Estimées d'entropie pour des modèles multi-échelles en rhéologie.

[Tony Lelièvre](http://cermics.enpc.fr/~lelievre)

CERMICS, Ecole des Pontes et projet MicMac, INRIA.

`http://cermics.enpc.fr/~lelievre`

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1D Micro-macro models for polymeric fluids

1E Conclusion and discussion

2 Mathematics and numerics

2A Generalities

2B Long-time behaviour

2C Free-energy dissipative schemes for macro models

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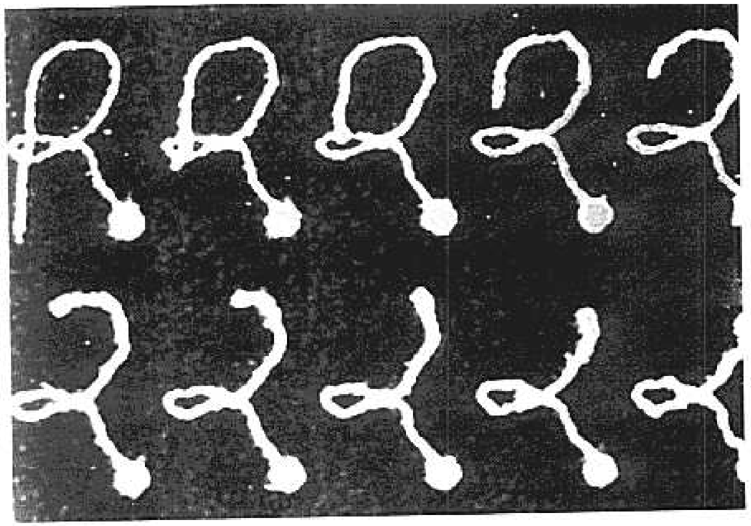
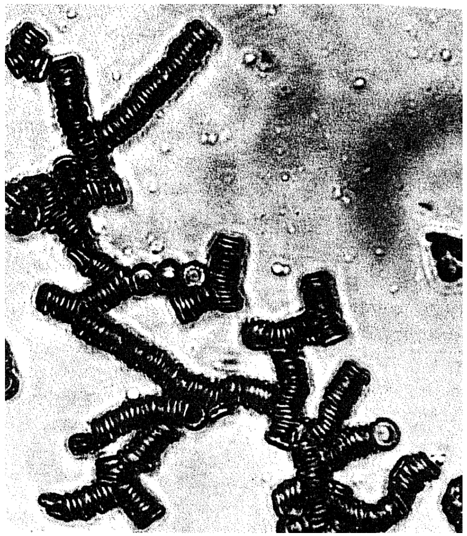
1A Experimental observations

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

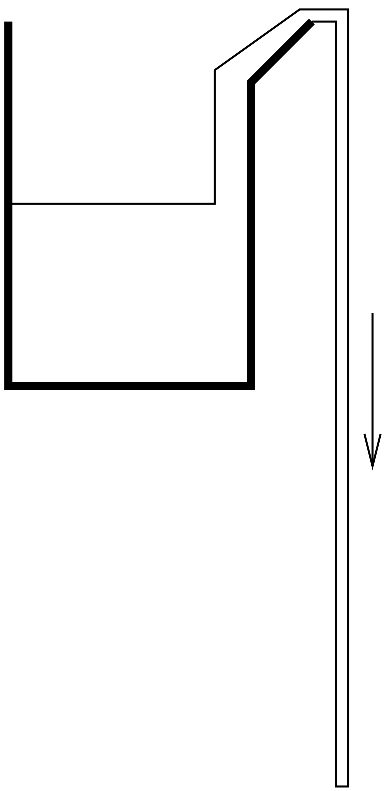
More precisely, we study the case when the microstructures are:

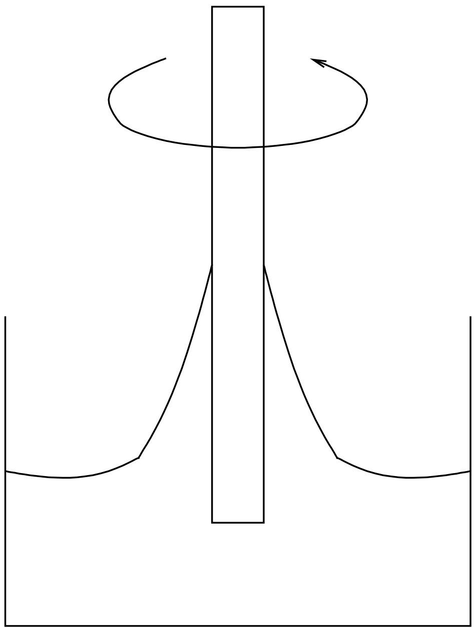
1. very numerous (statistical mechanics),
2. small and light (Brownian effects),
3. within a Newtonian solvent.

A prototypical example is dilute solution of polymers.

