Mathematical and numerical analysis of micro-macro models for polymeric fluids

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Outline

1. The physical model,
2. Numerical method and mathematical questions,
3. Sense and existence of solutions,
4. Convergence of the numerical scheme,
5. Dependency of the Brownian on the space variable,
6. Longtime behaviour: some remarks.

1 The physical model

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*.

1 The physical model

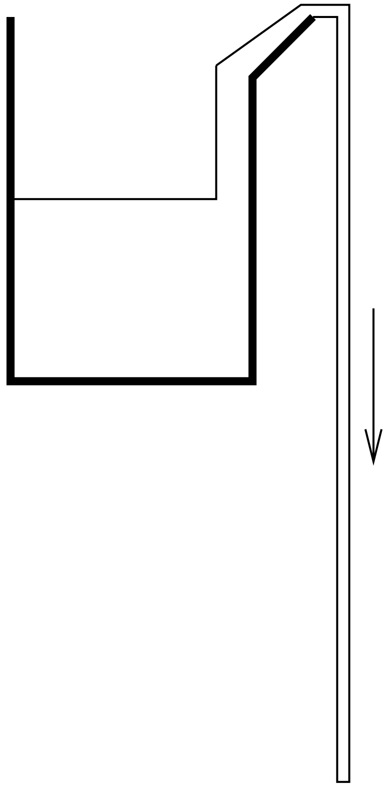
Polymeric liquids have non-Newtonian properties:

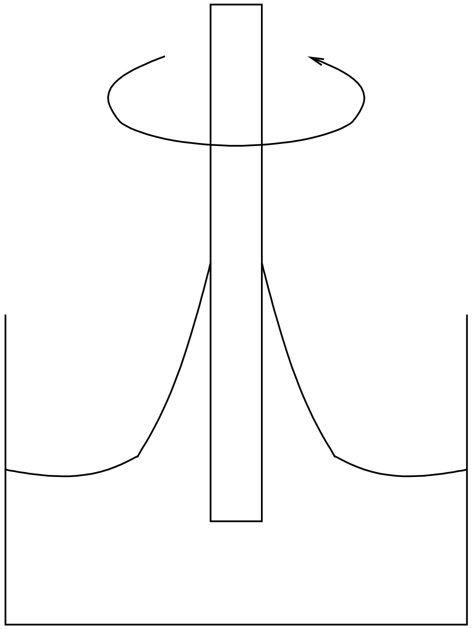
- Shear-rate dependent viscosity,
- Normal stresses in shear flows,
- Memory effects.

We are interested in models based on the modelling of the influence of the microstructures on the rheology of the fluid.

