Existence, equilibration and approximation of global weak solutions to kinetic models of dilute polymers

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in collaboration with

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1. Motivation: Newtonian fluids (Navier–Stokes eqs.)

Find $\underset{\sim}{u} : \Omega \times (0,\infty) \to \mathbb{R}^3$ and $p : \Omega \times (0,\infty) \to \mathbb{R}$ such that

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\partial_t \underset{\sim}{u} + (\underset{\sim}{u} \cdot \underset{\sim}{\nabla}_x)\underset{\sim}{u} - \nu \Delta_x \underset{\sim}{u} + \underset{\sim}{\nabla}_x p &= \underset{\sim}{f} && \text{in } \Omega \times (0,\infty),\\
\underset{\sim}{\nabla}_x \cdot \underset{\sim}{u} &= 0 && \text{in } \Omega \times (0,\infty),\\
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- Differential models: $\partial_t \underset{\approx}{\tau} + (\underset{\sim}{u} \cdot \nabla)\underset{\approx}{\tau} = \mathcal{F}(\underset{\approx}{\tau}, \underset{\sim}{\nabla}_x \underset{\sim}{u})$ — Oldroyd-B

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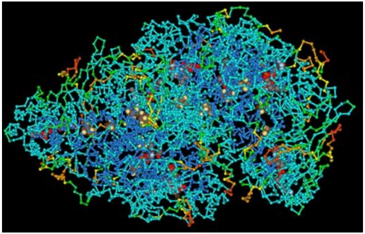
- Kinetic models for dilute polymers:
  $\underset{\approx}{\tau}$ is defined via partial differential equations from statistical physics.

Because of the high flexibility of chemical bonds that connect atoms, when a polymer molecule is dissolved in a solvent the entire molecule forms a coil structure with a large number of possible folding shapes.



Random coil of polypeptide.

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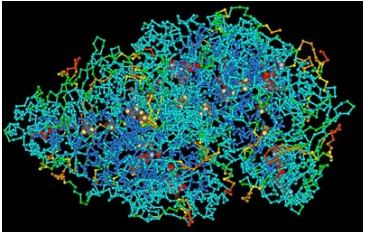

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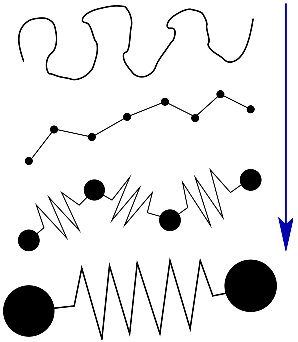
The presence of such large numbers of internal degrees of freedom makes it extremely difficult to study and simulate polymers at a microscopic level.

Coarse-graining: bead-rod chain → bead-spring chain → dumbbell



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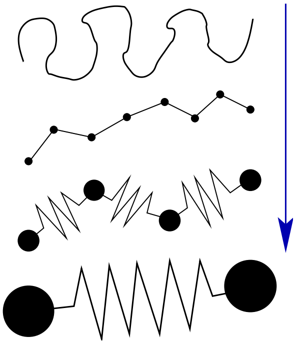

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Dynamics of Polymeric Liquids, Vol. II: Kinetic Theory. Wiley, 1987.

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

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

2. Formulation of the dumbbell model

Polymer chains, which are suspended in a solvent, are assumed not to interact with each other; i.e. a dilute polymer.

The solvent is an incompressible, viscous, isothermal Newtonian fluid in a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3, with Lipschitz boundary $\partial\Omega$.

Define $\quad \Omega_T := \Omega \times (0, T], \qquad \partial\Omega_T^* := \partial\Omega \times (0, T].$

Navier–Stokes equations, with the symmetric extra-stress tensor $\underset{\approx}{\tau}$ (i.e. the polymeric part of the Cauchy stress tensor), appearing as a source term.

Find:

the velocity field $\underset{\sim}{u} : (\underset{\sim}{x}, t) \in \Omega \times (0,T] \mapsto \underset{\sim}{u}(\underset{\sim}{x}, t) \in \mathbb{R}^d$

and the pressure $p : (\underset{\sim}{x}, t) \in \Omega \times (0,T] \mapsto p(\underset{\sim}{x}, t) \in \mathbb{R}$

of the fluid, such that:

$$
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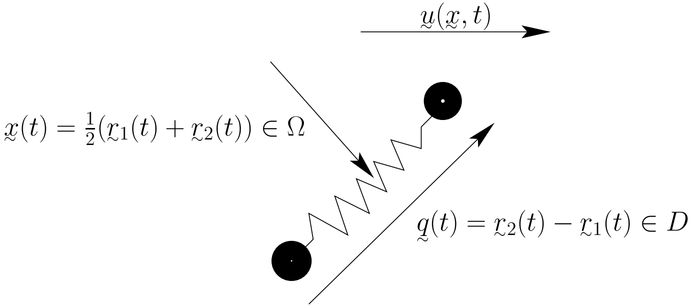
$\nu \in \mathbb{R}_{>0}$ is the given viscosity of the solvent, and $\underset{\sim}{f}$ is a given body force.

Definition of $\underset{\approx}{\tau}$: the dumbbell modell



Noninteracting polymer chains modelled by using dumbbells. A dumbbell is a pair of beads connected with an elastic spring, and is characterized by its centre of mass, $\underset{\sim}{x}(t) \in \Omega$, and its elongation vector $\underset{\sim}{q}(t) \in D$.

