Scaling of Fracture - An Application of Field Induced Percolation

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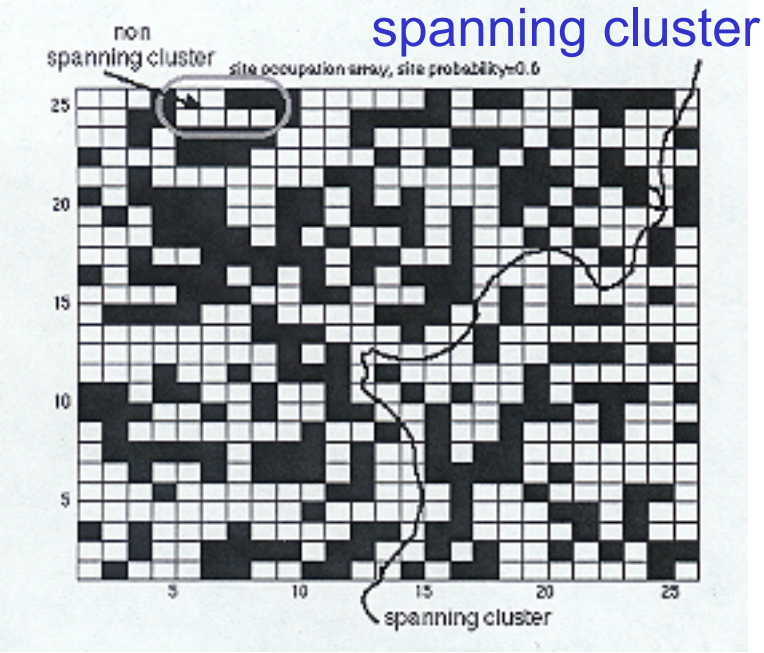
Percolation Basics

What is Percolation?

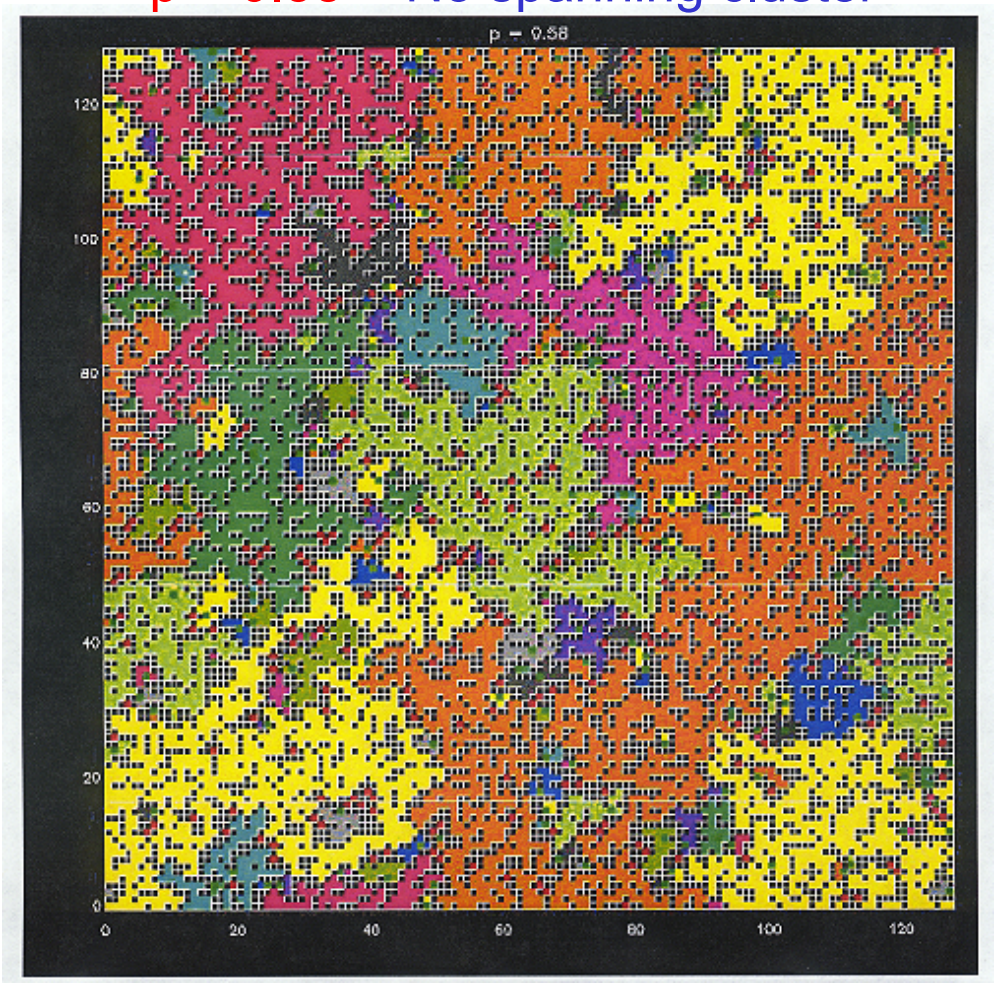
p = 0.60

spanning cluster



25 x 25 square lattice

p = 0.58 No spanning cluster



128 x 128 square lattice

Phase transition:

System changes from connected phase to disconnected phase as the critical point $p_c = 0.592746$ is approached from above

Why should we use Percolation Theory?

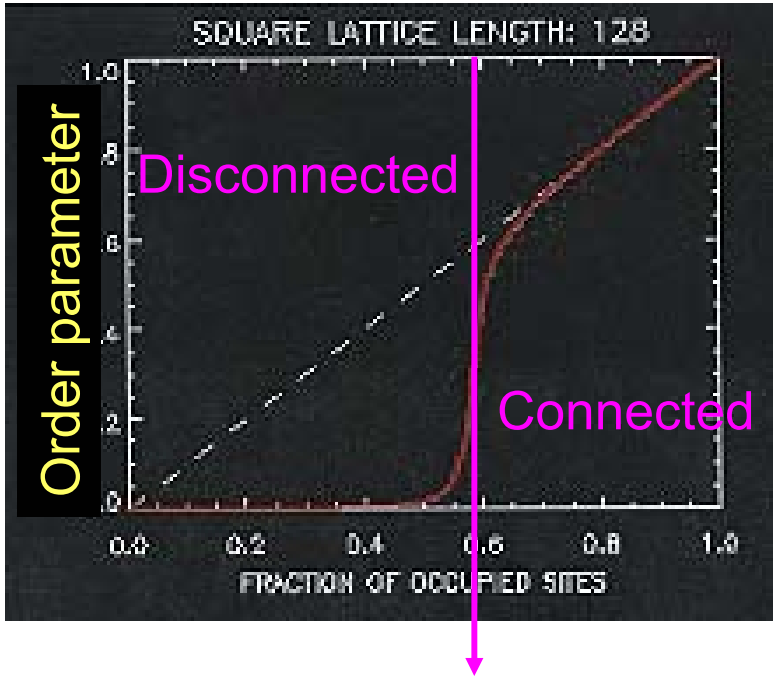
Percolation and Fracture Similarity

Fracture is a phase transition:
From a connected system to
a disconnected system

Stiffness of the system is the
Order parameter:

- non-zero in the connected phase
- zero in the disconnected phase

128 x 128 square lattice



critical percolation
threshold $p_c = 0.592746$

Percolation theory describes how
system approaches criticality

Scaling Laws

System behavior with change in length scale
- couples meso- and macro- phenomena

System size effect

Field Induced Percolation

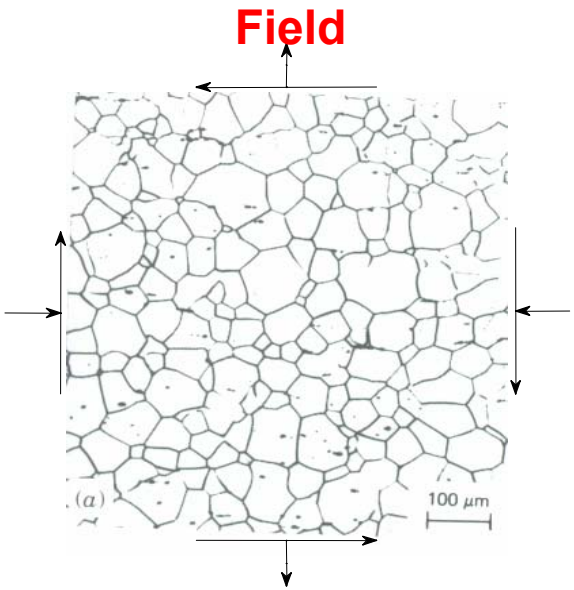
But, really, fracture is not a random percolation!
Stress distribution plays a significant role.

