Multiscale modelling of complex fluids: a mathematical initiation.

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Reference (with Matlab programs, see Section 5):

`http://hal.inria.fr/inria-00165171`.

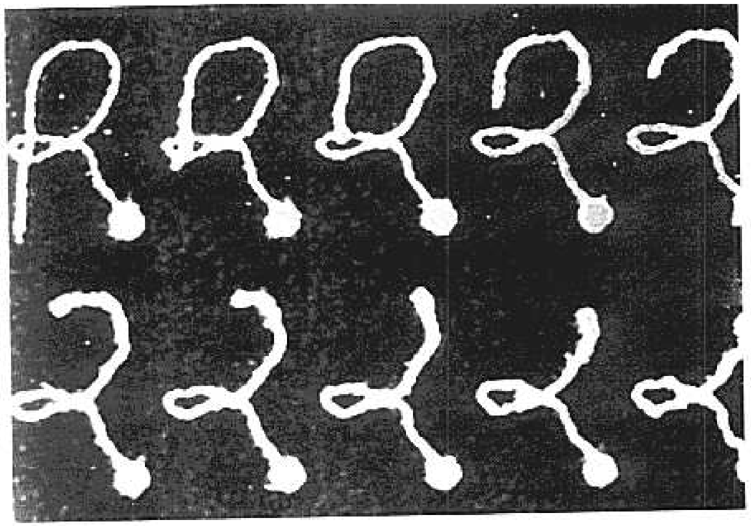
Outline

Outline

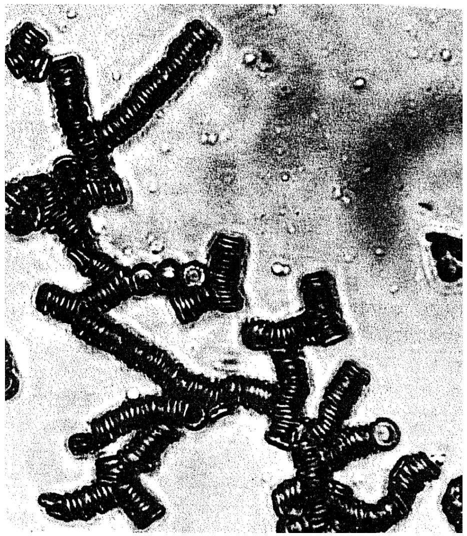
1A Experimental observations

We are interesting in complex fluids, whose non-Newtonian behaviour is due to some microstructures.

Cover page of *Science*, may 1994



Journal of Statistical Physics, **29** (1982) 813-848



1A Experimental observations

More precisely, we study the case when the microstructures are:

1. very numerous (statistical mechanics),
2. small and light (Brownian effects),
3. within a Newtonian solvent.

This is not the case of granular materials.

A prototypical example is dilute solution of polymers.

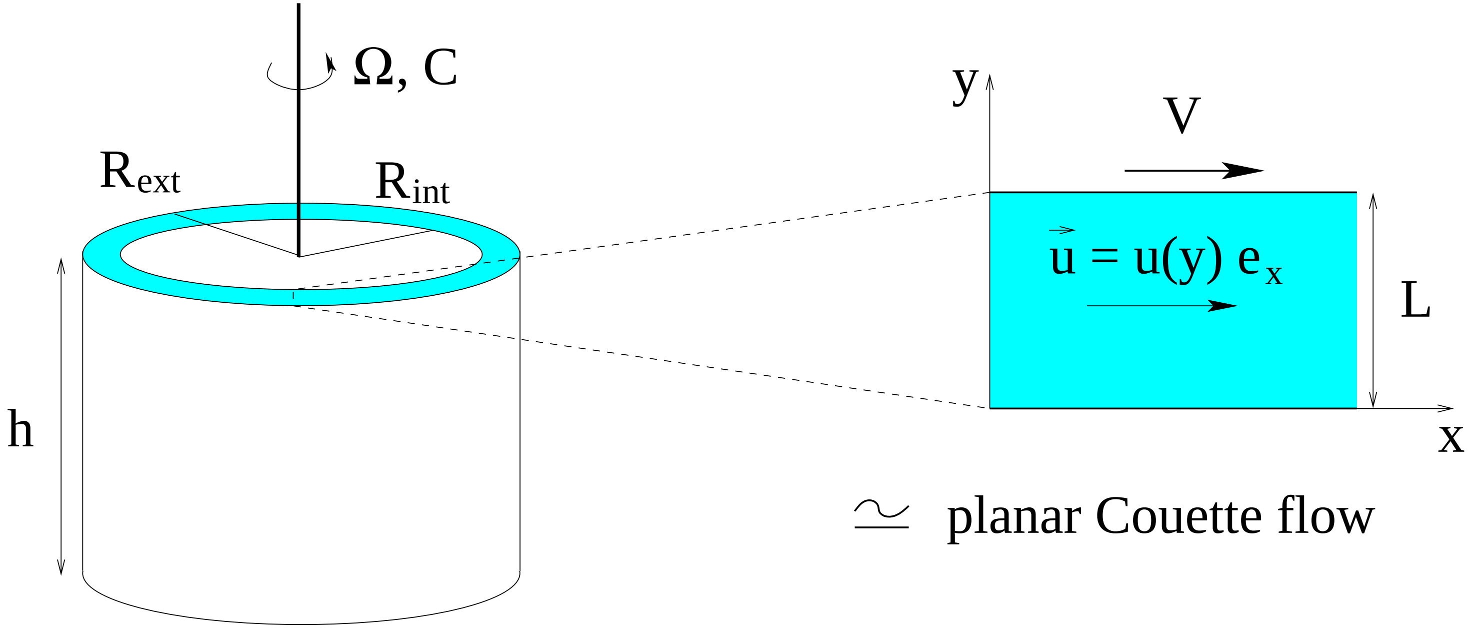
1A Experimental observations

Some examples of complex fluids:

- food industry: mayonnaise, egg white, jellies
- materials industry: plastic (especially during forming), polymeric fluids
- biology-medicine: blood, synovial liquid
- civil engineering: fresh concrete, paints
- environment: snow, muds, lava
- cosmetics: shaving cream, toothpaste, nail polish

1A Experimental observations

Shearing experiments in a rheometer:



$\simeq$ planar Couette flow

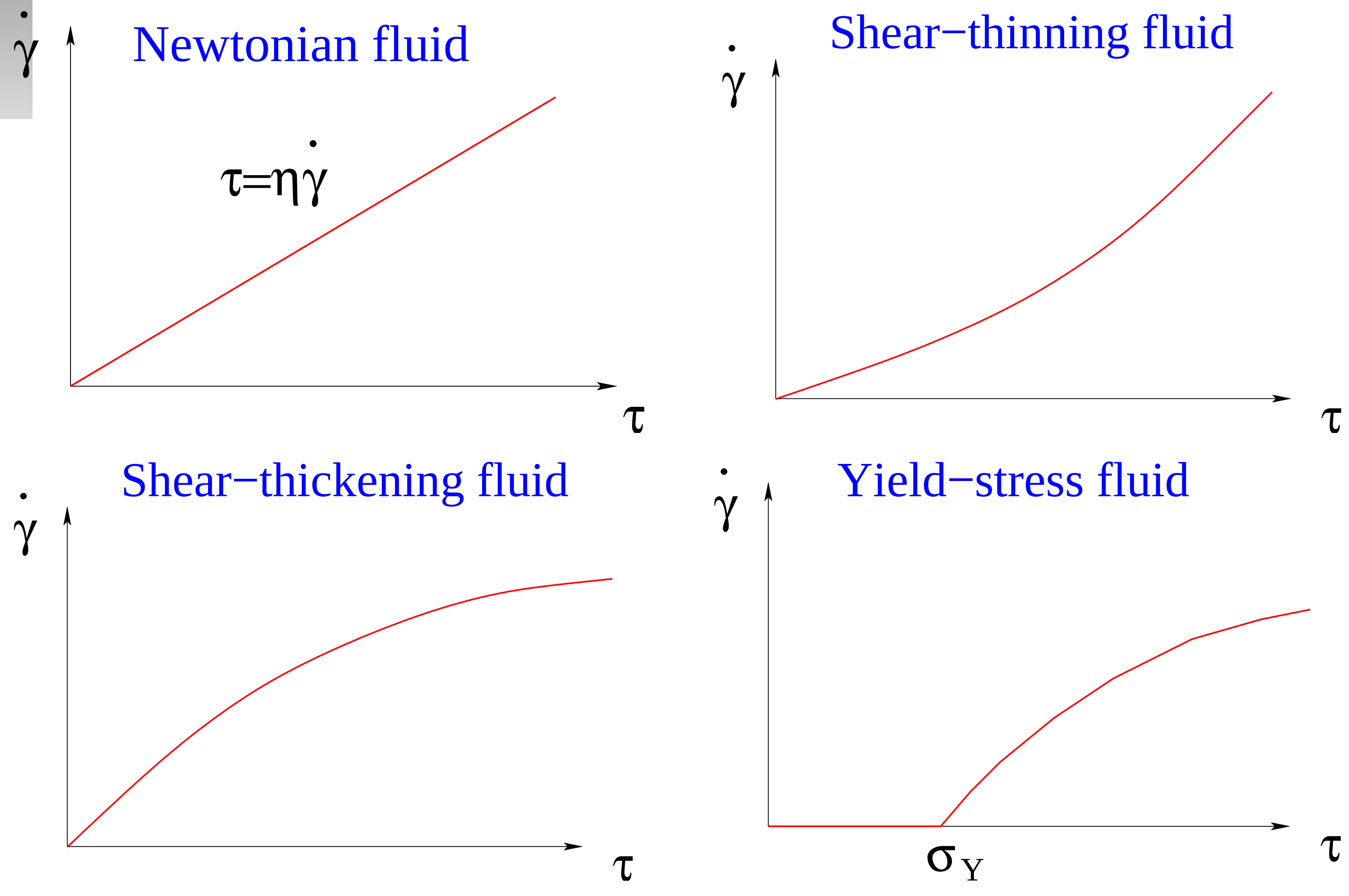
$$\dot{\gamma} = \frac{V}{L} = \frac{R_{int}\Omega}{R_{ext}-R_{int}}$$

$$(\Omega, C) \iff (\dot{\gamma}, \tau)$$

$$\tau = \frac{C}{2\pi R_{int}^2 h}$$

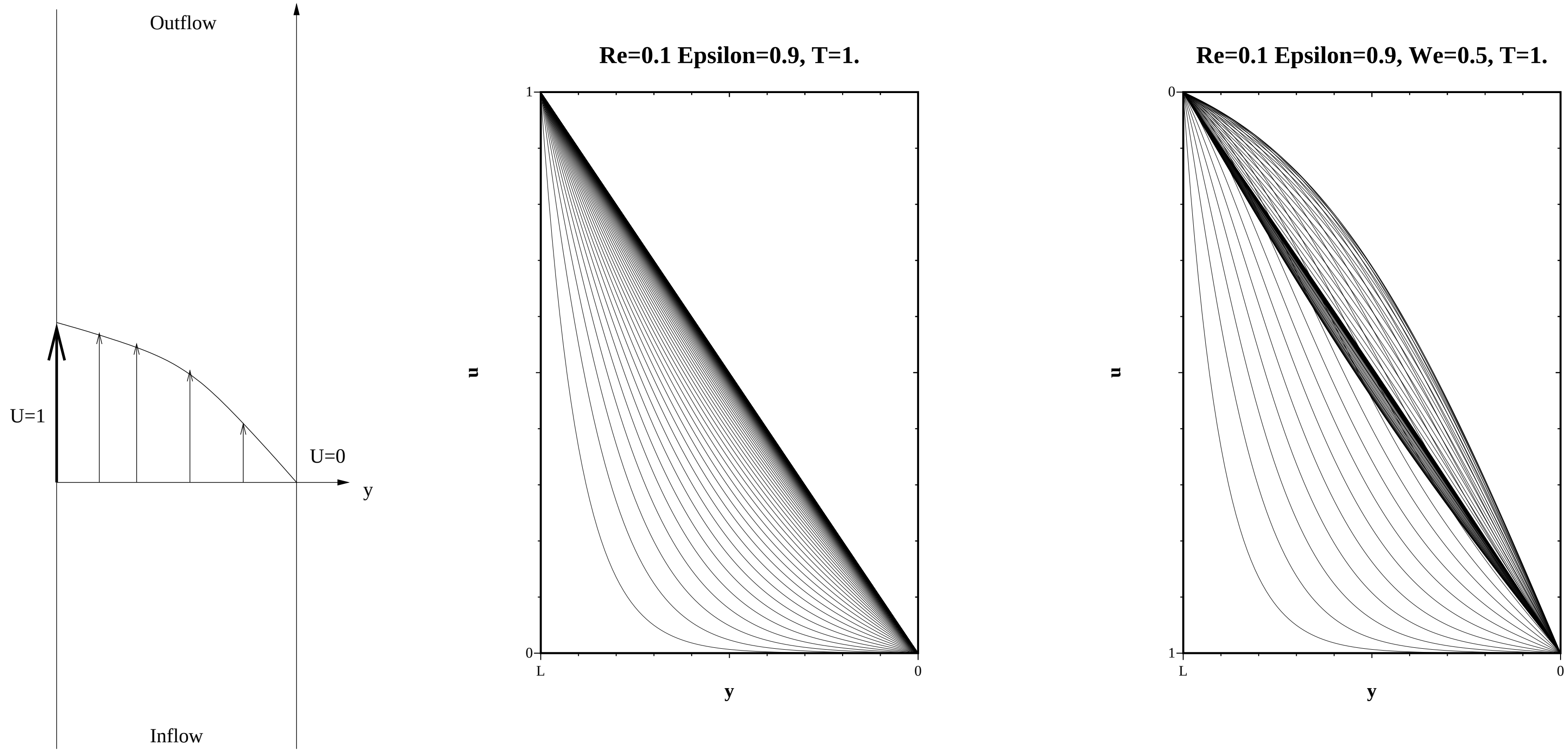
1A Experimental observations

At stationary state:



1A Experimental observations

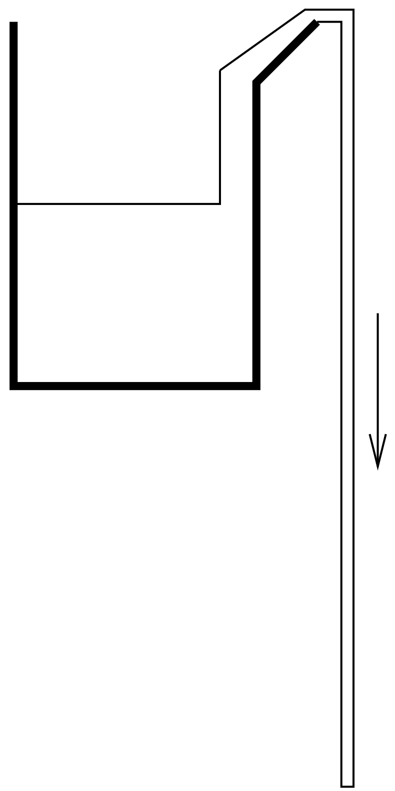
A simple dynamics effect: the velocity overshoot for the start-up of shear flow.

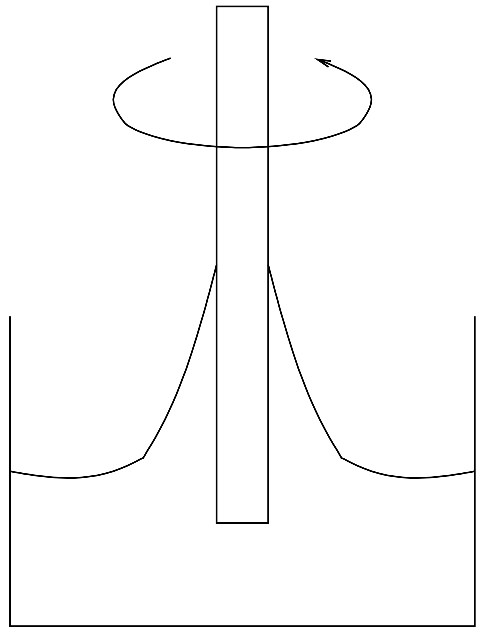


Velocity profile as time evolves: Newtonian fluid *vs* Hookean dumbbell model.

1A Experimental observations

These are two typical non-Newtonian effects : the open syphon effect and the rod climbing effect.





Outline

1 Modeling

1A Experimental observations

1B Multiscale modeling

1C Microscopic models for polymer chains

1D Micro-macro models for polymeric fluids

1E Conclusion and discussion

2 Mathematics and numerics

2A Generalities

2B Some existence results

2C Convergence of the CONNFFESSIT method

2D Dependency of the Brownian on the space variable

2E Long-time behaviour

2F Free-energy dissipative schemes for macro models

Momentum equations (incompressible fluid):

$$\rho\left(\partial_t + \mathbf{u}.\nabla\right)\mathbf{u} = -\nabla p + \mathrm{div}(\boldsymbol{\sigma}) + \mathbf{f}_{ext},$$

$$\mathrm{div}(\mathbf{u}) = 0.$$

Newtonian fluids (Navier-Stokes equations):

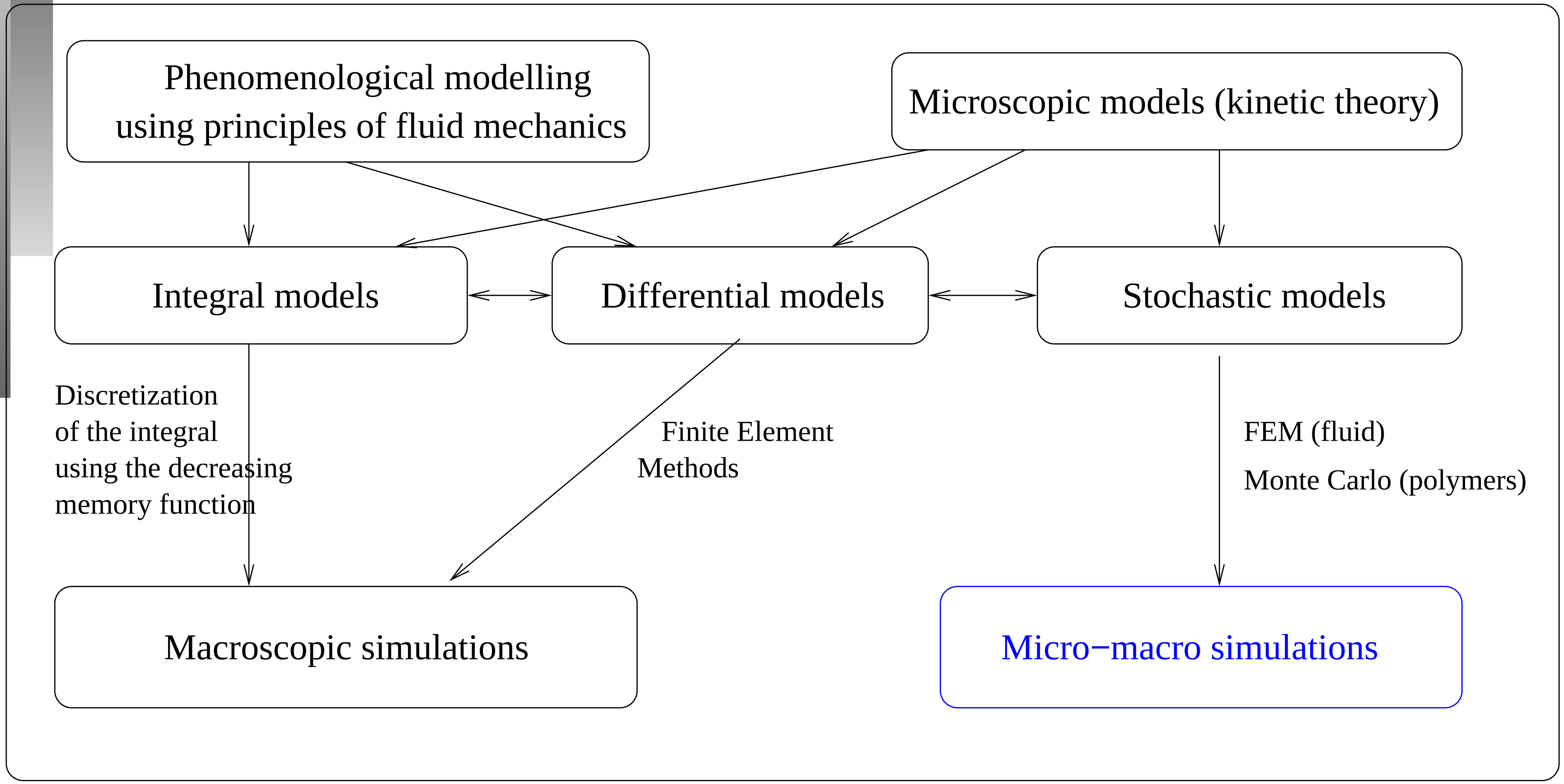
$$\boldsymbol{\sigma} = \eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right),$$

Non-Newtonian fluids:

$$\boldsymbol{\sigma} \;=\; \eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) + \boldsymbol{\tau},$$

$\boldsymbol{\tau}$ depends on *the history of the deformation*.

