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Mathematical and numerical analysis for multiscale simulations of suspensions

[Claude Le Bris]

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including mathematical works with and by E. Cancès, I. Catto, Y. Gati,

numerical works with A.T. Patera (MIT) and S. Boyaval,

in collaboration with Ph. Coussot (LCPC), F. Lequeux (ESPCI).

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Modelling of suspensions

- The Hébraud-Lequeux model

  A mesoscale model describing shear flows of concentrated suspensions

- A multiscale model based on the HL model

- Long-time existence and uniqueness
- Long-time limit (convergence to steady states)
- Numerical simulation (deterministic and stochastic approaches)

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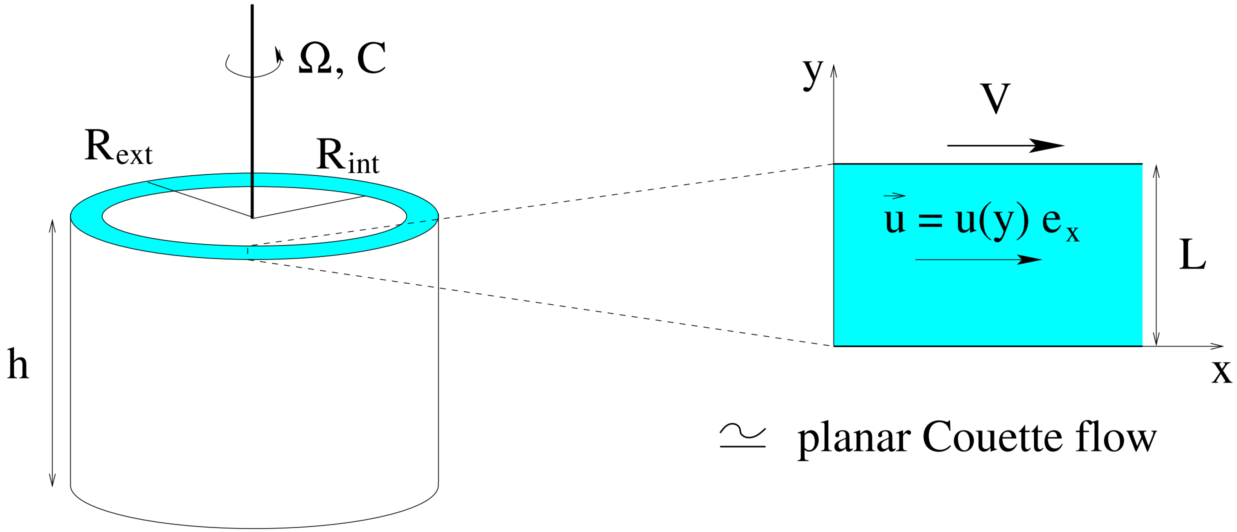
Shear-stress experiments



$$\begin{pmatrix} \Omega \\ C \end{pmatrix} \leftrightarrow \begin{pmatrix} \dot{\gamma} \\ \tau \end{pmatrix}$$

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

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

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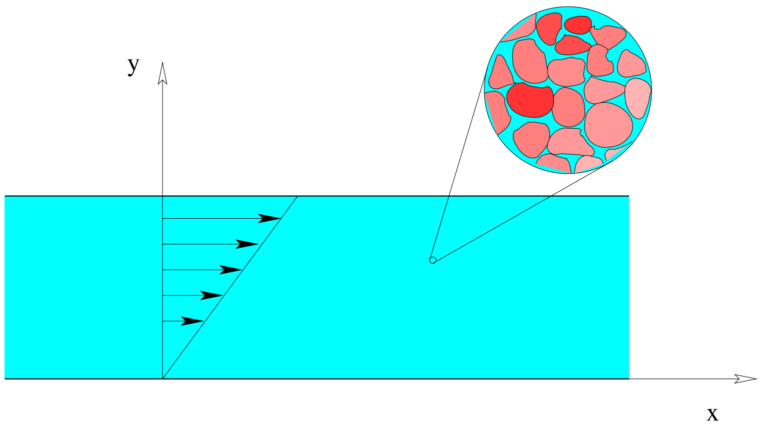
Phys. Rev. Lett. 1998

- Planar Couette flow: $\vec{u}(x,y,t) = u(y,t)\,\vec{e}_x$
- Shear rate $\dot{\gamma} = \partial_y u$ uniform in space



- A sample of matter: assembly of blocks, each of them carrying some shear stress σ.

