

Correlated Site Percolation: a Microscopic Gibbs Field Model for the Macroscopic Behaviour of a Viscoplastic Fluid

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March 26, 2015

- 1 Yield-stress or Viscoplastic Materials
- 2 Correlated Site Percolation micro-mechanistic IPS model

What are they and why study them?



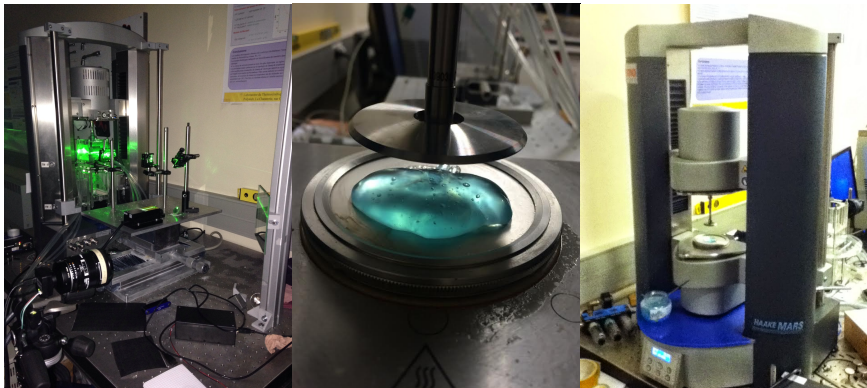
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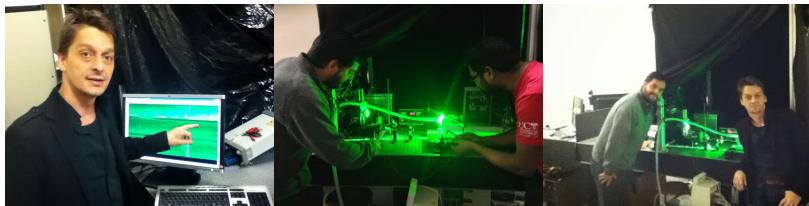


- Basically, solid-like until stressed past a yield-stress point.
- Correct material characterisation will bring understanding to unsteady processes found in the oil, food, cosmetic and bio-medical industries.

Measurements – Complex Fluids Lab, Nantes



Co-Researchers & their Collaborative Roles

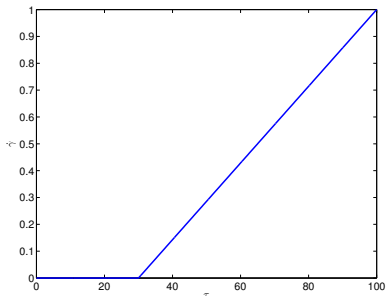


- An Experimental Complex-Fluids Physicist (TB)
- A Non-Newtonian Fluid Dynamicist (MM-G)
- A Statistician (RS)

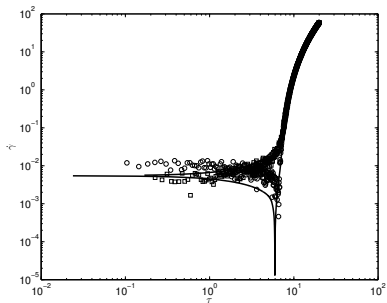
Need for a Richer Law/Model – Hysteretic Data

Why the “Bingham model” (solid below yield-stress and liquid above it) is not adequate for some situations?

applied stress (x) Vs. experienced strain or deformation rate (y)

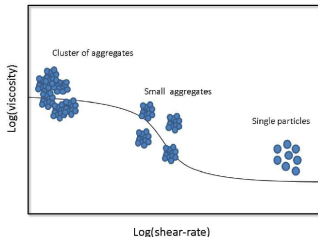


Physical Gel (Hair gel)



Empirical Data reveals hysteresis for unsteady flows

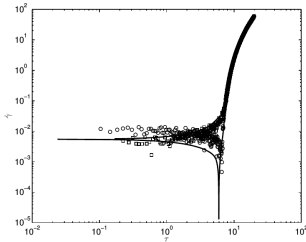
Microscopic Insight: Viscosity Depends on Micro-Structure



- Consider the material as a concentrated dispersion of structural units (SU).
- These units can form a loose association of particles that can be destroyed by shearing but re-establishes itself on standing.
- The driving force for microstructural change in flow is the result of the competition between break down due to flow stresses; build up due to in flow collisions and Brownian motion.
- To describe the complex behavior of the microstructure one can introduce a structural variable into the model and let rheological parameters to depend on it.

A Phenomenological Model Fits Better (Putz & Burghlea, 2009)

Please don't try to understand this right now!



Elastoviscoplastic fluid

$$\tau + \lambda_H(\Phi)\mu(\dot{\gamma}) \overset{\nabla}{\tau} = \mu(\dot{\gamma})\dot{\gamma}$$

and

$$\frac{D\Phi}{Dt} = -g(\tau)\Phi + f(\tau)(1 - \Phi).$$

with

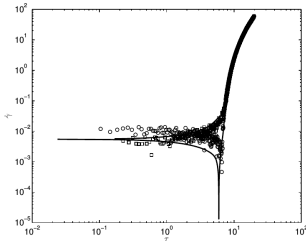
$$g(\tau) = K_d \left(1 + \tanh \left(\frac{\tau - \tau_y}{w} \right) \right)$$

$$f(\tau) = K_r \left(1 - \tanh \left(\frac{\tau - \tau_y}{w} \right) \right)$$

- This phenomenological model is not thermodynamically valid.

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- This phenomenological model is not thermodynamically valid.
- We make a simple thermodynamically valid model with observed macroscopic behaviours from microscopic structural considerations.

MOVIE before MATHS/STATS

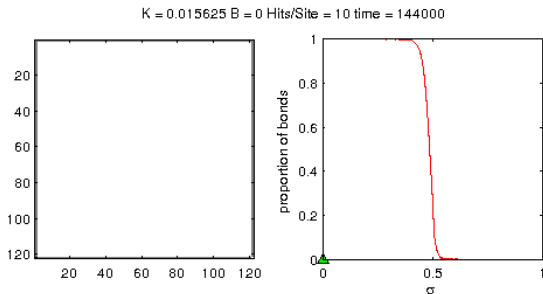
MOVIE TIME!