1B Multiscale modeling

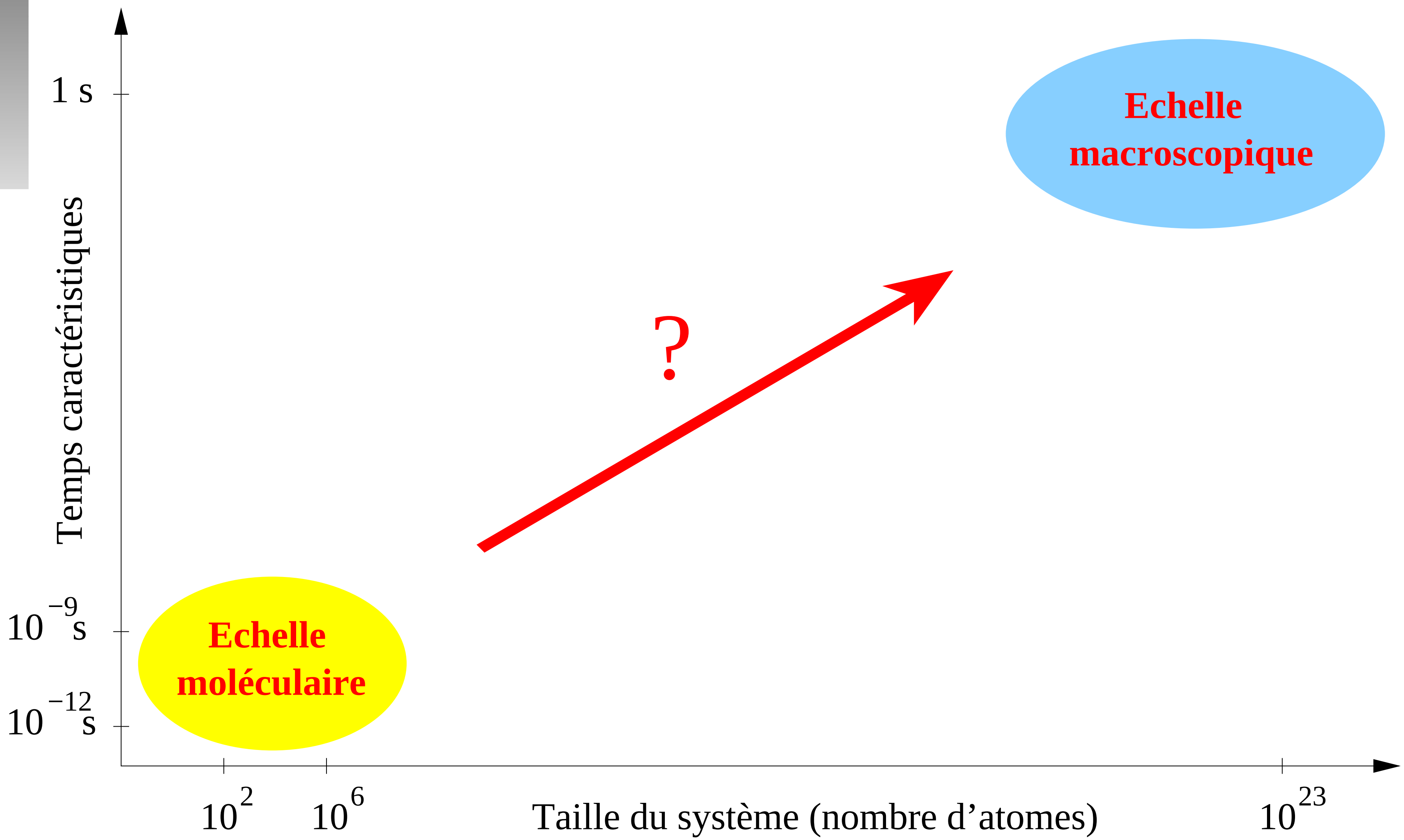


Differential models : $\frac{D\boldsymbol{\tau}}{Dt} = f(\boldsymbol{\tau}, \nabla \mathbf{u}),$

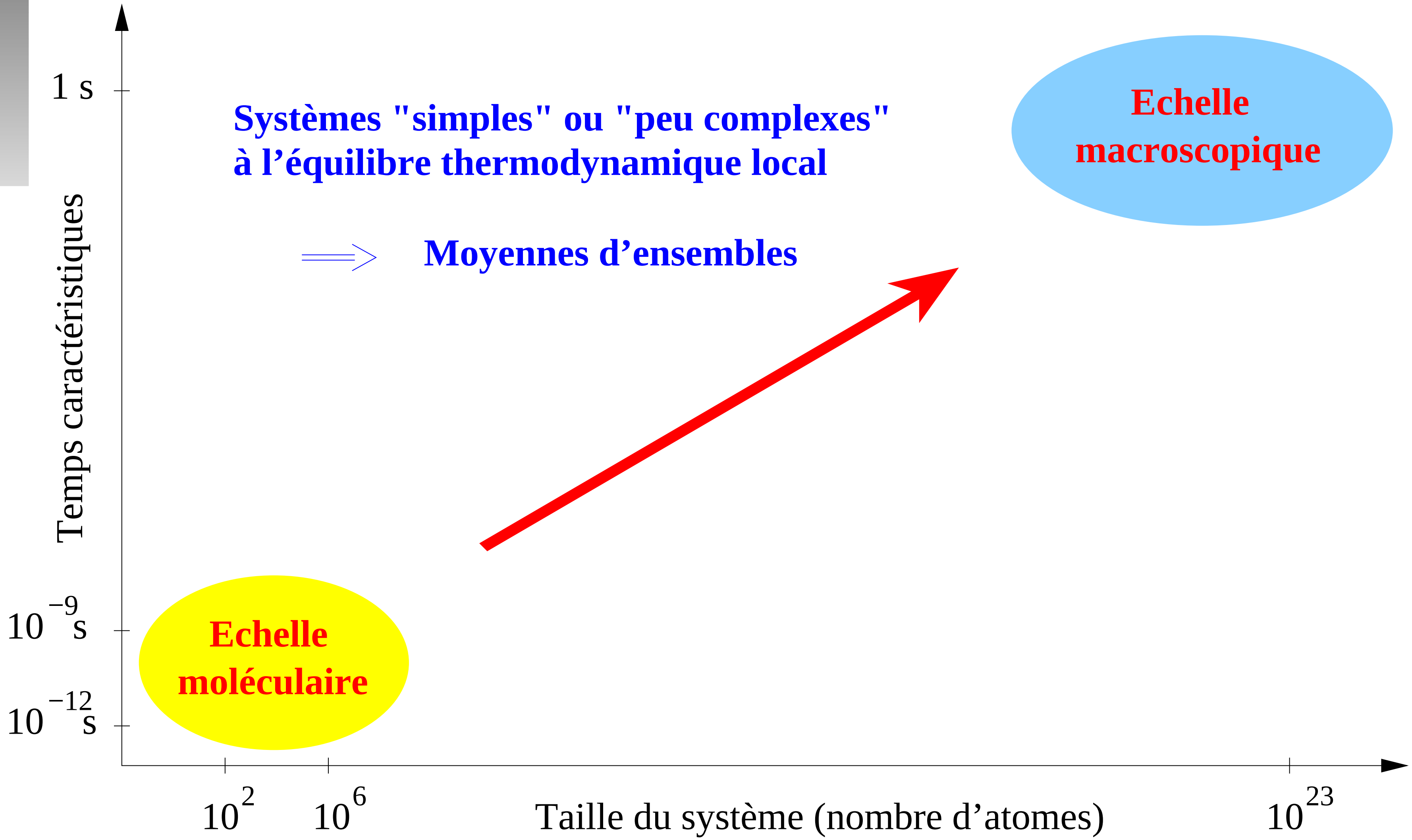
Integral models : $\boldsymbol{\tau} = \int_{-\infty}^{t} m(t-t')\mathbf{S}_t(t')\, dt'.$

(Macroscopic approach: R. Keunings & al., B. van den Brule & al., M. Picasso & al.)

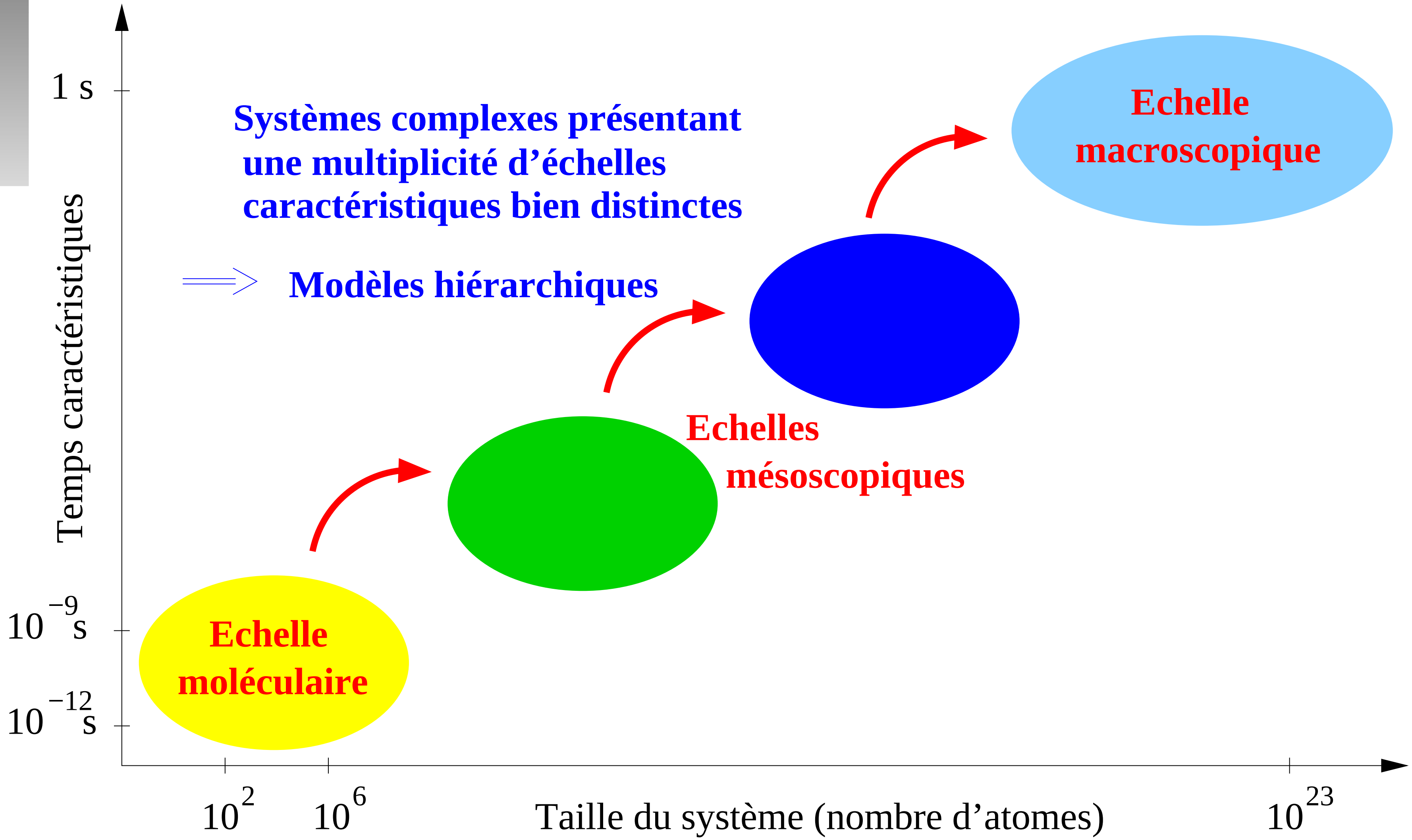
1B Multiscale modeling



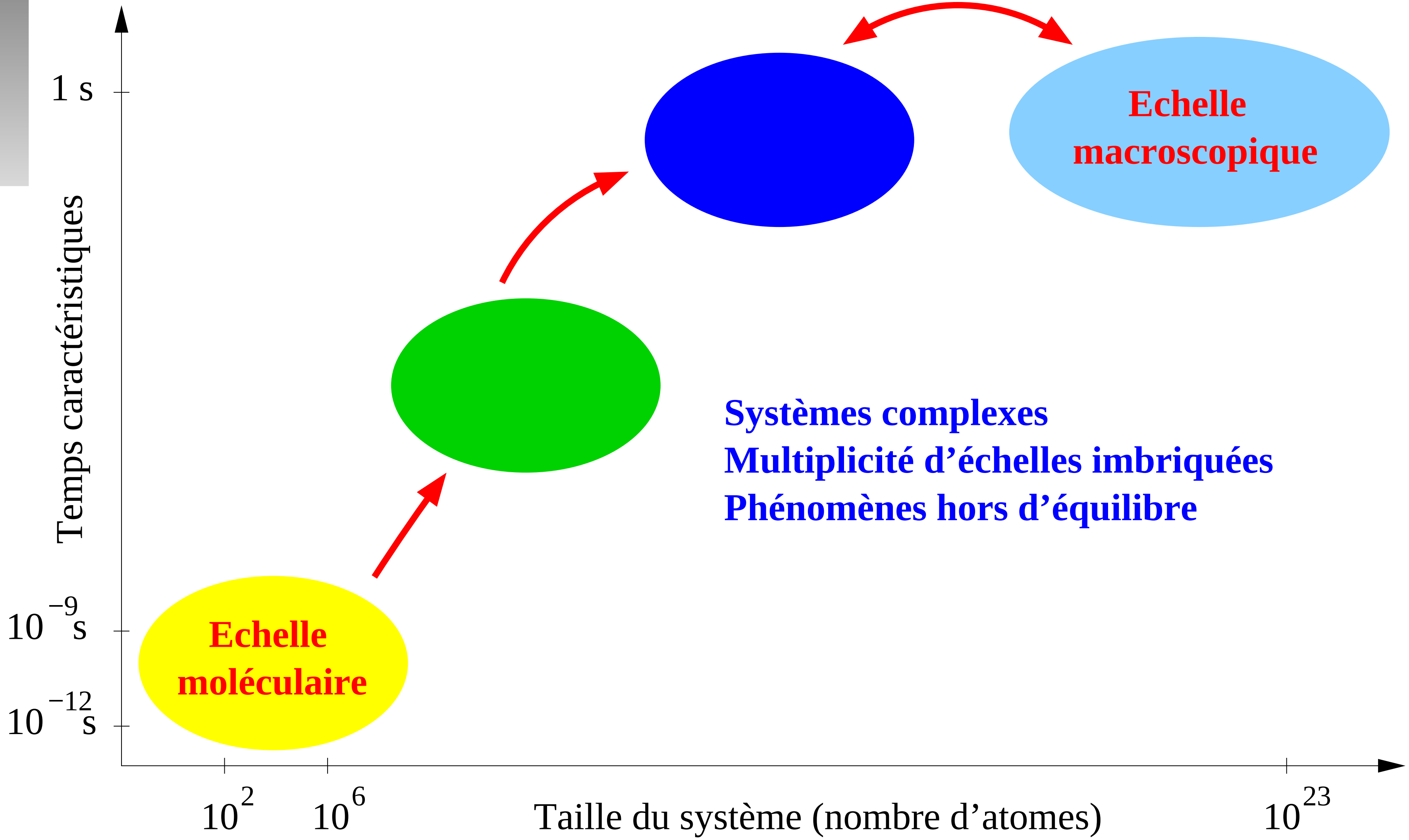
1B Multiscale modeling



1B Multiscale modeling

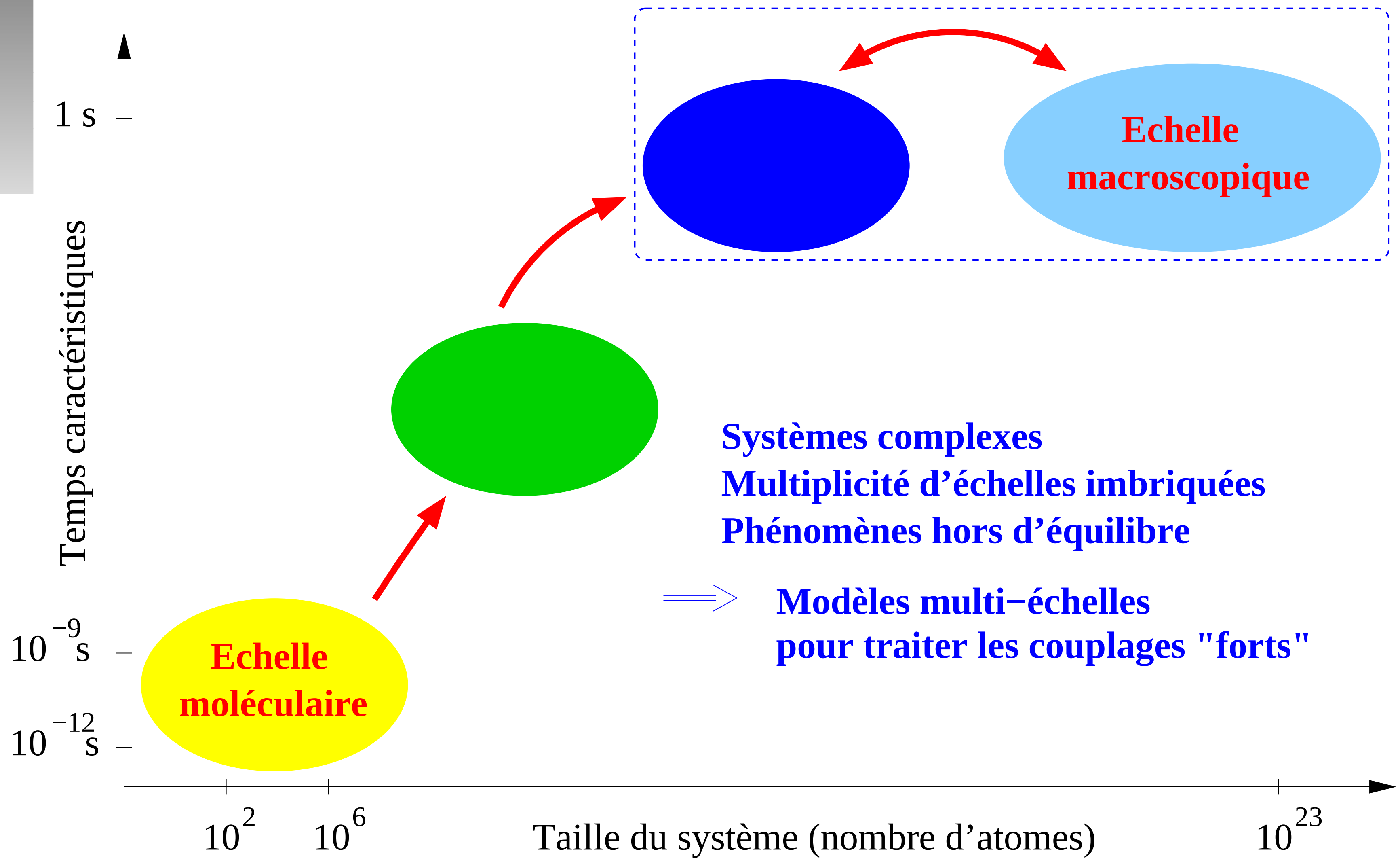


1B Multiscale modeling



Systèmes complexes
Multiplicité d'échelles imbriquées
Phénomènes hors d'équilibre

1B Multiscale modeling



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- 1A Experimental observations
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- 1C Microscopic models for polymer chains
- 1D Micro-macro models for polymeric fluids
- 1E Conclusion and discussion

2 Mathematics and numerics
- 2A Generalities
- 2B Some existence results
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1C Microscopic models for polymer chains

Micro-macro models require a microscopic model couped to a macroscopic description: difficulties wrt timescales and length scales.

The coupling requires some concepts from statistical mechanics: compute macroscopic quantities (stress, reaction rates, diffusion constants) from microscopic descriptions.

One needs a coarse description of the microstructures. How to model a microstructure evolving in a solvent ? Answer : molecular dynamics and the Langevin equations.

In Section 1C, we assume that the velocity field of the solvent is given (and is zero in a first stage).

1C Microscopic models for polymer chains

Microscopic model: N particles (atoms, groups of atoms) with positions $(\boldsymbol{q}_1, ..., \boldsymbol{q}_N) = \boldsymbol{q} \in \mathbb{R}^{3N}$, interacting through a potential $V(\boldsymbol{q}_1, ..., \boldsymbol{q}_N)$. Typically,

$$V(\boldsymbol{q}_1, ..., \boldsymbol{q}_N) = \sum_{i<j} V_{\mathrm{paire}}(\boldsymbol{q}_i, \boldsymbol{q}_j) + \sum_{i<j<k} V_{\mathrm{triplet}}(\boldsymbol{q}_i, \boldsymbol{q}_j, \boldsymbol{q}_k) + \dots$$

For a polymer chain, for example, a fine description would be to model the conformation by the position of the carbon atoms (backbone atoms). The potential V typically includes some terms function of the dihedral angles along the backbone.

1C Microscopic models for polymer chains

Molecular dynamics (solvent at rest): Langevin dynamics

$$\begin{cases} d\mathbf{Q}_t = M^{-1}\mathbf{P}_t\,dt, \\ d\mathbf{P}_t = -\nabla V(\mathbf{Q}_t)\,dt - \zeta M^{-1}\mathbf{P}_t\,dt + \sqrt{2\zeta\beta^{-1}}d\mathbf{W}_t, \end{cases}$$

where P_t is the momentum, M is the mass tensor, ζ is a friction coefficient and $\beta^{-1} = kT$.

Origin of the Langevin dynamics: description of a colloidal particle in a liquid (Brown).

1C Microscopic models for polymer chains

The Langevin dynamics is a thermostated Newton dynamics: The fluctuation ($\sqrt{2\zeta\beta^{-1}}d\mathbf{W}_t$) dissipation ($-\zeta M^{-1}\mathbf{P}_t\,dt$) terms are such that the Boltzmann-Gibbs measure is left invariant:

$$\nu(d\mathbf{p}, d\mathbf{q}) = \overline{Z}^{-1} \exp\left(-\beta\left(\frac{\mathbf{p}^T M^{-1}\mathbf{p}}{2} + V(\mathbf{q})\right)\right) d\mathbf{p}d\mathbf{q}.$$

To explain this in a simpler context, let us make the following simplification $M/\zeta \to 0$:

$$d\mathbf{Q}_t = -\nabla V(\mathbf{Q}_t)\zeta^{-1}\,dt + \sqrt{2\zeta^{-1}\beta^{-1}}d\mathbf{W}_t.$$

This dynamics leaves invariant the Boltzmann-Gibbs measure: $\mu(d\mathbf{q}) = Z^{-1}\exp\left(-\beta V(\mathbf{q})\right)d\mathbf{q}$.

