Kinetic models of dilute polymeric fluids: analysis and approximation

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Dedicated to the memory of John W. Barrett

29 June 1955 Wimbledon – 30 June 2019 Wimbledon

ICIAM 2023 TOKYO

Overview

- Mathematical analysis of kinetic models of dilute polymeric fluids (Navier–Stokes–Fokker–Planck (NSFP) systems):

  $\longrightarrow$ existence of global-in-time large-data weak solutions
  $\longrightarrow$ rigorous macroscopic closure

- Numerical approximation of Navier–Stokes–Fokker–Planck systems

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R.B. Bird, C.F. Curtiss, R.C. Armstrong, O. Hassager:
Dynamics of Polymeric Liquids, Vol. II: Kinetic Theory. Wiley, 1987.

Masao Doi: Introduction to Polymer Physics. OUP, 1995.

Toshihiro Kawakatsu: Statistical Physics of Polymers. Springer, 2004.

H.C. Öttinger: Stochastic Processes in Polymeric Fluids. Springer, 1996.

Incompressible Newtonian fluid (Navier–Stokes equations)

Find $u : \Omega \times [0,T] \to \mathbb{R}^d$ and $p : \Omega \times (0,T] \to \mathbb{R}$ such that:

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\begin{aligned}
\nabla_x \cdot u &= 0 && \text{in } \Omega \times (0,T], \\
\frac{\partial(\rho\, u)}{\partial t} + \nabla_x \cdot (\rho\, u \otimes u) - \nabla_x \cdot (2\mu\, D(u) - pI) &= \rho f && \text{in } \Omega \times (0,T], \\
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Notation:

ρ	mass density	u	velocity	$\mu > 0$	dynamic viscosity
p	pressure	f	density of body forces	$D(u) = \frac{1}{2}\left((\nabla_x u) + (\nabla_x u)^{\mathrm{T}}\right)$	

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History:

Navier (1822)
Poisson (1829)
} – based on molecular arguments

Saint Venant (1843)
Stokes (1845)
} – based on continuum mechanics arguments

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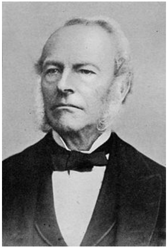
Claude Louis Marie Henri Navier

1785–1836



George Gabriel Stokes

1819–1903

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Jean Leray
1906–1998

Eberhard Hopf
1902–1983

Olga Ladyzhenskaya
1922–2004

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Formal energy identity:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \frac{1}{2}\, \rho |u(x,t)|^2 \,\mathrm{d}x + 2\mu \int_\Omega |D(u(x,t))|^2 \,\mathrm{d}x = \int_\Omega \rho f(x,t) \cdot u(x,t) \,\mathrm{d}x$$

for all $t \in (0,T]$.

Compressible Newtonian fluid (Navier–Stokes equations)

Compressible, barotropic, viscous, isothermal Newtonian fluid in a bounded domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, and $T > 0$. Find:

$$\begin{aligned} &\text{density} \quad \rho : (x,t) \in \Omega \times [0,T] \mapsto \rho(x,t) \in \mathbb{R}, \\ &\text{velocity} \quad u : (x,t) \in \overline{\Omega} \times [0,T] \mapsto u(x,t) \in \mathbb{R}^d, \qquad \text{such that} \end{aligned}$$

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Balance of mass:

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$$u = 0 \qquad \text{on } \partial\Omega \times (0,T],$$
$$(\rho\, u)(x,0) = (\rho_0\, u_0)(x) \qquad x \in \Omega.$$

$S(u)$ is the stress tensor, defined by

$$S(u) := 2\mu^S \left[D(u) - \tfrac{1}{d}(\nabla_x \cdot u)\, I\right] + \mu^B\, (\nabla_x \cdot u)\, I,$$

where I is the $d \times d$ identity matrix,

$$D(u) := \tfrac{1}{2}(\nabla_x\, u + (\nabla_x\, u)^{\mathrm{T}})$$

and $\mu^S > 0$, $\mu^B \geq 0$ are the shear- and bulk-viscosity coefficient.

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Existence of global weak solutions ($d = 3$):

- P.-L. Lions (1998, $\gamma \geq \frac{9}{5}$), E. Feireisl (2001, $\gamma > \frac{3}{2}$).

