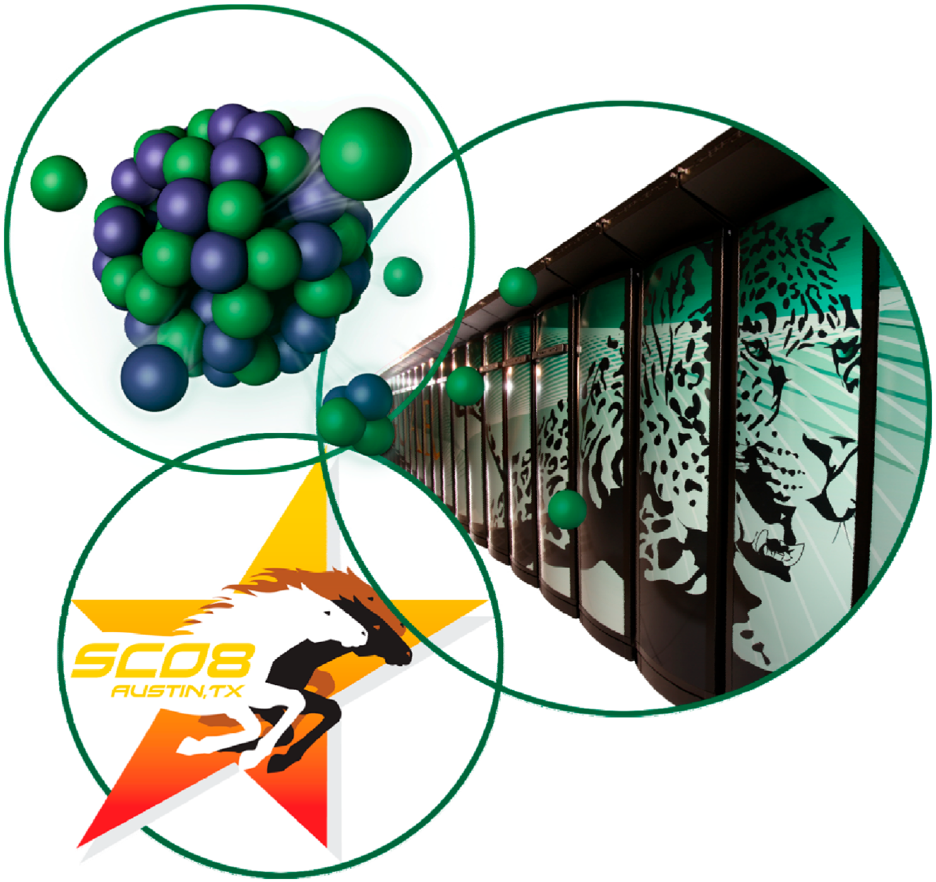
Statistical Physics of Fracture:
Recent Advances through High-Performance Computing



Presented by

Thomas C. Schulthess

Computer Science and Mathematics Division
Center for Nanophase Materials Sciences