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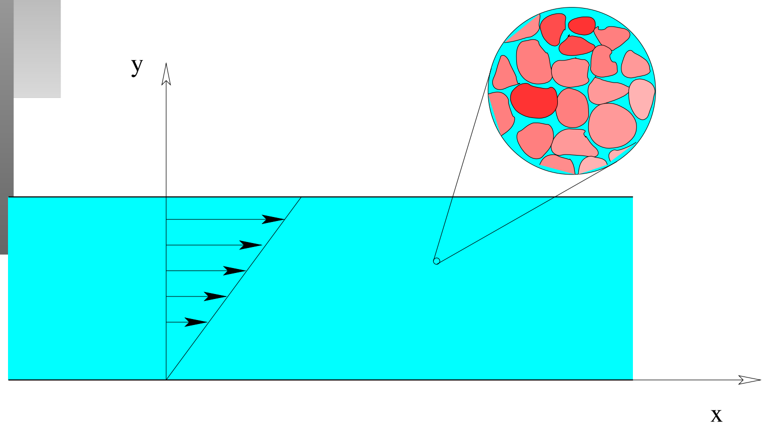
Modelling of suspensions

The probability density $p(t, \sigma)$ for a block carry shear-stress σ at time t is independent of x and y.



Macroscopic shear stress in the fluid

$$\tau(t) = \int_{\mathbf{R}} \sigma \, p(\sigma, t) \, d\sigma$$

Modelling of suspensions

- Elasticity of individual blocks (shear modulus G_0)
- Relaxation beyond a given threshold σ_c
  (T_0: characteristic relaxation time)
- Collective effect: relaxation induced rearrangement

$$\partial_t p(t,\sigma) = -G_0 \dot{\gamma}(t)\ \partial_\sigma p(t,\sigma) + D(p(t))\ \partial^2_{\sigma\sigma} p(t,\sigma) - \frac{\chi_{\mathbf{R}\setminus[-\sigma_c,\sigma_c]}(\sigma)}{T_0}\ p(t,\sigma) + \frac{1}{T_0}\left(\int_{|\sigma|>\sigma_c} p(t,\sigma)\, d\sigma\right)\ \delta_0(\sigma)$$

with

$$D(f) = \frac{\alpha}{T_0} \int_{|\sigma|>\sigma_c} f(\sigma)\, d\sigma$$

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Modelling of suspensions

Hébraud-Lequeux (HL) equation

$$\begin{aligned}\partial_t p(t,\sigma) &= -G_0 \dot{\gamma}(t)\, \partial_\sigma p(t,\sigma) + D(p(t))\, \partial_{\sigma\sigma} p(t,\sigma) \\ &\quad - \frac{\chi_{\mathbf{R}\setminus[-\sigma_c,\sigma_c]}(\sigma)}{T_0}\, p(t,\sigma) + \frac{D(p(t))}{\alpha} \delta_0(\sigma)\end{aligned}$$

$$D(f) = \frac{\alpha}{T_0} \int_{|\sigma|>\sigma_c} f(\sigma)\, d\sigma$$

Nonlinear (nonlocal) parabolic equation, which can degenerate into a linear advection equation

Nonlinear drift-diffusion process (in the sense of Mc-Kean) with jumps.

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Mesoscopic equation: steady-state

$\dot{\gamma}$ being given, search the solutions $p(\sigma)$ to

$$-G_0\dot{\gamma}\,\partial_\sigma p + D(p)\,\partial_{\sigma\sigma} p - \frac{\chi_{\mathbf{R}\setminus[-\sigma_c,\sigma_c]}(\sigma)}{T_0}\,p + \frac{D(p)}{\alpha}\delta_0(\sigma) = 0$$

with

$$D(p) = \frac{\alpha}{T_0}\int_{|\sigma|>\sigma_c} p(\sigma)\,d\sigma$$

such that

$$p \geq 0, \qquad \int_{\mathbf{R}} p(\sigma)\,d\sigma = 1$$

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Mesoscopic equation: steady-state

Proposition (E. Cancès, I. Catto, Y. Gati). For a given set of parameters α, G_0, T_0, and σ_c,

- For $\dot{\gamma} \neq 0$ fixed, there exists a unique steady state $p(\sigma)$, and therefore a unique τ
- For $\dot{\gamma} = 0$, any function $p(\sigma)$ supported in $[-\sigma_c, \sigma_c]$ is a steady-state.

