Multiscale modelling of complex fluids: a mathematical initiation.

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Reference (with Matlab programs, see Section 5):

C. Le Bris, TL, *Multiscale modelling of complex fluids: A mathematical initiation*,

in Multiscale Modeling and Simulation in Science Series, B. Engquist, P. Lötstedt, O. Runborg, eds.,

LNCSE 66, Springer, p. 49-138, (2009)

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

Outline

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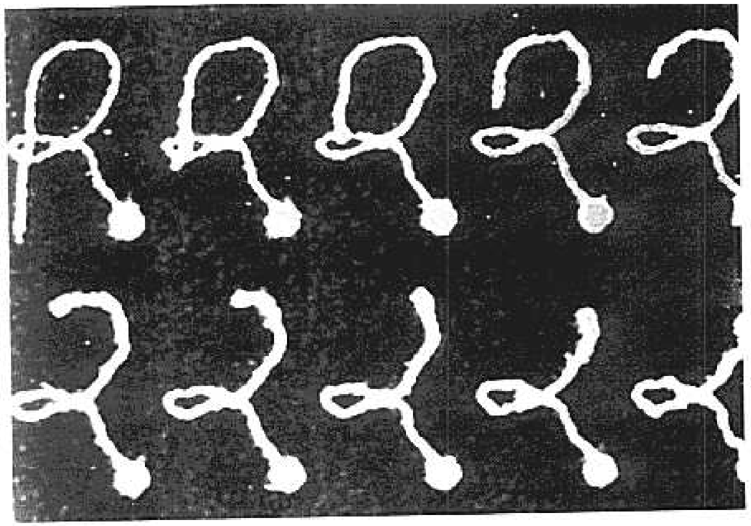
1 Modeling

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

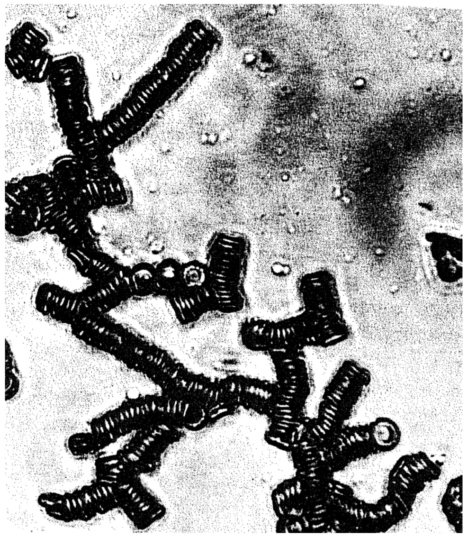
1A Experimental observations

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 for all non-Newtonian fluids with microstructures (granular materials).

A prototypical example is dilute solution of polymers.

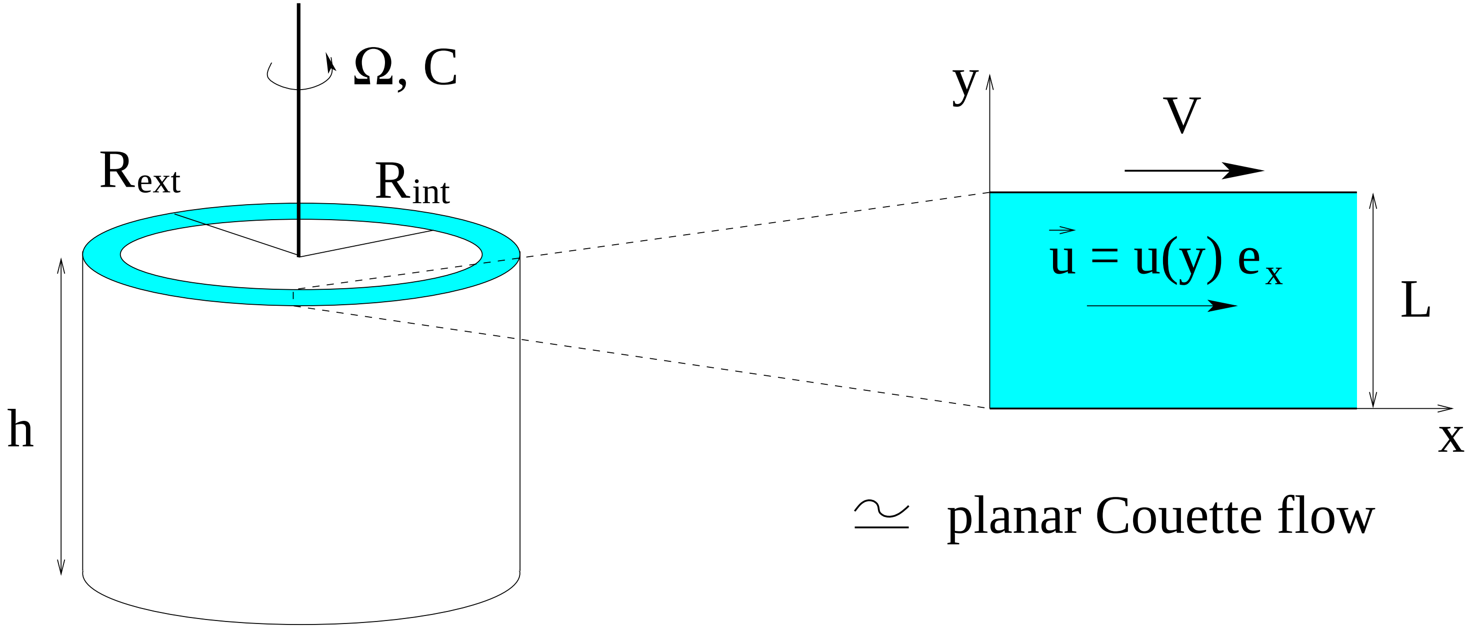
1A Experimental observations

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:



≃ planar Couette flow

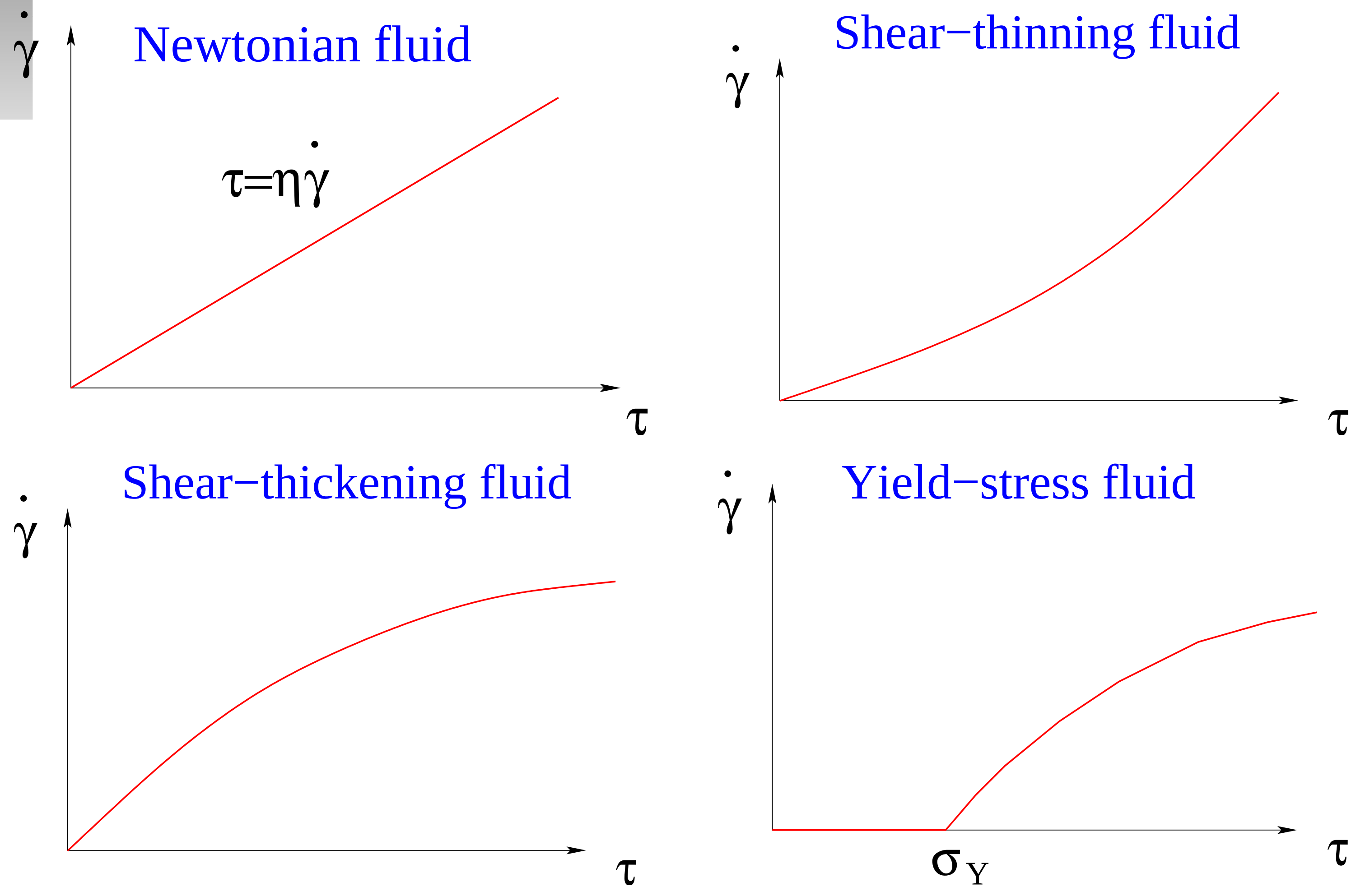
$$\dot\gamma = \frac{V}{L} = \frac{R_{int}\Omega}{R_{ext}-R_{int}}$$