Managed by UT-Battelle
for the Department of Energy

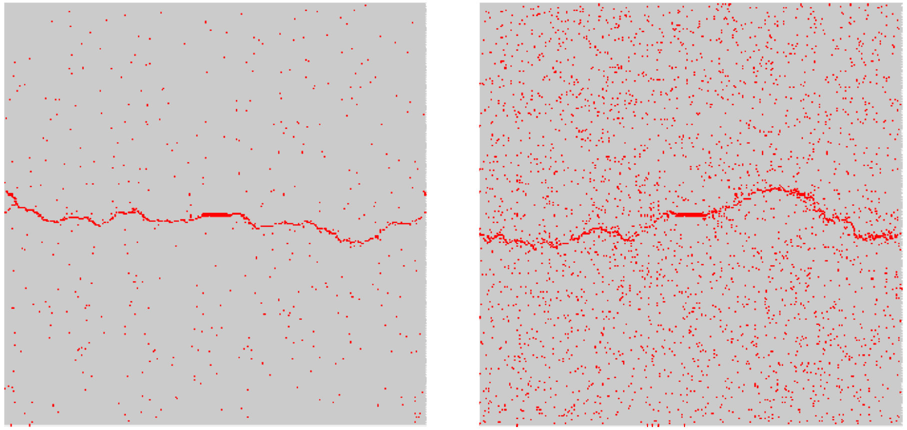
OAK RIDGE
National Laboratory

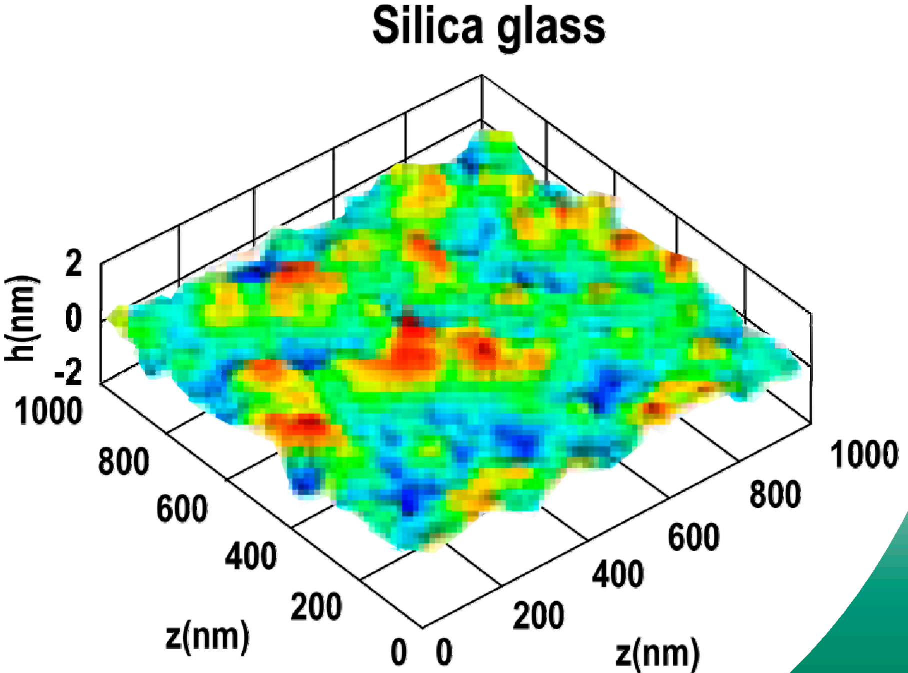
Acknowledgments

- MICS DOE Office of Science
- INCITE award: Computer resources on BG/L at ANL
- Leadership Computing Facility allocation on Cray XT4 Jaguar at ORNL
- Relevant journal publications:
  - J. Phys. Math. Gen. 36 (2003); 37 (2004); IJNME 62 (2005)
  - European Physical Journal B 37 (2004)
  - JSTAT, P08001 (2004); JSTAT (2006)
  - Phys. Rev. E 71 (2005a, 2005b, c); 73 (2006a 2006b)
  - Adv. Phys. (2006); Int. J. Fracture (2006)
  - Phys. Rev. E (2007); Phys. Rev. B (2007); IJNME (2007)
  - Phys. Rev. Lett. (2008); Phys. Rev. E (2008); Int. J. Fracture (2008a, 2008b)

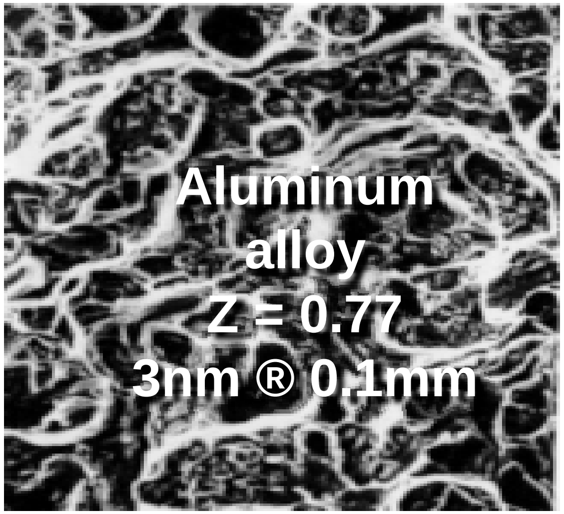
Motivation

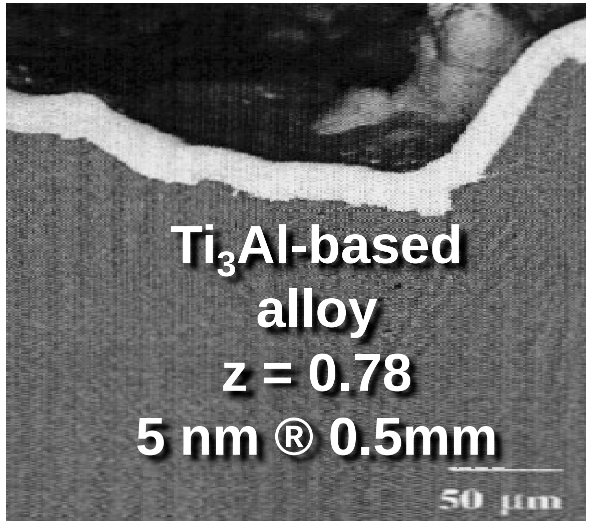
- **What are the size effects and scaling laws of fracture of disordered materials?**
- **What are the signatures of approach to failure?**
- **What is the relation between toughness and crack surface roughness?**
- **How can the fracture surfaces of materials as different as metallic alloys and glass, for example, be so similar?**