1C Micro models: some probabilistic background

The Stochastic Differential Equation

$$d\mathbf{Q}_t = -\nabla V(\mathbf{Q}_t)\zeta^{-1}\,dt + \sqrt{2\zeta^{-1}\beta^{-1}}d\mathbf{W}_t$$

is discretized by the Euler scheme (with time step Δt):

$$\overline{\mathbf{Q}}_{n+1} - \overline{\mathbf{Q}}_n = -\nabla V(\overline{\mathbf{Q}}_n)\zeta^{-1}\,\Delta t + \sqrt{2\zeta^{-1}\beta^{-1}\Delta t}\boldsymbol{G}_n$$

where $(G_n^i)_{1\leq ile3, n\geq 0}$ are i.i.d. Gaussian random variables with zero mean and variance one. Indeed

$$(\boldsymbol{W}_{(n+1)\Delta t} - \boldsymbol{W}_{n\Delta t})_{n\geq 0} \stackrel{\mathcal{L}}{=} \sqrt{\Delta t}(\boldsymbol{G}_n)_{n\geq 0}.$$

1C Micro models: some probabilistic background

The Itô formula. Let ϕ be a smooth test function. Then

$$d\phi(\mathbf{Q}_t) = \nabla\phi(\mathbf{Q}_t)\cdot d\mathbf{Q}_t + \Delta\phi(\mathbf{Q}_t)\zeta^{-1}\beta^{-1}\,dt.$$

Proof (dimension 1):

$$dX_t = b(X_t)\,dt + \sigma(X_t)\,dW_t$$

$$\overline{X}_{n+1} - \overline{X}_n = b(\overline{X}_n)\Delta t + \sigma(\overline{X}_n)\sqrt{\Delta t}G_n$$

and thus

$$\begin{aligned}\phi(\overline{X}_{n+1}) &= \phi\left(\overline{X}_n + b(\overline{X}_n)\Delta t + \sigma(\overline{X}_n)\sqrt{\Delta t}G_n\right)\\ &= \phi(\overline{X}_n) + \phi'(\overline{X}_n)(b(\overline{X}_n)\Delta t + \sigma(\overline{X}_n)\sqrt{\Delta t}G_n)\\ &\quad + \frac{1}{2}\phi''(\overline{X}_n)\sigma^2(\overline{X}_n)\Delta t G_n^2 + o(\Delta t).\end{aligned}$$

1C Micro models: some probabilistic background

Then, summing over n and in the limit $\Delta t \to 0$,

$$\phi(X_t) = \phi(X_0) + \int_0^t \phi'(X_s)(b(X_s)ds + \sigma(X_s)\, dW_s)$$

$$+\frac{1}{2}\int_0^t \sigma^2(X_s)\phi''(X_s)\, ds,$$

$$= \phi(X_0) + \int_0^t \phi'(X_s)dX_s + \frac{1}{2}\int_0^t \sigma^2(X_s)\phi''(X_s)\, ds,$$

which is exactly

$$d\phi(X_t) = \phi'(X_t)dX_t + \frac{1}{2}\sigma^2(X_t)\phi''(X_t)\, dt.$$

1C Micro models: some probabilistic background

The Fokker-Planck equation. At fixed time t, $\mathbf{Q}_t$ has a density $\psi(t, \mathbf{q})$. The function ψ satisfies the PDE:

$$\zeta \partial_t \psi = \operatorname{div}(\nabla V \psi + \beta^{-1} \nabla \psi).$$

Proof (dimension 1):

$$dX_t = b(X_t)\, dt + \sigma(X_t)\, dW_t,$$

and we show that $X_t \stackrel{\mathcal{L}}{=} \psi(t, x)\, dx$ with

$$\partial_t \psi = \partial_x \left(-b\psi + \partial_x(\sigma\psi) \right).$$

We recall the Itô formula:

$$\phi(X_t) = \phi(X_0) + \int_0^t \phi'(X_s) dX_s + \frac{1}{2} \int_0^t \sigma^2(X_s) \phi''(X_s)\, ds.$$

1C Micro models: some probabilistic background

By definition of ψ, $\mathbf{E}(\phi(X_t)) = \int \phi(x)\psi(t,x)\,dx$. Thus, we have

$$\int \phi\psi(t,\cdot) = \int \phi\psi(0,\cdot) + \int_0^t \int \phi' b\psi(s,\cdot)ds + \frac{1}{2}\int_0^t \int \sigma^2\phi''\psi(s,\cdot)ds.$$

We have used the fact that

$$\begin{aligned}\mathbf{E}\int_0^t \phi'(X_s)dX_s &= \mathbf{E}\int_0^t \phi'(X_s)b(X_s)\,ds + \mathbf{E}\int_0^t \phi'(X_s)\sigma(X_s)\,dW_s \\ &= \int_0^t \mathbf{E}(\phi'(X_s)b(X_s))\,ds\end{aligned}$$

since
$\mathbf{E}\int_0^t \phi'(X_s)\sigma(X_s)\,dW_s \simeq \mathbf{E}\sum_{k=0}^n \phi'(\overline{X}_k)\sigma(\overline{X}_k)\sqrt{\Delta t}G_k = 0.$

1C Micro models: some probabilistic background

Thus the Boltzmann-Gibbs measure

$$\mu(d\mathbf{q}) = Z^{-1} \exp(-\beta V(\mathbf{q}))\, d\mathbf{q}$$

is invariant for the dynamics

$$d\mathbf{Q}_t = -\nabla V(\mathbf{Q}_t)\zeta^{-1}\, dt + \sqrt{2\zeta^{-1}\beta^{-1}} d\mathbf{W}_t.$$

Proof: We know that $\mathbf{Q}_t$ has a density ψ which satisfies:

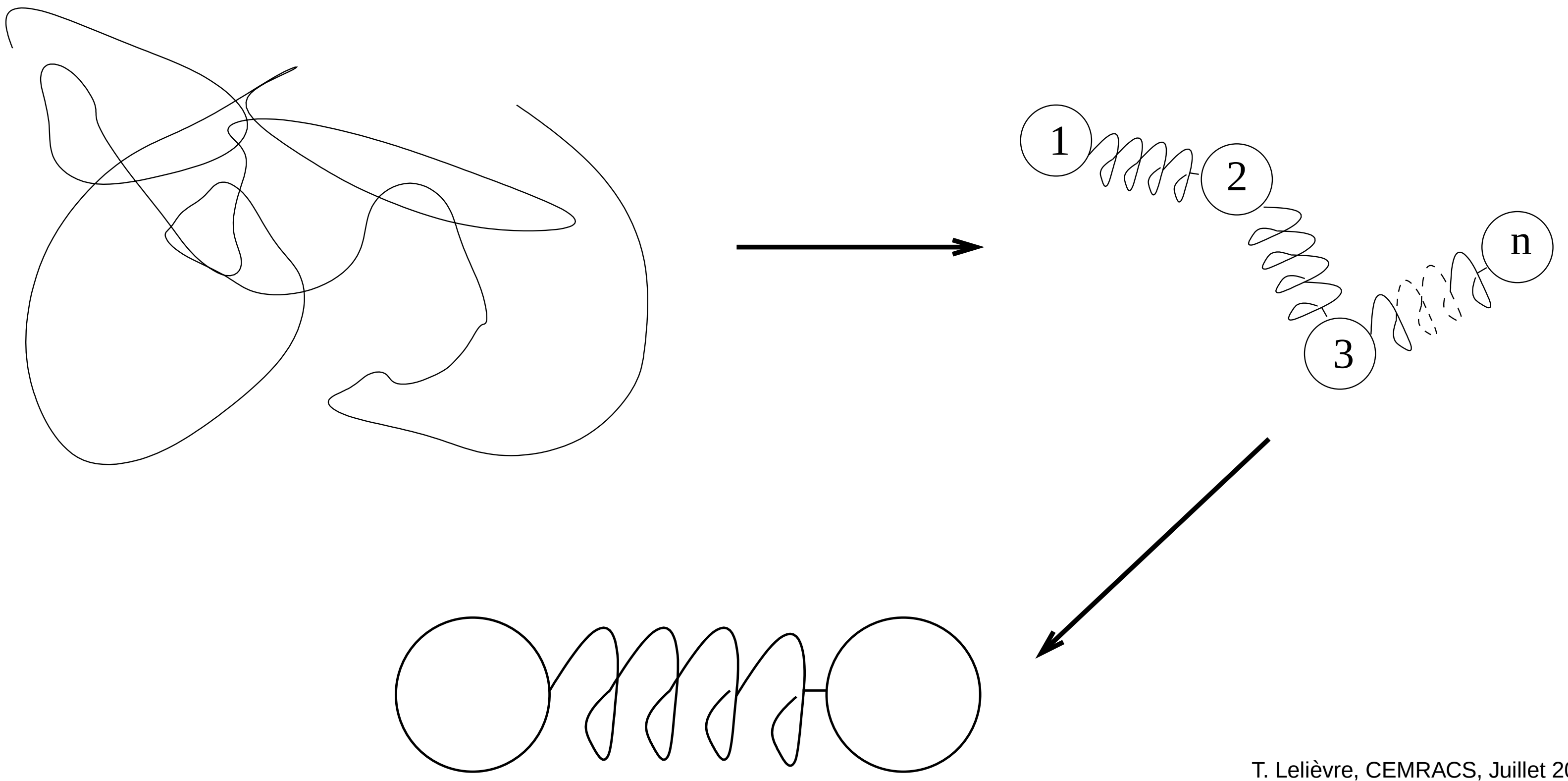
$$\zeta \partial_t \psi = \mathrm{div}(\nabla V \psi + \beta^{-1} \nabla \psi).$$

If $\psi(0,\cdot) = \exp(-\beta V)$, then $\forall t \geq 0$, $\psi(t,\cdot) = \exp(-\beta V)$.

A similar derivation can be done for the Langevin dynamics.

1C Microscopic models for polymer chains

Back to polymers. Which description ? The fine description is not suitable for micro-macro coupling (computer cost, time scale). We need to coarse-grain. Idea : consider blobs (1 blob $\simeq$ 20 CH_2 groups). The basic model (the dumbbell model): only two blobs. The conformation is given by the "end-to-end vector".



1C Microscopic models for polymer chains

Coarse-graining at equilibrium: use the image of the Boltzmann-Gibbs measure by the end-to-end vector mapping ("collective variable"):

$$\xi : \begin{cases} \mathbb{R}^{3N} & \to & \mathbb{R}^3 \\ \mathbf{q} = (\mathbf{q}_1, \dots, \mathbf{q}_N) & \mapsto & \mathbf{x} = \mathbf{q}_N - \mathbf{q}_1 \end{cases}$$

namely:

$$\xi * \left(Z^{-1} \exp(-\beta V(\mathbf{q}))\, d\mathbf{q} \right) = \exp(-\beta \Pi(\mathbf{x}))\, d\mathbf{x}.$$

Thus

$$\Pi(\mathbf{x}) = -\beta^{-1} \ln \left(\int \exp(-\beta V(\mathbf{q})) \delta_{\xi(\mathbf{q}) - \mathbf{x}}(d\mathbf{q}) \right).$$

Coarse-graining for polymers: W. Briels, V.G. Mavrantzas.

1C Microscopic models for polymer chains

Typically, two forces $\mathbf{F} = -\nabla \Pi$ are used:

$$\mathbf{F}(\mathbf{X}) = H\mathbf{X} \qquad \text{Hookean dumbbell,}$$

$$\mathbf{F}(\mathbf{X}) = \frac{H\mathbf{X}}{1 - \|\mathbf{X}\|^2/(bkT/H)} \qquad \text{FENE dumbbell,}$$

(FENE = Finite Extensible Nonlinear Elastic).

Notice that this effective potential Π ("free energy") is correct wrt statistical properties at equilibrium:
$\int \phi(\mathbf{x}) \exp(-\beta \Pi(\mathbf{x}))\, d\mathbf{x} = Z^{-1} \int \phi(\xi(\mathbf{q})) \exp(-\beta V(\mathbf{q}))\, d\mathbf{q}$.

We are now in position to write the basic model (the Rouse model).

References: R.B. Bird, C.F. Curtiss, R.C. Armstrong and O. Hassager, *Dynamic of Polymeric Liquids*, Wiley / M. Doi, S.F. Edwards, *The theory of polymer dynamics*, Oxford Science Publication) / H.C. Öttinger, *Stochastic processes in polymeric fluids*, Springer.

1C Microscopic models for polymer chains

Forces on bead i ($i = 1$ or 2) of coordinate vector $\mathbf{X}_t^i$ in a velocity field $\mathbf{u}(t, \boldsymbol{x})$ of the solvent (Langevin equation with negligible mass):

- Drag force:

$$-\zeta \left(\frac{d\mathbf{X}_t^i}{dt} - \mathbf{u}(t, \mathbf{X}_t^i) \right),$$

- Entropic force between beads 1 and 2 $(\mathbf{X} = (\mathbf{X}^2 - \mathbf{X}^1))$:

$$\mathbf{F}(\mathbf{X}) = H\mathbf{X} \qquad \text{Hookean dumbbell,}$$

$$\mathbf{F}(\mathbf{X}) = \frac{H\mathbf{X}}{1 - \|\mathbf{X}\|^2/(bkT/H)} \qquad \text{FENE dumbbell,}$$

1C Microscopic models for polymer chains

- “Brownian force”: $\mathbf{F}_b^i(t)$ such that

$$\int_0^t \mathbf{F}_b^i(s)\,ds = \sqrt{2kT\zeta}\,\mathbf{B}_t^i$$

with $\mathbf{B}_t^i$ a Brownian motion.

We introduce the end-to-end vector $\mathbf{X}_t = \left(\mathbf{X}_t^2 - \mathbf{X}_t^1\right)$ and the position of the center of mass $\mathbf{R}_t = \frac{1}{2}\left(\mathbf{X}_t^1 + \mathbf{X}_t^2\right)$.

We have:

$$\begin{cases} d\mathbf{X}_t^1 = \mathbf{u}(t, \mathbf{X}_t^1)\,dt - \zeta^{-1}\mathbf{F}(\mathbf{X}_t)\,dt + \sqrt{2kT\zeta^{-1}}d\mathbf{B}_t^1 \\ d\mathbf{X}_t^2 = \mathbf{u}(t, \mathbf{X}_t^2)\,dt + \zeta^{-1}\mathbf{F}(\mathbf{X}_t)\,dt + \sqrt{2kT\zeta^{-1}}d\mathbf{B}_t^2 \end{cases}$$

1C Microscopic models for polymer chains

By linear combinations of the two Langevin equations on X^1 and X^2, one obtains:

$$\begin{cases} d\mathbf{X}_t = \left(\mathbf{u}(t,\boldsymbol{X}_t^2) - \mathbf{u}(t,\boldsymbol{X}_t^1)\right)\,dt - \dfrac{2}{\zeta}\mathbf{F}(\mathbf{X}_t)\,dt + 2\sqrt{\dfrac{kT}{\zeta}}d\mathbf{W}_t^1, \\ d\boldsymbol{R}_t = \dfrac{1}{2}\left(\mathbf{u}(t,\boldsymbol{X}_t^1) + \mathbf{u}(t,\boldsymbol{X}_t^2)\right)\,dt + \sqrt{\dfrac{kT}{\zeta}}d\mathbf{W}_t^2, \end{cases}$$

where $\boldsymbol{W}_t^1 = \frac{1}{\sqrt{2}}\left(\boldsymbol{B}_t^2 - \boldsymbol{B}_t^1\right)$ and $\boldsymbol{W}_t^2 = \frac{1}{\sqrt{2}}\left(\boldsymbol{B}_t^1 + \boldsymbol{B}_t^2\right)$.

Approximations:

- $\mathbf{u}(t,\mathbf{X}_t^i) \simeq \mathbf{u}(t,\mathbf{R}_t) + \nabla\mathbf{u}(t,\mathbf{R}_t)(\mathbf{X}_t^i - \mathbf{R}_t)$,
- the noise on R_t is zero.

1C Microscopic models for polymer chains

We finally get

$$\begin{cases} d\mathbf{X}_t = \nabla \mathbf{u}(t, \boldsymbol{R}_t)\mathbf{X}_t \, dt - \frac{2}{\zeta}\mathbf{F}(\mathbf{X}_t)\, dt + \sqrt{\frac{4kT}{\zeta}} d\mathbf{W}_t, \\ d\boldsymbol{R}_t = \mathbf{u}(t, \boldsymbol{R}_t)\, dt. \end{cases}$$

Eulerian version:

$$d\mathbf{X}_t(\boldsymbol{x}) + \mathbf{u}(t, \boldsymbol{x}).\nabla \mathbf{X}_t(\boldsymbol{x})\, dt =$$

$$\nabla \mathbf{u}(t, \boldsymbol{x})\mathbf{X}_t(\boldsymbol{x})\, dt - \frac{2}{\zeta}\mathbf{F}(\mathbf{X}_t(\boldsymbol{x}))\, dt + \sqrt{\frac{4kT}{\zeta}} d\mathbf{W}_t.$$

$\mathbf{X}_t(\boldsymbol{x})$ is a function of time t, position x, and probability variable ω.

1C Microscopic models for polymer chains

Discussion of the modelling (1/2).

Discussion of the coarse-graining procedure:

- The construction of Π has been done for zero velocity field ($\mathbf{u} = 0$). How do the two operations : $\mathbf{u} \neq 0$ and “coarse-graining” commute ?
- Imagine $\mathbf{u} = 0$. The dynamics

$$d\mathbf{X}_t = -\frac{2}{\zeta}\mathbf{F}(\mathbf{X}_t)\,dt + \sqrt{\frac{4kT}{\zeta}}d\mathbf{W}_t$$

  is certainly correct wrt the sampled measure ($\exp(-\beta\Pi)$). But what to say about the correctness of the dynamics ?

1C Microscopic models for polymer chains

Discussion of the modelling (2/2).

Discussion of the approximations:

- the expansion used on the velocity requires some regularity on $\mathbf{u}$: the term $\nabla \mathbf{u}$ leads to some mathematical difficulties in the mathematical analysis.
- if the noise on $\mathbf{R}_t$ is not neglected, a diffusion term in space ($\mathbf{x}$-variable) in the Fokker-Planck equation gives more regularity.

1C Microscopic models for polymer chains

We have presented a suitable model for *dilute solution of polymers*.

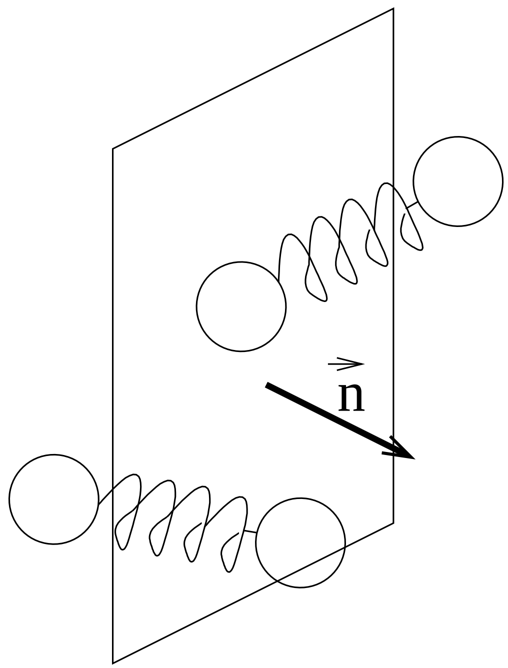
Similar descriptions (kinetic theory) have been used to model:

- rod-like polymers and liquid crystals (Onsager, Maier-Saupe),
- polymer melts (de Gennes, Doi-Edwards),
- concentrated suspensions (Hébraud-Lequeux),
- blood (Owens).

Outline

1D Micro-macro models for polymeric fluids

To close the system, an expression of the stress tensor $\boldsymbol{\tau}$ in terms of the polymer chain configuration is needed. This is the Kramers expression (assuming homogeneous system):



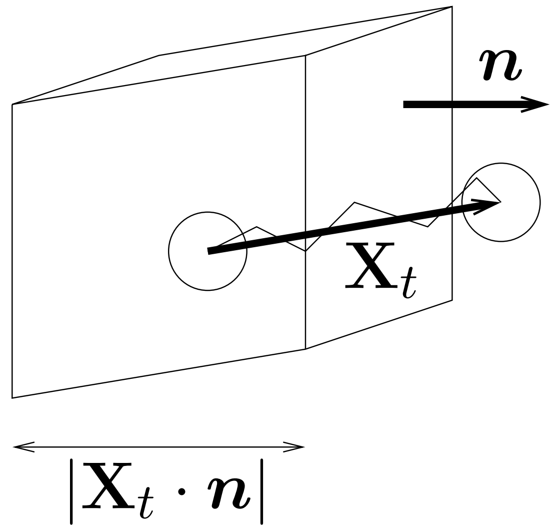
$$\boldsymbol{\tau}(t,\boldsymbol{x}) = n_p\Big(-kT\boldsymbol{I} + \mathbf{E}\left(\mathbf{X}_t(\boldsymbol{x}) \otimes \mathbf{F}(\mathbf{X}_t(\boldsymbol{x}))\right)\Big).$$

1D Micro-macro models for polymeric fluids

How to derive this formula ? One approach is to use the principle of virtual work. Another idea is to go back to the definition of stress:

$$\boldsymbol{\tau}\boldsymbol{n}\,dS = \mathbf{E}\left(\text{sgn}(\mathbf{X}_t\cdot\boldsymbol{n})\mathbf{F}(\mathbf{X}_t)1_{\{\mathbf{X}_t\text{ intersects plane}\}}\right).$$

Since the system is assumed to be homogeneous, given $\mathbf{X}_t$, the probability that $\mathbf{X}_t$ intersects the plane is $N_p\frac{dS|\mathbf{X}_t\cdot\boldsymbol{n}|}{V}$.



1D Micro-macro models for polymeric fluids

Thus we have:

$$\begin{aligned}
\boldsymbol{\tau}\boldsymbol{n}\, dS &= \mathbf{E}\left(\text{sgn}(\mathbf{X}_t \cdot \boldsymbol{n})\mathbf{F}(\mathbf{X}_t) 1_{\{\mathbf{X}_t \text{ intersects plane}\}}\right) \\
&= \mathbf{E}\left(\text{sgn}(\mathbf{X}_t \cdot \boldsymbol{n})\mathbf{F}(\mathbf{X}_t)\mathbf{P}(\mathbf{X}_t \text{ intersects plane}|\mathbf{X}_t)\right) \\
&= n_p \mathbf{E}\left(\text{sgn}(\mathbf{X}_t \cdot \boldsymbol{n})\mathbf{F}(\mathbf{X}_t)|\mathbf{X}_t \cdot \boldsymbol{n}|\right)\, dS \\
&= n_p \mathbf{E}\left(\mathbf{X}_t \otimes \mathbf{F}(\mathbf{X}_t)\right) \boldsymbol{n}\, dS,
\end{aligned}$$

where $n_p = N_p / V$.

1D Micro-macro models for polymeric fluids

This is the complete coupled system:

$$\left\{\begin{array}{l}\rho\left(\partial_t + \mathbf{u}.\nabla\right)\mathbf{u} = -\nabla p + \eta\Delta\mathbf{u} + \operatorname{div}(\boldsymbol{\tau}) + \mathbf{f}_{ext},\\ \operatorname{div}(\mathbf{u}) = 0,\\ \boldsymbol{\tau} = n_p\Big(-kT\boldsymbol{I} + \mathbf{E}\left(\mathbf{X}_t \otimes \mathbf{F}(\mathbf{X}_t)\right)\Big),\\ d\mathbf{X}_t + \mathbf{u}.\nabla_{\boldsymbol{x}}\mathbf{X}_t\,dt = \left(\nabla\mathbf{u}\mathbf{X}_t - \frac{2}{\zeta}\mathbf{F}(\mathbf{X}_t)\right)dt + \sqrt{\frac{4kT}{\zeta}}d\mathbf{W}_t.\end{array}\right.$$

The S(P)DE is posed at each macroscopic point $\boldsymbol{x}$.
The random process $\mathbf{X}_t$ is space-dependent: $\mathbf{X}_t(\boldsymbol{x})$.