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

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

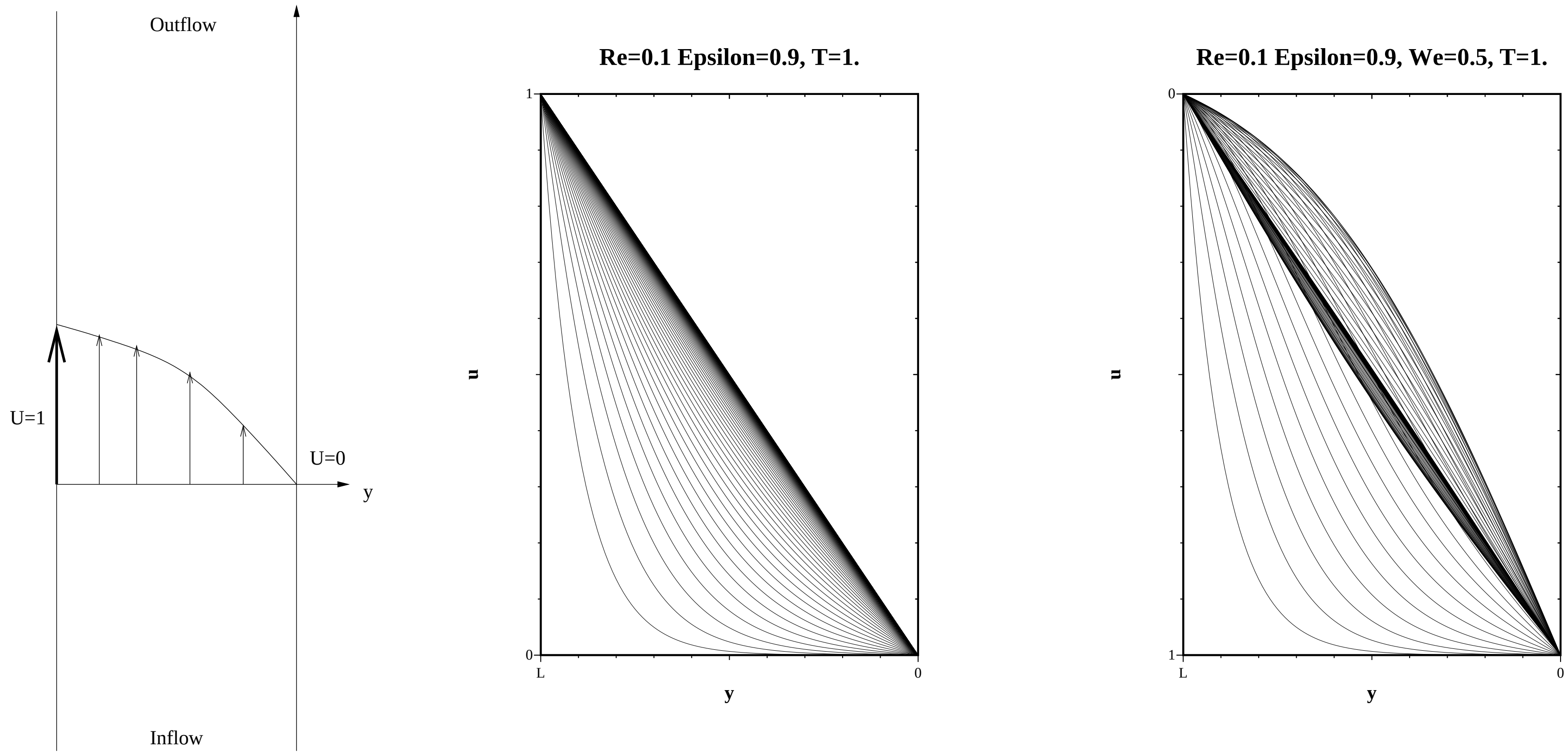
1A Experimental observations

At stationary state:



1A Experimental observations

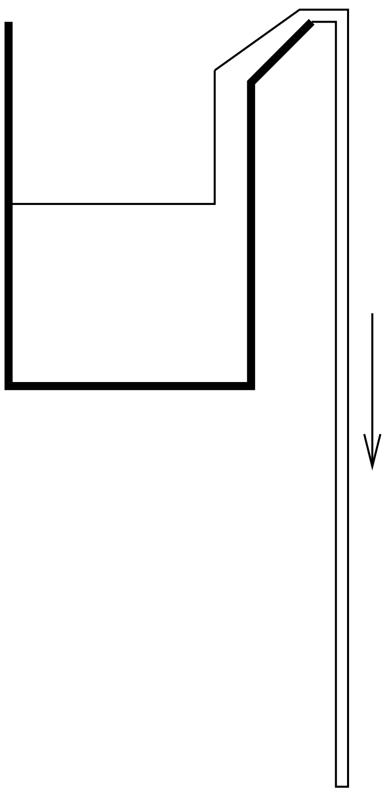
A simple dynamics effect: the velocity overshoot for the start-up of shear flow.

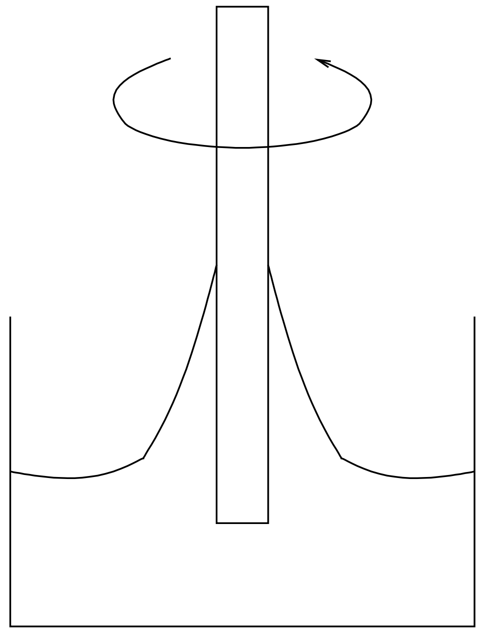


Velocity profile as time evolves: Newtonian fluid *vs* Hookean dumbbell model.

1A Experimental observations

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





Outline

Momentum equations (incompressible fluid):

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

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

Newtonian fluids (Navier-Stokes equations):

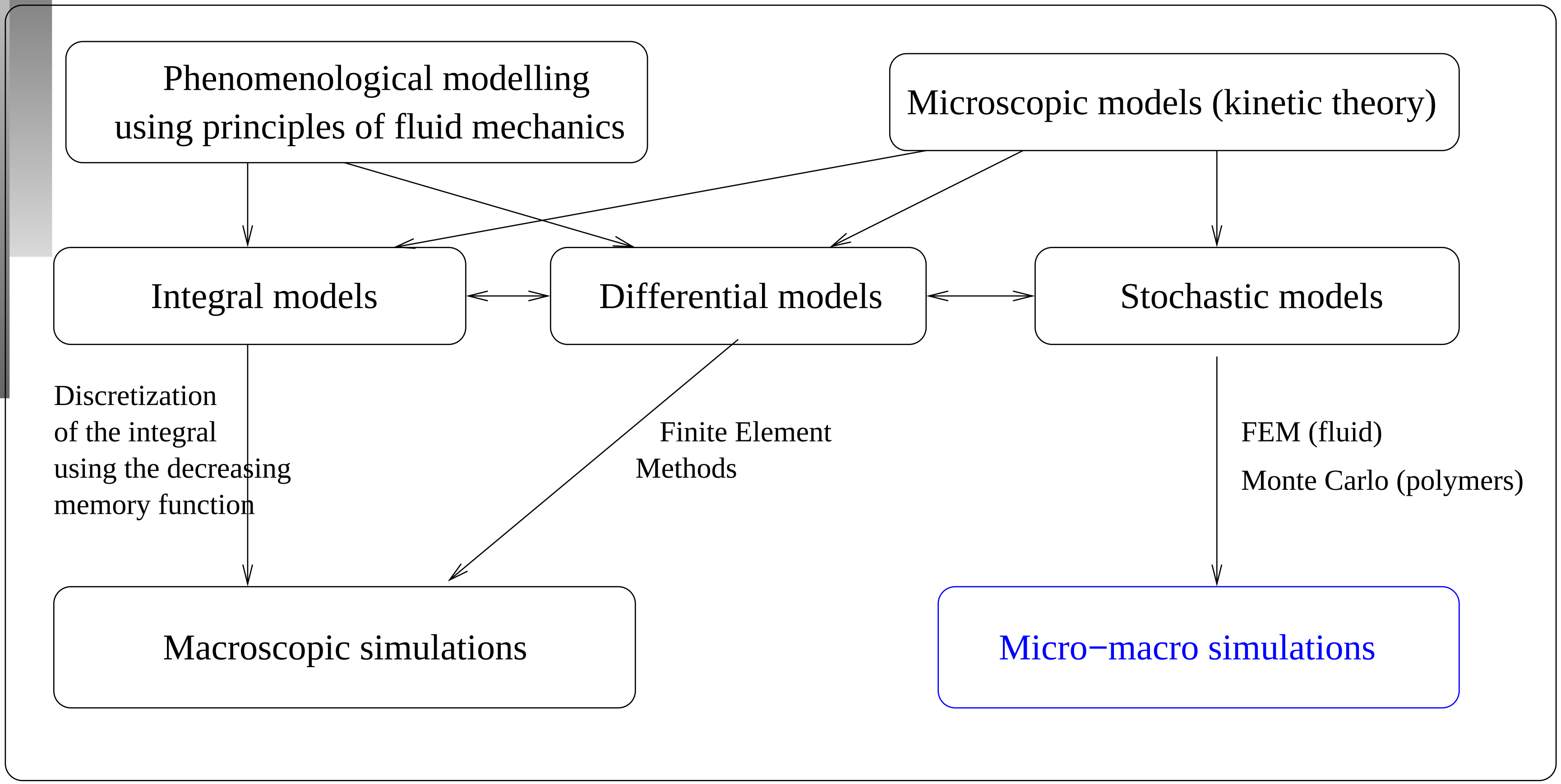
$$\boldsymbol{\sigma} = \eta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right),$$