Formal energy identity

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left[\frac{1}{2}\rho\,|u|^2 + P(\rho)\right]\mathrm{d}x + 2\mu^S\int_\Omega \left|D(u) - \frac{1}{d}\left(\nabla_x \cdot u\right) I\right|^2 \mathrm{d}x + \mu^B\int_\Omega |\nabla_x \cdot u|^2\,\mathrm{d}x = \int_\Omega \rho\, f\cdot u\,\mathrm{d}x$$

for all $t \in (0, T]$, with

$$P(\rho) := \frac{p(\rho)}{\gamma - 1}.$$

Part 1.

The mathematical model: kinetic theory of dilute polymers

Navier–Stokes–Fokker–Planck systems

M. Renardy (1991, SIAM J. Math. Anal.):
An existence theorem for model equations from kinetic theories of polymer solutions

B. Jourdain, T. Lelièvre, C. Le Bris (2004, J. Funct. Anal.):
Existence of solution for a micro-macro model of polymeric fluid: the FENE model

W. E, T. Li, P. Zhang (2004, Comm. Math. Phys.):
Well-posedness for the dumbbell model of polymeric fluids

J.W. Barrett, C. Schwab, E. Süli (2005, M3AS):
Existence of global weak solutions for some polymeric flow models

P. Constantin (2005, Comm. Math. Sci.):
Nonlinear Fokker–Planck–Navier–Stokes systems

P.-L. Lions, N. Masmoudi (2007, C. R. Math. Acad. Sci. Paris):
Global existence of weak solutions to some micro-macro models

F. Otto, T. Tzavaras (2008, Comm. Math. Phys.):
Continuity of velocity gradients in suspensions of rod-like molecules

N. Masmoudi (2012, Invent. Mathem.):
Global existence of weak solutions to the FENE dumbbell model of polymeric flows

The mathematical model

The solvent is a compressible, barotropic, viscous, isothermal Newtonian fluid in a bdd. domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, and $T > 0$. Find:

density $\quad \rho : (x, t) \in \Omega \times [0, T] \mapsto \rho(x, t) \in \mathbb{R}$,

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Balance of linear momentum (Navier–Stokes equation + elastic effects):

$$\begin{aligned} \frac{\partial (\rho\, u)}{\partial t} + \nabla_x \cdot (\rho\, u \otimes u) - \nabla_x \cdot S(u) + \nabla_x\, p(\rho) &= \rho\, f + \nabla_x \cdot \tau && \text{in } \Omega \times (0,T], \\ u &= 0 && \text{on } \partial\Omega \times (0,T], \\ (\rho\, u)(x,0) &= (\rho_0\, u_0)(x) && x \in \Omega. \end{aligned}$$

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BUT WHAT IS τ ?

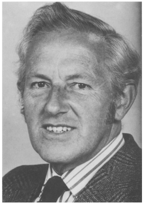
a) Macroscopic approach: Oldroyd-B model

On the formulation of rheological equations of state

By J. G. Oldroyd, *Courtaulds Limited, Research Laboratory, Maidenhead, Berks.*

(*Communicated by A. H. Wilson, F.R.S.—Received* 26 *July* 1949—
Revised 4 *November* 1949)

The invariant forms of rheological equations of state for a homogeneous continuum, suitable for application to all conditions of motion and stress, are discussed. The right invariance properties can most readily be recognized if the frame of reference is a co-ordinate system convected with the material, but it is necessary to transform to a fixed frame of reference in order to solve the equations of state simultaneously with the equations of continuity and of motion. An illustration is given of the process of formulating equations of state suitable for universal application, based on non-invariant equations obtained from a simple experiment or structural theory. Anisotropic materials, and materials whose properties depend on previous rheological history, are included within the scope of the paper.



James G. Oldroyd
1921–1982

J.G. Oldroyd: On the formulation of rheological equations of state.
Proc. Royal Soc., Ser. A, Math. & Phys. Sci., 200 (1063): 523–541, 1950.