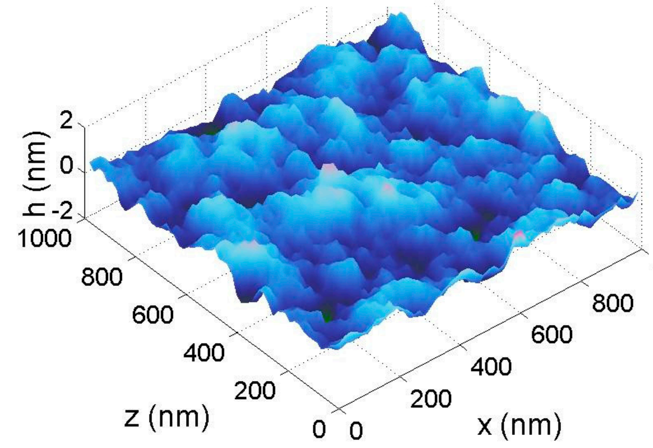


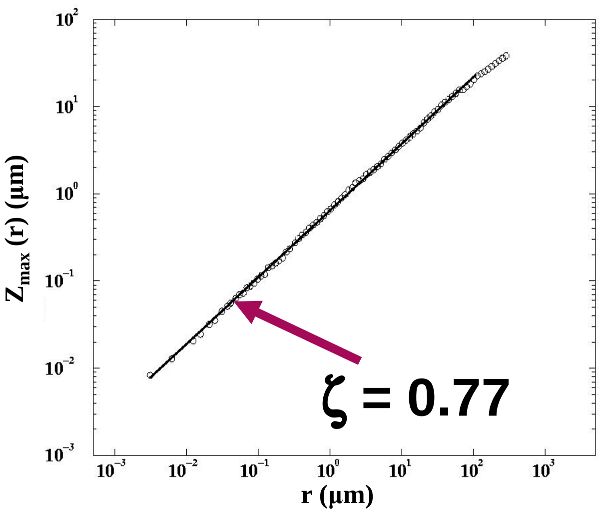
Universality of roughness

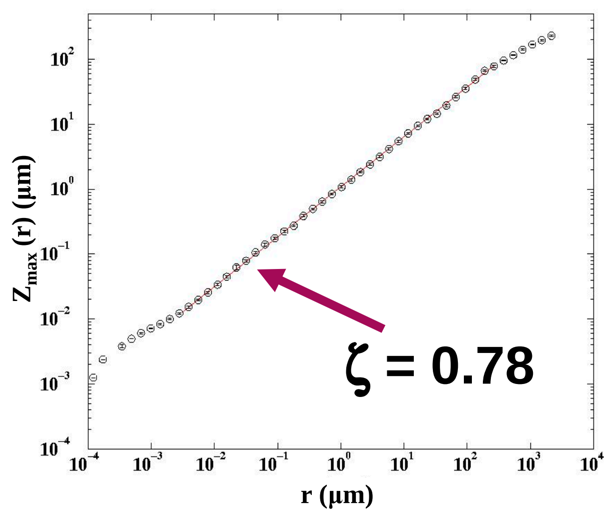


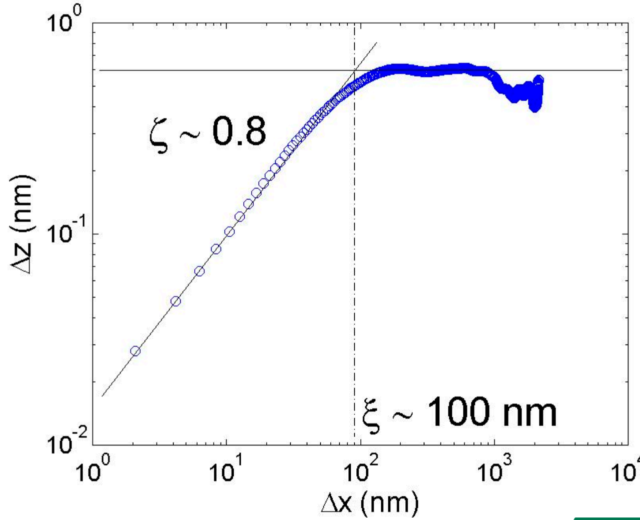


Amorphous silica







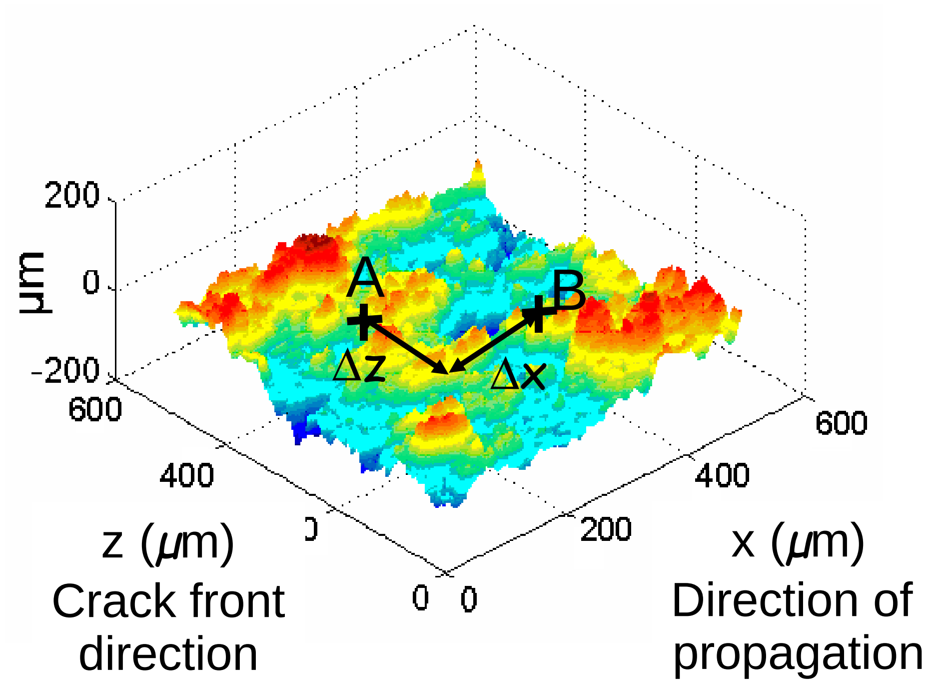


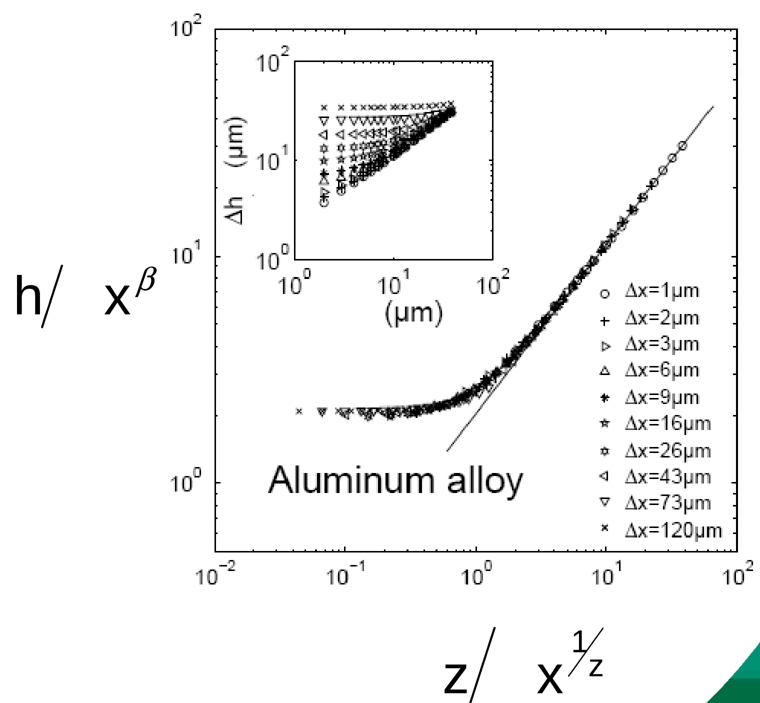
