Thesis Defense Presentation

Correlated Percolation in the Fracture Dynamics on a Network of Ionomer Bundles

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Committee Members: Dr. Michael Eikerling, Barbara Frisken
Examiner: Dr. Steven Holdcroft
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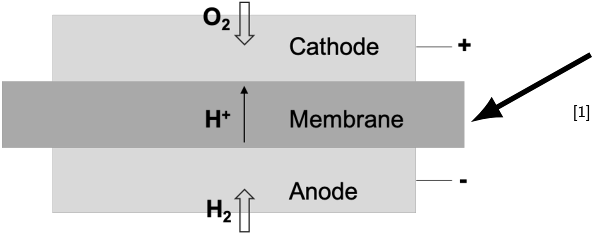
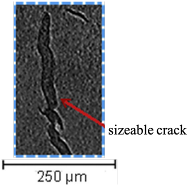
Burnaby
December 17th, 2020

Polymer Electrolyte Membranes (PEMs) in Fuel Cells

PEMs: transport-selective proton conductors
Fractures allow crossover fluxes of reactant gases, failure of the cell $\Rightarrow$ lifetime





[1] X-ray image of an Nafion PEM fractures

$$H_2 \longrightarrow 2H^+ + 2e^- \qquad \text{Anode}$$

$$2H^+ + \frac{1}{2}O_2 + 2e^- \longrightarrow H_2O \qquad \text{Cathode}$$

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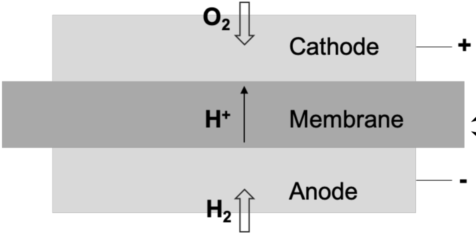

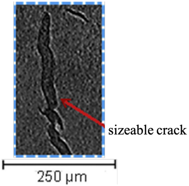

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[2] cross-linked PEM polymer network

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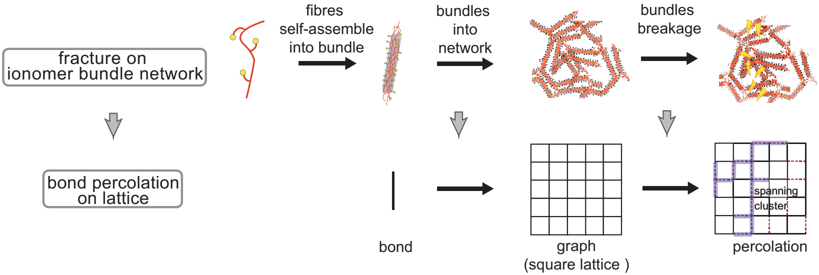
Mapping Polymer Networks to Bond Percolation Model



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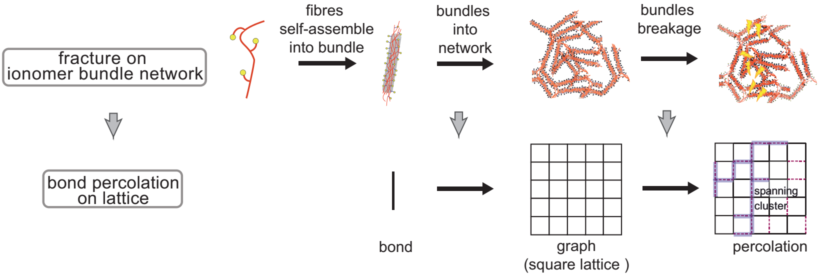
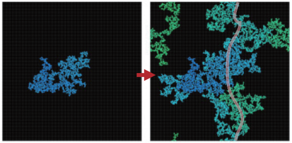


Fracture Mechanisms, Correlated Percolation

Providing insights for fracture systems

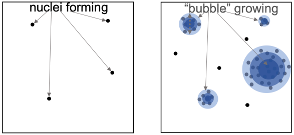
Fracture Systems – physical phenomena

- Percolation



[1]

- Nucleation and growth ($\Rightarrow$ random regime vs N & G regime)



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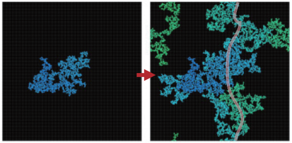

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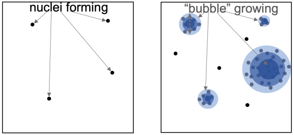
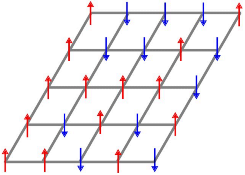


General statistical physics systems:

complex networks or classical physical disordered systems:
e.g. small-world, Ising models



Ising model
(Wald, 2017)

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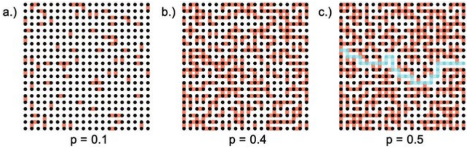
[2] C. Wald., Thermalisation and Relaxation of Quantum Systems. Université de Lorraine. 2017.