  In addition, if $\alpha > \alpha_c = 1/2$, there exists a unique steady state $p(\sigma)$ with $D(p) > 0$.

  No such state exists for $\alpha \leq \alpha_c$.

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Mesoscopic equation

$\dot{\gamma}(t)$ and p_0 such that $p_0 \geq 0$ and $\int_{\mathbf{R}} p_0 = 1$ being given, search the solutions $p(t,\sigma)$ to the HL equation

$$\begin{aligned} \partial_t p(t,\sigma) &= -G_0 \dot{\gamma}(t)\, \partial_\sigma p(t,\sigma) + D(p(t))\, \partial_{\sigma\sigma} p(t,\sigma) \\ &\quad - \frac{\chi_{\mathbf{R}\setminus[-\sigma_c,\sigma_c]}(\sigma)}{T_0}\, p(t,\sigma) + \frac{D(p(t))}{\alpha} \delta_0(\sigma) \end{aligned}$$

with $p(0,\sigma) = p_0(\sigma)$.

$$D(f) = \frac{\alpha}{T_0} \int_{|\sigma|>\sigma_c} f(\sigma)\, d\sigma$$

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Mesoscopic equation

A priori estimates ($G_0 = 1$, $T_0 = 1$, $\sigma_c = 1$)

$\int_{\mathbf{R}}$ (HL equation)

$$\frac{d}{dt}\int_{\mathbf{R}} p = 0$$

$\int_{\mathbf{R}}$ (HL equation) $\times\, p$

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbf{R}} p^2 + D(p(t))\int_{\mathbf{R}} |\partial_\sigma p|^2 + \int_{|\sigma|>1} p^2 = \frac{D(p(t))}{\alpha} p(t,0)$$

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Mesoscopic equation

Maximum principle $H_1 = \chi_{\mathbf{R}\setminus[-1,1]}$

$$\begin{cases} \partial_t p = -\dot\gamma\,\partial_\sigma p + D(p)\,\partial_{\sigma\sigma} p - H_1 p + \frac{D(p)}{\alpha}\delta_0 \ ; \\ p(0,\sigma) = p_0(\sigma)\ , \end{cases}$$

$$\begin{cases} \partial_t p_- = -\dot\gamma\,\partial_\sigma p_- + D(p)\,\partial_{\sigma\sigma} p_- - p_- \ ; \\ p_-(0,\sigma) = p_0(\sigma)\ , \end{cases}$$

$$\begin{cases} \partial_t p_+ = -\dot\gamma\,\partial_\sigma p_+ + D(p)\,\partial_{\sigma\sigma} p_+ + \dfrac{D(p)}{\alpha}\,\delta_0(\sigma) \ ; \\ p_+(0,\sigma) = p_0(\sigma)\ , \end{cases}$$

$$p_- \le p \le p_+$$

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Mesoscopic equation

Heat kernel

$$\begin{cases} \mathcal{G}_t(\sigma) = \dfrac{1}{\sqrt{4\pi t}} \exp\left(-\dfrac{\sigma^2}{4\,t}\right) & \text{if } t > 0\ ; \\ \mathcal{G}_0 = \delta_0\ . \end{cases}$$

Total shear

$$\chi(t) = \int_0^t \dot{\gamma}(s)\, ds \qquad \left[\in H^1_{\mathrm{loc},\,t} \hookrightarrow C^0_t\right]$$

$$p_- = e^{-t}\, \tau_{\chi(t)} p_0 \star \mathcal{G}_{\int_0^t D(p)}$$

$$p_+ = \tau_{\chi(t)} p_0 \star \mathcal{G}_{\int_0^t D(p)} + \frac{1}{\alpha} \int_0^t D(p(s))\, \mathcal{G}_{\int_s^t D(p)}\, (\cdot - \chi(t) + \chi(s))\ ds$$

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Mesoscopic equation

$$
\begin{aligned}
p(t,\sigma) &\leq p_+(t,\sigma) \\
&\leq \|\tau_{\chi(t)} p_0 \star \mathcal{G}_{\int_0^t D(p)}\|_{L^\infty} + \frac{1}{\alpha}\int_0^t \frac{D(p(s))}{\sqrt{4\pi \int_s^t D(p)}}\, ds \\
&\leq \|p_0\|_{L^\infty} + \frac{1}{\alpha\sqrt{\pi}}\sqrt{\int_0^t D(p)}
\end{aligned}
$$

$$
D(p) = \alpha \int_{|\sigma|>\sigma_c} p \leq \alpha \int_{\mathbf{R}} p = \alpha
$$

Therefore

$$
0 \leq p(t,\sigma) \leq \|p_0\|_{L^\infty} + \sqrt{\frac{t}{\alpha\pi}}
$$

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Mesoscopic equation

The subsolution p_- is used to prove that, if $D(p_0) > 0$, then $D(p(t))$ is bounded away from zero on finite time intervals.

