Parallel Wave Propagation and Topological Operators for Fragmentation Simulation

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Acknowledgments

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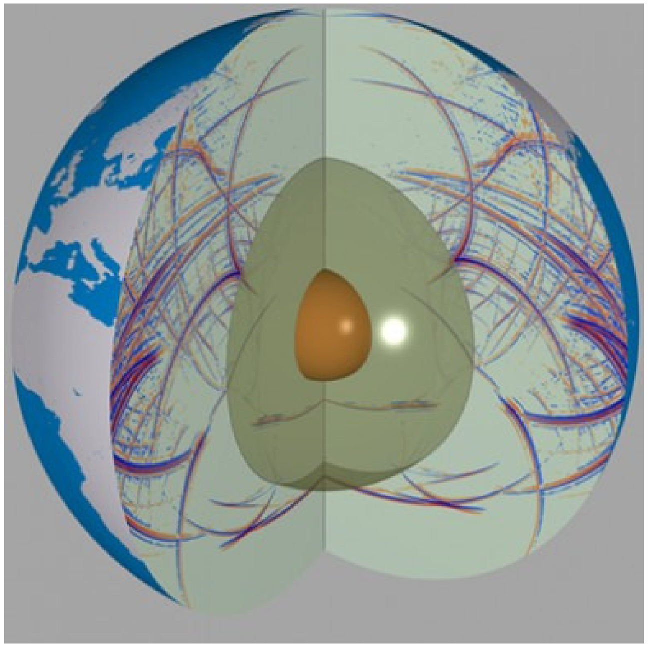
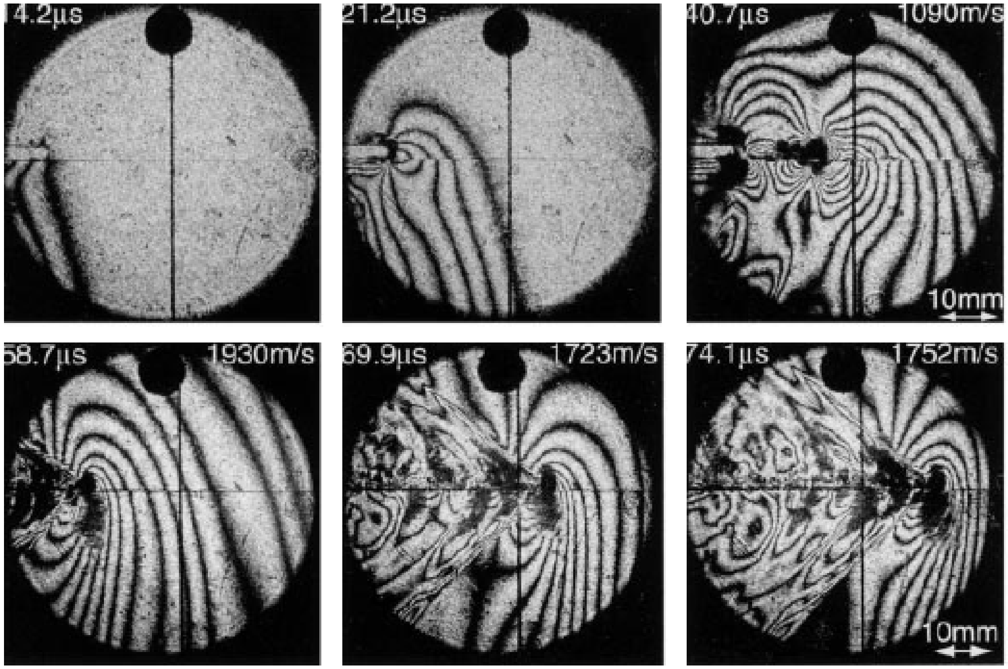
- Mr. Rodrigo Espinha (PUC-Rio)

Waves

Stress waves





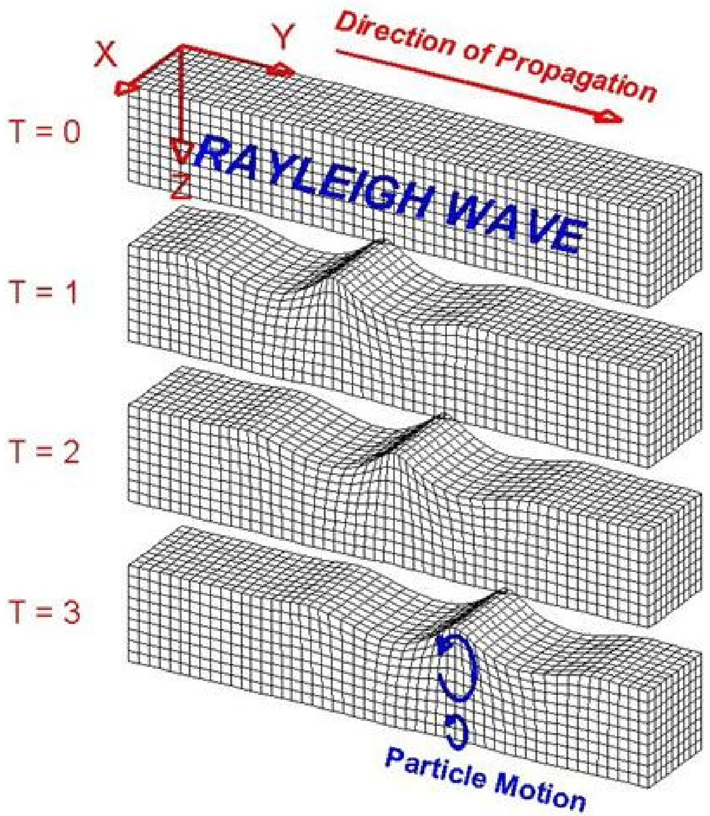
Rosakis AJ, Samudrala O, Coker D, 1999, Science 284

Outline

- Waves
- **Wave Propagation**
  - Rayleigh wave
  - Parallel computing: ParFUM
  - Results: Geological simulation
- Dynamic Fracture
  - Cohesive zone modeling
  - Node Perturbation & Edge-Swap Operation
  - Results: Fracture & Compact compression tests
- Summary
- Future Work

Wave Propagation: Rayleigh Wave

- Surface Wave
- Lord Rayleigh, 1885
- Seismology, Geology, Material Science, etc
- Homogeneous & Orthotropic materials (2005)
- Large-Scale 3D Analysis for Graded media



• Rayleigh L. 1885, On waves propagated along the plane surface of an elastic solid, Proc. R. Soc. Lond. A 17, 4-11

• Vinh PC, Ogden RW. 2005, On the Rayleigh wave speed in orthotropic elastic solids, Meccanica 40, 147-161.

Parallel Computing: ParFUM

Lawler OS, Chakravorty S, Wilmarth TL, Choudhury N, Dooley I, Zheng G, Kale LV, 2006, ParFUM: a parallel framework for unstructured meshes for scalable dynamic physics applications, *Engineering with Computers* 22, 215-235.