Fields:

- mechanical: stress, strain
- thermal
- electrical
- magnetic

Microstructure (cluster) evolution:

- microcracks
- second-phases



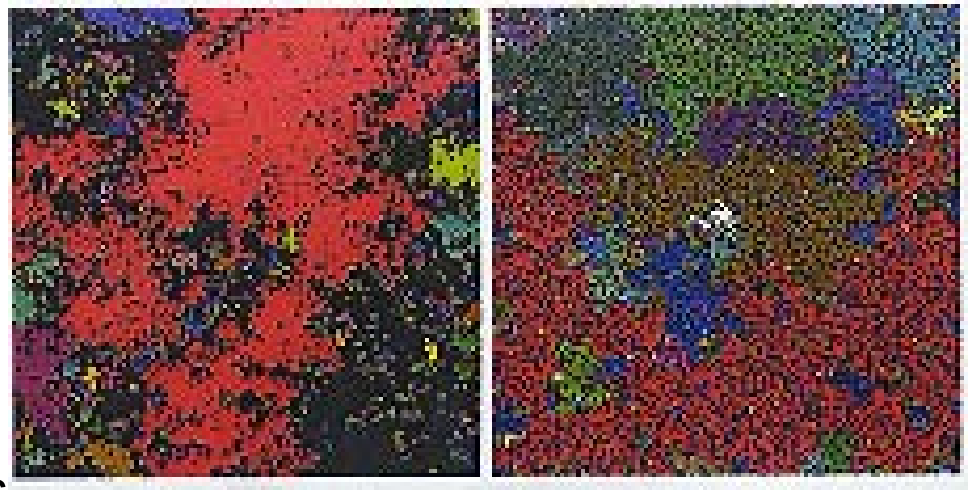
Microstructure evolution

Geometric percolation:

- clusters formed with randomly occurring events

Field induced percolation:

- current event is dependent on the past history of events
- applied field introduces a bias in the occurrence of events



Correlated Uncorrelated

General Applications

Materials Science Applications

Thermo-Mechanical Fields:

- Nucleation and growth of damage
  - Intergranular and transgranular cracking
- Dynamic recrystallization
- Stress induced boundary migration
  - Migration of both low and high angle flat boundaries
  - Twinning in ferromagnetic shape memory alloys

Electrical and Magnetic Fields:

- Evolution of magnetic domains
- Magnetic Fields in Solidification
  - Electromagnetic stirring (Dendrite morphology)
- Electro-migration of interfaces
  - Boundary migration related to grain boundary potential

Chemical Bond Fields:

- Polymer gelation, vulcanization; Glass transition

General Applications

Thermal Fields:

- Boiling of water: liquid-gas phase transition
- Paramagnetic to ferromagnetic phase transition

Electrical Fields:

- Fuse problem: conducting to non-conducting transition
- Dielectric breakdown: non-conducting to conducting transition

Fluid Flow: Geological Applications

- Flow through fractured rocks and porous media
- Earthquakes, fracture and fault patterns

Traffic Flow: Transportation Applications

- Traffic flow on a network

Information Flow on www: Computer Science Applications

- Information flow on www network
- Overloading of computer network within a massively parallel system

Graph Theory:

- Structural failure of a highly redundant system

Common Theme

System Behavior: undergoes phase transition at a critical point

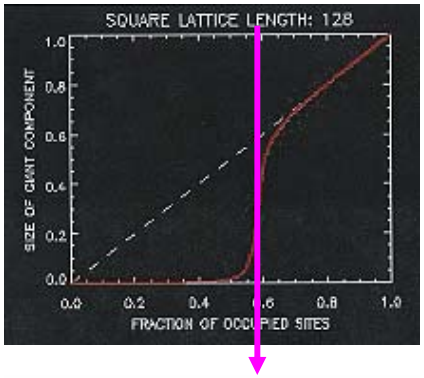
System Model: random graph with vertices, mutual interactions as bonds

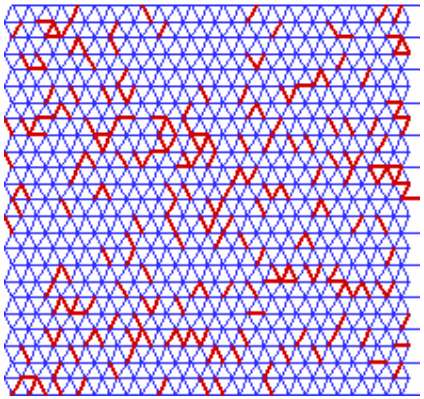
System Evolution: approaches criticality through a change in the interaction strength

Redistribution: underlying physics governs the redistribution of the applied field

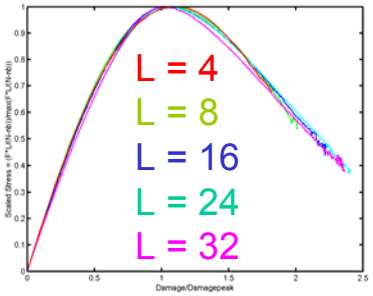
Scaling Laws: comparison of system behavior at different length scales is possible

System size effect on system behavior





Conservation laws; Kirchhoff equations

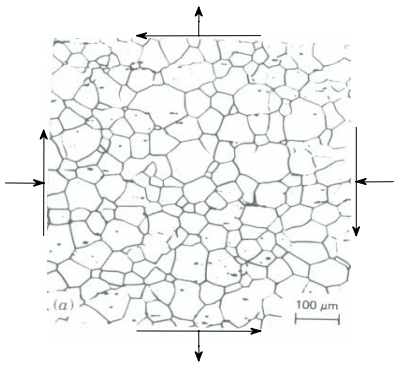


Damage Evolution in Brittle Materials

Motivation: Stress Induced Microcracking Evolution

Macroscopic properties and behavior of quasi-brittle materials are significantly affected by the internal microstructure and damage/microcracking evolution

Stress Field



Microcracking evolution

Phenomenological Material Models:

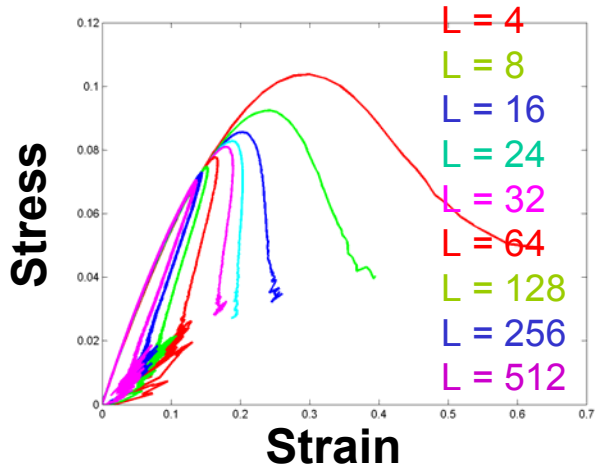
- microstructure-insensitive
- valid only for moderate damage levels
- local stress field fluctuations and interactions are not considered

Modeling at the mesoscale will lead to a fundamental understanding of the effect of microstructural features on the microcracking evolution in brittle materials

Motivation (cont'd): Scaling Laws in Fracture

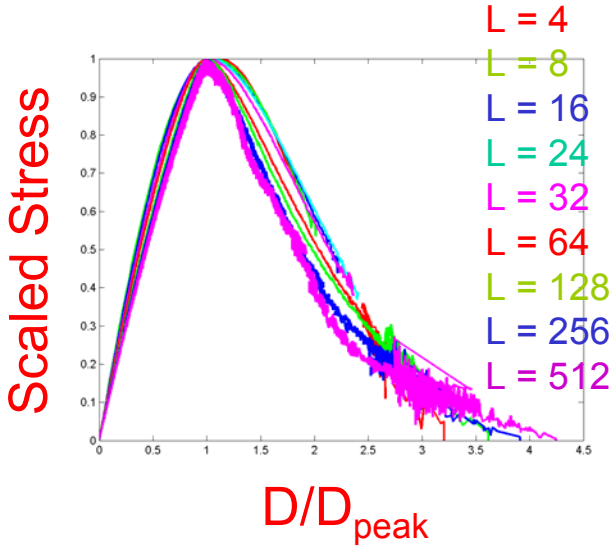
Mesoscale Damage Evolution:

- depends on the system size L
- computationally intractable $\approx \mathcal{O}(L^4)$



Material response is size dependent

Scaling laws are required to obtain a "normalized" response that couple mesoscopic and continuum length scales



Objective

Relevant Questions?:

- How does a disordered solid breakdown?

- What is the size effect and scaling laws of failure?

- How does one quantify damage? and how do we compare the extent of damage between two specimens?

- What is the connection between mesoscopic damage and the phenomenological continuum damage evolution?

