A Gibbs Field Model for the Microscopic Yielding of a Viscoplastic Fluid

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November 12, 2013

Outline

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- Deterministic Macroscopic Models of Viscoplastic Fluids

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- Stochastic Microscopic Model

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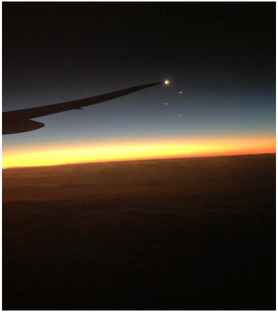
- Acknowledgments

**Brief outline of the collaboration
on the transfer phenomena in viscoplastic fluids:**

BEYOND THE DATE LINE



PEOPLE INVOLVED IN THE COLLABORATION

LTN Nantes (Experiments)

C. Castelain
(our boss, yes!)

Teo Burghelea

The recently founded Complex Fluids Team
(since October 2010)

UC, New Zealand (theory, modelling)

Miguel Moyers-Gonzalez

Phil Wilson

Raazesh Sainudiin

Projects (past and ongoing)

(1) Hydrodynamic stability of an elasto-visco plastic material

J. Non-Newtonian Fluid Mech. 166 (2011) 515–531

Contents lists available at ScienceDirect

Journal of Non-Newtonian Fluid Mechanics

journal homepage: www.elsevier.com/locate/jnnfm

ELSEVIER

Journal of Non-Newtonian Fluid Mechanics

Linear stability analysis for plane-Poiseuille flow of an elastoviscoplastic fluid with internal microstructure for large Reynolds numbers

Miguel Moyers-Gonzalez[a,*], Teodor I. Burghelea[b], Julian Mak[c]

[a] Department of Mathematics and Statistics, University of Canterbury, Private Bag 4800, Christchurch 8140, New Zealand
[b] Université de Nantes, Nantes Atlantique Universités, CNRS, Laboratoire de Thermocinétique de Nantes, UMR 6607, La Chantrerie, Rue Christian Pauc, B.P. 50609, F-44306 Nantes Cedex 3, France
[c] School of Mathematics, University of Leeds, Leeds LS2 9JT, UK

(2) Thermorheological properties of a Carbopol gel under shear

Journal of Non-Newtonian Fluid Mechanics 183–184 (2012) 14–24

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Thermorheological properties of a Carbopol gel under shear

Eva Weber [a], Miguel Moyers-González [b], Teodor I. Burghelea [c,*]

[a] *Institute of Polymer Materials, Friedrich-Alexander-University Erlangen-Nürnberg, D-91058 Erlangen, Germany*
[b] *Department of Mathematics and Statistics, University of Canterbury, Private Bag 4800, Christchurch 8041, New Zealand*
[c] *Université de Nantes, Nantes Atlantique Universités, CNRS, Laboratoire de Thermocinétique de Nantes, UMR 6607, La Chantrerie, Rue Christian Pauc, B.P. 50609, F-44306 Nantes Cedex 3, France*

(3) Unsteady flows of a Carbopol gel (being reviewed at JNNFM)

Unsteady laminar flows of a Carbopol® gel in the presence of wall slip

Antoine Poumaere

LUNAM Université, Université de Nantes, CNRS, Laboratoire de Thermocinétique, UMR 6607, La Chantrerie, Rue Christian Pauc, B.P. 50609, F-44306 Nantes Cedex 3, France

Miguel Moyers-González

Department of Mathematics and Statistics, University of Canterbury, Private Bag 4800, Christchurch, 8041, NZ

Cathy Castelain

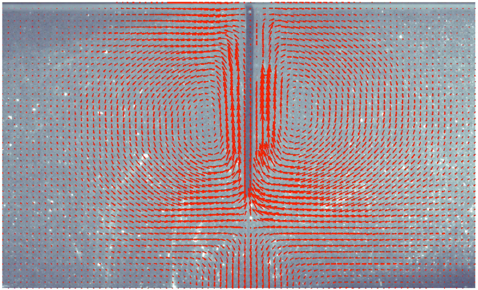
Cathy.Castelain@univ-nantes.fr

Teodor Burghelea

LUNAM Université, Université de Nantes, CNRS, Laboratoire de Thermocinétique, UMR 6607, La Chantrerie, Rue Christian Pauc, B.P. 50609, F-44306 Nantes Cedex 3, France