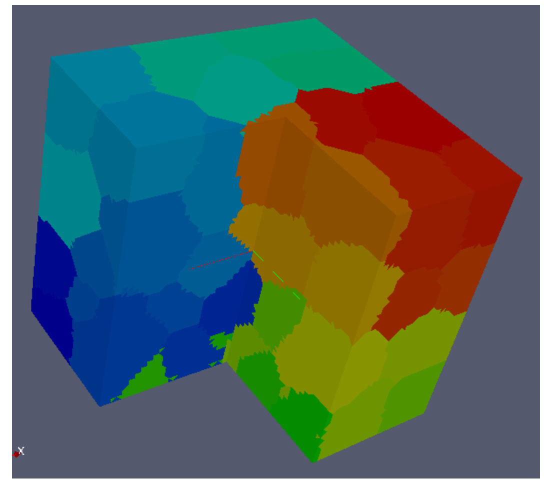
- **Finite Element Analysis**
- **Bill Gropp: Very "Easy to write code that scales and performs poorly."**
- **Time Integration**
  - Central difference method

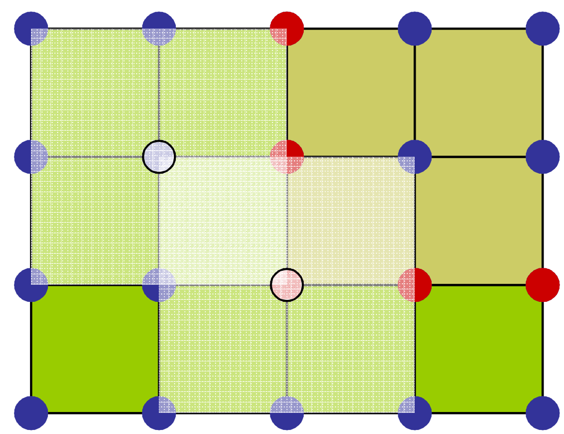
$$\mathbf{u}_{n+1} = \mathbf{u}_n + \Delta t \dot{\mathbf{u}}_n + \frac{1}{2}\Delta t^2 \ddot{\mathbf{u}}_n$$

$$\ddot{\mathbf{u}}_{n+1} = \mathbf{M}^{-1}(\mathbf{R}^{ext}_{n+1} - \mathbf{R}^{int}_{n+1})$$

$$\dot{\mathbf{u}}_{n+1} = \dot{\mathbf{u}}_n + \frac{\Delta t}{2}(\ddot{\mathbf{u}}_n + \ddot{\mathbf{u}}_{n+1})$$

- **Communications**
  - Update $\mathbf{R}^{int}$
  - Shared-node summation operation





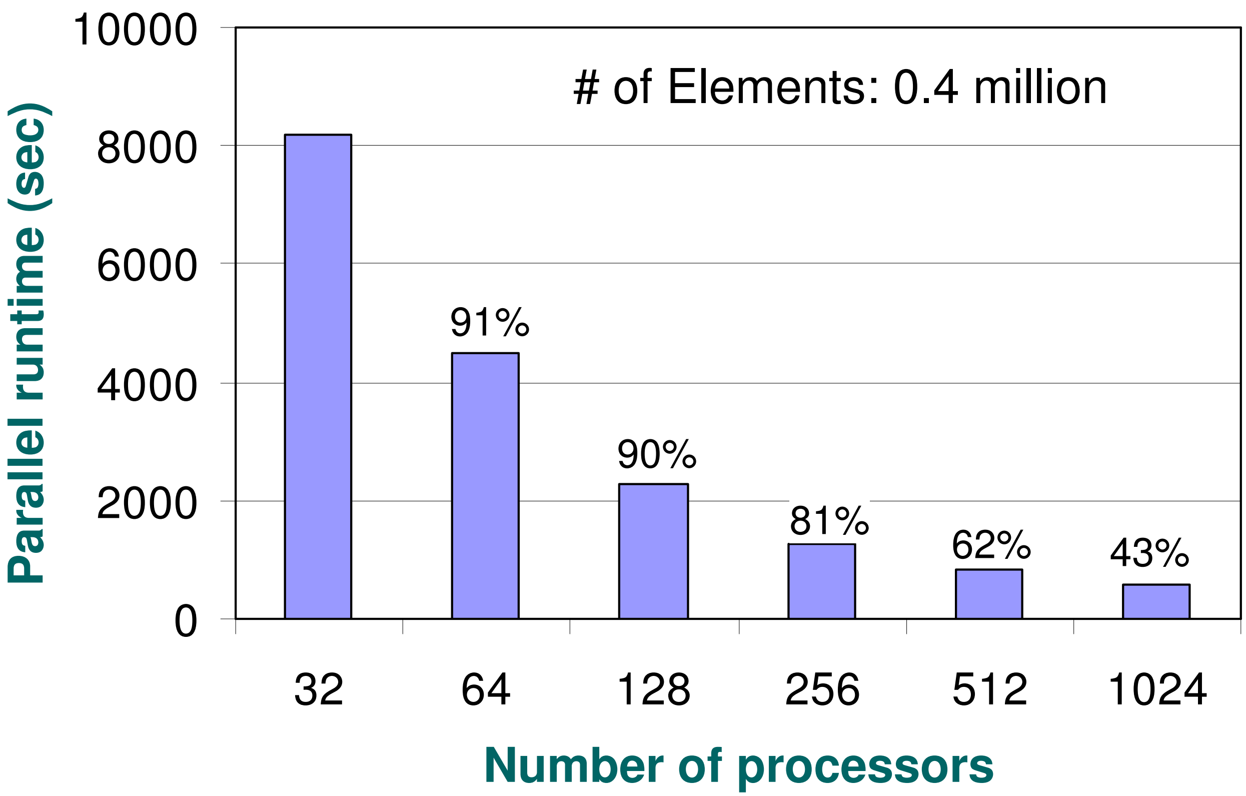
Machine Specification

- **Dell Cluster [Abe]**
  - Peak FLOPS: 89.47 TF
  - Number of Blades (nodes): 1200
  - Number of CPUs (cores): 9600
  - Processor: Intel 64 2.33GHz dual socket quad core
  - 8 MB L2 cache (2 MB)
  - Memory: 8GB (1GB) → Total: 9600 GB

- **Dell Xeon Cluster [Tungsten]**
  - Peak FLOPS: 16.38 TF
  - Number of nodes: 1280
  - Number of processors: 2560
  - Processor: Intel Xeon 3.2 GHz (32-bit)
  - Memory: 1.5 GB → Total: 3840 GB

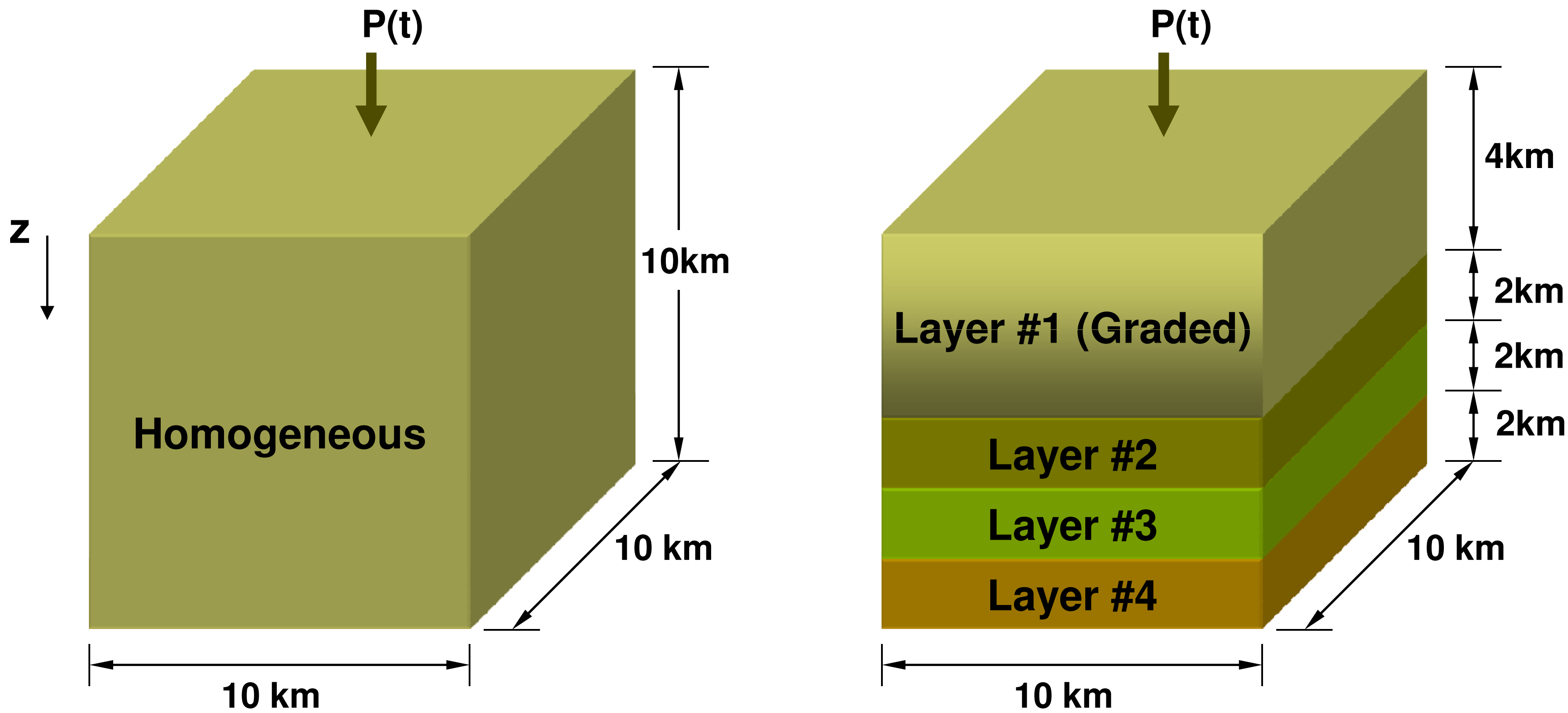
Runtime Performance

- Dell Cluster [Abe]