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

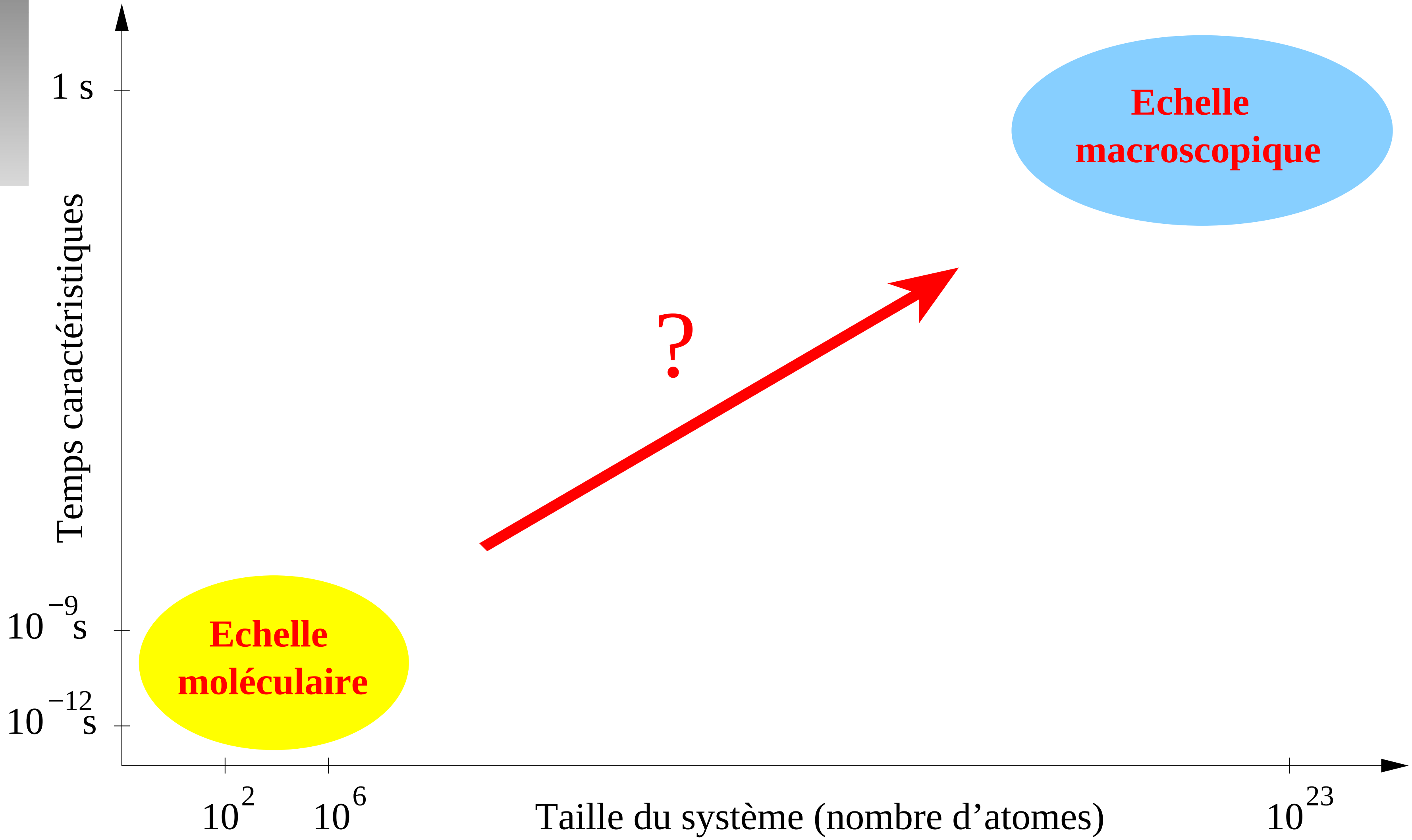


Differential models : $\frac{D\boldsymbol{\tau}}{Dt} = f(\boldsymbol{\tau}, \nabla \mathbf{u}),$

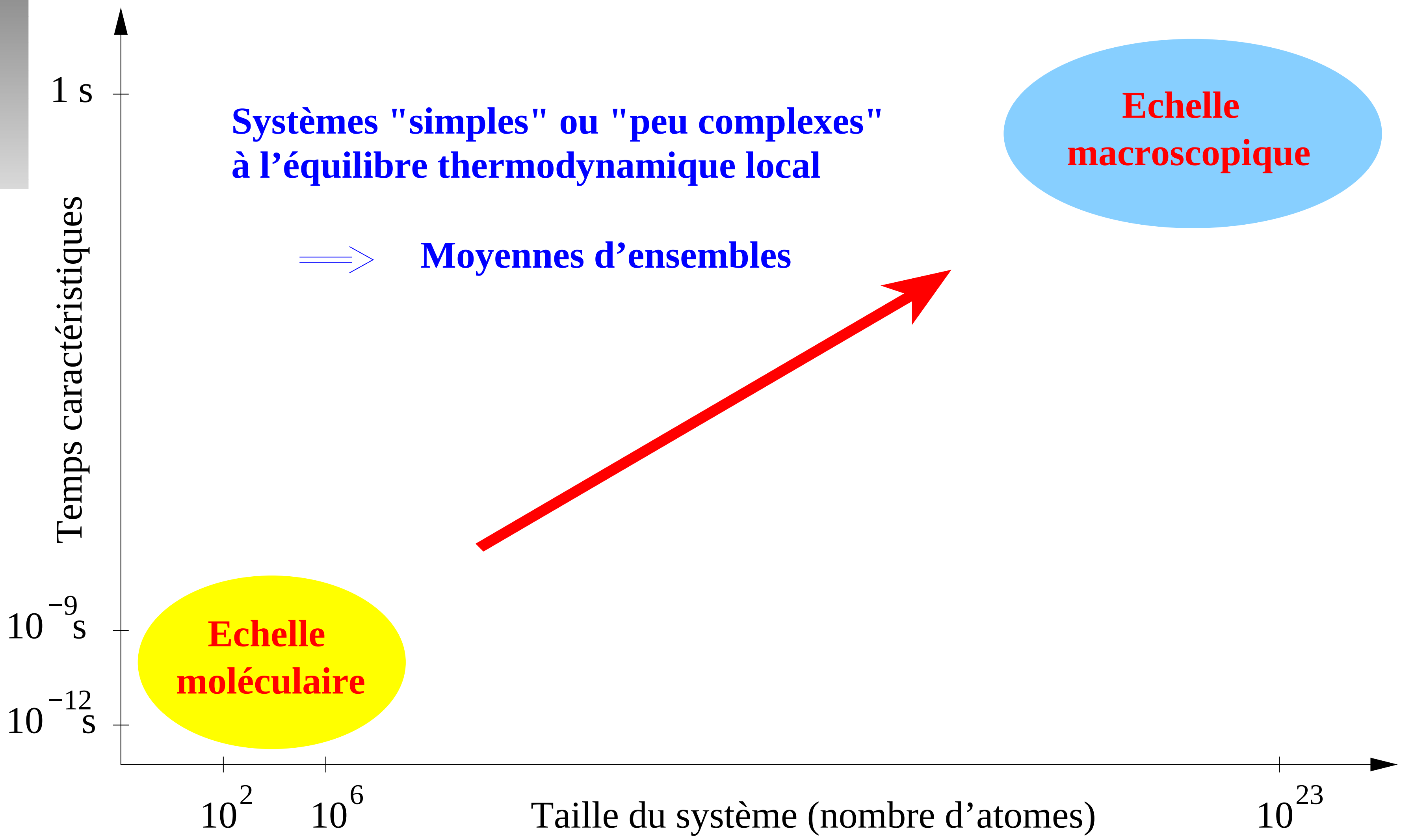
Integral models : $\boldsymbol{\tau} = \int_{-\infty}^{t} m(t-t')\mathbf{S}_t(t')\,dt'.$