Objective:

Describe continuum damage evolution based on mesoscopic modeling using scaling laws

Solution:

Explicit modeling of material microstructure combined with the scaling theory accounts for size effects and local stress field interactions during damage/microcrack evolution

Outline

- Numerical Methodology
- Typical Lattice Response
- Scaling Theory (Renormalization Group)
- Numerical Results
- Summary

Numerical Methodology

Mesoscopic Simulation: Discrete Lattice Models

Focus of the study is not on any particular material

But, in capturing the generic features of damage evolution

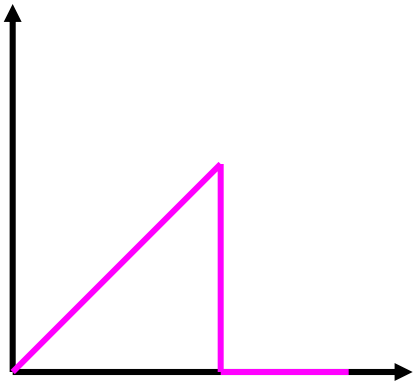
Essential ingredients of breakage process:

- Initial material disorder (inhomogeneities)
- redistribution of stresses due to damage evolution

Discrete Lattice Models:

- disorder in bond strength and stiffness
- elastic response characteristics of the bonds
- bond breaking rule (failure criteria)

Perfectly brittle bond



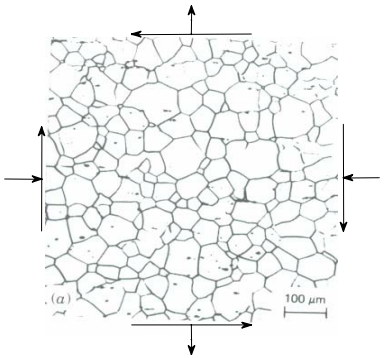
Any realistic damage evolution description must be capable of reproducing the behavior of these idealized discrete lattice models

Mesoscopic Modeling Approach

Failure of a bond is governed by

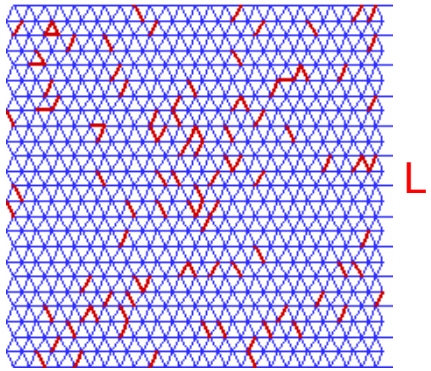
- weakest bond of the disordered medium
- stress concentration around material inhomogenities

Stress



Discretization with random disorder distributions

Lattice system with disorder



Disorder Type

+

Lattice Topology

+

Lattice Bond Model

Applied Stress

Failure Criteria

Mesoscopic Damage Evolution

Analysis Procedure

Procedure:

Step 0: For each bond in the lattice system, assign unit stiffness and random force threshold f_i^{th}

Step 1: Impose a unit macroscopic displacement

Step 2: Calculate the force f_i in each bond through lattice equilibrium

$$K = \sum_i f_i^2$$

K Global stiffness

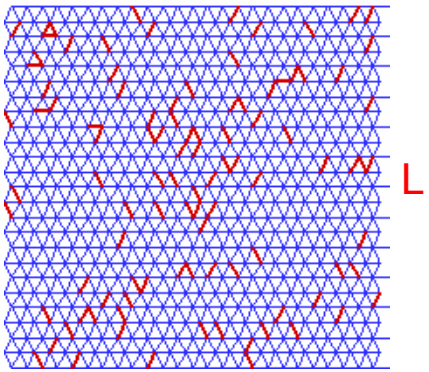
Step 3: Determine the bond i_c for which

$$\frac{1}{\lambda} = \max_i \left(\frac{f_i}{f_i^{th}} \right)$$

Step 4: Record the lattice displacement and force $(\lambda, K\lambda)$

Step 5: Remove the bond i_c and repeat steps 1-4, until the entire lattice system breaks apart