(4) The Landau-Levich coating problem with a yield stress fluid (in preparation)

(Miguel Moyers-Gonzalez, Phil Wilson, Cathy Castelain, Teo Burghelea)



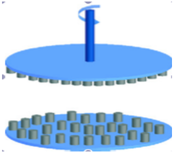
The QUEST:
Understand the flows of viscoplastic materials through a multi scale approach

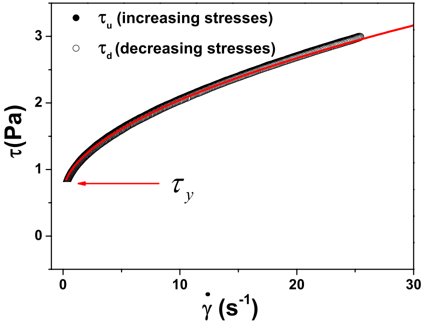
Viscoplastic Material:

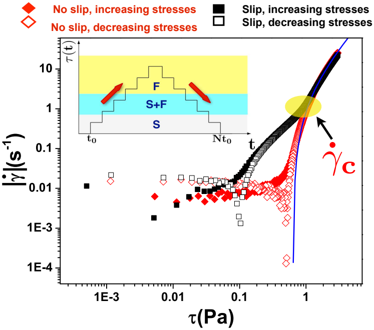
A material that behaves as a solid at low applied stresses and as a fluid beyond a threshold value of the applied stress

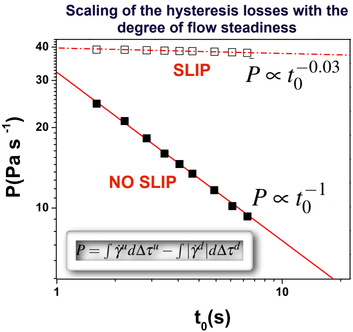
Yielding and flow of a gel at a macroscopic scale
(Teo, Cathy, Miguel, Phil)

The common “religion” of yielding: H-B









An unsteady rheological test takes us from paradise to hell in several ways...

- Rheological hysteresis

- Gradual Solid-Fluid transition coupled to the wall slip

- NO STEADY STATE REACHABLE IN THE PRESENCE OF WALL SLIP

The rheological hysteresis for a Carbopol gel is a new (and still subject of some controversy) observation:

Rheol Acta
DOI 10.1007/s00397-009-0365-9
ORIGINAL CONTRIBUTION

The solid–fluid transition in a yield stress shear thinning physical gel

Andreas M. V. Putz · Teodor I. Burghelea

Received: 28 May 2008 / Accepted: 23 April 2009

Other groups observed it as well

Soft Matter
Dynamic Article Links View Online
Cite this: DOI: 10.1039/c1sm05607g
www.rsc.org/softmatter
PAPER

From stress-induced fluidization processes to Herschel-Bulkley behaviour in simple yield stress fluids

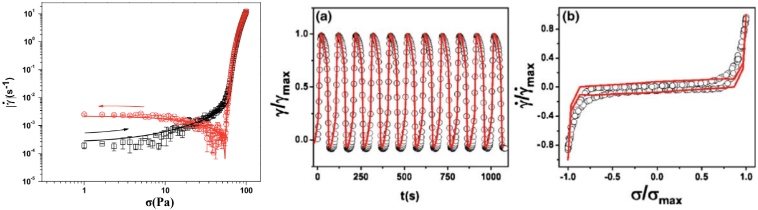
Thibaut Divoux,*[a] Catherine Barentin[b] and Sébastien Manneville[a]

Received 6th April 2011, Accepted 25th May 2011
DOI: 10.1039/c1sm05607g

RECONCILE THE "HEAVEN" AND THE "HELL": THE POOR MAN APPROACH AND BEYOND

$$\frac{d\Phi}{dt} = R_d(\Phi, t, \Gamma) + R_r(\Phi, t, \Gamma) + \delta \qquad R_d(\Phi, t, \Gamma) = -K_1 \Gamma \Phi, \quad \Gamma = \frac{\sigma}{\sigma_2}$$

$$R_r(\Phi, t, \Gamma) = f(\Gamma)\Phi(1-\Phi) \quad with\ f(\Gamma) = K_r\left[1 - tanh\left(\frac{\Gamma - 1}{w}\right)\right]$$



Can this novel yielding picture be validated at a microscopic scale (and automatically validated from a thermodynamical standpoint)?