Fracture surfaces are self-affine with a universal roughness of ζ = 0.78 over five decades

Universal roughness scaling law

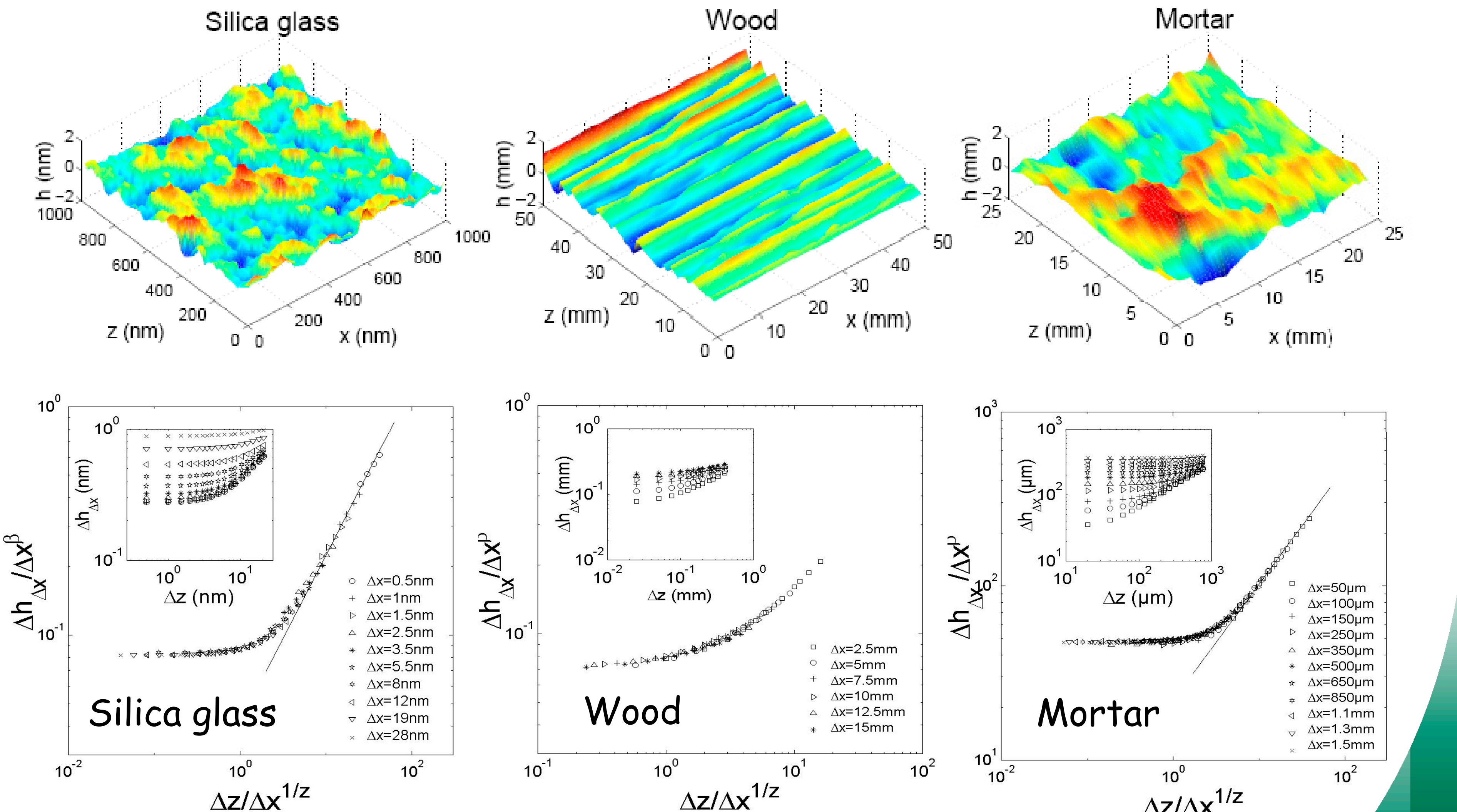
$$\Delta h_{2D}(\Delta z, \Delta x) = (\langle (h(z_A + \Delta z, x_A + \Delta x) - h(z_A, x_A))^2 \rangle)^{1/2}$$