Uncorrelated Percolation

Static Model

Each bond (or site) has equal occupation probability p.
Critical p_c: percolation threshold



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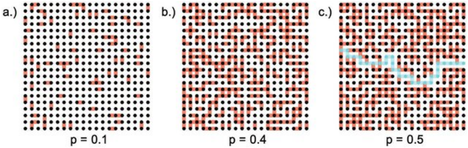

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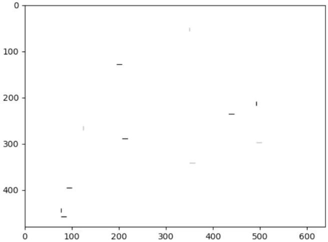
Kinetic Model

Bonds (or sites) are generated one by one randomly; p: concentration.
p_c: critical concentration



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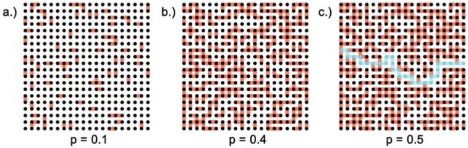

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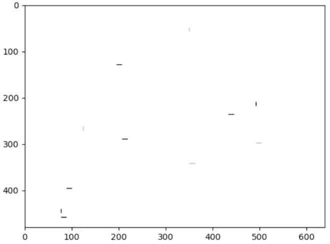
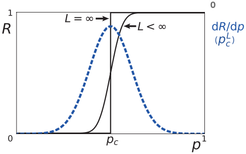
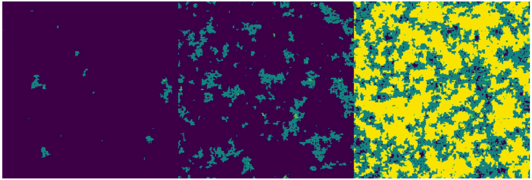




L: finite $\to \infty$
wrapping probability R: continuous $\to$ step-function
$\mathrm{d}R/\mathrm{d}p$ (p_c^L): Gaussian-like distribution $\to$ δ-like function

Correlated Percolation

Real physical systems, correlated random elements, e.g. epidemic spread



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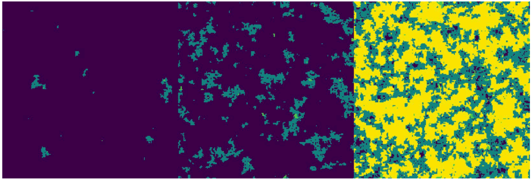

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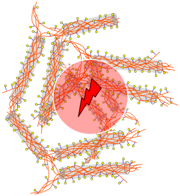

correlated failure events

Correlated Percolation

Instinctive expectation: reduction of percolation threshold p_c with increasing correlation strength.

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Theoretically, construct a correlation function (static percolation) $\langle u(\boldsymbol{r})u(\boldsymbol{r}+\boldsymbol{R})\rangle$, e.g.

$$\langle u(\boldsymbol{r})u(\boldsymbol{r}+\boldsymbol{R})\rangle \sim |\boldsymbol{R}|^{-\lambda}$$

Renault (1991)[1] and Mendelson (1997)[2], etc.: indeed, p_c reduce with λ.

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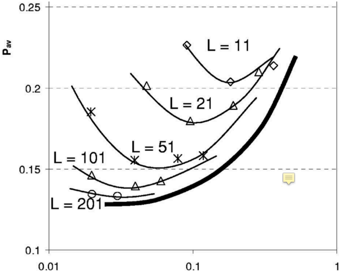
Exception, Harter (2005)[3]: p_c increase again, after reduction.



average p_c varies with normalized λ

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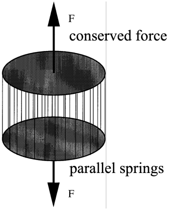
[3] T. Harter, Phys. Rev. E 72, 026120 (2005).

Correlated Percolation

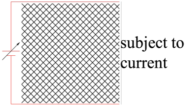
Instinctively, expectation of a reduction of percolation threshold p_c with increasing correlation strength.

How does p_c change with correlation strength in a more realistic system, i.e., a fracture system?