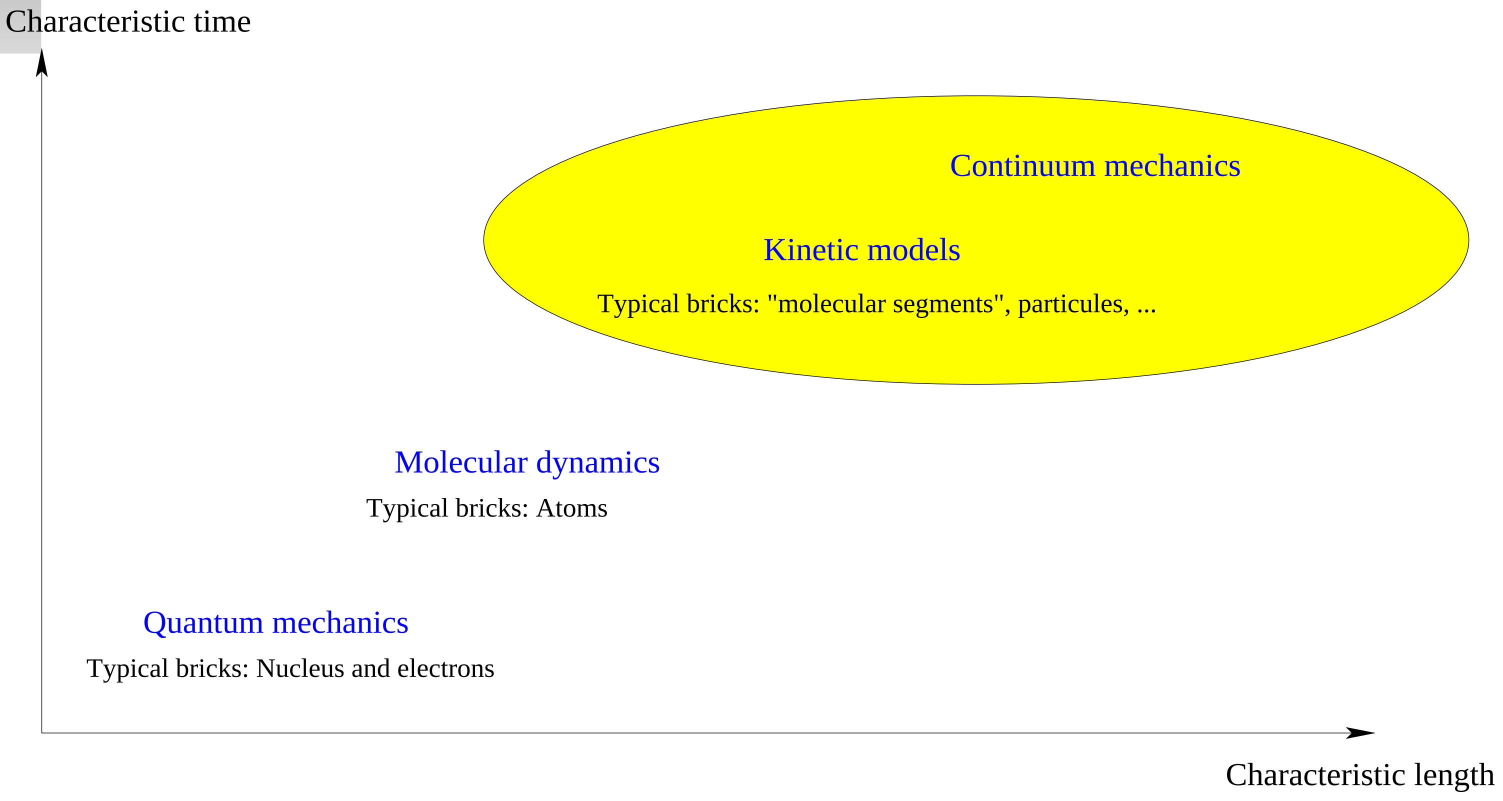
1 The physical model

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

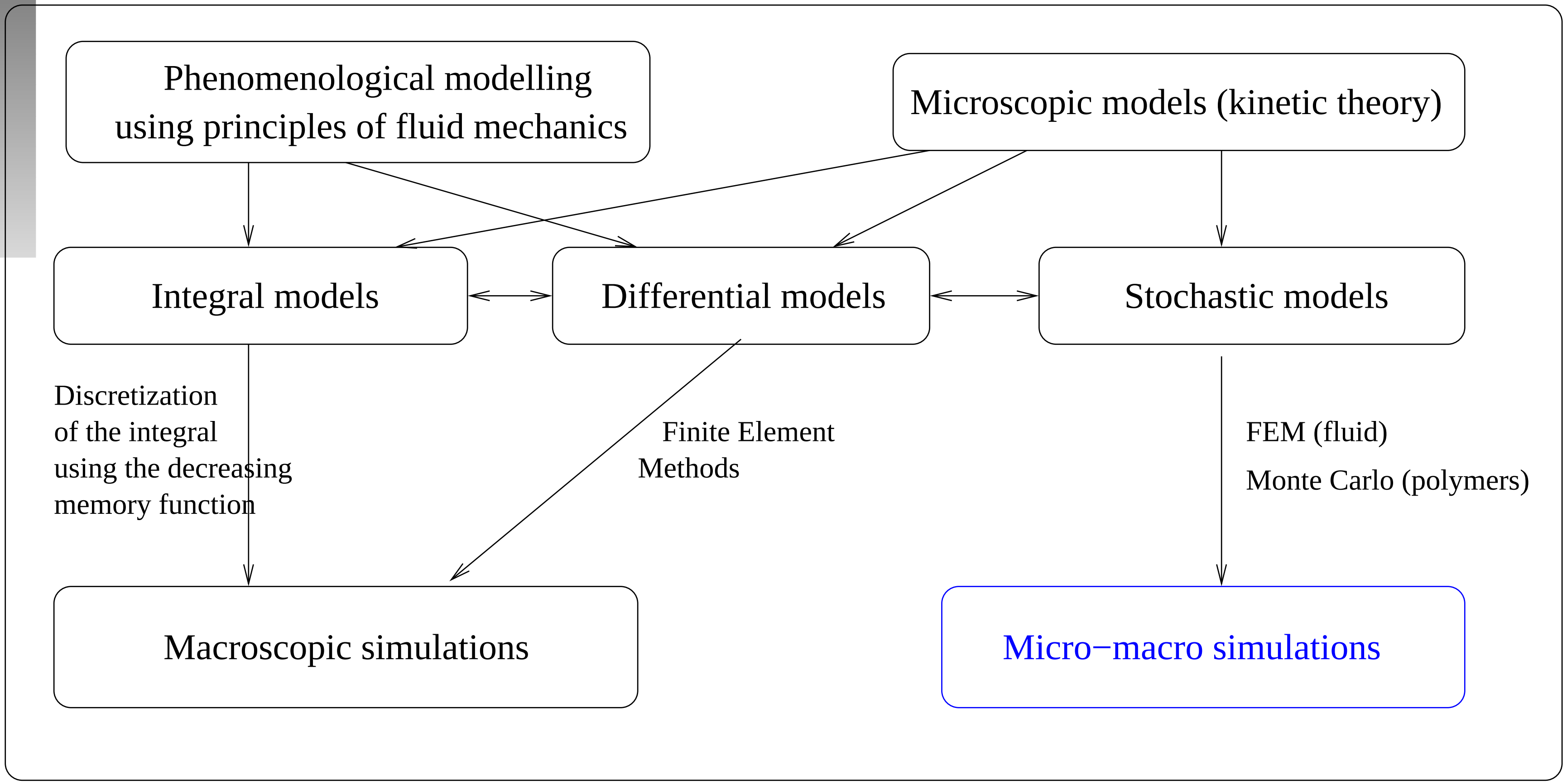




Micro-macro modelling domain:



1 The physical model



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.)