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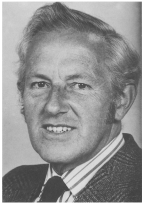

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$$\tau + \lambda_1 \overset{\nabla}{\tau} = 2\mu_p D(u) \qquad \begin{cases} \lambda_1 = \text{characteristic relaxation time} > 0 \\ \mu_p = \text{polymeric viscosity} > 0 \end{cases}$$

$$\overset{\nabla}{\tau} := \frac{\partial \tau}{\partial t} + u \cdot \nabla_x \tau - (\nabla_x u)\tau - \tau(\nabla_x u)^{\mathrm{T}}.$$

[Upper-convected (Oldroyd) derivative]

Hence the Oldroyd-B evolution equation for the polymeric stress tensor is:

$$\tau + \lambda_1 \left(\frac{\partial \tau}{\partial t} + u \cdot \nabla_x \tau - (\nabla_x u)\tau - \tau(\nabla_x u)^{\mathrm{T}} \right) = 2\mu_p D(u).$$

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M. Renardy and B. Thomases. A mathematician's perspective on the Oldroyd-B model: progress and future challenges. J. Non-Newton. Fluid Mech. 293 (2021).

The diffusive Oldroyd-B model ($\varepsilon > 0$ stress-diffusion coefficient):

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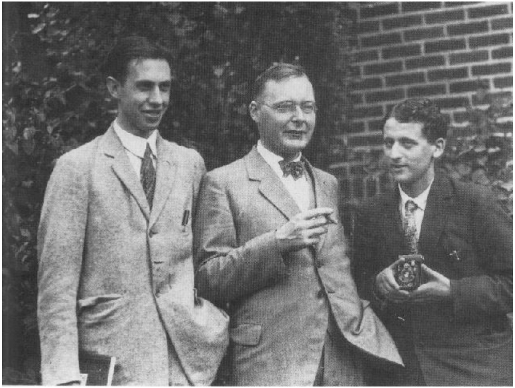
A.W. El-Kareh, L.G. Leal. Existence of solutions for all Deborah numbers for a non-Newtonian model modified to include diffusion. J. Non-Newton. Fluid Mech. 33 (1989).

J. Málek, V. Průša, T. Skřivan, E. Süli. Thermodynamics of viscoelastic rate-type fluids with stress-diffusion. Physics of Fluids, 30, 023101 (2018).

b) Microscopic approach: Kinetic theory of dilute polymers

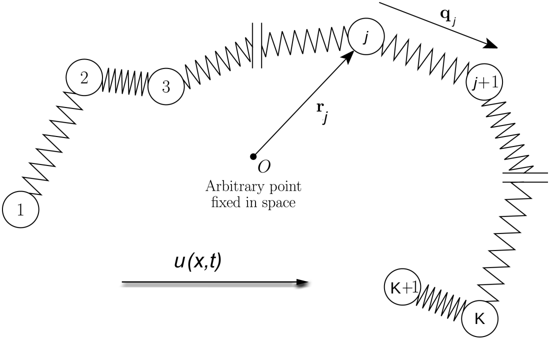


George Uhlenbeck, Hans Kramers and Samuel Goudsmit
(Ann Arbor, Michigan – around 1928).

Werner Kuhn. Über die Gestalt von Fadenmolekülen in Lösung. Experientia. vol. 3, pp. 315–318 (1947) [Original paper: Kolloid-Zeitschrift (1934)].

Hans A. Kramers: The viscosity of macromolecules in a streaming fluid, Physica, 11, 1944.

Definition of the elastic extra stress tensor τ



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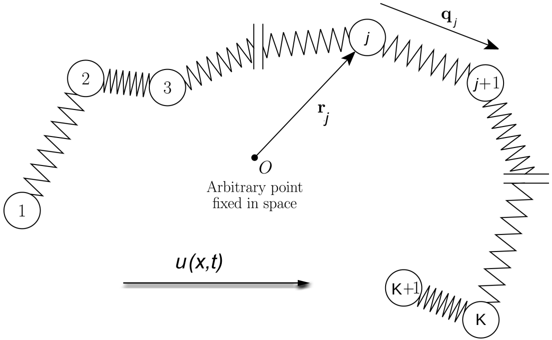

In the absence of external forces and neglecting inertial effects Langevin's equation for the i-th bead in this model is, for $i = 1, \ldots, K+1$:

$$0 = \underbrace{-\zeta \left(\mathrm{d}r_i - u(r_i, \cdot)\,\mathrm{d}t \right)}_{\text{Hydrodynamic drag force}} + \underbrace{\sum_{j=1}^{K} G_{ij}\, F_j(q_j)\,\mathrm{d}t}_{\text{Intramolecular force}} + \underbrace{\sqrt{2\, k_B\, \mathtt{T}\, \zeta}\;\mathrm{d}W_i}_{\text{Brownian force}}\,.$$