Simplified Fracture Models



Fiber Bundle Model (FBM)
(Kloster *et al.*, 1997)



Random Fuse Network (RFN)
(Shekhawat *et al.*, 2013)

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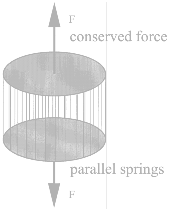
Random vs Correlated Fracture



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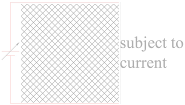

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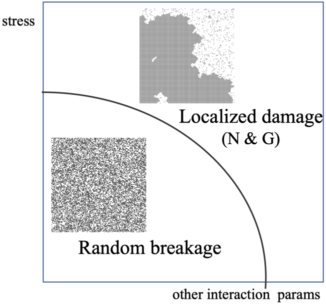

Exploration of phase diagram between random and localization regime

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Correlated Fracture Behavior Characterized by Stress Field $\boldsymbol{\sigma}$

Probabilistic Model:

Sequential failure, the probability of next fracture element:

$$p\{\text{failure at } \boldsymbol{x} \mid \text{failure history}\} \propto \kappa(\sigma(\boldsymbol{x}))$$

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$$\kappa_{\mathrm{p}}(\sigma) \propto \left(\frac{\sigma}{\sigma_0}\right)^{\rho}$$

(corresponding to Weibull distribution)

$$\kappa_e(\sigma) \propto e^{\beta(a\sigma - E_{\mathrm{a}})}$$

β: $1/(k_{\mathrm{B}}T)$; E_a: activation energy

(corresponding to Gumbel distribution)

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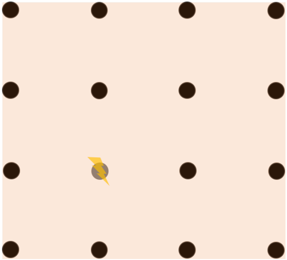
thermally activated (e.g., polymer fiber)

Stress Redistribution $\Rightarrow$ Evolution of Dynamic Stress Field

Failing element(s) distribute(s) stress load to others

Limiting stress sharing schemes:

- Equal Load Sharing (ELS)



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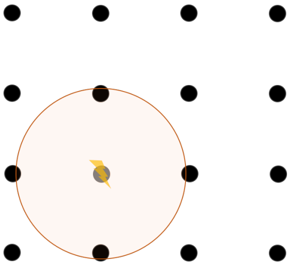

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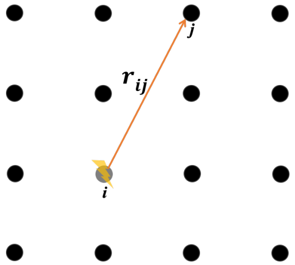

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Real material:

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$$\sigma_{add} \sim r^{-\gamma}$$

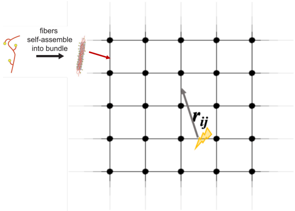
Hidalgo, Moreno, Kun and Herrmann, 2002, in FBM

ELS: $\gamma \to 0$; LLS: $\gamma \to \infty$

Hidalgo *et al.*, Phys. Rev. E 65, 046148 (2002).

Previous Work on Fiber-Bundle-Network

Fracture behaviors in fiber-bundle-network



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thermally activated exponential decay rate of an ionomer fiber

$$\kappa_{\mathrm{f}}(\sigma_{\mathrm{f}}) = \tau_0^{-1} \exp\left(-\beta\left(E_{\mathrm{a}} - \nu\sigma_{\mathrm{f}}\right)\right),$$

activation volume ν

- Assume ELS within a bundle
  $\Rightarrow$ lifetime of a bundle of fibers

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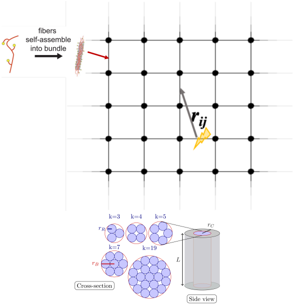

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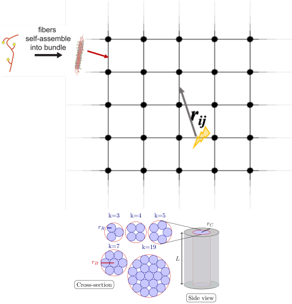

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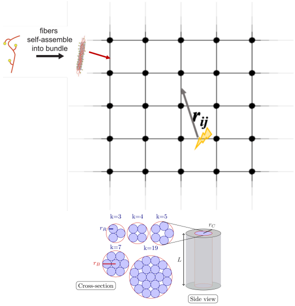
- Random breakage of bundles in the network (cubic lattice)



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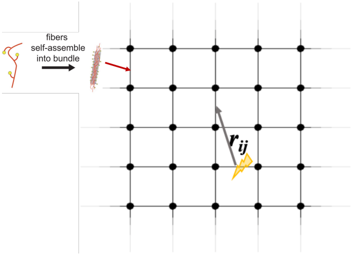
- Adopt simplified exponential form of bundle breakage rate

$$\kappa_{\rm b}(\sigma) = \alpha_k \exp\left(\eta_k \sigma\right)$$



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$$\sigma_j(t+\tau) = \sigma_j(t+\tau-1) + \sigma_i(t+\tau-1)F\left(r_{ij},\gamma\right)$$