$\psi : \Omega \times D \times [0,T] \mapsto \psi(\underset{\sim}{x}, \underset{\sim}{q}, t) \in \mathbb{R}$ is a probability density function: — the probability at time t of there being a dumbbell with centre of mass at $\underset{\sim}{x}$ and elongation $\underset{\sim}{q}$ — and satisfies the Fokker–Planck equation:

$$\frac{\partial \psi}{\partial t} + (\underset{\sim}{u} \cdot \underset{\sim}{\nabla}_x)\psi + \underset{\sim}{\nabla}_q \cdot ((\underset{\approx}{\nabla}_x \underset{\sim}{u})\underset{\sim}{q}\psi) = \frac{1}{2\lambda} \underset{\sim}{\nabla}_q \cdot (\underset{\sim}{\nabla}_q \psi + U' \underset{\sim}{q} \psi) \quad \text{in } \Omega_T \times D,$$

$\lambda = \mathrm{Wi} > 0$: elastic relaxation constant of the fluid (Weissenberg number).

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$$\psi(\underset{\sim}{x}, \underset{\sim}{q}, 0) = \psi^0(\underset{\sim}{x}, \underset{\sim}{q}) \geq 0 \qquad \forall (\underset{\sim}{x}, \underset{\sim}{q}) \in \Omega \times D;$$

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where $\underset{\sim}{n}_{\partial D}$ is $\perp$ to ∂D, and $\int_D \psi^0(\underset{\sim}{x},\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q} = 1$ for a.e. $\underset{\sim}{x}\in\Omega$.

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b.c. $\Rightarrow$ $\int_D \psi(\underset{\sim}{x}, \underset{\sim}{q}, t)\,\mathrm{d}\underset{\sim}{q} = 1$ for a.e. $(\underset{\sim}{x}, t) \in \Omega_T$.

$D \subset \mathbb{R}^d$, $d = 2$ or 3: the set of admissible elongation vectors $\underset{\sim}{q}$.

U is the potential for the elastic force $\underset{\sim}{F} : D \to \mathbb{R}^d$ of the dumbbell spring (U strictly monotonic increasing):

$$\underset{\sim}{F}(\underset{\sim}{q}) := U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)\,\underset{\sim}{q}.$$

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Gibbs measure $\mathrm{d}\mu := M(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q}$; normalised Maxwellian:

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We have the following symmetrization of the Ornstein–Uhlenbeck operator:

$$\underset{\sim}{\nabla}_q \cdot (\underset{\sim}{\nabla}_q \psi + U' \underset{\sim}{q} \psi) \equiv \underset{\sim}{\nabla}_q \cdot \left(M \underset{\sim}{\nabla}_q \left(\frac{\psi}{M} \right) \right).$$

Kolmogorov (1931), Da Prato & Lunardi (2004)

Finally, the symmetric extra stress tensor, due to the dumbbells, on the RHS of the Navier–Stokes equations is

$$\underset{\approx}{\tau}(\psi) := \mu \left(\underset{\approx}{C}(\psi) - \rho(\psi)\, \underset{\approx}{I} \right), \qquad \text{Kramers expression.}$$

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$\mu \in \mathbb{R}_{>0}$ is the product of the Boltzmann constant and the temperature,

$\underset{\approx}{I}$ is the unit $d \times d$ tensor,

$$\underset{\approx}{C}(\psi)(\underset{\sim}{x},t) := \int_D \psi(\underset{\sim}{x},\underset{\sim}{q},t)\,U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)\,\underset{\sim}{q}\,\underset{\sim}{q}^{\mathrm{T}}\,\mathrm{d}\underset{\sim}{q}$$

and

$$\rho(\psi)(\underset{\sim}{x},t) := \int_D \psi(\underset{\sim}{x},\underset{\sim}{q},t)\,\mathrm{d}\underset{\sim}{q}.$$

Examples

Hookean model:

$D = \mathbb{R}^d$,

$U(s) = s \quad \Rightarrow \quad U'(s) = 1 \quad$ and $\quad \mathrm{e}^{-U(\frac{1}{2}|\underset{\sim}{q}|^2)} = \mathrm{e}^{-\frac{1}{2}|\underset{\sim}{q}|^2}$.

Boundary condition on ∂D replaced by decay conditions as $|\underset{\sim}{q}| \to \infty$.

Note that $M(\underset{\sim}{q}) \propto \mathrm{e}^{-\frac{1}{2}|\underset{\sim}{q}|^2} \to 0$ as $|\underset{\sim}{q}| \to \infty$.

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FENE (Finitely Extensible Nonlinear Elastic) model:

$D = B(\underset{\sim}{0}, b^{\frac{1}{2}})$,

$U(s) = -\frac{b}{2}\ln(1 - \frac{2s}{b}) \quad \Rightarrow \quad U'(s) = (1 - \frac{2s}{b})^{-1}$,

$$M(\underset{\sim}{q}) \propto \mathrm{e}^{-U(\frac{1}{2}|\underset{\sim}{q}|^2)} = \left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{\frac{b}{2}} \quad \Rightarrow \quad M = 0 \text{ on } \partial D.$$

Note that $b \to \infty \quad \Rightarrow$ Hookean model.

Remark

In the Hookean model, as $U' = 1$, one can eliminate $\psi(\underset{\sim}{x}, \underset{\sim}{q}, t)$, leading to a closed macroscopic model (Oldroyd-B model) for $\underset{\sim}{u}(\underset{\sim}{x}, t)$, $\rho(\underset{\sim}{x}, t)$, $\underset{\approx}{\tau}(\underset{\sim}{x}, t)$:

Navier–Stokes for $\underset{\sim}{u}$ with extra stress tensor $\underset{\approx}{\tau}$ plus

$$\frac{\partial \rho}{\partial t} + (\underset{\sim}{u} \cdot \underset{\sim}{\nabla}_x)\, \rho = 0 \qquad \text{in } \Omega_T\,,$$

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where

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is the upper-convected time derivative.