1D Micro-macro models for polymeric fluids

One can replace the SDE by the Fokker-Planck equation, which rules the evolution of the density probability function $\psi(t,\boldsymbol{x},\mathbf{X})$ of $\mathbf{X}_t(\boldsymbol{x})$:

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla_{\boldsymbol{x}} \psi = -\operatorname{div}_{\mathbf{X}} \left(\left(\nabla \mathbf{u} \, \mathbf{X} - \frac{2}{\zeta} \mathbf{F}(\mathbf{X}) \right) \psi \right) + \frac{2kT}{\zeta} \Delta_{\mathbf{X}} \psi,$$

and then:

$$\boldsymbol{\tau}(t,\boldsymbol{x}) = -n_p \, k \, T \boldsymbol{I} + n_p \int_{\mathbb{R}^d} (\mathbf{X} \otimes \mathbf{F}(\mathbf{X})) \, \psi(t,\boldsymbol{x},\mathbf{X}) \, d\mathbf{X}.$$

1D Micro-macro models for polymeric fluids

Once non-dimensionalized, we obtain:

$$\left\{\begin{array}{l}\text{Re}\,(\partial_t + \mathbf{u}\cdot\nabla)\,\mathbf{u} = -\nabla p + (1-\epsilon)\Delta\mathbf{u} + \mathrm{div}(\boldsymbol{\tau}) + \mathbf{f}_{ext},\\ \mathrm{div}(\mathbf{u}) = 0,\\ \boldsymbol{\tau} = \frac{\epsilon}{\mathrm{We}}(\mu\mathbf{E}(\mathbf{X}_t\otimes\mathbf{F}(\mathbf{X}_t)) - \boldsymbol{I}),\\ d\mathbf{X}_t + \mathbf{u}\cdot\nabla_{\boldsymbol{x}}\mathbf{X}_t\,dt = \left(\nabla\mathbf{u}\cdot\mathbf{X}_t - \frac{1}{2\mathrm{We}}\mathbf{F}(\mathbf{X}_t)\right)dt + \frac{1}{\sqrt{\mathrm{We}\,\mu}}d\mathbf{W}_t,\end{array}\right.$$

with the following non-dimensional numbers:

$$\text{Re} = \frac{\rho U L}{\eta},\ \mathrm{We} = \frac{\lambda U}{L},\ \epsilon = \frac{\eta_p}{\eta},\ \mu = \frac{L^2 H}{k_b T},$$

and $\lambda = \frac{\zeta}{4H}$: a relaxation time of the polymers,
$\eta_p = n_p k T\lambda$: the viscosity associated to the polymers,
U and L: characteristic velocity and length. Usually, L is chosen so that $\mu = 1$.

1D Micro-macro models for polymeric fluids

Link with macroscopic models. the Hookean dumbbell model is equivalent to the Oldroyd-B model: if $\mathbf{F}(\mathbf{X}) = \mathbf{X}$, $\boldsymbol{\tau}$ satisfies:

$$\frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u}.\nabla \boldsymbol{\tau} = \nabla \mathbf{u} \boldsymbol{\tau} + \boldsymbol{\tau} (\nabla \mathbf{u})^T + \frac{\epsilon}{\mathrm{We}} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{1}{\mathrm{We}} \boldsymbol{\tau}.$$

There is no macroscopic equivalent to the FENE model. However, using the closure approximation

$$\mathbf{F}(\mathbf{X}) = \frac{H\mathbf{X}}{1 - \|\mathbf{X}\|^2/(bkT/H)} \simeq \frac{H\mathbf{X}}{1 - \mathbf{E}\|\mathbf{X}\|^2/(bkT/H)}$$

one ends up with the FENE-P model.

1D Micro-macro models for polymeric fluids

The FENE-P model:

$$\begin{cases} \lambda\left(\dfrac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u}\cdot\nabla\boldsymbol{\tau} - \nabla\mathbf{u}\boldsymbol{\tau} - \boldsymbol{\tau}(\nabla\mathbf{u})^T\right) + Z(\mathrm{tr}(\boldsymbol{\tau}))\boldsymbol{\tau} \\ -\lambda\left(\boldsymbol{\tau} + \dfrac{\eta_p}{\lambda}\boldsymbol{I}\right)\left(\left(\dfrac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\ln\left(Z(\mathrm{tr}(\boldsymbol{\tau}))\right)\right) = \eta_p(\nabla\mathbf{u} + (\nabla\mathbf{u})^T), \end{cases}$$

with

$$Z(\mathrm{tr}(\boldsymbol{\tau})) = 1 + \frac{d}{b}\left(1 + \lambda\frac{\mathrm{tr}(\boldsymbol{\tau})}{d\,\eta_p}\right),$$

where d is the dimension.

Remark: The derivative $\frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u}\cdot\nabla\boldsymbol{\tau} - \nabla\mathbf{u}\boldsymbol{\tau} - \boldsymbol{\tau}(\nabla\mathbf{u})^T$ is called the Upper Convected derivative.

Outline

1E Conclusion and discussion

This system coupling a PDE and a SDE can be solved by adapted numerical methods. The interests of this micro-macro approach are:

- kinetic modelling is reliable and based on some clear assumptions (macroscopic models usually derive from kinetic models (e.g. Oldroyd B), sometimes *via* closure approximations, but some microscopic models have no macroscopic equivalent (e.g FENE)),
- it enables numerical explorations of the link between microscopic properties and macroscopic behaviour,
- the parameters of these models have a physical meaning and can be evaluated,
- it seems that the numerical methods based on this approach are more robust.

1E Conclusion and discussion

However, micro-macro approaches are not the solution:

- One of the main difficulties for the computation of viscoelastic fluid is the High Weissenberg Number Problem (HWNP). This problem is still present in micro-macro models (highly refined meshes would be needed ?).
- The computational cost is very high. Discretization of the Fokker-Planck equation rather than the set of SDEs may help, but this is restrained to low-dimensional space for the microscopic variables.

The main interest of micro-macro approaches as compared to macro-macro approaches lies at the modelling level.

1E Conclusion and discussion

Macro-macro approach:

$$\begin{cases} \dfrac{D\mathbf{u}}{Dt} & = & \mathcal{F}(\boldsymbol{\tau}_p, \mathbf{u}), \\ \dfrac{D\boldsymbol{\tau}_p}{Dt} & = & \mathcal{G}(\boldsymbol{\tau}_p, \mathbf{u}). \end{cases}$$

Multiscale, or micro-macro approach:

$$\begin{cases} \dfrac{D\mathbf{u}}{Dt} & = & \mathcal{F}(\boldsymbol{\tau}_p, \mathbf{u}), \\ \boldsymbol{\tau}_p & = & \text{average over } \Sigma, \\ \dfrac{D\Sigma}{Dt} & = & \mathcal{G}_\mu(\Sigma, \mathbf{u}). \end{cases}$$

1E Conclusion and discussion

Pros and cons for the macro-macro and micro-macro approaches:

	MACRO	MICRO-MACRO	
modelling capabilities	low	high	
current utilization	industry	laboratories	
		discretization by Monte Carlo	discretization of Fokker-Planck
computational cost	low	high	moderate
computational bottleneck	HWNP	variance, HWNP	dimension, HWNP

Outline

The main difficulties for mathematical analysis: transport and (nonlinear) coupling.

$$\begin{cases} \text{Re}\left(\dfrac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = (1-\epsilon)\Delta\mathbf{u} - \nabla p + \mathrm{div}(\boldsymbol{\tau}) \, , \\ \mathrm{div}(\mathbf{u}) = 0 \, , \\ \boldsymbol{\tau} = \dfrac{\epsilon}{\text{We}}(\mathbf{E}(\mathbf{X}\otimes\mathbf{F}(\mathbf{X})) - \boldsymbol{I}) \, , \\ d\mathbf{X} + \mathbf{u}\cdot\nabla\mathbf{X} dt = \left(\nabla\mathbf{u}\mathbf{X} - \dfrac{1}{2\text{We}}\mathbf{F}(\mathbf{X})\right) dt + \dfrac{1}{\sqrt{\text{We}}} d\mathbf{W}_t . \end{cases}$$

Similar difficulties with macro models (Oldroyd-B):

$$\frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u}.\nabla\boldsymbol{\tau} = \nabla\mathbf{u}\boldsymbol{\tau} + \boldsymbol{\tau}(\nabla\mathbf{u})^T + \frac{\epsilon}{\text{We}}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{1}{\text{We}}\boldsymbol{\tau}.$$

The state-of-the-art mathematical well-posedness analysis is local-in-time existence and uniqueness results, both for macro-macro and micro-macro models.
One exception (P.L Lions, N. Masmoudi) concerns models with co-rotational derivatives rather than upper-convected derivatives, for which global-in-time existence results have been obtained. It consists in replacing

$$\frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u}.\nabla \boldsymbol{\tau} - \nabla \mathbf{u} \boldsymbol{\tau} - \boldsymbol{\tau} (\nabla \mathbf{u})^T$$

by

$$\frac{\partial \boldsymbol{\tau}}{\partial t} + \mathbf{u}.\nabla \boldsymbol{\tau} - W(\mathbf{u}) \boldsymbol{\tau} - \boldsymbol{\tau} W(\mathbf{u})^T,$$

where $W(\mathbf{u}) = \frac{\nabla \mathbf{u} - \nabla \mathbf{u}^T}{2}$.

These better results come from additional *a priori* estimates based on the fact that $\left(W(\mathbf{u})\boldsymbol{\tau} + \boldsymbol{\tau} W(\mathbf{u})^T\right) : \boldsymbol{\tau} = 0$.

For micro-macro models, it consists in using the SDE:

$$d\mathbf{X}_t + \mathbf{u} \cdot \nabla \mathbf{X}_t dt = \left(\frac{\nabla \mathbf{u} - \nabla \mathbf{u}^T}{2} \mathbf{X}_t - \frac{1}{2\mathrm{We}} \mathbf{F}(\mathbf{X}_t) \right) dt + \frac{1}{\sqrt{\mathrm{We}}} d\mathbf{W}_t.$$

However, these models are not considered as good models. For example, $\psi \propto \exp(-\Pi)$ is a stationary solution to the Fokker Planck equation whatever $\mathbf{u}$.

Well-posedness results for micro-macro models:

- The uncoupled problem: SDE or FP.
  - SDE in the FENE case (B. Jourdain, TL: OK for $b \geq 2$),
  - the case of non smooth velocity field, transport term in the SDE or FP (C. Le Bris, P.L Lions).
- The coupled problem: PDE + SDE or PDE + FP.
  - PDE+SDE: shear flow for Hookean or FENE (C. Le Bris, B. Jourdain, TL / W. E, P. Zhang),
  - PDE+FP: FENE case (M. Renardy / J.W. Barrett, C. Schwab, E. Süli: (mollification) OK for $b \geq 10$ / N. Masmoudi, P.L. Lions).

Another interesting (not only) theoretical issue is the long-time behaviour.

2A Generalities

For numerics, the main difficulties both for micro-macro and macro-macro models are:

- An inf-sup condition is needed between the discretization space for $\boldsymbol{\tau}$ and that for $\mathbf{u}$ (in the limit $\epsilon \to 1$). $\longrightarrow$ use of special discretization spaces, use stabilization methods
- The discretization of the advection terms needs to be done properly. $\longrightarrow$ use stabilization methods, use numerical characteristic method.
- The discretization of the nonlinear term raises difficulties.

For High Weissenberg, difficulties are observed numerically in some geometries: instabilities, convergence under mesh refinement. As applied mathematicians, we would like to build safe numerical schemes, *e.g.* schemes which do not bring spurious "energy" (which one ?) in the system.

In the following, we focus on the specificities of discretization for micro-macro models. Two approaches: discretizing the Fokker-Planck equation, or discretizing the SDEs.

The basic method is called CONNFFESSIT (Laso, Öttinger / Hulsen, van Heel, van den Brule: BCF) (Calculation Of Non-Newtonian Flow: Finite Elements and Stochastic SImulation Technique.)

2A Generalities

Numerical analysis in fluid mechanics

Numerical analysis of SDEs

The problem

Discretization in space : convergence of finite element approximations for solutions of PDEs : $O(\delta y)$.

Discretization in time : convergence of finite difference schemes for time-dependent ODEs or SDEs : $O(\Delta t)$.

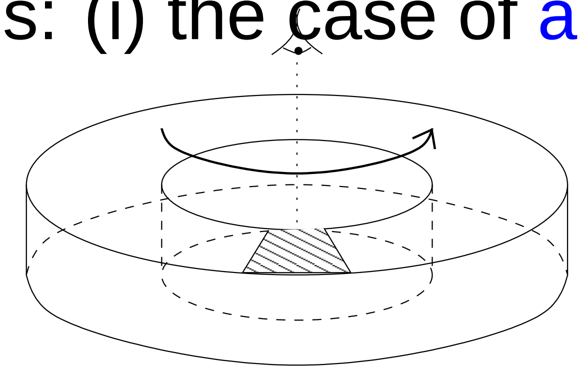
Discretization by Monte Carlo methods : generalization of the law of large number : $O\left(\frac{1}{\sqrt{M}}\right)$.

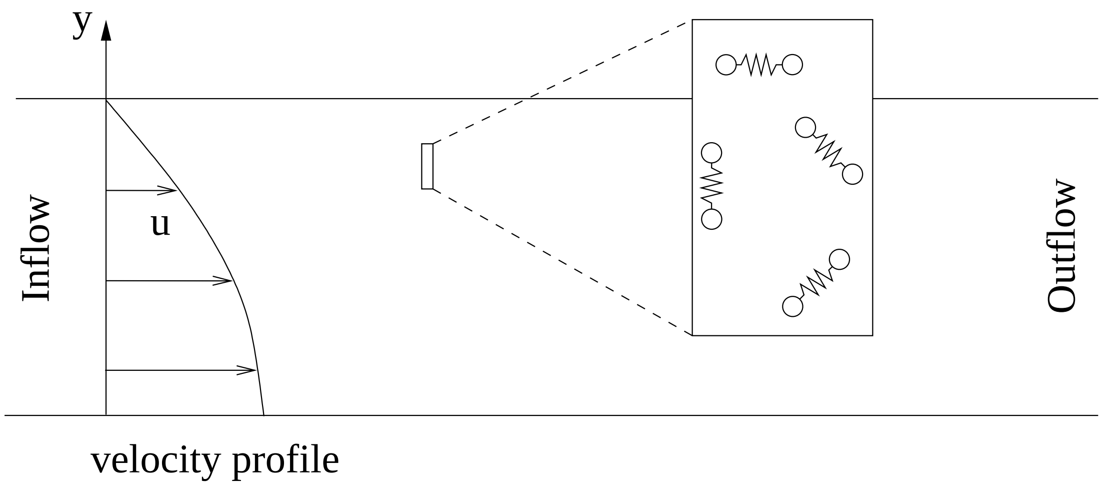
$$\left\|u(t_n) - \overline{u}_h^n\right\|_{L^2_y(L^2_\omega)} + \left\|\mathbb{E}(X_{t_n} Y_{t_n}) - \frac{1}{M}\sum_{j=1}^M \overline{X}_{h,n}^j \overline{Y}_n^j\right\|_{L^1_y(L^1_\omega)} \leq C\left(\delta y + \Delta t + \frac{1}{\sqrt{M}}\right).$$

Numerical questions:

- The uncoupled problem: SDE or FP.
  - SDE: Variance reduction by control variate methods (M. Picasso), the FENE-P model as a control variate (B. Jourdain, TL),
  - FP: Finite-difference methods, spectral methods, the bead-spring model (high-dimensional problem) (C. Liu / Q. Du / C. Chauvière/ R. Owens / A. Lozinski).
- The coupled problem
  - PDE+SDE: Convergence of the MC / Euler / FE discretization (C. Le Bris, B. Jourdain, TL / P. Zhang),
  - PDE+SDE: Dependency of the B.M on space (C. Le Bris, B. Jourdain, TL).

Two simplifications: (i) the case of a plane shear flow.





We keep the coupling, but we get rid of the transport (since $\mathbf{u}.\nabla = 0$).

The equations in this case read ($0 \le t \le T$, $y \in \mathcal{O} = (0,1)$):

$$\begin{cases} \partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \tau(t,y) + f_{ext}(t,y), \\ \tau(t,y) = \mathbf{E}\left(X_t(y)\, F_2(X_t(y), Y_t(y))\right) = \mathbf{E}\left(Y_t(y)\, F_1(X_t(y), Y_t(y))\right) \\ dX_t(y) = \left(-\frac{1}{2} F_1(X_t(y), Y_t(y)) + \partial_y u(t,y) Y_t(y)\right) dt + dV_t, \\ dY_t(y) = \left(-\frac{1}{2} F_2(X_t(y), Y_t(y))\right) dt + dW_t, \end{cases}$$

- $\mathbf{F}(\mathbf{X}_t) = \mathbf{X}_t = (X_t, Y_t)$ (Hookean), or
- $\mathbf{F}(\mathbf{X}_t) = \frac{\mathbf{X}_t}{1 - \frac{\|\mathbf{X}_t\|^2}{b}} = \left(\frac{X_t}{1 - \frac{X_t^2 + Y_t^2}{b}}, \frac{Y_t}{1 - \frac{X_t^2 + Y_t^2}{b}} \right)$ (FENE),

where $\mathbf{u}(t,x,y) = (u(t,y), 0)$, $\boldsymbol{\tau} = \begin{bmatrix} * & \tau \\ \tau & * \end{bmatrix}$,

and $\mathbf{F}(\mathbf{X}_t) = (F_1(X_t, Y_t), F_2(X_t, Y_t))$.

(ii) the case of a homogeneous velocity field:

$$\mathbf{u}(t, \boldsymbol{x}) = \boldsymbol{\kappa}(t)\boldsymbol{x}.$$

In this case, $\mathbf{X}_t$ does not depend on $\boldsymbol{x}$ and the polymer does not influence the flow (since $\mathrm{div}(\boldsymbol{\tau}) = 0$).
Therefore, we simply have to study the following SDE:

$$d\mathbf{X} = \left(\boldsymbol{\kappa}(t)\mathbf{X} - \frac{1}{2\mathrm{We}}\mathbf{F}(\mathbf{X})\right) dt + \frac{1}{\sqrt{\mathrm{We}}} d\mathbf{W}_t.$$

Outline

2B Some existence results

$$
\begin{cases}
\text{Re}\left(\dfrac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = (1-\epsilon)\Delta\mathbf{u} - \nabla p + \mathrm{div}(\boldsymbol{\tau}) , \\
\mathrm{div}(\mathbf{u}) = 0 , \\
\boldsymbol{\tau} = \dfrac{\epsilon}{\mathrm{We}}(\mathbf{E}(\mathbf{X}_t \otimes \mathbf{F}(\mathbf{X}_t)) - \boldsymbol{I}) , \\
d\mathbf{X}_t + \mathbf{u}\cdot\nabla\mathbf{X}_t dt = \left(\nabla\mathbf{u}\mathbf{X}_t - \dfrac{1}{2\mathrm{We}}\mathbf{F}(\mathbf{X}_t)\right) dt + \dfrac{1}{\sqrt{\mathrm{We}}} d\mathbf{W}_t .
\end{cases}
$$

Adopted approach :

- The SDEs are posed at each macroscopic point $\boldsymbol{x}$ (we need a pointwise defined $\nabla\mathbf{u}$),
- The PDEs are posed in a distributional sense (we need $\boldsymbol{\tau}$ to be in L^1_{loc}).

2B Some existence results

Fundamental *a priori* estimate ($\mathbf{F} = \nabla \Pi$):

$$(1) \quad \frac{\mathrm{Re}}{2} \int_{\mathcal{D}} |\mathbf{u}|^2 + (1-\epsilon) \int_0^t \int_{\mathcal{D}} |\nabla \mathbf{u}|^2$$

$$= \frac{\mathrm{Re}}{2} \int_{\mathcal{D}} |\mathbf{u}_0|^2 - \frac{\epsilon}{\mathrm{We}} \int_0^t \int_{\mathcal{D}} \mathbf{E}(\mathbf{X}_s \otimes \mathbf{F}(\mathbf{X}_s)) : \nabla \mathbf{u}.$$

$$(2) \int_{\mathcal{D}} \mathbf{E}(\Pi(\mathbf{X}_t)) + \frac{1}{2\mathrm{We}} \int_0^t \int_{\mathcal{D}} \mathbf{E}(\|\mathbf{F}(\mathbf{X}_s)\|^2)$$

$$= \int_{\mathcal{D}} \mathbf{E}(\Pi(\mathbf{X}_0)) + \int_0^t \int_{\mathcal{D}} \mathbf{E}(\mathbf{F}(\mathbf{X}_s).\nabla \mathbf{u} \mathbf{X}_s) + \frac{1}{2\mathrm{We}} \int_0^t \int_{\mathcal{D}} \Delta \Pi(\mathbf{X}_s).$$

$$(1) + \frac{\epsilon}{\mathrm{We}}(2) \Longrightarrow \frac{\mathrm{Re}}{2} \frac{d}{dt} \int_{\mathcal{D}} |\mathbf{u}|^2 + (1-\epsilon) \int_{\mathcal{D}} |\nabla \mathbf{u}|^2 + \frac{\epsilon}{\mathrm{We}} \frac{d}{dt} \int_{\mathcal{D}} \mathbf{E}(\Pi(\mathbf{X}_t))$$

$$+ \frac{\epsilon}{2\mathrm{We}^2} \int_{\mathcal{D}} \mathbf{E}(\|\mathbf{F}(\mathbf{X}_t)\|^2) = \frac{\epsilon}{2\mathrm{We}^2} \int_{\mathcal{D}} \Delta \Pi(\mathbf{X}_t).$$

2B Some existence results: Hookean

The Hookean dumbbell case in a shear flow: $\mathbf{F}(\mathbf{X}) = \mathbf{X}$

$$\begin{cases} \partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \tau(t,y) + f_{ext}(t,y), \\ \tau(t,y) = \mathbf{E}\left(X(t,y)Y(t)\right), \\ dX(t,y) = \left(-\frac{1}{2}X(t,y) + \partial_y u(t,y)Y(t)\right) dt + dV_t, \\ dY(t) = -\frac{1}{2}Y(t)\, dt + dW_t, \end{cases}$$

with appropriate initial and boundary conditions.

No problem to solve the SDE.

The process Y_t can be computed externally. The nonlinearity of the coupling term $\partial_y u Y_t$ disappears: global-in-time existence result.

Notion of solution:

Let us be given $u_0 \in L^2_y$, $f_{ext} \in L^1_t(L^2_y)$, X_0 and (V_t, W_t).