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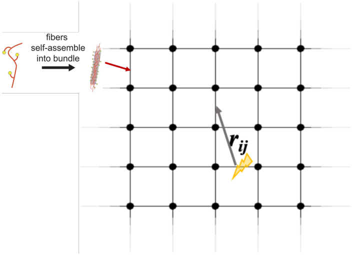

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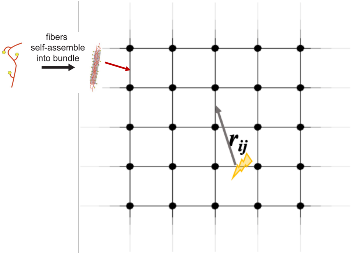

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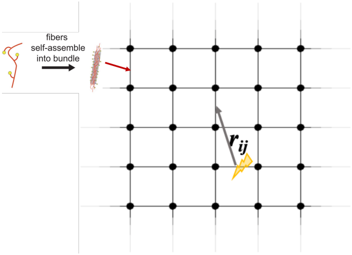

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(initial uniform stress & effective stress transfer range)

random percolation: $\sigma^0 \to 0$ or $\gamma \to 0$
strong correlation: high σ^0 or γ

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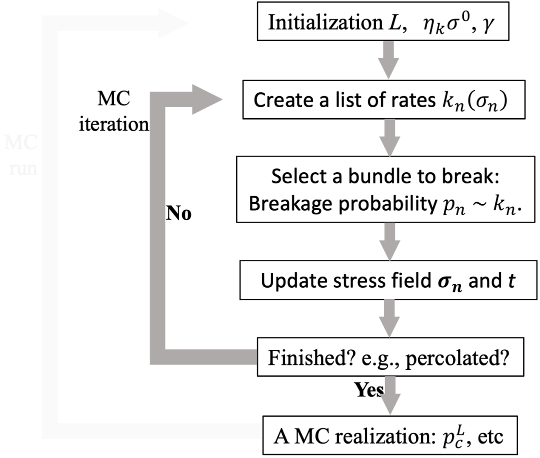
$$F\left(r_{ij},\gamma\right) = r_{ij}^{-\gamma}\left(\sum_{j\in I} r_{ij}^{-\gamma}\right)^{-1}$$

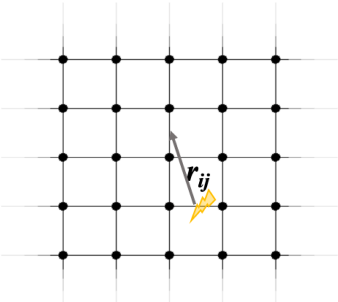
Simulation Process

$p\{$failure at $\boldsymbol{x}$ | current network structure, load field, ongoing failing element$\} \propto \kappa(\sigma(\boldsymbol{x}))$.

$\Rightarrow$ kinetic Monte Carlo

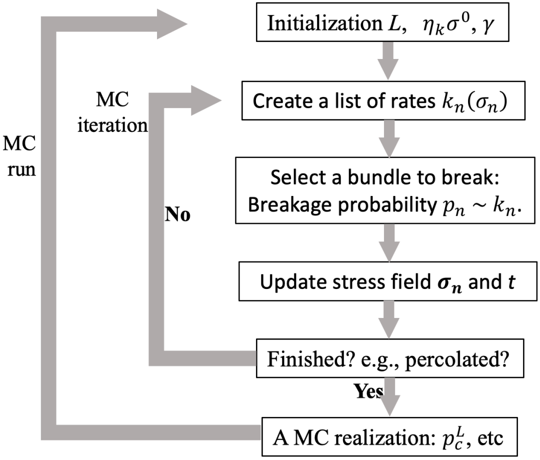
Rejection-Free Monte Carlo Method

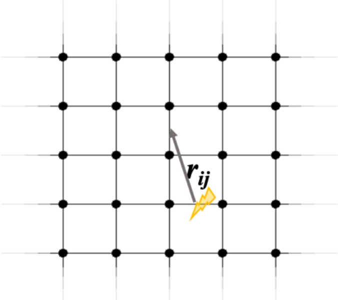




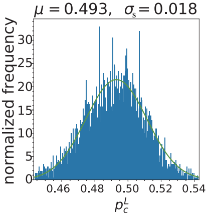
square lattice bundle network

Rejection-Free Monte Carlo Method





square lattice bundle network



$L = 50$, $\gamma = 0$ and $\eta_k\sigma = 0.45$

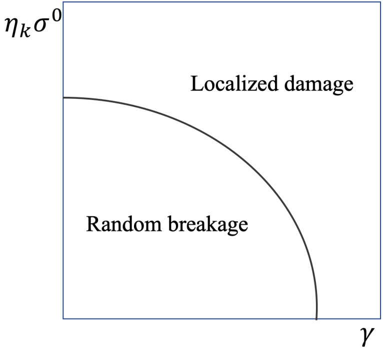
Framework of the Model

- Square lattice bond percolation
- Exponential breakage rate of bundles (network bonds)
- Stress Transfer: $\sigma_{\text{add}} \sim r^{-\gamma}$, stress conservation assumption