Let us try to watch sample paths of the material going from solid to liquid and back now.

$\beta = 0$: Site Percolation Configurations

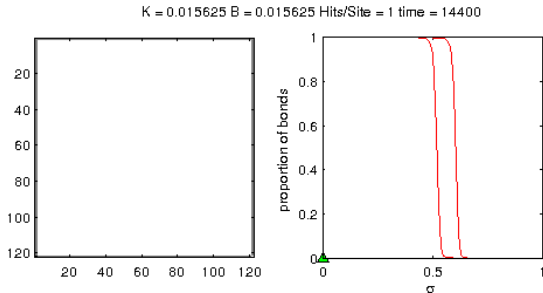
& Bonded Fraction \bar{b} on a $\tilde{\sigma}$ -stress Ramp \implies No Hysteresis; site-gelling prob. $p = 1/(1 + e^{\tilde{\sigma}})$

Open Problem: find critical p^* when a *percolation cluster* appears ($p_c \cong 0.5927$).



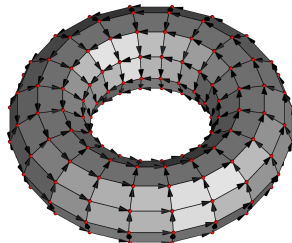
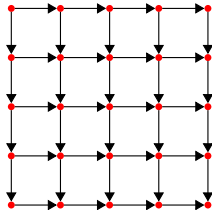
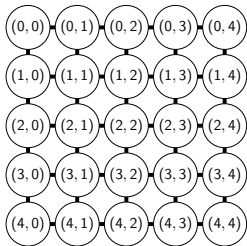
$\beta > 0$: Correlated Site Percolation Configurations

& Bonded Fraction \bar{b} on a σ -stress Ramp \implies Hysteresis; site-gelling prob $p_i = 1/(1 + e^{\tilde{\sigma} - i\beta})$



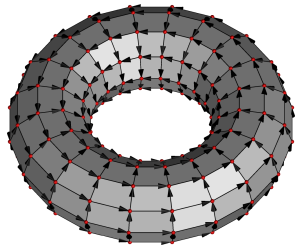
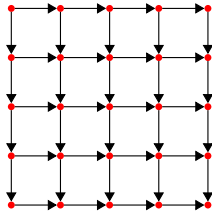
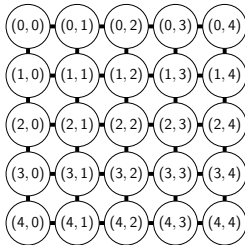
State Space

- \mathcal{G} = regular graph (2D toroidal square lattice)



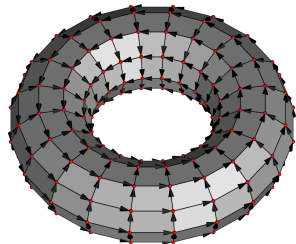
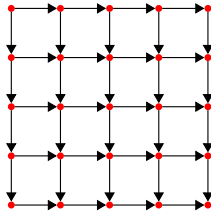
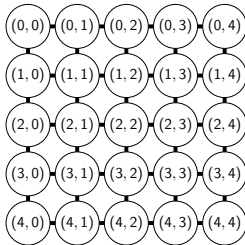
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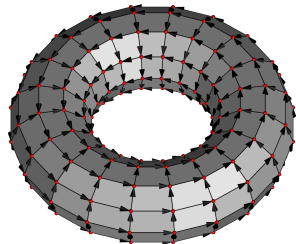
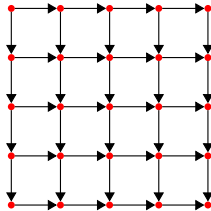
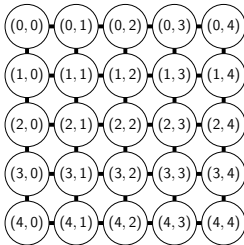
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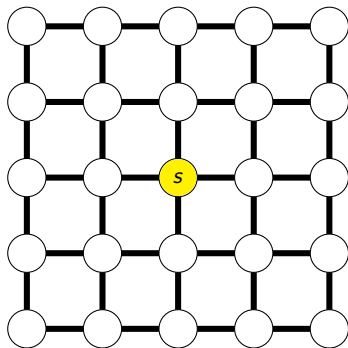
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- As $n \rightarrow \infty$ we study system behaviour on the boundary-free self-dual limiting square lattice



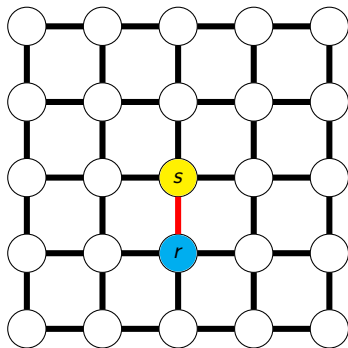
State Space Interpretation

- each site $s \in \mathbb{S}_n$ represents a *microscopic clump* of particles



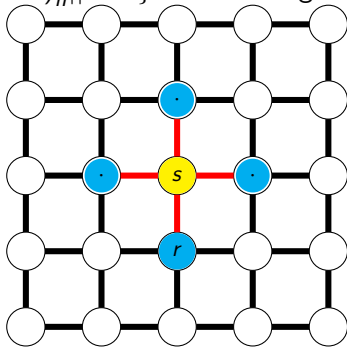
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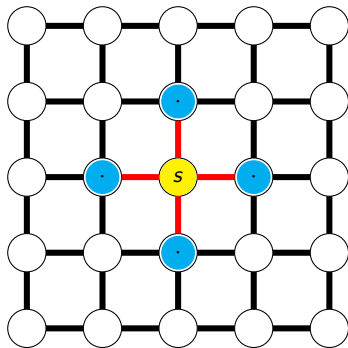
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- $N_s = \{r : \|\overline{(r - s)}_n\| = 1\}$ denotes neighbours of a site s



