Analysis of micro-macro models for polymeric fluids

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Summary

1 The physical model

Navier-Stokes equations :

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

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

Newtonian fluids :

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

Non-Newtonian fluids :

$$\begin{aligned}\sigma &= \eta\left(\nabla\mathbf{u} +^t \nabla\mathbf{u}\right) + \tau \\ \tau(x,t) &= f((\nabla u(s,x))_{0\leq s\leq t})\end{aligned}$$

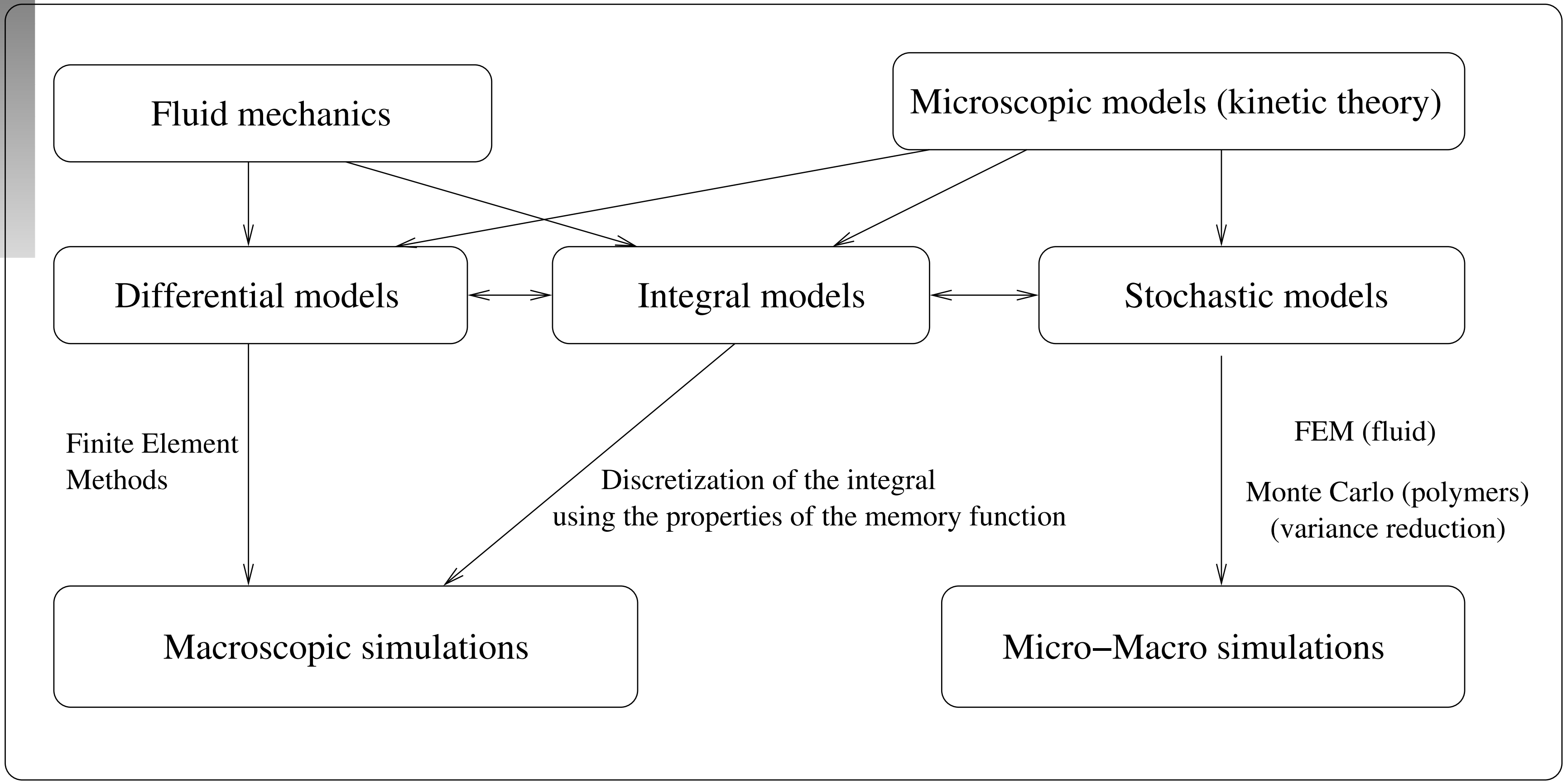
1 The physical model

Polymeric liquids have non-Newtonian properties :

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

We are interesting in numerical methods using some physically-realistic models for these kinds of fluids.