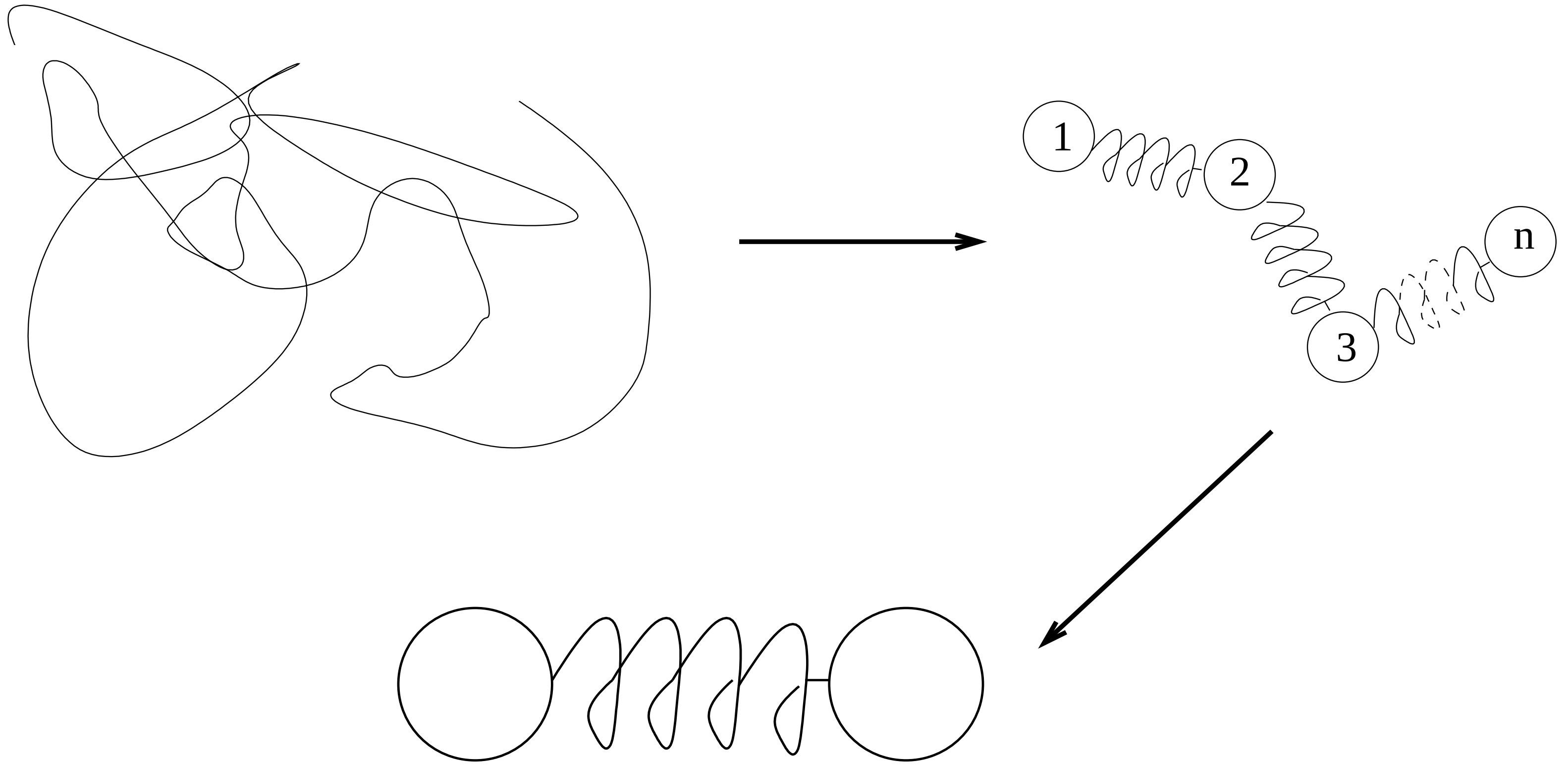
1 The physical model

Mesoscopic approach. It is based upon kinetic theory. The basic model is the Rouse model.

(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)



1 The physical model

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 $(\mathbf{X} = (\mathbf{X}^2 - \mathbf{X}^1))$:

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

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

1 The physical model

- "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 $\mathbf{R}_t = \frac{1}{2}\left(\mathbf{X}_t^1 + \mathbf{X}_t^2\right)$.

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 $\mathbf{R}_t$ is zero.

1 The physical model

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

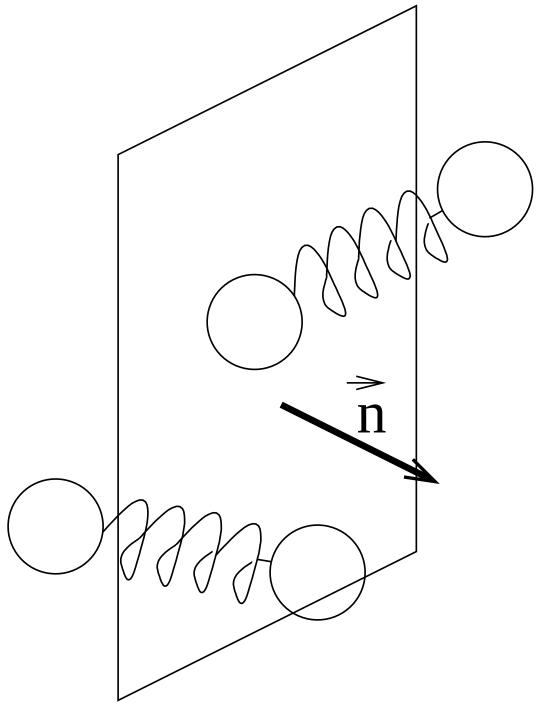
$$\begin{cases} d\mathbf{X}_t = \nabla \mathbf{u}(t, \boldsymbol{R}_t)\mathbf{X}_t \, dt - \dfrac{2}{\zeta}\mathbf{F}(\mathbf{X}_t) \, dt + \sqrt{\dfrac{4kT}{\zeta}} d\mathbf{W}_t, \\ d\boldsymbol{R}_t = \mathbf{u}(t, \boldsymbol{R}_t) \, dt. \end{cases}$$