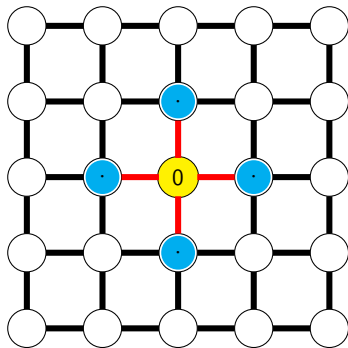
Phases of Sites

- $x(s) \in \Lambda = \{0, 1\}$ denotes the phase of the clump at site s



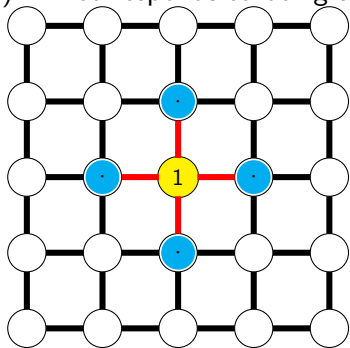
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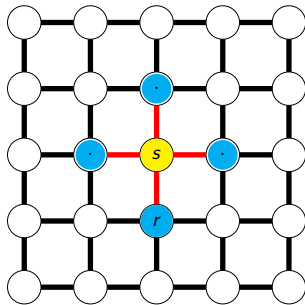
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Phases of Edges from Phases of Sites

$$y(\langle s, r \rangle) = \begin{cases} 1 & \text{if } r \in N_s \text{ and } x(r)x(s) = 1 \\ 0 & \text{if } r \in N_s \text{ and } x(r)x(s) = 0 \end{cases}$$

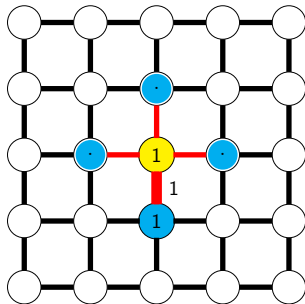
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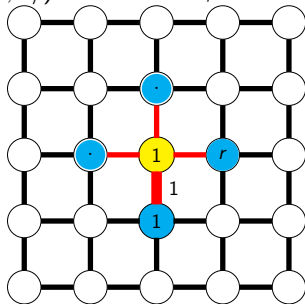
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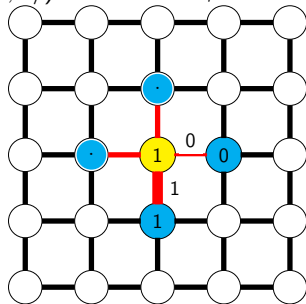
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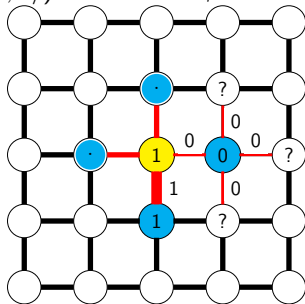
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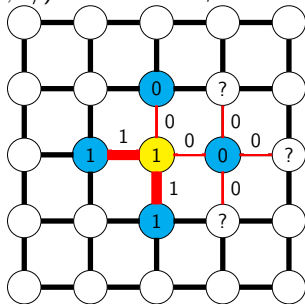
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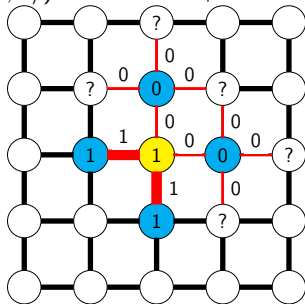
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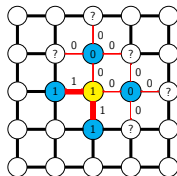
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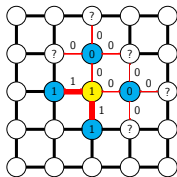
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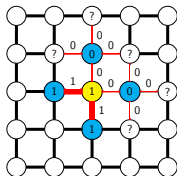
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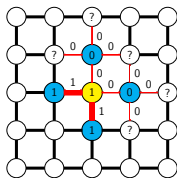
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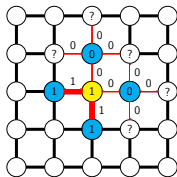
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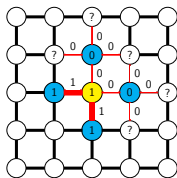
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- Will ODE \cong 'te $\mathbf{E}(\bar{A})$, where $\bar{A} = n^{-2} \sum_{s \in \mathbb{S}_n} X(s)$ is the gelled fraction



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By $X \sim \pi$, we mean that the random site configuration X has probability distribution π , i.e.,

$$\Pr(X = x) = \begin{cases} \pi(x) & \text{if } x \in \mathbb{X}_n \\ 0 & \text{otherwise} \end{cases}.$$

π is a Gibbs distribution

\therefore our neighbourhoods $\{N_s : s \in \mathbb{S}_n\}$ have only two clique types.

Given parameters α and β for the material's rheology, where:

- $\alpha \geq 0$ is the *site-specific threshold*,
- $\beta \in (-\infty, \infty)$ is the *interaction constant* of neighboring sites,
- and parameter $\sigma \geq 0$ for the externally applied stress,

\therefore the Gibbs potential over the singleton clique $\{s\}$ is:

$$V_{\{s\}}(x) = (\sigma - \alpha)x_s = \begin{cases} 0 & \text{if } x_s = 0 \\ \sigma - \alpha & \text{if } x_s = 1 \end{cases},$$

and over the doubleton clique $\langle s, r \rangle$ with $r \in N_s$ is:

$$V_{\langle s, r \rangle}(x) = -\beta x_s x_r = \begin{cases} 0 & \text{if } (x_s, x_r) = (0, 0) \\ 0 & \text{if } (x_s, x_r) = (1, 0) \\ 0 & \text{if } (x_s, x_r) = (0, 1) \\ -\beta & \text{if } (x_s, x_r) = (1, 1) \end{cases},$$

The energy function of this potential is

$$\begin{aligned}
 \mathcal{E}(x) &= \sum_C V_C(x) \\
 &= \sum_{s \in \mathbb{S}_n} V_{\{s\}}(x) + \sum_{\langle s,r \rangle \in \mathbb{E}_n} V_{\langle s,r \rangle}(x) \\
 &= \left(-\beta \sum_{\langle s,r \rangle \in \mathbb{E}_n} x_s x_r + (\sigma - \alpha) \sum_{s \in \mathbb{S}_n} x_s \right) .
 \end{aligned}$$

$\therefore \mathcal{E}(x)$ only depends on β and the difference $(\sigma - \alpha)$, we can reparameterize by $\tilde{\sigma} := \sigma - \alpha \geq -\alpha$ for convenience

$$\mathcal{E}(x) = \left(-\beta \sum_{\langle s,r \rangle \in \mathbb{E}_n} x_s x_r + \tilde{\sigma} \sum_{s \in \mathbb{S}_n} x_s \right) ,$$

through $(\tilde{\sigma}, \beta) \in [-\alpha, \infty) \times (-\infty, \infty)$.