As $D(p_0) > 0$, p_0 is not supported in $[-1, 1]$.

As $t \mapsto \chi(t)$ is continuous, $p_-(t) = e^{-t}\,\tau_{\chi(t)} p_0 \star \mathcal{G}_{\int_0^t D(p)}$ is not supported in $[-1, 1]$ for any $0 \leq t < t^*$.

In fact, for any $T < t^*$,

$$\forall 0 \leq t \leq T, \quad D(p(t)) \geq D(p_-(t)) \geq \frac{\alpha}{2} e^{-T} \min_{0 \leq t \leq T} \int_{|\sigma+\chi(t)|>1} p_0$$

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Mesoscopic equation

As $\int_0^{t^*} D(p(t))\,dt = \mathcal{D} > 0$, the support of

$$p_-(t^*) = e^{-t^*}\,\tau_{\chi(t^*)}p_0 \star \mathcal{G}_{\mathcal{D}}$$

is the whole real line.

Therefore, so is the support of

$$p_-(t) = e^{-(t-t^*)}\,\tau_{\chi(t-t^*)}p_-(t^*) \star \mathcal{G}_{\int_{t^*}^t D(p)}$$

for any $t \geq t^*$, and $D(p(t)) > 0$ for any t.

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Mesoscopic equation

Theorem (E. Cancès, I. Catto, Y. Gati). Let $\dot{\gamma} \in L^2_{\rm loc}(\mathbf{R}_+)$ and let the initial data p_0 satisfy the conditions

$$p_0 \in L^1 \cap L^\infty(\mathbf{R}), \quad p_0 \geq 0, \quad \int_{\mathbf{R}} p_0 = 1, \quad \int_{\mathbf{R}} |\sigma|\, p_0 < +\infty$$

and be such that $D(p_0) > 0$.

Then, there exists a unique global solution $p(t,\sigma)$ to the HL equation in $L^\infty_{\rm loc,\ t}(L^1_\sigma \cap L^2_\sigma) \cap L^2_{\rm loc,\ t}(H^1_\sigma)$.

Moreover, $p \in L^\infty_{\rm loc,\ t}(L^\infty_\sigma) \cap C^0_t(L^1_\sigma \cap L^2_\sigma)$

SIAM Journal on Mathematical Analysis, 37, pp 60-82, 2005,

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Mesoscopic equation

In addition,

- For all $t \geq 0$, $\quad p(t, \cdot) \geq 0$, $\qquad \int_{\mathbf{R}} p(t, \sigma)\, d\sigma = 1$
- $D(p) \in C^0_t$ and for all $T > 0$

$$\min_{0 \leq t \leq T} D(p(t)) > 0$$

- $\sigma\, p \in L^\infty_t(L^1_\sigma)$ so that the macroscopic shear-stress

$$\tau(t) = \int_{\mathbf{R}} \sigma\, p(t, \sigma)\, d\sigma$$

is well-defined in $L^\infty_{\mathrm{loc},\, t}$

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Sketch of the proof

- Step 1. For any $0 < \epsilon \leq 1$, equation

$$\begin{cases} \partial_t p_\epsilon = -\dot{\gamma}\, \partial_\sigma p_\epsilon + (D(p_\epsilon) + \epsilon)\, \partial_{\sigma\sigma} p_\epsilon - H_1 p_\epsilon + \frac{D(p_\epsilon)}{\alpha} \delta_0 \; ; \\ p_\epsilon(0, \sigma) = p_0(\sigma) \; , \end{cases}$$

  has a solution p_ϵ (a priori bounds + Schauder for local existence, growth control on $\int_{\mathbf{R}} |\sigma| p_\epsilon$ for global existence).

- Step 2. Up to extraction (p_ϵ) converges toward a solution of the HL equation when ϵ goes to zero.