1 The physical model



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

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

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

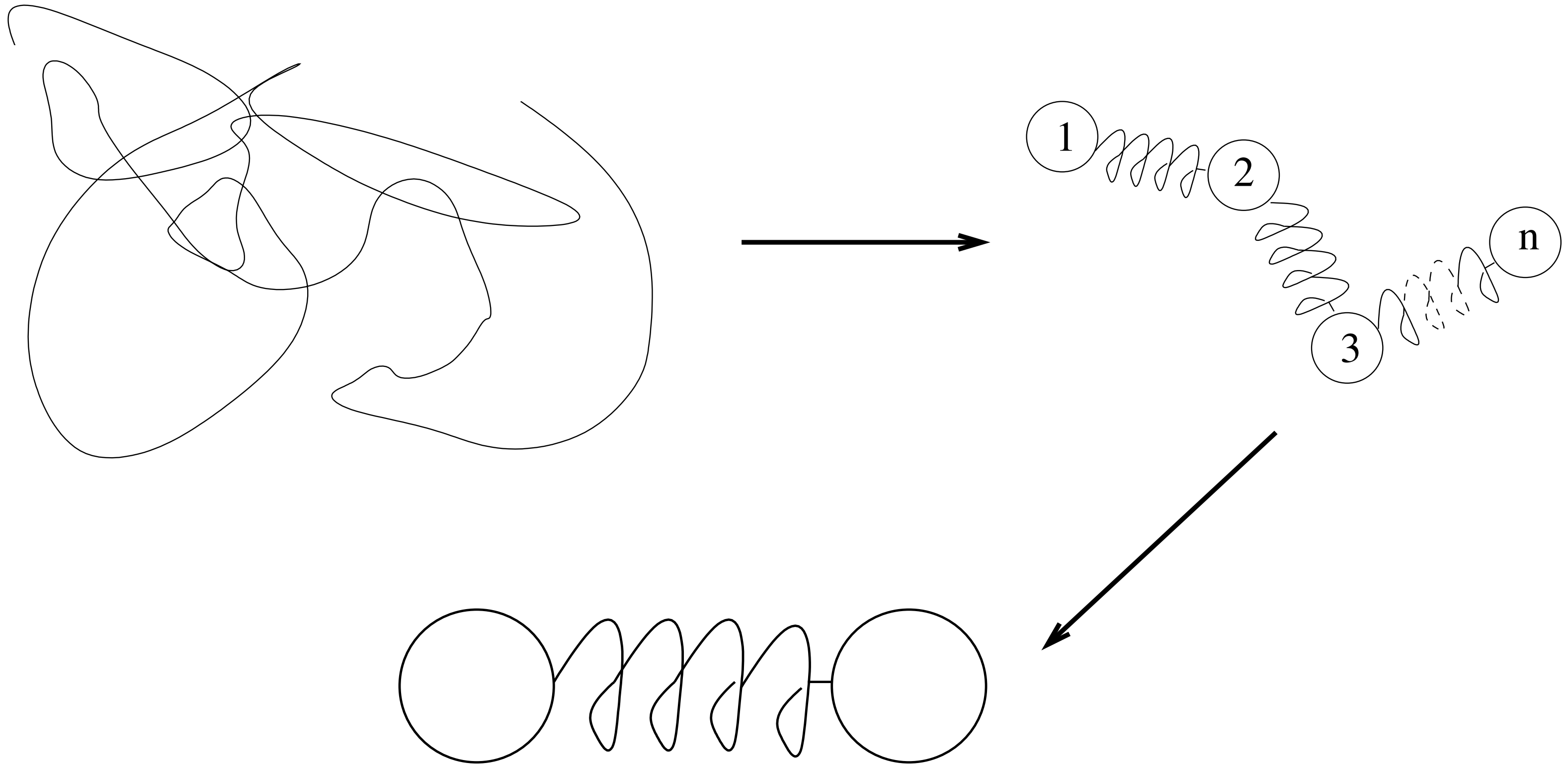
1 The physical model

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

(R.B. Bird, C.F. Curtiss, R.C. Armstrong and O. Hassager, *Dynamic of Poymeric 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 one bead i of coordinate vector $\mathbf{X}_t^i$ in a velocity field $\mathbf{u}(t,x)$ of the solvent (Langevin equation) :

- Drag force :

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

- Entropic force between two beads i and $(i-1)$ $(\mathbf{X}=\left(\mathbf{X}^i-\mathbf{X}^{i-1}\right))$:

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

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

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

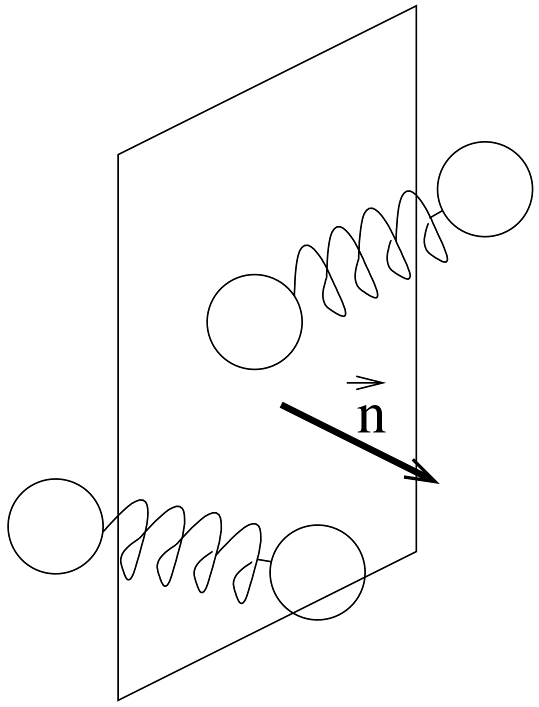
with $\mathbf{W}_t^i$ a Wiener process.