Eulerian version:

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

1 The physical model

The stress tensor is then computed using Kramers expression:



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

1 The physical model

This yields the following system:

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

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

1 The physical model

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

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

and then:

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

Once non-dimensionalized, we obtain, for the Hookean dumbbell model:

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

with the following non-dimensional numbers:

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

and $\lambda = \frac{\zeta}{4H}$: a relaxation time of the polymers,
$\eta_p = n_p k T \lambda$: the viscosity associated to the polymers,

U and L: characteristic velocity and length.

1 The physical model

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.

2 Numerical method and mathematical questions

The main difficulties: transport and coupling.

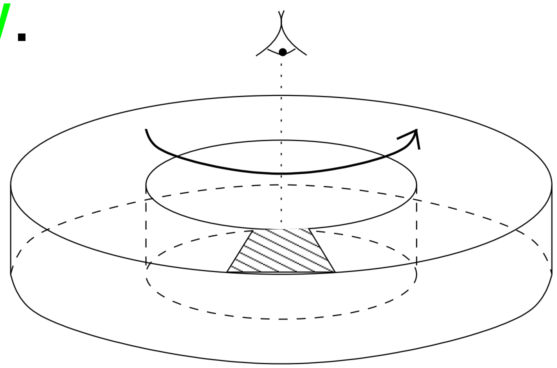
$$\begin{cases} \mathrm{Re}\left(\dfrac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = (1-\epsilon)\Delta\mathbf{u} - \nabla p + \mathrm{div}\,(\boldsymbol{\tau})\,, \\ \mathrm{div}\,(\mathbf{u}) = 0\,, \\ \boldsymbol{\tau} = \dfrac{\epsilon}{\mathrm{We}}(\mu\mathbf{E}(\mathbf{X}\otimes\mathbf{F}(\mathbf{X}))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

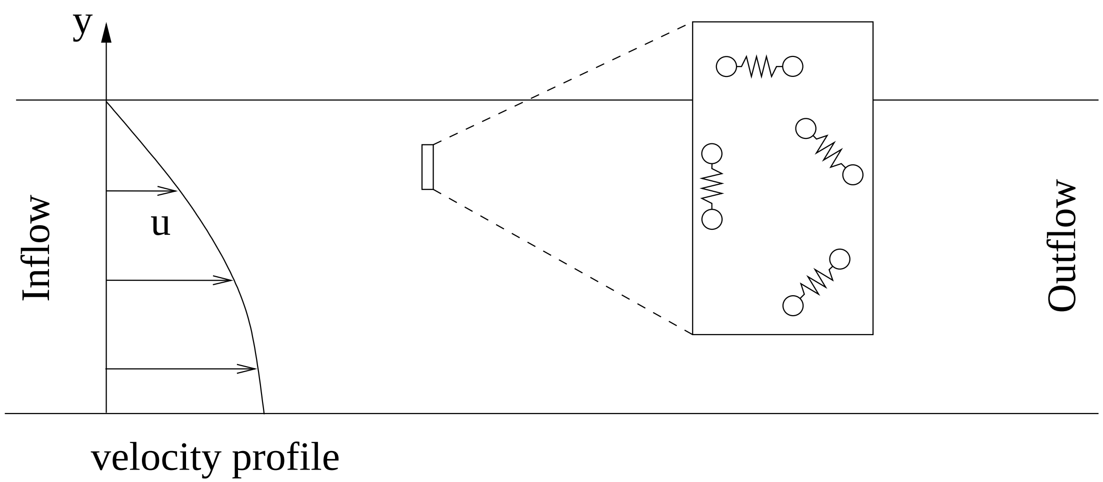
If $\mathbf{F}(\mathbf{X}) = \mathbf{X}$, we have equivalently (Oldroyd-B):

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

2 Numerical method and mathematical questions

In the following, we will especially consider the case of a plane shear flow.