$$\Delta h_{2D}(\Delta x, \Delta z) = \Delta x^{\beta} f\left(\frac{\Delta z}{\Delta x^{1/z}}\right) \qquad f(u) \propto \begin{cases} 1 \; if \; u << 1 \\ u^{\zeta} \; if \; u >> 1 \end{cases}$$





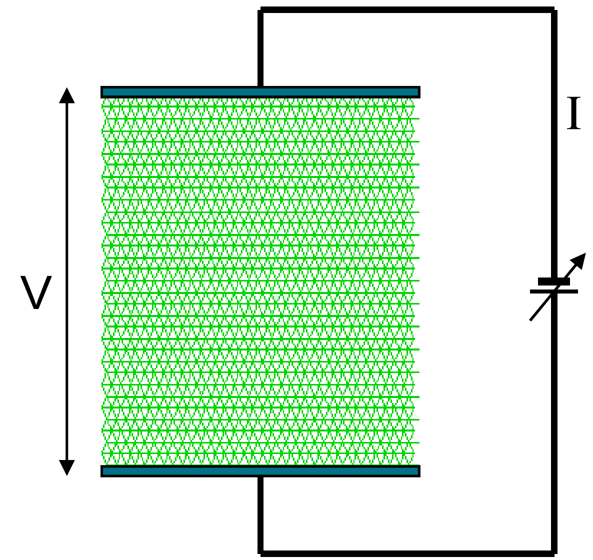
Anisotropic roughness scaling

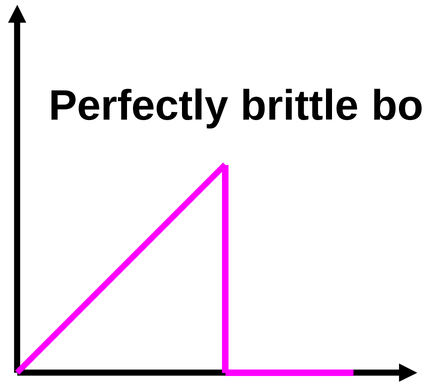


$\zeta=0.75 \pm 0.05$ $\beta=0.6 \pm 0.05$ $z=\zeta/\beta=1.25 \pm 0.1$

Random thresholds fuse model

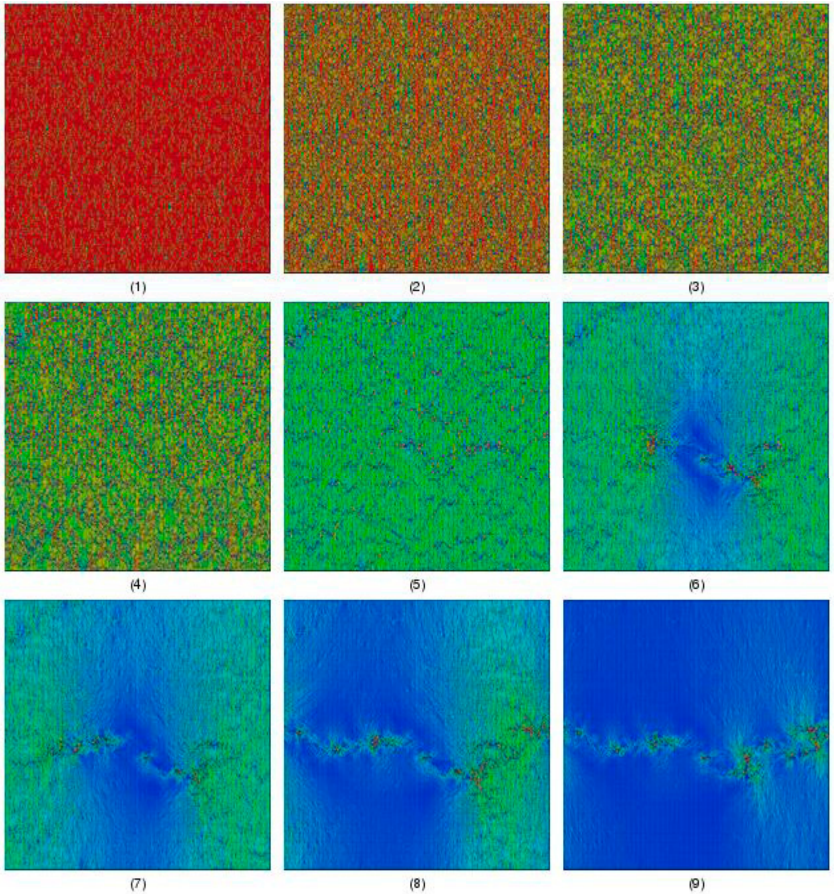
- Scalar or electrical analogy
- For each bond, assign unit conductance, and the thresholds are prescribed based on a random thresholds distribution
