Polymeric multi-scale models

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Various approaches. FENE model

Navier-Stokes-Fokker-Planck system (finitely extensible nonlinear elastic type model):

$$\frac{\partial u}{\partial t} + (u \cdot \nabla_x)u - \nu\Delta_x u + \nabla_x p = \mathrm{div}_x \tau(\psi) + f,$$

$$\mathrm{div}_x u = 0$$

AND

$$\frac{\partial \psi}{\partial t} + (u \cdot \nabla_x)\psi + \nabla_q \cdot \Big[(\nabla_x u)q\psi\Big]$$

$$= \nabla_q \cdot \left(\nabla_q \psi + U'\left(\frac{|q|^2}{2}\right)\right) + \varepsilon\Delta_x\psi$$

where $\psi(t, x, q)$ is a probability density function.

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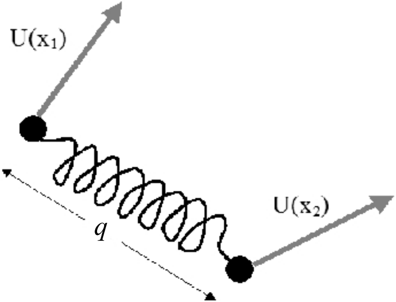
Dumbbell models: polymer chains $\sim$ dumbbell



We describe polymer chains as two beads connected by a spring, q is the vector connecting the beads.

FENE model - continuation

Extra stress tensor

$$\tau(\psi) = \int_D q \otimes q \; U'\left(\frac{|q|^2}{2}\right) \psi(t, x, q)\, dq$$

Spring potentials U:

- Hookean potential $U\left(\frac{|q|^2}{2}\right) = \frac{|q|^2}{2}$
- FENE $U\left(\frac{|q|^2}{2}\right) = \frac{b}{2} \ln\left(1 - \frac{|q|^2}{b}\right), \; |q| \leq \sqrt{b}$

Navier-Stokes-Fokker-Planck references:

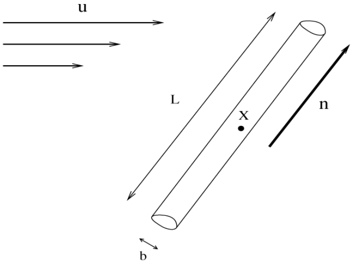
1. Barrett, J.W., Schwab, C., Süli, E., Existence of global weak solutions for some polymeric flow models. Math. Models Methods Appl. Sci. 15 (2005).
2. Barrett, J.W., Süli, E., Existence of global weak solutions to some regularized kinetic models of dilute polymers. SIAM Multiscale Modelling and Simulation 6 (2007).
3. Barrett, J.W., Süli, E., Existence of global weak solutions to dumbbell models for dilute polymers with microscopic cut-off. Mathematical Models and Methods in Applied Sciences 18 (2008).
4. Arnold, A.; Carrillo, J. A.; Manzini, C. Refined long-time asymptotics for some polymeric fluid flow models. Commun. Math. Sci. 8 (2010)

Modifications of the model

1 N. Masmoudi. Global existence of weak solutions to the FENE dumbbell model of polymeric flows. Invent. Math., 191 (2013)

2 Bulíček, M.; Málek, J.; Süli, E. Existence of global weak solutions to implicitly constituted kinetic models of incompressible homogeneous dilute polymers. Comm. Partial Differential Equations 38 (2013),

Different approaches - Doi model



We describe polymer chains as rigid rods

Various approaches. Doi model

Doi model for rod-like molecules

$$\partial_t u - \Delta_x u + \nabla_x p - \mathrm{div}\tau = 0, \quad \mathrm{div} u = 0$$

and

$$\partial_t f = -u \cdot \nabla_x f - \nabla_n \cdot (P_{n^\perp} \nabla_x u\, nf) + D\Delta_x f + D_r \Delta_n f$$

Here $\nabla_n, \nabla_n \cdot, \Delta_n$ denote gradient, divergence and Laplacian on S^2 and $P_{n^\perp} \nabla_x un = \nabla_x un - (n \cdot \nabla_x un)n$ denotes the projection of the vector $\nabla_x un$ on the tangent space in n. The last two terms on the right-hand side describe the Brownian effects: translational and rotational diffusion respectively.