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- Step 3. Uniqueness: let p_1 and p_2 be two solutions of the HL equations. Let $q = p_2 - p_1$.

  Maximum principle: $p \geq p_- \quad \Rightarrow \quad \forall T > 0,\ \exists \nu(T) > 0$ depending only on α and p_0 such that

$$\min_{0 \leq t \leq T} D(p(t)) \ \geq \ \nu(T).$$

$$\frac{1}{2}\frac{d}{dt}\|q\|^2_{L^2_\sigma} \leq \left(\frac{1}{\nu(T)} + \frac{\alpha^2}{\nu(T)} \|\partial_\sigma p_1\|^2_{L^2_\sigma} + \frac{\nu(T)}{2} \right) \|q\|^2_{L^2_\sigma}$$

$$\text{Gronwall} \quad \Rightarrow \quad q = 0$$

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Proposition (E. Cancès, I. Catto, Y. Gati). Let the initial data p_0 satisfy the conditions

$$p_0 \in L^1 \cap L^\infty(\mathbf{R}), \quad p_0 \geq 0, \quad \int_{\mathbf{R}} p_0 = 1, \quad \int_{\mathbf{R}} |\sigma|\, p_0 < +\infty$$

and be such that

$$D(p_0) = 0 \ .$$

Then, the HL equation has at least one solution, but may have an infinity of solutions.

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Mesoscopic equation: long-time behaviour

Theorem (E. Cancès and CLB). For α large enough, for $\dot\gamma_\infty$ small enough, for $\mathcal{C}$ small enough, if

$$|\dot\gamma(t) - \dot\gamma_\infty| \leq \mathcal{C} f(t) \quad \text{with} \quad |f(t)| \leq 1 \quad \text{and} \quad f(t) \underset{t \to +\infty}{\longrightarrow} 0,$$

and if p_0 is close enough to p_∞ [unique steady state associated with $\dot\gamma_\infty$ for which $D(p_\infty) > 0$], then

$$p(t, \cdot) \underset{t \to +\infty}{\longrightarrow} p_\infty \qquad \text{at least in } L^2_{loc}(\mathbf{R}) \cap L^1(\mathbf{R}).$$

If moreover, $\dot\gamma(t)$ converges exponentially fast to $\dot\gamma_\infty$, then $p(t, \cdot)$ converges exponentially fast to p_∞.

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Mesoscopic equation: long-time behaviour

The proof makes use of the entropy function

$$S_2(t) = \int_{\mathbf{R}} \left(\frac{p(t,\sigma)}{p_\infty(\sigma)} - 1 \right)^2 p_\infty(\sigma)\, d\sigma$$

The assumption "p_0 close enough to p_∞" means

$$S_2(0) = \int_{\mathbf{R}} \left(\frac{p_0(\sigma)}{p_\infty(\sigma)} - 1 \right)^2 p_\infty(\sigma)\, d\sigma$$

small enough.

Multiscale model

It is observed in experiments that the shear rate $\partial_y u$ is not uniform in space. We therefore propose the following multiscale model:

$$\left\{ \begin{aligned} \rho \partial_t u(t,y) &= \mu \partial_{yy} u(t,y) + \partial_y \tau(t,y), \qquad u(t,0)=0, \quad u(t,L)=V(t), \\ \partial_t p(t,y,\sigma) &= -G_0\, \partial_y u(t,y)\, \partial_\sigma p(t,y,\sigma) \;+\; D(t,y)\, \partial^2_{\sigma\sigma} p(t,y,\sigma) \\ &\quad - \frac{\chi_{\mathbf{R}\setminus[-\sigma_c,\sigma_c]}(\sigma)}{T_0}\, p(t,y,\sigma) \;+\; \frac{1}{T_0} \left(\int_{|\sigma'|>\sigma_c} p(t,y,\sigma')\, d\sigma' \right) \delta_0(\sigma) \\ \tau(t,y) &= \int_{\mathbf{R}} \sigma\, p(t,y,\sigma)\, d\sigma, \\ D(t,y) &= \frac{\alpha}{T_0} \int_{|\sigma|>\sigma_c} p(t,y,\sigma)\, d\sigma. \end{aligned} \right.$$