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

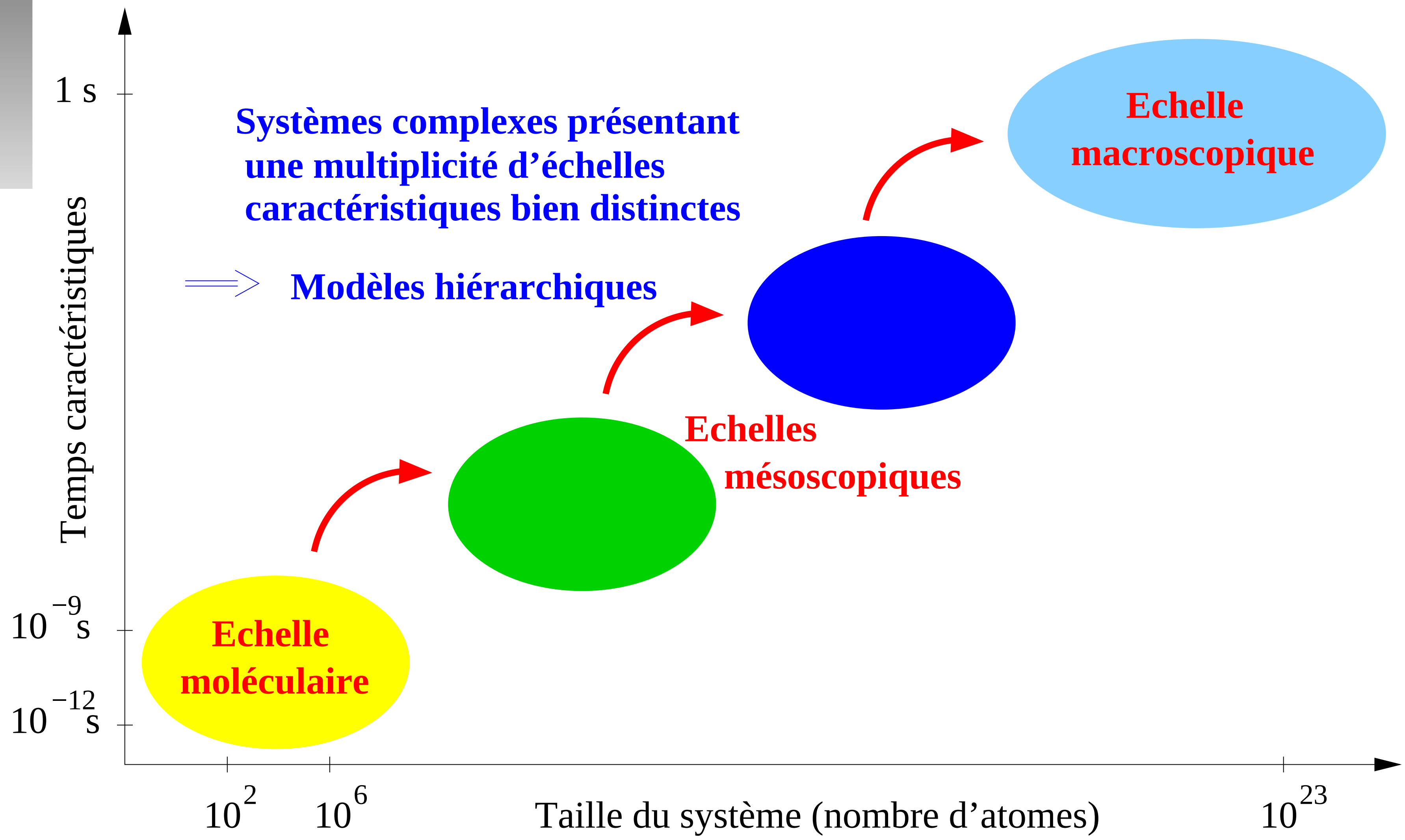
1B Multiscale modeling



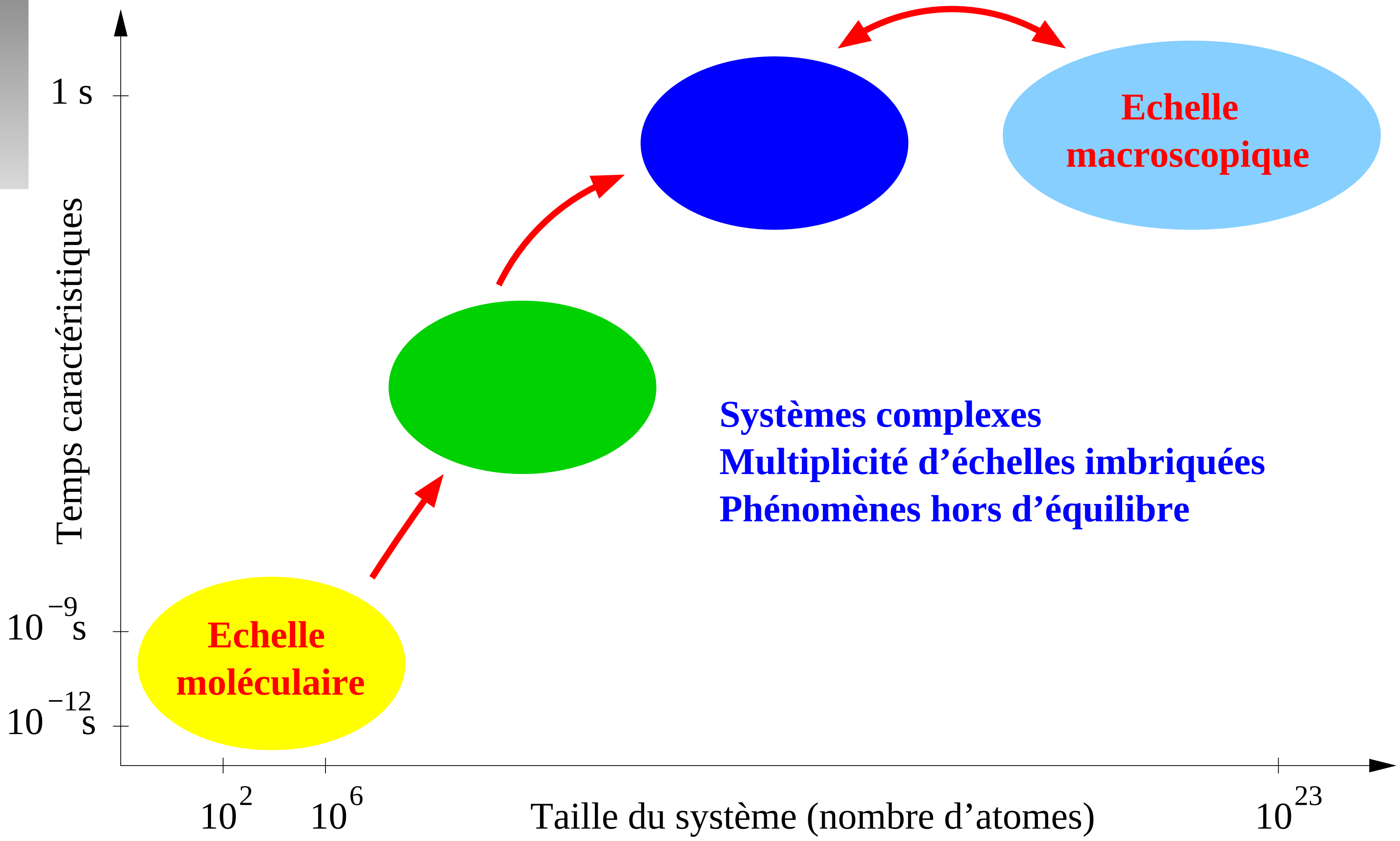
1B Multiscale modeling



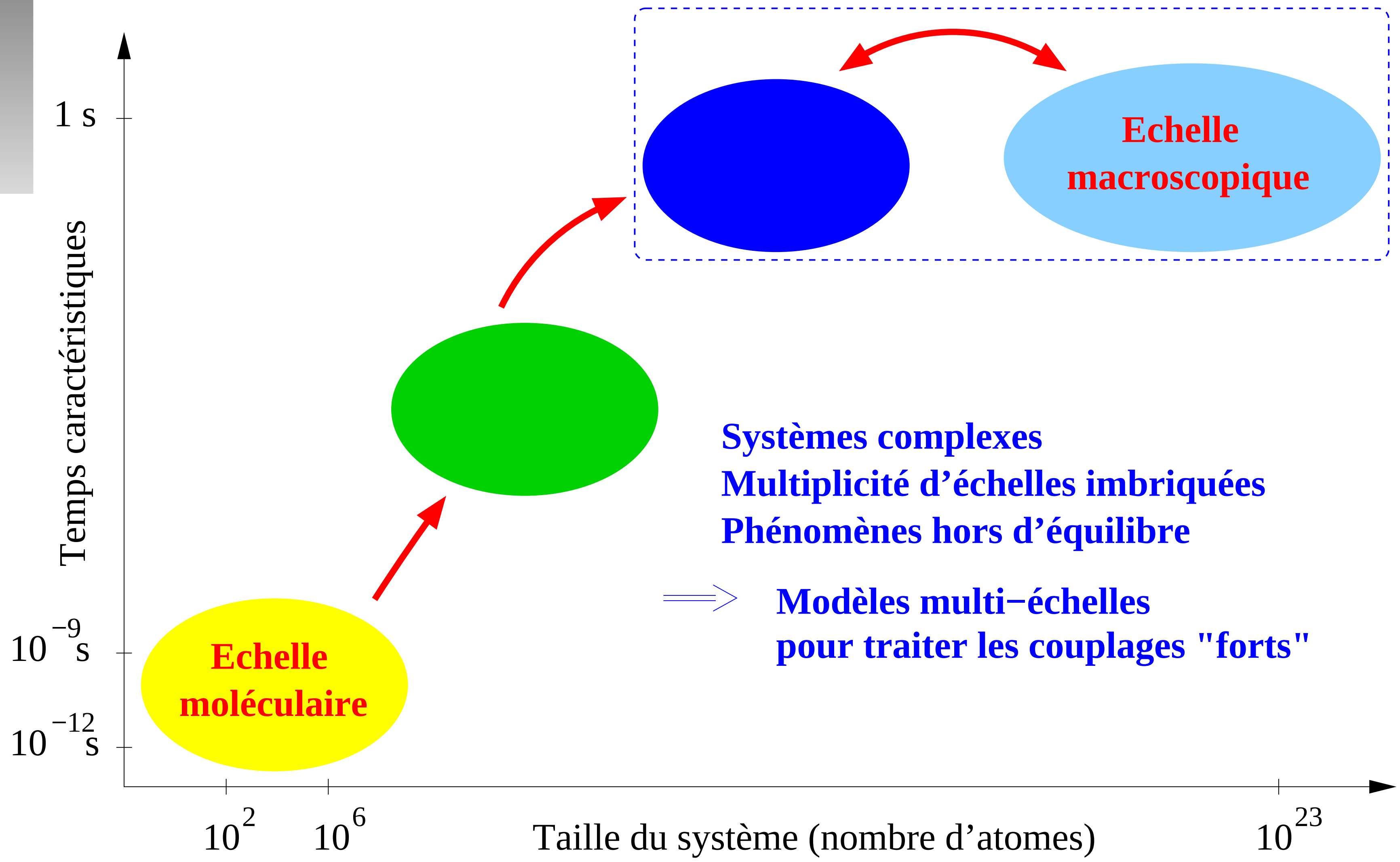
1B Multiscale modeling



1B Multiscale modeling



1B Multiscale modeling



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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,

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

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 $\Delta t \to 0$,

$$
\begin{aligned}
\phi(X_t) = \phi(X_0) &+ \int_0^t \phi'(X_s)(b(X_s)ds + \sigma(X_s)\, dW_s) \\
&+ \frac{1}{2}\int_0^t \sigma^2(X_s)\phi''(X_s)\, ds, \\
&= \phi(X_0) + \int_0^t \phi'(X_s)dX_s + \frac{1}{2}\int_0^t \sigma^2(X_s)\phi''(X_s)\, ds,
\end{aligned}
$$

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:

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

Proof (dimension 1):

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

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

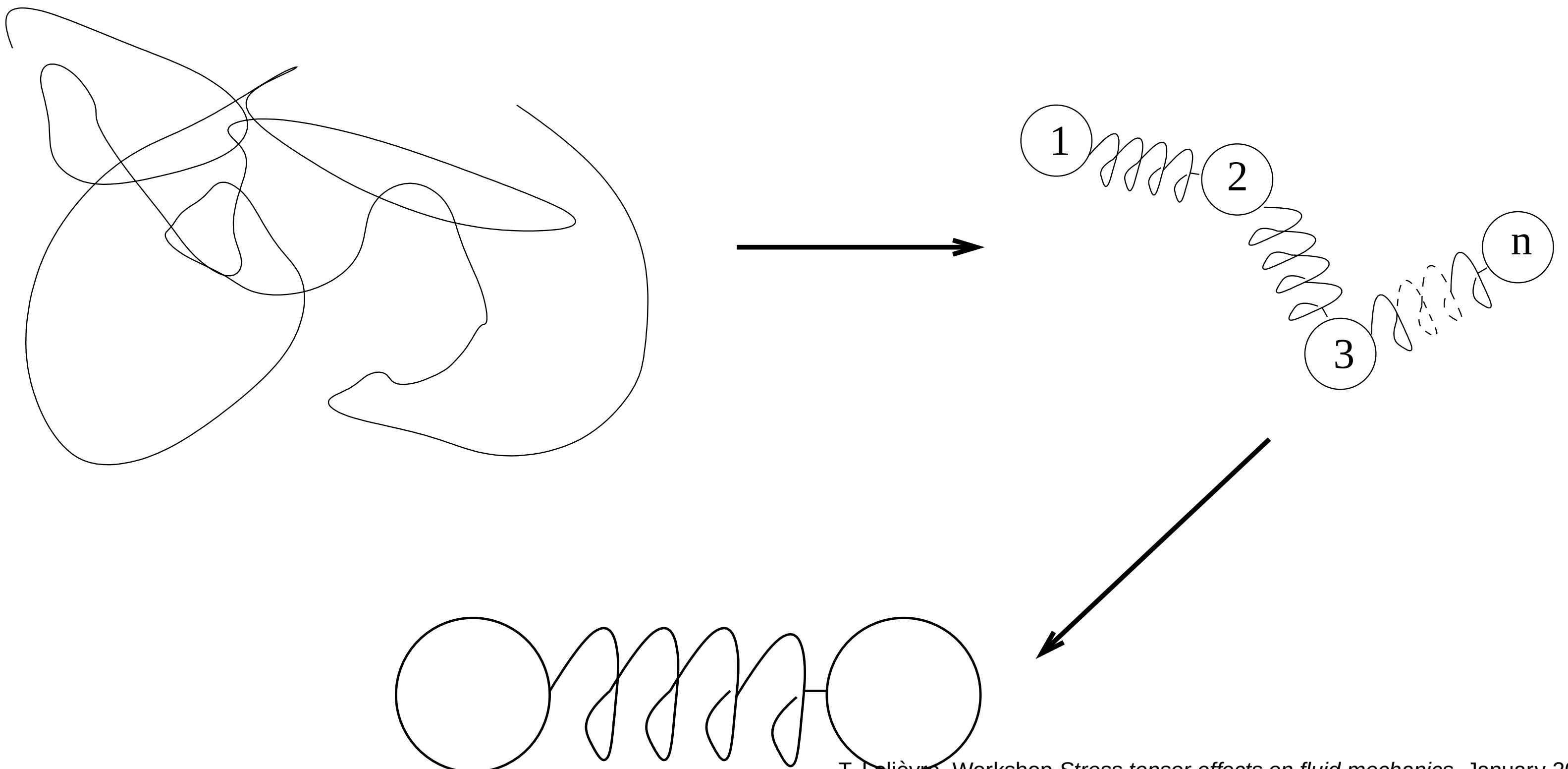
$$\zeta \partial_t \psi = \mathrm{div}(\nabla V \psi + \beta^{-1} \nabla \psi).$$