In the dumbbell case (2 beads : $\mathbf{X} = (\mathbf{X}^2 - \mathbf{X}^1)$), one obtains (mass negligible) :
$0 = -\zeta \left(d\mathbf{X}_t - \left(\mathbf{u}(t, \mathbf{X}_t^2) - \mathbf{u}(t, \mathbf{X}_t^1) \right) \, dt \right) - 2\mathbf{F}(\mathbf{X})\, dt + \sqrt{2k_B T\zeta}\, d(\mathbf{W}_t^2 - \mathbf{W}_t^1)$

$$d\mathbf{X}_t = \left(\nabla_x \mathbf{u}(t,x)\mathbf{X}_t - \frac{2}{\zeta}\mathbf{F}(\mathbf{X}_t) \right) \, dt + \sqrt{\frac{4k_B T}{\zeta}} d\mathbf{W}_t$$

1 The physical model

The stress tensor is then computed using Kramers expression :



$$\tau = n_p \left(-k_B T \,\mathsf{Id} + \mathbf{E}\left(\mathbf{X} \otimes \mathbf{F}(\mathbf{X})\right)\right)$$

1 The physical model

This yields the following system :

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

Or, more precisely :

$$d\mathbf{X}_t + \mathbf{u}.\nabla_x\mathbf{X}_t\, dt = \left(\nabla_x \mathbf{u}(t,x)\mathbf{X}_t - \frac{2}{\zeta}\mathbf{F}(\mathbf{X}_t)\right)\, dt + \sqrt{\frac{4k_BT}{\zeta}} d\mathbf{W}_t$$

(C. Le Bris, P.L. Lions, adaptation of Di Perna-Lions theory)

1 The physical model

One can try to solve directly this coupled system of equations. The physical interest of this micro-macro approach :

- the macroscopic models usually derive from kinetic models (e.g. Oldroyd B), sometimes *via* closure approximations,
- some microscopic models do not have a macroscopic equivalent model (e.g. FENE model),
- a better insight in the physical model,
- the parameters of these models have a physical meaning and can be computed.

1 The physical model

The questions we try to address on these models :

- Sense and existence of solutions,

  (M. Renardy, *An existence theorem for model equations resulting from kinetic theories of polymer solutions*, SIAM J. Math. Anal. 22-2, (1997) : a local-in-time existence result on the Fokker-Planck equation coupled with Navier-Stokes, with $\eta = 0$, in $\mathbb{R}^3$, which does not apply in the case of FENE)

- Convergence of the numerical methods,
- Improvement of the numerical methods (variance reduction).

  (J. Bonvin and M. Picasso, J. Non-Newtonian Fluid Mech., 84, (1999)))

2 The numerical method on a simple model

The discretization of the system coupling Navier-Stokes and the SDE uses :

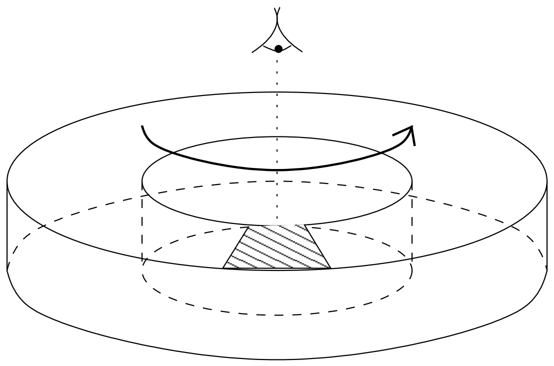
- Euler in time,
- Finite Elements in space,
- Monte Carlo for the expectation value.

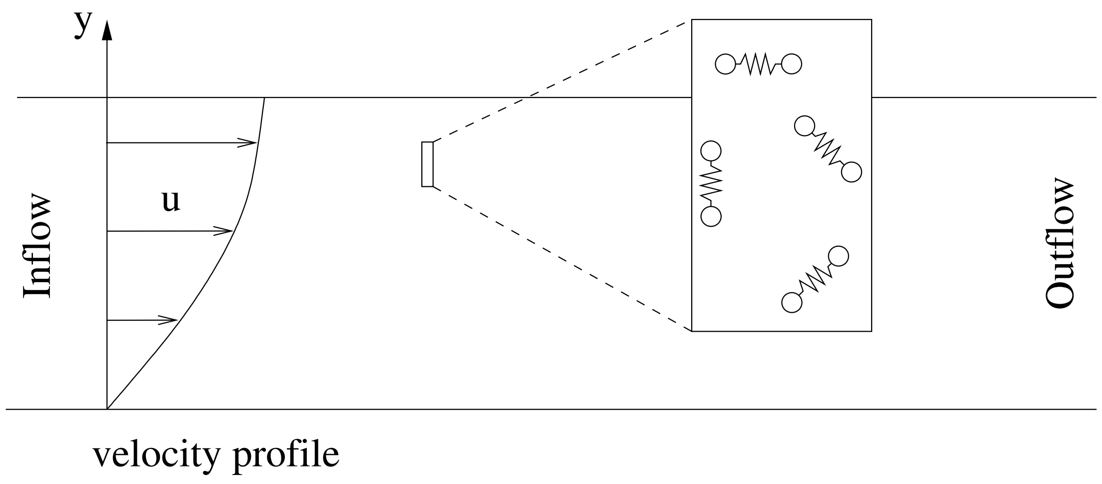
This is the CONNFFESSIT approach (Calculation of Non-Newtonian Fluids : Finite Elements and Stochastic Simulation Techniques.)