(u, X) is said to be a solution if: $u \in L^\infty_t(L^2_y) \cap L^2_t(H^1_{0,y})$ and $X \in L^\infty_t(L^2_y(L^2_\omega))$ are s.t.,

in $\mathcal{D}'([0,T) \times \mathcal{O})$,

$$\partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \mathbf{E}\left(X(t,y)Y(t)\right) + f_{ext}(t,y),$$

for a.e. (y, ω), $\forall t \in (0,T)$,

$$X_t(y) = e^{-\frac{t}{2}} X_0 + \int_0^t e^{\frac{s-t}{2}} \, dV_s + \int_0^t e^{\frac{s-t}{2}} \partial_y u(s,y) Y_s \, ds,$$

where $Y_t = Y_0 \, e^{-t/2} + \int_0^t e^{\frac{s-t}{2}} dW_s$.

2B Some existence results: Hookean

Theorem 1 *[B. Jourdain, C. Le Bris, TL 02]*
Global-in-time existence and uniqueness.

Assuming $u_0 \in L^2_y$ and $f_{ext} \in L^1_t(L^2_y)$, this problem admits a unique solution (u, X) on $(0, T)$, $\forall T > 0$.
In addition, the following estimate holds:

$$\|u\|^2_{L^\infty_t(L^2_y)} + \|u\|^2_{L^2_t(H^1_{0,y})} + \|X_t\|^2_{L^\infty_t(L^2_y(L^2_\omega))} + \|X_t\|^2_{L^2_t(L^2_y(L^2_\omega))}$$
$$\leq C\left(\|X_0\|^2_{L^2_y(L^2_\omega)} + \|u_0\|^2_{L^2_y} + T + \|f_{ext}\|^2_{L^1_t(L^2_y)}\right).$$

Remarks:

- The "$+T$" comes from Itô's formula,
- For more regular data, one can obtain more regular solutions.

2B Some existence results: Hookean

Sketch of the proof

- *a priori* estimate,
$$\frac{1}{2}\int_{\mathcal{O}} u(t,y)^2 - \frac{1}{2}\int_{\mathcal{O}} u_0(y)^2 + \int_0^t \int_{\mathcal{O}} (\partial_y u)^2 = -\int_0^t \int_{\mathcal{O}} \mathbb{E}(X_s(y)Y_s)\partial_y u(s,y) + \int_0^t \int_{\mathcal{O}} f_{ext}(s,y)u(s,y),$$
$$\frac{1}{2}\int_{\mathcal{O}} \mathbb{E}(X_t^2(y)) - \frac{1}{2} = \int_0^t \int_{\mathcal{O}} \mathbb{E}(X_s(y)Y_s)\partial_y u(s,y) - \frac{1}{2}\int_0^t \int_{\mathcal{O}} \mathbb{E}(X_s^2(y)) + \frac{1}{2}t,$$
- Galerkin method (space discretization in a finite dimensional space V^m), (fixed point to find a solution u^m to the space-discretized problem),
- Convergence of the discretized problem. Difficulty: $\int_{\mathcal{O}} \mathbf{E}(Y_t X_t^m(y))\partial_y v_i$, where $X_t^m = e^{-\frac{t}{2}}X_0 + \int_0^t e^{\frac{s-t}{2}}\,dV_s + \int_0^t e^{\frac{s-t}{2}}\partial_y u^m(s,y)Y_s\,ds$.

2B Some existence results: Hookean

We use an explicit expression of τ (cf. Hookean Dumbbell = Oldroyd B): $\int_{\mathcal{O}} \mathbf{E}(Y_t X_t^m(y)) w = \int_{\mathcal{O}} \mathbf{E}\left(Y_t \int_0^t e^{\frac{s-t}{2}} \partial_y u^m Y_s \, ds \right) w$
and $\partial_y u^m \rightharpoonup \partial_y u$ in $L^2_t(L^2_y)$,

- Uniqueness: the problem is essentially linear, so the uniqueness of weak solution holds.

2B Some existence results: FENE

The FENE dumbbell case in a shear flow: $\mathbf{F}(\mathbf{X}) = \frac{\mathbf{X}}{1-\|\mathbf{X}\|^2/b}$

$$\left\{\begin{array}{l} \partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \tau(t,y) + f_{ext}(t,y), \\ \tau(t,y) = \mathbf{E}\left(\frac{X_t^y Y_t^y}{1-\frac{(X_t^y)^2+(Y_t^y)^2}{b}}\right), \\ dX_t^y = \left(-\frac{1}{2}\frac{X_t^y}{1-\frac{(X_t^y)^2+(Y_t^y)^2}{b}} + \partial_y u(t,y) Y_t^y\right) dt + dV_t, \\ dY_t^y = \left(-\frac{1}{2}\frac{Y_t^y}{1-\frac{(X_t^y)^2+(Y_t^y)^2}{b}}\right) dt + dW_t. \end{array}\right.$$

New difficulties:

- An explosive drift term in the SDE, which however yields a bound on the stochastic processes,
- The system is nonlinear (due to the term $\partial_y u Y_t^y$), and both X and Y depend on the space variable.

2B Some existence results: FENE

Two remarks:

- The global *a priori* estimate $u \in L^\infty_t(L^2_y) \cap L^2_t(H^1_{0,y})$ is not sufficient to pass to the limit in the nonlinear term $\partial_y u \, Y^y_t$,
- What is the regularity of τ in function of the regularity of $\partial_y u$?

Notion of solution:

Let us be given $u_0 \in H^1_y$, $f_{ext} \in L^2_t(L^2_y)$, (X_0, Y_0) and (V_t, W_t).

(u, X, Y) is said to be a solution if:

$u \in L^\infty_t(H^1_{0,y}) \cap L^2_t(H^2_y)$ is s.t., in $\mathcal{D}'([0,T) \times \mathcal{O})$,

$$\partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \mathbf{E}\left(\frac{X^y_t Y^y_t}{1 - \frac{(X^y_t)^2 + (Y^y_t)^2}{b}}\right) + f_{ext}(t,y),$$

and for a.e. (y,ω), $\forall t \in (0,T)$, $\int_0^t \left| \frac{1}{1 - \frac{(X^y_s)^2 + (Y^y_s)^2}{b}} \right| ds < \infty$ and

$$\begin{aligned} X^y_t &= X_0 + \int_0^t \left(-\frac{1}{2} \frac{X^y_s}{1 - \frac{(X^y_s)^2 + (Y^y_s)^2}{b}} + \partial_y u Y^y_s \right) ds + V_t, \\ Y^y_t &= Y_0 + \int_0^t -\frac{1}{2} \frac{Y^y_s}{1 - \frac{(X^y_s)^2 + (Y^y_s)^2}{b}} ds + W_t. \end{aligned}$$

2B Some existence results: FENE

Theorem 2 *[B. Jourdain, C. Le Bris, TL 03]*
Local-in-time existence and uniqueness.

Under the assumptions $b > 6$, $f_{ext} \in L^2_t(L^2_y)$ *and* $u_0 \in H^1_y$, $\exists T > 0$ *(depending on the data) s.t. the system admits a unique solution* (u, X, Y) *on* $[0, T)$*. This solution is such that* $u \in L^\infty_t(H^1_{0,y}) \cap L^2_t(H^2_y)$*. In addition, we have:*

- $\mathbf{P}(\exists t > 0, ((X^y_t)^2 + (Y^y_t)^2) = b) = 0$,
- (X^y_t, Y^y_t) *is adapted /* $\mathcal{F}^{V,W}_t$.

2B Some existence results: FENE

Sketch of the proof

Existence of solution to the SDE

For $g \in L^1_{\text{loc}}(\mathbb{R}_+)$, $b \geq 2$, the following system

$$\begin{cases} dX_t^g = \left(-\frac{1}{2} \frac{X_t^g}{1 - \frac{(X_t^g)^2 + (Y_t^g)^2}{b}} + g(t)\, Y_t^g \right) dt + dV_t, \\ dY_t^g = \left(-\frac{1}{2} \frac{Y_t^g}{1 - \frac{(X_t^g)^2 + (Y_t^g)^2}{b}} \right) dt + dW_t, \end{cases}$$

admits a unique strong solution, which is with values in $B = \mathcal{B}(0, \sqrt{b})$.

The proof follows from general results on multivalued SDE (E. Cépa) and the fact that the FENE force derivates from a convex potential Π.

2B Some existence results: FENE

More precisely, one can show that:

- As soon as $b > 0$, there exists a unique solution with value in $\overline{B}$.
- If $0 < b < 2$, the stochastic process hits the boundary of B in finite time: one can thus build many solutions to the SDE.
- If $b \geq 2$, the stochastic process does not hit the boundary, and one thus has a unique strong solution to the SDE. Yamada Watanabe theorem then shows that there exists a unique weak solution.

2B Some existence results: FENE

Using Girsanov theorem, one can build a weak solution to the SDE using the solution (X_t, Y_t) for $g = 0$:

$$\begin{cases} dX_t = \left(-\frac{1}{2} \frac{X_t}{1 - \frac{(X_t)^2 + (Y_t)^2}{b}} \right) dt + dV_t, \\ dY_t = \left(-\frac{1}{2} \frac{Y_t}{1 - \frac{(X_t)^2 + (Y_t)^2}{b}} \right) dt + dW_t, \end{cases}$$

By Girsanov, under P^g defined by
$\left.\frac{d\mathrm{P}^g}{d\mathrm{P}}\right|_{\mathcal{F}_t} = \mathcal{E}\left(\int_0^\bullet g(s) Y_s \, dV_s\right)_t =$
$\exp\left(\int_0^t g(s) Y_s \, dV_s - \frac{1}{2}\int_0^t (g(s) Y_s)^2 \, ds\right)$,
$(X_t, Y_t, V_t - \int_0^t g(s) Y_s \, ds, W_t, \mathbf{P}^g)$ is a weak solution of the SDE.

2B Some existence results: FENE

Regularity of τ in space

We choose $g(t) = \partial_y u(t)$ (y is fixed). By Girsanov, under $\mathbf{P}^y$ defined by

$$\left.\frac{d\mathbf{P}^y}{d\mathbf{P}}\right|_{\mathcal{F}_t} = \mathcal{E}\left(\int_0^\bullet \partial_y u(s,y) Y_s \, dV_s\right)_t =$$

$$\exp\left(\int_0^t \partial_y u Y_s \, dV_s - \frac{1}{2}\int_0^t (\partial_y u Y_s)^2 \, ds\right),$$

$(X_t, Y_t, V_t - \int_0^t \partial_y u Y_s \, ds, W_t, \mathbf{P}^y)$ is a weak solution to the initial SDE, so that:

$$\begin{aligned}
\tau &= \mathbf{E}\left(\frac{X_t^y Y_t^y}{1 - \frac{(X_t^y)^2 + (Y_t^y)^2}{b}}\right) = \mathbf{E}^y\left(\frac{X_t Y_t}{1 - \frac{X_t^2 + Y_t^2}{b}}\right), \\
&= \mathbf{E}\left(\left(\frac{X_t Y_t}{1 - \frac{X_t^2 + Y_t^2}{b}}\right) \mathcal{E}\left(\int_0^\bullet \partial_y u(s,y) Y_s \, dV_s\right)_t\right).
\end{aligned}$$

2B Some existence results: FENE

Therefore, one has (for a.e. y):

$$\begin{aligned}
|\tau| &= \left| \mathbf{E}\left(\left(\frac{X_t Y_t}{1 - \frac{X_t^2 + Y_t^2}{b}} \right) \mathcal{E}\left(\int_0^\bullet \partial_y u(s,y) Y_s \, dV_s \right)_t \right) \right| \\
&\leq \mathbf{E}\left(\left(\frac{1}{X_0^2 + Y_0^2} \right)^{\frac{q}{q-1}} \right)^{\frac{q-1}{q}} \mathbf{E}\left(\mathcal{E}\left(\int_0^\bullet \partial_y u Y_s \, dV_s \right)_t^q \right)^{1/q} \\
&\leq C_q \exp\left((q-1) \int_0^t |\partial_y u(s,y)|^2 \, ds \right)
\end{aligned}$$

where C_q depends on b, q and $\mathbf{E}\left(\left(\frac{1}{X_0^2+Y_0^2} \right)^{\frac{q}{q-1}} \right)$.

One can derive the same kind of estimate on $\partial_y \tau$.

2B Some existence results: FENE

Back to the coupled problem

- *a priori* estimates:
  global-in-time

$$\|u\|_{L^\infty_t(L^2_y)} + \|\partial_y u\|_{L^2_t(L^2_y)} + \|\Pi(X,Y)\|_{L^\infty_t(L^1_y(L^1_\omega))}$$
$$+\|\Upsilon(X,Y)\|_{L^2_t(L^2_y(L^2_\omega))} \leq C(T, \|u_0\|_{L^2_y}, \|f_{ext}\|_{L^1_t(L^2_y)})$$

where Π is a potential from which derivates the FENE force : $\Pi(x,y) = -\frac{b}{2}\ln\left(1 - \frac{x^2+y^2}{b}\right)$ and $\Upsilon(x,y) = \frac{\sqrt{x^2+y^2}}{1-\frac{x^2+y^2}{b}}$,

local-in-time

$$\|u\|_{L^\infty_t(H^1_y)} + \|u\|_{L^2_t(H^2_y)} \leq C(\|\partial_y u_0\|_{L^2_y}, \|f_{ext}\|_{L^2_t(L^2_y)}).$$

(we use $H^1 \hookrightarrow L^\infty$: dimension 1 !)

2B Some existence results: FENE

- Galerkin method (Picard theorem to find a solution u^m to the space-discretized problem).
  Remark: Using the first *a priori* estimate, the space-discretized solution is defined on $[0,T]$.
- Convergence of the space-discretized problem. Difficulty:

$$\int_{\mathcal{O}} \mathbf{E}\left(\left(\frac{X_t Y_t}{1-\frac{X_t^2+Y_t^2}{b}}\right)\mathcal{E}\left(\int_0^{\bullet} \partial_y u^m Y_s \, dV_s\right)_T\right)\partial_y v_i$$

  where v_i is a test function. We need a strong convergence of $\partial_y u^m$ (convergence a.e.) and therefore, we need a $L^2_t(H^1_y)$ estimate on $\partial_y u$...
- Uniqueness follows from the estimates.

Outline

2C Convergence of the CONNFFESSIT method

We consider again Hookean dumbbell: $\mathbf{F}(\mathbf{X}) = \mathbf{X}$ in shear flow

$$\begin{cases} \partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \tau(t,y) + f_{ext}(t,y), \\ \tau(t,y) = \mathbf{E}\left(X(t,y)Y(t)\right), \\ dX(t,y) = \left(-\frac{1}{2}X(t,y) + \partial_y u(t,y)Y(t)\right)\,dt + dV_t, \\ dY(t) = -\frac{1}{2}Y(t)\,dt + dW_t, \end{cases}$$

with appropriate initial and boundary conditions.

Remember: The process Y_t can be computed externally. The nonlinearity of the coupling term $\partial_y u Y_t$ disappears: global-in-time existence result.

2C Convergence of the CONNFFESSIT method

The numerical scheme: $\mathbf{P}1$ finite element on u, Monte Carlo discretization for τ, Euler schemes in time.

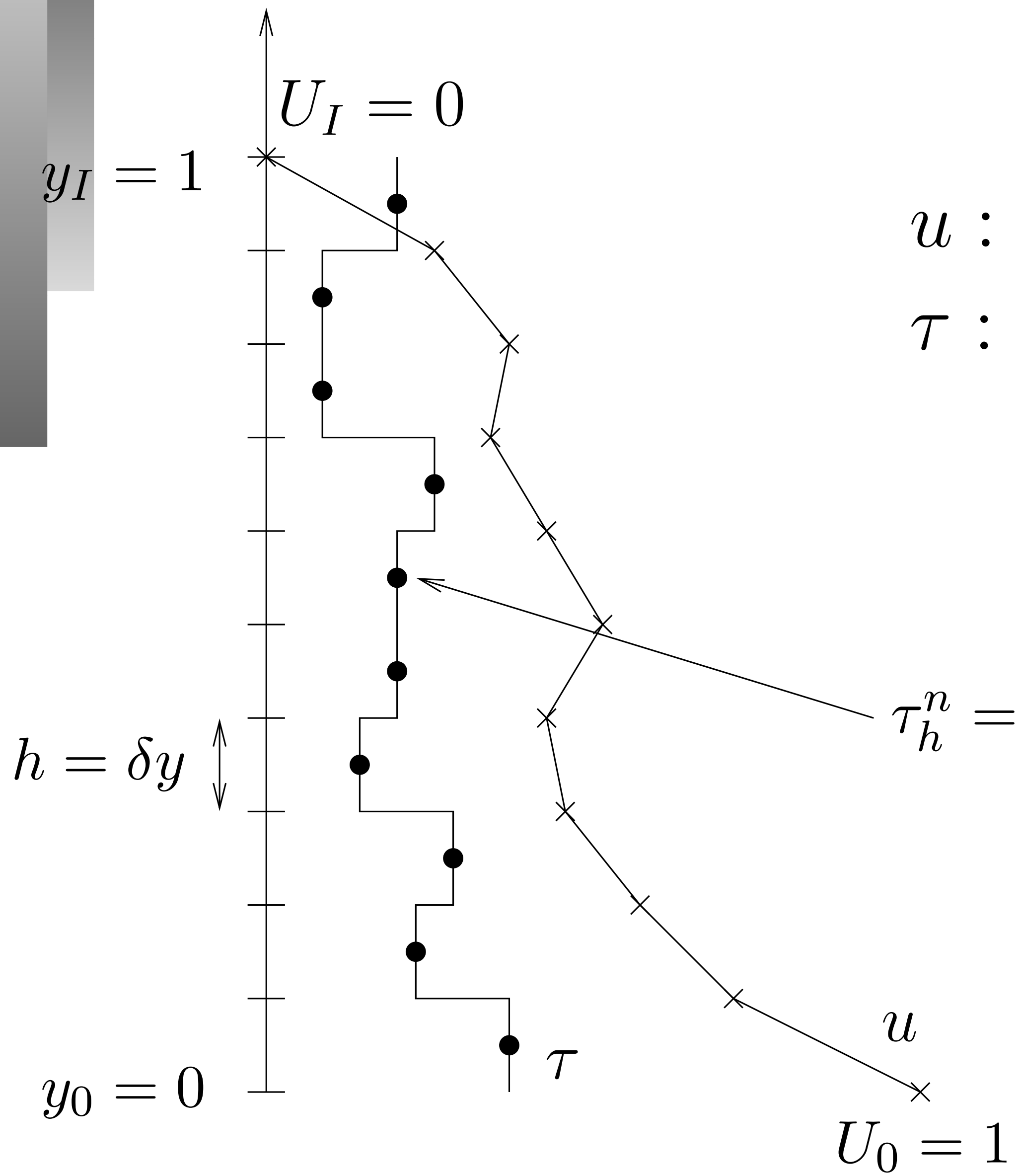
Spacestep: $h = \delta y$, timestep: Δt, number of realizations: M.

$$
\begin{cases}
\frac{1}{\Delta t} \int_{\mathcal{O}} \left(\overline{u}_h^{n+1} - \overline{u}_h^n \right) v_h + \int_{\mathcal{O}} \partial_y \overline{u}_h^{n+1} \partial_y v_h = - \int_{\mathcal{O}} \overline{\tau}_h^n \partial_y v_h + F_{ext}, \forall v_h \in V_h, \\
\overline{\tau}_h^n = \frac{1}{M} \sum_{j=1}^M \left(\overline{X}_h^{j,n} \overline{Y}^{j,n} \right), \\
\overline{X}_h^{j,n+1} = \overline{X}_h^{j,n} + \left(-\frac{1}{2} \overline{X}_h^{j,n} + \partial_y \overline{u}_h^{n+1} \overline{Y}^{j,n} \right) \Delta t + \left(V_{t_{n+1}}^j - V_{t_n}^j \right), \\
\overline{Y}^{j,n+1} = \overline{Y}^{j,n} + \left(-\frac{1}{2} \overline{Y}^{j,n} \right) \Delta t + \left(W_{t_{n+1}}^j - W_{t_n}^j \right).
\end{cases}
$$

We obtain a system of interacting particles.
Difficulties:

- the $\overline{X}_{h,n}^j$ are not independent (mean field interaction),
- $\overline{u}_h^n$ is a random variable.

2C Convergence of the CONNFFESSIT method



$u : \mathbb{P}1$

$\tau : \mathbb{P}0$

$\tau_h^n = \frac{1}{M}\sum_{j=1}^{M}(X_h^{j,n}Y^{j,n})$

2C Convergence of the CONNFFESSIT method

Theorem 3 *[B. Jourdain, C. Le Bris, TL 02]*
Convergence of the numerical scheme.

Assuming $u_0 \in H^2_y$*,* $f_{ext} \in L^1_t(H^1_y)$*,* $\partial_t f_{ext} \in L^1_t(L^2_y)$ *and* $\Delta t < \frac{1}{2}$*, we have (for* $V_h = \mathbf{P}1$*):* $\forall n < \frac{T}{\Delta t}$*,*

$$\left\| u(t_n) - \overline{u}_h^n \right\|_{L^2_y(L^2_\omega)} + \left\| \mathbf{E}(X_{t_n} Y_{t_n}) - \frac{1}{M} \sum_{j=1}^{M} \overline{X}^j_{h,n} \overline{Y}^j_n \right\|_{L^1_y(L^1_\omega)} \leq C \left(\delta y + \Delta t + \frac{1}{\sqrt{M}} \right).$$

Remark: [TL 02] One can actually show that the convergence in space is optimal:

$$\left\| u(t_n) - \overline{u}_h^n \right\|_{L^2_y(L^2_\omega)} \leq C \left(\delta y^2 + \Delta t + \frac{1}{\sqrt{M}} \right).$$

2C Convergence of the CONNFFESSIT method

Sketch of the proof

- $\mathbf{P}1$ discretization in space: $O(\delta y)$,
- Euler discretization in time: $O(\Delta t)$,
- Monte Carlo discretization: $O\left(\frac{1}{\sqrt{M}}\right)$.

Basic idea: use the following *a priori* estimate,

$$\frac{1}{2}\int_{\mathcal{O}} u(t,y)^2 - \frac{1}{2}\int_{\mathcal{O}} u_0(y)^2 + \int_0^t \int_{\mathcal{O}} (\partial_y u)^2 = -\int_0^t \int_{\mathcal{O}} \mathbb{E}(X_s(y)Y_s)\partial_y u(s,y) + \int_0^t \int_{\mathcal{O}} f_{ext}(s,y)u(s,y),$$

$$\frac{1}{2}\int_{\mathcal{O}} \mathbb{E}(X_t^2(y)) - \frac{1}{2} = \int_0^t \int_{\mathcal{O}} \mathbb{E}(X_s(y)Y_s)\partial_y u(s,y) - \frac{1}{2}\int_0^t \int_{\mathcal{O}} \mathbb{E}(X_s^2(y)) + \frac{1}{2}t,$$

Main difficulty in the stability proof: we need that $\Delta t \frac{1}{M}\sum_{j=1}^M (\overline{Y}_n^j)^2 < 1$. We introduce a cut-off.