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is the upper-convected time derivative.

$$\int_D \psi^0(\underset{\sim}{x}, \underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q} = 1 \text{ for a.e. } \underset{\sim}{x} \in \Omega \quad \Rightarrow \quad \rho(\underset{\sim}{x}, t) \equiv 1.$$

3. Analysis of Navier–Stokes/Fokker–Planck systems

We denote the above coupled Navier–Stokes/Fokker–Planck system for $\underset{\sim}{u}(\underset{\sim}{x},t)$ and $\psi(\underset{\sim}{x},\underset{\sim}{q},t)$ by (P): — a microscopic-macroscopic polymer model.

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The term that causes all the mathematical difficulties in establishing the existence of global weak solutions is the drag term in Fokker–Planck eq.:

$$\frac{\partial\psi}{\partial t} + (\underset{\sim}{u}\cdot\underset{\sim}{\nabla}_x)\psi + \underset{\sim}{\nabla}_q\cdot((\underset{\approx}{\nabla}_x\underset{\sim}{u})\,\underset{\sim}{q}\,\psi)$$
$$= \frac{1}{2\lambda}\underset{\sim}{\nabla}_q\cdot\left(M\underset{\sim}{\nabla}_q\left(\frac{\psi}{M}\right)\right) \qquad \text{in } \Omega_T\times D\,.$$

A mathematically simpler model is the COROTATIONAL model.

Splitting the tensor $\quad \underset{\approx}{\nabla}_x \underset{\sim}{u} = \underset{\approx}{D}(\underset{\sim}{u}) + \underset{\approx}{\omega}(\underset{\sim}{u})$

into its symmetric and skew-symmetric parts

$$\underset{\approx}{D}(\underset{\sim}{u}) = \frac{1}{2}\,[\underset{\approx}{\nabla}_x \underset{\sim}{u} + (\underset{\approx}{\nabla}_x \underset{\sim}{u})^{\mathrm{T}}], \quad \underset{\approx}{\omega}(\underset{\sim}{u}) = \frac{1}{2}\,[\underset{\approx}{\nabla}_x \underset{\sim}{u} - (\underset{\approx}{\nabla}_x \underset{\sim}{u})^{\mathrm{T}}],$$

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The two cases are then:

(i)	the corotational case	$\underset{\approx}{\sigma}(\underset{\sim}{u}) = \underset{\approx}{\omega}(\underset{\sim}{u})\,,$
(ii)	the general noncorotational case	$\underset{\approx}{\sigma}(\underset{\sim}{u}) = \underset{\approx}{\nabla}_x \underset{\sim}{u}\,.$

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Splitting the tensor $\underset{\approx}{\nabla}_x \underset{\sim}{u} = \underset{\approx}{D}(\underset{\sim}{u}) + \underset{\approx}{\omega}(\underset{\sim}{u})$

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$$\underset{\approx}{D}(\underset{\sim}{u}) = \tfrac{1}{2}\,[\underset{\approx}{\nabla}_x \underset{\sim}{u} + (\underset{\approx}{\nabla}_x \underset{\sim}{u})^{\mathrm{T}}], \quad \underset{\approx}{\omega}(\underset{\sim}{u}) = \tfrac{1}{2}\,[\underset{\approx}{\nabla}_x \underset{\sim}{u} - (\underset{\approx}{\nabla}_x \underset{\sim}{u})^{\mathrm{T}}],$$

the difficult drag term is written as

$$\underset{\sim}{\nabla}_q \cdot (\underset{\approx}{\sigma}(\underset{\sim}{u})\, \underset{\sim}{q}\, \psi)\,.$$

The two cases are then:

(i)	the corotational case	$\underset{\approx}{\sigma}(\underset{\sim}{u}) = \underset{\approx}{\omega}(\underset{\sim}{u})\,,$
(ii)	the general noncorotational case	$\underset{\approx}{\sigma}(\underset{\sim}{u}) = \underset{\approx}{\nabla}_x \underset{\sim}{u}\,.$

(i) is mathematically easier (... but physically justified?) :
upper-convected time derivative $\rightarrow$ Jaumann (corotational) derivative.

(ii) is the original, difficult, case.

Existence of global weak solution

P.-L. Lions & Masmoudi (2001) have shown the existence of global-in-time weak solutions to the COROTATIONAL Oldroyd-B model.

P.-L. Lions & Masmoudi (2007) have shown the existence of global-in-time weak solutions to the COROTATIONAL FENE model.

In both cases $\underset{\approx}{\sigma}(\underset{\sim}{u}) = \underset{\approx}{\omega}(\underset{\sim}{u}) = \frac{1}{2}\,[\underset{\approx}{\nabla}_x\,\underset{\sim}{u} - (\underset{\approx}{\nabla}_x\,\underset{\sim}{u})^{\mathrm{T}}\,]$ was assumed.

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Our contribution:
We prove the existence of global-in-time weak solutions, for a large class of FENE type bead-spring chain models for dilute polymers, under minimal regularity conditions on the data, WITHOUT assuming corotationality.

J.W. Barrett & E. Süli (Submitted to M3AS; March 2010)
http://arxiv.org/abs/1004.1432

Two relevant remarks

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1. We consider FENE type models with centre-of-mass diffusion,

$$\varepsilon \Delta_x \psi = \varepsilon \underset{\sim}{\nabla}_x \cdot \left(M \underset{\sim}{\nabla}_x \left(\frac{\psi}{M} \right) \right)$$

in the Fokker–Planck equation, with no-flux boundary condition. The term *does appear* in the derivation of the model, but is usually dropped because ε is very small ($\in [10^{-9}, 10^{-7}]$) for typical molecules.