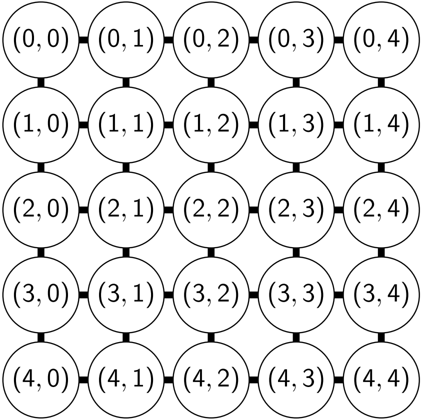
Yielding and flow of a gel at a microscopic scale:

A Gibbs field model for the microscopic yielding of a gel

Raaz, we are all ears!

Stochastic Microscopic Model – 1

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



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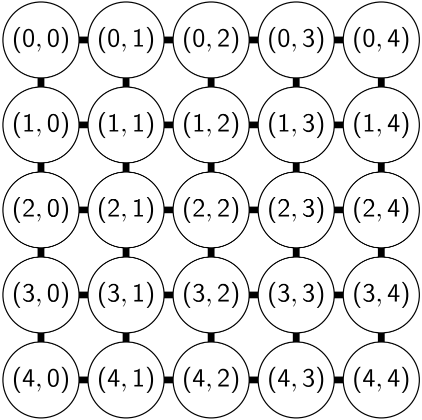
- $\mathcal{G}$ = regular graph (2D toroidal square lattice)
- $\mathbb{S}_n = \{0, 1, 2, \ldots, n-1\}^2$ = set of nodes or sites



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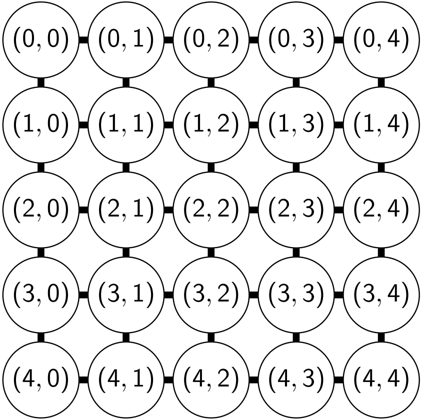
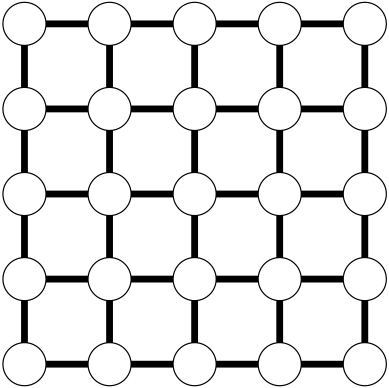
- $\mathbb{E}_n \subset \mathbb{S}_n^2$ = set of edges between pairs of sites



Microscopic Models (Stochastic) – 2

- each site $s \in \mathbb{S}_n$ represents a polymer molecule



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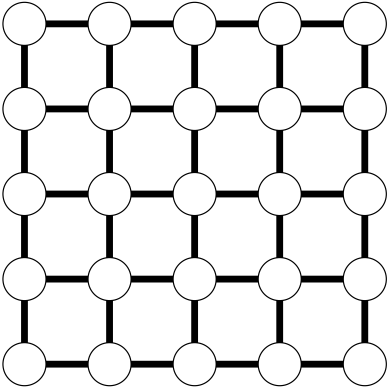
- each edge $\langle s, t \rangle \in \mathbb{E}_n$ represents a potential bond between neighbouring molecules at sites s and t.