$\Delta = 1$



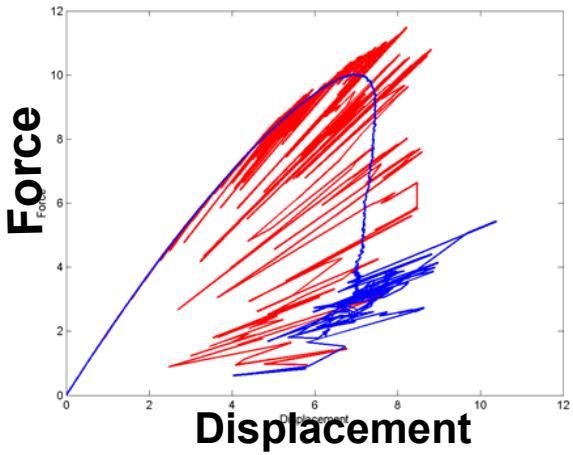
Lattice system with disorder

Typical Lattice Response

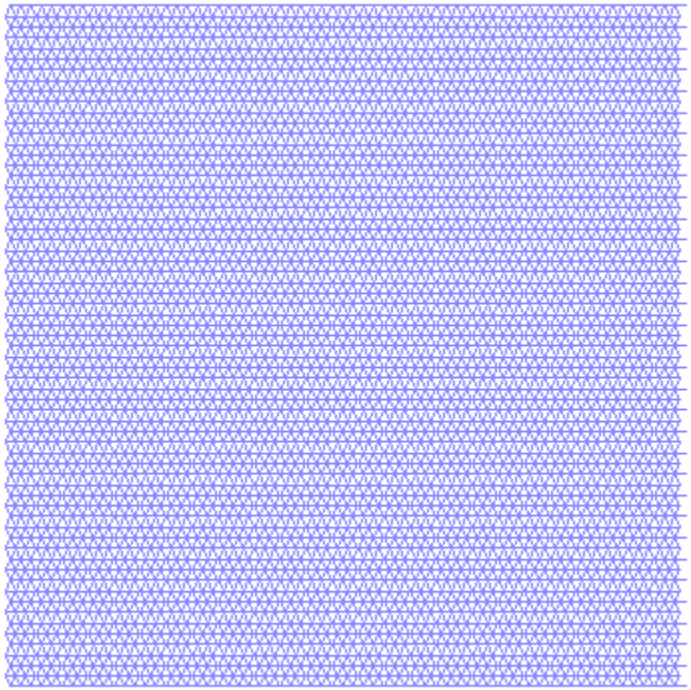
Typical Loading Response

Single lattice response (64 x 64)
Lattice response averaged
over 5000 samples

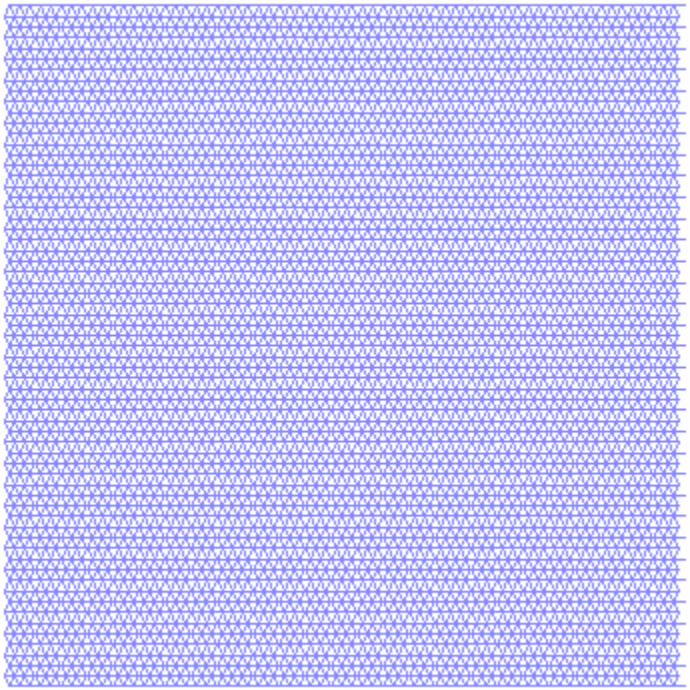
512 x 512



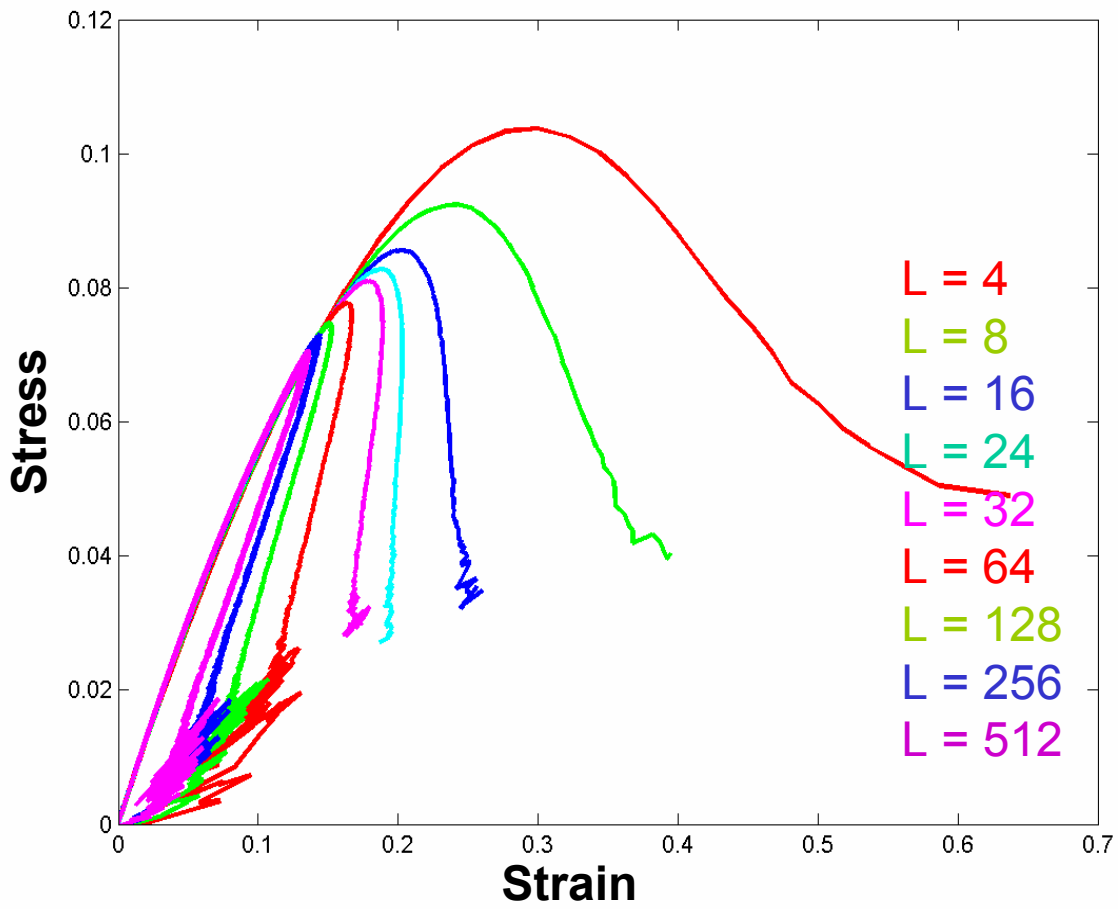
At Failure



At Peak Load

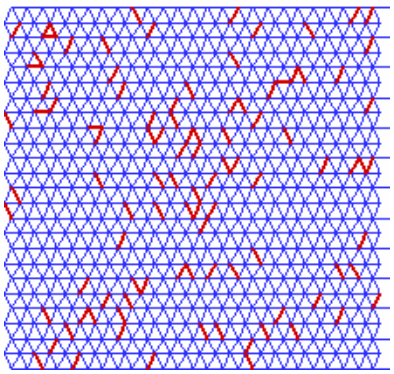


Lattice Response versus System Size

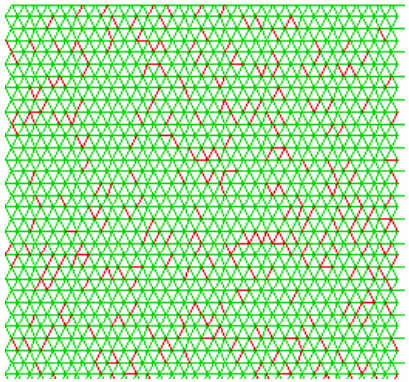


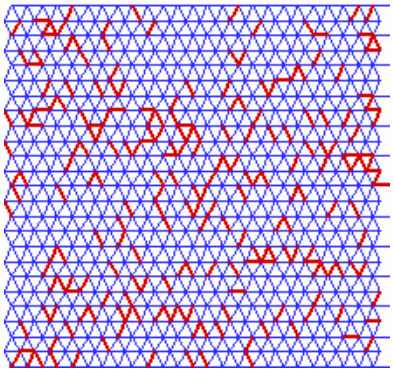
- Lattice response depends on the system size
- Scaling laws are required to obtain a “normalized” response that couples the mesoscopic scale response to the continuum scale response

What is the Intensive Measure of Damage?

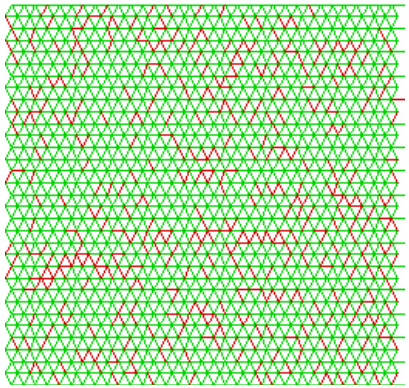


Nucleation Phase:
Diffusive Damage

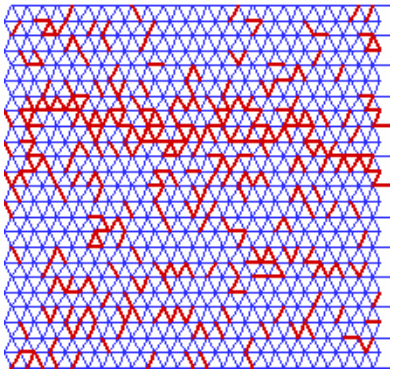




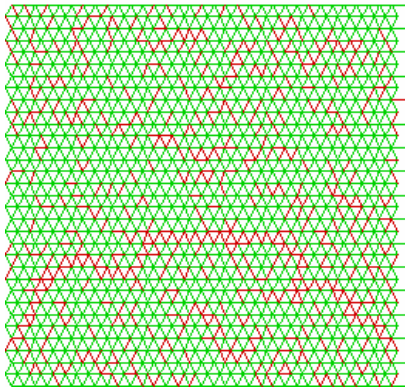
Growth Phase:
Stress Concentration effects are dominant