We shall retain the centre-of-mass diffusion term in the model.

J. Schieber (J. Non-Newtonian Fluid Fluid. Mech., (2006))

J.W. Barrett & E. Süli (Multiscale Model. Simul., (2007))

P. Degond, H. Liu (Networks & Heterogenous Media, (2009))

P. Degond, A. Lozinski, R. Owens (J. Non-Newtonian Fluid Mechanics, (2010))

Two relevant remarks

1. We consider FENE type models with centre-of-mass diffusion,

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We shall retain the centre-of-mass diffusion term in the model.

2. Motivated by the above, we change variable from ψ to $\widehat{\psi} := \psi / M$.

(P) Find $\utilde{u} : (\utilde{x}, t) \in \overline{\Omega} \times [0,T] \mapsto \utilde{u}(\utilde{x},t) \in \mathbb{R}^d$, $p : (\utilde{x}, t) \in \Omega \times (0,T] \mapsto p(\utilde{x},t) \in \mathbb{R}$:

$$
\begin{aligned}
\frac{\partial \utilde{u}}{\partial t} + (\utilde{u} \cdot \utilde{\nabla}_x) \utilde{u} - \nu \Delta_x \utilde{u} + \utilde{\nabla}_x p & \\
= \utilde{f} + \utilde{\nabla}_x \cdot \utilde{\utilde{\tau}}(M \widehat{\psi}) & \qquad \text{in } \Omega_T, \\
\utilde{\nabla}_x \cdot \utilde{u} = 0 & \qquad \text{in } \Omega_T, \\
\utilde{u} = \utilde{0} & \qquad \text{on } \partial\Omega_T^*, \\
\utilde{u}(\utilde{x}, 0) = \utilde{u}^0(\utilde{x}) & \qquad \forall \utilde{x} \in \Omega;
\end{aligned}
$$

where

$$
\utilde{\utilde{\tau}}(M \widehat{\psi}) = \mu \left(\utilde{\utilde{C}}(M \widehat{\psi}) - \rho(M \widehat{\psi}) \utilde{\utilde{I}} \right);
$$

and $\widehat{\psi} : (\underset{\approx}{x}, \underset{\sim}{q}, t) \in \Omega \times D \times [0,T] \mapsto \widehat{\psi}(\underset{\approx}{x}, \underset{\sim}{q}, t) \in \mathbb{R}$ is s.t.

$$M \frac{\partial \widehat{\psi}}{\partial t} + (\underset{\approx}{u} \cdot \underset{\sim}{\nabla}_x)(M\widehat{\psi}) + \underset{\sim}{\nabla}_q \cdot (\underset{\approx}{\sigma}(\underset{\approx}{u})\,\underset{\sim}{q}\,M\widehat{\psi})$$

$$= \frac{1}{2\lambda} \underset{\sim}{\nabla}_q \cdot (M \underset{\sim}{\nabla}_q \widehat{\psi}) + \varepsilon M \Delta_x \widehat{\psi} \qquad \text{in } \Omega_T \times D,$$

$$M \left[\frac{1}{2\lambda} \underset{\sim}{\nabla}_q \widehat{\psi} - [\underset{\approx}{\sigma}(\underset{\approx}{u})\,\underset{\sim}{q}]\,\widehat{\psi} \right] \cdot \underset{\approx}{n}_{\partial D} = 0 \qquad \text{on } \Omega_T \times \partial D,$$

$$\varepsilon M \underset{\sim}{\nabla}_x \widehat{\psi} \cdot \underset{\approx}{n}_{\partial \Omega} = 0 \qquad \text{on } \partial\Omega_T^* \times D,$$

$$M \widehat{\psi}(\underset{\approx}{x}, \underset{\sim}{q}, 0) = \psi^0(\underset{\approx}{x}, \underset{\sim}{q}) \geq 0 \qquad \forall (\underset{\approx}{x}, \underset{\sim}{q}) \in \Omega \times D;$$

where $\underset{\approx}{n}_{\partial D}$ is $\perp$ to ∂D, and $\underset{\approx}{n}_{\partial \Omega}$ is $\perp$ to $\partial \Omega$.

Formal Energy Bounds for (P):

Testing the Navier–Stokes equation with $\underset{\sim}{u}$, integrating over $\Omega \Rightarrow$

$$
\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_\Omega |\underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x}\right] + \nu \int_\Omega |\underset{\approx}{\nabla}_x \underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x} - \int_\Omega \underset{\sim}{f}\cdot \underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x} \\
= -\int_\Omega \underset{\approx}{\tau}(M\widehat{\psi}) : \underset{\approx}{\nabla}_x \underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x} \\
= -\mu \int_\Omega \underset{\approx}{C}(M\widehat{\psi}) : \underset{\approx}{\nabla}_x \underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x} \\
\leq \frac{\nu}{2}\int_\Omega |\underset{\approx}{\nabla}_x \underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x} + \frac{\mu^2}{2\nu}\int_\Omega |\underset{\approx}{C}(M\widehat{\psi})|^2 \,\mathrm{d}\underset{\sim}{x}.
\end{aligned}
$$