- The bond breaks irreversibly whenever the current (stress) in the fuse exceeds the prescribed thresholds value
- Currents (stresses) are redistributed instantaneously
- The process of breaking one bond at a time is repeated until the lattice falls apart





Fracture of a 2-D lattice system

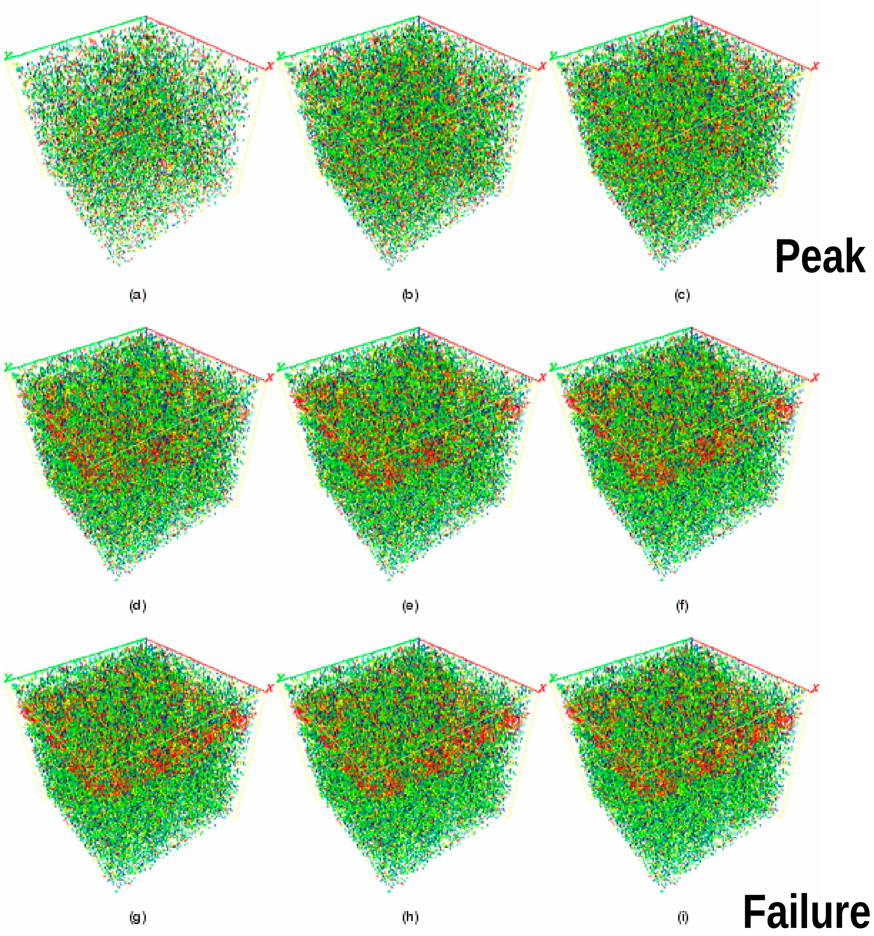
- **CPU ~ O(L4.5)**
- **Capability issue: Previous simulations have been limited to a system size of L = 128**
- **Largest 2-D lattice system (L = 1024) analyzed for investigating fracture and damage evolution**
- **Effective computational gain ~ 80 times**