Doi model - continuation

A velocity gradient $\nabla_x v$ distorts an isotropic distribution f which leads to an increase in entropy. Thermodynamic consistency requires that this is balanced by a stress tensor given by

$$\tau(t,x) = \nu k_B T \int_{S^2} (3n \otimes n - \mathrm{id}) f(t,x,n)\, dn.$$

Doi model - references

1. Otto, Felix; Tzavaras, Athanasios, Continuity of velocity gradients in suspensions of rod-like molecules. Comm. Math. Phys. 277 (2008),
2. Bae, Hantaek; Trivisa, Konstantina, On the Doi model for the suspensions of rod-like molecules: global-in-time existence. Commun. Math. Sci. 11 (2013),
3. Bae, Hantaek; Trivisa, Konstantina, On the Doi model for the suspensions of rod-like molecules in compressible fluids. Math. Models Methods Appl. Sci. 22 (2012)

Summary of the presented models

- FENE model
- Doi model

Structure

- Equation for macroscopic quantities v, p (Navier-Stokes), with microscopic quantities appearing in the additive stress tensor
- Equation for microscopic quantities (Fokker-Planck)

What is still not captured?

- polimerization
- fragmentation

Monomers-polymers models, e.g. prion proliferation

ψ is the distribution function of polymers of the length $r > r_0$ solving the following equation

$$\partial_t \psi(t,r) + \tau\phi(t)\partial_r \psi(t,r) = -\beta(r)\psi(t,r) + 2\int_r^\infty \beta(\tilde{r})\kappa(r,\tilde{r})\psi(t,\tilde{r})\, d\tilde{r}$$

- $\tau\phi(t)\partial_r\psi(t,r)$ – the gain in length of polymer chains due to polymerization with rate $\tau > 0$,
- $\beta(r)$ is the fragmentation rate, namely the length-dependent likelihood of splitting of polymers to monomers
- $\kappa(r,\tilde{r})$ is the probablity that a polymer will split into two polymers of length r and $\tilde{r} - r$,
- $-\beta(r)\psi(t,r)$ is the loss of polymers, subject to the splitting rate $\beta(r)$
- the last term is the count of all the polymers of length r resulting from the splitting of polymers of length greater than r.

Equation for monomers

The function $\phi(t,x)$ is the concentration of free monomers satisfying the equation

$$\partial_t \phi(t,x) = 2\int_0^{r_0} r \int_r^{\infty} \beta(\tilde{r})\kappa(r,\tilde{r})\psi(t,\tilde{r})\,d\tilde{r}\,dr - \phi(t,x)\int_{r_0}^{\infty} \tau\psi(t,r)\,dr.$$

- $2\int_0^{r_0} r \int_r^{\infty} \beta(\tilde{r})\kappa(r,\tilde{r})\psi(t,\tilde{r})\,d\tilde{r}\,dr$ represents the monomers gained when a polymer splits with at least one polymer shorter than the minimum length r_0
- $-\phi(t,x)\int_{r_0}^{\infty} \tau\psi(t,r)\,dr$ – the loss of monomers as they are polymerized

References for monomers-polymers models

1 Greer, Meredith L.; Pujo-Menjouet, Laurent; Webb, Glenn F. A mathematical analysis of the dynamics of prion proliferation. J. Theoret. Biol. 242 (2006)

2 Calvez, Vincent; Lenuzza, Natacha; Oelz, Dietmar; Deslys, Jean-Philippe; Laurent, Pascal; Mouthon, Franck; Perthame, Benoît. Size distribution dependence of prion aggregates infectivity. Math. Biosci. 217 (2009)

New approach: we couple the equation describing fluid flow with the equations capturing the process of (de-)polymerization.

Idea

The length of polymer chains influences viscosity of the fluid. Then the viscosity is not constant (non-newtonian fluid), but depends also on microscopic quantities.

Results

We show existence of weak solutions under the assumption of polynomial growth conditions of the Cauchy stress tensor.