L = 24



Coalescence:
Localization of damage to form a percolating crack

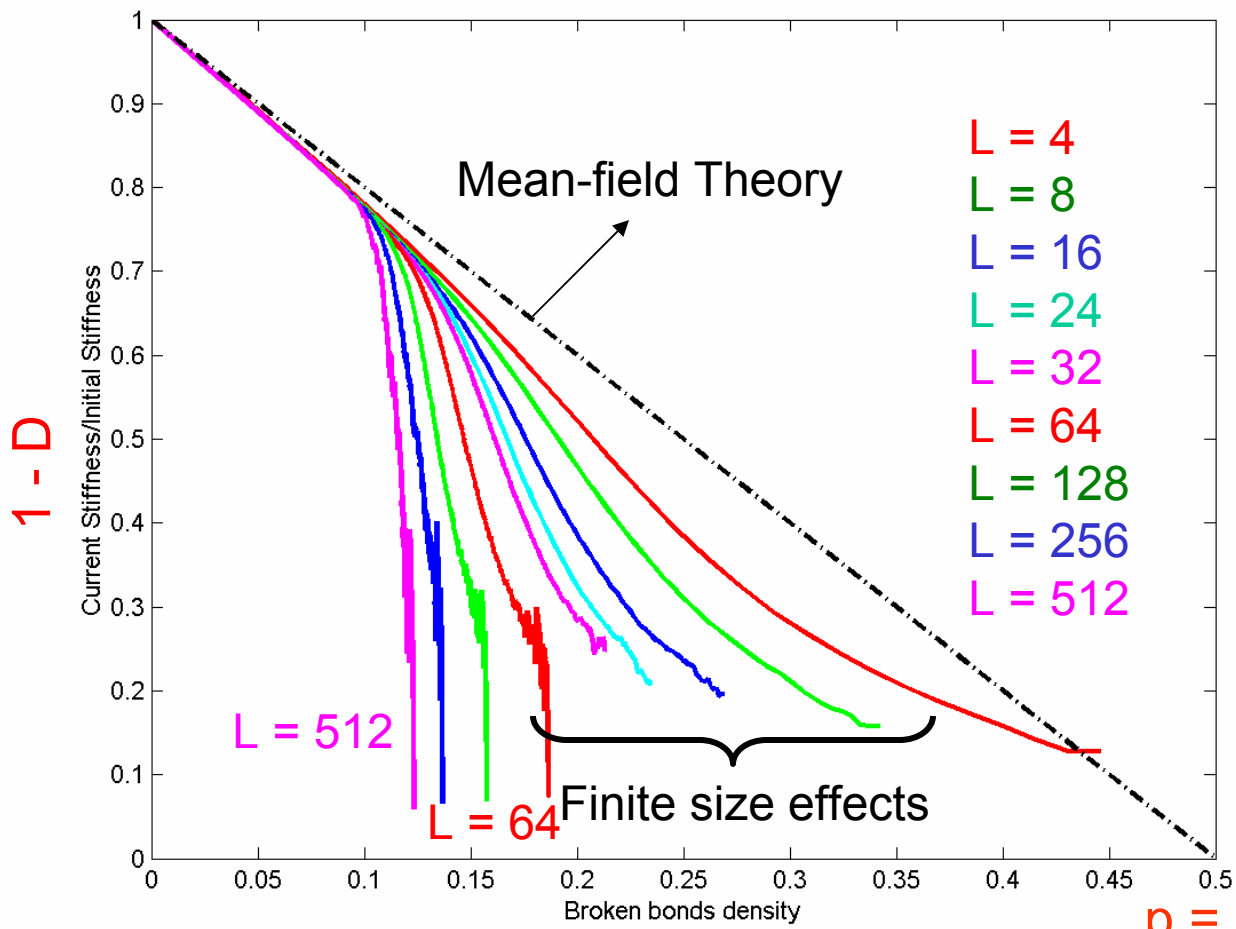


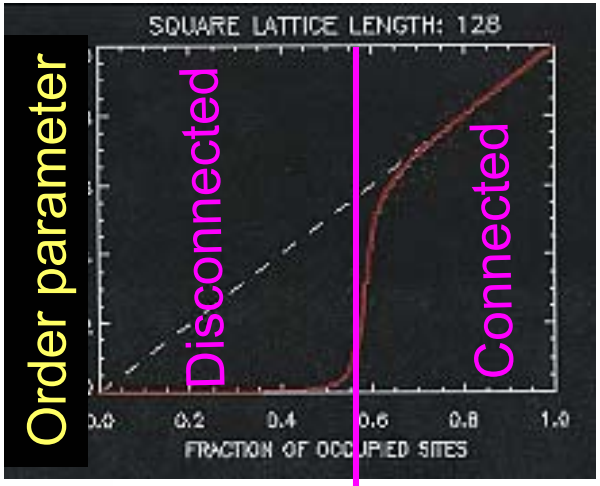
L = 32

Damage Definition Based on Stiffness Degradation

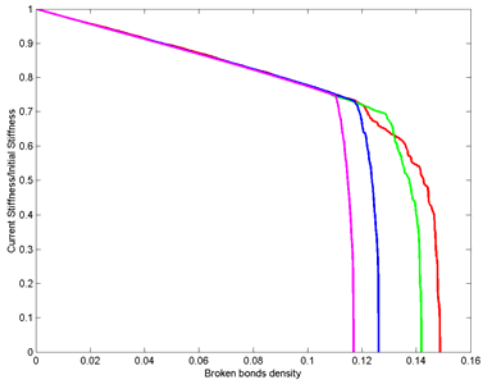
$$\text{Damage Variable} = \left\{ 1 - \frac{\text{Current Stiffness}}{\text{Initial Stiffness}} \right\}$$

→ Close to being intensive!



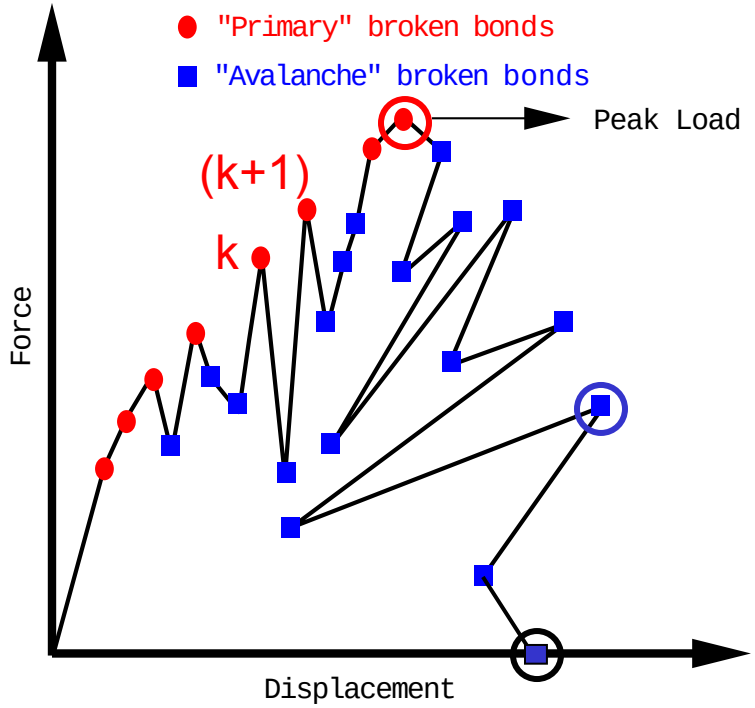


$$p = \frac{n_b}{L^d}$$



Typical Stiffness Degradation

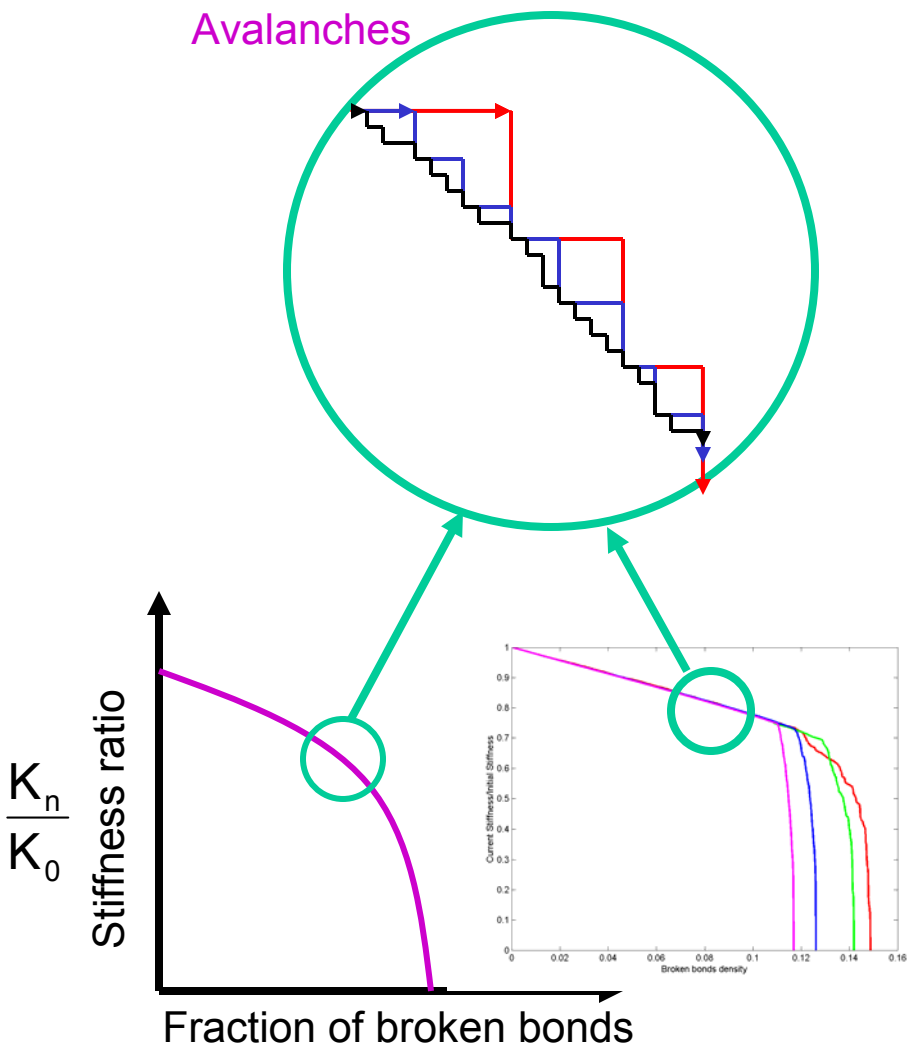
Material Breakdown: Avalanche Process



Load Controlled

Displacement Controlled

Bond Failure Controlled



Scaling Theory

RG Theory:

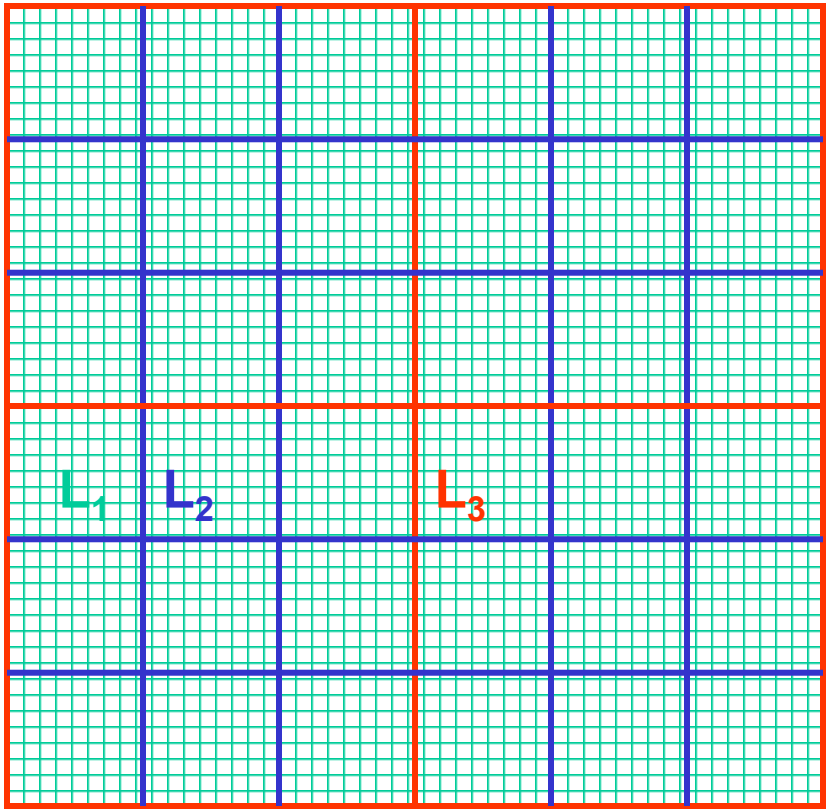
Coarse graining followed by rescaling of lengths such that the probability of failure under the influence of external load remains the same at both scales