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"):

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

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 can be said about the correctness of the dynamics ?

  F. Legoll, TL, http://fr.arXiv.org/abs/0906.4865

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).

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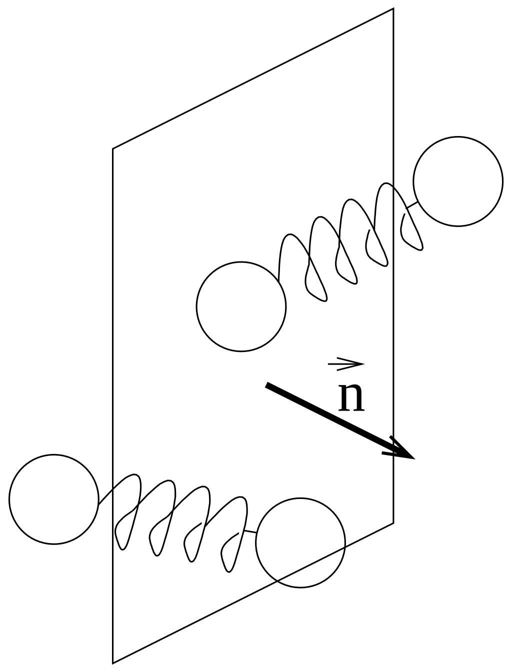
1D Micro-macro models for polymeric fluids

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):



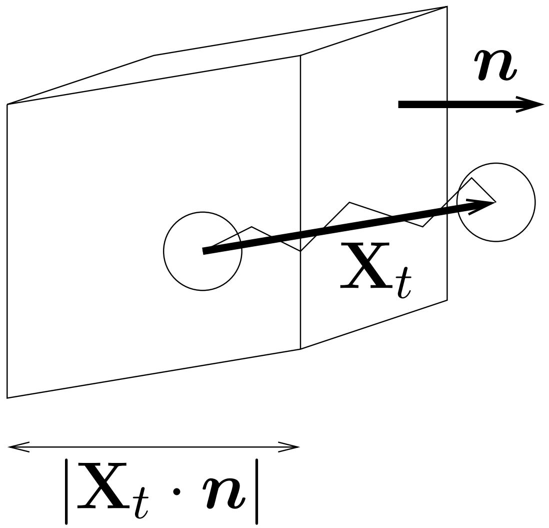
$$\boldsymbol{\tau}(t,\boldsymbol{x}) = n_p\Big(-kT\boldsymbol{I} + \mathbf{E}\left(\mathbf{X}_t(\boldsymbol{x}) \otimes \mathbf{F}(\mathbf{X}_t(\boldsymbol{x}))\right)\Big).$$

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:

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

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:

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

with the following non-dimensional numbers:

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

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:

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

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

Outline

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

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.

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

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 $\mathbf{u}$.

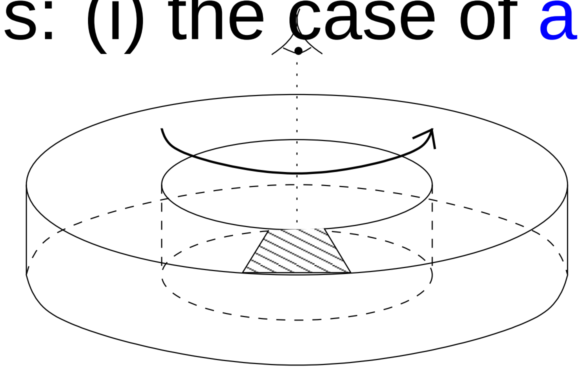
Well-posedness results for micro-macro models:

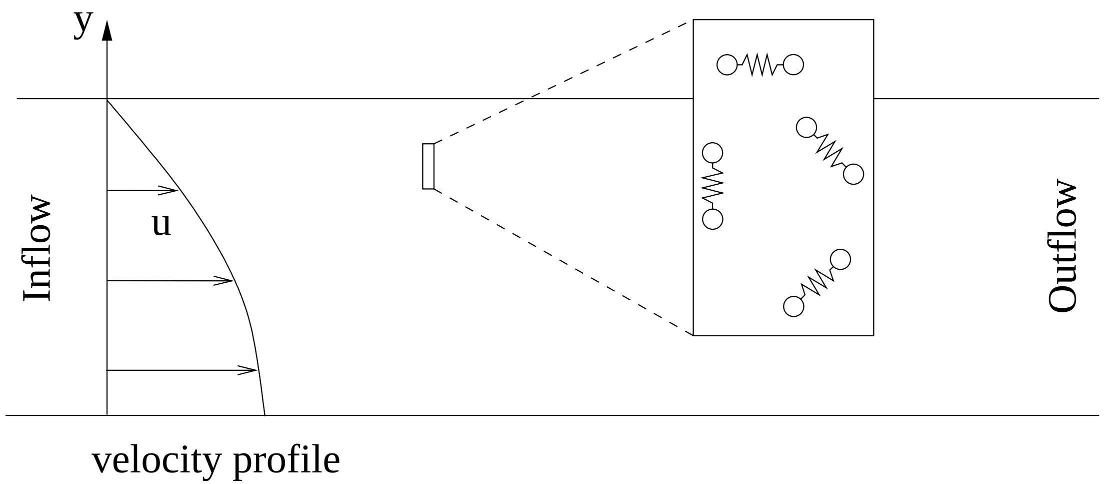
- The uncoupled problem: SDE or FP.
  - SDE in the FENE case (B. Jourdain, TL: OK for $b \geq 2$),
  - the case of non smooth velocity field, transport term in the SDE or FP (C. Le Bris, P.L Lions).
- The coupled problem: PDE + SDE or PDE + FP.
  - PDE+SDE: shear flow for Hookean or FENE (C. Le Bris, 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

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, 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:

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

The separation between the coupling term and the transport term is actually somehow misleading: all these terms are transport terms.
For Oldroyd-B

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

Let $y(t,Y)$ satisfy $y(0,Y)=Y$ and

$$\frac{dy(t,Y)}{dt} = u(t, y(t,Y)).$$

Let us consider the deformation tensor $G(t,y(t,Y)) = \frac{\partial y}{\partial Y}(t,Y)$. Then G satisfies:

$$\partial_t G + \mathbf{u} \cdot \nabla G = \nabla \mathbf{u} G.$$

Thus, if $\sigma(t,y) = G(t,y)\sigma_0 G^T(t,y)$, then

$$\frac{\partial \sigma}{\partial t} + \mathbf{u}.\nabla\sigma - \nabla\mathbf{u}\sigma - \sigma(\nabla\mathbf{u})^T = 0.$$

Likewise, for the Fokker-Planck equation:

$$\frac{\partial \psi}{\partial t} + \mathbf{u}\cdot\nabla_{\boldsymbol{x}}\psi + \mathrm{div}_{\mathbf{X}}\,(\nabla_{\boldsymbol{x}}\mathbf{u}\,\mathbf{X}\psi) = \frac{1}{2\mathrm{We}}\,\mathrm{div}_{\mathbf{X}}\,(\nabla\Pi(\mathbf{X})\psi + \nabla_{\mathbf{X}}\psi)\,,$$

one can check that

$$\frac{d}{dt}\Big(\psi(t,y(t,Y),G(t,Y)\mathbf{X})\Big)$$
$$= \Big(\partial_t\psi + \mathbf{u}\cdot\nabla_{\boldsymbol{x}}\psi + \mathrm{div}_{\mathbf{X}}\,(\nabla_{\boldsymbol{x}}\mathbf{u}\,\mathbf{X}\psi)\Big)(t,y(t,Y),G(t,Y)\mathbf{X}).$$

(Notice that $\mathrm{div}_{\mathbf{X}}\,(\nabla_{\boldsymbol{x}}\mathbf{u}\,\mathbf{X}\psi) = \nabla_{\boldsymbol{x}}\mathbf{u}\,\mathbf{X}\cdot\nabla_{\mathbf{X}}\psi$.)

2A Generalities

This fact is well-known in the literature (C. Liu, P. Zhang, L. Chupin, ...) but is seems that it does not help to get better existence results.

Remark: I am not aware of any numerical method using this feature (characteristic method).

Outline

2B Some existence results

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

Adopted approach :

- The SDEs are posed at each macroscopic point 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}).

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

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

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

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

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

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

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

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.

2B Some existence results: Hookean

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: $\int_{\mathcal{O}} \mathbb{E}(Y_t X_t^m(y))\partial_y v_i$, 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:

$\mathbf{F}(\mathbf{X}) = \frac{\mathbf{X}}{1-\|\mathbf{X}\|^2/b}$

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

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 $\partial_y u \, Y_t^y$,
- For a given regularity of $\partial_y u$, what is the regularity of τ ?