$\rho > 0$, $\mu > 0$

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Theorem (E. Cancès, I. Catto, Y. Gati and CLB). Let the initial data p_0 satisfy the conditions

$$\begin{cases} p_0 \geq 0 \,, & \displaystyle\int_{\mathbf{R}} p_0(y,\sigma)\, d\sigma = 1, \quad \forall y \in \Omega =]0,L[\,, \\ p_0 \in L^\infty(\Omega \times \mathbf{R}) \,, & \displaystyle\int_{\mathbf{R}} |\sigma|\, p_0\, d\sigma \ \in \ L^2(\Omega) \,; \end{cases}$$

together with

$$\inf_{y\in\Omega,\ \chi\in\mathbf{R}} \int_{|\sigma+\chi|>\sigma_c} p_0(y,\sigma)\, d\sigma = \eta > 0 \,.$$

Let $V \in H^1_{\mathrm{loc},t}$ and $u_0 \in H^1(0,L)$ such that $u_0(0) = 0$ and $u_0(L) = V(0)$.

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Multiscale model

Then, there exists a unique global solution $(u; p)$ of the multiscale HL system such that

$$u \in C_t^0\left(L_y^2\right) \cap L^2_{\mathrm{loc},\,t} H_y^1 \,,$$

$$p \in L^\infty_{\mathrm{loc},\,t}\left(L_y^\infty\left(L_\sigma^1\right) \cap \, L^\infty_{y,\sigma}\right) \cap L_y^\infty\left(C_t^0\left(L_\sigma^2\right) \cap L^2_{\mathrm{loc},\,t} H_\sigma^1\right)$$

and

$$\tau \in L_y^2\left(L^\infty_{\mathrm{loc},\,t}\right) \cap C_t^0\left(L_y^2\right).$$

Moreover,

$$p \geq 0 \qquad \text{and} \qquad \int_{\mathbf{R}} p(t, y, \sigma)\, d\sigma = 1, \qquad \forall (t, y)$$

SIAM Multiscale Modeling and Simulation, vol. 4, No. 4, pp 1041-1058, 2005,

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- Step 1. Change of variable $v(t,y) = u(t,y) - \frac{V(t)}{L} y$

$$
\left\{
\begin{aligned}
\rho \partial_t v(t,y) &= \mu \partial_{yy} v(t,y) + \partial_y \tau(t,y) - \frac{V'(t)}{L} y, \\
v(t,0) &= 0, \quad v(t,L) = 0, \\
\partial_t p(t,y,\sigma) &= -G_0 \left(\partial_y v(t,y) + \frac{V(t)}{L} \right) \partial_\sigma p(t,y,\sigma) + D(t,y)\, \partial^2_{\sigma\sigma} p(t,y,\sigma) \\
&\quad - \frac{\chi_{\mathbf{R} \setminus [-\sigma_c, \sigma_c]}(\sigma)}{T_0} p(t,y,\sigma) + \frac{1}{T_0} \left(\int_{|\sigma'|>\sigma_c} p(t,y,\sigma')\, d\sigma' \right) \delta_0(\sigma) \\
\tau(t,y) &= \int_{\mathbf{R}} \sigma\, p(t,y,\sigma)\, d\sigma, \\
D(t,y) &= \frac{\alpha}{T_0} \int_{|\sigma|>\sigma_c} p(t,y,\sigma)\, d\sigma.
\end{aligned}
\right.
$$

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- Step 2. Short time existence and uniqueness

For $T > 0$ we define the mappings

$$\begin{array}{rccc} \mathcal{F}_1 : & L^2\left(0,T;H_0^1(\Omega)\right) & \longrightarrow & L^\infty\left(0,T;L^2(\Omega)\right) \\ & v & \longmapsto & \tau \end{array}$$

and

$$\begin{array}{rccc} \mathcal{F}_2 : & L^\infty\left(0,T;L^2(\Omega)\right) & \longrightarrow & L^2\left(0,T;H_0^1(\Omega)\right) \\ & \tau & \longmapsto & v\ , \end{array}$$

For $T > 0$ small enough, $\mathcal{F} = \mathcal{F}_2 \circ \mathcal{F}_1$ is contractive.

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- Step 3. Global and time existence and uniqueness

Let $[0, t^*[$ be the maximal time interval on which the solution $(u; p)$ is defined.