Renormalization Approach for Scaling

Let $L_1 < L_2 < L_3$

p fraction of broken bonds at scale L_1

p' fraction of broken bonds at scale L_2



Coarse Graining*

$$p' = R_l(p) \quad \text{where} \quad l = \frac{L_2}{L_1}$$

$$p' - p_\infty = R_l(p) - R_l(p_\infty)$$

$$= \left.\frac{\partial R_l}{\partial p}\right|_{p=p_\infty} (p - p_\infty)$$

$$= \Lambda_l (p - p_\infty)$$

where $\Lambda_l = l^{-\alpha} \Rightarrow p_L - p_\infty = c_\infty L^{-\alpha}$

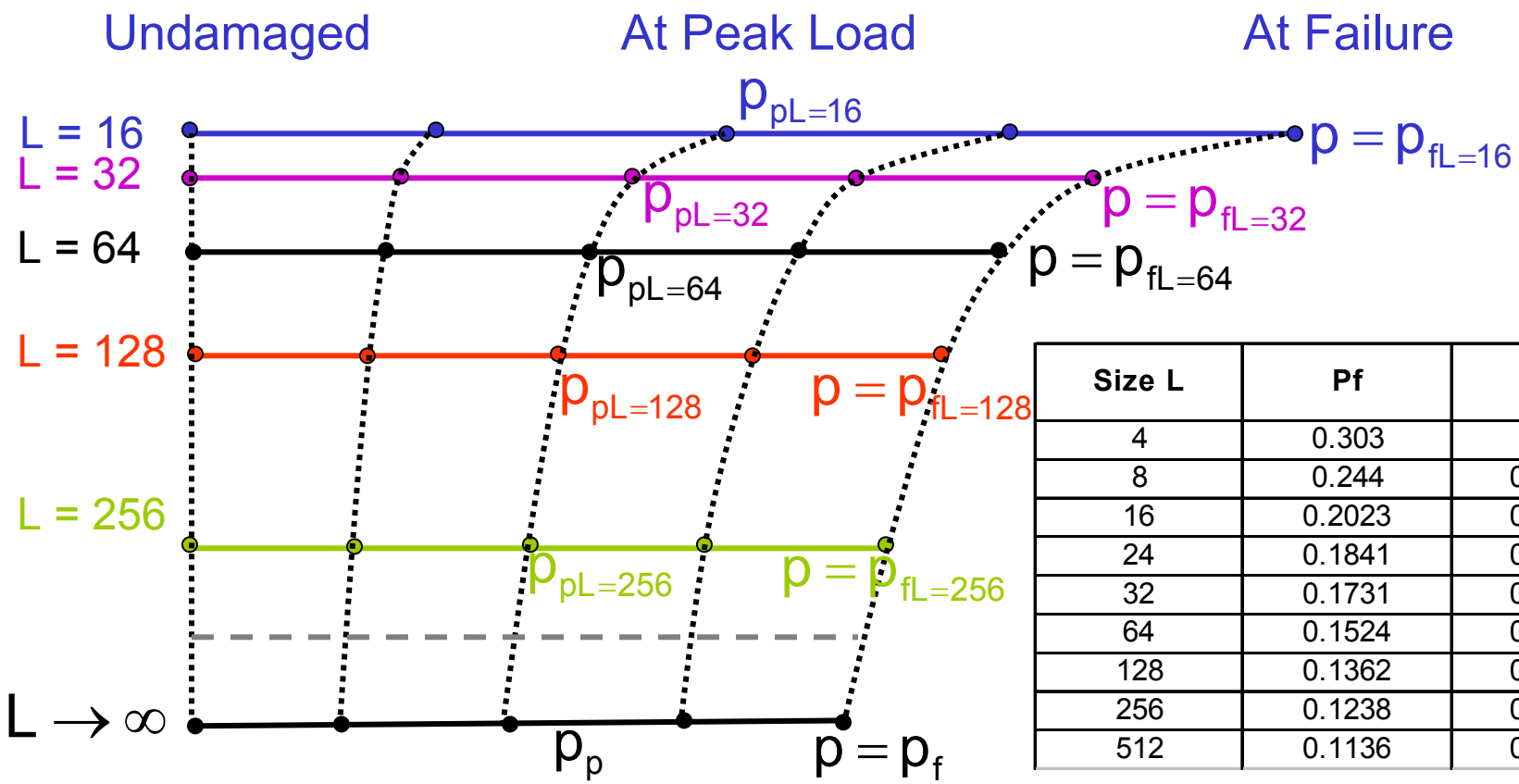
(* such that the probability of failure under the influence of external load remains the same at both scales)

non-zero p_∞ indicates critical crack size needed for macroscopic fracture

Intensive Definition of Damage

$$p_L - p_\infty = c_\infty L^{-\alpha} \quad \Rightarrow \quad n_L = N_{el}\left(p_\infty + c_\infty L^{-\alpha}\right)$$

$$c_\infty = c(p_\infty)$$



Size L	Pf	Pp
4	0.303	0.207
8	0.244	0.1813
16	0.2023	0.1612
24	0.1841	0.1513
32	0.1731	0.1451
64	0.1524	0.1325
128	0.1362	0.1222
256	0.1238	0.1142
512	0.1136	0.1072

Scaling of Number of Broken Bonds

$$p_f - p_\infty = c_\infty L^{-\alpha} \quad \Rightarrow \quad n_f = N_{el}\left(p_\infty + c_\infty L^{-\alpha}\right)$$

In the literature, power laws have been fitted for n_f versus L

$$n_f \propto L^{1.71\pm0.1} \quad \Rightarrow \quad p_f = \frac{n_f}{N_{el}} \propto \frac{L^{1.71\pm0.1}}{L^2} \xrightarrow{\text{Limit } L\to\infty} 0$$

Maximum crack size:

$$a_c \propto \varphi(p_f) \quad \text{and} \quad a_c \to 0 \quad \text{as} \quad p_f \to 0$$

Notes:

- Eliminates inconsistencies associated with the conventional power-law expressions
- Non-zero critical threshold $p_f \to p_\infty$ as $L \to \infty$

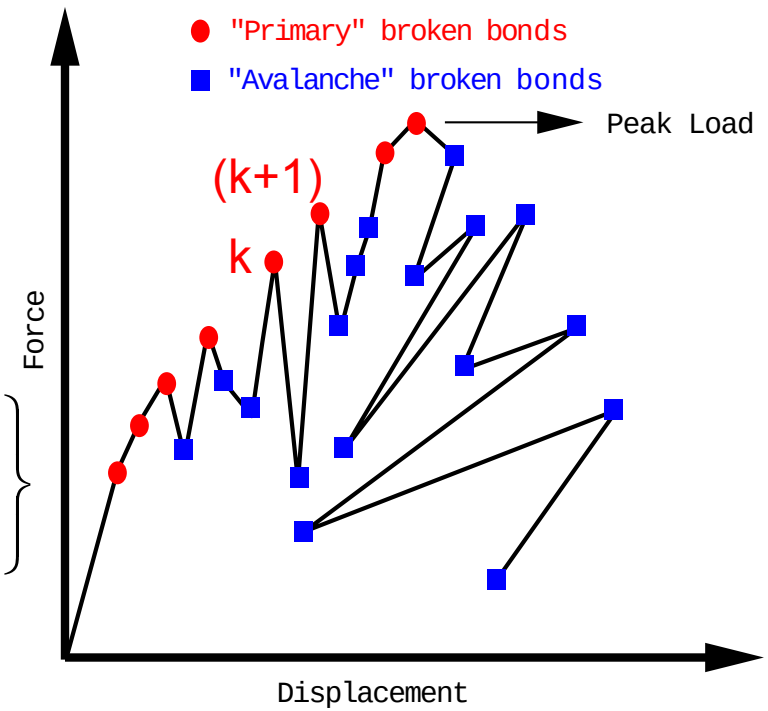
Failure Load Distribution

Let B_k = {set of k "primary" broken bonds}

Probability $f_{(k+1)}$ that $(k+1)^{th}$ "primary" bond fails

$$f_{(k+1)} = \prod_{j \in B_k} f_j$$

Define $G = \left\{ g_j = \dfrac{\sigma_j}{\sigma_{(j-1)}} \quad \forall j \in B_k \text{ and } g_1 = 1 \right\}$



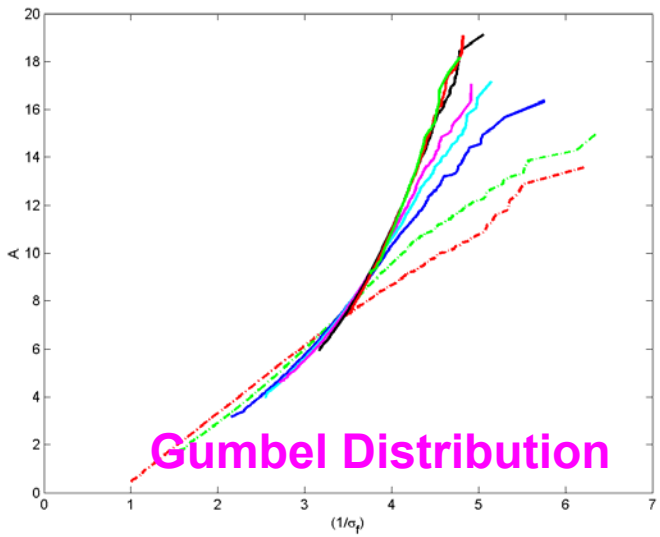
- g_j are independently distributed random variables.