1A Experimental observations

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





Outline

Momentum equations (incompressible fluid):

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

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

Newtonian fluids (Navier-Stokes equations):

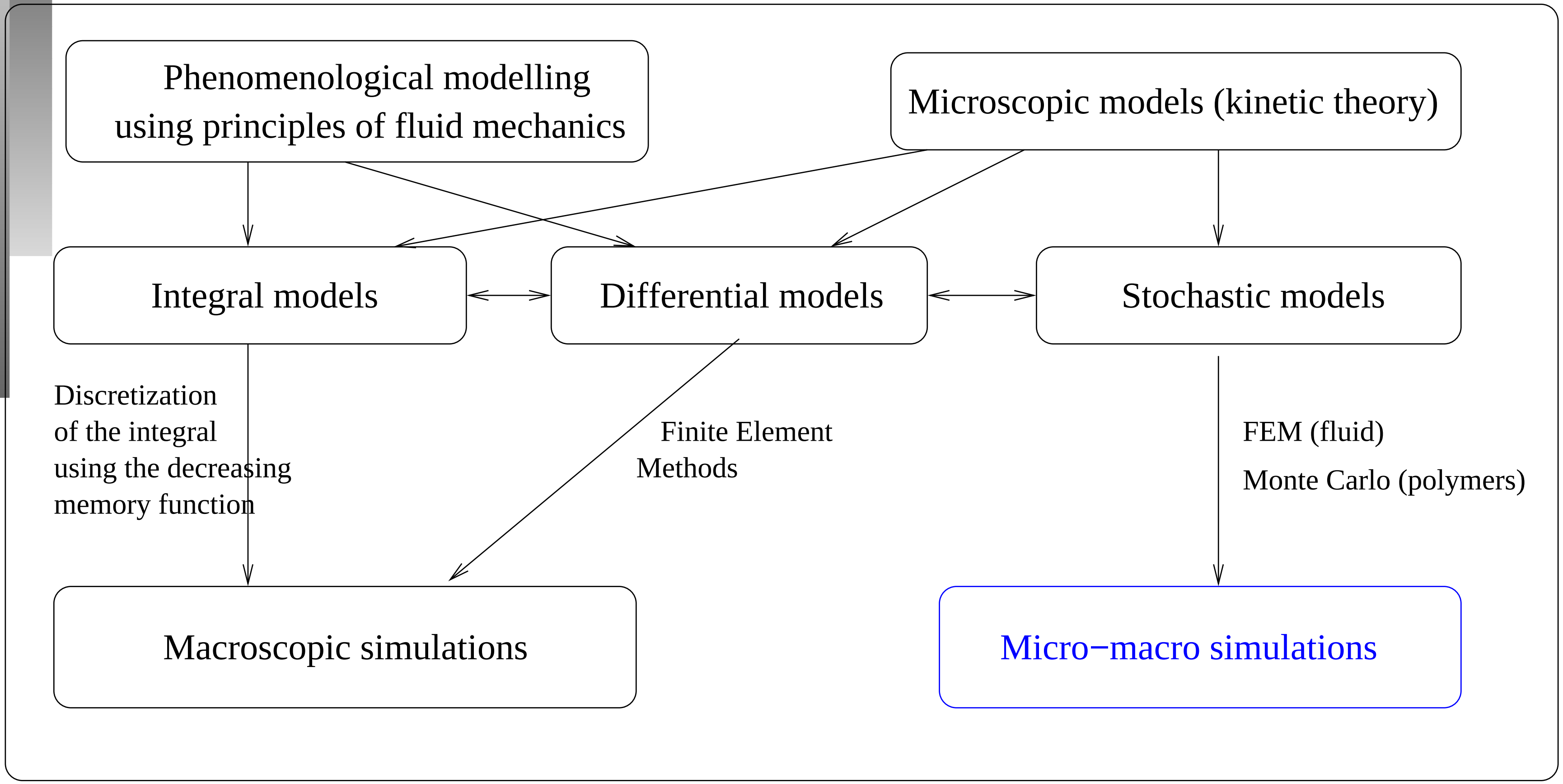
$$\boldsymbol{\sigma} = \eta \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right),$$

Non-Newtonian fluids:

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

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

1B Multiscale modeling

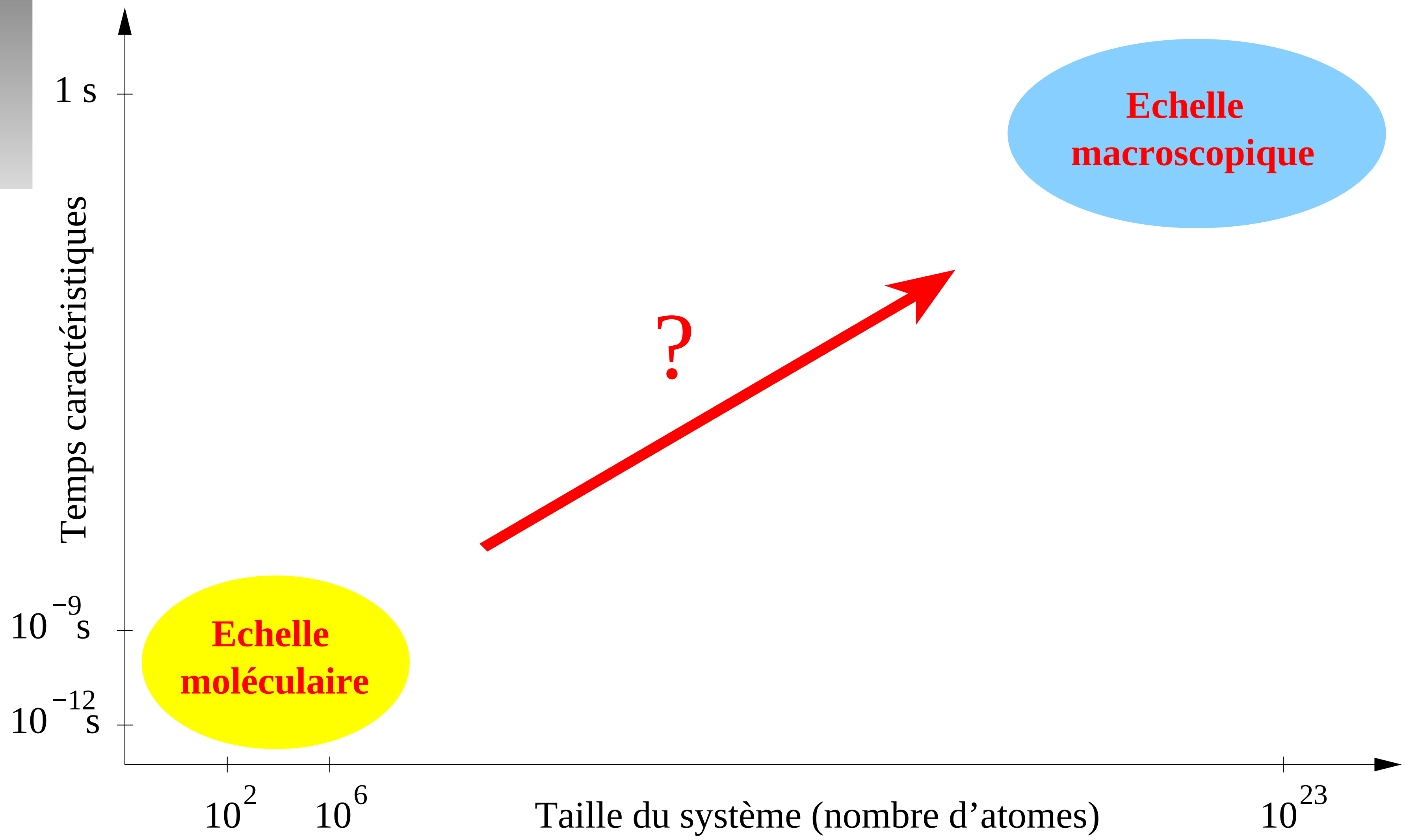


Differential models : $\frac{D\boldsymbol{\tau}}{Dt} = f(\boldsymbol{\tau}, \nabla \mathbf{u}),$

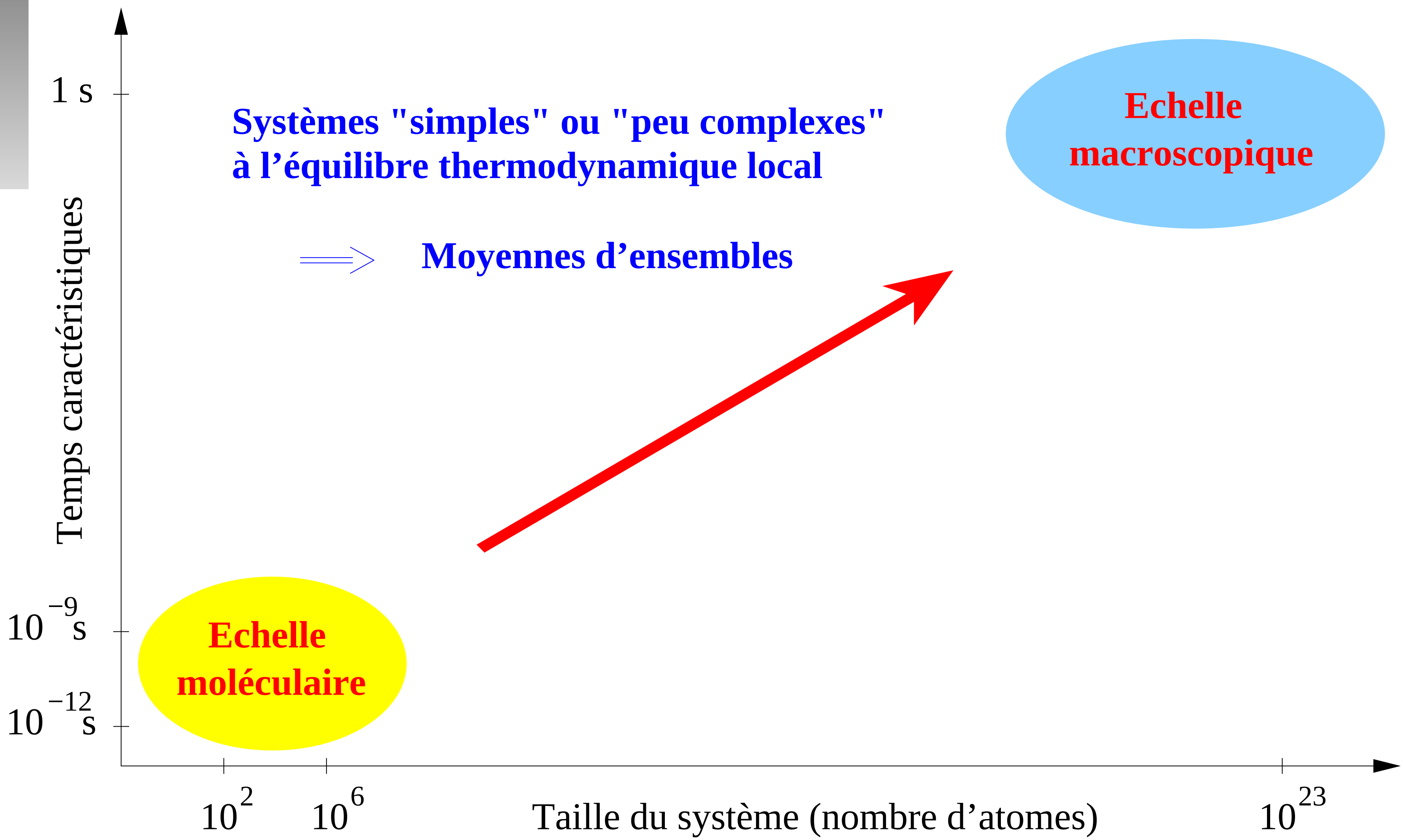
Integral models : $\boldsymbol{\tau} = \int_{-\infty}^{t} m(t-t')\mathbf{S}_t(t')\, dt'.$