Stress redistribution in the lattice due to progressive damage/crack propagation

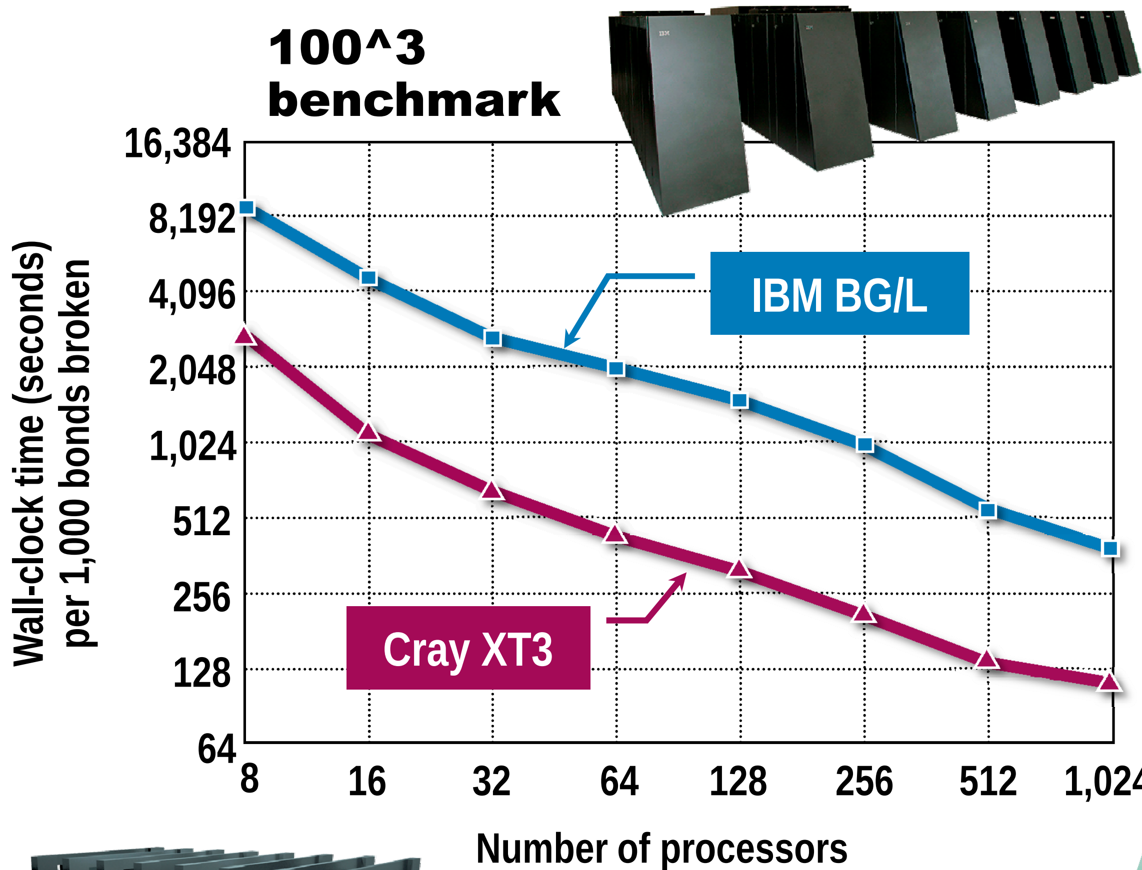
Fracture of 3-D lattice system

- CPU ~ O(L6.5)
- Largest cubic lattice system analyzed for investigating fracture and damage evolution in 3-D systems (L = 64)
- On a single processor, a 3-D system of size L = 64 requires 15 days of CPU time!



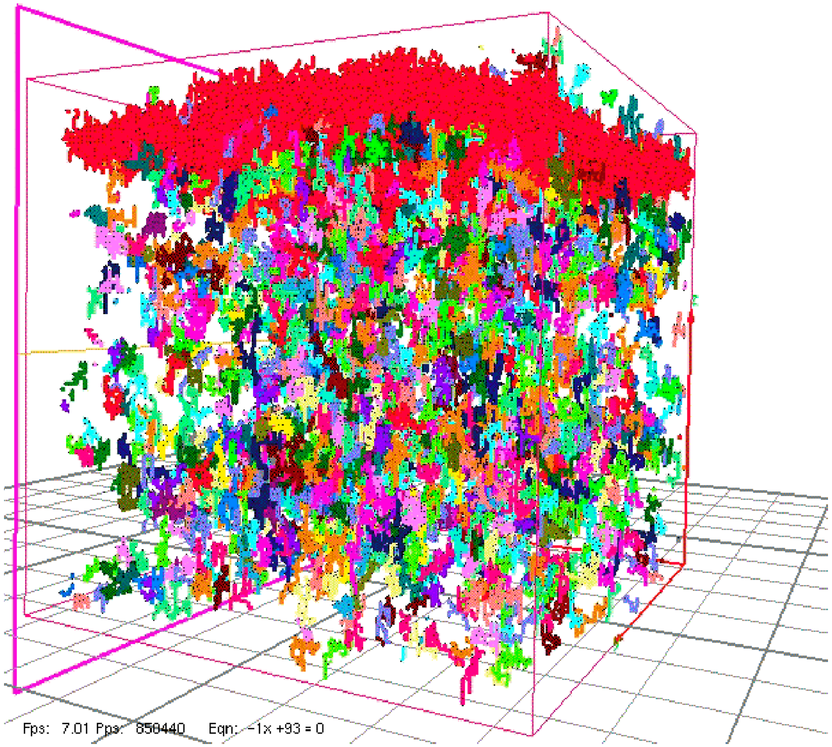
High-performance computing

High-performance computing	Processing time
L = 64 on 128	3 hours
L = 100 on 1024	12 hours
L = 128 on 1024	3 days
L = 200 on 2048	20 days (est.)