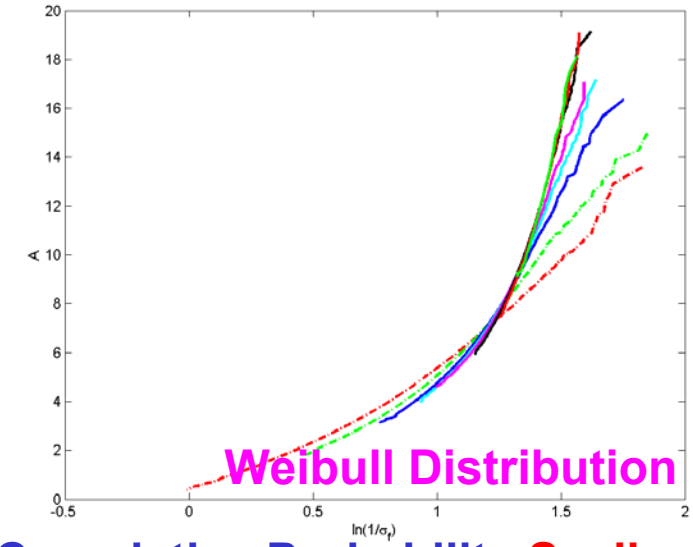
Stress $\sigma_{(k+1)}$ required to break $(k+1)^{th}$ "primary" bond $\sigma_{(k+1)} = \left(\prod_{j \in B_k} g_j \right) \sigma_1$

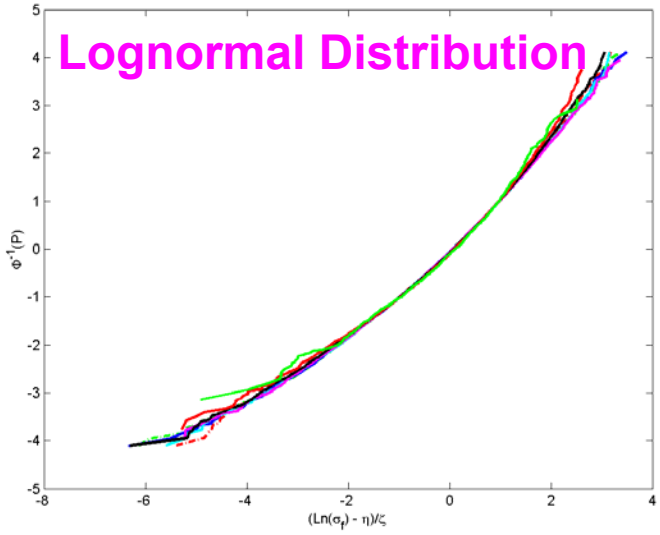
$\Rightarrow$ $\text{Prob}\left[\sigma_{(k+1)} \le \sigma\right] \approx \text{LN}$

Numerical Results

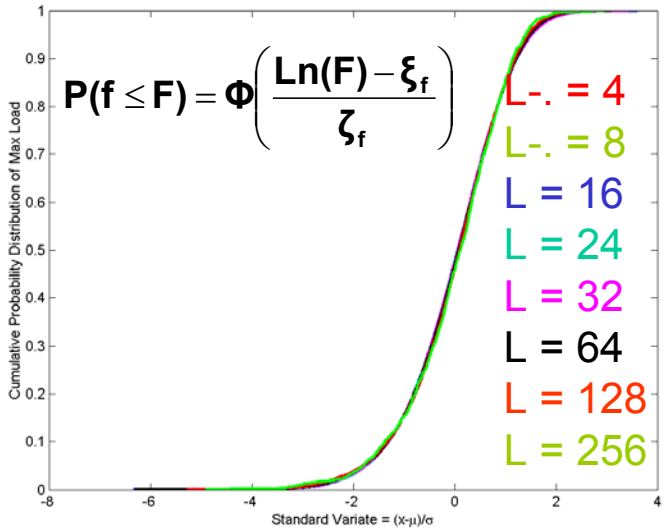
Scaling of Failure Load Distribution





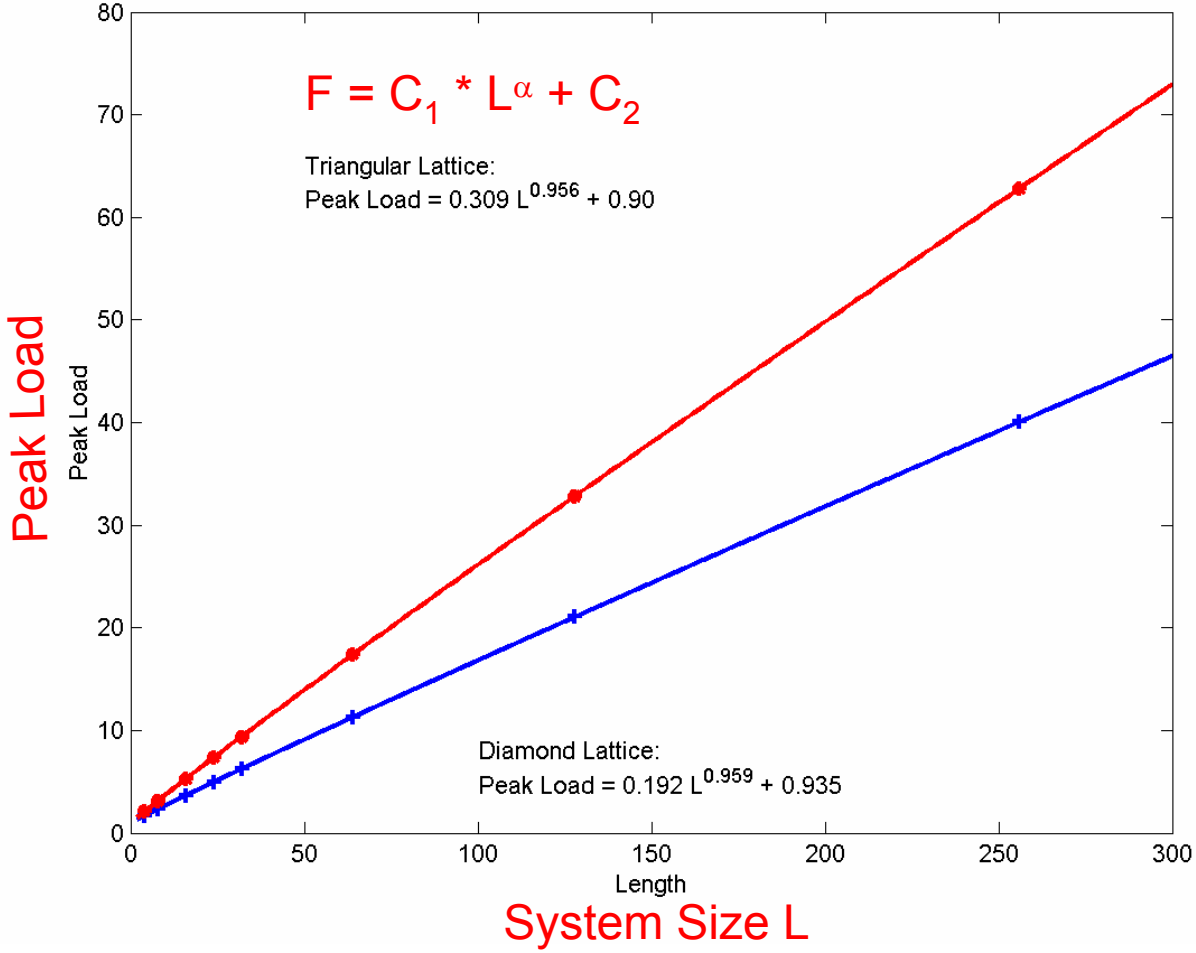


- **Cumulative Probability Scaling Law**



Standard Variate = (Ln(F)-ξ)/ζ

Size Effect on the Mean Failure Load



$$\sigma_{peak} = C_1 L^{(\alpha-1)} + \frac{C_2}{L}$$

Since

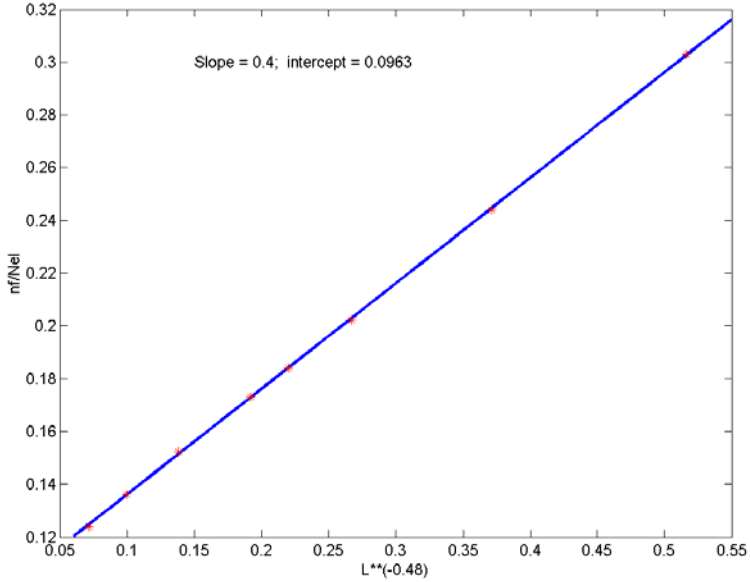
$$(1-\alpha) << 1 \Rightarrow L^{(1-\alpha)} \approx (\log(L))^{-\psi}$$

