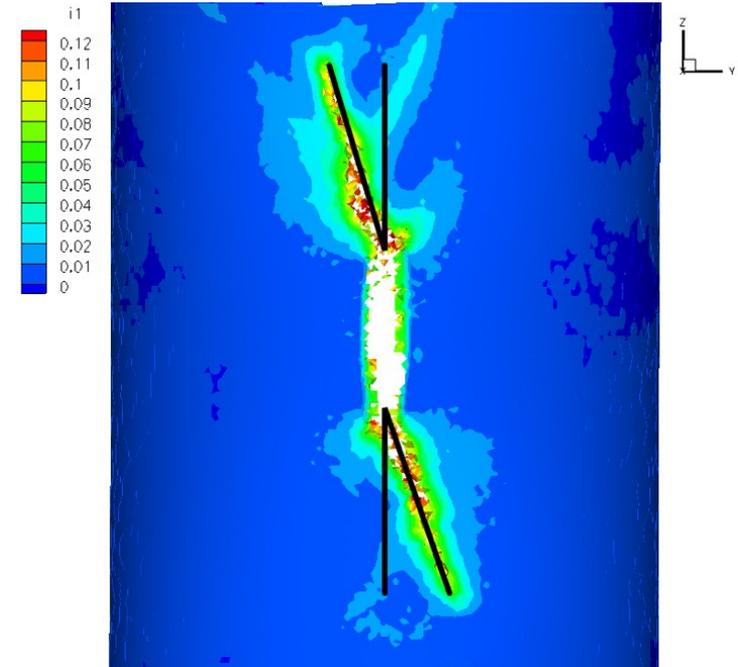
# Crack Angles



Serial simulation  
Peak pressure: 6.1 MPa  
Crack kink angle ~ 14 degrees

Peak pressure [MPa]	Crack angle [degrees]
6.1	7
5.1	13
4.1	38
3.3	50

Experimental results  
(Chao and Shepherd, 2004)



Parallel simulation  
Peak pressure: 6.1 MPa  
Crack kink angle ~ 16 degrees

# Conclusions

- Graphs allow fracture by simple, repetitive operations.
- The use of the Boost library reduced the work load significantly.
- Localized fracture operations suitable for parallel implementation.
- Time complexity reduced practically from quadratic to linear.
- Non-manifold cases handled correctly.



# Future Work

- Extend graph representation for CW complexes.
- Run very large fracture problems.
- Reuse graph mesh representation for serial and parallel contact.
- Replace connectivity arrays and use the graph for all FE computations.
- Mesh subdivision.