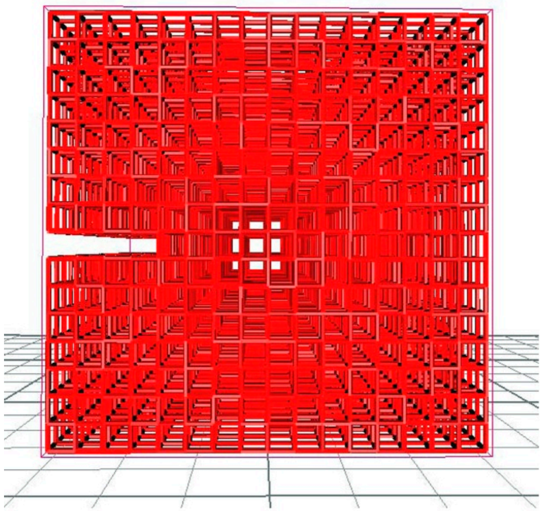
Roughness 3-D crack

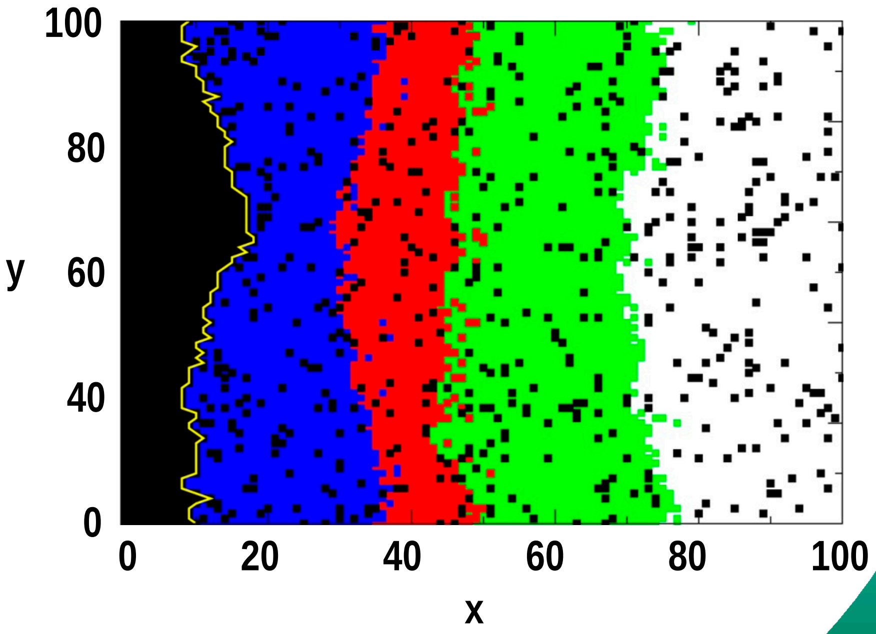
- Study the roughness properties of a crack surface
- Largest ever 3-D lattice system (L = 128) used
- For the first time, roughness exhibits anomalous scaling, as observed in experiments
- Local roughness ~ 0.4
- Global roughness ~ 0.5



Interfacial cracks

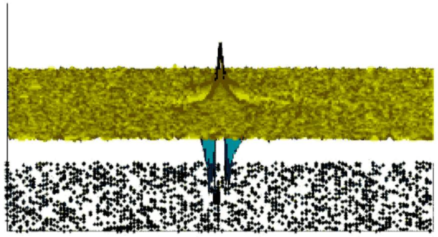
- Study the roughness properties of an interfacial crack front
- Largest ever 3-D lattice system (L = 128) used for studying interfacial fracture
- Figures show crack fronts at various damage levels
- Roughness exponent is equal to 0.3





Scaling law for material strength

- **Study the size-effect and scaling law of material strength**
- **Largest ever 2-D (L = 1024) and 3-D lattice systems (L = 128) used for studying size-effect of fracture**
- **Figures show crack propagation and fracture process zone**
- **A novel scaling law for material strength is obtained in the disorder-dominated regime**



Summary of accomplishments

FY 2006

- 7 refereed journal publications
  - 150-page review article
- 3 refereed conference proceedings
- 13 conference presentations (6 invited)
  - SciDAC 06 (invited)
  - Multiscale Mathematics and Materials (invited)
- INCITE award for 1.5 million hours on Blue Gene/L

FY 2007

- 6 refereed journal publications
- 14 conference presentations (8 invited)
  - StatPhys 23 (invited)
  - Multiscale Modeling (invited)
- INCITE award for 1.1 million hours on Blue Gene/L

FY 2008

- 6 refereed journal publications
- 2 refereed conference proceedings
- 10 conference presentations (6 invited)

Contacts

Phani Nukala

Oak Ridge National Laboratory
(865) 574-7472
nukalapk@ornl.gov

Srdjan Simunovic

Oak Ridge National Laboratory
(865) 241-3863
simunovics@ornl.gov

Thomas Schulthess

Oak Ridge National Laboratory
(865) 574-4344
schulthesstc@ornl.gov