Geology Simulation: Rayleigh Wave

$$P(t) = \sin(2\pi t) \qquad (0 \le t \le 2)$$
$$P(t) = 0 \qquad (t > 2)$$

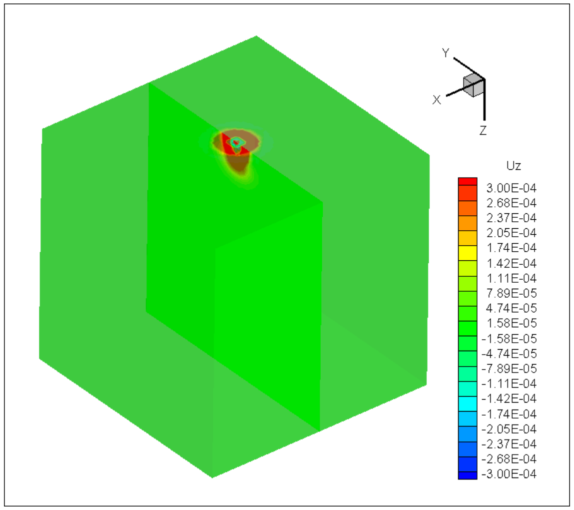


V. Pereyra, E. Richardson, S. E. Zarantonello, Large scale calculations of 3D elastic wave propagation in a complex geology, Proceedings of the 1992 ACM/IEEE conference on Supercomputing, Minneapolis, Minnesota, 301-309.