(M. Laso, H.C. Öttinger, J. Non-Newtonian Fluid Mech., 47, (1993))

2 The numerical method on a simple model

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





2 The numerical method on a simple model

The equations in this case are ($0 \leq t \leq T$, $0 \leq y \leq 1$) :

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

with

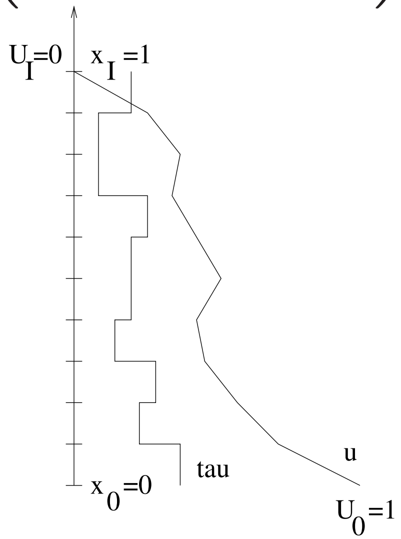
- $\mathbf{F}(x, y) = (x, y)$ (Hookean dumbbells), or
- $\mathbf{F}(x, y) = \left(\frac{x}{1 - \frac{x^2+y^2}{b}}, \frac{y}{1 - \frac{x^2+y^2}{b}} \right)$ (FENE dumbbells).

2 The numerical method on a simple model

Discretization : find $u_h \in V_h$ such that :

$$\left\{\begin{aligned}
&\frac{1}{\delta t}\int_{\mathcal{O}}\left(u_h^{n+1}-u_h^n\right)v_h+\int_{\mathcal{O}}\partial_y u_h^{n+1}\partial_y v_h=-\int_{\mathcal{O}}\tau_h^n\partial_y v_h+F_{ext}, \forall v_h\in V_h\\
&\tau_h^n=\frac{1}{M}\sum_{j=1}^M\left(X_h^{j,n}\mathbf{F}_y(X_h^{j,n},Y_h^{j,n})\right)=\frac{1}{M}\sum_{j=1}^M\left(Y_h^{j,n}\mathbf{F}_x(X_h^{j,n},Y_h^{j,n})\right)\\
&X_h^{j,n+1}=X_h^{j,n}+\left(-\frac{1}{2}\mathbf{F}_x(X_h^{j,n},Y_h^{j,n})+\partial_y u_h^{n+1}Y_h^{j,n}\right)\delta t+\left(V_{t_{n+1}}^j-V_{t_n}^j\right)\\
&Y_h^{j,n+1}=Y_h^{j,n}+\left(-\frac{1}{2}\mathbf{F}_y(X_h^{j,n},Y_h^{j,n})\right)\delta t+\left(W_{t_{n+1}}^j-W_{t_n}^j\right)
\end{aligned}\right.$$

e.g., $V_h=\mathbf{P}1$, and
therefore $\tau_h^n\in\mathbf{P}0$



3 The case of Hookean dumbbells

Existence and uniqueness

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

with

$u(0,y) = u_0(y),$ $u(t,0) = f_0(t)$ and $u(t,1) = f_1(t),$

$$\left.\begin{array}{l} X_0 \text{ and } Y_0 \sim \mathcal{N}(0,1) \\ (V_t, W_t) \text{ Brownian} \end{array}\right\} \text{independent variables.}$$

3 The case of Hookean dumbbells

We have en explicit solution for Y (Ornstein Uhlenbeck) :

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

For X, we have :

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

One can suppose $f_0 = 0$ and $f_1 = 0$ (modyfing f_{ext} and translating u and X).

3 The case of Hookean dumbbells

Weak formulation : find $u \in L^\infty_t(L^2_y) \cap L^2_t(H^1_{0,y})$ and $X \in L^\infty_t(L^2_y(L^2_\omega))$ s.t., $\forall v \in H^1_{0,y}$,

$$\frac{d}{dt}\int_{\mathcal{O}} uv + \int_{\mathcal{O}} \partial_y u \partial_y v = -\int_{\mathcal{O}} \mathbf{E}(X_t(y) Y_t) \partial_y v + \int_{\mathcal{O}} f_{ext}(t,x) v,$$

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

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

3 The case of Hookean dumbbells

Theorem 1 *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)*.*
Moreover, one has the following estimate :

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

Remark : The "$+T$" comes from Itô's formula.

3 The case of Hookean dumbbells

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 : $\int_{\mathcal{O}} \mathbb{E}(Y_t X_t^m(x))\partial_y v_i$, where $X_t^m = e^{-\frac{t}{2}} X_0 + \int_0^t e^{\frac{s-t}{2}}\, dV_s + \int_0^t e^{\frac{s-t}{2}} \partial_y u^m(s,x) Y_s\, ds$.

3 The case of Hookean dumbbells

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

- Uniqueness : the problem is “quasi”-linear.