After nondimensionalization and the linear change of variables:

$$x := \frac{1}{K+1}\sum_{i=1}^{K+1} r_i, \qquad q_i := r_{i+1} - r_i, \quad i = 1, \dots, K,$$

the probability density function ψ solves the following Fokker–Planck eqn.:

$$\frac{\partial \psi}{\partial t} + \nabla_x \cdot (u\,\psi) + \sum_{i=1}^{K} \nabla_{q_i} \cdot \left((\nabla_x u)\, q_i\, \psi - \frac{1}{4\lambda}\sum_{j=1}^{K} A_{ij}\, F_i(q_j)\psi \right)$$
$$= \underline{\varepsilon\, \Delta_x \psi} + \frac{1}{4\,\lambda}\sum_{i=1}^{K}\sum_{j=1}^{K} A_{ij} \nabla_{q_i} \cdot \left(\nabla_{q_j}\, \psi\right).$$

After nondimensionalization and the linear change of variables:

$$x := \frac{1}{K+1}\sum_{i=1}^{K+1} r_i, \qquad q_i := r_{i+1} - r_i, \quad i = 1, \ldots, K,$$

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A. Bhave, R.C. Armstrong, R.A. Brown. Kinetic theory and rheology of dilute, non-homogeneous polymer solutions. J. Chem. Phys., 95 (4), 2988–3000 (1991).

M. Dostalík, J. Málek, V. Průša, E. Süli. A simple approach to thermodynamically consistent modelling of non-isothermal flows of dilute compressible polymeric fluids. Fluids, 5(3), 29 pp. (2020).

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$$= \underline{\varepsilon\, \Delta_x \psi} + \frac{1}{4\,\lambda} \sum_{i=1}^{K} \sum_{j=1}^{K} A_{ij} \nabla_{q_i} \cdot \left(\nabla_{q_j} \psi \right).$$

$\varepsilon := \frac{1}{4\,\lambda\,(K+1)} \left(\frac{\ell_0}{L_0} \right)^2$ is the centre-of-mass diffusion coefficient;

$\lambda := (\zeta/4\mathtt{H})(U_0/L_0) = \mathrm{De}$ is the Deborah number;

$F_i(q_i) = H\, U_i'(\frac{1}{2}|q_i|^2) q_i$, $i = 1, \dots, K$: spring forces; $H > 0$ the spring constant;

$A := G^{\mathrm{T}} G \in \mathbb{R}^{K \times K}_{\mathsf{symm}}$: Rouse matrix.

A) Finitely extensible nonlinear elastic (FENE) model by Warner (1972):

$$U_i(\tfrac{1}{2}|q_i|^2) := -\frac{1}{2} b_i \log\left(1 - \frac{|q_i|^2}{b_i}\right) \to +\infty \quad \text{as} \quad |q_i|^2 \nearrow b_i < \infty,$$

defined on

$$D_i := \{q_i \in \mathbb{R}^d \,:\, |q_i|^2 < b_i\}, \qquad b_i > 0, \quad i = 1, \dots, K.$$

B) Hookean model: $U_i(\frac{1}{2}|q_i|^2) = \frac{1}{2}|q_i|^2$ for $q_i \in D_i = \mathbb{R}^d$, $i = 1, \dots, K$.

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The Maxwellian is defined by

$$M(q) := \prod_{i=1}^{K} M_i(q_i), \qquad q := (q_1, \dots, q_K) \in D := \bigtimes_{i=1}^{K} D_i.$$

where

$$M_i(q_i) := \frac{\mathrm{e}^{-U_i(\frac{1}{2}|q_i|^2)}}{\int_{D_i} \mathrm{e}^{-U_i(\frac{1}{2}|q_i|^2)}\, \mathrm{d}q_i}, \qquad i = 1, \dots, K.$$

Thus the Fokker–Planck equation then becomes:

Fokker–Planck equation:

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$$= \underline{\varepsilon\,\Delta_x \psi} + \frac{1}{4\,\lambda} \sum_{i=1}^{K} \sum_{j=1}^{K} A_{ij} \nabla_{q_i} \cdot \left(M\, \nabla_{q_j} \left(\frac{\psi}{M} \right) \right) \quad \text{on } \Omega \times D \times (0,T].$$

Kramers–Kirkwood stress tensor:

$$\tau(\psi)(x,t) := k\Bigg(\sum_{i=1}^{K}\int_D \psi(x,q,t)\, q_i\, q_i^{\mathrm{T}}\, U_i'\left(\tfrac{1}{2}|q_i|^2\right)\mathrm{d}q - (K+1)I\int_D \psi(x,q,t)\,\mathrm{d}q\Bigg) - \left(\int_{D\times D}\gamma(q,q')\,\psi(x,q,t)\,\psi(x,q',t)\;\mathrm{d}q\;\mathrm{d}q'\right)I.$$

Here, $\gamma : D\times D \to \mathbb{R}_{\geq 0}$ is a smooth, time-independent, x-independent and ψ-independent interaction kernel, which we shall henceforth consider to be

$$\gamma(q,q') \equiv \mathfrak{z} \geq 0,$$

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$K = 1 \longrightarrow$ dumbbell model

Part 2.

Mathematical analysis of the model: existence of global weak solutions

to Navier–Stokes–Fokker–Planck systems

Formal energy identity

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left[\frac{1}{2}\rho\,|u|^2 + P(\rho) + \mathfrak{z}\left(\int_D \psi\,\mathrm{d}q\right)^2 + k\int_D M\,\mathcal{F}\left(\frac{\psi}{M}\right)\,\mathrm{d}q\right]\mathrm{d}x \\
&\quad + 2\mu^S\int_\Omega \left|D(u) - \frac{1}{d}\left(\nabla_x\cdot u\right) I\right|^2\mathrm{d}x + \mu^B\int_\Omega |\nabla_x\cdot u|^2\,\mathrm{d}x \\
&\quad + 2\varepsilon\,\mathfrak{z}\int_\Omega \left|\nabla_x\left(\int_D \psi\,\mathrm{d}q\right)\right|^2\mathrm{d}x + \varepsilon\,k\int_{\Omega\times D} M\left|\nabla_x\sqrt{\frac{\psi}{M}}\right|^2\mathrm{d}q\,\mathrm{d}x \\
&\quad + \frac{k}{4\lambda}\sum_{i=1}^{K}\sum_{j=1}^{K} A_{ij}\int_{\Omega\times D} M\,\nabla_{q_j}\sqrt{\frac{\psi}{M}}\cdot\nabla_{q_i}\sqrt{\frac{\psi}{M}}\,\mathrm{d}q\,\mathrm{d}x \\
&\qquad = \int_\Omega \rho\,f\cdot u\,\mathrm{d}x \qquad \text{for all } t\in(0,T],
\end{aligned}
$$

where $\mathcal{F}(s) := s(\log s - 1) + 1$ for $s \geq 0$ and $\mathfrak{z} > 0$.

Formal energy identity $\longrightarrow$ Existence of global weak solutions

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left[\frac{1}{2}\rho\,|u|^2 + P(\rho) + \mathfrak{z}\left(\int_D \psi\,\mathrm{d}q\right)^2 + k\int_D M\,\mathcal{F}\left(\frac{\psi}{M}\right)\,\mathrm{d}q\right]\mathrm{d}x \\
&\quad + 2\mu^S\int_\Omega \left|D(u) - \frac{1}{d}\,(\nabla_x\cdot u)\,I\right|^2 \mathrm{d}x + \mu^B\int_\Omega |\nabla_x\cdot u|^2\,\mathrm{d}x \\
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$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left[\frac{1}{2}\rho\,|u|^2 + P(\rho) + \mathfrak{z}\left(\int_D \psi\,\mathrm{d}q\right)^2 + k\int_D M\,\mathcal{F}\left(\frac{\psi}{M}\right)\,\mathrm{d}q\right]\mathrm{d}x$$

$$+\ 2\mu^S\int_\Omega \left|D(u) - \frac{1}{d}\,(\nabla_x\cdot u)\,I\right|^2\mathrm{d}x + \mu^B\int_\Omega |\nabla_x\cdot u|^2\,\mathrm{d}x$$