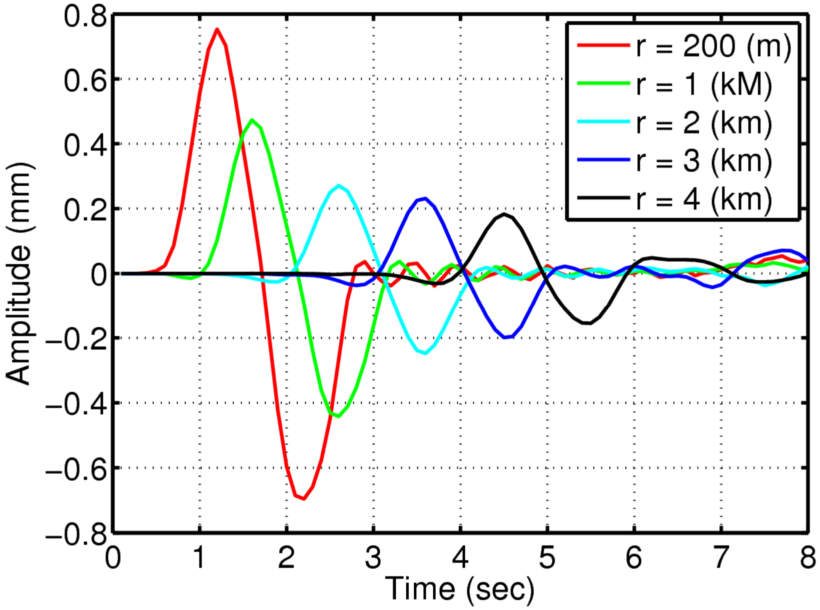
Homogeneous Media

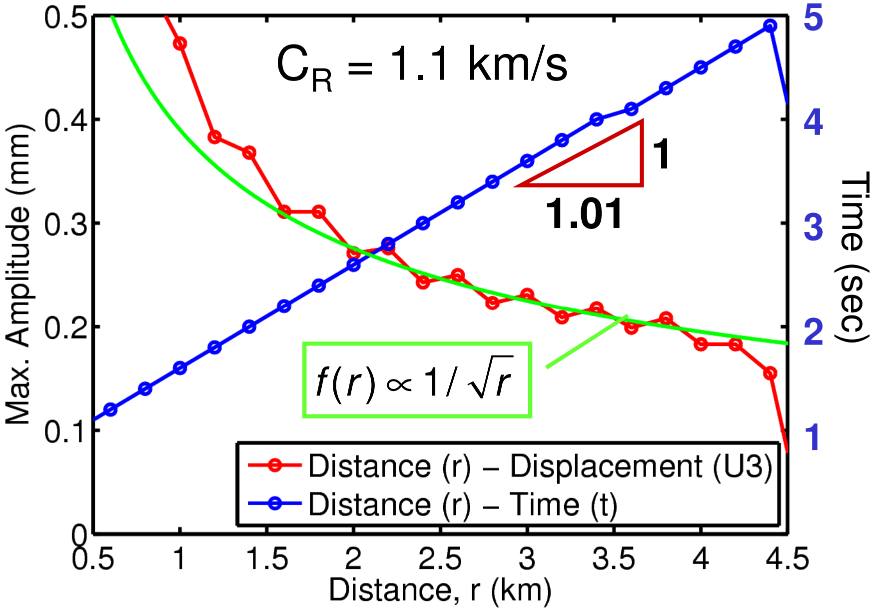
Material Properties

	C_P (km/s)	C_S (km/s)	ρ (kg/m³)	E (MPa)	v
Media	2	1.2	2	7.02	0.219



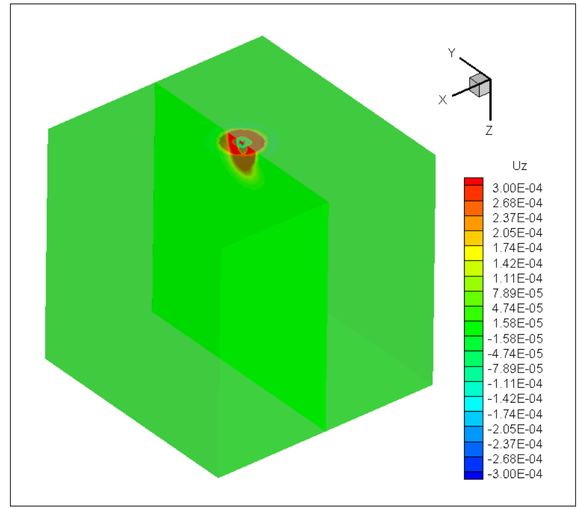
Dynamic Responses

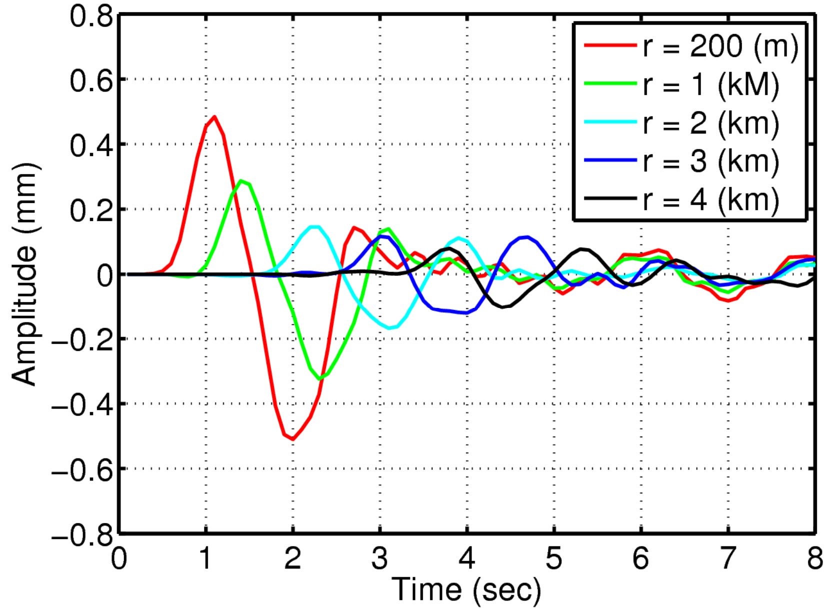


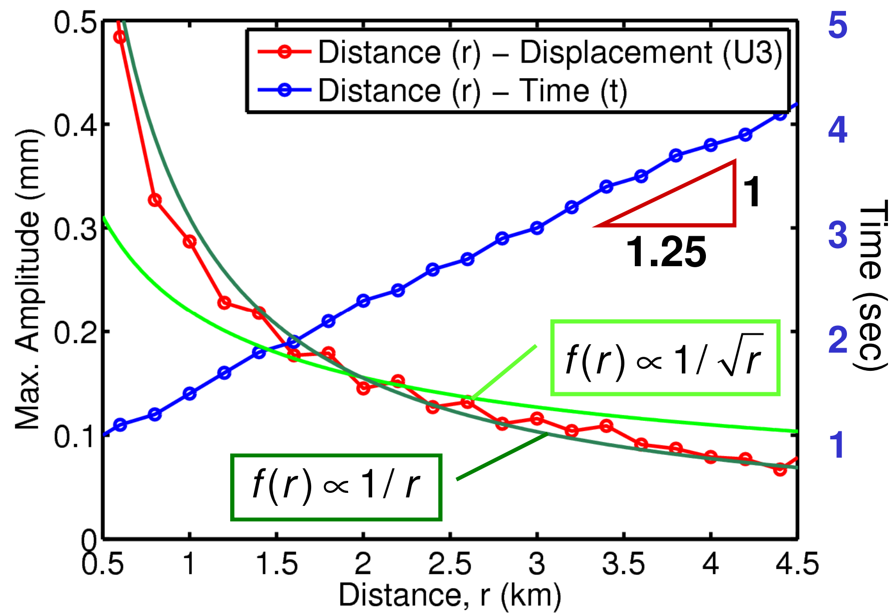


Graded & Layered Media

	C_P (km/s)	C_S (km/s)	ρ (kg/m³)	E (MPa)	ν
Graded Layer #1	2 3.6	1.2 2.16	2 3.6	7.02 40.94	0.219 0.219
Layer #2	3.5	2.1	2.3	24.7	0.336
Layer #3	4.5	2.1	2.3	27.6	0.361
Layer #4	5.5	2.1	2.3	28.7	0.430







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  - Parallel computing: ParFUM
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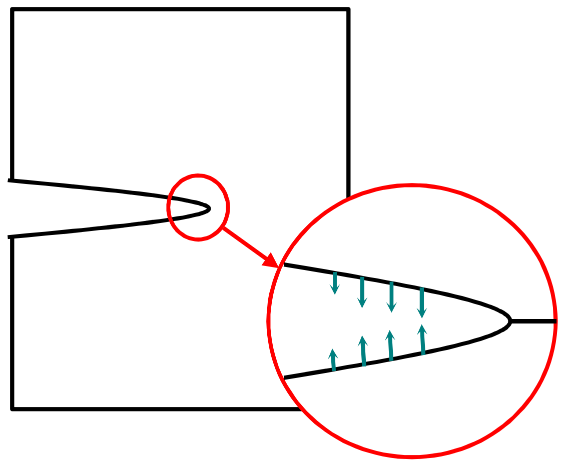
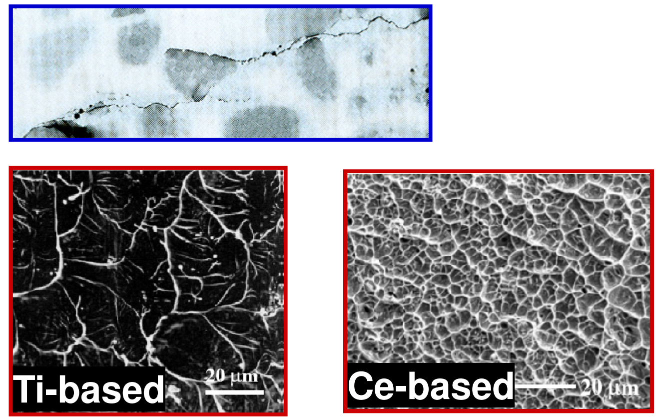
Dynamic Fracture: Cohesive Zone

Cohesive Zone Model





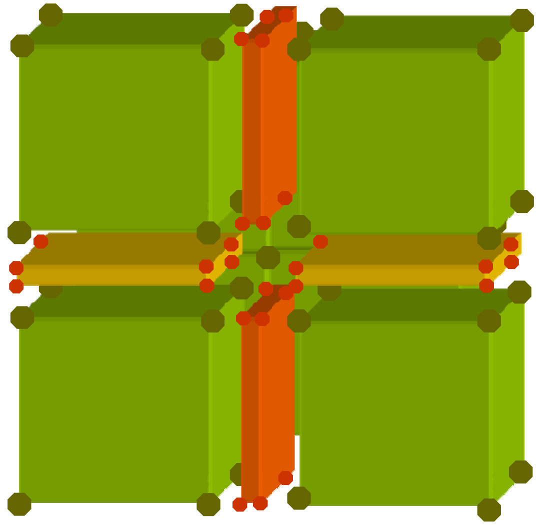
Xi XK et al., 2005,, *Physical Review Letters*, 94, 125510

Computational Simulation

- TRULY Extrinsic cohesive surface elements
- Several claims of extrinsic simulations in the literature are NOT truly extrinsic (e.g. activated elements are not extrinsic)

Topology-based Data Structure

- Complete Topological Data
- Reduced Representation
- Support for Adaptive Analysis



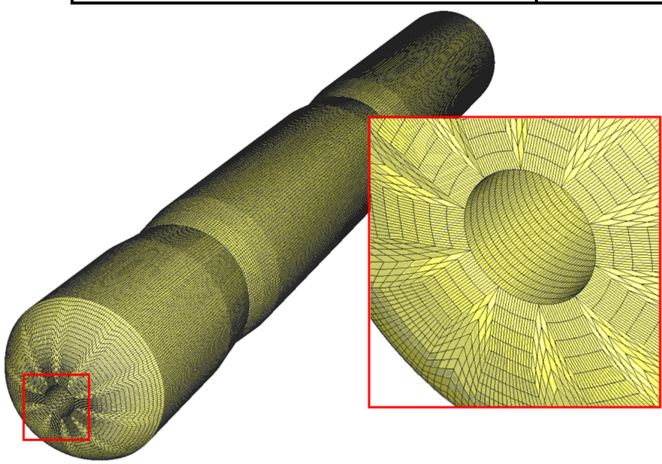
• W. Celes, G.H. Paulino, R. Espinha, 2005, Efficient handling of implicit entities in reduced mesh representations, Journal of Computing and Information Science in Engineering 5 (4), 348-359.