3 The case of Hookean dumbbells

Convergence of the numerical scheme

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

with $\overline{Y}^{j,n+1}=\max(-A,\min(A,Y^{j,n+1}))$, where

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

Two types of result :

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

3 The case of Hookean dumbbells

Theorem 2 *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* $V_h = \mathbf{P}1$*) :*

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

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

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

Two types of results :

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

3 The case of Hookean dumbbells

Sketch of the proof

- Discretization in space : $O(h)$,
- Discretization in time : $O(\delta t)$ (because diffusion is constant),
- Monte Carlo discretization : $O\left(\delta t + \frac{1}{\sqrt{M}}\right)$.

Remarks :

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

Main difficulty in the stability proof :

$$\int_{\mathcal{O}} \mathbb{E}\left(\left(\frac{9}{10} - \delta t \frac{1}{M}\sum_{j=1}^{M}(\overline{Y}_n^j)^2\right)\partial_y \overline{u}_{n+1}^2 1_{\mathcal{A}_n}\right).$$

4 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 $(V_t(y), W_t(y))$?

Remarks :

- The deterministic continuous solution (u, X) does not depend on the correlation function ϕ in space,
- The convergence result we have shown still holds.

But the variance of the numerical results depend on ϕ.

4 Dependency of the Brownian on the space variable

The correlation function in space ϕ is such that :

$$\begin{aligned} K(s,x,t,y) &= \mathbf{E}(V_t(x)V_t(y)), \\ &= s \wedge t \int_z \phi(x-z)\phi(y-z)\, dz. \end{aligned}$$

Remark : If $\phi = \delta$, $W_t(y)$ and $W_t(y)$ ($x \neq y$) are independent.

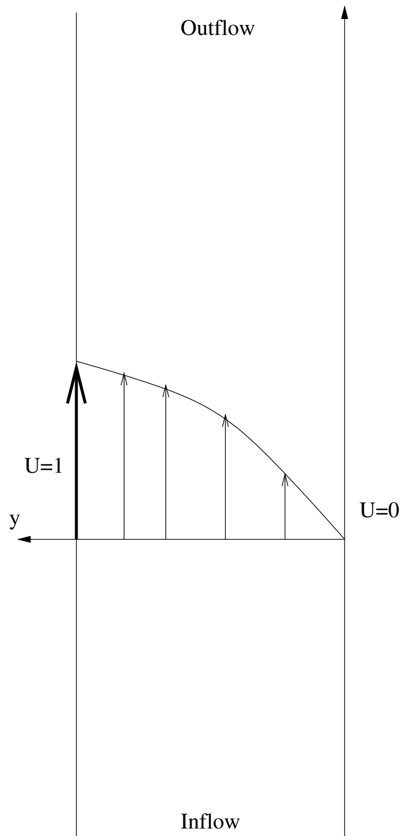
Discretization :

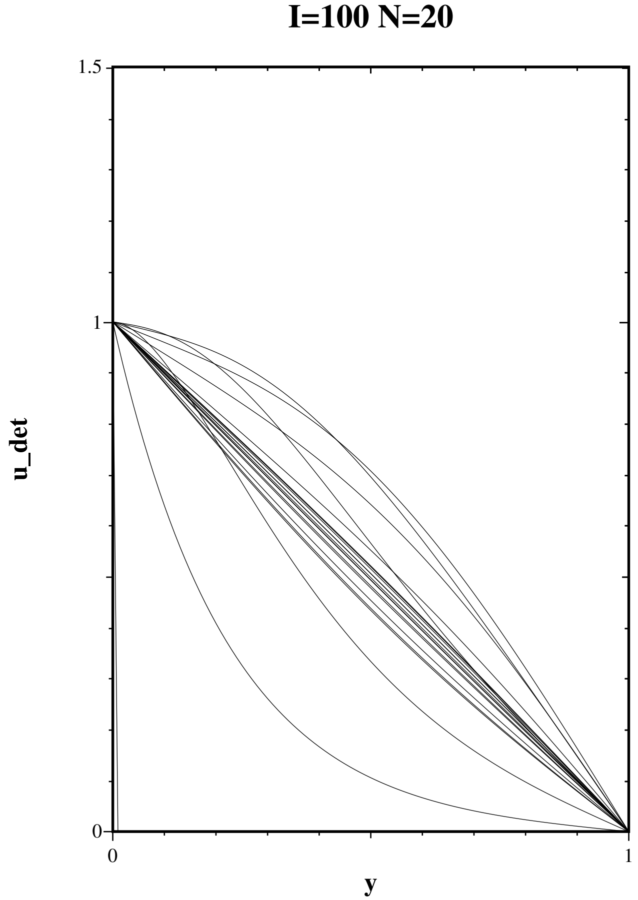
$$V_{t_n}(y_i) = \sum_{m<n} \sum_j \phi(y_i - y_j)\xi_{m,j},$$

with $\xi_{m,j}$ i.i.d. $\sim \mathcal{N}(0,1)$.