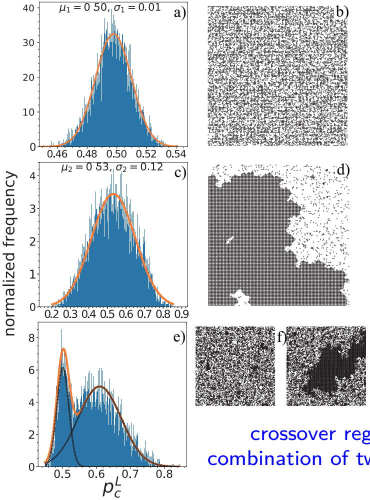
Results Overlook

Part (a): fixed finite-size ($L = 100$)
Part (b): varying size

- random regime & localized damage regime
  $\Rightarrow$ phase diagram over $\eta_k \sigma^0$ and γ
  (order parameter?)
- Variation of percolation threshold
- Lifetime



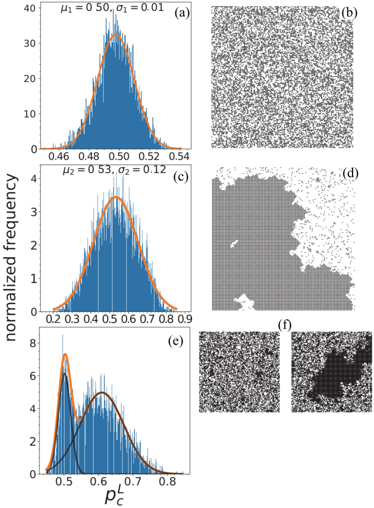
Distribution of Percolation Thresholds: Fracture Regimes



crossover region,
combination of two peaks

(a,b) random breakage; (c,d) localized damage; (e,f) crossover

Order Parameter ξ



(a,b) random breakage; (c,d) localized damage; (e,f) crossover

Order parameter:

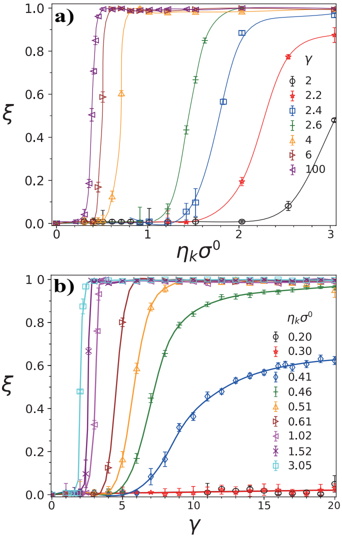
$$\xi = \frac{A_2}{A_1 + A_2}$$

A_1: area of left peak
A_2: area of right peak

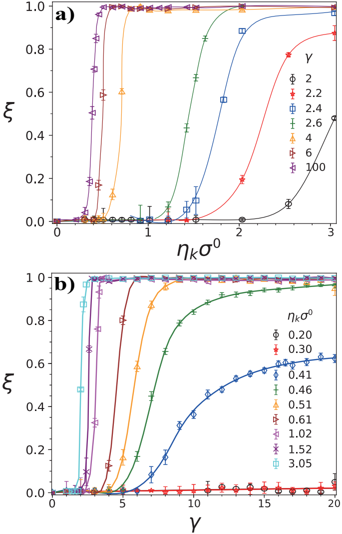
to describe

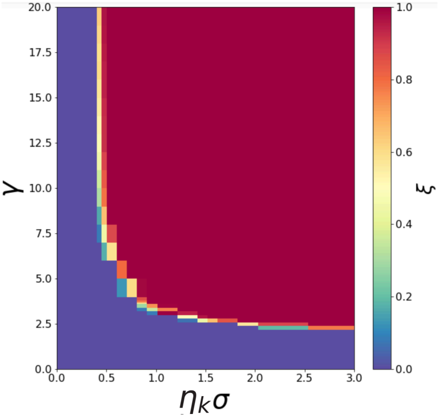
* correlation strength
* random breakage $\Leftrightarrow$ localization
  $(\xi \sim 0)$ $(\xi \sim 1)$