2C Convergence of the CONNFFESSIT method

Let $A > 0$. We set $\overline{Y}^{j,n+1} = \max(-A, \min(A, Y^{j,n+1}))$, where

$$Y^{j,n+1} = Y^{j,n} + \left(-\frac{1}{2}Y^{j,n}\right)\Delta t + \left(W^j_{t_{n+1}} - W^j_{t_n}\right).$$

Two types of result :

- $A = \infty$: without cut-off,
- $0 < A < \sqrt{\frac{3}{5\Delta t}}$: with cut-off.

The precise result is the following:

$$\left\| u(t_n) - \overline{u}_h^n 1_{\mathcal{A}_n} \right\|_{L^2_y(L^2_\omega)} + \left\| \mathbb{E}(X_{t_n} Y_{t_n}) - \frac{1}{M}\sum_{j=1}^M \overline{X}^j_{h,n} \overline{Y}^j_n 1_{\mathcal{A}_n} \right\|_{L^1_y(L^1_\omega)} \le C\left(\delta y + \Delta t + \frac{1}{\sqrt{M}}\right),$$

with $\mathcal{A}_n = \left\{ \forall k \le n,\ \frac{1}{M}\sum_{j=1}^M (\overline{Y}^j_k)^2 < \frac{13}{20}\frac{1}{\Delta t} \right\}$.

2C Convergence of the CONNFFESSIT method

Two types of results:

without cut-off:

$A = \infty$: $\overline{Y}^{j,n} = Y^{j,n}$ but $\mathcal{A}_n \subsetneq \Omega$,

with cut-off:

$0 < A < \sqrt{\frac{3}{5\Delta t}}$: $\mathcal{A}_n = \Omega$ but $\overline{Y}^{j,n} \neq Y^{j,n}$.

without cut-off: $\mathcal{A}_n$ is s.t. for $\Delta t < \frac{13}{40}$, $\mathbf{P}(\mathcal{A}_n) \geq 1 - \frac{1}{\Delta t} \exp\left(-\frac{M}{2}\left(\frac{13}{40\Delta t} - 1 - \ln\left(\frac{13}{40\Delta t}\right)\right)\right)$. Notice that $\mathbf{P}\left(\mathcal{A}_{\lfloor \frac{t}{\Delta t} \rfloor}\right) \longrightarrow 1$ as $\Delta t \longrightarrow 0$, or as $M \longrightarrow \infty$.

with cut-off: one can show that the cut-off is used with very small probability for a “reasonable” timestep.

Generalizations: T. Li and P. Zhang.

2C The CONNFFESSIT method: variance reduction

One important question in Monte Carlo methods is variance reduction.
Recall that for $(Q_n)_{n\geq 1}$ i.i.d. random variables, we have (CLT)

$$\frac{1}{N}\sum_{n=1}^{N} f(Q_n) \in \left[\mathbf{E}(f(Q_1)) \pm 1.96\sqrt{\frac{\mathrm{Var}(f(Q_1))}{N}}\right].$$

How to reduce the variance in multiscale models ?
One idea is to use control variate method with, as a control variate (Bonvin, Picasso):

- the system at equilibrium,
- or a “close” model which has a macroscopic equivalent.

2C The CONNFFESSIT method: variance reduction

For example, for the FENE model, one writes:

$$\mathbf{E}\left(\frac{\mathbf{X}_t \otimes \mathbf{X}_t}{1-\|\mathbf{X}_t\|^2/b}\right) = \mathbf{E}\left(\frac{\mathbf{X}_t \otimes \mathbf{X}_t}{1-\|\mathbf{X}_t\|^2/b} - \tilde{\mathbf{X}}_t \otimes \tilde{\mathbf{F}}(\tilde{\mathbf{X}}_t)\right) + \mathbf{E}\left(\tilde{\mathbf{X}}_t \otimes \tilde{\mathbf{F}}(\tilde{\mathbf{X}}_t)\right),$$

with suitable $\tilde{\mathbf{F}}$ and $\tilde{\mathbf{X}}_t$, like

- $\tilde{\mathbf{F}} = \mathbf{F}$ and
  $d\tilde{\mathbf{X}}_t + \mathbf{u} \cdot \nabla \tilde{\mathbf{X}}_t \, dt = -\frac{1}{2\mathrm{We}} \tilde{\mathbf{F}}(\tilde{\mathbf{X}}_t) \, dt + \frac{1}{\sqrt{\mathrm{We}}} d\mathbf{W}_t$.
- $\tilde{\mathbf{F}}(\tilde{\mathbf{X}}) = \tilde{\mathbf{X}}$ and
  $d\tilde{\mathbf{X}}_t + \mathbf{u} \cdot \nabla \tilde{\mathbf{X}}_t \, dt = \left(\nabla \mathbf{u} \tilde{\mathbf{X}}_t - \frac{1}{2\mathrm{We}} \tilde{\mathbf{F}}(\tilde{\mathbf{X}}_t)\right) dt + \frac{1}{\sqrt{\mathrm{We}}} d\mathbf{W}_t$.

The Brownian motion driving $\tilde{\mathbf{X}}_t$ needs to be the same as the Brownian motion driving $\mathbf{X}_t$.

Outline

2D Dependency of the Brownian on the space variable

We consider Hookean dumbbells in a shear flow.

$$\begin{cases} \partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \tau(t,y) + f_{ext}(t,y), \\ \tau(t,y) = \mathbf{E}\left(X(t,y)Y(t)\right), \\ dX(t,y) = \left(-\frac{1}{2}X(t,y) + \partial_y u(t,y) Y(t)\right)\, dt + dV_t, \\ dY(t) = -\frac{1}{2}Y(t)\, dt + dW_t. \end{cases}$$

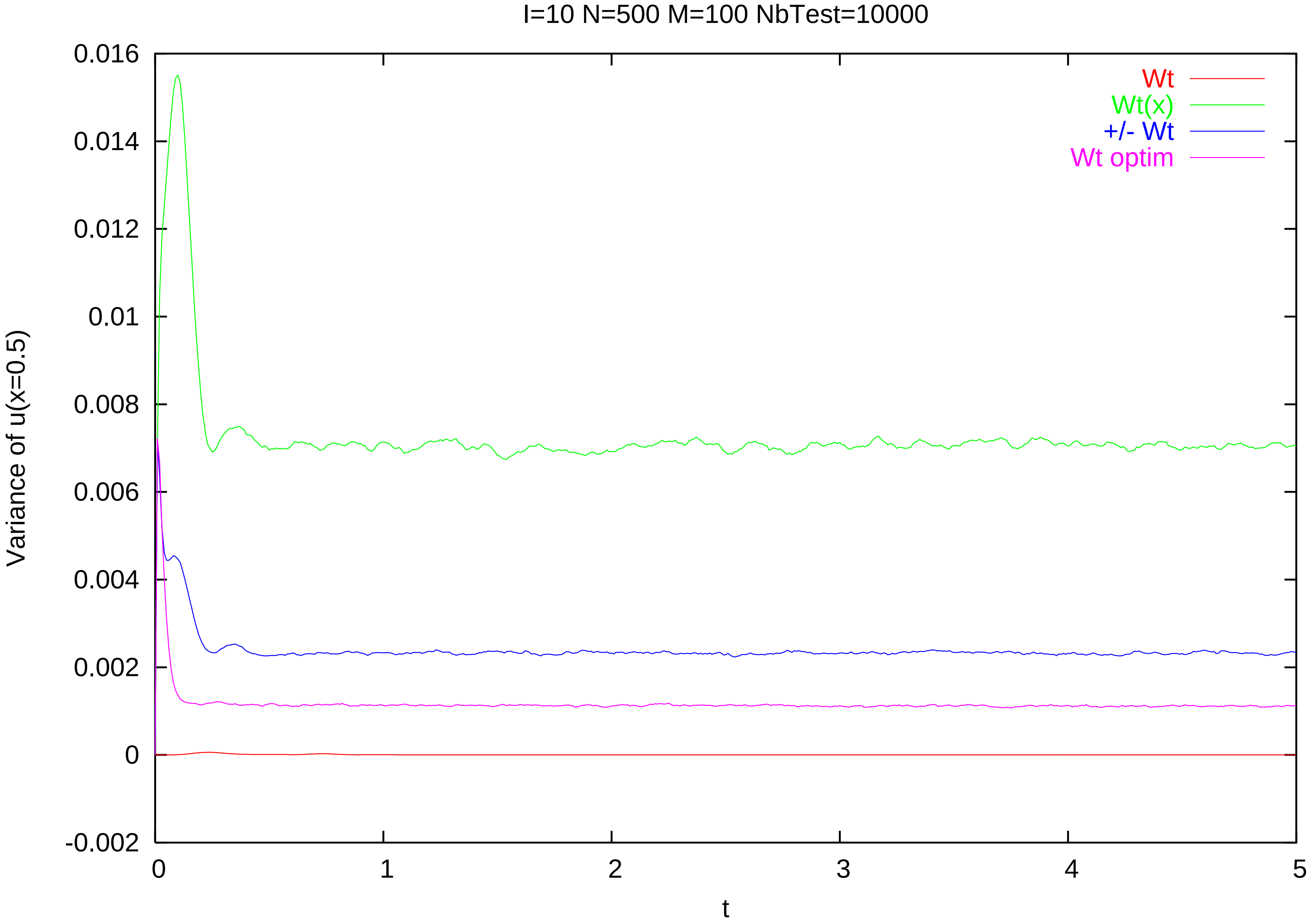
Question: (V_t, W_t) or $(V_t(y), W_t(y))$?

- The convergence result still holds,
- The deterministic continuous solution (u,τ) does not depend on the correlation in space of the Brownian motions,

but the variance of the numerical results is sensitive to this dependency (Keunings / Bonvin, Picasso).

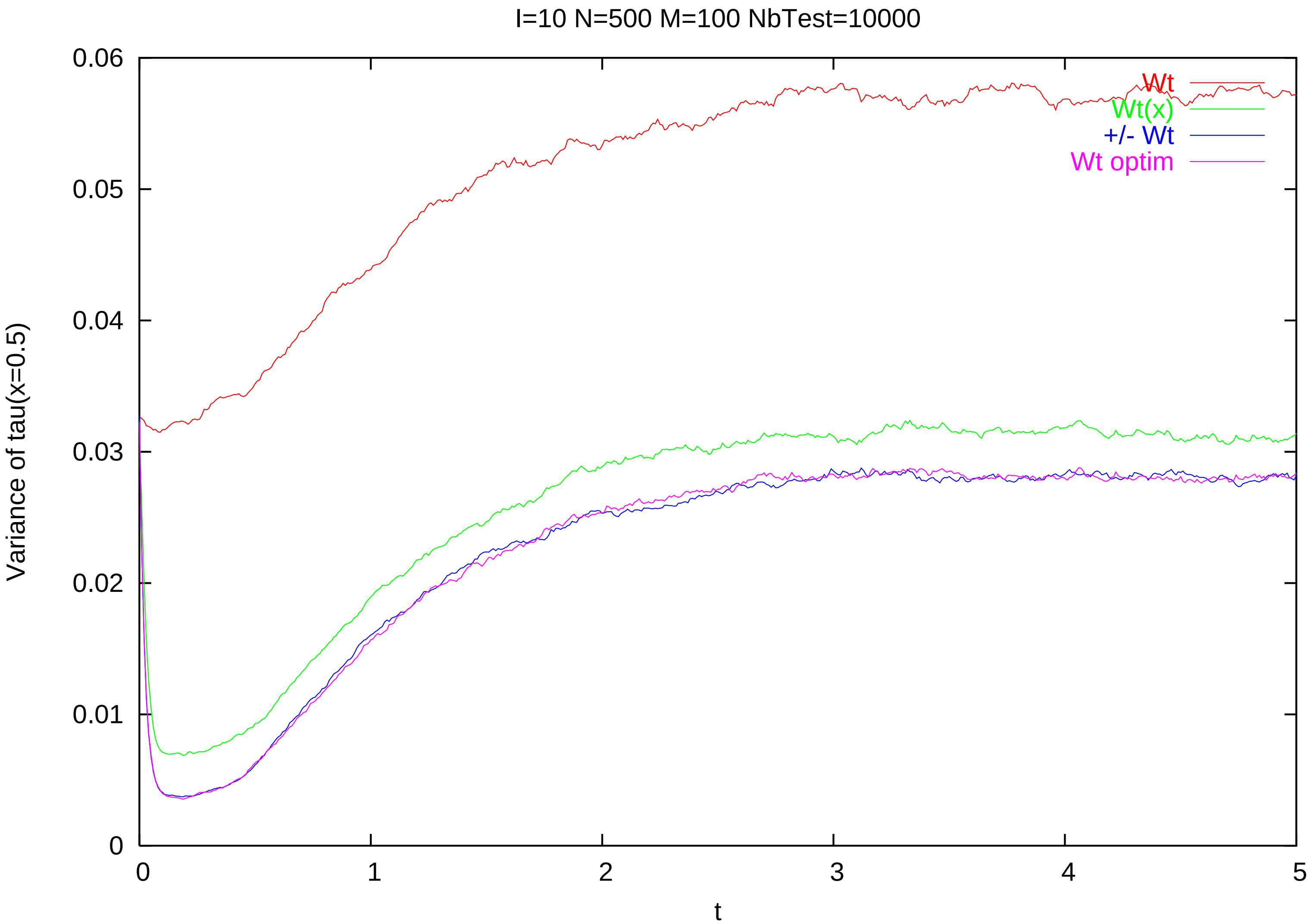
2D Dependency of the Brownian on the space variable

Variance of u



2D Dependency of the Brownian on the space variable

Variance of τ



2D Dependency of the Brownian on the space variable

Two cases: A B.M. not depending on space (V_t) and a B.M. uncorrelated from one cell to another ($V_t(y)$).

	Going from V_t to $V_t(y)$
$\mathrm{Var}(u)$	Variance increases (short time : $*15$ - long time : $*1000$)
$\mathrm{Var}(\tau)$	Variance decreases (short time : $/4$ - long time : $/2$)

Can we “explain” this phenomenon ?

On u, the equation contains a derivative in space:

$$\int_{\mathcal{O}} \partial_t u_h(t) v_h + \int_{\mathcal{O}} \partial_y u_h(t) \partial_y v_h = - \int_{\mathcal{O}} \frac{1}{R} \sum_{j=1}^{R} \left(\overline{X}_h^j(t) \overline{Y}^j(t) \right) \partial_y v_h + F_{ext}.$$

If $V_t(y)$ is a random process w.r.t. y, one derives this process and it is therefore natural to expect large variances. But on τ ?

2D Dependency of the Brownian on the space variable

Once discretized in space, we have (stationary solution) :

$$\begin{aligned} -MU(t) &= Y_t B X_t + \mathrm{bc}, \\ dX_t &= \left(Y_t C U(t) + \mathrm{bc} Y_t - \frac{X_t}{2} \right) dt + dV_t, \\ Y_t &= e^{-\frac{t}{2}} Y_0 + \int_0^t e^{\frac{s-t}{2}} \, dW_s, \end{aligned}$$

with (on a uniform mesh)

- M matrix of Δ,
- B, $C = -{}^t B$ discretizations of div and ∇,
- bc : vectors depending on boundary conditions.

We want to compute $\mathrm{Covar}(U(t))$ and $\mathrm{Covar}(X_t)$ where $\mathrm{Covar}(v) := \mathbf{E}(v \otimes v) - \mathbf{E}(v) \otimes \mathbf{E}(v)$.

2D Dependency of the Brownian on the space variable

With the (unnecessary) simplifying assumption $Y_t^2 = 1$, we have:

$$\begin{aligned}\mathrm{Covar}(X(t)) &= \mathrm{Covar}\left(\exp(At)X_0 + \int_0^t \exp(A(t-s))\mathrm{bc}Y_s\,ds\right.\\ &\quad \left.+ \int_0^t \exp(A(t-s))\,dV_s\right),\\ \mathrm{Covar}(U(t)) &= M^{-1}B\mathrm{Covar}\left(X(t)\right)\left({}^t(M^{-1}B)\right),\end{aligned}$$

with $A = -CM^{-1}B - \frac{1}{2}Id$. We have $BC = M$, and $CM^{-1}B = Id - P$ where P is a projector on $\mathrm{Ker}(B)$.
Idea: $\nabla\Delta^{-1}\,\mathrm{div}$ is a projector on irrotational fields.

$$\exp(As) = \left(\exp\left(-\frac{s}{2}\right) - \exp\left(-\frac{3s}{2}\right)\right)P + \exp\left(-\frac{3s}{2}\right)Id.$$

2D Dependency of the Brownian on the space variable

We can now understand the behaviour of the variance on τ. In $\mathrm{Covar}(X_t)$, there is a term involving PdV_s, i.e.

$$\sum_{i=1}^{I} (V_i(t_{n+1}) - V_i(t_n))$$

(in the case of a uniform space step) with $V_i(t)$ the Brownian motion in the i-th cell of discretization. And it is clear that :

$$\mathrm{Var}\left(\sum_{i=1}^{I} G^i\right) < \mathrm{Var}\left(\sum_{i=1}^{I} G\right)$$

if G^i i.i.d., so that $\mathrm{Covar}(X_t)$ decreases using $V_t(y)$.

2D Dependency of the Brownian on the space variable

In the limit $t \longrightarrow \infty$, we finally obtain :

$$\mathrm{Covar}(X_t) = 2\mathrm{bc} \otimes \mathrm{bc} + \frac{1}{3}\left(K + PK + PKP\right),$$

$$\mathrm{Covar}(U(t)) = \frac{1}{3} M^{-1} B K({}^t(M^{-1}B)),$$

with

$$K = \frac{1}{t}\mathbf{E}(V_t \otimes V_t),$$

the discrete space correlation matrix of V_t.
We can use these results to understand the behaviour in the cases $K = Id$ and $K = J$, and also to find the optimal K in some sense.

2D Dependency of the Brownian on the space variable

In the case of a uniform discretization in space, $K = Id$ in the case V_t and $K = J$ in the case $V_t(y)$ so that

$t \longrightarrow \infty$	$\mathrm{Covar}(X_t)$	$\mathrm{Covar}(U(t))$
V_t	$2\mathrm{bc} \otimes \mathrm{bc} + J$	0
$V_t(y)$	$2\mathrm{bc} \otimes \mathrm{bc} + \frac{2\delta y}{3} J + \frac{1}{3} Id$	$-\frac{1}{3} M^{-1}$

Remark: in the limit $\delta y \to 0$, with $V_t(y)$, U becomes deterministic !

2D Dependency of the Brownian on the space variable

[B. Jourdain, C. Le Bris, TL, 04]:

- the variance of the results comes from an interplay between the space discretized operators and the dependency of the Brownian motion on space,
- the minimum of the variance of u is obtained for a Brownian constant in space,
- the minimum of the variance of τ is NOT obtained with some Brownian motions independent from one cell to another. One can further reduce the variance by using a Brownian motion W_t multiplied alternatively by $+1$ or -1 from one cell to another.

Generalizations: R. Kupferman, Y. Shamai

Outline

2E Long-time behaviour: FP

We are interested in the long-time behaviour of the coupled system. More precisely, we want to prove exponential convergence of $(\mathbf{u}, \boldsymbol{\tau})$ to $(\mathbf{u}_\infty, \boldsymbol{\tau}_\infty)$, or $(\mathbf{u}, \psi)$ to $(\mathbf{u}_\infty, \psi_\infty)$.

Outline:

- preliminary: the decoupled case: FP (entropy methods) and SDE (coupling methods),
- the coupled case: PDE-SDE and PDE-FP.

2E Long-time behaviour: FP

When dealing with the FP equation itself, a classical approach is the following (see e.g. A. Arnold, P. Markowich, G.Toscani and A. Unterreiter, Comm. Part. Diff. Eq., 2001):

$$\frac{\partial \psi}{\partial t} = \mathrm{div}_{\mathbf{X}} \left(\left(-\boldsymbol{\kappa} \mathbf{X} + \frac{1}{2\mathrm{We}} \nabla \Pi(\mathbf{X}) \right) \psi \right) + \frac{1}{2\mathrm{We}} \Delta_{\mathbf{X}} \psi.$$

Let h be a convex function s.t. $h(1) = h'(1) = 0$ and

$$H(t) = \int h\left(\frac{\psi}{\psi_\infty}\right) \psi_\infty(\mathbf{X})\, d\mathbf{X},$$

where ψ_∞ is defined as a stationary solution. The relative entropy H is zero iff $\psi = \psi_\infty$. Some examples of admissible functions h: $h(x) = x\ln(x) - x + 1$ or $h(x) = (x-1)^2$.

2E Long-time behaviour: FP

Differentiating H w.r.t. t, one obtains (using the fact that ψ_∞ is a stationary solution)

$$\frac{d}{dt}\int h\left(\frac{\psi}{\psi_\infty}\right)\psi_\infty = -\frac{1}{2\mathrm{We}}\int h''\left(\frac{\psi}{\psi_\infty}\right)\left|\nabla\left(\frac{\psi}{\psi_\infty}\right)\right|^2\psi_\infty.$$

Then, one uses a functional inequality: $\forall\phi\geq 0$, $\int\phi=1$,

$$\int h\left(\frac{\phi}{\psi_\infty}\right)\psi_\infty \leq C\int h''\left(\frac{\phi}{\psi_\infty}\right)\left|\nabla\left(\frac{\phi}{\psi_\infty}\right)\right|^2\psi_\infty,$$

to show exponential decay of H,

$$H(t)\leq H(0)\exp(-t/(2C\mathrm{We})).$$

2E Long-time behaviour: FP

Example 1: If $h(x) = (x-1)^2$, one needs a Poincaré inequality: $\forall f, \int |\nabla f|^2 \psi_\infty < \infty$,

$$\int \left| f - \int f \psi_\infty \right|^2 \psi_\infty \leq C \int |\nabla f|^2 \psi_\infty,$$

with $f = \psi/\psi_\infty - 1$, and obtains convergence in L^2-norm.

Example 2: If $h(x) = x\ln(x) - x + 1$, one needs a log-Sobolev inequality: $\forall f, \int |\nabla f|^2 \psi_\infty < \infty$,

$$\int f^2 \ln\left(\frac{f^2}{\int f^2 \psi_\infty}\right) \psi_\infty \leq C \int |\nabla f|^2 \psi_\infty,$$

with $f = \sqrt{\psi/\psi_\infty}$, and obtains convergence in L^1-norm.

Remark: (LSI) implies (PI), but $L^2 \subset L^1 \ln(L^1)$.