Non-Newtonian-Smoluchowski fragmentation model, joint work in progress with E. Süli and M. Bulíček

Consider in $(0,T)\times\Omega$ the equations for the fluid solvent

$$\begin{aligned}\partial_t u(t,x)+&\mathrm{div}_x(u(t,x)\otimes u(t,x))+\nabla_x p(t,x)\\ &-\mathrm{div}_x\mathbf{S}(\psi(t,x,r),\mathbf{D}_x u(t,x))=f,\\ &\mathrm{div}_x u(t,x)=0,\end{aligned}$$

where the stress tensor is given by the formula

$$\mathbf{S}(\psi(t,x,r),\mathbf{D}_x u(t,x)):=\nu(\psi(t,x,r),\mathbf{D}_x u(t,x))\mathbf{D}_x u(t,x)$$

and $\nu:\mathbb{R}_+\times\mathbb{R}_+\to\mathbb{R}_+$ is the generalized viscosity which depends on the shear rate and $\psi:(0,T)\times\Omega\times\mathbb{R}_+\to\mathbb{R}_+$ is the distribution function of polymers.

Non-Newtonian-Smoluchowski fragmentation model

$\psi : (0, T) \times \Omega \times \mathbb{R}_+ \to \mathbb{R}_+$ is the distribution function of polymers solving the following equation

$$\begin{aligned}\partial_t \psi(t,x,r) + u(t,x)\nabla_x \psi(t,x,r) + \tau\phi(t,x)\partial_r \psi(t,x,r) \\ - A(r)\Delta_x \psi(t,x,r) = -\beta(r,u,\mathbf{D}_x u)\psi(t,x,r) \\ + 2\int_r^\infty \beta(\tilde{r},u,\mathbf{D}_x u)\kappa(r,\tilde{r})\psi(t,x,\tilde{r})\,d\tilde{r},\end{aligned}$$

- $\tau > 0$ is the polimerization rate,
- $\beta(r,\cdot,\cdot)$ is the fragmentation rate of polymers of size r, which depends also on macroscopic quantities, namely on the velocity of the solvent and the shear rate,
- $A(r) \to 0$ as $r \to \infty$

Non-Newtonian-Smoluchowski fragmentation model - cont.

The function $\phi(t,x)$ is the concentration of free monomers satisfying

$$\partial_t \phi(t,x) + u(t,x)\nabla_x \phi(t,x) - A_0 \Delta_x \phi(t,x) \\ = -\,\phi(t,x) \int_0^\infty \tau \psi(t,x,r)\,dr.$$

Conservation of mass

For showing

$$\frac{d}{dt}\left[\int_\Omega \phi(t,x)\,dx + \int_0^\infty r\int_\Omega \psi(t,x,r)\,dx\,dr\right] = 0$$

it is important that for $\kappa(r,\tilde{r})$ – the probablity that a polymer will split into two polymers of length r and $\tilde{r}-r$ it holds

$$\int_0^{\tilde{r}} \kappa(r,\tilde{r})\,dr = 1, \quad \int_0^{\tilde{r}} r\kappa(r,\tilde{r})\,dr = \frac{\tilde{r}}{2}.$$

Toy model for situation $A(r) = 0$, big amount of monomers and small amount of polymers

Navier-Stokes size-structured model:

$$\frac{\partial u(t,x)}{\partial t} + \mathrm{div}_x(u(t,x) \otimes u(t,x)) + \nabla_x p(t,x) = \mathrm{div}_x \mathbf{S}(\psi, D_x u(t,x)) + f(t,x),$$

$$\mathrm{div}_x u(t,x) = 0,$$

with Dirichlet BC for u **AND**

$$\mathbf{S}(\psi, D_x u(t,x)) := \nu \left(\int_0^\infty \gamma(r)\psi(t,x,r)dr, |D_x u(t,x)| \right) D_x u(t,x),$$

$\nu \in C(\mathbb{R};\mathbb{R})$ where $\psi(t,x,r)$ is the function representing density of the polymer molecules of length r at time t at x.