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

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

$$Y^y_t = Y_0 + \int_0^t -\frac{1}{2} \frac{Y^y_s}{1 - \frac{(X^y_s)^2 + (Y^y_s)^2}{b}} ds + W_t.$$

2B Some existence results: FENE

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

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

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

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 is associated to 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 $\mathbf{P}^g$ defined by

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

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

$(X_t, Y_t, V_t - \int_0^t g(s) Y_s \, ds, W_t, \mathbf{P}^g)$ is a weak solution of the SDE.

Regularity of τ in space

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

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

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

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

$$\tau = \mathbf{E}\left(\frac{X_t^y Y_t^y}{1 - \frac{(X_t^y)^2 + (Y_t^y)^2}{b}}\right) = \mathbf{E}^y\left(\frac{X_t Y_t}{1 - \frac{X_t^2 + Y_t^2}{b}}\right),$$

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

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 the potential associated to 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

2 Mathematics analysis

2A Generalities

2B Some existence results

2C Long-time behaviour

2D Free-energy for macro models

2C Long-time behaviour

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.

2C 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):

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

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 $h(x) = (x-1)^2$.

2C 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,

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

2C 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 $L^2 \subset L^1 \ln(L^1)$.

2C 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 $H''(t)$.

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 skew-symmetric, $\psi_\infty \propto \exp(-\Pi)$ 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.

2C 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 $\mathrm{osc}\left(\ln\left(\frac{\psi_\infty}{\exp(-\Pi)}\right)\right) < \infty$.
For FENE dumbbell, we will prove that there exists such a stationary solution if $\boldsymbol{\kappa} + \boldsymbol{\kappa}^T$ is small enough.

2C 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):

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

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

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

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 $\kappa \in L^p_t, 1 \le p < \infty$) or FENE dumbbells (for $\kappa \in L^2_t + L^\infty_t$ and b sufficiently large).

2C 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 $\mathbf{X}_0^\infty \sim \psi_\infty(\mathbf{X})\, d\mathbf{X}$.

2C Long-time behaviour: SDE

Then (using α-convexity of Π),

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

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.

2C 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.

2C 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.

2C 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^∞, $f_0, f_1 \in W^{1,1}_{loc}(\mathbb{R}_+)$ *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 ?

2C Long-time behaviour: PDE-FP

The Fokker-Planck version of the coupled system is:

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

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

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

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

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).

2C Long-time behaviour: PDE-FP

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

We introduce the kinetic energy:

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

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

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

2C Long-time behaviour: PDE-FP

Let us introduce $F(t) = E(t) + \frac{\epsilon}{\mathrm{We}} H(t)$. One has, by differentiating F w.r.t. time:

$$\frac{d}{dt}\left(\frac{\mathrm{Re}}{2}\int_{\mathcal{D}} |\mathbf{u}|^2 + \frac{\epsilon}{\mathrm{We}}\int_{\mathcal{D}}\int_{\mathbb{R}^d} \psi \ln\left(\frac{\psi}{\psi_\infty}\right)\right)$$

$$= \quad -(1-\epsilon)\int_{\mathcal{D}} |\nabla \mathbf{u}|^2 - \frac{\epsilon}{2\mathrm{We}^2}\int_{\mathcal{D}}\int_{\mathbb{R}^d} \psi \left|\nabla \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 .$$

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 $\psi = \psi_\infty \propto \exp(-\Pi)$.

2C 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 $t \to \infty$.

2C 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. $h(x) = x\ln(x)$.

2C 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 $L^\infty_{\mathbf{X}}$.

2C 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).

2C Long-time behaviour: PDE-FP

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

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

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_∞.

2C 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:

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

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 skew-symmetric, take $\psi_\infty \propto \exp(-\Pi)$ and one obtains exponential decay.

2C Long-time behaviour: PDE-FP

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

For Hookean dumbbells, this term can be handled using moment estimates (Arnold et al.).

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

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

2C Long-time behaviour: PDE-FP

Then, for FENE dumbbells:

Theorem 3 *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 $\int_{\mathcal{D}} \int_{\mathcal{B}} \psi \ln \left(\frac{\psi}{\psi_\infty} \right)$, 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.

2C 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:

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

2C Long-time behaviour: PDE-FP

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

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

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).

2C Long-time behaviour: PDE-FP

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

Theorem 4 *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_∞*.*

2C 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 ?

General question: convergence to equilibrium for Fokker-Planck equations, of the form

$$\partial_t \psi = \mathrm{div}(b\psi + \nabla\psi)$$

using a decomposition of b in gradient part, and divergence free part.

Outline

2 Mathematics analysis

2A Generalities

2B Some existence results

2C Long-time behaviour

2D Free-energy for macro models

2D Free-energy 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:

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

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

2D Free-energy for macro models

Compared to the "classical" estimate:

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

the interest is that

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

while we have no sign on

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

2D Free-energy for macro models

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

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

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

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

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

2D Free-energy 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...

2D Free-energy for macro models

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

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

$$0\le -\ln(\det(M))-b\ln(1-\text{tr}(M)/b)+(b+d)\ln\left(\frac{b}{b+d}\right)$$
$$\le\left(\frac{\text{tr}(M)}{(1-\text{tr}(M)/b)^2}-\frac{2d}{1-\text{tr}(M)/b}+\text{tr}(M^{-1})\right).$$

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

2D Free-energy 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.

Outline

3 Numerical methods and numerical analysis

- 3A Generalities
- 3B Convergence of the CONNFFESSIT method
- 3C Dependency of the Brownian on the space variable
- 3D Free-energy dissipative schemes for macro models
- 3E Variance reduction and reduced basis method

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.)

3A Generalities

Numerical analysis in fluid mechanics

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 : $O(\Delta t)$.

Numerical analysis of SDEs

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

The problem

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

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), RB (S. Boyaval, 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).

Outline

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3B 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.

3B Convergence of the CONNFFESSIT method

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

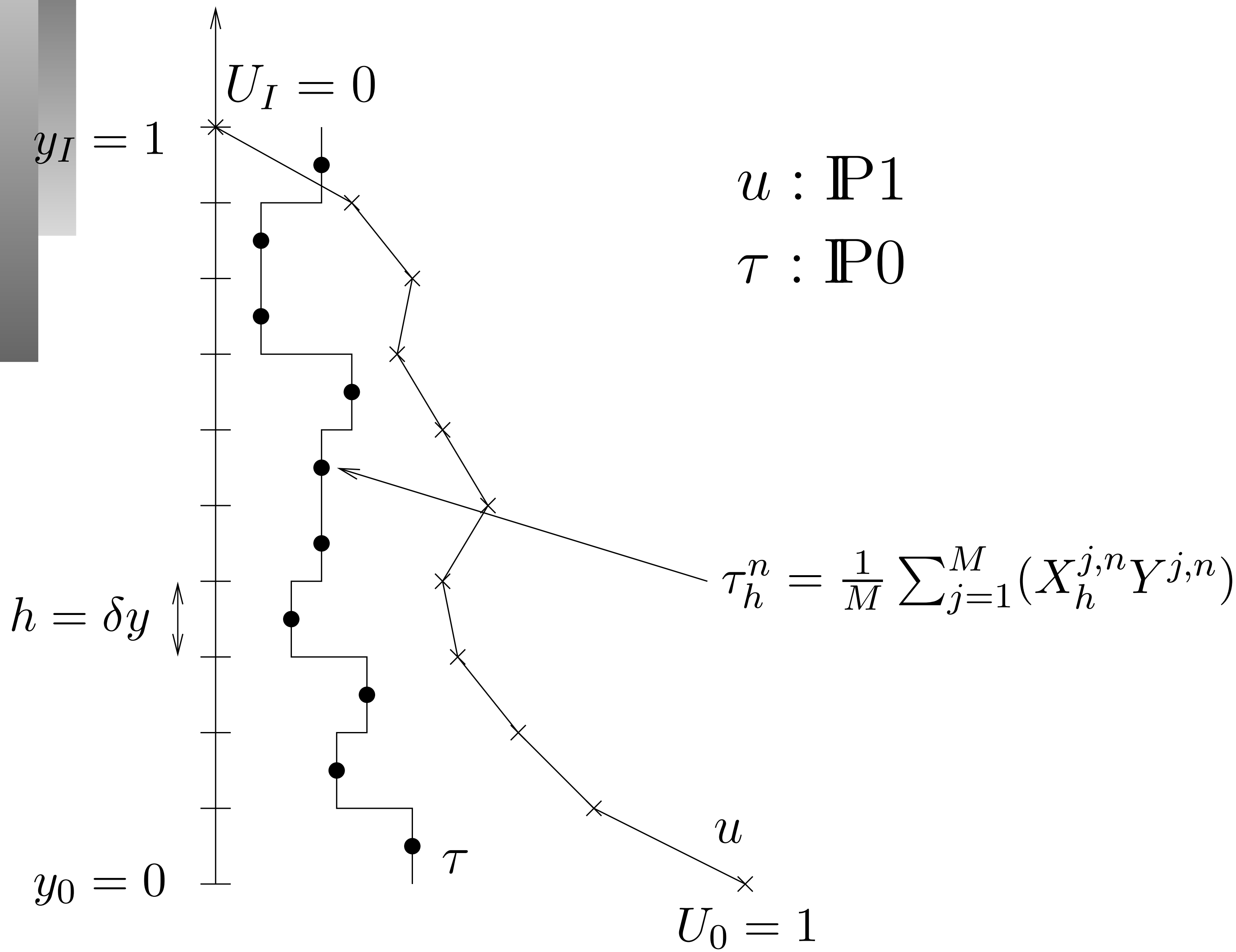
Spacestep: $h = \delta y$, timestep: Δt, number of realizations: M.

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

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.

3B Convergence of the CONNFFESSIT method



3B Convergence of the CONNFFESSIT method

Theorem 5 *[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:

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

3B Convergence of the CONNFFESSIT method

Sketch of the proof:

- $\mathbb{P}1$ 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.

3B 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:

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

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

3B 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.

3B 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.

3B 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

- (control variate at equilibrium) $\tilde{\mathbf{F}} = \mathbf{F}$ and $d\tilde{\mathbf{X}}_t + \mathbf{u} \cdot \nabla \tilde{\mathbf{X}}_t \, dt = -\frac{1}{2\mathrm{We}} \tilde{\mathbf{F}}(\tilde{\mathbf{X}}_t) \, dt + \frac{1}{\sqrt{\mathrm{We}}} d\mathbf{W}_t$.
- (Hook. dumbbell as control variate) $\tilde{\mathbf{F}}(\tilde{\mathbf{X}}) = \tilde{\mathbf{X}}$ 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 $\mathbf{X}_t$.