4 Dependency of the Brownian on the space variable

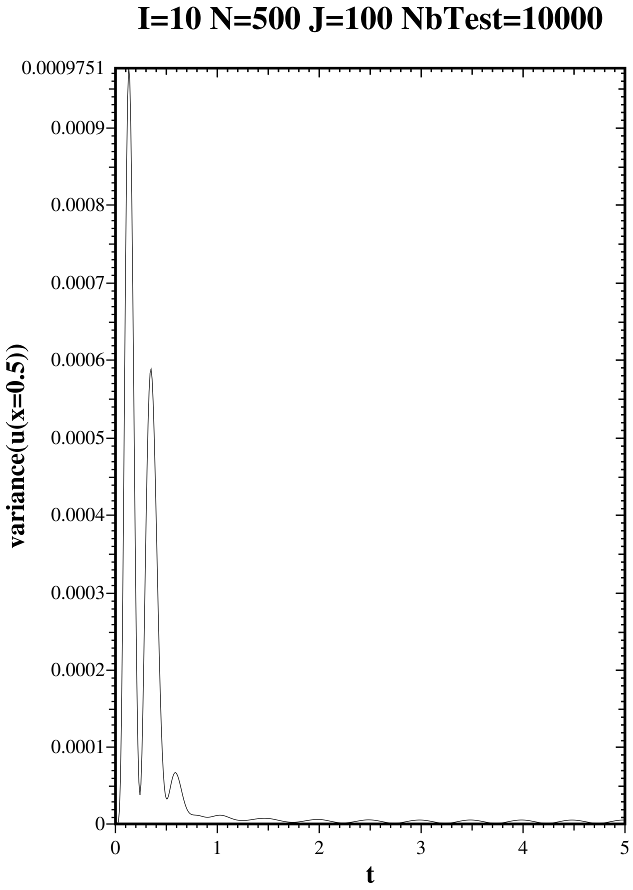
Numerical results

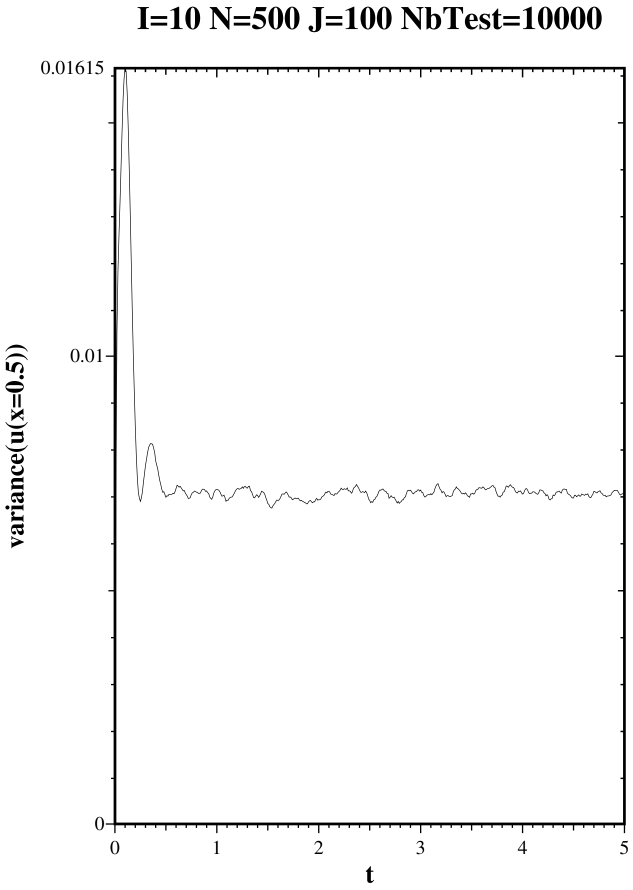




Velocity profile as time evolves.

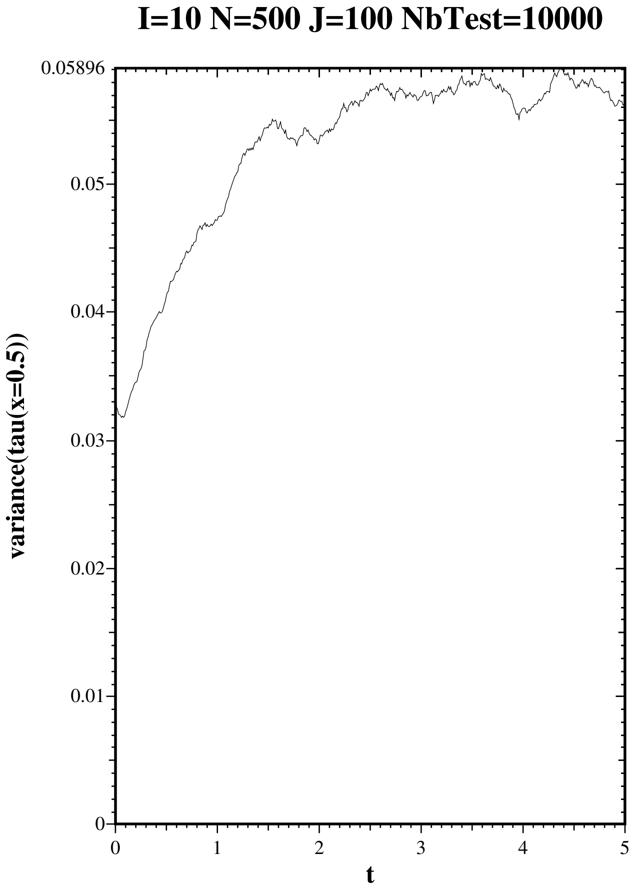
4 Dependency of the Brownian on the space variable