Maxwellian-weighted Sobolev norm (degenerate weight M)

$$\|\widehat{\varphi}\|_{\mathrm{H}^1(\Omega\times D;M)} := \left\{ \int_{\Omega\times D} M \left[|\widehat{\varphi}|^2 + \left|\underset{\sim}{\nabla}_q \widehat{\varphi}\right|^2 + \left|\underset{\sim}{\nabla}_x \widehat{\varphi}\right|^2 \right] \mathrm{d}\underset{\sim}{q}\, \mathrm{d}\underset{\sim}{x} \right\}^{\frac{1}{2}},$$

and Maxwellian-weighted H^1 space:

$$\widehat{X} \equiv \mathrm{H}^1(\Omega \times D; M).$$

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Lemma

$$\mathrm{H}^1_M(D) \hookrightarrow\!\!\!\rightarrow \mathrm{L}^2_M(D) \quad \textit{and} \quad \mathrm{H}^1(\Omega \times D; M) \hookrightarrow\!\!\!\rightarrow \mathrm{L}^2(\Omega \times D; M).$$

For all $\widehat{\varphi} \in \widehat{X}$, we have that

$$\int_\Omega |\underset{\approx}{C}(M\widehat{\varphi})|^2 \, \mathrm{d}\underset{\sim}{x}$$

$$= \int_\Omega \sum_{i=1}^{d} \sum_{j=1}^{d} \left(\int_D M \widehat{\varphi} U' q_i q_j \, \mathrm{d}\underset{\sim}{q} \right)^2 \mathrm{d}\underset{\sim}{x}$$

$$\leq d \left(\int_D M |U'|^2 |\underset{\sim}{q}|^4 \, \mathrm{d}\underset{\sim}{q} \right) \left(\int_{\Omega \times D} M |\widehat{\varphi}|^2 \, \mathrm{d}\underset{\sim}{q} \, \mathrm{d}\underset{\sim}{x} \right)$$

$$\leq C \left(\int_{\Omega \times D} M |\widehat{\varphi}|^2 \, \mathrm{d}\underset{\sim}{q} \, \mathrm{d}\underset{\sim}{x} \right) < \infty.$$

Multiplying the Fokker–Planck equation with $\widehat{\psi}$, integrating over $\Omega \times D$:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_{\Omega\times D} M\,|\widehat{\psi}|^2\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\right] + \frac{1}{2\lambda}\int_{\Omega\times D} M\,|\underset{\sim}{\nabla}_q\,\widehat{\psi}|^2\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} + \varepsilon\int_{\Omega\times D} M\,|\underset{\sim}{\nabla}_x\,\widehat{\psi}|^2\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} = \int_{\Omega\times D} M\,(\underset{\approx}{\sigma}(\underset{\sim}{u})\,\underset{\sim}{q}\,\widehat{\psi})\cdot\underset{\sim}{\nabla}_q\,\widehat{\psi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\,.$$

3.1. The corotational case (skew-symmetric $\underset{\approx}{\sigma}$)

$$\underset{\approx}{\sigma}(\underset{\sim}{v}) = \underset{\approx}{\omega}(\underset{\sim}{v}) \qquad \Rightarrow \qquad \underset{\sim}{q}^{\mathrm{T}} \underset{\approx}{\omega}(\underset{\sim}{v})\, \underset{\sim}{q} = 0 \qquad \forall \underset{\sim}{q} \in \mathbb{R}^d\,.$$

3.1. The corotational case (skew-symmetric $\underset{\approx}{\sigma}$)

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Hence we have for all $\widehat{\varphi} \in \widehat{X}$ and $\underset{\sim}{v} \in [\mathrm{W}^{1,\infty}(\Omega)]^d$ that

$$\begin{aligned}
&\int_{\Omega\times D} M\left(\underset{\approx}{\omega}(\underset{\sim}{v})\, \underset{\sim}{q}\, \widehat{\varphi}\right) \cdot \underset{\sim}{\nabla}_q \widehat{\varphi}\, \mathrm{d}\underset{\sim}{q}\, \mathrm{d}\underset{\sim}{x} \\
&\qquad = \tfrac{1}{2} \int_{\Omega\times D} M\left(\underset{\approx}{\omega}(\underset{\sim}{v})\, \underset{\sim}{q}\right) \cdot \underset{\sim}{\nabla}_q \left(\widehat{\varphi}^2\right) \mathrm{d}\underset{\sim}{q}\, \mathrm{d}\underset{\sim}{x} \\
&\qquad = \tfrac{1}{2} \int_{\Omega\times \partial D} M\left(\underset{\approx}{\omega}(\underset{\sim}{v})\, \underset{\sim}{q}\right) \cdot \underset{\sim}{n}_{\partial D}\, \widehat{\varphi}^2\, \mathrm{d}s\, \mathrm{d}\underset{\sim}{x} \\
&\qquad\qquad + \tfrac{1}{2} \int_{\Omega\times D} M\left(\underset{\sim}{q}^{\mathrm{T}} \underset{\approx}{\omega}(\underset{\sim}{v})\, \underset{\sim}{q}\right) U'\, \widehat{\varphi}^2\, \mathrm{d}\underset{\sim}{q}\, \mathrm{d}\underset{\sim}{x} = 0 ,
\end{aligned}$$

since $\quad \underset{\sim}{n}_{\partial D} = \dfrac{\underset{\sim}{q}}{|\underset{\sim}{q}|}, \quad \underset{\sim}{\nabla}_q M = -M\, U'\, \underset{\sim}{q} \quad$ and $\quad \underset{\sim}{q}^{\mathrm{T}} \underset{\approx}{\omega}(\underset{\sim}{v}) \underset{\sim}{q} = 0.$