2E Long-time behaviour: FP

The case $\boldsymbol{\kappa} = 0$:

In the case $\boldsymbol{\kappa} = 0$, we have $\psi_\infty \propto \exp(-\Pi)$ which satisfies the detailed balance:

$$\left(-\boldsymbol{\kappa}\mathbf{X} + \frac{1}{2\mathrm{We}}\nabla\Pi\right)\psi_\infty + \frac{1}{2\mathrm{We}}\nabla\psi_\infty = 0.$$

and not only $-\,\mathrm{div}\,(\bullet) = 0$. In this case, one can actually "directly" prove that:

$$H(t) \leq H(0)\exp(-t/(2C\mathrm{We}))$$

without using the functional inequality, but using the fact that: $(1/h'')'' \leq 0$, Π is α-convex, ψ_∞ satisfies the detailed balance. Proof: compute $H''(t)$.

2E Long-time behaviour: FP

The exponential decay $H(t) \leq H(0)\exp(-t/(2C\mathrm{We}\,))$ then implies that the functional inequality holds:

$$\int h\left(\frac{\phi}{\psi_\infty}\right)\psi_\infty \leq C\int h''\left(\frac{\phi}{\psi_\infty}\right)\left|\nabla\left(\frac{\phi}{\psi_\infty}\right)\right|^2\psi_\infty,$$

for $\phi = \psi_\infty(t=0)$.

Proof: expansion of the inequality $H(t) \leq H(0)\exp(-t/(2C\mathrm{We}\,))$ around $t = 0$.

Thus we obtain that a LSI or a PI holds with respect to a density ψ_∞ if $-\ln(\psi_\infty)$ is α-convex (with $C \leq \frac{1}{2\alpha}$).

The case $\boldsymbol{\kappa} \neq 0$:
If $\boldsymbol{\kappa}$ is antisymmetric, $\psi_\infty \propto \exp(-\Pi)$ is a stationary solution so that, by using the LSI inequality w.r.t. ψ_∞, $H(t) \leq H(0)\exp(-t/2C)$. Here, ψ_∞ does not satisfy the detailed balance.

To treat other cases, we need the perturbation result:

Lemma 1 *Suppose that*

- *a LSI holds for* $\psi_\infty \propto \exp(-\Pi)$,
- $\tilde{\Pi}$ *is a bounded function,*

then a LSI holds for the density $\widetilde{\psi_\infty} \propto \exp(-\Pi + \tilde{\Pi})$. *Moreover,* $C_{\mathrm{LSI}}(\widetilde{\psi_\infty}) \leq C_{\mathrm{LSI}}(\psi_\infty)\exp(2\mathrm{osc}(\tilde{\Pi}))$ *where* $\mathrm{osc}(\tilde{\Pi}) = \sup(\tilde{\Pi}) - \inf(\tilde{\Pi})$.

The same lemma holds for PI.

2E Long-time behaviour: FP

If $\boldsymbol{\kappa}$ is symmetric, we have again an explicit expression for a stationary solution:

$$\psi_\infty(\mathbf{X}) \propto \exp(-\Pi(\mathbf{X}) + \mathrm{We}\ \mathbf{X}^T \boldsymbol{\kappa} \mathbf{X}).$$

For FENE dumbbells, Lemma 1 shows that a LSI holds for ψ_∞, and therefore, one obtains $H(t) \leq H(0) \exp(-t/2C)$.

For Hookean dumbbells, OK if $\int \exp(-\Pi(\mathbf{X}) + \mathrm{We}\ \mathbf{X}^T \boldsymbol{\kappa} \mathbf{X}) < \infty$.

For a general $\boldsymbol{\kappa}$, exponential decay is obtained if ψ_∞ is a stationary solution such that $\operatorname{osc}\left(\ln\left(\frac{\psi_\infty}{\exp(-\Pi)}\right)\right) < \infty$.

For FENE dumbbell, we will prove that there exists such a stationary solution if $\boldsymbol{\kappa} + \boldsymbol{\kappa}^T$ is small enough.

2E Long-time behaviour: FP

Convergence of the stress tensor: in this decoupled framework, we can deduce from the exponential convergence of ψ to ψ_∞ (Csiszar-Kullback inequality):

$$\int |\psi - \psi_\infty| \leq C \exp(-\lambda t)$$

and the fact that there exists a polynomial $P(t)$ s.t.

$$\mathbf{E}(\mathbf{X}_t \otimes \nabla \Pi(\mathbf{X}_t)) \leq P(t)$$

that $\boldsymbol{\tau}$ converges exponentially fast to $\boldsymbol{\tau}_\infty$. Proof: use Hölder inequality.

The polynomial growth in time of $\mathbf{E}(\mathbf{X}_t \otimes \nabla \Pi(\mathbf{X}_t))$ holds for Hookean (for $\kappa \in L^p_t, 1 \leq p < \infty$) or FENE dumbbells (for $\kappa \in L^2_t + L^\infty_t$ and b sufficiently large).

2E Long-time behaviour: SDE

Thinking of the Monte-Carlo / Euler discretized problem, let us now try to do the same on the SDE (here, we suppose $\mathbf{u} = 0$. This can be generalized to an exponentially fast decaying $\nabla \mathbf{u}$):

$$d\mathbf{X}_t = -\frac{1}{2\mathrm{We}} \nabla \Pi(\mathbf{X}_t)\, dt + \frac{1}{\sqrt{\mathrm{We}}}\, d\mathbf{W}_t.$$

Let us introduce

$$d\mathbf{X}_t^\infty = -\frac{1}{2\mathrm{We}} \nabla \Pi(\mathbf{X}_t^\infty)\, dt + \frac{1}{\sqrt{\mathrm{We}}}\, d\mathbf{W}_t,$$

with $\mathbf{X}_0^\infty \sim \psi_\infty(\mathbf{X})\, d\mathbf{X}$.

2E Long-time behaviour: SDE

Then (using α-convexity of Π),

$$\begin{aligned} d|\mathbf{X}_t - \mathbf{X}_t^\infty|^2 &= -\frac{1}{2\mathrm{We}} \left(\nabla\Pi(\mathbf{X}_t) - \nabla\Pi(\mathbf{X}_t^\infty)\right).\left(\mathbf{X}_t - \mathbf{X}_t^\infty\right) dt \\ &\leq -\frac{\alpha}{2\mathrm{We}} |\mathbf{X}_t - \mathbf{X}_t^\infty|^2, \end{aligned}$$

and therefore $\mathbf{E}(\phi(\mathbf{X}_t)) - \mathbf{E}(\phi(\mathbf{X}_t^\infty))$ goes exponentially fast to 0 (for ϕ Lipschitz-continuous e.g.).

Since $\mathbf{E}(\phi(\mathbf{X}_t)) = \int \phi(\mathbf{X})\psi(t,\mathbf{X})\, d\mathbf{X}$ and $\mathbf{E}(\phi(\mathbf{X}_t^\infty)) = \int \phi(\mathbf{X})\psi_\infty(\mathbf{X})\, d\mathbf{X}$, this also means exponentially fast (weak) convergence of $\psi(t,\mathbf{X})$ to $\psi_\infty(\mathbf{X})$.

Here again, the α-convexity of Π plays a crucial role.

2E Long-time behaviour: PDE-SDE

Let us now consider the coupled system.
If we consider the coupled PDE-SDE system (with zero boundary conditions on $\mathbf{u}$), we have the following estimate:

$$\frac{\text{Re}}{2}\frac{d}{dt}\int_{\mathcal{D}}|\mathbf{u}|^2+(1-\epsilon)\int_{\mathcal{D}}|\nabla\mathbf{u}|^2+\frac{\epsilon}{\text{We}}\frac{d}{dt}\int_{\mathcal{D}}\mathbf{E}(\Pi(\mathbf{X}_t))$$
$$+\frac{\epsilon}{2\text{We}^2}\int_{\mathcal{D}}\mathbf{E}(\|\mathbf{F}(\mathbf{X}_t)\|^2)=\frac{\epsilon}{2\text{We}^2}\int_{\mathcal{D}}\mathbf{E}(\Delta\Pi(\mathbf{X}_t)).$$

The r.h.s. is positive: it seems difficult to use such kinds of estimate to study the limit $t\to\infty$.
It is actually possible to combine this kind of estimate with the former SDE approach, but for Hookean dumbbells in shear flow.

2E Long-time behaviour: PDE-SDE

$$\begin{cases} \partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \tau(t,y) + f_{ext}(t,y), \\ \tau(t,y) = \mathbf{E}\left(X(t,y) Y(t)\right), \\ dX(t,y) = \left(-\frac{1}{2} X(t,y) + \partial_y u(t,y) Y(t)\right) dt + dV_t, \\ dY(t) = -\frac{1}{2} Y(t)\, dt + dW_t, \end{cases}$$

IC: $u(0,y) = u_0(y)$, $(X_0(y), Y_0(y))$, BC: $u(t,0) = f_0(t) \to a_0$, $u(t,1) = f_1(t) \to a_1$, as $t \to \infty$.

$$\begin{cases} -\partial_{y,y} u_\infty(y) = \partial_y \tau_\infty, \\ \tau_\infty = \mathbf{E}\left(X_t^\infty Y_t^\infty\right), \\ dX_t^\infty = (-\frac{1}{2} X_t^\infty + \partial_y u_\infty(y) Y_t^\infty)\, dt + dV_t, \\ dY_t^\infty = -\frac{1}{2} Y_t^\infty\, dt + dW_t, \end{cases}$$

$u_\infty(y) = a_0 + y(a_1 - a_0)$, (X_t^∞, Y_t^∞) is a stationary Gaussian process not depending on y.

2E Long-time behaviour: PDE-SDE

Lemma 2 *Long-time behaviour for Hookean.*

We assume that $\forall y$, $Y_0(y)$ *is independent from* Y_0^∞*,* $f_0, f_1 \in W^{1,1}_{\mathrm{loc}}(\mathbb{R}_+)$ *and* $\lim_{t\to\infty} \dot{f}_0(t) = \lim_{t\to\infty} \dot{f}_1(t) = 0$*. Then,*

$$\lim_{t\to\infty} \|u(t,y) - u_\infty(y)\|_{L^2_y} = 0,$$

$$\lim_{t\to\infty} \|X_t(y) - X_t^\infty\|_{L^2_y(L^2_\omega)} + \|Y_t(y) - Y_t^\infty\|_{L^2_y(L^2_\omega)} = 0,$$

$$\lim_{t\to\infty} \|\mathbf{E}(X_t(y)Y_t(y)) - (a_1 - a_0)\|_{L^1_y} = 0.$$

Remark: The convergence is exponential if the convergences on f_0, f_1, $\dot{f}_0$ and $\dot{f}_1$ are exponential.

How to proceed for general geometry and nonlinear force ?

2E Long-time behaviour: PDE-FP

The Fokker-Planck version of the coupled system is:

$$\text{Re}\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u}\right) = (1-\epsilon)\Delta\mathbf{u} - \nabla p + \operatorname{div}\boldsymbol{\tau}$$

$$\operatorname{div}(\mathbf{u}) = 0$$

$$\boldsymbol{\tau} = \frac{\epsilon}{\text{We}}\left(\int_{\mathbb{R}^d} (\mathbf{X}\otimes\nabla\Pi(\mathbf{X}))\psi\, d\mathbf{X} - \boldsymbol{I}\right)$$

$$\frac{\partial \psi}{\partial t} + \mathbf{u}\cdot\nabla_{\boldsymbol{x}}\psi = -\operatorname{div}_{\mathbf{X}}\left(\left(\nabla_{\boldsymbol{x}}\mathbf{u}\,\mathbf{X} - \frac{1}{2\text{We}}\nabla\Pi(\mathbf{X})\right)\psi\right) + \frac{1}{2\text{We}}\,\Delta_{\mathbf{X}}\psi.$$

We suppose $\boldsymbol{x}\in\mathcal{D}$ (bounded domain of $\mathbb{R}^d$) and that $\Pi(\mathbf{X}) = \pi(\|\mathbf{X}\|)$ (so that $\boldsymbol{\tau}$ is symmetric).

2E Long-time behaviour: PDE-FP

Let us start with the case $\mathbf{u} = 0$ on $\partial\mathcal{D}$.

We introduce the kinetic energy:

$$E(t) = \frac{\mathrm{Re}}{2} \int_{\mathcal{D}} |\mathbf{u}|^2$$

and the entropy:

$$\begin{aligned} H(t) &= \int_{\mathcal{D}} \int_{\mathbb{R}^d} \Pi\psi + \int_{\mathcal{D}} \int_{\mathbb{R}^d} \psi \ln(\psi) + C \\ &= \int_{\mathcal{D}} \int_{\mathbb{R}^d} \psi \ln\left(\frac{\psi}{\psi_\infty}\right) \end{aligned}$$

with

$$\psi_\infty(\mathbf{X}) \propto \exp(-\Pi(\mathbf{X})).$$

2E Long-time behaviour: PDE-FP

Let us introduce $F(t) = E(t) + H(t)$. One has, by differentiating F w.r.t. time:

$$\begin{aligned} &\frac{d}{dt}\left(\frac{\text{Re}}{2}\int_{\mathcal{D}} |\mathbf{u}|^2 + \int_{\mathcal{D}}\int_{\mathbb{R}^d} \psi \ln\left(\frac{\psi}{\psi_\infty}\right)\right) \\ &\quad = \; -(1-\epsilon)\int_{\mathcal{D}} |\nabla \mathbf{u}|^2 - \frac{\epsilon}{2\text{We}^{\,2}}\int_{\mathcal{D}}\int_{\mathbb{R}^d} \psi \left|\nabla \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2. \end{aligned}$$

This yields a new energy estimate, which holds on $\mathbb{R}_+$.

First consequence: The stationary solutions of the coupled problem are $\mathbf{u} = \mathbf{u}_\infty = 0$ and $\psi = \psi_\infty \propto \exp(-\Pi)$.

2E Long-time behaviour: PDE-FP

Moreover, using the following inequalities:

- Poincaré inequality:

$$\int |\mathbf{u}|^2 \leq C \int |\nabla \mathbf{u}|^2$$

- Sobolev logarithmic inequality for ψ_∞ (which holds *e.g.* for α-convex potentials Π):

$$\int \psi \ln \left(\frac{\psi}{\psi_\infty} \right) \leq C \int \psi \left| \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2$$

we obtain $\frac{dF}{dt} \leq -CF$ so that:

Second consequence: The free energy F (and thus the velocity $\mathbf{u}$) decreases exponentially fast to 0 when $t \to \infty$.

2E Long-time behaviour: PDE-FP

Remark: If one considers a more general entropy $H(t) = \int h\left(\frac{\psi}{\psi_\infty}\right)\psi_\infty$, one ends up with (written here for a shear flow with Re $= 1/2$, $\mathrm{We} = 1$, $\epsilon = 1/2$):

$$\frac{dF}{dt} = -\int_{\mathcal{D}} |\partial_y u|^2 - \frac{1}{2}\int_{\mathcal{D}}\int_{\mathbb{R}^2} \left|\nabla\left(\frac{\psi}{\psi_\infty}\right)\right|^2 h''\left(\frac{\psi}{\psi_\infty}\right)\psi_\infty$$
$$-\int_{\mathcal{D}}\int_{\mathbb{R}^2} Y\,\psi\,\partial_y u\,\partial_X \Pi\left(1 - h'\left(\frac{\psi}{\psi_\infty}\right) - h\left(\frac{\psi}{\psi_\infty}\right)\frac{\psi_\infty}{\psi}\right).$$

Sufficient condition to have exponential decay:
$h'(x) - h(x)/x = 0$ i.e. $h(x) = x\ln(x)$.

2E Long-time behaviour: PDE-FP

Convergence of the stress tensor:

- for FENE dumbbells: ($b > 2$)

$$\int_0^\infty \int_{\mathcal{D}} |\boldsymbol{\tau}(t,\boldsymbol{x}) - \boldsymbol{\tau}_\infty(\boldsymbol{x})| < \infty.$$

- for Hookean dumbbells:

$$\int_{\mathcal{D}} |\boldsymbol{\tau}(t,\boldsymbol{x}) - \boldsymbol{\tau}_\infty(\boldsymbol{x})| \leq C e^{-\beta t}.$$

For FENE dumbbell, the difficulty comes from the fact that we have only $L^2_{\boldsymbol{x}}(L^1_{\mathbf{X}})$ exponential convergence of ψ to ψ_∞, and $\mathbf{X} \otimes \nabla \Pi(\mathbf{X})$ is not $L^\infty_{\mathbf{X}}$.

2E Long-time behaviour: PDE-FP

Let us now consider the case $\mathbf{u} \neq 0$ on $\partial\mathcal{D}$ (constant). We introduce (Re $= 1/2$, $\mathrm{We} = 1$, $\epsilon = 1/2$)

$$\begin{aligned} E(t) &= \frac{1}{2}\int_{\mathcal{D}} |\overline{\mathbf{u}}|^2(t,\boldsymbol{x}), \\ H(t) &= \int_{\mathcal{D}}\int_{\mathbb{R}^d} \psi(t,\boldsymbol{x},\mathbf{X}) \ln\left(\frac{\psi(t,\boldsymbol{x},\mathbf{X})}{\psi_\infty(\boldsymbol{x},\mathbf{X})}\right), \\ F(t) &= E(t) + H(t), \end{aligned}$$

where $\overline{\mathbf{u}}(t,\boldsymbol{x}) = \mathbf{u}(t,\boldsymbol{x}) - \mathbf{u}_\infty(\boldsymbol{x})$.

Here, $(\mathbf{u}_\infty, \psi_\infty)$ is a stationary solution (no *a priori* explicit expressions).

2E Long-time behaviour: PDE-FP

By differentiating F w.r.t. time, one obtains:

$$\begin{aligned}
\frac{d}{dt}\left(\frac{1}{2}\int_{\mathcal{D}}|\overline{\mathbf{u}}|^2+\int_{\mathcal{D}}\int_{\mathbb{R}^d}\psi\ln\left(\frac{\psi}{\psi_\infty}\right)\right) \\
= \quad -\int_{\mathcal{D}}|\nabla\overline{\mathbf{u}}|^2-\frac{1}{2}\int_{\mathcal{D}}\int_{\mathbb{R}^d}\psi\left|\nabla_{\mathbf{X}}\ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 \\
-\int_{\mathcal{D}}\overline{\mathbf{u}}.\nabla\mathbf{u}_\infty\overline{\mathbf{u}}-\int_{\mathcal{D}}\int_{\mathbb{R}^d}\overline{\mathbf{u}}.\nabla_{\boldsymbol{x}}(\ln\psi_\infty)\overline{\psi} \\
-\int_{\mathcal{D}}\int_{\mathbb{R}^d}\left(\nabla_{\mathbf{X}}(\ln\psi_\infty)+\nabla\Pi(\mathbf{X})\right).\nabla\overline{\mathbf{u}}\mathbf{X}\,\overline{\psi},
\end{aligned}$$

where $\overline{\psi}(t,\boldsymbol{x},\mathbf{X})=\psi(t,\boldsymbol{x},\mathbf{X})-\psi_\infty(\boldsymbol{x},\mathbf{X})$. Difficulties: (i) estimate these 3 additional terms, (ii) prove a LSI w.r.t. to ψ_∞.

2E Long-time behaviour: PDE-FP

We consider the case of homogeneous stationary flows: $\mathbf{u}_\infty(\boldsymbol{x}) = \nabla \mathbf{u}_\infty \boldsymbol{x}$. ψ_∞ is defined as a stationary solution which does not depend on $\boldsymbol{x}$.
Then, the only remaining term is:

$$
\begin{aligned}
& - \int_{\mathcal{D}} \int_{\mathbb{R}^d} \left(\nabla_{\mathbf{X}} (\ln \psi_\infty) + \nabla \Pi(\mathbf{X})\right) . \nabla \overline{\mathbf{u}} \mathbf{X} \, \overline{\psi} \\
= \quad & - \int_{\mathcal{D}} \int_{\mathbb{R}^d} \nabla_{\mathbf{X}} \ln \left(\frac{\psi_\infty}{\exp(-\Pi)} \right) (\mathbf{X}) . \nabla \overline{\mathbf{u}} \mathbf{X} \, \overline{\psi}
\end{aligned}
$$

We need a $L^\infty_{\mathbf{X}}$ estimate on $\left\| \nabla_{\mathbf{X}} \ln \left(\frac{\psi_\infty}{\exp(-\Pi)} \right) \right\| \|\mathbf{X}\|$.

If $\nabla \mathbf{u}_\infty$ is antisymmetric, take $\psi_\infty \propto \exp(-\Pi)$ and one obtains exponential decay.

2E Long-time behaviour: PDE-FP

Let us now consider non-antisymmetric $\nabla \mathbf{u}_\infty$.

For Hookean dumbbells, it seems difficult to control this term.

For FENE dumbbells, a $L^\infty_{\mathbf{X}}$ estimate on $\left\| \nabla_{\mathbf{X}} \ln \left(\frac{\psi_\infty}{\exp(-\Pi)} \right) \right\|$ is sufficient, and also yields a LSI w.r.t. to ψ_∞, by Lemma 1.

If $\nabla \mathbf{u}_\infty$ is symmetric, take $\psi_\infty \propto \exp(-\Pi + \mathbf{X}^T \nabla \mathbf{u}_\infty \mathbf{X})$. The only remaining term in the right hand side is

$$
\begin{aligned}
& -\int_{\mathcal{D}} \int_{\mathbb{R}^d} \nabla_{\mathbf{X}} \ln \left(\frac{\psi_\infty}{\exp(-\Pi)} \right) (\mathbf{X}). \nabla \overline{\mathbf{u}} \mathbf{X} \, \overline{\psi} \\
= & \; -2 \int_{\mathcal{D}} \int_{\mathbb{R}^d} \nabla \mathbf{u}_\infty \mathbf{X}. \nabla \overline{\mathbf{u}} \mathbf{X} \overline{\psi}.
\end{aligned}
$$

2E Long-time behaviour: PDE-FP

Then, for FENE dumbbells:

Theorem 4 *In the case of a stationary potential homogeneous flow ($\mathbf{u}_\infty(\boldsymbol{x}) = \boldsymbol{\kappa}\boldsymbol{x}$ with $\boldsymbol{\kappa} = \boldsymbol{\kappa}^T$) in the FENE model, if*

$$C_{\mathrm{PI}}(\mathcal{D})|\boldsymbol{\kappa}| + 4b^2|\boldsymbol{\kappa}|^2 \exp(4b|\boldsymbol{\kappa}|) < 1,$$

then $\mathbf{u}$ converges exponentially fast to $\mathbf{u}_\infty$ in $L^2_{\boldsymbol{x}}$ norm and the entropy $\displaystyle\int_{\mathcal{D}}\int_{\mathcal{B}} \psi \ln\left(\frac{\psi}{\psi_\infty}\right)$, where $\psi_\infty \propto \exp(-\Pi(\mathbf{X}) + \mathbf{X}.\boldsymbol{\kappa}\mathbf{X})$, converges exponentially fast to 0. Therefore ψ converges exponentially fast in $L^2_{\boldsymbol{x}}(L^1_{\mathbf{X}})$ norm to ψ_∞.