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

2 Numerical method and mathematical questions

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

2 Numerical method and mathematical questions

Numerical analysis in fluid mechanics

Numerical analysis of SDEs

The problem

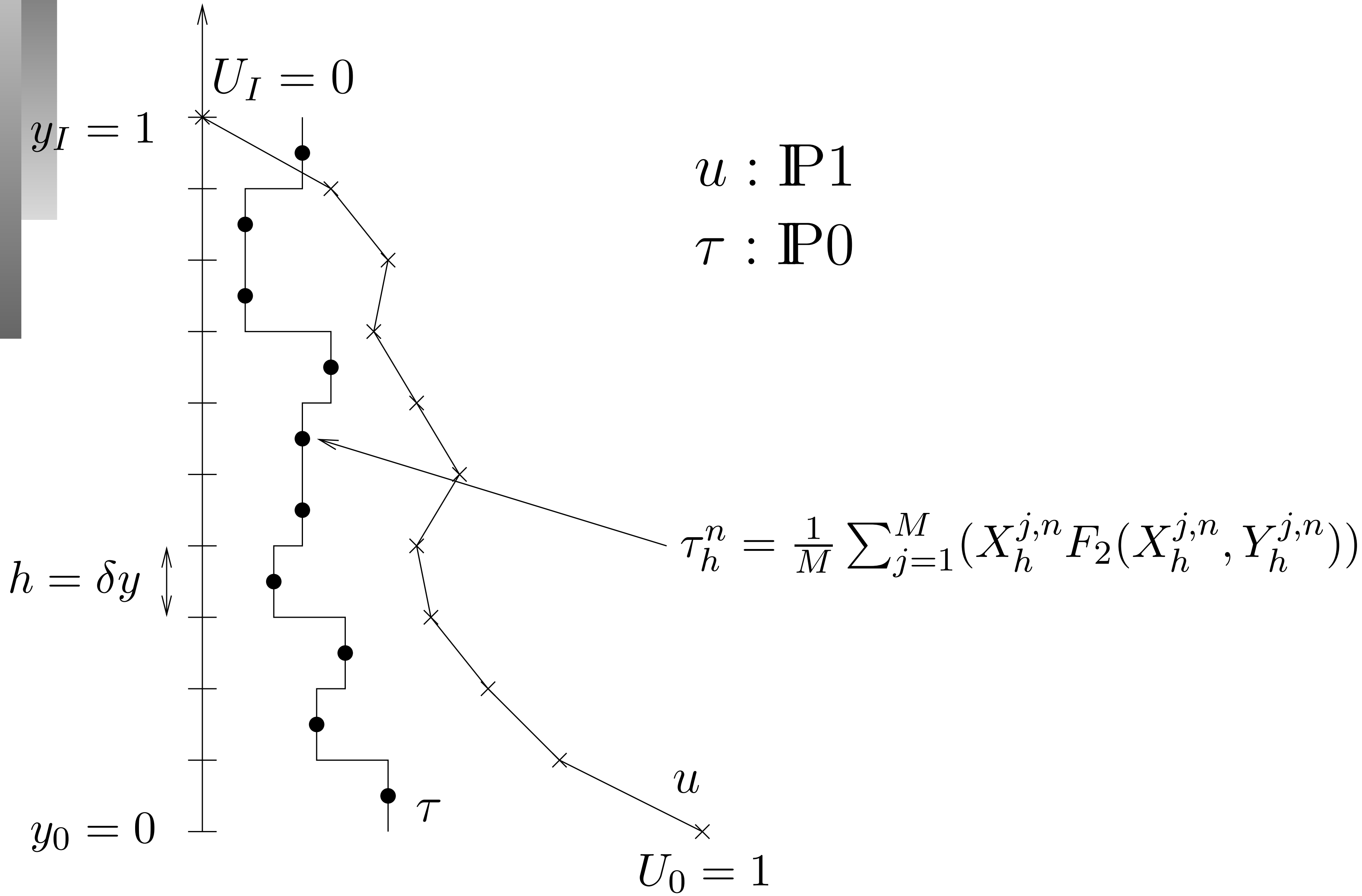
Discretization in space : convergence of finite element approximations for solutions of PDEs : $O(\delta y)$.