Hence in the corotational case, we have the formal estimates:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_\Omega |\underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x}\right] + \nu \int_\Omega |\underset{\approx}{\nabla}_x \underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x} - 2\int_\Omega \underset{\sim}{f}\cdot\underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x}$$
$$\leq \frac{\mu^2}{\nu}\int_\Omega |\underset{\approx}{C}(M\widehat{\psi})|^2 \,\mathrm{d}\underset{\sim}{x} \leq C\int_{\Omega\times D} M\,|\widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x};$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_{\Omega\times D} M\,|\widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\right] + \frac{1}{\lambda}\int_{\Omega\times D} M\,|\underset{\sim}{\nabla}_q \widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}$$
$$+\ 2\varepsilon\int_{\Omega\times D} M\,|\underset{\sim}{\nabla}_x \widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} = 0.$$

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$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_{\Omega\times D} M\,|\widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\right] + \frac{1}{\lambda}\int_{\Omega\times D} M\,|\underset{\sim}{\nabla}_q \widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}$$
$$+\, 2\varepsilon\int_{\Omega\times D} M\,|\underset{\sim}{\nabla}_x \widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} = 0.$$

Further formal estimates are needed on the time derivatives of $\underset{\sim}{u}$ and $\widehat{\psi}$.

Hence in the corotational case, we have the formal estimates:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_\Omega |\underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x}\right] + \nu \int_\Omega |\underset{\approx}{\nabla}_x \underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x} - 2\int_\Omega \underset{\sim}{f}\cdot \underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x}$$
$$\leq \frac{\mu^2}{\nu}\int_\Omega |\underset{\approx}{C}(M\widehat{\psi})|^2 \,\mathrm{d}\underset{\sim}{x} \leq C\int_{\Omega\times D} M\,|\widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x};$$

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$$+\ 2\varepsilon\int_{\Omega\times D} M\,|\underset{\sim}{\nabla}_x \widehat{\psi}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} = 0.$$

Aubin–Lions Compactness Theorem: Let $\mathcal{B}_0$, $\mathcal{B}$ and $\mathcal{B}_1$ be Banach spaces, $\mathcal{B}_i$, $i=0,1$, reflexive, with $\mathcal{B}_0 \hookrightarrow\!\!\!\to \mathcal{B} \hookrightarrow \mathcal{B}_1$. Then, for $\alpha_i > 1$, $i=0,1$,

$$\{\,\eta \in \mathrm{L}^{\alpha_0}(0,T;\mathcal{B}_0) : \frac{\partial\eta}{\partial t} \in \mathrm{L}^{\alpha_1}(0,T;\mathcal{B}_1)\,\} \hookrightarrow\!\!\!\to \mathrm{L}^{\alpha_0}(0,T;\mathcal{B}).$$

3.2. The general noncorotational case

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The trick is to choose the testing procedure so as to cancel the extra stress term in the Navier–Stokes eq. with the drag term in the Fokker–Planck eq;

Barrett, Schwab & Süli (2005);
Jourdain, Lelièvre, Le Bris & Otto (2006); Lin, Liu & Zhang (2007).

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Barrett, Schwab & Süli (2005);
Jourdain, Lelièvre, Le Bris & Otto (2006); Lin, Liu & Zhang (2007).

As before, for the Navier–Stokes equations tested with $\underset{\sim}{u}$, we have that

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_\Omega |\underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x}\right] + \nu \int_\Omega |\underset{\approx}{\nabla}_x \underset{\sim}{u}|^2 \,\mathrm{d}\underset{\sim}{x} = \int_\Omega \underset{\sim}{f}\cdot\underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x} - \mu \int_\Omega \underset{\approx}{C}(M\widehat{\psi}) : \underset{\approx}{\nabla}_x \underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x}.$$

Let $\mathcal{F}(s) := s(\ln s - 1) + 1 \in \mathbb{R}_{\geq 0}$ for $s \geq 0$.

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Multiplying the Fokker–Planck equation with $\mathcal{F}'(\widehat{\psi}) \equiv \ln \widehat{\psi}$, assuming that $\widehat{\psi} > 0$, integrating over $\Omega \times D$ $\Rightarrow$

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_{\Omega\times D} M\,\mathcal{F}(\widehat{\psi})\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\right] \\
&\quad + \frac{1}{2\lambda}\int_{\Omega\times D} M\,\underset{\sim}{\nabla}_q\widehat{\psi}\cdot\underset{\sim}{\nabla}_q[\mathcal{F}'(\widehat{\psi})]\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} \\
&\quad + \varepsilon\int_{\Omega\times D} M\,\underset{\sim}{\nabla}_x\widehat{\psi}\cdot\underset{\sim}{\nabla}_x[\mathcal{F}'(\widehat{\psi})]\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} \\
&\quad = \int_{\Omega\times D} M\,\widehat{\psi}\,[(\underset{\approx}{\nabla}_x\underset{\sim}{u})\,\underset{\sim}{q}]\cdot\underset{\sim}{\nabla}_q[\mathcal{F}'(\widehat{\psi})]\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}.
\end{aligned}$$

Note that $\mathcal{F}''(s) = s^{-1} > 0$ for $s > 0$.

Noting that

$$\widehat{\psi}\,\underset{\sim}{\nabla}_q\,[\mathcal{F}'(\widehat{\psi})] = \underset{\sim}{\nabla}_q\,\widehat{\psi}, \quad \underset{\sim}{\nabla}_q M = -M\,U'\,\underset{\sim}{q}, \quad M = 0 \text{ on } \partial D, \quad \underset{\sim}{\nabla}_x \cdot \underset{\sim}{u} = 0:$$