Thermodynamic Validity by Gibbs Construction

Let the expectation of $g : \mathbb{X}_n \rightarrow \mathbb{R}$, with respect to π , be

$$\mathbf{E}_\pi(g) := \sum_{x \in \mathbb{X}_n} g(x) \pi(x)$$

then the *internal energy* of the system is

$$\mathcal{U} = \mathbf{E}_\pi(\mathcal{E}) = \sum_{x \in \mathbb{X}_n} \mathcal{E}(x) \pi(x) ,$$

and the *free energy* of the system is

$$\mathcal{F} = -kT \ln(Z_{kT}) .$$

Our model satisfies the standard thermodynamic equality:

$$-T^2 \frac{\partial}{\partial T} \left(\frac{\mathcal{F}}{T} \right) = \mathcal{U} .$$

We sometimes emphasize the dependence upon α , β and σ by:

$$\mathcal{E}(x) = \mathcal{E}_{\alpha, \beta, \sigma}(x) \quad \text{and} \quad \pi(x) = \pi_{\alpha, \beta, \sigma}(x) .$$

Local Specification $\pi_s(x)$ from Local Energy $\mathcal{E}_s(x)$

The *local energy* at site s of configuration x is

$$\begin{aligned}
 \mathcal{E}_s(x) &= \sum_{C \ni s} V_C(x) \\
 &= V_{\{s\}}(x) + \sum_{r \in N_s} V_{\langle s,r \rangle}(x) \\
 &= (\sigma - \alpha)x_s - \beta \sum_{r \in N_s} x_s x_r \\
 &= x_s \left((\sigma - \alpha) - \beta \sum_{r \in N_s} x_r \right) \\
 &= x_s (\tilde{\sigma} - \beta i) .
 \end{aligned}$$

where $i := \sum_{r \in N_s} x_r$ is the # of neighbouring sites of s in phase 1

Local Specification $\pi_s(x)$ from Local Energy $\mathcal{E}_s(x)$

Then the *local specification* is

$$\begin{aligned}\pi_s(x) &= \frac{\exp(-\frac{1}{kT}\mathcal{E}_s(x))}{\sum_{\lambda \in \Lambda} \exp(-\frac{1}{kT}\mathcal{E}_s(\lambda, x(\mathbb{S} \setminus s)))} \\ &= \begin{cases} \frac{\theta}{1+\theta} & \text{if } x_s = 0 \\ \frac{1}{1+\theta} & \text{if } x_s = 1 \end{cases},\end{aligned}\quad (1)$$

where, $(\lambda, x(\mathbb{S} \setminus s)) \in \mathbb{X}_n$ has phase λ at s and identical to x elsewhere, and

$$\theta = \theta(s, \alpha, \beta, \sigma) = \exp\left(-\frac{1}{kT}(\beta x_{N_s} - (\sigma - \alpha))\right). \quad (2)$$

Local Specification $\pi_s(x)$ from Local Energy $\mathcal{E}_s(x)$

Then the *local specification* is

$$\begin{aligned} \pi_s(x) &= \frac{\exp\left(-\frac{1}{kT}\mathcal{E}_s(x)\right)}{\sum_{\lambda \in \Lambda} \exp\left(-\frac{1}{kT}\mathcal{E}_s(\lambda, x(\mathbb{S} \setminus s))\right)} \\ &= \begin{cases} \frac{\theta}{1+\theta} & \text{if } x_s = 0 \\ \frac{1}{1+\theta} & \text{if } x_s = 1 \end{cases}, \end{aligned} \quad (1)$$

where, $(\lambda, x(\mathbb{S} \setminus s)) \in \mathbb{X}_n$ has phase λ at s and identical to x elsewhere, and

$$\theta = \theta(s, \alpha, \beta, \sigma) = \exp\left(-\frac{1}{kT}(\beta x_{N_s} - (\sigma - \alpha))\right). \quad (2)$$

In this work we focus on the effect of varying external stress σ at a constant ambient temperature, and therefore without loss of generality, we take $kT = 1$ and work with $\pi(x) = Z_1^{-1} \exp(-\mathcal{E}(x))$.

Markov chain on configuration space

Our model is an \mathbb{X}_n -valued Markov chain $\{X(m)\}_{m \in \{0,1,2,\dots\}}$ with the initial distribution $\delta_{x(0)}$. Then the m -step transition probability is:

$$\Pr \{ X(m) | X(0) = x(0) \} = \delta_{x(0)} (P_{\alpha,\beta,\sigma})^m, \quad (3)$$

with the 1-step transition probability matrix $P_{\alpha,\beta,\sigma}$ over any pair of configurations $(x, x') \in \mathbb{X}_n \times \mathbb{X}_n$ given by:

$$P_{\alpha,\beta,\sigma}(x, x') = \begin{cases} \frac{1}{n^2} \frac{1}{1+\theta} & \text{if } \|x - x'\| = 1, 0 = x_s \neq x'_s = 1 \\ \frac{1}{n^2} \frac{\theta}{1+\theta} & \text{if } \|x - x'\| = 1, 1 = x_s \neq x'_s = 0 \\ \frac{1}{n^2} \frac{1}{1+\theta} & \text{if } \|x - x'\| = 0, 1 = x_s = x'_s = 1 \\ \frac{1}{n^2} \frac{\theta}{1+\theta} & \text{if } \|x - x'\| = 0, 0 = x_s = x'_s = 0 \\ 0 & \text{otherwise} . \end{cases} \quad (4)$$

with **self** and **non-self-at-s** transitions & $\theta = \theta(s, \alpha, \beta, \sigma)$ is indeed a function of the site s and the three parameters: α , β and σ .