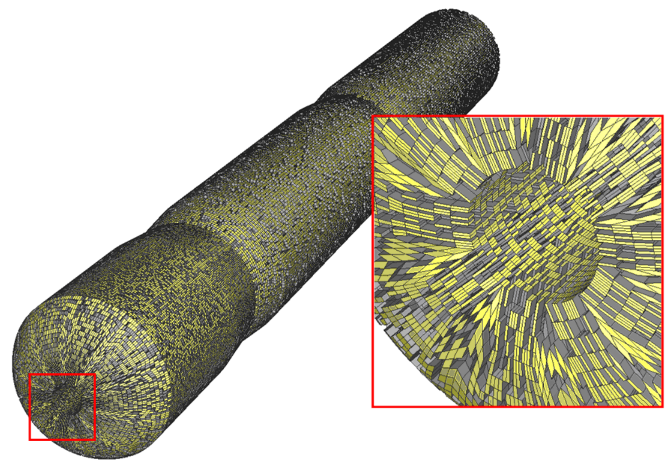
• W. Celes, G.H. Paulino, R. Espinha, 2005, A compact adjacency-based topological data structure for finite element mesh representation, IJNME 64(11), 1529-1556

• G. H. Paulino, W. Celes, R. Espinha, Z. Zhang, 2008, A general topology-based framework for adaptive insertion of cohesive elements in finite element meshes, EWC 24, 59-78

Entity Enumeration

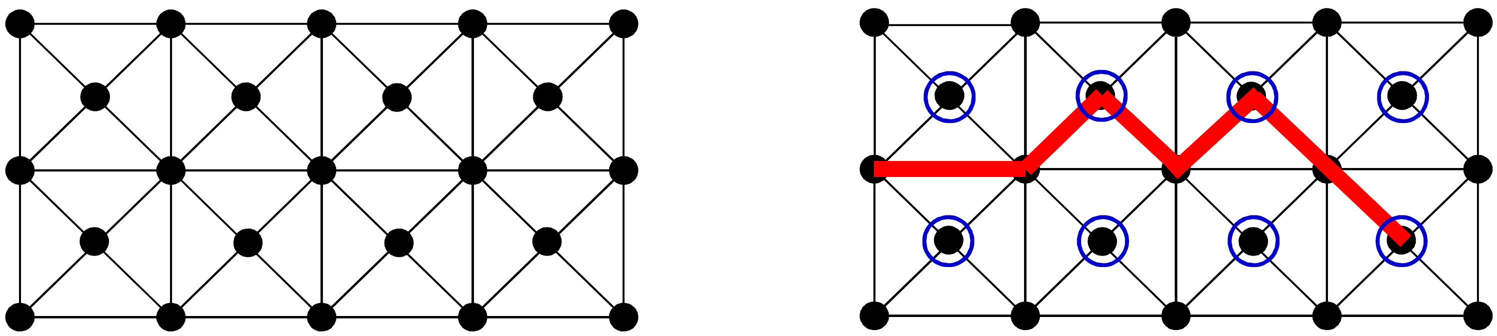
Model	*Entity information*		*Elapsed time (s)*
	Topological entity	*Number of entities*	
Titan IV model (linear hexahedral mesh)	Element	1,738,240	0.097
	Node	1,845,640	0.046
	Facet	5,321,600	0.219
	Edge	5,429,000	0.292
	Vertex	1,845,640	0.186





W. Celes, G.H. Paulino, R. Espinha, 2005, Efficient handling of implicit entities in reduced mesh representations, Journal of Computing and Information Science in Engineering 5 (4), 348-359.

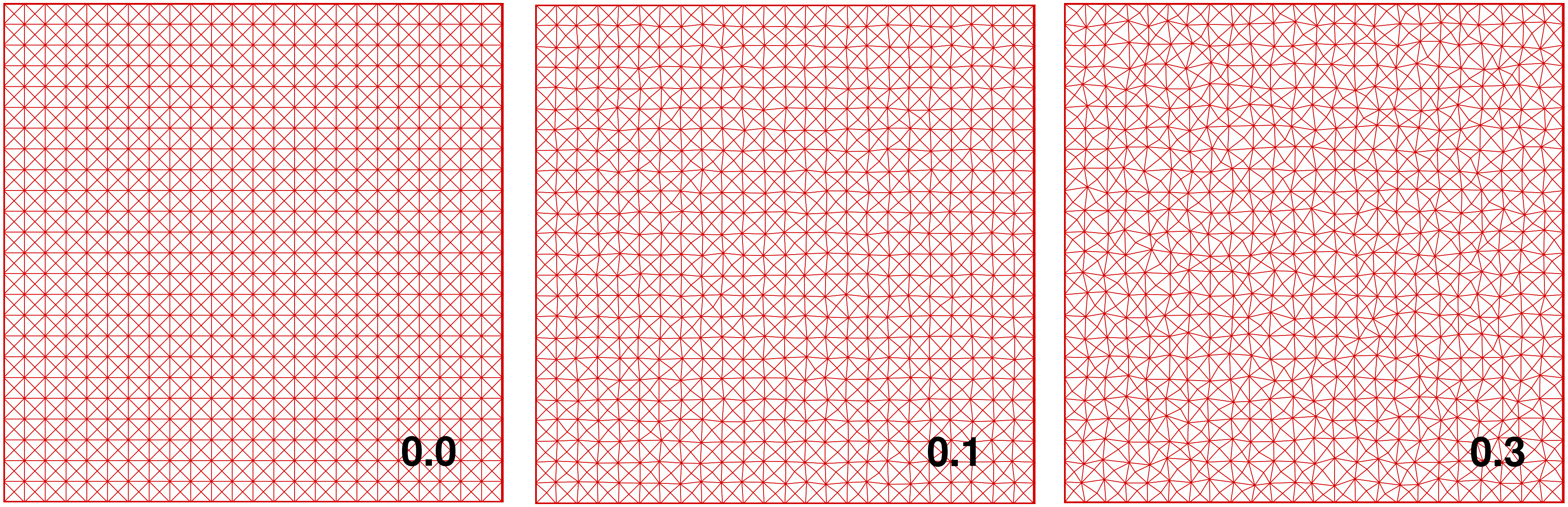
4K Structured Mesh



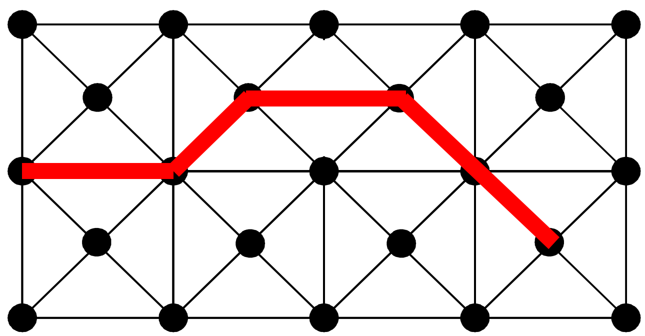
- **Mesh Orientation Dependence**
  - 4 direction → Maximum error: 45º
  - 8 direction → Maximum error: 22.5º
  - Undesirable crack pattern

Proposed Remediation

- Node Perturbation



- Edge Swap

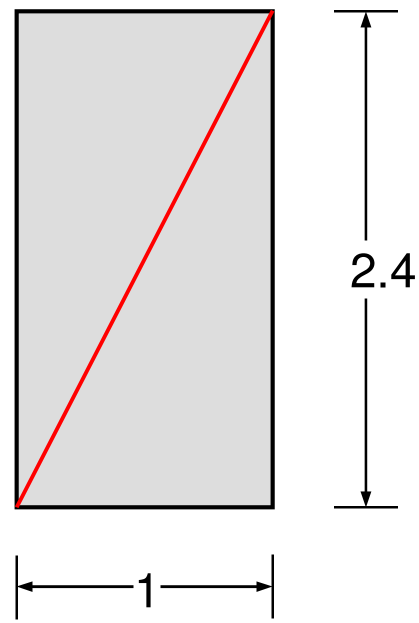


Crack Length Convergence

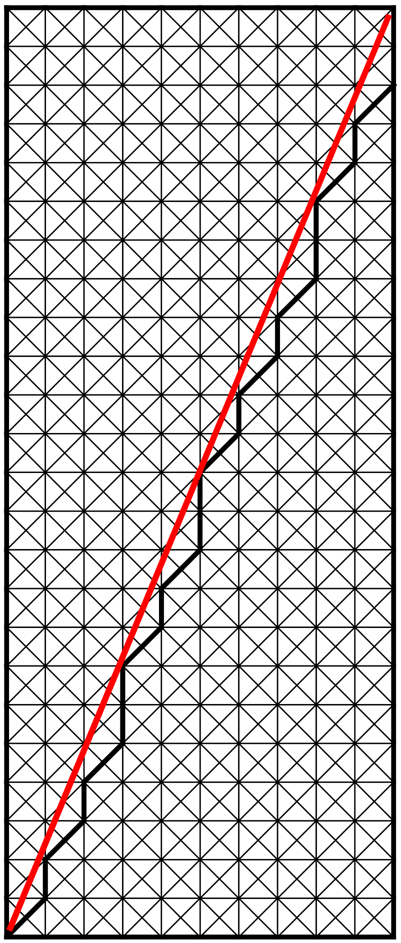
- **Simulation Outline**
  - Find the shortest path (e.g. MAPQUEST)
  - Node Perturbation (NP) Factor: 0.3
  - Edge Swap
  - Square 4K structured mesh
  - Element size: 0.1
  - Simulate 100 randomly perturbed meshes for each node perturbation factor