$$\begin{aligned}
\int_{\Omega\times D} & M\,\widehat{\psi}\,[(\underset{\approx}{\nabla}_x\,\underset{\sim}{u})\,\underset{\sim}{q}] \cdot \underset{\sim}{\nabla}_q\,[\mathcal{F}'(\widehat{\psi})]\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} \\
&= \int_{\Omega\times D} M\,[(\underset{\approx}{\nabla}_x\,\underset{\sim}{u})\,\underset{\sim}{q}] \cdot \underset{\sim}{\nabla}_q\,\widehat{\psi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} \\
&= \int_{\Omega\times D} M\,U'\,\underset{\sim}{q} \cdot [(\underset{\approx}{\nabla}_x\,\underset{\sim}{u})\,\underset{\sim}{q}]\,\widehat{\psi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} \\
&= +\int_{\Omega} \underset{\approx}{C}(M\,\widehat{\psi}) : \underset{\approx}{\nabla}_x\,\underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x},
\end{aligned}$$

on recalling that

$$\underset{\approx}{C}(M\,\widehat{\psi})(\underset{\sim}{x},t) \quad = \int_D M\,\widehat{\psi}(\underset{\sim}{x},\underset{\sim}{q},t)\,U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)\,\underset{\sim}{q}\,\underset{\sim}{q}^{\mathrm{T}}\,\mathrm{d}\underset{\sim}{q}\,.$$

We deduce the following formal energy identity:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \mathcal{A}(\underset{\sim}{u},\widehat{\psi})\,\mathrm{d}\underset{\sim}{x} + \int_\Omega \mathcal{B}(\underset{\sim}{u},\widehat{\psi})\,\mathrm{d}\underset{\sim}{x} = \int_\Omega \underset{\sim}{f}\cdot\underset{\sim}{u}\,\mathrm{d}\underset{\sim}{x},$$

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where

$$\mathcal{A}(\underset{\sim}{u},\widehat{\psi}) := \frac{1}{2}|\underset{\sim}{u}|^2 + \mu\int_D M\,\mathcal{F}(\widehat{\psi})\,\mathrm{d}\underset{\sim}{q},$$

$$\mathcal{B}(\underset{\sim}{u},\widehat{\psi}) := \nu\,|\nabla_x \underset{\sim}{u}|^2 + \frac{2\mu}{\lambda}\int_D M\left|\nabla_q\sqrt{\widehat{\psi}}\right|^2 \mathrm{d}\underset{\sim}{q} + 4\,\varepsilon\mu\int_D M\left|\nabla_x\sqrt{\widehat{\psi}}\right|^2 \mathrm{d}\underset{\sim}{q},$$

We deduce the following formal energy identity:

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with $\widehat{\psi}\geq 0$ and $\mathcal{F}(s) := s\,(\ln s - 1) + 1$.

Remark

Consider the strictly convex function

$$\mathcal{F}(s) := s(\ln s - 1) + 1 \in \mathbb{R}_{\geq 0} \qquad \text{for } s \geq 0.$$

Note that

$$M\mathcal{F}(\widehat{\psi}) = M\mathcal{F}\left(\frac{\psi}{M}\right) = \psi \log \frac{\psi}{M} - \psi + M.$$

Remark

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Note that

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The Kullback–Leibler relative entropy of ψ with respect to M is:

$$S(\psi \mid M) := \int_D \left(\psi \log \frac{\psi}{M} - \psi + M\right) \mathrm{d}\underset{\sim}{q} = \int_D M\mathcal{F}(\widehat{\psi})\, \mathrm{d}\underset{\sim}{q}.$$

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The Fisher information:

$$I(\widehat{\psi}) := \int_D \left|\nabla_q \log \widehat{\psi}\right|^2 \widehat{\psi}(\underset{\sim}{q}) M(\underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q} = 4 \int_D \left|\nabla_q \sqrt{\widehat{\psi}}\right|^2 M(\underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q}.$$

The two are related by a log-Sobolev inequality.

Making it all rigorous...

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... is a difficult exercise.

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STEP 1.

We discretize the system with respect to t, using a time step Δt. Has to be done in a way that retains the special cancellation property between the Navier–Stokes and Fokker–Planck equations.

Making it all rigorous...

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STEP 3.

We use Schauder's fixed point theorem to show that the nonlinear elliptic system resulting at each time step has a solution.

In the course of the Schauder argument, we are forced to truncate the upper-truncated entropy $\mathcal{F}^L$ from below also, using another positive cut-off parameter $\delta \in (0,1)$; ditto for $\widehat{\psi}$ in the drag term. Call it: $\mathcal{F}^L_\delta$.

STEP 4.

We test the Fokker–Planck equation using the derivative $[\mathcal{F}_\delta^L]'$ of the doubly-truncated entropy function, and use a weak-compactness argument to pass to the limit $\delta \to 0_+$ with the lower cut-off, *with Δt and L kept fixed.*

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(c) We use these, and the time-discrete equations, to derive L and Δt independent bounds on the sequences of approximate time derivatives.

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A further problem is that passage to the limit requires specially prepared initialization of the Fokker–Planck equation, with finite relative entropy and finite Fisher information. We use de la Valée-Poussin's theorem and the Dunford–Pettis theorem to generate the correct initialization.

STEP 9.

We pass to the weak limits in the time-discrete equations with $L \to \infty$ and $\Delta t = o(L^{-1})$.

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We use a weak lower-semicontinuity argument to pass to the limit in the time-discrete energy estimate...

... and obtain the following Theorem.