In English, $\{X(m)\}$ evolves by these locally specified rules

This is our **Simulation Algorithm** (Glauber Dynamics or Gibbs Sampler)

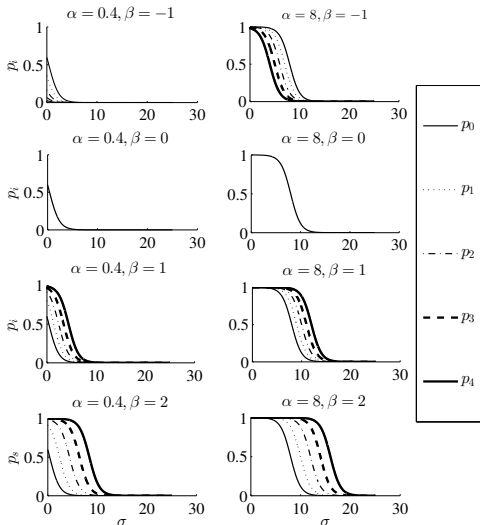
- given the current configuration x , we first choose one of the n^2 sites in \mathbb{S}_n uniformly at random with probability n^{-2} ,
- denote this chosen site by s and let the number of bondable neighbors of s be $i \in \{0, 1, 2, 3, 4\}$, and
- finally change the phase at s to 1, i.e., set $x_s = 1$ with probability

$$p_i := (1 + \theta)^{-1} = (1 + \theta(s, \alpha, \beta, \sigma))^{-1} = 1/(1 + e^{(\sigma - \alpha - i\beta)}) \quad (5)$$

and set $x_s = 0$ with probability $1 - p_i$.

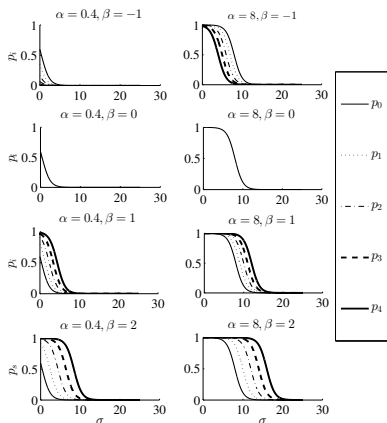
p_i as a function of σ , with $\alpha \in \{0.4, 8\}$ & $\beta \in \{-1, 0, 1, 2\}$

$p_i = \Pr\{\text{site } s \text{ with } i \text{ neighbors in phase 1, is also in phase 1}\}$



p_i as a function of σ , with $\alpha \in \{0.4, 8\}$ & $\beta \in \{-1, 0, 1, 2\}$

$p_i = \Pr\{\text{site } s \text{ with } i \text{ neighbors in phase 1, is also in phase 1}\}$



α translates & β controls the distance between p_i 's.

So $p_i = p_i(\beta, \tilde{\sigma})$, recall $\tilde{\sigma} = \sigma - \alpha$

Three β -dependent Behavioural Regimes

agglomerative interactions

$$\beta > 0 \implies 0 < p_0 < p_1 < p_2 < p_3 < p_4 < 1 .$$

\therefore the probability of a site being in phase 1 increases with the number of its neighboring sites also being in phase 1.

non-interactive (classical site percolation model)

$$\beta = 0 \implies 0 < p = p_0 = p_1 = p_2 = p_3 = p_4 = 1 / (1 + e^{\sigma - \alpha}) < 1 .$$

\therefore the probability of a site being in phase 1 is independent of the phase of the neighboring sites and identically p at each site.

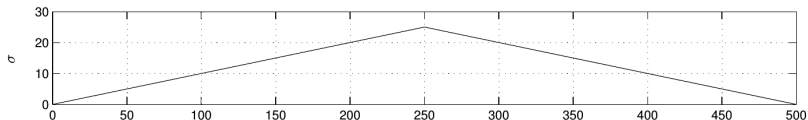
anti-agglomerative interactions

$$\beta < 0 \implies 1 > p_0 > p_1 > p_2 > p_3 > p_4 > 0 .$$

\therefore the probability of a site being in phase 1 decreases with the number of its neighboring sites also being in phase 1.

A Time-inhomogeneous Version for Temporal Stress Ramps

If σ varies as a function of time-blocks of length $\underline{h} = \lfloor hn^2 \rfloor$ and given by the function $\sigma(m)$ for each time-block $m = 0, 1, \dots, M$



then we have the time-inhomogeneous Markov chain $\{X(k)\}_{k=0}^{M\underline{h}}$ with the transition probability matrix at time k given by

$$P(k) = P_{\alpha,\beta,\sigma(\lfloor k/\underline{h} \rfloor)} ,$$

and the k -step configuration probability, with $k < M\underline{h}$ is

$$\begin{aligned} & \Pr \{ X(k) = x(k) \mid X(0) = x(0) \} \\ &= \delta_{x(0)} \left(\prod_{m=0}^{\lfloor k/\underline{h} \rfloor} (P_{\alpha,\beta,\sigma(m)})^{\underline{h}} \right) (P_{\alpha,\beta,\sigma(\lfloor k/\underline{h} \rfloor + 1)})^{\overline{(k)}_{\underline{h}}}, \quad \overline{(k)}_{\underline{h}} \text{ is } k \bmod \underline{h} . \end{aligned}$$

Sufficient Statistics are $\bar{a}(x)$ and $\bar{b}(x)$

Gelled fraction, the fraction of gelled sites:

$$\bar{a}(x) := n^{-2} \sum_{s \in \mathbb{S}_n} x_s \quad \text{and} \quad ,$$

Bonded fraction, the fraction of connected pairs of neighbouring sites:

$$\bar{b}(x) := (2n^2)^{-1} \sum_{\langle s, r \rangle \in \mathbb{E}_n} x_r x_s .$$