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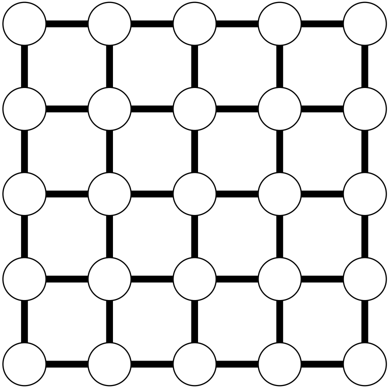
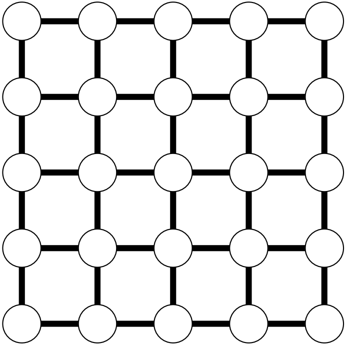
- $N_s = \{t : |t - s| = 1\}$ denotes neighbours of a site s



Microscopic Models (Stochastic) – 3

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



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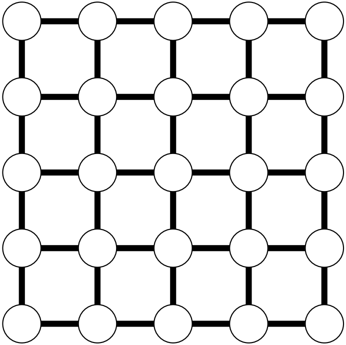

Microscopic Models (Stochastic) – 3

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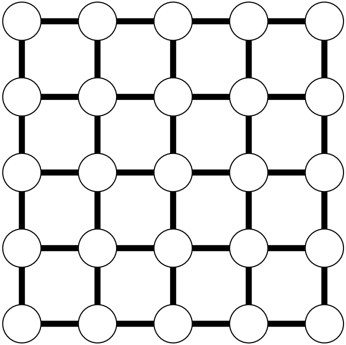
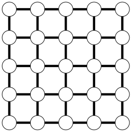
- phase 1 corresponds to possibly being bonded with at least one of its neighbours



Phases at Sites and Bonds

We say a bond exists between molecules at sites s and t and denote it by

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



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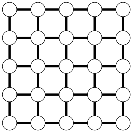

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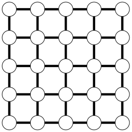

- every site configuration $x \in \mathbb{X}_n := \Lambda^{\mathbb{S}_n}$ has an associated bond configuration $y \in \mathbb{Y}_n := \Lambda^{\mathbb{E}_n}$
- Note that $Y(x) : \mathbb{X}_n \to \mathbb{Y}_n$ is neither injective nor surjective

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$$V_{\langle s,t \rangle}(x) = -\frac{B}{k} x(s)x(t) = \begin{cases} 0 & \text{if } (x(s), x(t)) = (0,0) \\ 0 & \text{if } (x(s), x(t)) = (1,0) \\ 0 & \text{if } (x(s), x(t)) = (0,1) \\ -\frac{B}{k} & \text{if } (x(s), x(t)) = (1,1) \end{cases}$$

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where $\langle s, t\rangle$ is the two element clique with $t \in N_s$ and B is the internal energy of a bond-pair (between two polymer molecules).

Total, Internal and Free Energy – 1

Thus, the energy function corresponding to this potential is

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$$\begin{aligned}\mathcal{E}(x) = \sum_C V_C(x) &= \sum_{s \in \mathbb{S}_n} V_{\{s\}}(x) + \sum_{\langle s,t \rangle \in \mathbb{E}_n} V_{\langle s,t \rangle}(x) \\ &= \frac{1}{k} \left(-B \sum_{\langle s,t \rangle \in \mathbb{E}_n} x(s)x(t) + (\sigma - \sigma_0) \sum_{s \in \mathbb{S}_n} x(s) \right)\end{aligned}$$

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$$= \frac{1}{k} \left(-B \sum_{\langle s,t \rangle \in \mathbb{E}_n} x(s)x(t) + (\sigma - \sigma_0) \sum_{s \in \mathbb{S}_n} x(s) \right)$$

Let the expectation of a function $g : \mathbb{X}_n \to \mathbb{R}$, w.r.t. π, be

$$\langle g \rangle := \sum_{x \in \mathbb{X}_n} g(x)\pi(x)$$

Total, Internal and Free Energy – 2

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

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

Energy $\mathcal{E}$ and Gibbs Distribution π over Site Configurations

Let $\mathcal{E}(x)$, the energy of a site configuration x be

$$\mathcal{E}(x) = \frac{1}{k}\left(-B \sum_{\langle s,t\rangle \in \mathbb{E}_n} x(s)x(t) + (\sigma - \sigma_0) \sum_{s \in \mathbb{S}_n} x(s) \right)$$