$$+\,2\varepsilon\,\mathfrak{z}\int_\Omega\left|\nabla_x\left(\int_D\psi\,\mathrm{d}q\right)\right|^2\mathrm{d}x + \varepsilon\,k\int_{\Omega\times D} M\left|\nabla_x\sqrt{\frac{\psi}{M}}\right|^2\mathrm{d}q\,\mathrm{d}x$$

$$+\ \frac{k}{4\lambda}\sum_{i=1}^K\sum_{j=1}^K A_{ij}\int_{\Omega\times D} M\,\nabla_{q_j}\sqrt{\frac{\psi}{M}}\cdot\nabla_{q_i}\sqrt{\frac{\psi}{M}}\,\mathrm{d}q\,\mathrm{d}x$$

$$=\int_\Omega \rho\,f\cdot u\,\mathrm{d}x \qquad \text{for all } t\in(0,T],$$

where $\mathcal{F}(s) := s(\log s - 1) + 1$ for $s \geq 0$.

Idea: construct an approximating sequence obeying an energy inequality

Formal energy identity $\longrightarrow$ Existence of global weak solutions

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left[\frac{1}{2}\rho\,|u|^2 + P(\rho) + \mathfrak{z}\left(\int_D \psi\,\mathrm{d}q\right)^2 + k\int_D M\,\mathcal{F}\left(\frac{\psi}{M}\right)\,\mathrm{d}q\right]\mathrm{d}x \\
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$\longrightarrow$ Energy inequality yields weak convergence of the approximating sequence

Formal energy identity $\longrightarrow$ Existence of global weak solutions

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$$+\ \frac{k}{4\lambda}\sum_{i=1}^{K}\sum_{j=1}^{K} A_{ij}\int_{\Omega\times D} M\,\nabla_{q_j}\sqrt{\frac{\psi}{M}}\cdot\nabla_{q_i}\sqrt{\frac{\psi}{M}}\,\mathrm{d}q\,\mathrm{d}x$$

$$= \int_\Omega \rho\,f\cdot u\,\mathrm{d}x \qquad \text{for all } t\in(0,T],$$

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Idea: construct an approximating sequence obeying an energy inequality

$\longrightarrow$ Energy inequality yields weak convergence of the approximating sequence

$\longrightarrow$ Most difficult step: passage to limit in nonlinear terms requires strong convergence

Theorem

For any FENE-type spring-potential, the compressible NSFP system has a global-in-time large-data entropy-dissipative weak solution.

J.W. Barrett, E. Süli:
Existence of global weak solutions to compressible barotropic finitely extensible nonlinear bead-spring chain models for dilute polymers. M3AS 26(3) (2016) 469–568.

E. Feireisl, Y. Lu, E. Süli:
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What about the Hookean model and its rigorous macroscopic closure?

Part 3.

The problem of rigorous macroscopic closure

Hookean Navier–Stokes–Fokker–Planck system $\longrightarrow$ diffusive Oldroyd-B system

$$\int_{\mathbb{R}^d} \text{(Fokker–Planck equation)}\; q\, q^{\mathrm{T}}\, \mathrm{d}q = \text{diffusive Oldroyd-B model (?)}$$

- J. W. Barrett, E. Süli. Existence of global weak solutions to the kinetic Hookean dumbbell model for incompressible dilute polymeric fluids. J. Nonlin. Anal., Ser. B: Real World Applications. 36 (2018) 362–395.
- T. Dębiec, E. Süli. Corotational Hookean models of dilute polymeric fluids: existence of global weak solutions, weak-strong uniqueness, equilibration and macroscopic closure. SIAM J. Math. Anal. 55(1) (2023).
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Theorem