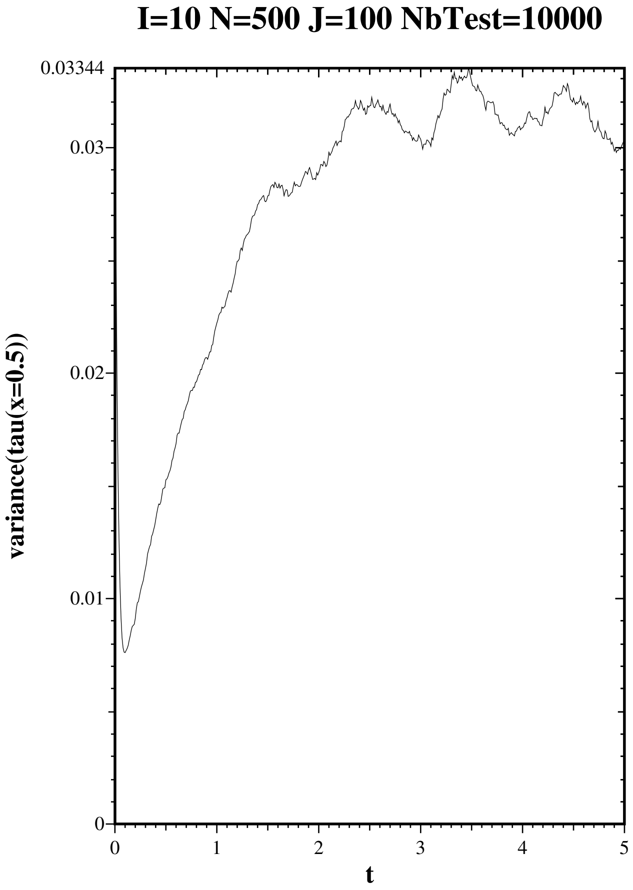




Variance on u : on the left, W_t ; on the right, $W_t(y)$.

4 Dependency of the Brownian on the space variable





Variance on τ : on the left, W_t ; on the right, $W_t(y)$.

4 Dependency of the Brownian on the space variable

	$W_t \longrightarrow W_t(y)$
$\mathrm{Var}(u)$	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 : $\forall v_h \in V_h$

$$\int_{\mathcal{O}} \partial_t u_h(t) v_h + \int_{\mathcal{O}} \partial_y u_h(t) \partial_y v_h = -\int_{\mathcal{O}} \frac{\mathbf{1}}{\mathbf{M}} \sum_{\mathbf{j}=\mathbf{1}}^{\mathbf{M}} \left(\overline{\mathbf{X}}_{\mathbf{h}}^{\mathbf{j}}(\mathbf{t}) \overline{\mathbf{Y}}^{\mathbf{j}}(\mathbf{t}) \right) \partial_{\mathbf{y}} \mathbf{v}_{\mathbf{h}} + F_{ext}.$$

“We derive a brownian...”

But on τ ?

4 Dependency of the Brownian on the space variable

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

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

with

- M matrix of Δ,
- B and C the two discretizations of ∇,
- bc : boundary conditions.

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

4 Dependency of the Brownian on the space variable

Simplifying assumption : $Y_t^2 = 1$ and $Y_t = 0$.

(cf. Y_t and W_t independent.)

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

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 $\mathrm{Ker}(B)$.
This yields :

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

4 Dependency of the Brownian on the space variable

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

$$\mathrm{Covar}(X_t) = \frac{1}{3}PKP + \frac{1}{6}(PK + KP) + \frac{1}{3}K$$

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

with

$$K = \frac{1}{t}\mathrm{Var}(W_t \otimes W_t)$$

the discrete space correlation matrix.

4 Dependency of the Brownian on the space variable

In the case of a uniform discretization in space, we obtain :

Case W_t ($K = Id$) :

- $\mathrm{Covar}(X_t) = J$,
- $\mathrm{Covar}(U(t)) = 0$.

Case $W_t(y)$ ($K = J$) :

- $\mathrm{Covar}(X_t) = \frac{2\delta y}{3} J + \frac{1}{3} Id$,
- $\mathrm{Covar}(U(t)) = -\frac{1}{3} M^{-1}$.

with $J = \begin{bmatrix} 1 & \dots & 1 \\ \vdots & & \vdots \\ 1 & \dots & 1 \end{bmatrix}$

4 Dependency of the Brownian on the space variable

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

An "answer" :

in $\mathrm{Covar}(X_t)$, there is a term $\sum_{i=1}^{I} \left(W_i(t_{n+1}) - W_i(t_n)\right)$ with $W_i(t)$ the i-th coordinate of the brownian W_t.

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.

4 Dependency of the Brownian on the space variable

What can we deduce from this approach ?

For example, the dependency of the variance on the space step δy :

$t \longrightarrow \infty$	$\mathrm{Covar}(Q_t)$	$\mathrm{Covar}(U(t))$
W_t	$O(1)$	0
$W_t(y)$	$O(1)$	$O(\delta y)$

Remark : In the case $W_t(y)$, in the limit $\delta y \to 0$, u is deterministic.