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

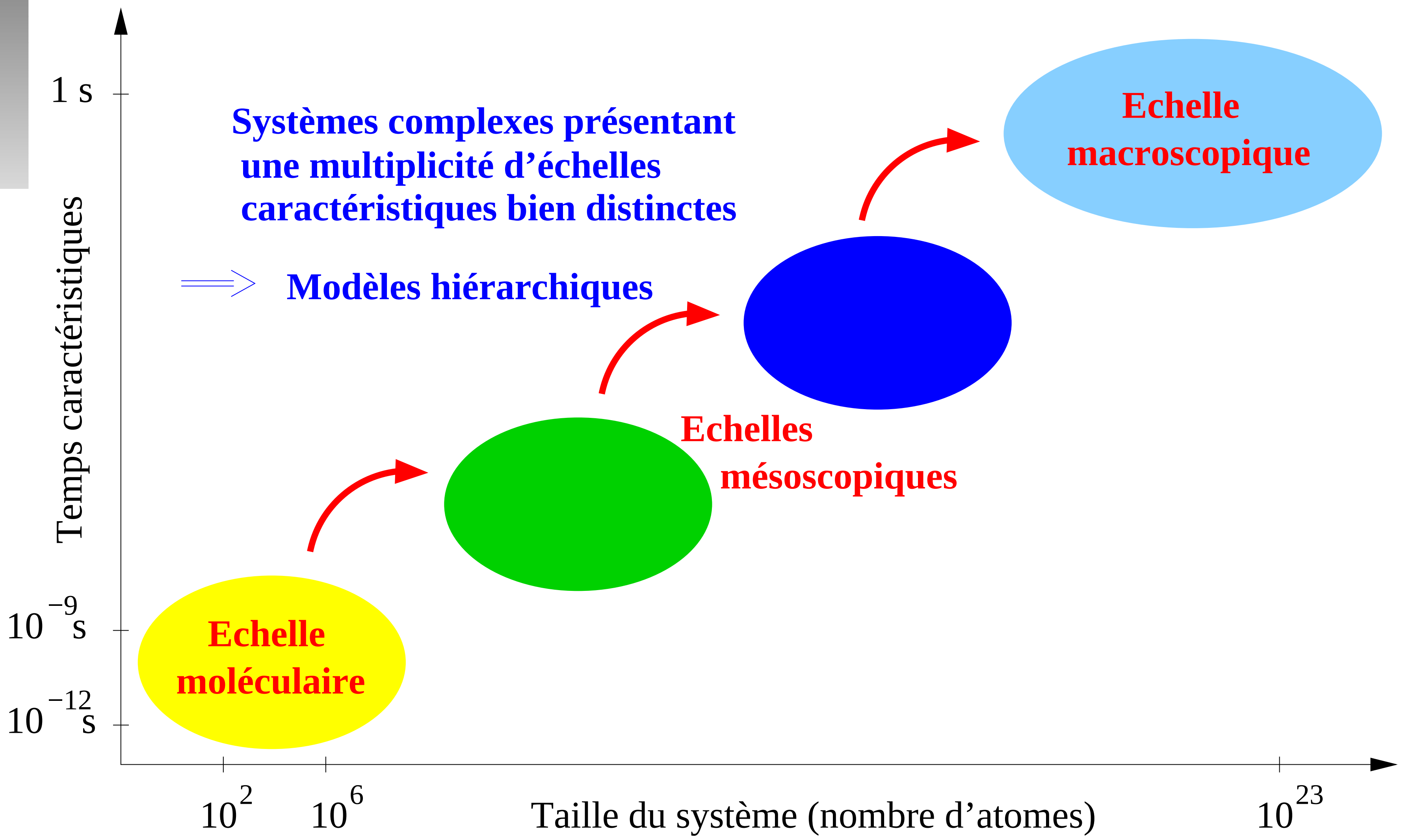
1B Multiscale modeling



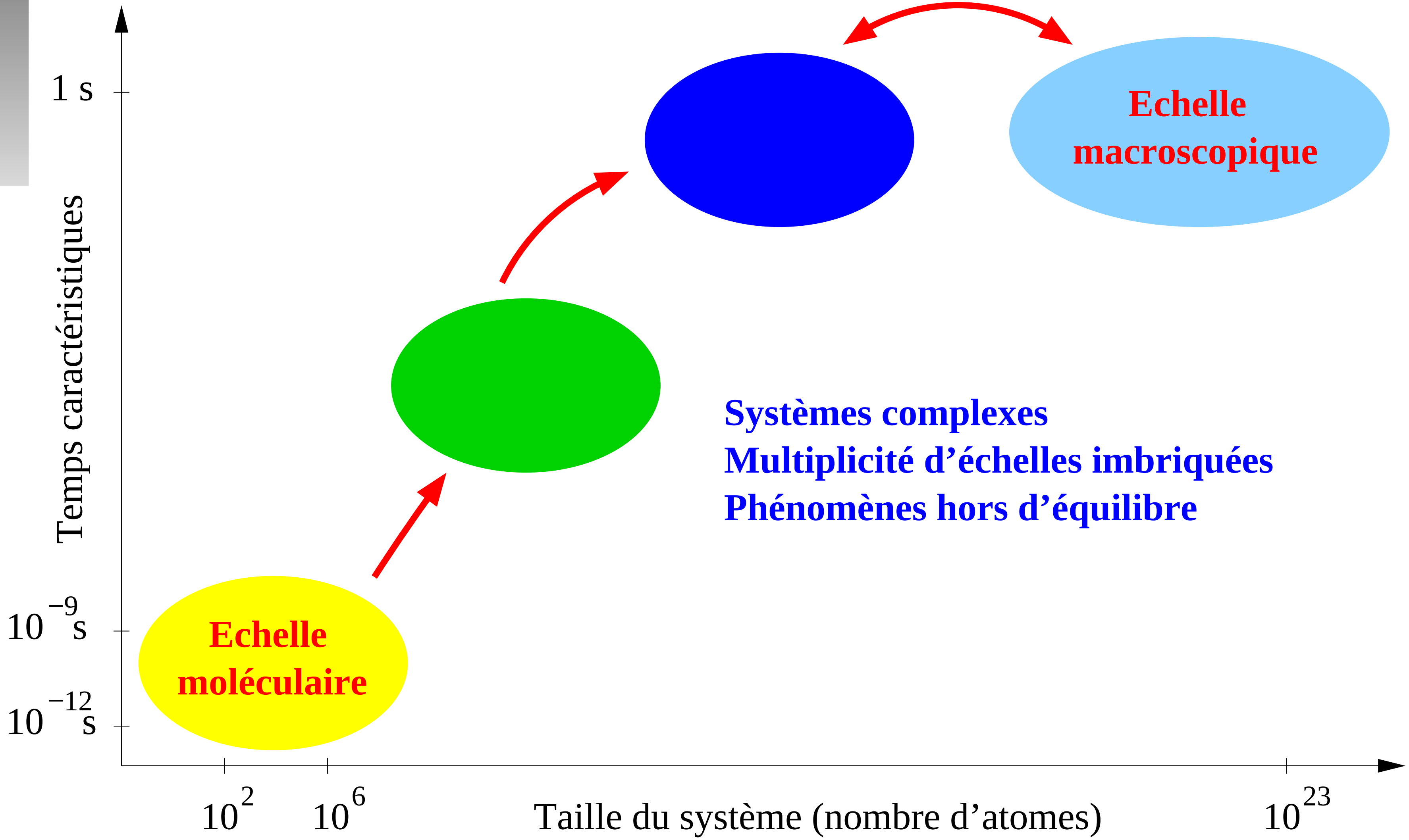
1B Multiscale modeling



1B Multiscale modeling

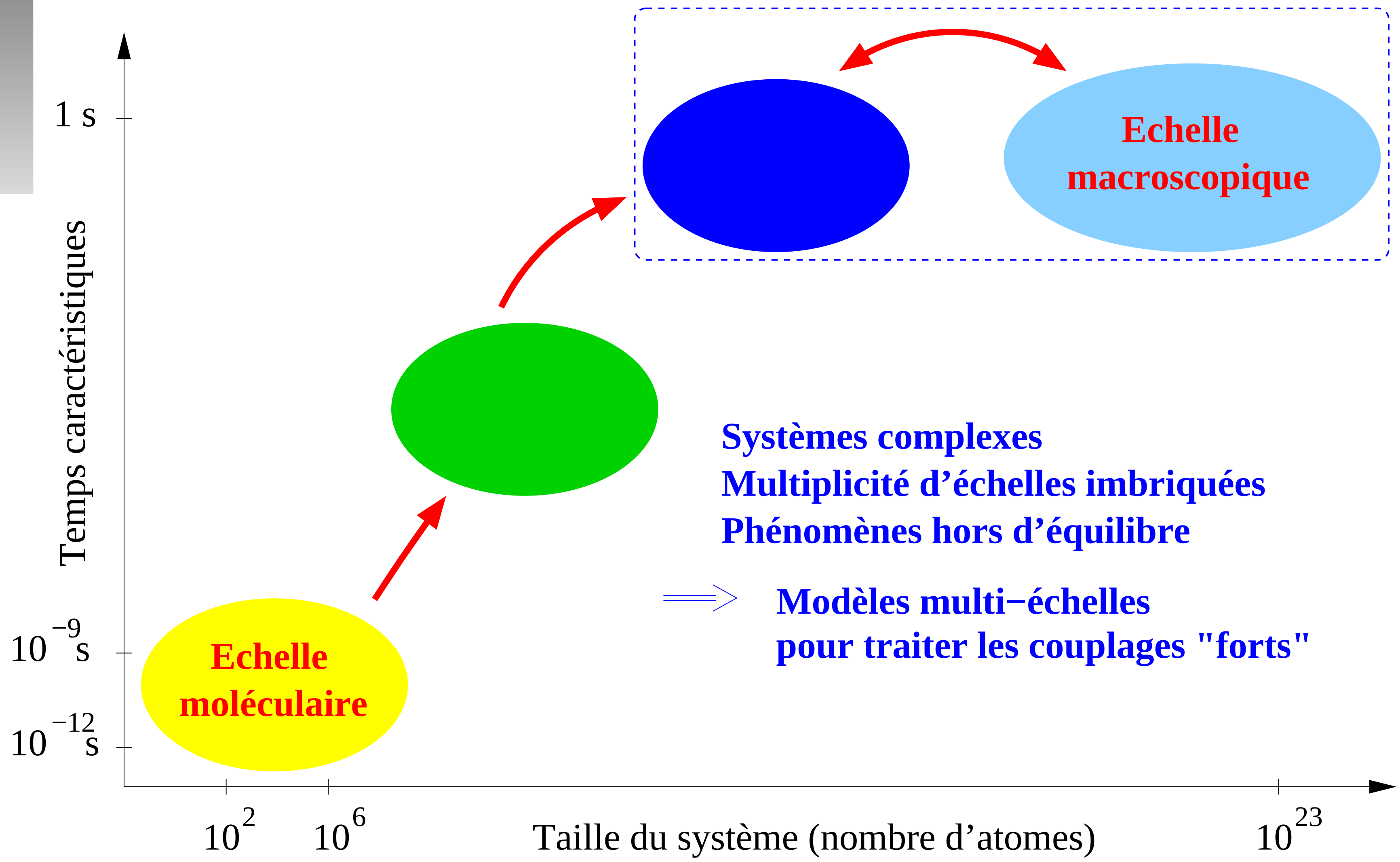