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Size-structure of a polymer molecule

$\psi(t,x,r)$ is the function representing density of polymer molecules of length r at time t at x.

$$\partial_t \psi(t,x,r) + \mathrm{div}_x(u(t,x)\psi(t,x,r))$$

$$= \tau(r)\partial_r \psi(t,x,r) - \beta(r)\psi(t,x,r) + 2\int_r^\infty \beta(\tilde{r})\kappa(r,\tilde{r})\psi(t,x,\tilde{r})d\tilde{r}$$

- $\beta(r)$ - the rate of fragmentation

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Weak sequential stability

It is essential to show that

$$\int_0^\infty \gamma(r)\psi^n(t,x,r)dr \to \int_0^\infty \gamma(r)\psi(t,x,r)dr$$

a.e. in Q_T. For this purpose consider the reduced problem for $\mu : [0,T] \times \mathbb{R}_+ \to \mathbb{R}_+$ (without the transport term)

$$\frac{\partial}{\partial t}\mu(t,r) = \tau(r)\frac{\partial}{\partial r}\mu(t,r) - \beta(r)\mu(t,r) + 2\int_z^\infty \beta(r)\kappa(r,\tilde{r})\mu(t,\tilde{r})d\tilde{r}$$

$$\mu(0,z) = \mu_0$$

Dual problem to the reduced problem

The dual problem (backward in time) to the reduced problem

$$\partial_t \varphi(t,r)$$

$$= \partial_r(\tau(r)\varphi(t,r)) + \beta(r)\varphi(t,r) - 2\int\limits_0^\infty \beta(\tilde{r})\kappa(\tilde{r},r)\varphi(t,\tilde{r})d\tilde{r}$$

$$\varphi(T_1,z) = \gamma(r)$$

where $T_1 \in [0, T]$ and

$$\frac{d}{dt}\int_0^\infty \mu(t,r)\varphi(t,r)dr = 0$$

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We multiply the original equation for ψ

$$\partial_t \psi + \mathrm{div}_x(u\psi) = \partial_r(\tau\psi) - \beta\psi + 2\int_r^\infty \beta(\tilde{r})\kappa(r,\tilde{r})\psi(t,x,\tilde{r})\; d\tilde{r}$$

by the solution to the dual problem to the reduced problem, namely by φ and integrate over $(0,\infty)$ w.r.t. r to obtain

$$\partial_t \left(\int_0^\infty \varphi\psi\, dr\right) - \int_0^\infty \psi\partial_t\varphi\, dr + u\cdot\nabla_x \left(\int_0^\infty \varphi\psi\, dr\right)$$
$$= \int_0^\infty \varphi\tau\partial_r\psi\, dr - \int_0^\infty \varphi\beta\psi\, dr + 2\int_0^\infty \psi \int_0^\infty \beta(\tilde{r})\kappa(\tilde{r},r)\varphi(t,r)\, d\tilde{r}\, dr$$

Denoting

$$g_\varphi(t,x) := \int_0^\infty \varphi(t,r)\psi(t,x,r)\,dr$$

we get

$$\partial_t g_\varphi + u\cdot\nabla_x g_\varphi =$$
$$\int_0^\infty \psi\left(\partial_t\varphi - \partial_r(\tau\varphi) - \varphi\beta + 2\int_0^\infty \beta(\tilde r)\kappa(\tilde r, r)\varphi(t,\tilde r)\,d\tilde r\right)dr$$

which is the homogeneous linear transport equation

$$\partial_t g_\varphi + u\cdot\nabla_x g_\varphi = 0$$

for which the renormalization techniques can be used.

What was essential in this procedure?

Reduced problem for $\mu : [0, T] \times \mathbb{R}_+ \to \mathbb{R}_+$ (without the transport term)

$$\partial_t \mu(t, r) = \tau(r)\partial_r \mu(t, r) - \beta(r)\mu(t, r) + 2\int_r^\infty \beta(r)\kappa(r, \tilde{r})\mu(t, \tilde{r})d\tilde{r}$$

$$\mu(0, z) = \mu_0$$

τ, β are independent of x

Integral operators

$$\partial_t \psi(t,x) + u(t,x) \cdot \nabla_x \psi(t,x) = \int \gamma(x,y)\psi(t,x)dy,$$

$$\psi(0,x) = \bar{\psi}(x).$$

The equation for a renormalized quantity $\beta(\psi)$ is not a linear equation anymore.

Thank you for your attention!