ξ vs σ^0 and γ

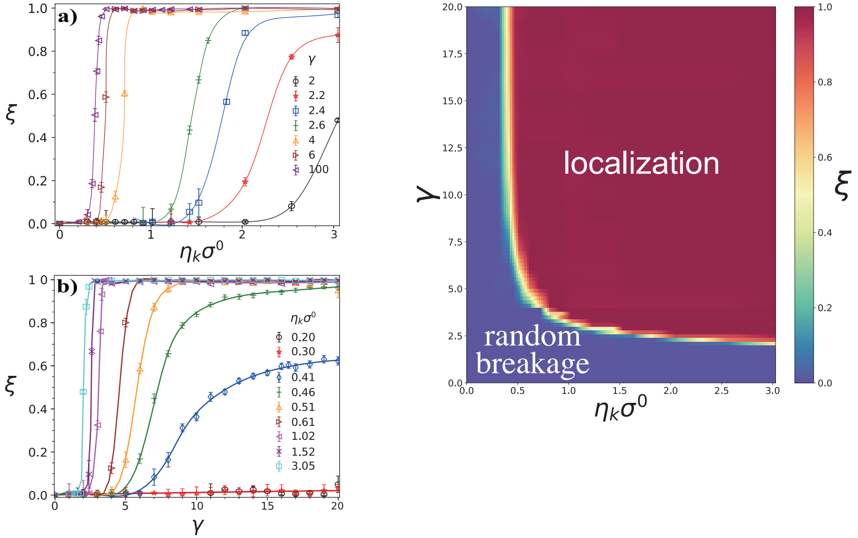


Phase Diagram

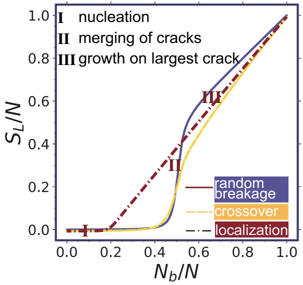




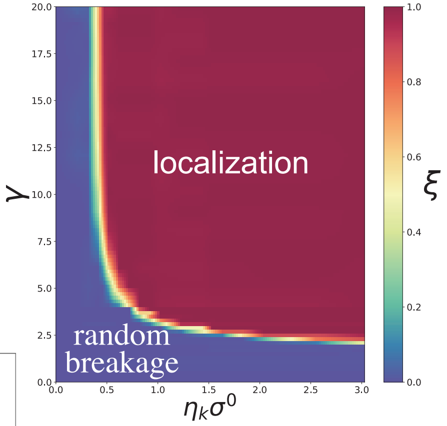
Phase Diagram

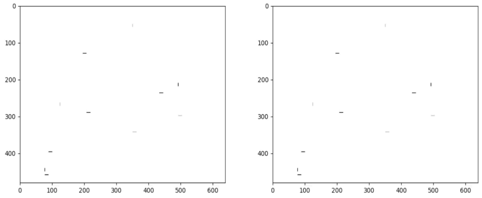


Phase Diagram



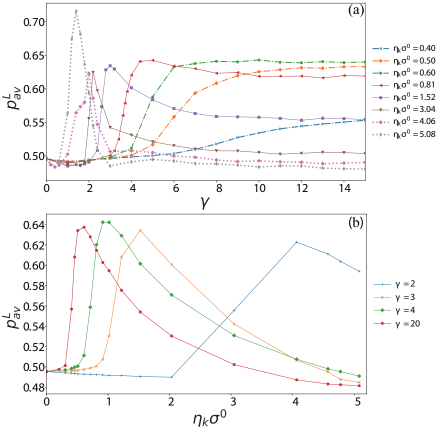
Dynamic analysis: largest crack size S_L growth





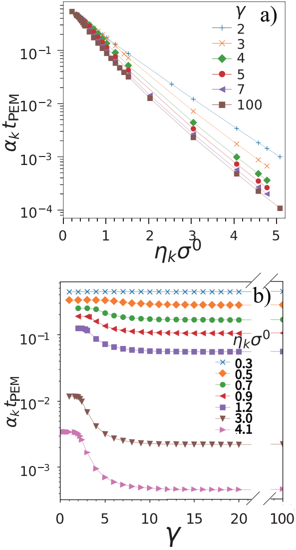
Animation: weak-correlated vs localization

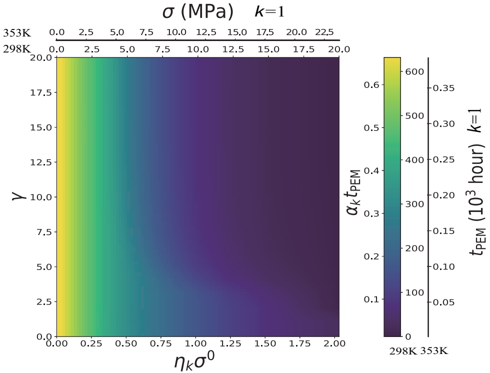
Variation of Percolation Thresholds p_c^L



Average percolation threshold p_c^{av}: drops, rises, drops again as ξ rises from 0 to 1.