1B Multiscale modeling



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

1B Multiscale modeling



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1C Microscopic models for polymer chains

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

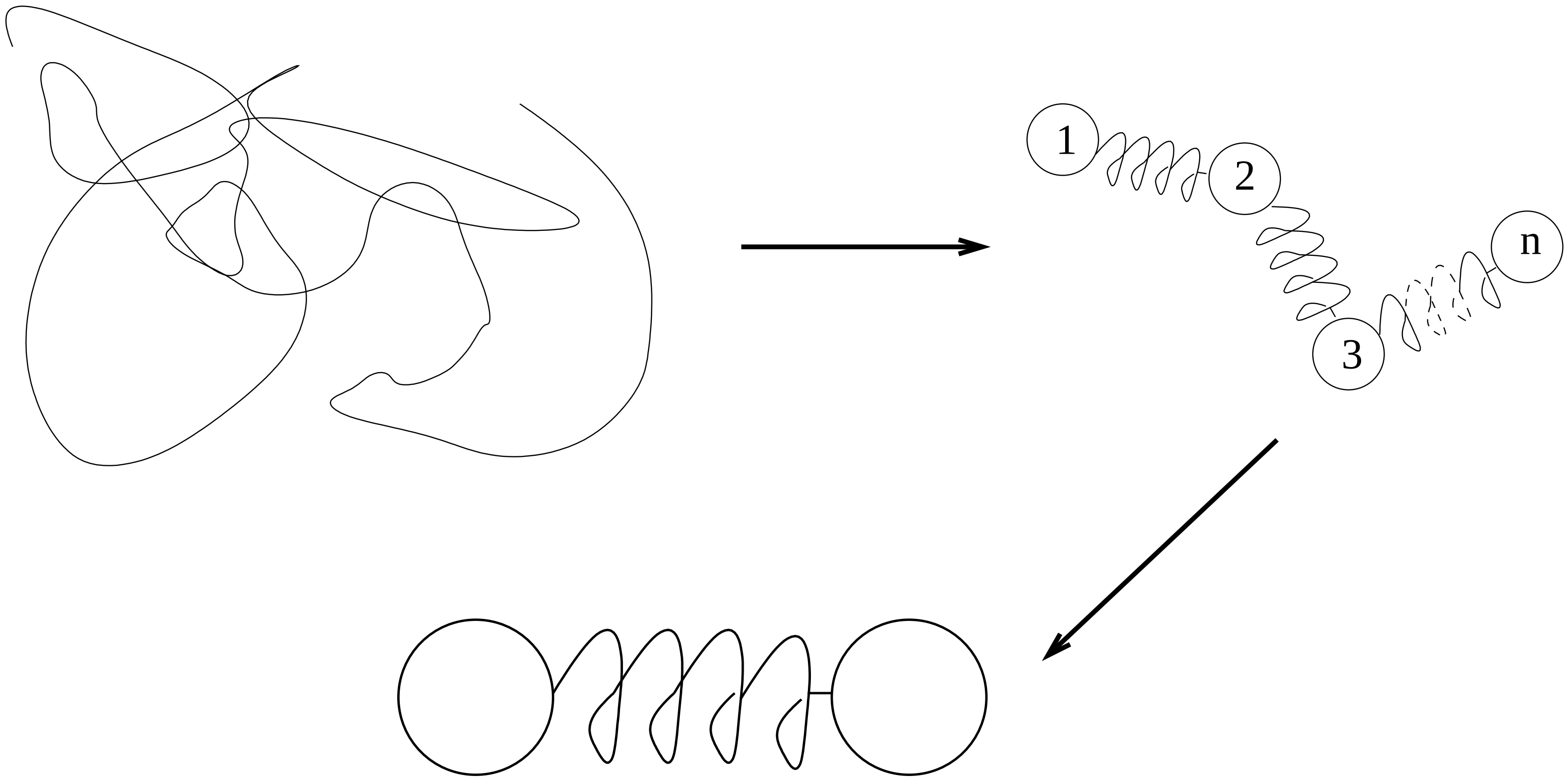
The coupling requires some concepts from statistical mechanics: compute macroscopic quantities (stress, reaction rates, diffusion constants) from microscopic descriptions.