\therefore the energy of a configuration x is re-expressible in terms of $\bar{a}(x)$ and $\bar{b}(x)$ as

$$\mathcal{E}(x) = -\beta 2n^2 \bar{b}(x) + (\sigma - \alpha) n^2 \bar{a}(x) ,$$

and therefore

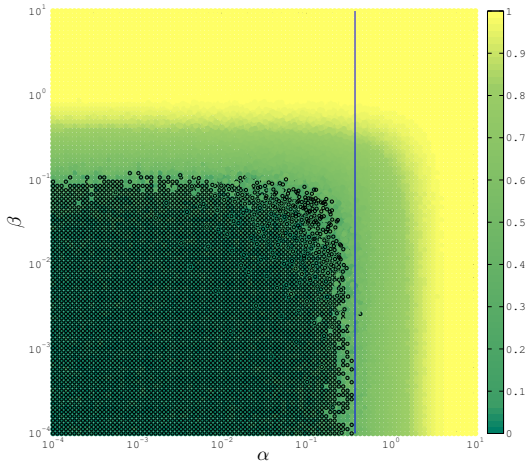
$$\mathcal{E}(x) \propto -2\beta \bar{b}(x) + \tilde{\sigma} \bar{a}(x) .$$

These Chains are our Correlated Site percolation Model

PICTURE TIME!

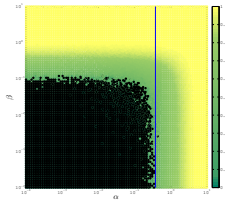
Let us try to see sample paths of the time-homogeneous chains via the Gibbs sampler now.

Phase Transition Without Stress, $\sigma = 0$, on $(\alpha, \beta) \in [10^{-4}, 10^1]^2$ as the appearance of the percolation cluster (Simulation – not known exactly in $[0, 1]$ even if $\beta = 0$)



Phase Transition Without Stress, $\sigma = 0$, on $(\alpha, \beta) \in [10^{-4}, 10^1]^2$

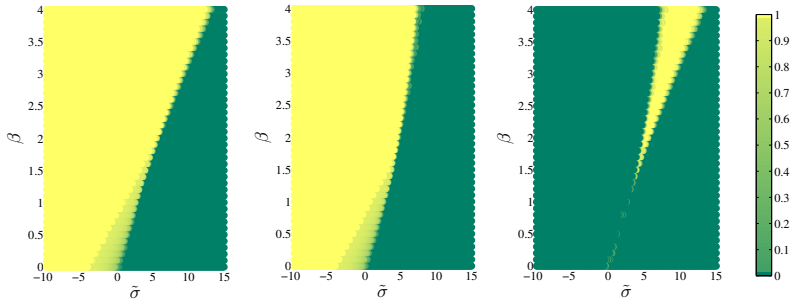
as the appearance of the percolation cluster (Simulation – not known exactly in $[0, 1]$ even if $\beta = 0$)



The shading of the circle at each (α, β) indicates $F_{x(100)}^{(*)}$, the proportion of the lattice occupied by the largest cluster of gelled sites at rescaled time $t = 100$ after having initialized from the all fluid configuration $\mathbf{0}$. Parameter values that do not lead to a percolation cluster (vertically spanning largest cluster) after each one of the $n^2 = 10^4$ sites has undergone 100 transitions (on average), i.e. with $F_{x(100)}^{(*)} < 1$, are highlighted by black-edged circles.

Phase Transition With Constant Time-Asymptotic Stress

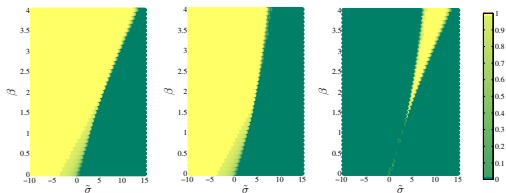
(solid) $\mathbf{1} \leftrightarrow \mathbf{0}$ (fluid) initialized with δ_1, δ_0 , and their hysteretic difference
 over $(\sigma - \alpha) =: \tilde{\sigma} \in [-10, 15]$ (Simulation)



Phase Transition With Constant Time-Asymptotic Stress

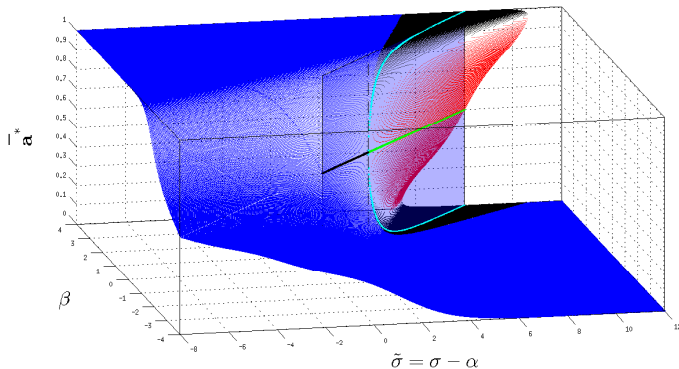
(solid) $\mathbf{1} \leftrightarrow \mathbf{0}$ (fluid) initialized with δ_1, δ_0 , and their hysteretic difference

over $(\sigma - \alpha) =: \tilde{\sigma} \in [-10, 15]$ (Simulation)



The value of \bar{a} , gelled fraction, at rescaled time $t = 100$ for fixed parameters $(\tilde{\sigma}, \beta)$ when initialized from $\mathbf{1}$ (left subplot) and from $\mathbf{0}$ (middle sub-plot). The difference in \bar{a} between left and middle sub-plots is shown in the right sub-plot.