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

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

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

2 Numerical method and mathematical questions

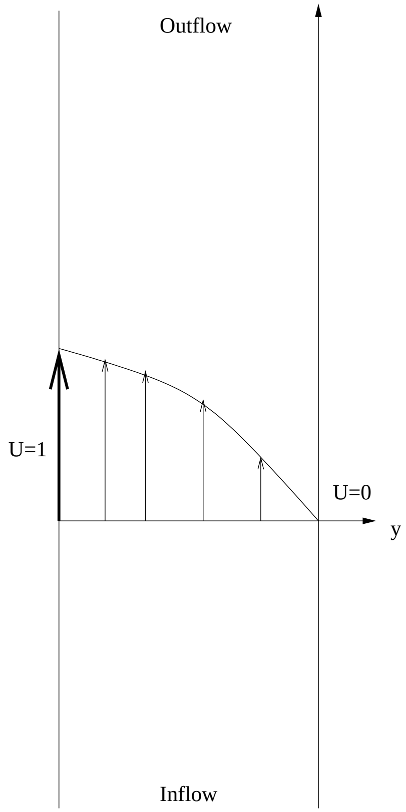


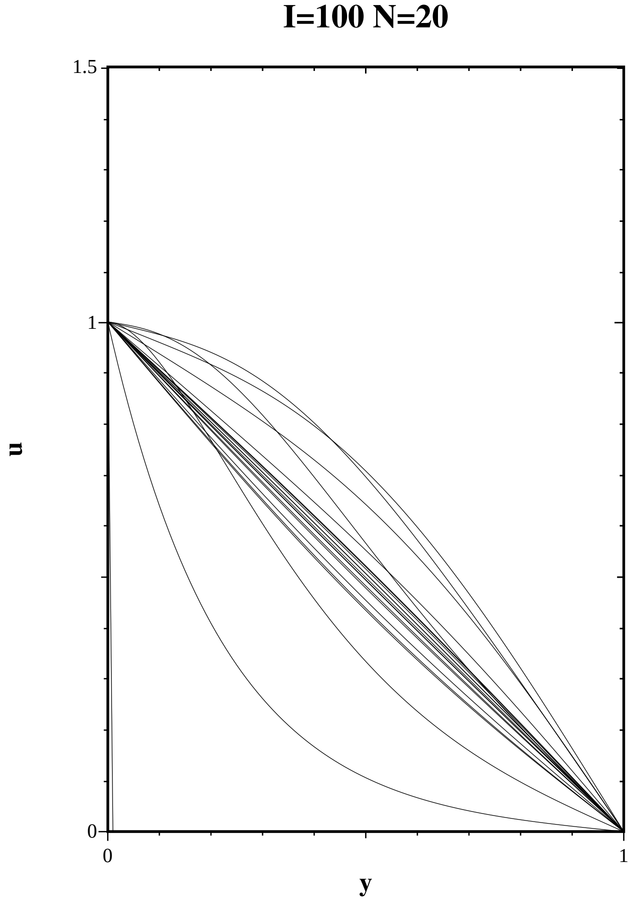
$u : \mathbb{P}1$

$\tau : \mathbb{P}0$

2 Numerical method and mathematical questions

Numerical results





Velocity profile as time evolves.

2 Numerical method and mathematical questions

Mathematical and numerical questions:

- Sense and existence of solutions

  Hookean dumbbell : B. Jourdain, TL, C. Le Bris, M^3AS, 2002.

  FENE dumbbell : B. Jourdain, TL, C. Le Bris, JFA, 2003 / B. Jourdain, TL, About the FENE SDE / M. Renardy SIAM J. Math, 1997.

  Advective term in the SDE : C. Le Bris, P.L. Lions, Annali di Matematica pura ed applicata, 2004.

- Convergence of numerical methods

  Numerical analysis of the Hookean dumbbell model : B. Jourdain, TL, C. Le Bris, M^3AS, 2002 / TL, Computers and Fluids, 2003.

  The FENE-P model : B. Jourdain, TL, 2004.

- Analysis and improvement of these methods

  Variance reduction methods : B. Jourdain, TL, C. Le Bris, JNNFM, 2004 / J. Bonvin and M. Picasso, JNNFM, 1999.

3 Sense and existence of solutions

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

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}).

3 Sense and existence of solutions

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

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

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

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

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

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

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

3 Sense and existence of solutions

The Hookean dumbbell case: $\mathbf{F}(\mathbf{X}) = \mathbf{X}$

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

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.

3 Sense and existence of solutions: 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 $Y_t = Y_0\, e^{-t/2} + \int_0^t e^{\frac{s-t}{2}} dW_s$.

3 Sense and existence of solutions: Hookean

Theorem 1 *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).
In addition, the following estimate holds:

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

Remarks:

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

3 Sense and existence of solutions: Hookean

Sketch of the proof

- *a priori* estimate,

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

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

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

3 Sense and existence of solutions: 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.

3 Sense and existence of solutions: FENE

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

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

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.

3 Sense and existence of solutions: FENE

Two remarks:

- The global *a priori* estimate $u \in L_t^\infty(L_y^2) \cap L_t^2(H_{0,y}^1)$ is not sufficient to pass to the limit in the nonlinear term $\partial_y u \, Y_t^y$,
- What is the regularity of τ in function of the regularity of $\partial_y u$?

3 Sense and existence of solutions: FENE

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

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

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

3 Sense and existence of solutions: FENE

Theorem 2 *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* / $\mathcal{F}_t^{V,W}$.

3 Sense and existence of solutions: 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

$$\begin{cases} dX^g_t = \left(-\frac{1}{2} \frac{X^g_t}{1 - \frac{(X^g_t)^2 + (Y^g_t)^2}{b}} + g(t)\, Y^g_t \right) dt + dV_t, \\ dY^g_t = \left(-\frac{1}{2} \frac{Y^g_t}{1 - \frac{(X^g_t)^2 + (Y^g_t)^2}{b}} \right) dt + dW_t, \end{cases}$$

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 derives from a convex potential Π.

3 Sense and existence of solutions: 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.

3 Sense and existence of solutions: FENE

Regularity of τ in space

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

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

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

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

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

3 Sense and existence of solutions: 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 et $\mathbf{E}\left(\left(\frac{1}{X_0^2+Y_0^2} \right)^{\frac{q}{q-1}} \right)$.

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

3 Sense and existence of solutions: FENE

Back to the coupled problem

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

$$||u||_{L_t^\infty(L_y^2)} + ||\partial_y u||_{L_t^2(L_y^2)} + ||\Pi(X,Y)||_{L_t^\infty(L_y^1(L_\omega^1))}$$
$$+||\Upsilon(X,Y)||_{L_t^2(L_y^2(L_\omega^2))} \leq C(T, ||u_0||_{L_y^2}, ||f_{ext}||_{L_t^1(L_y^2)})$$

where Π is a potential from which derives 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

$$||u||_{L_t^\infty(H_y^1)} + ||u||_{L_t^2(H_y^2)} \leq C(||\partial_y u_0||_{L_y^2}, ||f_{ext}||_{L_t^2(L_y^2)}).$$

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

3 Sense and existence of solutions: 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.

4 Convergence of the numerical scheme

For Hookean dumbbell: $\mathbf{F}(\mathbf{X}) = \mathbf{X}$

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.