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3C Dependency of the Brownian on the space variable

We consider Hookean dumbbells in a shear flow.

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

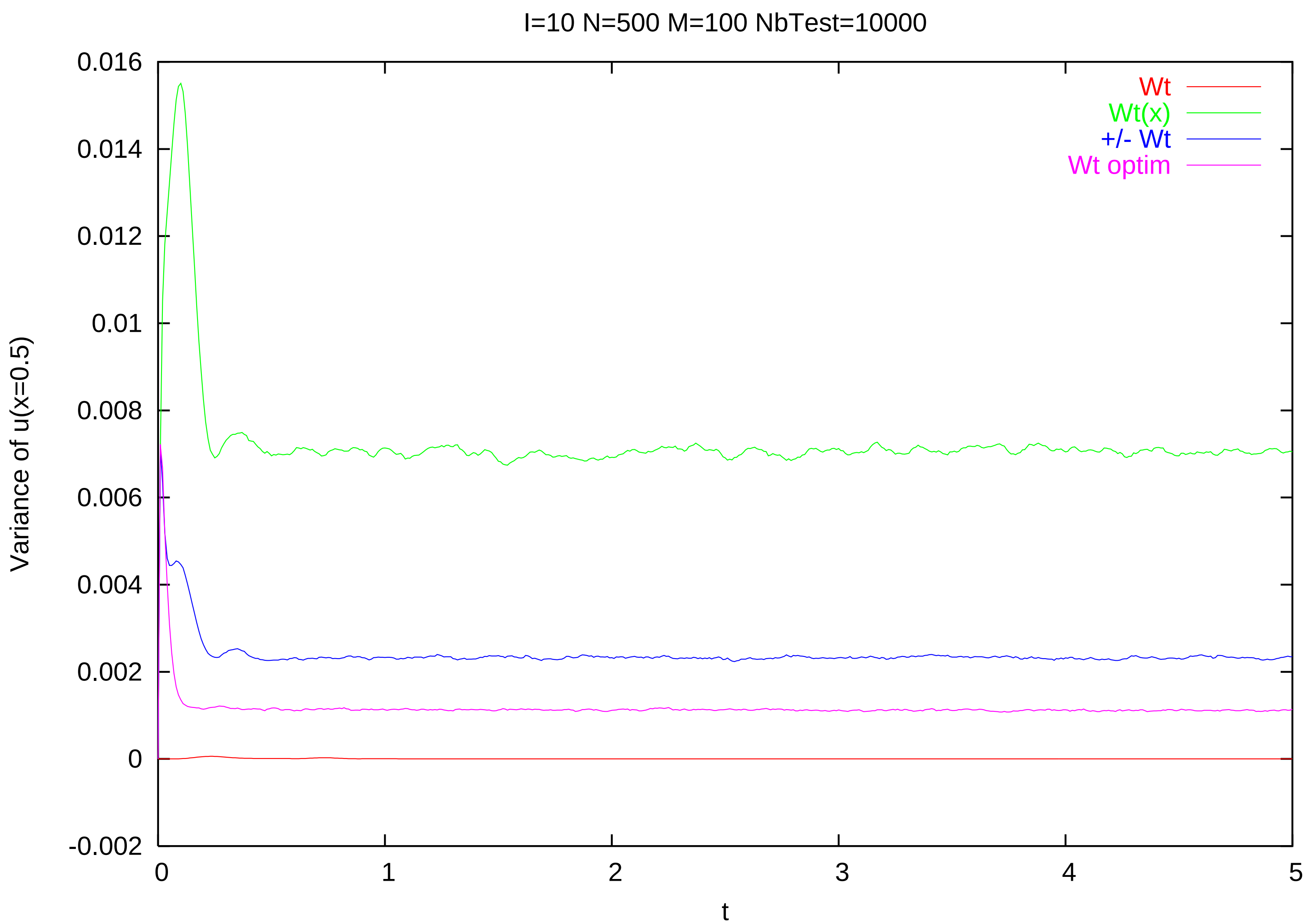
Question: (V_t, W_t) or $(V_t(y), W_t(y))$?

- 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).

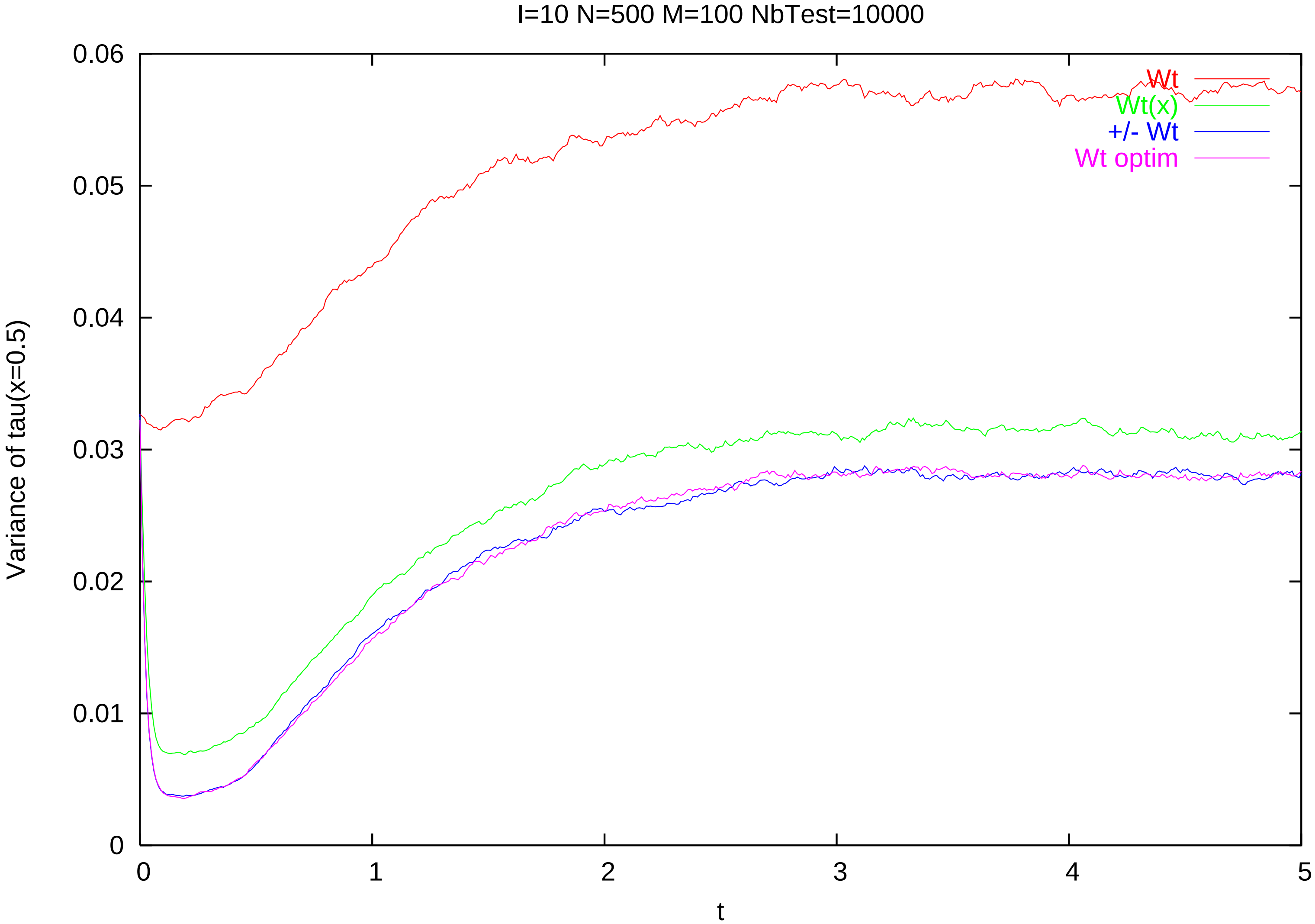
3C Dependency of the Brownian on the space variable

Variance of u



3C Dependency of the Brownian on the space variable

Variance of τ



3C 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 ?

3C 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 $\mathrm{Covar}(v) := \mathbf{E}(v \otimes v) - \mathbf{E}(v) \otimes \mathbf{E}(v)$.

3C 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.

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

3C 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 $V_t(y)$.

3C Dependency of the Brownian on the space variable

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

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

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

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.

3C 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 !

3C 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

3 Numerical methods and numerical analysis

- 3A Generalities
- 3B Convergence of the CONNFFESSIT method
- 3C Dependency of the Brownian on the space variable
- 3D Free-energy dissipative schemes for macro models
- 3E Variance reduction and reduced basis method

3D Free-energy dissipative schemes for macro models

Recall the free energy estimate for the Oldroyd-B model:

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

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

Aim: Analyze the stability of numerical schemes using this free energy estimate. Indeed, if one is able to build numerical scheme such that the free energy $\frac{\mathrm{Re}}{2}\int_{\mathcal{D}}|\mathbf{u}|^2+\frac{\varepsilon}{2\mathrm{We}}\int_{\mathcal{D}}(-\ln(\det(\boldsymbol{A}))-d+\mathrm{tr}(\boldsymbol{A}))$ decreases in time, one ensures “some” stability of the numerical scheme.

3D Free-energy dissipative schemes for macro models

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

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

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

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

3D Free-energy dissipative schemes for macro models

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

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

where

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

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

3D Free-energy dissipative schemes for macro models

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...

3D Free-energy dissipative schemes for macro models

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:

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

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

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

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

3D Free-energy dissipative schemes for macro models

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:

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

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

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

3D Free-energy dissipative schemes for macro models

Key ingredients for the proof:

- Take as test functions (since $\boldsymbol{\sigma}_h^{n+1} \in (\mathbb{P}_0)^3$): $\left(\boldsymbol{u}_h^{n+1}, p_h^{n+1}, \frac{\varepsilon}{2\mathrm{We}}\left(\boldsymbol{I} - (\boldsymbol{\sigma}_h^{n+1})^{-1}\right)\right)$.
- 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 $\int_{\mathcal{D}} \operatorname{tr}\ln(\boldsymbol{\sigma}_h^n \circ X^n(t^n)) = \int_{\mathcal{D}} \operatorname{tr}\ln(\boldsymbol{\sigma}_h^n)$.