$\tan^{-1}(2.4) = 67.38^{\circ}$

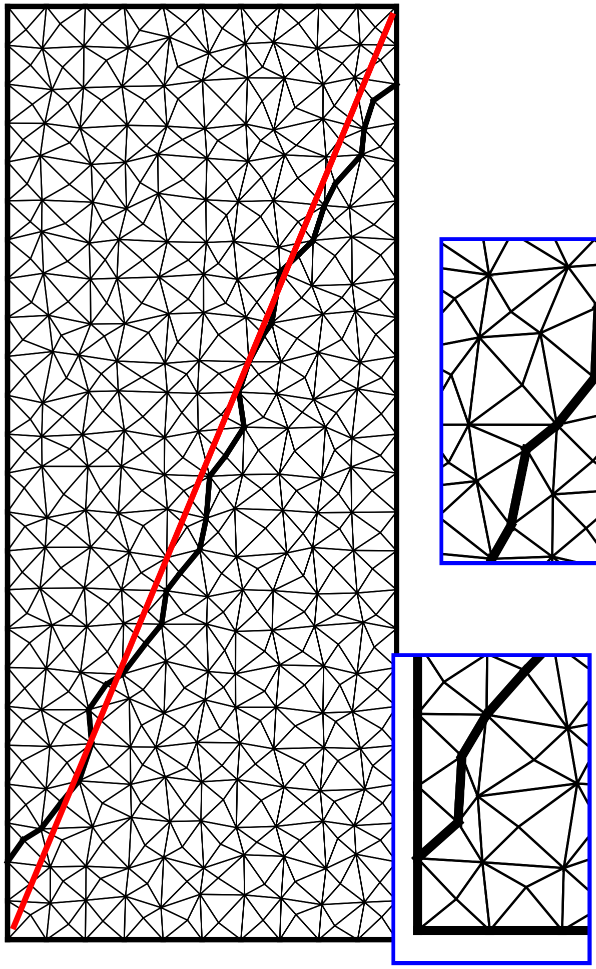
$L_{Exact} = 2.6$



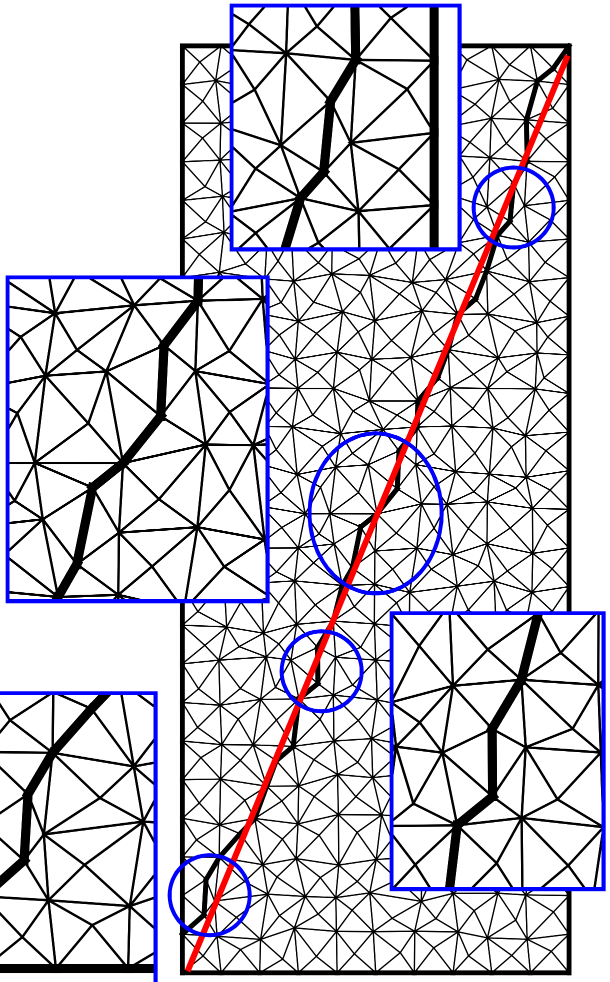
Results



NP0, Error = 8.2%

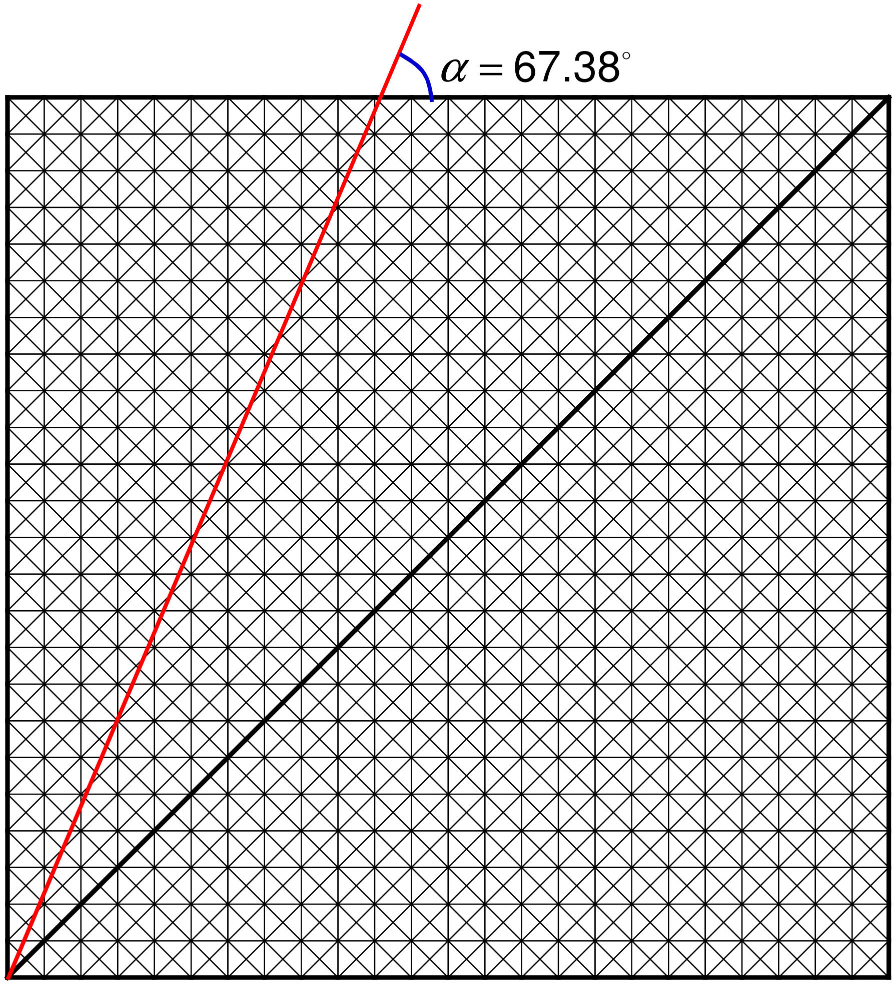


NP 0.3
Avg. Error = 5.5%

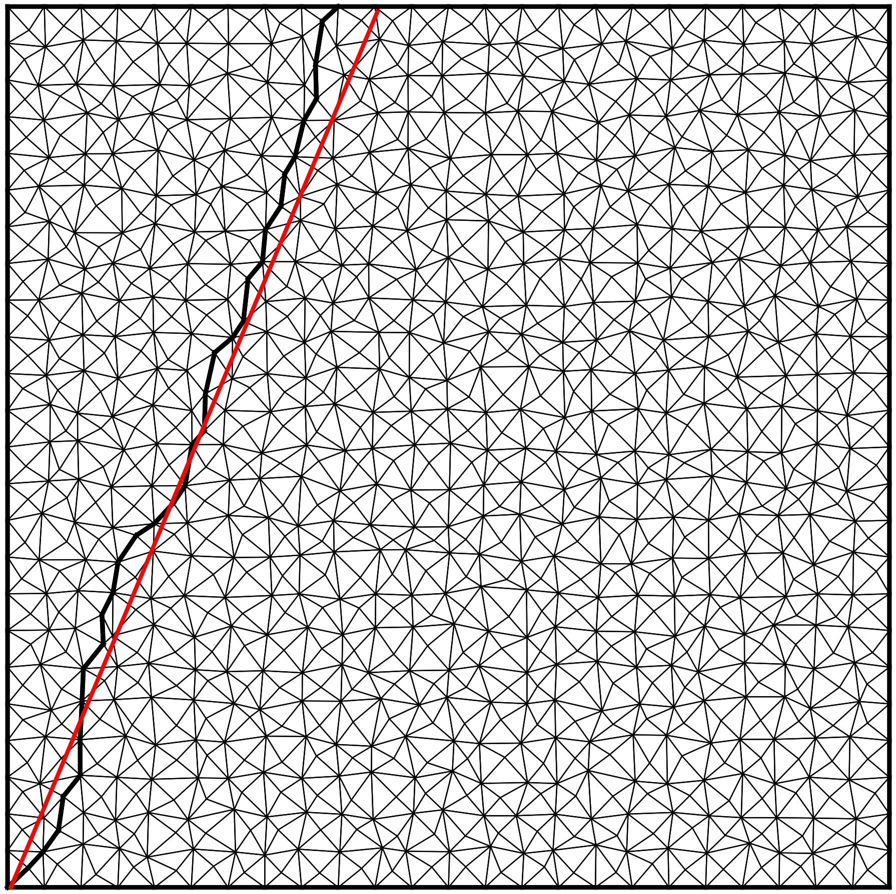


NP 0.3 & Edge Swap
Avg. Error = 4.5%