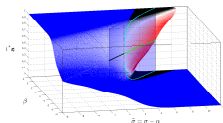
A bi-parametric Quartic ODE for \approx 'ing $\bar{a}(t) := \mathbf{E}_{\tilde{\sigma}, \beta}(\bar{A}(t))$



A bi-parametric Quartic ODE for \approx 'ing $\bar{a}(t) := \mathbf{E}_{\tilde{\sigma}, \beta}(\bar{A}(t))$

Let continuous time t be discrete time m in units of n^2 , i.e. $m = \lfloor tn^2 \rfloor$

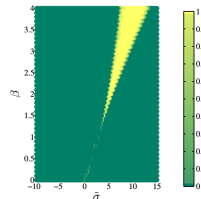
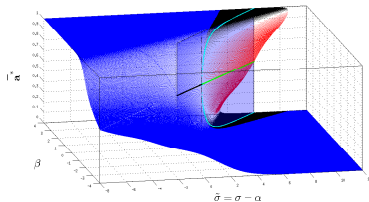
$$\begin{aligned} \dot{\bar{a}}(t) &:= \lim_{\Delta_t \rightarrow 0} \mathbf{E} \left(\frac{\overbrace{\bar{A}(t + \Delta_t) - \bar{A}(t)}^{\Delta_a}}{\Delta_t} \middle| \bar{A}(t) \right) \\ &= p_0 - (4p_0 - 4p_1 + 1)\bar{a} + 6(p_0 - 2p_1 + p_2)\bar{a}^2 \\ &\quad - 4(p_0 - 3p_1 + 3p_2 - p_3)\bar{a}^3 \\ &\quad + (p_0 - 4p_1 + 6p_2 - 4p_3 + p_4)\bar{a}^4. \end{aligned}$$



where, $p_i := 1/(1 + \exp(\underbrace{(\sigma - \alpha)}_{\tilde{\sigma}} - i\beta))$.

from an $\bar{a}, 1 - \bar{a}$ mixture of p_i -weighted combinations of Bernstein polynomials of degree 4 as $n^2 \rightarrow \infty, \Delta_t = O(1/n^2) \rightarrow 0, \Delta_a \rightarrow 0 : \Pr\{\Delta_a/\Delta_t \in \{0, -1, +1\}\} \rightarrow 1$ (cf. §3.2 of preprint). Fixed point map is CAPA: extended interval Newton operator.

A bi-parametric Quartic ODE for \approx 'ing $\bar{\mathbf{a}}(t) := \mathbf{E}_{\tilde{\sigma}, \beta}(\bar{\mathbf{A}}(t))$



The fixed points $\bar{\mathbf{a}}^*$ as a set-valued function of the parameters $\tilde{\sigma} = \sigma - \alpha$ and β . The blue, black and azure points are the stable fixed points while the red and green points are the unstable fixed points of the system. There is a pitch-fork bifurcation along $\tilde{\sigma} = 2\beta$ that starts at $(2.589145, 1.2945725)$ where the fixed point at 0.5 becomes unstable with two stable fixed points on either side. Compare the black triangle (from ODE) on left with yellow triangle on right (simulation with $h = 100$)

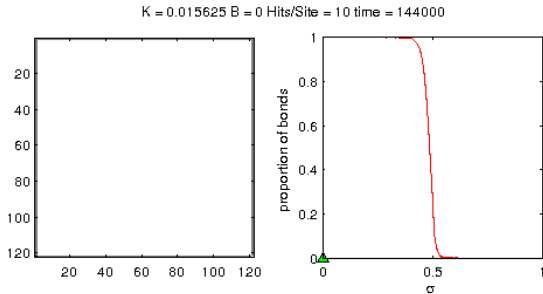
These Chains are our Correlated Site percolation Model

MOVIE TIME AGAIN!

Let us try to watch sample paths of the time-inhomogeneous chains via the Gibbs sampler now.

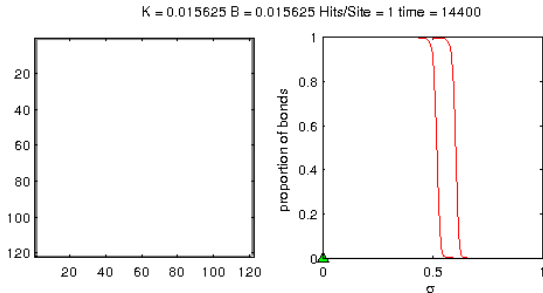
$\beta = 0$: Bonded Fraction \bar{b} on a Stress Ramp

\implies No Hysteresis



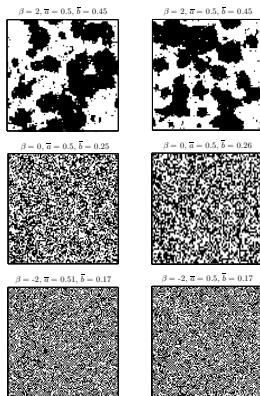
$\beta > 0$: Bonded Fraction \bar{b} on a Stress Ramp

\Rightarrow Hysteresis



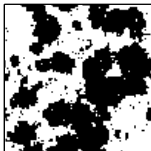
Two Samples each for $\beta \in \{2, 0, -2\}$, $\alpha = 8$ at $\bar{a} \approx 1/2$

Let's see sample configurations over 100^2 sites in phase 0 (black) and 1 (white) at **the solid-fluid interface** when the realized gelled fraction $\bar{a} \approx 1/2$.

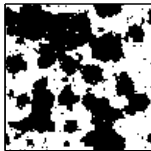


Two Samples each for $\beta \in \{2, 0, -2\}$, $\alpha = 8$ at $\bar{a} \cong 1/2$

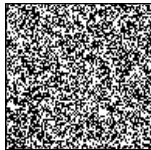
$\beta = 2, \bar{a} = 0.5, \bar{b} = 0.45$



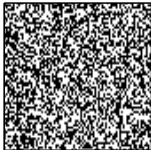
$\beta = 2, \bar{a} = 0.5, \bar{b} = 0.45$



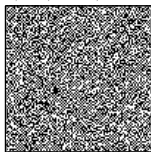
$\beta = 0, \bar{a} = 0.5, \bar{b} = 0.25$



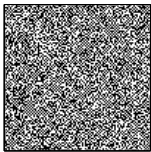
$\beta = 0, \bar{a} = 0.5, \bar{b} = 0.26$