For all $0 \leq t < t^*$,

- $$\left\| \int_{\mathbf{R}} |\sigma| p(t) \, d\sigma \right\|_{L^2_y} \leq \left\| \int_{\mathbf{R}} |\sigma| p_0 \, d\sigma \right\|_{L^2_y} + C_{p_0} \left(1 + t^{3/2}\right)$$
- $$\inf_{y \in \Omega, \ \chi \in \mathbf{R}} \int_{|\sigma + \chi| > \sigma_c} p(t, y, \sigma) \, d\sigma \geq \frac{\eta}{2\alpha} e^{-t}$$

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Multiscale model: long-time behaviour

$$\left\{\begin{aligned}
\rho\partial_t u &= \mu\partial_{yy}u(y,t) + \partial_y\tau(y,t), \qquad u(t,0)=0, \quad u(t,L)=V(t),\\
\partial_t p(y,\sigma,t) &= -G_0\,\partial_y u(y,t)\,\partial_\sigma p(y,\sigma,t) \;+\; D(y,t)\,\partial^2_{\sigma\sigma}p(y,\sigma,t)\\
&\quad -\frac{\chi_{\mathbf{R}\setminus[-\sigma_c,\sigma_c]}(\sigma)}{T_0}\,p(y,\sigma,t) \;+\; \frac{1}{T_0}\left(\int_{|\sigma'|>\sigma_c} p(y,\sigma',t)\,d\sigma'\right)\delta_0(\sigma)\\
\tau(y,t) &= \int_{\mathbf{R}} \sigma\, p(y,\sigma,t)\,d\sigma,\\
D(y,t) &= \frac{\alpha}{T_0}\int_{|\sigma|>\sigma_c} p(y,\sigma,t)\,d\sigma.
\end{aligned}\right.$$

If $V(t) \underset{t\to+\infty}{\longrightarrow} V_\infty$, does $(u;p)$ converge to some (u_∞, p_∞)?

$$u_\infty = u_\infty(y) = \frac{V_\infty}{L}y, \qquad p_\infty = p_\infty(\sigma)$$

Multiscale model: long-time behaviour

Compute u from τ (thus from p):

$$\frac{\partial u}{\partial y}(t,y) = -\frac{1}{\eta}\tau(t,y) + \frac{1}{\eta L}\int_0^L \tau(t,y')\,dy' + \frac{1}{L}V(t).$$

Insert in the mesoscopic equation

$$\begin{aligned}\frac{\partial p}{\partial t}(t,y,\sigma) \quad = \quad & -\left[-\frac{1}{\eta}\int_{\mathbf{R}} \sigma p(t,y,\sigma)\,d\sigma + \frac{1}{L}V(t)\right. \\ & \left. + \frac{1}{\eta L}\int_0^L \int_{\mathbf{R}} \sigma p(t,y',\sigma)\,d\sigma\,dy'\right] \frac{\partial p}{\partial \sigma}(t,y,\sigma) \\ & + D(p)\,\frac{\partial^2 p}{\partial \sigma^2}(t,y,\sigma) - H_1 p(t,y,\sigma) + \frac{D(p)}{\alpha}\delta_0,\end{aligned}$$

Family indexed by $y \in]0,L[$ of PDE in (t,σ) coupled through the term $\int_0^L \int_{\mathbf{R}} \sigma p(t,y',\sigma)\,d\sigma\,dy'$.

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Theorem (E. Cancès and CLB). For $\rho = 0$.

- Existence and uniqueness. For $V \in H^1_t$ and p_0 such that $D(p_0(y)) > 0$ for all y, the multiscale model has a unique solution $(u; p)$.
- Long-time limit. For α large enough, for V_∞ small enough, for $\mathcal{C}$ small enough, if

$$|V(t) - V_\infty| \leq \mathcal{C} f(t) \quad \text{with} \quad |f(t)| \leq 1 \quad \text{and} \quad f(t) \underset{t\to+\infty}{\longrightarrow} 0,$$

and if p_0 is close enough to p_∞ [unique steady state associated with V_∞/L for which $D(p_\infty) > 0$], then

$$(u(t), p(t)) \underset{t\to+\infty}{\longrightarrow} (u_\infty; p_\infty) \qquad \text{at least in } L^1_y \times L^1_{y,\sigma}.$$

Discrete and Continuous dynamical Systems B, Vol. 6, No. 3, pp 449-470, 2006,

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Multiscale model: long-time behaviour