The NSFP system with a Hookean spring model has a large-data global-in-time generalised dissipative solution (u, ψ, m_{NS}) *in both 2D and 3D, where* $m_{NS} \in L^\infty(0,T;\mathcal{M}^+(\overline{\Omega};\mathbb{R}^{d\times d}))$ *is a defect measure. This solution is entropy-dissipative, i.e., for a.e.* $t \in (0,T)$*:*

$$\frac{1}{2}\int_\Omega |u(t)|^2 \,\mathrm{d}x + \int_{\Omega\times\mathbb{R}^d} M\mathcal{F}(\psi(t)/M)\,\mathrm{d}q\,\mathrm{d}x + 2\mu\int_0^t\int_\Omega |D(u(s))|^2\,\mathrm{d}x\,\mathrm{d}s$$
$$+ 4\int_0^t\int_{\Omega\times\mathbb{R}^d} M\left(\varepsilon\left|\nabla_x\sqrt{\psi/M}\right|^2 + \left|\nabla_q\sqrt{\psi/M}\right|^2\right)\mathrm{d}q\,\mathrm{d}x\,\mathrm{d}s$$
$$\leq \frac{1}{2}\int_\Omega |u_0|^2\,\mathrm{d}x + \int_{\Omega\times\mathbb{R}^d} M\mathcal{F}(\psi_0/M)\,\mathrm{d}q\,\mathrm{d}x.$$

Theorem

- *If* $\boxed{d=2}$, *then*

$$\sigma(\psi) + m_{NS}, \qquad \textit{where} \qquad \sigma(\psi)(x,t) := \int_{\mathbb{R}^2} \psi(x,q,t)\, q\, q^{\mathrm{T}}\, \mathrm{d}q,$$

  satisfies the diffusive Oldroyd-B stress evolution equation. Furthermore, if $u_0 \in W^{1,2}(\Omega;\mathbb{R}^2)$ *and* $\sigma(\psi_0) \in W_n^{1/2,4/3}(\Omega;\mathbb{R}^{2\times 2})$*, then* $m_{NS} = 0$ *and:*
  - (u,ψ) *is a weak solution to the Hookean NSFP system;*
  - $(u,\sigma(\psi))$ *is the unique weak solution to the diffusive Oldroyd-B system.*

- *If* $\boxed{d=3}$, $\partial_t u \in L^1(0,T;L^2(\Omega;\mathbb{R}^3))$ *and* $\nabla_x u \in L^1(0,T;C(\overline{\Omega};\mathbb{R}^{3\times 3}))$*, then* $m_{NS} = 0$ *and* (u,ψ) *is a weak solution to the Hookean NSFP system.*

Part 4.

Numerical approximation

of Navier–Stokes–Fokker–Planck systems

Challenges

The construction of a provably convergent numerical method for the coupled Navier–Stokes–Fokker–Planck system is a nontrivial problem.

J. W. Barrett, E. Süli. Finite element approximation of finitely extensible nonlinear elastic dumbbell models for dilute polymers. ESAIM M2AN 46 (2012), 949–978.

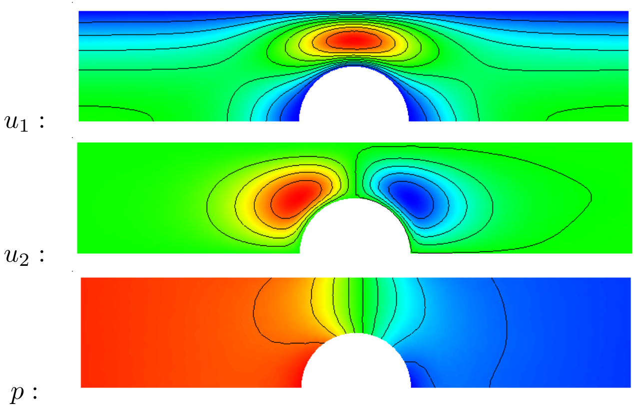
The Fokker–Planck equation is a high-dimensional parabolic PDE
⇝ curse of dimensionality:

$$\frac{\partial\psi}{\partial t} + \nabla_x \cdot (u\,\psi) + \sum_{i=1}^{K} \nabla_{q_i} \cdot ((\nabla_x u)\, q_i\, \psi)$$
$$= \varepsilon\,\Delta_x\psi + \frac{1}{4\,\lambda} \sum_{i=1}^{K}\sum_{j=1}^{K} A_{ij} \nabla_{q_i} \cdot \left(M\, \nabla_{q_j} \frac{\psi}{M} \right) \quad \text{on } \Omega \times D \times (0,T]$$

$\Omega \subset \mathbb{R}^d$ and $D \subset \mathbb{R}^{K\,d}$ $\longrightarrow$ PDE in $(K+1)d$ space dimensions!