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.

1C Microscopic models for polymer chains

A coarse-grained description: 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”.



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

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

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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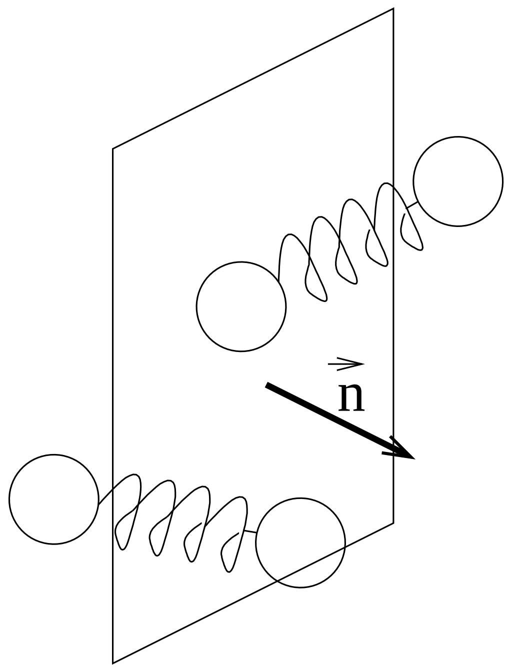
1D Micro-macro models for polymeric fluids

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

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 $\mathbf{X}_t(\boldsymbol{x})$:

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

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:

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

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.

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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.
- 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.

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2A Generalities

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

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

Similar difficulties with macro models (Oldroyd-B):

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

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:

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

one can check that

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

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

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: For numerical counterparts (characteristic method), see Lee, Xu.

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.

Remark: There are global-in-time existence results for other time-derivatives: co-rotational derivative (P.L. Lions, N. Masmoudi): 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 $W(\mathbf{u}) = \dfrac{\nabla \mathbf{u} - \nabla \mathbf{u}^T}{2}$.

$\longrightarrow$ Additional *a priori* estimates based on the fact that $\left(W(\mathbf{u})\boldsymbol{\tau} + \boldsymbol{\tau} W(\mathbf{u})^T\right) : \boldsymbol{\tau} = 0$.

Well-posedness results for micro-macro models:

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

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

2A Generalities

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

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

2A Generalities

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.

The origin of these instabilities is not clearly understood: absence of stationary state / modeling problems / numerical problems ?

Outline

2B 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:

- Starting point: a bad energy estimate.
- Preliminary: the decoupled case.
- The coupled case with $u = 0$ on $\partial\mathcal{D}$.
- The coupled case with $u \neq 0$ on $\partial\mathcal{D}$.

A "bad" energy estimate (recall $\mathbf{F} = \nabla \Pi$):

$$(1) \quad \frac{\mathrm{Re}}{2} \int_{\mathcal{D}} \|\mathbf{u}\|^2 + (1-\epsilon) \int_0^t \int_{\mathcal{D}} \|\nabla \mathbf{u}\|^2 = \frac{\mathrm{Re}}{2} \int_{\mathcal{D}} \|\mathbf{u}_0\|^2 - \frac{\epsilon}{\mathrm{We}} \int_0^t \int_{\mathcal{D}} \mathbf{E}(\mathbf{X}_s \otimes \mathbf{F}(\mathbf{X}_s)) : \nabla \mathbf{u}.$$

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

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

2B Long-time behaviour: decoupled case

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

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

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

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

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

2B Long-time behaviour: decoupled case

Differentiating H w.r.t. t, one obtains (using only 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,

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

2B Long-time behaviour: decoupled case

Example 1: If $h(x) = (x-1)^2$, one needs a Poincaré inequality: $\forall \psi$ pdf,

$$\int \left| \frac{\psi}{\psi_\infty} - 1 \right|^2 \psi_\infty \leq C \int \left| \nabla \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi_\infty.$$

$\longrightarrow$ Convergence of ψ/ψ_∞ in L^2-norm.

Example 2: If $h(x) = x\ln(x) - x + 1$, one needs a logarithmic-Sobolev inequality: $\forall \psi$ pdf,

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

$\longrightarrow$ Convergence of ψ/ψ_∞ in $L^1 \ln(L^1)$-norm.

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

2B Long-time behaviour: decoupled case

The case $\boldsymbol{\kappa} = 0$:
Then, we have $\psi_\infty \propto \exp(-\Pi)$. It is known that if Π is α-convex, then the functional inequality holds (Bakry-Emery criterion):

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

for all p.d.f. ϕ, with

$$C = \frac{1}{2\alpha}.$$

The case $\boldsymbol{\kappa} \neq 0$:
If $\boldsymbol{\kappa}$ is skew-symmetric, $\psi_\infty \propto \exp(-\Pi)$ is again a stationary solution so that, by using the LSI inequality w.r.t. ψ_∞, $H(t) \le H(0)\exp(-t/2C)$.