The long-time limit is obtained by using the entropy function

$$S_2(y,t) = \int_{\mathbf{R}} \left(\frac{p(t,y,\sigma)}{p_\infty(\sigma)} - 1 \right)^2 p_\infty(\sigma)\, d\sigma$$

and by writing an equation of the form

$$\frac{d\mathcal{S}}{dt} + \epsilon \mathcal{S} \leq C \, |V(t) - V_\infty|$$

for the quantity

$$\mathcal{S}(t) = \int_0^L \sqrt{S_2(t,y)}\, dy$$

Numerical issues

We recall the mesoscopic equation is a parabolic equation which is

- nonlinear,
- nonlocal,
- possibly degenerate,
- with a singular r.h.s.,
- set on an unbounded domain.

$$\partial_t p = -\partial_\sigma p + D(p)\,\partial_{\sigma\sigma} p - \chi_{\mathbf{R}\setminus[-\sigma_c,\sigma_c]}(\sigma)\,p + D(p)\delta_0(\sigma)$$

$$D(p) = \int_{|\sigma|>\sigma_c} p$$

All constants to one, for simplicity.

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Numerical issues

Two approaches

- deterministic: finite-differences in space, operator splitting in time: advection (upwind, Lax-Friedrichs), diffusion (implicit Euler), source (exact)
- stochastic

Question: numerical analysis of time-splitting (say, Strang) for time-dependent operators $e^{S/2}e^{A/2}e^{D}e^{A/2}e^{S/2}$; Simpler situation, Take advection-diffusion

$$\partial_t p = -\partial_\sigma p + D(p(t), t, ...))\ \partial_{\sigma\sigma} p$$

What is the order of the usual splitting schemes?

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Numerical issues

Stochastic approach: simulate a diffusion process with jumps, nonlinear in the sense of McKean

$$\left\{\begin{array}{ll} \text{if} \quad |\sigma_{k,i}^n| < \sigma_c, \quad \text{then} \quad \sigma_{k,i}^{n+1} = \sigma_{k,i}^n + \frac{u_{k+1}^n - u_k^n}{\Delta y}\Delta t + \nu_k^n \sqrt{\Delta t}\, G_{k,i}^n, & \\ \text{otherwise} & \begin{array}{l} \text{if} \quad \omega_{k,i}^n \in [0, \Delta t] \quad \text{then} \quad \sigma_{k,i}^{n+1} = 0, \\ \text{otherwise} \quad \sigma_{k,i}^{n+1} = \sigma_{k,i}^n + \frac{u_{k+1}^n - u_k^n}{\Delta y}\Delta t + \nu_k^n \sqrt{\Delta t}\, G_{k,i}^n, \end{array} \end{array}\right.$$

where $\sigma_{k,i}^n$ is the state of constraint of the i-th “particle” at time $n\Delta t$, at the macropoint $(k+1/2)\Delta y$, and where $D_k^n = \frac{1}{N}\,\text{Card}\{i/ \quad |\sigma_{k,i}^n| > \sigma_c\}$, $\nu_k^n = \sqrt{2\nu D_k^n}$, $G_{k,i}^n$ and $\omega_{k,i}^n$ are two random variables following $\mathcal{N}(0,1)$ and the uniform law respectively.

Then the stress writes

$$T_k^n = \frac{1}{N}\sum_{i=1}^N \sigma_{k,i}^n.$$

See BenAlaya/Jourdain, J.Appl. Prob., to appear.

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Numerical issues

Solve at each macroscopic point (Gauss point) the mesoscopic equation, a PDE, parameterized by some macroscopic field

$$\partial_t p = -f(y,t))\, \partial_\sigma p + D(p)\, \partial_{\sigma\sigma} p - \chi_{\mathbf{R}\setminus[-\sigma_c,\sigma_c]}(\sigma)\, p + D(p)\delta_0(\sigma)$$

$(f(y,t) = -G_0\, \partial_y u(t,y))$.

Appropriate framework for Reduced Basis approaches (Maday/Patera/Rondqvist, Almroth et al. - 1970'-, Noor and Peters -1980'-)

Off-line: Solve the equation for a set of $f(y,t)$

On-line: use the solutions obtained as a basis set for expanding the solution for a general $f(y,t)$

Crucial ingredient: a-posteriori estimators to evaluate the quality of the solution, and possibly extend the basis on demand.

Preliminary tests (by S. Boyaval) on Fokker-Planck for polymeric fluids: very very (very) promising...

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Work in progress

- numerical analysis of the splitting scheme (dependence in time, issues of regularity)
- clarify mathematically the stochastic approach (coupled case)
- proceed with the reduced basis technology
- Extend the simulation (and, before, the model!) to dimensions 2 and 3

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