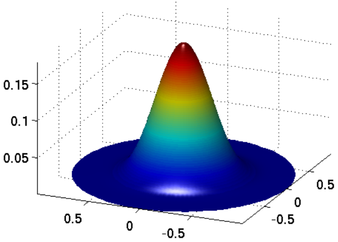
2D-NS/4D-FP macro-micro simulation — velocity field

- Standard benchmark problem: flow around a cylinder
- Stokes flow, parabolic inflow BCs on u_1, no-slip on stationary walls & cylinder
- Steady state solution (computed on 8 processors):



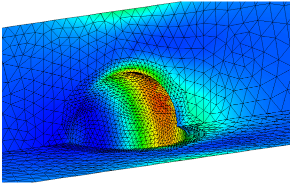
Computations by David Knezevic

2D-NS/4D-FP macro-micro simulation — PDF ψ

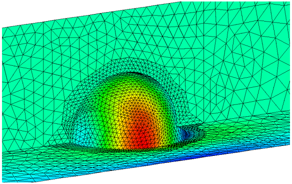


Computations by David Knezevic

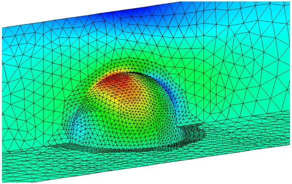
3D/6D: Flow past a ball in a channel: extra-stress tensor



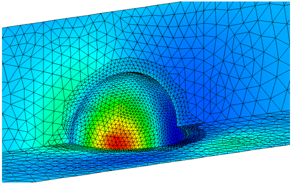
τ_{11}



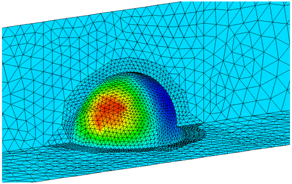
τ_{12}



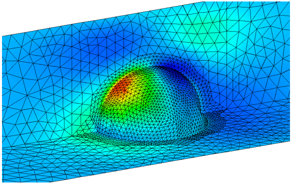
τ_{13}



τ_{22}



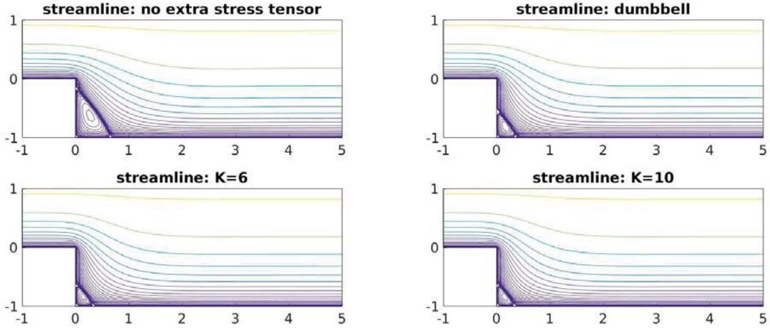
τ_{23}



τ_{33}

Computations by David Knezevic

Alternative: stochastic simulation



The contour plot of the velocity field at time $t = 5$.
Top left: no stress tensor; top right: dumbbell model;
bottom left: $K = 6$ springs; bottom right: $K = 10$ springs.

Computations by Shenghan Ye: Mixed finite element method + multilevel Monte Carlo method (cf. the work of Mike Giles)

Conclusions

- There exist large-data global-in-time entropy-dissipative weak solutions to the incompressible and compressible FENE NSFP systems.

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Conclusions

- There exist large-data global-in-time entropy-dissipative weak solutions to the incompressible and compressible FENE NSFP systems.

- The macroscopic closure of the incompressible Hookean NSFP system is the diffusive Oldroyd-B model involving a defect measure.
  - In 2D the defect measure vanishes, the Hookean NSFP model and the diffusive Oldroyd-B model have 'standard' weak solutions, and macroscopic closure holds.
  - In 3D generalised solutions (involving a defect measure) exist, and macroscopic closure holds assuming additional regularity of u.

Conclusions

- There exist large-data global-in-time entropy-dissipative weak solutions to the incompressible and compressible FENE NSFP systems.

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  - In 3D generalised solutions (involving a defect measure) exist, and macroscopic closure holds assuming additional regularity of u.

- The construction of (provably!) convergent numerical algorithms for NSFP systems remains a significant challenge.

  The same is true of the development of efficient deterministic numerical algorithms for the solution of high-dimensional Fokker–Planck equations.