Time-to-fractures

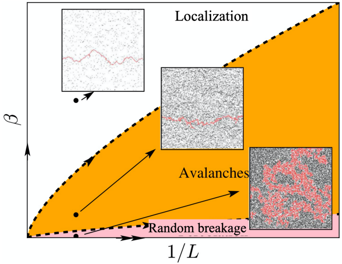




Now study the size effects

Why varying L?

- Phase diagram of random breakage and localization: localization dominates for larger L?
- Peculiar percolation threshold limited by size effects?

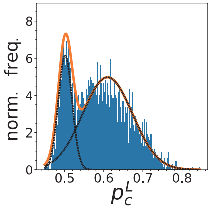


Phase diagram (RFN)
Shekhawat *et al.*, 2013

A. Shekhawat, *et al.* , Phys. Rev. Lett. 110, 185505 (2013).

Another Approach to Study Transition between Fracture Regimes

Limitation of the original approach, by ξ, to separate fracture regimes:

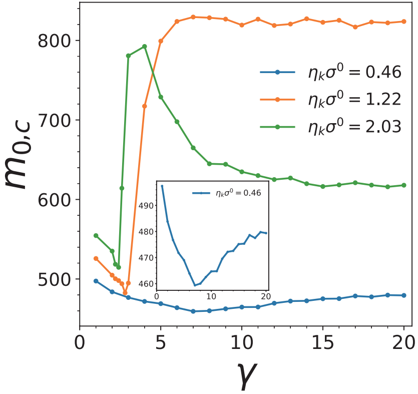


Adopt ξ,
determined by the areas of two peaks

- good for $L = 100$
  $*$ needs to complete more than 2000 MC runs for a set of L, $\eta_k\sigma^0$ and γ.
- But for $L > 250$? (a few hrs for a single MC run for a set of $L = 400$)

Another Approach to Study Transition between Fracture Regimes

m_0, 0th moment: the number of clusters
($*$ at least 100 MC runs per set)



Minimums of $m_{0,\mathrm{c}}$ to separate two regimes

Another Approach to Study Transition between Fracture Regimes

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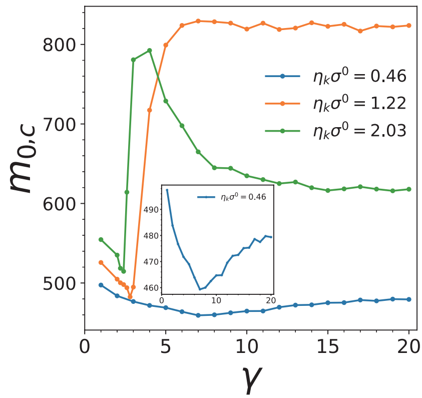
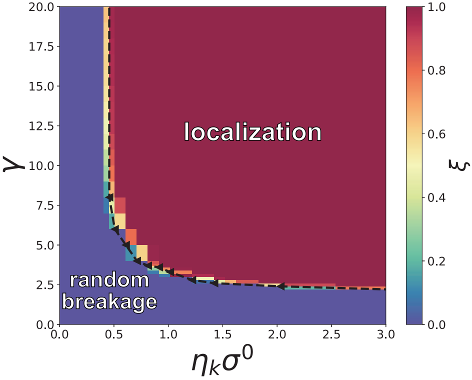
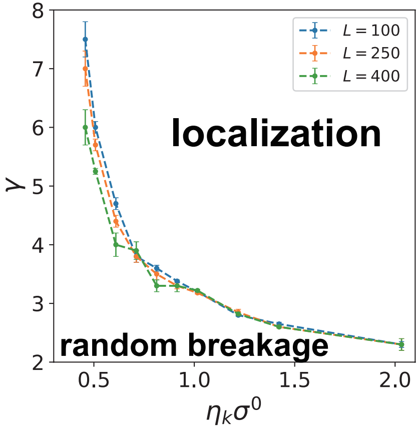