3D Free-energy dissipative schemes for macro models

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:

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

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

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

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

3D Free-energy dissipative schemes for macro models

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 $\{E_j\}$

3D Free-energy dissipative schemes for macro models

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 $(\mathbb{P}_0)^3$.

3D Free-energy dissipative schemes for macro models

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

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

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

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

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

3D Free-energy dissipative schemes for macro models

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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3E Variance reduction and reduced basis method

In the CONNFFESSIT method, we have to compute expected values:

$$\mathbf{E}(\mathbf{X}_t \otimes \mathbf{F}(\mathbf{X}_t))$$

where $\mathbf{X}_t$ satisfies the SDE:

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

This Monte Carlo calculation has to be done for many values of the velocity gradient.

Idea: Use this “many query” context to build a variance reduction method.

Two building blocks: The control variate method and the reduced basis method.

3E Variance reduction and reduced basis method

Variance reduction by control variate: Instead of approximating $\mathbf{E}(Z)$, approximate

$$\mathbf{E}(Z - \alpha Y)$$

where Y is a zero-mean random variable, and α is a deterministic parameter to be fixed. We want

$$\mathrm{Var}(Z - \alpha Y) \ll \mathrm{Var}(Z).$$

Optimal $\alpha = \alpha^* = \frac{\mathrm{Covar}(Z,Y)}{\mathrm{Var}(Y)}$ so that $\mathrm{Var}(Z - \alpha^* Y) = \mathrm{Var}(Z)(1 - \rho(Z,Y)^2)$ with

$$\rho(Z,Y) = \frac{\mathrm{Covar}(Z,Y)}{\sqrt{\mathrm{Var}(Y)\mathrm{Var}(Z)}} \in [-1,1].$$

3E Variance reduction and reduced basis method

Optimal case: $|\rho(Z,Y)| = 1$ (*i.e.* $Y = Z - \mathbf{E}(Z)$!).

Worst case: $\rho(Z,Y) = 0$ (uncorrelated Y and Z).

How to build a correlated random variable Y with zero mean ?

3E Variance reduction and reduced basis method

Reduced basis method Y. Maday, A.T. Patera: Assume one has to solve $-\operatorname{div}(A(\lambda)\nabla u) = f$ for many values of the parameter $\lambda \in \Lambda$.

Principle of the method:

- In an *offline stage*, build a reduced basis

$$X_N = \operatorname{span}(u(\lambda_1), \ldots, u(\lambda_N))$$

  for well chosen values of the parameter λ.

- In an *online stage*, look for a solution to the original problem in X_N.

3E Variance reduction and reduced basis method

Some practical details in the PDE context:

- For a given reduced basis X_N, the solution in X_N is computed using a Galerkin method.
- In the offline stage, the parameter values λ_i are computed using a greedy algorithm: choose a finite set $\Lambda_{\rm trial} \subset \Lambda$, and $\lambda_1 \in \Lambda_{\rm trial}$. Then, for $n \geq 0$

$$\lambda_{n+1} \in \arg \sup_{\lambda \in \Lambda_{\rm trial}} \Delta_n(\lambda)$$

  where $\Delta_n(\lambda)$ is an *a posteriori* estimator of the error made on the output, when approximating $u(\lambda)$ by $u_n(\lambda) \in {\rm span}(u(\lambda_1), \dots, u(\lambda_n))$.

This approach has proven to be useful in many contexts, with relatively small N ($N \sim 10$).

3E Variance reduction and reduced basis method

The main tools used in the RB methodology are:

- Two-stage offline-online strategy (many-query context, or real-time applications);
- Use some solutions at given values of the parameter to build a reduced basis;
- A procedure to select the best linear combination on a given reduced basis;
- A greedy algorithm to select offline the best samples among a trial sample;
- An *a posteriori* estimator used online and offline to evaluate the error;

We will use the same ideas to build a control variate to reduce the variance for Monte Carlo estimations by empirical means of parametrized random variables.

3E Variance reduction and reduced basis method

Approximate $\mathbf{E}(Z^\lambda)$ by

$$E_M((Z^\lambda - Y^\lambda)_i) = \frac{1}{M}\sum_{i=1}^{M}(Z_i^\lambda - Y_i^\lambda),$$

where $(Z_i^\lambda, Y_i^\lambda)$ are i.i.d. We use as an *a posteriori* estimator of the error the empirical variance

$$V_M((Z^\lambda - Y^\lambda)_i) = \frac{1}{M}\sum_{i=1}^{M}(Z_i^\lambda - Y_i^\lambda - E_M((Z^\lambda - Y^\lambda)_i))^2.$$

Recall the optimal control variate: $Y^\lambda = Z^\lambda - \mathbf{E}(Z^\lambda)$.

3E Variance reduction and reduced basis method

In the offline stage, optimal control variates are computed:

$$Y^{\lambda_n} = Z^{\lambda_n} - E_{M_{\mathrm{large}}}((Z^{\lambda_n})_i).$$

In the online stage, use as a control variate:

$$\tilde{Y}^{\lambda} = \sum_{n=1}^{N} \alpha_n^* Y^{\lambda_n}$$

where $(\alpha_n^*) = \arg\inf_{(\alpha_n)} \mathrm{Var}\left(Z^{\lambda} - \sum_{n=1}^{N} \alpha_n Y^{\lambda_n}\right)$. The optimal (α_n^*) are solution to a least square problem. In practice the expected values are approximated online using empirical means over $M_{\mathrm{small}} \ll M_{\mathrm{large}}$ i.i.d. replicas (typically $M_{\mathrm{large}} = 100 M_{\mathrm{small}}$).

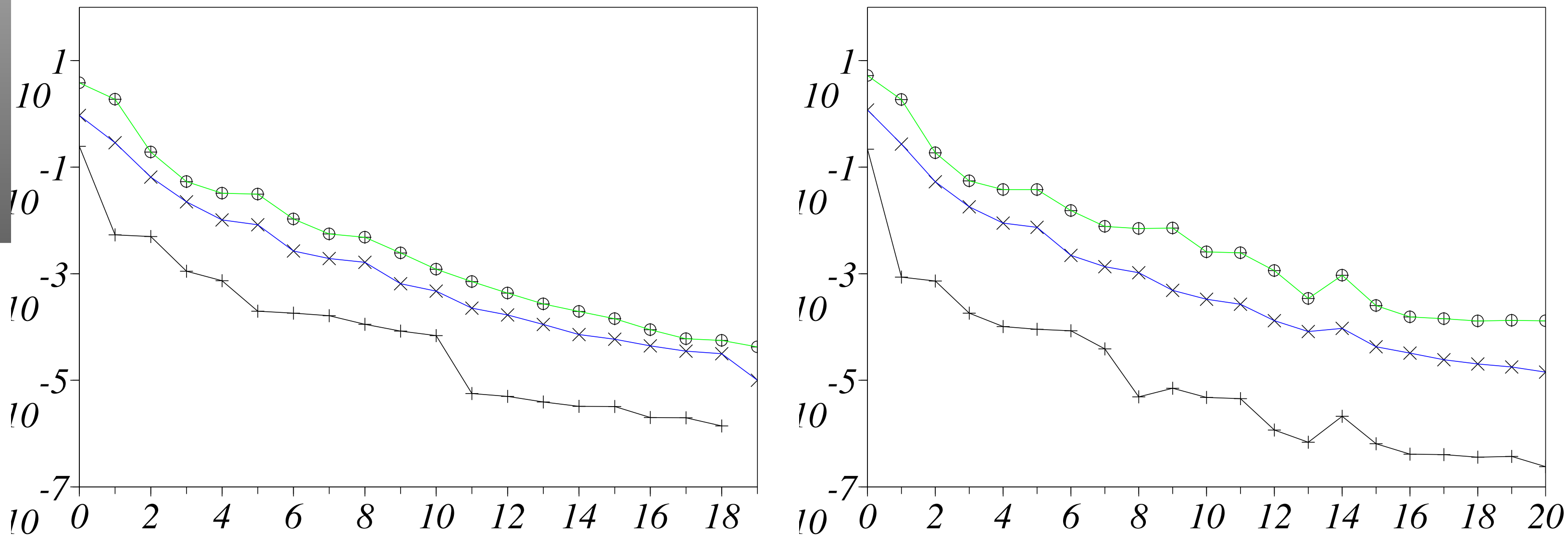
3E Variance reduction and reduced basis method

The parameters λ_n in the offline stage are computed using a greedy algorithm, in order to minimize the variance.

Remark: There exists another version of the algorithm specialized to the case when Z^λ is a function of some solution to a parametrized SDE.

Numerical results for the FENE model, the parameters being the gradient of the velocity field.

3E Variance reduction and reduced basis method



Max, med and min of the variance over the samples, in the offline stage, over $\Lambda_{\rm trial}$ (left) and in the online stage, over Λ (right), as a function of the size of the reduced basis.

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Some references

- BJ, TL, CLB, Numerical analysis of micro-macro simulations of polymeric fluid flows: a simple case, *M3AS*, **12(9)**, 1205–1243, (2002).
- BJ, TL, CLB, Existence of solution for a micro-macro model of polymeric fluid: the FENE model, *Journal of Functional Analysis*, **209**, 162–193, (2004).
- BJ, CLB, TL, On a variance reduction technique for micro-macro simulations of polymeric fluids, *J. Non-Newtonian Fluid Mech.*, **122**, 91–106, (2004).
- BJ, CLB, TL, An elementary argument regarding the long-time behaviour of the solution to a SDE, *Annals of Craiova University*, **32**, 39–47, (2005).
- BJ, CLB, TL, FO, Long-time asymptotics of a multiscale model for polymeric fluid flows, *Archive for Rational Mechanics and Analysis*, **181(1)**, 97–148, (2006).
- DH, TL, New entropy estimates for the Oldroyd-B model, and related models, *Commun. Math. Sci.*, **5(4)**, 909–916 (2007).
- SB, TL, CM, Free-Energy-dissipative schemes for the Oldroyd-B model, *Mathematical Modelling and Numerical Analysis*, **43**, 523–561, (2009).
- SB, TL, A variance reduction method for parametrized stochastic differential equations using the reduced basis paradigm, to appear in *Commun. Math. Sci.*
- CLB, TL, Multiscale modelling of complex fluids: a mathematical initiation, (B. Engquist, P. Lötstedt, O. Runborg, eds.), LNCSE **66**, Springer, 49–138, (2009).