The proof is based on the free energy estimate and on the perturbation result Lemma 1.

2E Long-time behaviour: PDE-FP

For a general $\nabla \mathbf{u}_\infty = \boldsymbol{\kappa}$, for FENE dumbbells, we have:

Proposition 1 *For FENE dumbbells, if $\boldsymbol{\kappa}$ is a traceless matrix such that $|\boldsymbol{\kappa}^s| < 1/2$, there exists a unique non negative solution $\psi_\infty \in \mathcal{C}^2(\mathcal{B}(0,\sqrt{b}))$ of*

$$-\operatorname{div}\left(\left(\boldsymbol{\kappa}\mathbf{X} - \frac{1}{2}\nabla\Pi(\mathbf{X})\right)\psi_\infty(\mathbf{X})\right) + \frac{1}{2}\Delta\psi_\infty(\mathbf{X}) = 0 \text{ in } \mathcal{B}(0,\sqrt{b}),$$

normalized by $\int_{\mathcal{B}(0,\sqrt{b})} \psi_\infty = 1$, and whose boundary behavior is characterized by:

$$\inf_{\mathcal{B}(0,\sqrt{b})} \frac{\psi_\infty}{\exp(-\Pi)} > 0, \qquad \sup_{\mathcal{B}(0,\sqrt{b})} \left|\nabla\left(\frac{\psi_\infty}{\exp(-\Pi)}\right)\right| < \infty.$$

2E Long-time behaviour: PDE-FP

Furthermore, it satisfies: $\forall \mathbf{X} \in \mathcal{B}(0, \sqrt{b})$*,*

$$\left| \nabla \left(\ln \left(\frac{\psi_\infty(\mathbf{X})}{\exp(-\Pi(\mathbf{X}))} \right) \right) - 2\boldsymbol{\kappa}^s \mathbf{X} \right| \leq \frac{2\sqrt{b}\, |[\boldsymbol{\kappa}, \boldsymbol{\kappa}^T]|}{1 - 2|\boldsymbol{\kappa}^s|},$$

where $\boldsymbol{\kappa}^s = (\boldsymbol{\kappa} + \boldsymbol{\kappa}^T)/2$ *and* $[.,.]$ *is the commutator bracket:* $[\boldsymbol{\kappa}, \boldsymbol{\kappa}^T] = \boldsymbol{\kappa}\boldsymbol{\kappa}^T - \boldsymbol{\kappa}^T \boldsymbol{\kappa}$*.*

The proof is based on an regularization procedure around the boundary, and on a *a priori* estimate based on a maximum principle on the equation satisfied by $\left| \nabla \ln \left(\frac{\psi_\infty(\mathbf{X})}{\exp(-\Pi(\mathbf{X}) + \mathbf{X}^T \boldsymbol{\kappa}^s \mathbf{X})} \right) \right|^2$ (Bernstein estimate).

2E Long-time behaviour: PDE-FP

For the stationary solution ψ_∞ we have obtained, using the free energy estimate, we have:

Theorem 5 *In the case of a stationary homogeneous flow for the FENE model, if* $|\boldsymbol{\kappa}^s| < \frac{1}{2}$*,* ψ_∞ *is the stationary solution built in Proposition 1 and*

$$M^2 b^2 \exp(4bM) + C_{\mathrm{PI}}(\mathcal{D})|\boldsymbol{\kappa}^s| < 1,$$

where $M = 2|\boldsymbol{\kappa}^s| + \frac{2\,|[\boldsymbol{\kappa},\boldsymbol{\kappa}^T]|}{1-2|\boldsymbol{\kappa}^s|}$*, then* $\mathbf{u}$ *converges exponentially fast to* $\mathbf{u}_\infty$ *in* $L^2_{\boldsymbol{x}}$ *norm and the entropy* $\displaystyle\int_{\mathcal{D}}\int_{\mathcal{B}} \psi \ln\left(\frac{\psi}{\psi_\infty}\right)$ *converges exponentially fast to 0. Therefore* ψ *converges exponentially fast in* $L^2_{\boldsymbol{x}}(L^1_{\mathbf{X}})$ *norm to* ψ_∞*.*

2E Long-time behaviour: PDE-FP

Open problems:

- Convergence of the stress tensor in the case $\mathbf{u} \neq 0$ on $\partial\mathcal{D}$?
- Extend the results in the PDE-SDE framework ?
- What about the Monte-Carlo discretized system ?

Outline

2F Free-energy dissipative schemes for macro models

- Some macroscopic models have microscopic interpretation.
- We have derived some entropy estimates for micro-macro models

It is thus natural to try to recast the entropy estimate for macroscopic models. For example, for the Oldroyd-B model, one obtains:

$$\frac{d}{dt}\left(\frac{\text{Re}}{2}\int_{\mathcal{D}}|\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}}\left(-\ln(\det(\boldsymbol{A}))-d+\mathrm{tr}(\boldsymbol{A})\right)\right)$$
$$+(1-\varepsilon)\int_{\mathcal{D}}|\nabla\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}^2}\int_{\mathcal{D}}\mathrm{tr}((\boldsymbol{I}-\boldsymbol{A}^{-1})^2\boldsymbol{A})=0,$$

where $\boldsymbol{A}=\frac{\mathrm{We}}{\varepsilon}\boldsymbol{\tau}+\boldsymbol{I}$ is the conformation tensor. In this section, $u=0$ on $\partial\mathcal{D}$.

2F Free-energy dissipative schemes for macro models

Compared to the “classical” estimate:

$$\frac{d}{dt}\left(\frac{\text{Re}}{2}\int_{\mathcal{D}}|\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}}\mathrm{tr}\boldsymbol{A}\right)$$
$$+(1-\varepsilon)\int_{\mathcal{D}}|\nabla\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}^{\,2}}\int_{\mathcal{D}}\mathrm{tr}(\boldsymbol{A}-\boldsymbol{I})=0,$$

the interest is that

$$\frac{d}{dt}\left(\frac{\text{Re}}{2}\int_{\mathcal{D}}|\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}}\left(-\ln(\det(\boldsymbol{A}))-d+\mathrm{tr}(\boldsymbol{A})\right)\right)\leq 0$$

while we have no sign on

$$\frac{d}{dt}\left(\frac{\text{Re}}{2}\int_{\mathcal{D}}|\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}}\mathrm{tr}\boldsymbol{A}\right).$$

2F Free-energy dissipative schemes for macro models

Moreover, since for any symmetric positive matrix M of size $d \times d$,

$$0 \leq -\ln(\det M) - d + \mathrm{tr} M \leq \mathrm{tr}((\boldsymbol{I} - M^{-1})^2 M)$$

we obtain from the free energy estimate exponential convergence to equilibrium:

$$\frac{d}{dt}\left(\frac{\mathrm{Re}}{2}\int_{\mathcal{D}} |\mathbf{u}|^2 + \frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}} (-\ln(\det(\boldsymbol{A})) - d + \mathrm{tr}(\boldsymbol{A}))\right) \leq C\exp(-\lambda t).$$

This is the result we obtained on the micro-macro Hookean dumbbells model, that we recast on the macro-macro Oldroyd-B model.

2F Free-energy dissipative schemes for macro models

The Oldroyd-B case can be use as a guideline to derive “free energy” estimates for other macroscopic models that are not equivalent to the “simple” micro-macro models we studied.
For example, for the FENE-P model

$$\boldsymbol{\tau} = \frac{\varepsilon}{\mathrm{We}} \left(\frac{\boldsymbol{A}}{1 - \mathrm{tr}(\boldsymbol{A})/b} - \boldsymbol{I} \right),$$

$$\frac{\partial \boldsymbol{A}}{\partial t} + \mathbf{u}.\nabla \boldsymbol{A} = \nabla \mathbf{u} \boldsymbol{A} + \boldsymbol{A}(\nabla \mathbf{u})^T - \frac{1}{\mathrm{We}} \frac{\boldsymbol{A}}{1 - \mathrm{tr}(\boldsymbol{A})/b} + \frac{1}{\mathrm{We}} \boldsymbol{I},$$

we have...

2F Free-energy dissipative schemes for macro models

$$\frac{d}{dt}\left(\frac{\mathrm{Re}}{2}\int_{\mathcal{D}}|\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}}\left(-\ln(\det \boldsymbol{A})-b\ln\left(1-\mathrm{tr}(\boldsymbol{A})/b\right)\right)\right)$$
$$+(1-\varepsilon)\int_{\mathcal{D}}|\nabla\mathbf{u}|^2$$
$$+\frac{\varepsilon}{2\mathrm{We}^2}\int_{\mathcal{D}}\left(\frac{\mathrm{tr}(\boldsymbol{A})}{(1-\mathrm{tr}(\boldsymbol{A})/b)^2}-\frac{2d}{1-\mathrm{tr}(\boldsymbol{A})/b}+\mathrm{tr}(\boldsymbol{A}^{-1})\right)=0.$$

Using the fact for any symmetric positive matrix M of size $d\times d$,

$$\begin{aligned}0 &\leq -\ln(\det(M))-b\ln\left(1-\mathrm{tr}(M)/b\right)+(b+d)\ln\left(\frac{b}{b+d}\right)\\ &\leq \left(\frac{\mathrm{tr}(M)}{(1-\mathrm{tr}(M)/b)^2}-\frac{2d}{1-\mathrm{tr}(M)/b}+\mathrm{tr}(M^{-1})\right).\end{aligned}$$

we again obtain that the “free energy” $\frac{\mathrm{Re}}{2}\int_{\mathcal{D}}|\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}}\left(-\ln(\det \boldsymbol{A})-b\ln\left(1-\mathrm{tr}(\boldsymbol{A})/b\right)\right)$ decreases exponentially fast to 0.

2F Free-energy dissipative schemes for macro models

The interest of this remark is twofold:

- *Theoretically*: Obtain new estimates for macroscopic models (longtime behaviour, existence and uniqueness result ?, etc...)
- *Numerically:* Analyze the stability of numerical schemes / build more stable numerical schemes.

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Let us recall the variational formulation for the Oldroyd-B model ($\boldsymbol{\sigma} = \boldsymbol{A}$ is the conformation tensor):

$$0 = \int_{\mathcal{D}} \mathrm{Re} \left(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} \right) \cdot \boldsymbol{v} + (1-\varepsilon) \boldsymbol{\nabla} \boldsymbol{u} : \boldsymbol{\nabla} \boldsymbol{v} - p \, \mathrm{div} \, \boldsymbol{v}$$

$$+ \frac{\varepsilon}{\mathrm{We}} \boldsymbol{\sigma} : \boldsymbol{\nabla} \boldsymbol{v} + q \, \mathrm{div} \, \boldsymbol{u}$$

$$+ \left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{\sigma} \right) : \boldsymbol{\phi} - ((\boldsymbol{\nabla} \boldsymbol{u}) \boldsymbol{\sigma} + \boldsymbol{\sigma} (\boldsymbol{\nabla} \boldsymbol{u})^T) : \boldsymbol{\phi} + \frac{1}{\mathrm{We}} (\boldsymbol{\sigma} - \boldsymbol{I}) : \boldsymbol{\phi}$$

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Taking as test functions $(\boldsymbol{v}, q, \boldsymbol{\phi}) = \left(\boldsymbol{u}, p, \frac{\varepsilon}{2\mathrm{We}}(\boldsymbol{I} - \boldsymbol{\sigma}^{-1})\right)$, one obtains the free energy estimate

$$\frac{d}{dt}F + (1-\varepsilon)\int_{\mathcal{D}} |\boldsymbol{\nabla u}|^2 + \frac{\varepsilon}{2\mathrm{We}^2}\int_{\mathcal{D}} \mathrm{tr}(\boldsymbol{\sigma} + \boldsymbol{\sigma}^{-1} - 2\boldsymbol{I}) = 0.$$

where

$$F(\boldsymbol{u}, p, \boldsymbol{\sigma}) = \frac{\mathrm{Re}}{2}\int_{\mathcal{D}} |\boldsymbol{u}|^2 + \frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}} \mathrm{tr}(\boldsymbol{\sigma} - \ln \boldsymbol{\sigma} - \boldsymbol{I}).$$

Moreover, using Poincaré inequality and the inequality $\mathrm{tr}(\boldsymbol{\sigma} - \ln \boldsymbol{\sigma} - \boldsymbol{I}) \leq \mathrm{tr}(\boldsymbol{\sigma} + \boldsymbol{\sigma}^{-1} - 2\boldsymbol{I})$, one obtains exponential decay of F to 0.

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Question: Is it possible to find a numerical scheme which yields similar estimates ?

Interest: Build more stable numerical schemes / get an insight on some instabilities observed in numerical simulations (?)

Difficulties: Time discretization, test functions in the Finite Element space...

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A numerical scheme for which everything works well: Scott-Vogelius finite elements and characteristic method. $(\boldsymbol{u}_h^{n+1}, p_h^{n+1}, \boldsymbol{\sigma}_h^{n+1}) \in (\mathbb{P}_2)^2 \times \mathbb{P}_{1,disc} \times (\mathbb{P}_0)^3$ solution to:

$$0 = \int_{\mathcal{D}} \mathrm{Re} \left(\frac{\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n}{\Delta t} + \boldsymbol{u}_h^n \cdot \boldsymbol{\nabla} \boldsymbol{u}_h^{n+1} \right) \cdot \boldsymbol{v} - p_h^{n+1} \operatorname{div} \boldsymbol{v} + q \operatorname{div} \boldsymbol{u}_h^{n+1}$$

$$+ (1-\varepsilon) \boldsymbol{\nabla} \boldsymbol{u}_h^{n+1} : \boldsymbol{\nabla} \boldsymbol{v} + \frac{\varepsilon}{\mathrm{We}} \boldsymbol{\sigma}_h^{n+1} : \boldsymbol{\nabla} \boldsymbol{v} + \frac{1}{\mathrm{We}} (\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{I}) : \boldsymbol{\phi}$$

$$+ \left(\frac{\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^n \circ X^n(t^n)}{\Delta t} \right) : \boldsymbol{\phi} - \left((\boldsymbol{\nabla} \boldsymbol{u}_h^{n+1}) \boldsymbol{\sigma}_h^{n+1} + \boldsymbol{\sigma}_h^{n+1} (\boldsymbol{\nabla} \boldsymbol{u}_h^{n+1})^T \right) : \boldsymbol{\phi},$$

$$\begin{cases} \frac{d}{dt} X^n(t) = \boldsymbol{u}_h^n(X^n(t)), \quad \forall t \in [t^n, t^{n+1}], \\ X^n(t^{n+1}) = x. \end{cases}$$

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One can prove that:

- for given $(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n)$ and $\boldsymbol{\sigma}_h^n$ spd, there exists $C_n > 0$ s.t. $\forall 0 < \Delta t < C_n$ there exists a unique solution $(\boldsymbol{u}_h^{n+1}, p_h^{n+1}, \boldsymbol{\sigma}_h^{n+1})$ with $\boldsymbol{\sigma}_h^{n+1}$ spd.
- such a solution satisfy a discrete free energy estimate:

$$F_h^{n+1} - F_h^n + \int_{\mathcal{D}} \frac{\mathrm{Re}}{2} |\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n|^2$$

$$+ \Delta t \int_{\mathcal{D}} (1-\varepsilon)|\boldsymbol{\nabla} \boldsymbol{u}_h^{n+1}|^2 + \frac{\varepsilon}{2\mathrm{We}^2} \operatorname{tr}\left(\boldsymbol{\sigma}_h^{n+1} + (\boldsymbol{\sigma}_h^{n+1})^{-1} - 2I\right) \leq 0$$

- And thus, there exists a C_0 such that $\forall 0 < \Delta t < C_0$, there exists a unique solution $(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n)$ $\forall n \geq 0$.

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Key ingredients for the proof:

- Take as test functions (since $\boldsymbol{\sigma}_h^{n+1} \in (\mathbb{P}_0)^3$): $\left(\boldsymbol{u}_h^{n+1}, p_h^{n+1}, \frac{\varepsilon}{2\text{We}}\left(\boldsymbol{I} - (\boldsymbol{\sigma}_h^{n+1})^{-1}\right)\right)$.
- Treatment of the advection term $(\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{\sigma}$:

$$\begin{aligned}\left(\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^n \circ X^n(t^n)\right) : (\boldsymbol{\sigma}_h^{n+1})^{-1} &= \operatorname{tr}\left([\boldsymbol{\sigma}_h^n \circ X^n(t^n)][\boldsymbol{\sigma}_h^{n+1}]^{-1} - \boldsymbol{I}\right)\\ &\geq \ln\det\left([\boldsymbol{\sigma}_h^n \circ X^n(t^n)][\boldsymbol{\sigma}_h^{n+1}]^{-1}\right)\\ &= \operatorname{tr}\ln(\boldsymbol{\sigma}_h^n \circ X^n(t^n)) - \operatorname{tr}\ln(\boldsymbol{\sigma}_h^{n+1})\end{aligned}$$

$\boldsymbol{\sigma}, \boldsymbol{\tau}$ spd $\Rightarrow \operatorname{tr}(\boldsymbol{\sigma}\boldsymbol{\tau}^{-1} - \boldsymbol{I}) \geq \ln\det(\boldsymbol{\sigma}\boldsymbol{\tau}^{-1}) = \operatorname{tr}\left(\ln\boldsymbol{\sigma} - \ln\boldsymbol{\tau}\right)$

- Strong incompressibility $\operatorname{div}\boldsymbol{u}_h = 0$ and thus $\int_{\mathcal{D}} \operatorname{tr}\ln(\boldsymbol{\sigma}_h^n \circ X^n(t^n)) = \int_{\mathcal{D}} \operatorname{tr}\ln(\boldsymbol{\sigma}_h^n)$.

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Another possible discretization: Scott-Vogelius finite elements and Discontinuous Galerkin Method.
$(\boldsymbol{u}_h^{n+1}, p_h^{n+1}, \boldsymbol{\sigma}_h^{n+1}) \in (\mathbb{P}_2)^2 \times \mathbb{P}_{1,disc} \times (\mathbb{P}_0)^3$ solution to:

$$0 = \sum_{k=1}^{N_K} \int_{K_k} \mathrm{Re} \left(\frac{\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n}{\Delta t} + \boldsymbol{u}_h^n \cdot \boldsymbol{\nabla} \boldsymbol{u}_h^{n+1} \right) \cdot \boldsymbol{v} - p_h^{n+1} \operatorname{div} \boldsymbol{v} + q \operatorname{div} \boldsymbol{u}$$

$$+ (1-\varepsilon) \boldsymbol{\nabla} \boldsymbol{u}_h^{n+1} : \boldsymbol{\nabla} \boldsymbol{v} + \frac{\varepsilon}{\mathrm{We}} \boldsymbol{\sigma}_h^{n+1} : \boldsymbol{\nabla} \boldsymbol{v} + \frac{1}{\mathrm{We}} (\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{I}) : \boldsymbol{\phi}$$

$$+ \left(\frac{\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^n}{\Delta t} \right) : \boldsymbol{\phi} - ((\boldsymbol{\nabla} \boldsymbol{u}_h^{n+1}) \boldsymbol{\sigma}_h^{n+1} + \boldsymbol{\sigma}_h^{n+1} (\boldsymbol{\nabla} \boldsymbol{u}_h^{n+1})^T) : \boldsymbol{\phi}$$

$$+ \sum_{j=1}^{N_E} \int_{E_j} \boldsymbol{u}_h^n \cdot \boldsymbol{n}_{E_j} [\![\boldsymbol{\sigma}_h^{n+1}]\!] : \boldsymbol{\phi}^+$$

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With this discretization a similar result can be proved under the weak incompressibility constraint $\int q \,\mathrm{div}(\boldsymbol{u}_h^n) = 0$.

Summary: what we need for discrete free energy estimates with piecewise constant $\boldsymbol{\sigma}_h$:

Advection for $\boldsymbol{\sigma}_h$:	Characteristic	DG
For $\boldsymbol{u}_h$:	$\mathrm{div}\, \boldsymbol{u}_h = 0$ ($\Rightarrow \det(\nabla_{\boldsymbol{x}} X^n) \equiv 1$) ($\Rightarrow$ $\boldsymbol{u}_h \cdot \boldsymbol{n}$ well defined on $\{E_j\}$)	$\int_{\mathcal{D}} q \,\mathrm{div}\, \boldsymbol{u}_h = 0$, $\forall q \in \mathbb{P}_0$ and $\boldsymbol{u}_h \cdot \boldsymbol{n}$ well defined on $\{E_j\}$

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These results can be extended to discontinuous piecewise affine discretization for $\boldsymbol{\sigma}$ using the projection operator π_h with values in $(\mathbb{P}_0)^3$ s.t.

$$\pi_h(\boldsymbol{\phi})|_{K_k} = \boldsymbol{\phi}(\theta_{K_k}),$$

where θ_{K_k} is the barycenter of the triangle K_k.

The properties we use:

- π_h commutes with nonlinear functional (like $^{-1}$)
- π_h coincides with L^2 orthogonal projection from $(\mathbb{P}_{1,disc})^3$ onto $(\mathbb{P}_0)^3$.

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Stability for the log-formulation (Fattal, Kupferman):
$\boldsymbol{\psi} = \ln(\boldsymbol{\sigma})$

$$\begin{cases} \text{Re}\left(\dfrac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u}\cdot\boldsymbol{\nabla}\boldsymbol{u}\right) = -\boldsymbol{\nabla} p + (1-\varepsilon)\Delta\boldsymbol{u} + \dfrac{\varepsilon}{\text{We}}\operatorname{div} e^{\boldsymbol{\psi}} \\ \operatorname{div}\boldsymbol{u} = 0 \\ \dfrac{\partial \boldsymbol{\psi}}{\partial t} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{\psi} = \Omega\boldsymbol{\psi} - \boldsymbol{\psi}\Omega + 2B + \dfrac{1}{\text{We}}(e^{-\boldsymbol{\psi}} - \boldsymbol{I}) \end{cases}$$

with decomposition ($\boldsymbol{\sigma}$ spd):

$$\boldsymbol{\nabla}\boldsymbol{u} = \Omega + B + N e^{-\boldsymbol{\psi}}$$

Ω, N antisymmetric, B symmetric and commutes with $e^{-\boldsymbol{\psi}}$.

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Since e^{ψ} naturally enforces spd-ness, one can prove (for Scott-Vogelius FEM and characteristic or DG method):

- $\forall \Delta t > 0$, there exists a solution $(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{\psi}_h^n)$ $\forall n \geq 0$. (no CFL, but no uniqueness !)

Proof : use free energy estimate and Brouwer fixed point theorem.

Is this related to the better stability properties that have been reported for the log-formulation ?

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