2B Long-time behaviour: decoupled case

To treat other cases, we need the perturbation result (Holley-Stroock): Suppose that

(i) a LSI holds for $\psi_\infty \propto \exp(-\Pi)$,

(ii) $\tilde{\Pi}$ is a bounded function,

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

Remarks:

- The same result holds for PI (and actually for any h).
- (ii) $\iff 0 < c \leq \dfrac{\psi_\infty}{\widetilde{\psi_\infty}} \leq C < \infty.$

2B Long-time behaviour: decoupled case

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

2B Long-time behaviour: coupled case

The Fokker-Planck version of the coupled system is:

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

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

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

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

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

2B Long-time behaviour: coupled case

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

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

2B Long-time behaviour: coupled case

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

2B Long-time behaviour: coupled case

Moreover, using the following inequalities:

- Poincaré inequality:

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

- Sobolev logarithmic inequality for ψ_∞ (recall Π is α-convex):

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

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 $t \to \infty$.

2B Long-time behaviour: coupled case

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 $= 1/2$, 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 (almost necessary !) condition to have exponential decay:
$h'(x) - h(x)/x = 0$ *i.e.* $h(x) = x\ln(x)$.

2B Long-time behaviour: coupled case

Let us now consider the case $\mathbf{u} \neq 0$ on $\partial\mathcal{D}$ (time-independant Dirichlet BC). 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).

2B Long-time behaviour: coupled case

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

$$\frac{d}{dt}\left(\frac{1}{2}\int_{\mathcal{D}}|\overline{\mathbf{u}}|^2+\int_{\mathcal{D}}\int_{\mathbb{R}^d}\psi\ln\left(\frac{\psi}{\psi_\infty}\right)\right)$$

$$= -\int_{\mathcal{D}}|\nabla\overline{\mathbf{u}}|^2-\frac{1}{2}\int_{\mathcal{D}}\int_{\mathbb{R}^d}\psi\left|\nabla_{\mathbf{X}}\ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2$$

$$-\int_{\mathcal{D}}\overline{\mathbf{u}}.\nabla\mathbf{u}_\infty\overline{\mathbf{u}}-\int_{\mathcal{D}}\int_{\mathbb{R}^d}\overline{\mathbf{u}}.\nabla_{\boldsymbol{x}}(\ln\psi_\infty)\overline{\psi}$$

$$-\int_{\mathcal{D}}\int_{\mathbb{R}^d}\left(\nabla_{\mathbf{X}}(\ln\psi_\infty)+\nabla\Pi(\mathbf{X})\right).\nabla\overline{\mathbf{u}}\mathbf{X}\,\overline{\psi},$$

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_∞.

2B Long-time behaviour: coupled case

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

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

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

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

2B Long-time behaviour: coupled case

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 Holley-Stroock.

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

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

2B Long-time behaviour: coupled case

Then, for FENE dumbbells:

Theorem 1 *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 of Holley-Stroock.

2B Long-time behaviour: coupled case

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:

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

2B Long-time behaviour: coupled case

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

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

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

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

2B Long-time behaviour: coupled case

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

Theorem 2 *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_∞.

2B Long-time behaviour: coupled case

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 ? (Simple coupling arguments work only in very specific cases)

Outline

2C Free-energy dissipative schemes for macro models

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

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

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

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

2C Free-energy dissipative schemes 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

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

2C Free-energy dissipative schemes for macro models

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

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

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

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

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

2C Free-energy dissipative schemes for macro models

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

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

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

we have...

2C Free-energy dissipative schemes for macro models

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

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

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

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

2C Free-energy dissipative schemes for macro models

The interest of this remark is twofold:

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

2C Free-energy dissipative schemes for macro models

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

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

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

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

2C 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

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

where

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

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

2C 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...

2C 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:

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

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

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

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

2C 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 $(\boldsymbol{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n)$ $\forall n \geq 0$.

2C Free-energy dissipative schemes for macro models

Key ingredients for the proof:

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

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

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

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

2C 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:

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

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

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

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

2C Free-energy dissipative schemes for macro models

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

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

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

2C Free-energy dissipative schemes for macro models

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

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

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

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

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

2C 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 ?

Perspectives and work in progress

- Analyze the long-time behaviour for rigid polymers (much richer dynamical behaviour, with time-periodic solutions).

$$dX_t = P(X_t)(\kappa X_t - \mathbb{E}(X_t \otimes X_t)X_t)\,dt + \sqrt{2}P(X_t) \circ dB_t$$

where $P(X) = \mathrm{Id} - \frac{X \otimes X}{\|X\|^2}$.

Doi closure:

$$\begin{aligned} dX_t &= (\kappa X_t - \mathbb{E}(X_t \otimes X_t)X_t)\ dt \\ &\quad - \frac{1}{\mathbb{E}(\|X_t\|^2)} (\kappa : \mathbb{E}(X_t \otimes X_t)\, X_t - \mathbb{E}(X_t \otimes X_t) : \mathbb{E}(X_t \otimes X_t)\, X_t)\ dt \\ &\quad + \sqrt{2} dB_t - n \frac{X_t}{\mathbb{E}(\|X_t\|^2)}\, dt. \end{aligned}$$

Perspectives and work in progress

- General analysis of the long-time behaviour of a Fokker-Planck equation

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

by using Helmholtz decomposition of b.

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