Crack Angle Convergence

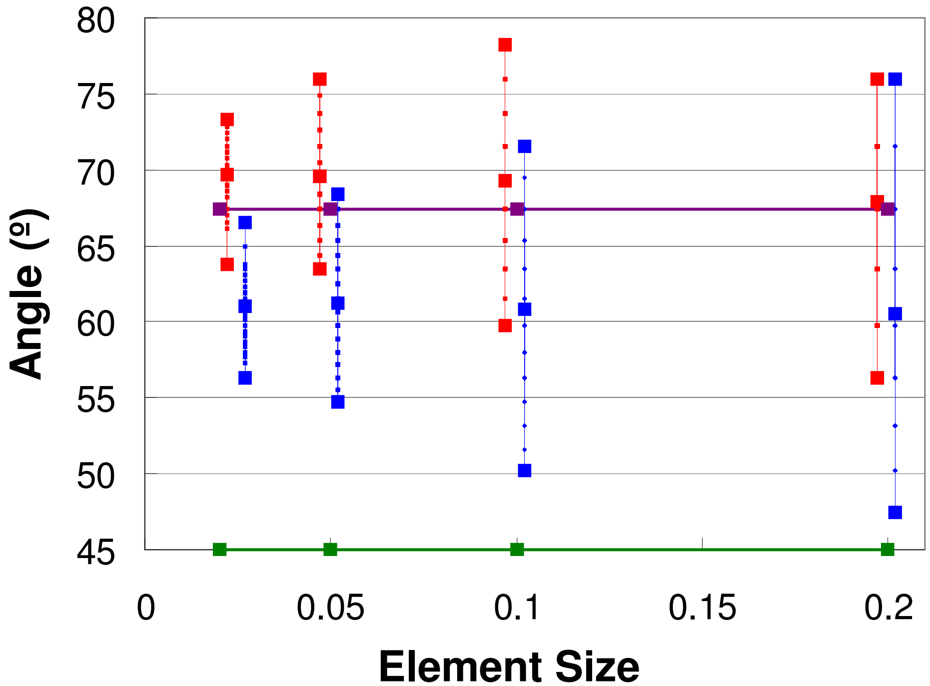


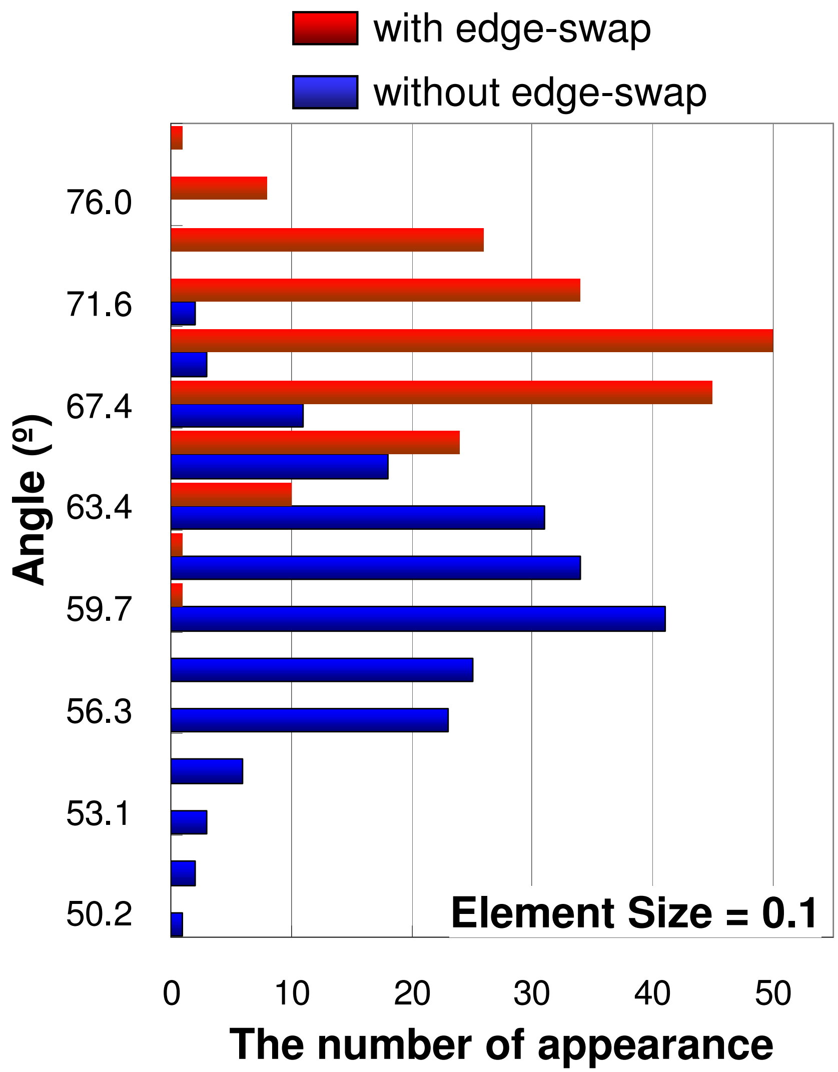
NP Factor = 0



NP Factor (0.3) & Edge swap

Effect of Element Size & Edge-Swap

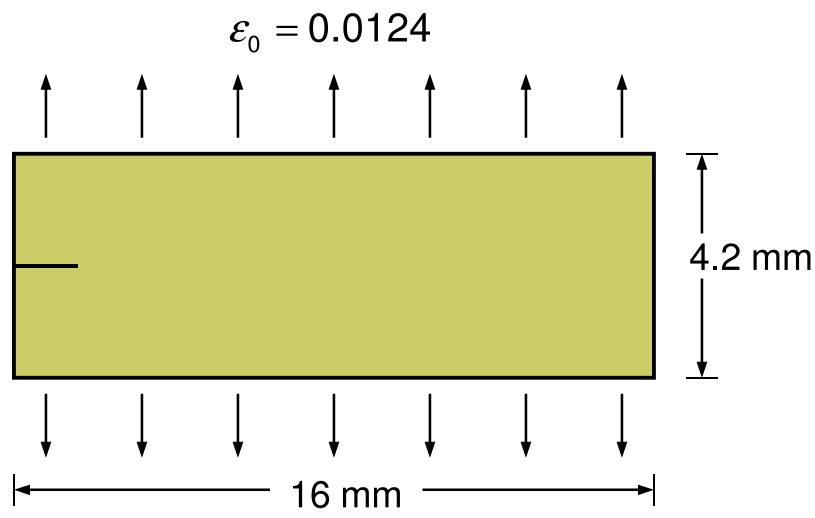




NP Factor = 0.3

- Given Angle (**α**)
- Without Edge Swap (ES)
- Activate Edge Swap (ES)