Minimums of $m_{0,c}$ to separate two regimes

Phase Diagrams vs L: a transition to localization regime for larger L

New phase diagrams



Phase Diagrams vs L: a transition to localization regime for larger L

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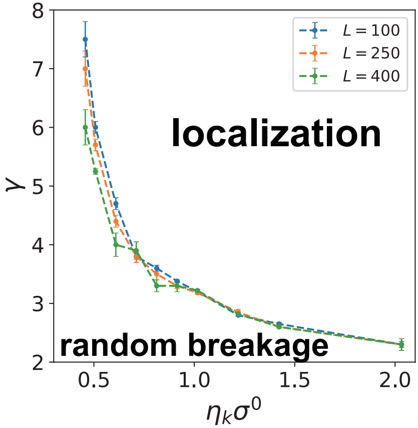
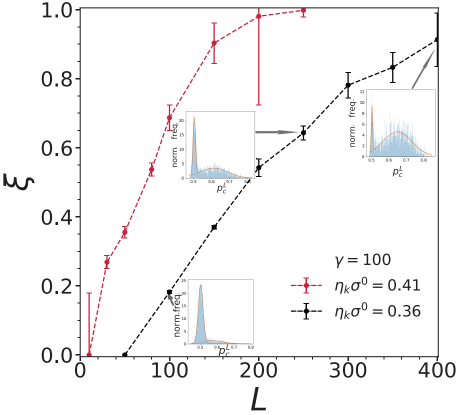


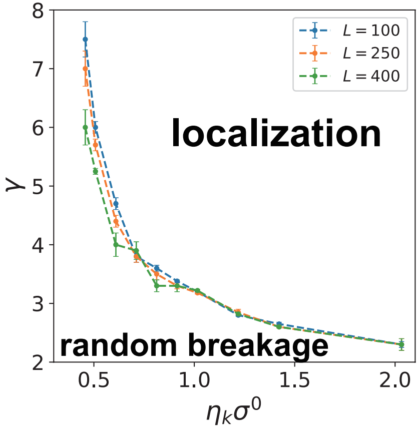
Check the (vicinity of) crossover region



ξ of two points in the (vicinity of) crossover as a function of L

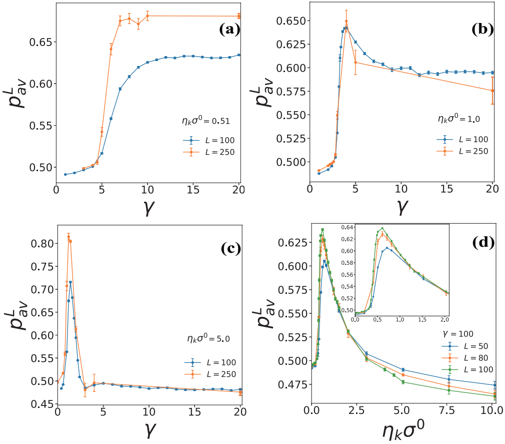
Phase Diagrams vs L: a transition to localization regime for larger L

New phase diagrams



Question:
Transition to Localization Regime for $L \to \infty$?

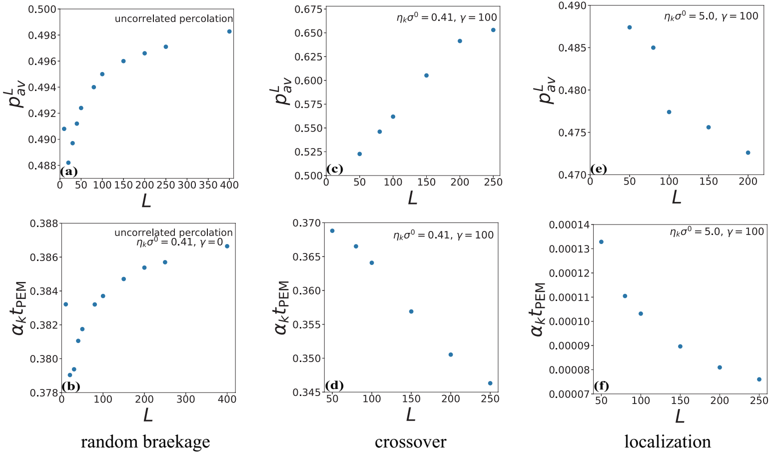
Percolation Thresholds vs L



p_{av}^L as a function of γ and $\eta_k\sigma^0$ for several L

Peculiar percolation phenomenon remains regardless of increase of L

Lifetimes vs L



Significant reduction as a function of L for localization regime.

Conclusions and Outlook

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- ∗ Two peaks in distribution of percolation thresholds in crossover
  ∗ Competition of the random breakage regime and localization regime
  ∗ Order parameter ξ

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- Percolation threshold: drops, rises, drops again.

Conclusions and Outlook

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- ∗ Two peaks in distribution of percolation thresholds in crossover
  ∗ Competition of the random breakage regime and localization regime
  ∗ Order parameter ξ
- ∗ Phase diagram over stress σ^0 and stress interaction range parameter γ
  ∗ For larger L: a transition to localization regime at crossover
- Percolation threshold: drops, rises, drops again.
- Lifetimes: similar phase diagram. Rapid decrease with L in the localization regime.

Conclusions and Outlook

Outlook

- Within same framework of model, exploration of smaller σ^0 and γ.
- Refine current stress conservation assumption: introduce the stress dissipation during stress transfer.
- 3D lattice; random network.

Thank you!

To my beloved mom!