$\beta = -2, \bar{a} = 0.51, \bar{b} = 0.17$



$\beta = -2, \bar{a} = 0.5, \bar{b} = 0.17$

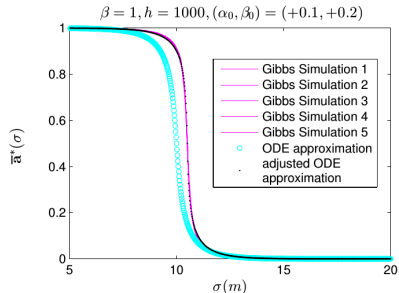
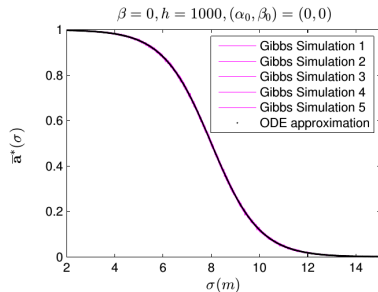


cowhide :
agglomerative,

random :
non-interactive,

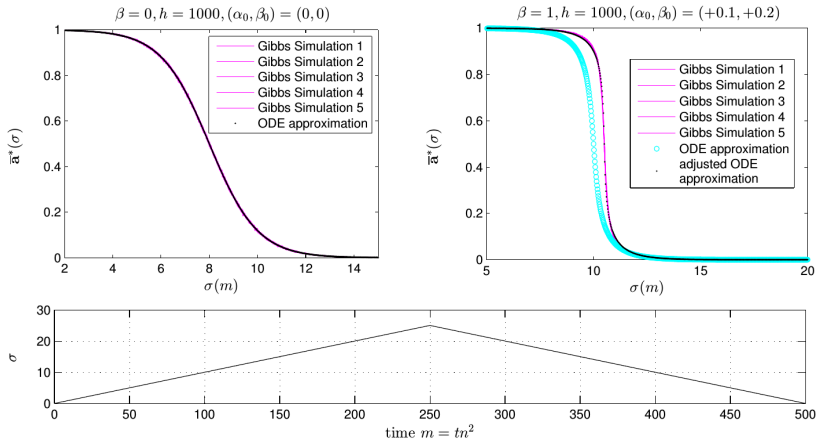
chess-board :
anti-agglomerative

Hysteresis in gelled fraction $\bar{a}(x)$ with $\alpha = 8$, $\beta \in \{0, 1\}$ as $h \rightarrow \infty$ at $\sigma(m) \forall m \in \{0, 1, \dots, M\}$



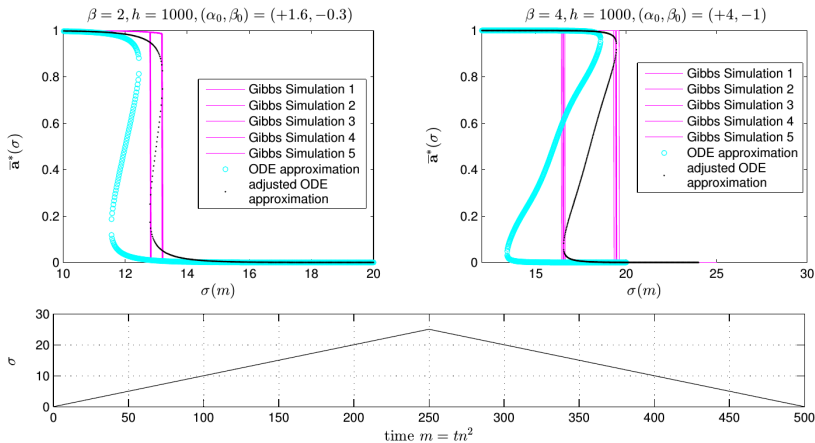
Gibbs field simulations, fixed points $\bar{\mathbf{a}}^*(\sigma; \alpha, \beta)$ of ODE with and without (α_0, β_0) -translation of vector field (adjusted ODE). σ was increased from 0 to 25 in units of 0.01 and decreased back to 0 with a holding time of $h = 1000$ (nearly asymptotic Gibbs state for each distinct stress) as x traversed $\mathbf{1} \rightarrow \mathbf{0} \rightarrow \mathbf{1}$.

Hysteresis in gelled fraction $\bar{a}(x)$ with $\alpha = 8, \beta \in \{0, 1\}$ as $h \rightarrow \infty$ at $\sigma(m) \forall m \in \{0, 1, \dots, M\}$



Now with the stress ramp shown.

Hysteresis in gelled fraction $\bar{a}(x)$ with $\alpha = 8$, $\beta \in \{2, 4\}$ as $h \rightarrow \infty$ at $\sigma(m) \forall m \in \{0, 1, \dots, M\}$



Some Concluding Remarks

- Using an Interacting Particle System Model We can fit data better
- Each material can be empirically identified by its rheological parameter $\alpha, \tilde{\sigma}$ for science / engineering applications
- It would be nice to use geometric perturbation theoretic ideas to better approximate the expected gelled fraction
- Ideally Find a large enough neighbourhood (larger than just the binomial neighbourhood configuration approximation done here) so that you can obtain a 2-parameter family of ODEs in terms of the gelled fraction and the bonded fraction, a sufficient statistic, which we are not modelling now!
- some more is done in the preprint... but time kills.

The End

Many thanks to:

- Steve Strogatz, Maths@Cornell for IGERT - Complex Non-linear Systems
- UC College of Engineering Sabbatical Grant Northern Fall 2014
- Michael Nussbaum, Maths@Cornell for being my Sabbatical host Northern Fall 2014
- Brendan Creutz for discussions on the discriminants of the quartic polynomial ODE with transcendental coefficients
- Rua Murray for discussions on geometric perturbation theoretic [future pursuits for a better 2D ODE (and justifying the 1D ODE formally)]
- Thanks for your Attention :)

Preprint

A Microscopic Gibbs Field Model for the Macroscopic Behavior of a Viscoplastic Fluid, Raazesh Sainudiin, Miguel Moyers-Gonzalez and Teodor Burghilea, UCDMS Research Report 2014/1, 2014

http://www.math.canterbury.ac.nz/~r.sainudiin/preprints/20140825_MicroNNF.pdf (5.6MB)