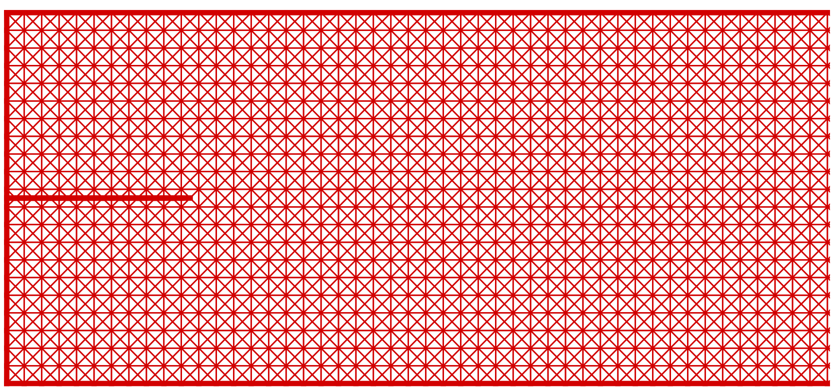
Fracture Test (Verification)

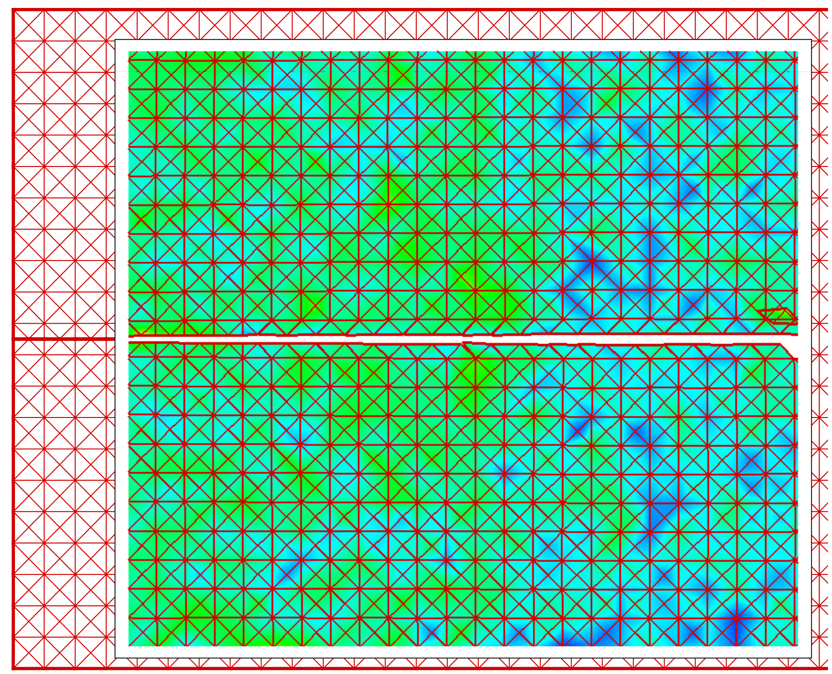


Material Properties

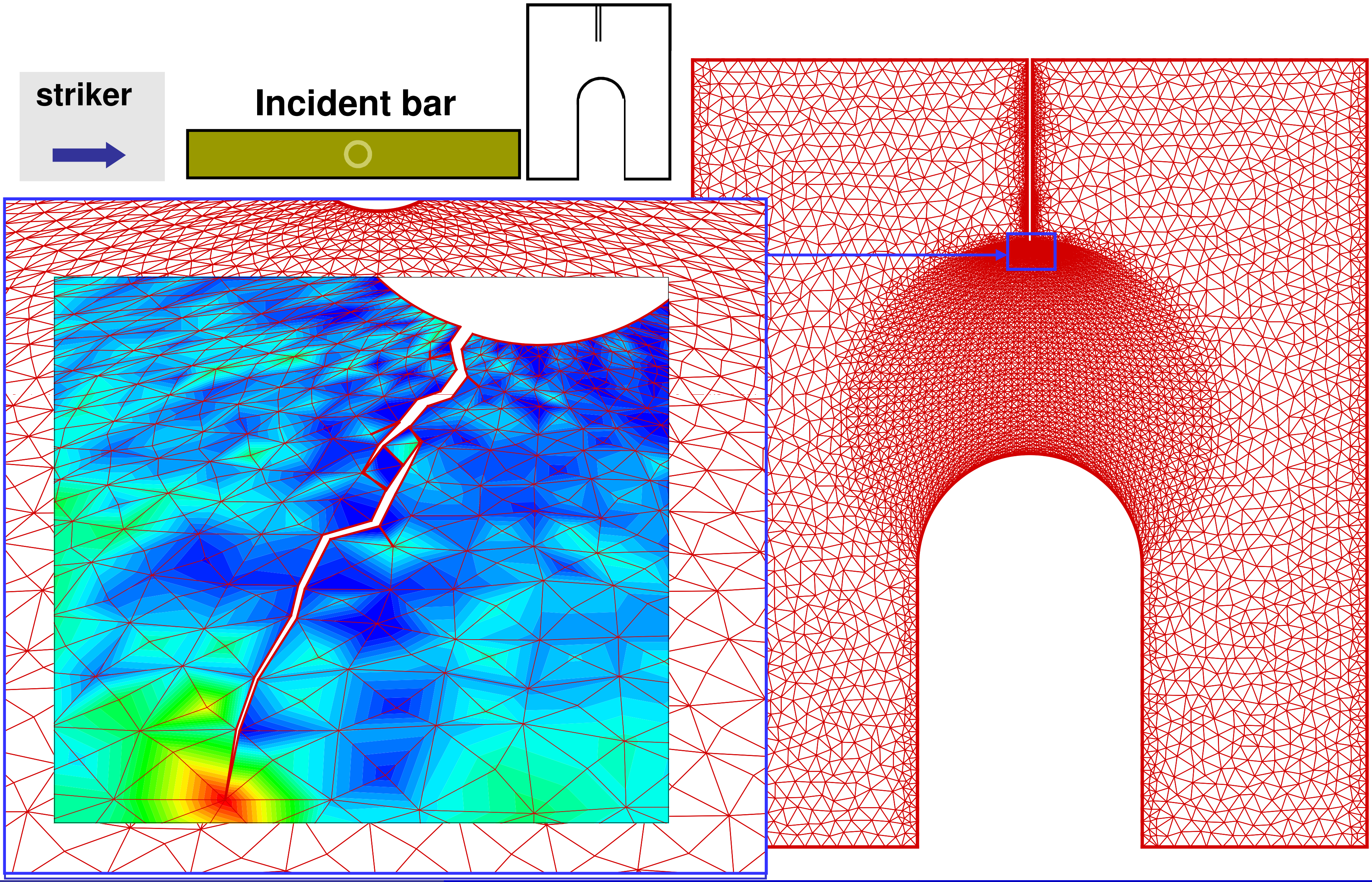
E = 3.24 GPa
ν = 0.35
ρ = 1190 kg/m^3
G_I = 352 N/m
σ_{max} = 129.6 MPa

4K structured mesh (80 X 21)





Compact Compression Specimen



Summary

- **Large-Scale Parallel Wave Propagation**
  - 1024 processors
- **Rayleigh Wave Speed in 3D Functionally Graded Media**
- **Crack Path Representation thru Topological representation**
  - Node perturbation & Edge swap operators
- **Adaptive Dynamic Fracture Simulation**
  - V & V

Future Work

- **Wave propagation for complex geology systems**
  - Provide guidance to estimate Rayleigh wave speed in smoothly graded heterogeneous media
- **Incorporate data from geological surveys**
- **Parallel Dynamic Fracture Simulation**
  - Parallel adaptive insertion of cohesive surface element
  - Dynamic adaptive load balancing

- **There is a lot of exciting work to do !**