We can also investigate :

- the dependency on the boundary condition,
- how to choose K in order to obtain the desired variance ou (u, τ).

5 The case of FENE dumbbells

FENE = Finite Extensible Nonlinear Elastic force.

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

New difficulties :

- A non-linearity in the SDE,
- Both components of $\mathbf{X}$ depend on the space variable,

but

- A uniform bound on the stochastic processes.

5 The case of FENE dumbbells

Weak formulation : find $u \in L^\infty_t(H^1_{0,y}) \cap L^2_t(H^2_y)$ s.t.,
$\forall v \in H^1_{0,y}$,

$$\frac{d}{dt}\int_{\mathcal{O}} uv + \int_{\mathcal{O}} \partial_y u \partial_y v = -\int_{\mathcal{O}} \tau \partial_y v + \int_{\mathcal{O}} f_{ext}(t,x) v,$$

with $\tau = \mathbf{E}\left(\frac{X_t Y_t}{1 - \frac{X_t^2 + Y_t^2}{b}}\right)$, and s.t. for a.e. (y,ω), $\forall t \in (0,T)$,

$$\begin{aligned} X_t &= X_0 + \int_0^t \left(-\frac{1}{2} \frac{X_s}{1 - \frac{X_s^2+Y_s^2}{b}} + \partial_y u Y_s \right) ds + V_t, \\ Y_t &= Y_0 + \int_0^t -\frac{1}{2} \frac{Y_s}{1 - \frac{X_s^2+Y_s^2}{b}} ds + W_t. \end{aligned}$$

5 The case of FENE dumbbells

Theorem 3 *Under the assumptions $b > 6$, $f_{ext} \in L^2_t(L^2_y)$ and $u_0 \in H^1_y$, the system admits a unique solution (u,τ) on a time interval $[0,T')$, with $T' < T$ depending on the datas. This solution is such that $u \in L^\infty_t(H^1_{0,y}) \cap L^2_t(H^2_y)$ and $\tau = \mathbf{E}\left(\left(\frac{X_tY_t}{1-\frac{X_t^2+Y_t^2}{b}}\right)\mathcal{E}\left(\int_0^{T'}\partial_y u(y) Y_s\, dV_s\right)\right)$, where the random processes X_t and Y_t are defined by :*

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

and

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

5 The case of FENE dumbbells

Sketch of the proof

- Assuming b is large enough, the system
$$\begin{cases} dX_t = \left(-\frac{1}{2}\frac{X_t}{1-\frac{X_t^2+Y_t^2}{b}}\right) dt + dV_t, \\ dY_t = \left(-\frac{1}{2}\frac{Y_t}{1-\frac{X_t^2+Y_t^2}{b}}\right) dt + dW_t, \end{cases}$$
admits a unique strong bounded solution such that $\mathbf{P}(\exists t > 0, (X_t^2 + Y_t^2) = b) = 0$ and (for $b > 2(p+1)$)
$$\mathbf{E}\left(\frac{1}{1-\frac{X_t^2+Y_t^2}{b}}\right)^p < \infty.$$

5 The case of FENE dumbbells

- By Girsanov Lemma, under $\mathbf{P}^y$ defined by

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

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

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

5 The case of FENE dumbbells

- *a priori* estimates :

  on $[0,T]$

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

where Π is a potential from which derives the FENE force :

$\Pi(x,y) = -\frac{b}{2}\ln\left(1 - \frac{x^2+y^2}{b}\right)$ and $\Upsilon(x,y) = \frac{\sqrt{x^2+y^2}}{1-\frac{x^2+y^2}{b}}$,

on $[0,T']$, with $T' < T$

$$||u||_{L^\infty_t(H^1_y)} + ||u||_{L^2_t(H^2_y)} \leq C(T', ||\partial_y u_0||_{L^2_y}, ||f_{ext}||_{L^2_t(L^2_y)}).$$

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

5 The case of FENE dumbbells

- Galerkin method (fixed point 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 :
  $$\int_{\mathcal{O}} \mathbf{E}\left(\left(\frac{X_t Y_t}{1-\frac{X_t^2+Y_t^2}{b}}\right)\mathcal{E}\left(\int_0^{T'} \partial_y u^m Y_s \, dV_s\right)\right)\partial_y v_i$$
  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 u...
- Uniqueness derives from the estimates.

Lemma 1 *The weak solution* $(X_t^y, Y_t^y, V_t^y, W_t^y, \mathbf{P}^y)$ *of the SDE obtained by Girsanov lemma is a strong solution.*

Sketch of the proof

We prove the uniqueness of a strong bounded solution (defined in $\mathcal{C}([0,T], B)$ where $B = \{(x,y) \in \mathrm{R}^2, x^2 + y^2 < b\}$) and use Yamada-Watanabe theorem.

Prospects

- Convergence of the numerical scheme on FENE,
- Long time on FENE (using the first energy estimate ?),
- Fokker-Planck approach (new estimates),
- In 2D : transport term $\mathbf{u}.\nabla$ (EDPS), Trudinger inequality to control the exponential martingale,
- Variance reduction schemes,
- Models with non-linear SDE,
- Models of reptation (Doi-Edwards).

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