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

Difficulties:

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

4 Convergence of the numerical scheme

Theorem 3 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 $V_h = \mathbf{P}1$): $\forall n < \frac{T}{\delta t}$,

$$\left\| u(t_n) - \overline{u}_h^n \right\|_{L^2_y(L^2_\omega)} + \left\| \mathbf{E}(X_{t_n} Y_{t_n}) - \frac{1}{M} \sum_{j=1}^{M} \overline{X}_{h,n}^j \overline{Y}_n^j \right\|_{L^1_y(L^1_\omega)}$$

$$\leq C \left(\delta y + \delta t + \frac{1}{\sqrt{M}} \right),$$

4 Convergence of the numerical scheme

Sketch of the proof

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

Main difficulty in the stability proof: we need that $\delta t \frac{1}{M} \sum_{j=1}^{M} (\overline{Y}_n^j)^2 < 1$.

Remark: On can actually show that the convergence in space is optimal:

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

5 Dependency of the Brownian on the space variable

We consider again Hookean dumbbells in a shear flow.

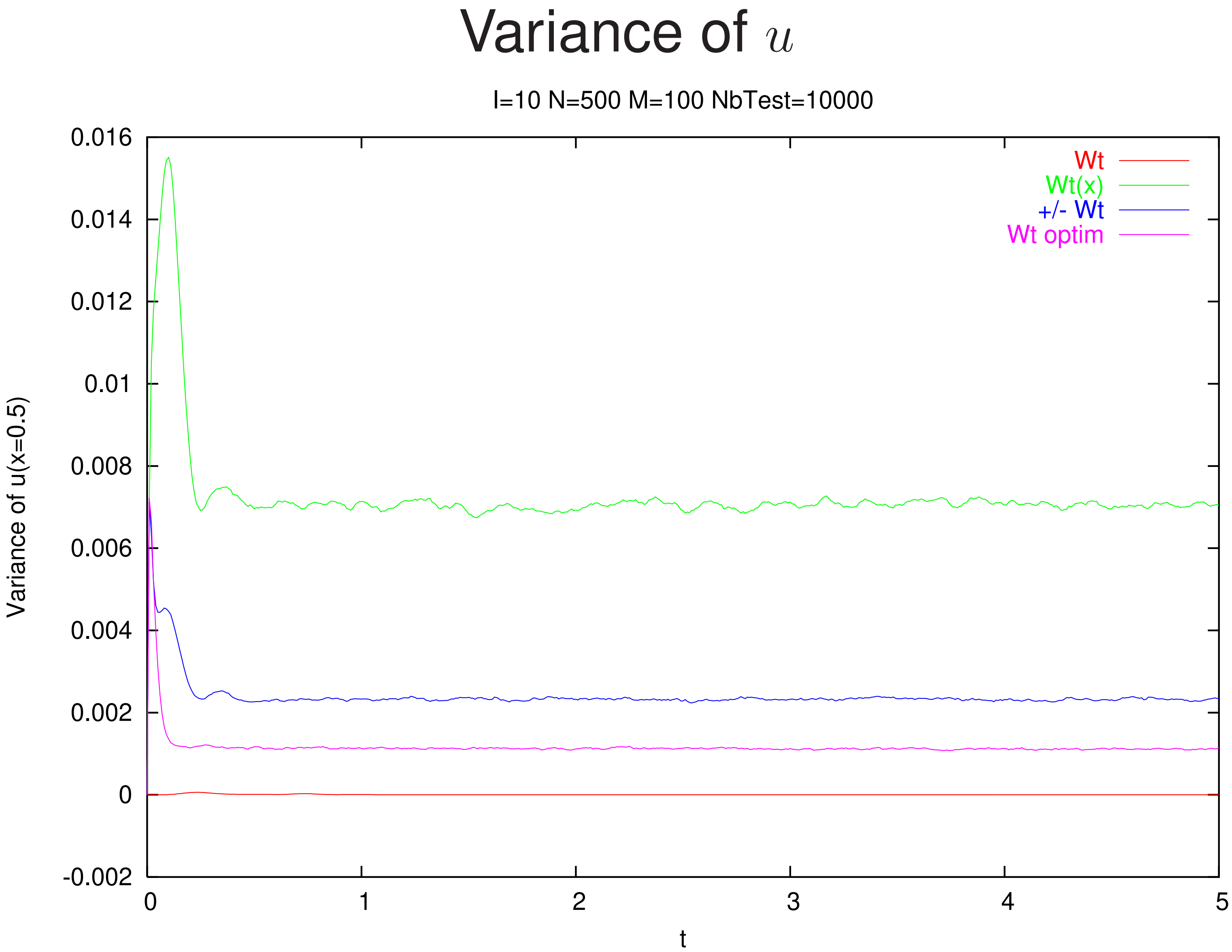
$$\begin{cases} \partial_t u(t,y) - \partial_{yy} u(t,y) = \partial_y \tau(t,y) + f_{ext}(t,y), \\ \tau(t,y) = \mathbf{E}\left(X(t,y)Y(t)\right), \\ dX(t,y) = \left(-\frac{1}{2}X(t,y) + \partial_y u(t,y)Y(t)\right)\, dt + dV_t, \\ dY(t) = -\frac{1}{2}Y(t)\, dt + dW_t. \end{cases}$$