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where Z_T is the normalising constant or partition function

$$Z_T = \sum_{x \in \mathbb{X}_n} \exp\left(-\frac{1}{T}\mathcal{E}\right).$$

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The average number of bondable polymers per site is

$$\bar{a} := |\mathbb{S}_n|^{-1} \langle a \rangle = n^{-2} \sum_{x \in \mathbb{X}_n} a(x)\pi(x) = n^{-2} \sum_{x \in \mathbb{X}_n} \left(\sum_{s \in \mathbb{S}_n} x(s) \right) \pi(x)$$

Two Informative Statistics of a Configuration x – 2

The number of bonds

$$b(x) = \sum_{\langle s,t \rangle \in \mathbb{E}_n} y(\langle s, t \rangle) = \sum_{\langle s,t \rangle \in \mathbb{E}_n} x(t)x(s)$$

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and the average number of bonds per edge (or pair of sites) is

$$\begin{aligned} \bar{b} &:= |\mathbb{E}_n|^{-1} \langle b \rangle = (2n^2)^{-1} \sum_{x \in \mathbb{X}_n} b(x)\pi(x) \\ &= \frac{n^{-2}}{2} \sum_{x \in \mathbb{X}_n} \left(\sum_{\langle s,t \rangle \in \mathbb{E}_n} x(t)x(s) \right) \pi(x) \end{aligned}$$

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$$\begin{aligned} \bar{b} &:= |\mathbb{E}_n|^{-1} \langle b \rangle = (2n^2)^{-1} \sum_{x \in \mathbb{X}_n} b(x)\pi(x) \\ &= \frac{n^{-2}}{2} \sum_{x \in \mathbb{X}_n} \left(\sum_{\langle s,t \rangle \in \mathbb{E}_n} x(t)x(s) \right) \pi(x) \end{aligned}$$

One of our primary interests is to study $\bar{a}$ and $\bar{b}$ as a function of extrenally applied stress σ.

Gibbs Sampler – 1

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We want to simulate configurations $x \in \mathbb{X}_n$ that are distributed according to π (for fixed $\sigma, \sigma_0, k, B, T$)

- We construct an $\mathbb{X}_n$-valued Markov chain $\{X_m\}_{m \geq 0}$, where $(X_m(s), s \in \mathbb{S}_n)$ and $X_m(s) \in \Lambda$, with stationary distribution π, i.e.,

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- This Monte Carlo Markov chain (MCMC) is called the Gibbs sampler.

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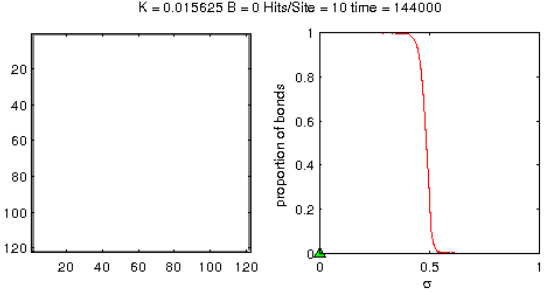
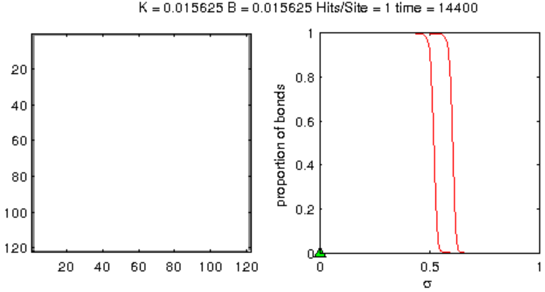
When $B = 0$


K = 0.015625 B = 0 Hits/Site = 10 time = 144000
20
40
60
80
100
120
20 40 60 80 100 120
proportion of bonds
0
0.2
0.4
0.6
0.8
1
0 0.5 1
σ

$B \neq 0$


K = 0.015625 B = 0.015625 Hits/Site = 1 time = 14400
20
40
60
80
100
120
20 40 60 80 100 120
1
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The End

- Many thanks to:
  - Teo and Cathy for inviting me here
  - UC for research travel funds
  - Thanks for your Attention :)