$$\sigma_{peak} = \frac{C_1}{(\log(L))^{\psi}} + \frac{C_2}{L}$$

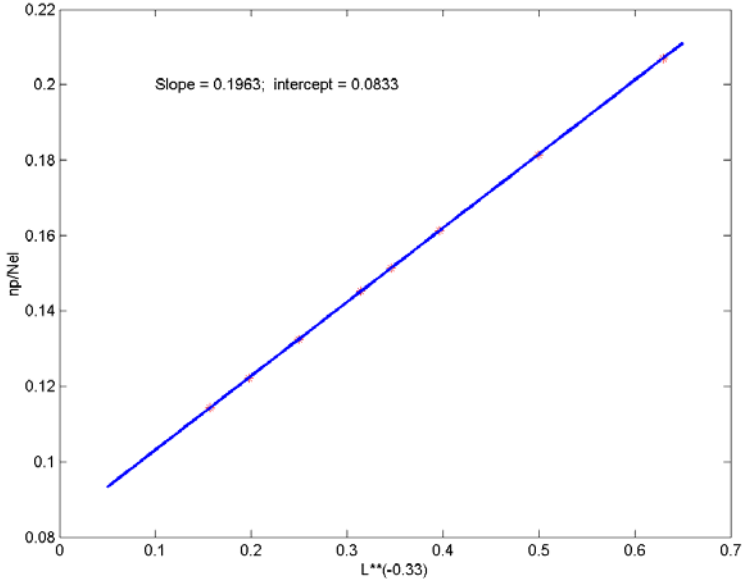
Mean fracture strength decreases very slowly with increasing system size L, and scales as $\sigma_{peak} \approx \frac{C_1}{(\log(L))^{\psi}}$ for very large L

Scaling of Number of Broken Bonds

At Failure



At Peak Load



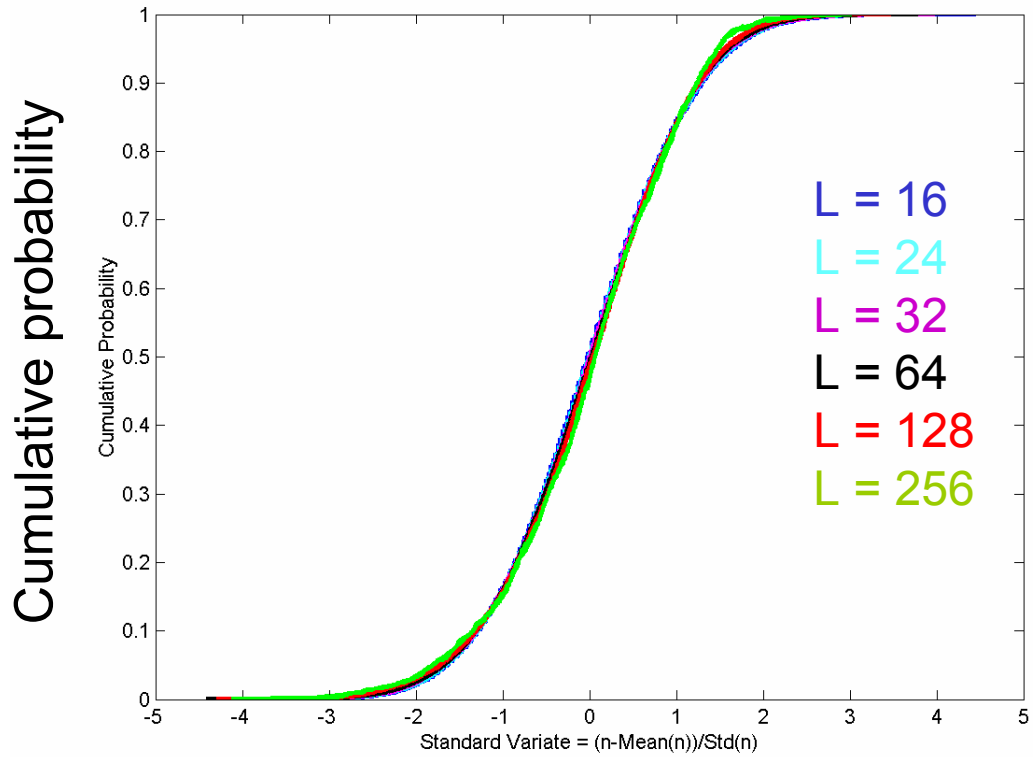
L = {4, 8, 16, 24, 32, 64, 128, 256, 512}

$$p_f - 0.096 = 0.4\ L^{-0.48}$$

$$p_p - 0.083 = 0.196\ L^{-0.33}$$

Probability Distributions for Fraction of Broken Bonds at Failure and at Peak Load

p_f = Mean fraction of broken bonds at failure
p_p = Mean fraction of broken bonds at peak load



Standard variate = (p – Mean(p)) / Std(p)

Probability distributions for fraction of broken bonds at failure as well as at peak load are identical and are normal

Computing Requirements

- Need to resolve after breaking a bond (intact lattice to total failure)
- Ensemble averaging of the response

Lattice Size (L)	CPU Time (sec)	CPU Time (sec)
	PCG Algorithm	New Algorithm
32	11.66	0.592
64	173.6	10.72
128	7473	212.2
256		5647
512		93779

CPU Time (sec) = $1.53 * 10^{-7}\ L^{4.36}$

For L = 1000 → Time ~ 21 days!

New Algorithm:

Direct Solver

- Breaking a bond is equivalent to rank-p update
- Use multiple-rank down-date algorithm of Cholesky factorization

Iterative Solver

- Laplacian on 2D and 3D lattice topology exhibits block structure
- Use block-circulant and optimal circulant preconditioners

Summary

For materials with broadly distributed heterogeneities,

- Scaling Law: $p_f - p_\infty = c_\infty L^{-\alpha}$
- Fraction of broken bonds p_f is finite:

$$p_f \to p_\infty \quad \text{as} \quad L \to \infty$$

- Fracture Strength: ~ Lognormal (LN)
- Mean fracture strength

$$\sigma_{peak} = \frac{C_1}{(\log(L))^\psi} + \frac{C_2}{L}$$

$$\Rightarrow \quad \sigma_{peak} \approx \frac{C_1}{(\log(L))^\psi} \quad \text{as} \quad L \to \infty$$

For materials with narrowly distributed heterogeneities,

- Weakest-link hypothesis
- p_f tends to zero threshold

$$p_f \to 0 \quad \text{as} \quad L \to \infty$$

- Fracture Strength: ~ Weibull or modified Gumbel
- Mean fracture strength

Weibull $\rightarrow$ $\sigma_{peak} = \dfrac{C_2}{L^\psi}$

Gumbel $\rightarrow$ $\sigma_{peak} \approx \dfrac{C_1}{(\log(L))^\psi}$

Mesoscopic Simulation: Discrete versus Continuum Models

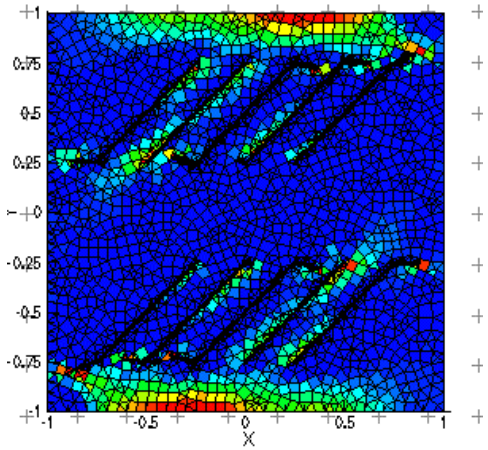
Discrete Lattice Models

- Suitable for studying the behavior of complex microstructures with heterogeneities
- Captures crack propagation and microstructure evolution with relative ease
- Ideal for studying statistical behavior including scaling and size effects
- Not readily applicable for capturing plasticity dominated phenomena

Continuum Models

- Suitable for studying the behavior of homogeneous solids
- Mesh size should be much smaller than typical inhomogeneity (crack, grain) size
- Captures inter-granular cracks using cohesive laws
- Not readily applicable for large number of heterogeneities
- Recent investigations on extended FE methods show promise in capturing inter- and trans-granular cracks and their interaction

Extended FE Models:
Multiple cracks, growth, interaction and coalescence



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