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

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

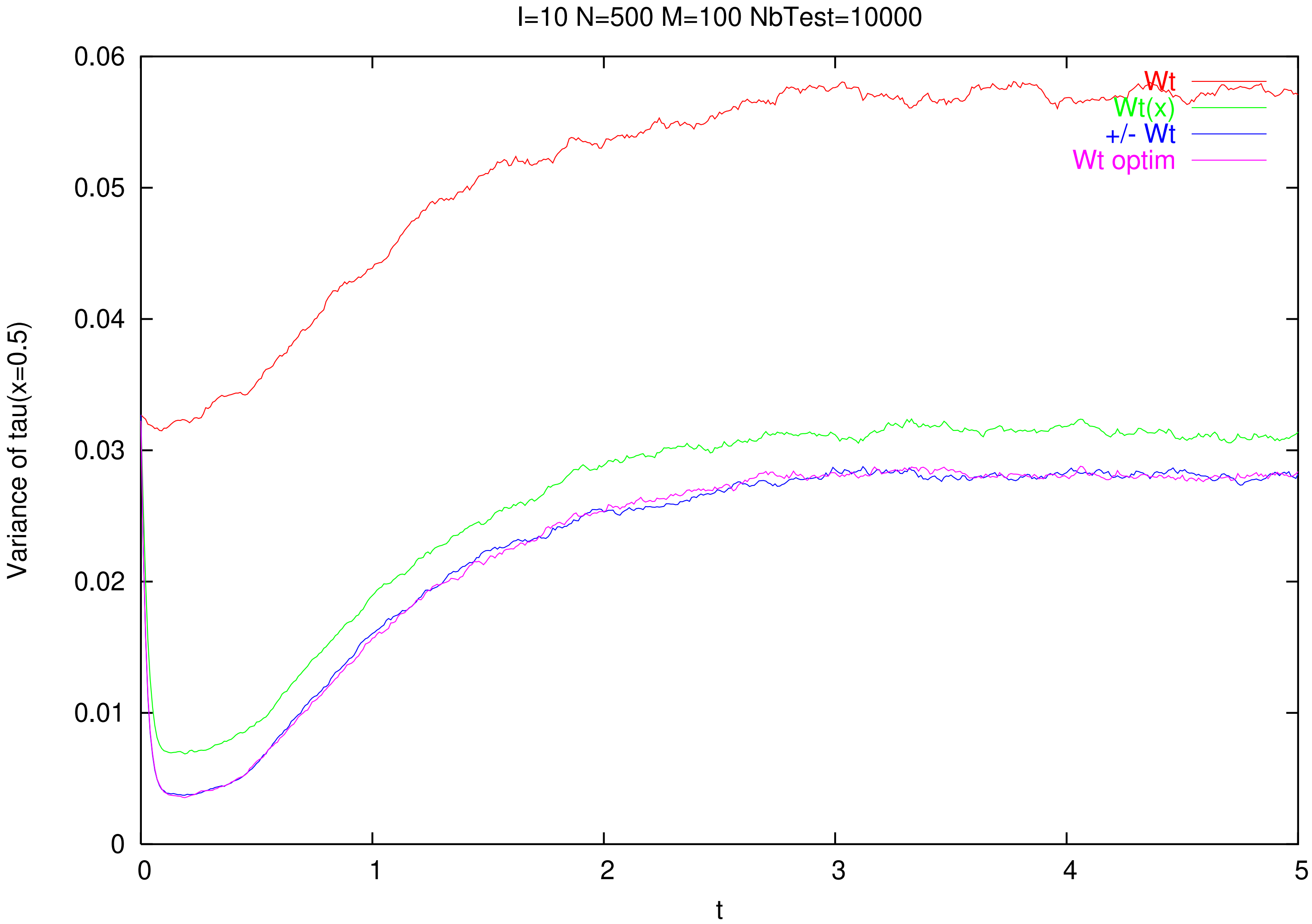
but the variance of the numerical results depends on it.

5 Dependency of the Brownian on the space variable



5 Dependency of the Brownian on the space variable

Variance of τ



5 Dependency of the Brownian on the space variable

We have shown that:

- 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 reduce the variance by using a Brownian motion W_t multiplied alternatively by $+1$ or -1 from one cell to another.

6 Longtime behaviour: some remarks

The Fokker-Planck version of the coupled system is ($\mu = 1$):

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

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

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

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

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

6 Longtime behaviour: some remarks

We introduce the kinetic energy:

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

and the entropy:

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

with

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

6 Longtime behaviour: some remarks

Let us introduce $F(t) = E(t) + H(t)$ (F is a free energy).
Assuming that $u = 0$ on $\partial \mathcal{D}$, one has:

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

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

6 Longtime behaviour: some remarks

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 $t \to \infty$.

6 Longtime behaviour: some remarks

The entropy is the right energy of the system (no Itô term). The free energy shows exponential decay to equilibrium ($\mathbf{u}_\infty = 0$ and $\psi_\infty \propto \exp(-\Pi)$).

But :

- Generalization to the case $\mathbf{u}_\infty \neq 0$?
- How to prove this convergence on the SDE version system ?
- How to perform these computations on the discrete system ?
- Exponential convergence of the stress tensor $\boldsymbol{\tau}$?

Work in progress

- Longtime behaviour (entropy method),
- Solving the Fokker-Planck equation in high dimension,
- Numerical analysis for FENE dumbbell,
- Local-in-time existence in dimension 2,
- Other models (liquid cristals, reptation models).

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