J.W. Barrett & E. Süli (Submitted to M3AS; March, 2010)
http://arxiv.org/abs/1004.1432

Existence of global weak solutions: bead-spring chain model

Theorem

Suppose that

$$\partial\Omega \in C^{0,1}; \quad \underset{\sim}{u}^0 \in \underset{\sim}{\mathrm{H}}; \quad \widehat{\psi}^0 := \frac{\psi^0}{M} \geq 0 \ \text{ a.e. on } \Omega \times D \quad \textit{with}$$

$$\mathcal{F}(\widehat{\psi}^0) \in L^1_M(\Omega \times D) \quad \textit{and} \quad \int_D M(\underset{\sim}{q})\, \widehat{\psi}^0(\underset{\sim}{x}, \underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q} = 1 \quad \textit{for a.e. } \underset{\sim}{x} \in \Omega;$$

$$\textit{and} \qquad \underset{\sim}{f} \in L^2(0,T;\underset{\sim}{\mathrm{V}}')\,.$$

Then, there exists a pair of functions $(\underset{\sim}{u}, \widehat{\psi})$*, such that*

$$\underset{\sim}{u} \in L^\infty(0,T;\underset{\sim}{\mathrm{L}}^2(\Omega)) \cap L^2(0,T;\underset{\sim}{\mathrm{V}}) \cap H^1(0,T;\underset{\sim}{\mathrm{V}}'_\sigma), \quad \sigma \geq \tfrac{1}{2}d,\ \sigma > 1,$$

and

$$\widehat{\psi} \in L^1(0,T;L^1_M(\Omega \times D)) \cap H^1(0,T;M^{-1}H^s(\Omega \times D)'), \quad s > 1 + \tfrac{1}{2}(K+1)d,$$

with ...

Theorem (Continued)

... $\widehat{\psi} \geq 0$ *a.e. on* $\Omega \times D \times [0,T]$,

$$\int_D M(\underset{\sim}{q})\,\widehat{\psi}(\underset{\sim}{x},\underset{\sim}{q},t)\,\mathrm{d}\underset{\sim}{q} = 1 \quad \textit{for a.e. } (x,t) \in \Omega \times [0,T],$$

and finite relative entropy and Fisher information, with

$$\mathcal{F}(\widehat{\psi}) \in L^\infty(0,T;L^1_M(\Omega \times D)) \quad \textit{and} \quad \sqrt{\widehat{\psi}} \in L^2(0,T;\widehat{X}),$$

such that the pair of functions $(\underset{\sim}{u},\widehat{\psi})$ *is a global weak solution to the problem in the sense that*

$$\int_0^T \left\langle \frac{\partial \underset{\sim}{u}}{\partial t}, \underset{\sim}{w} \right\rangle_V \mathrm{d}t + \int_0^T \int_\Omega \left[\left[(\underset{\sim}{u} \cdot \underset{\sim}{\nabla}_x)\underset{\sim}{u}\right] \cdot \underset{\sim}{w} + \nu \underset{\approx}{\nabla}_x \underset{\sim}{u} : \underset{\approx}{\nabla}_x \underset{\sim}{w}\right] \mathrm{d}\underset{\sim}{x}\,\mathrm{d}t$$

$$= \int_0^T \left[\langle \underset{\sim}{f}, \underset{\sim}{w}\rangle_V - \mu \sum_{i=1}^K \int_\Omega \underset{\approx}{C}_i(M\widehat{\psi}) : \underset{\approx}{\nabla}_x \underset{\sim}{w}\,\mathrm{d}\underset{\sim}{x}\right] \mathrm{d}t$$

$$\forall \underset{\sim}{w} \in L^2(0,T;\underset{\sim}{\mathrm{V}}_\sigma), \quad \sigma \geq \tfrac{1}{2}d,\ \sigma > 1;$$

Theorem (Continued)

$$\int_0^T \left\langle M \frac{\partial \widehat{\psi}}{\partial t}, \widehat{\varphi} \right\rangle_{\widehat{X}} \mathrm{d}t$$
$$+ \int_0^T \int_{\Omega \times D} M \left[\varepsilon \underset{\sim}{\nabla}_x \widehat{\psi} - \underset{\sim}{u} \widehat{\psi} \right] \cdot \underset{\sim}{\nabla}_x \widehat{\varphi} \, \mathrm{d}\underset{\sim}{q} \, \mathrm{d}\underset{\sim}{x} \Delta t$$
$$+ \frac{1}{2\lambda} \int_0^T \int_{\Omega \times D} M \sum_{i=1}^K \sum_{j=1}^K A_{ij} \underset{\sim}{\nabla}_{q_j} \widehat{\psi} \cdot \underset{\sim}{\nabla}_{q_i} \widehat{\varphi} \, \mathrm{d}\underset{\sim}{q} \, \mathrm{d}\underset{\sim}{x} \Delta t$$
$$- \int_0^T \int_{\Omega \times D} M \sum_{i=1}^K [\underset{\approx}{\sigma}(\underset{\sim}{u}) \underset{\sim}{q}_i] \widehat{\psi} \cdot \underset{\sim}{\nabla}_{q_i} \widehat{\varphi} \, \mathrm{d}\underset{\sim}{q} \, \mathrm{d}\underset{\sim}{x} \Delta t = 0$$
$$\forall \widehat{\varphi} \in L^2(0,T; H^s(\Omega \times D)) \quad \textit{with } s > 1 + \tfrac{1}{2}(K+1)d.$$

The initial conditions $\underset{\sim}{u}(\cdot,0) = \underset{\sim}{u}^0(\cdot)$ *and* $\widehat{\psi}(\cdot,\cdot,0) = \widehat{\psi}^0(\cdot,\cdot)$ *are satisfied in the sense of weakly continuous functions, in the function spaces* $C_w([0,T]; \underset{\sim}{L}^2(\Omega))$ *and* $C_w([0,T]; L^1_M(\Omega \times D))$*, respectively.*

Theorem (Continued)

The weak solution $(\underset{\sim}{u}, \widehat{\psi})$ *obeys the following energy inequality for* $t \in [0, T]$*:*

$$
\begin{aligned}
&\|\underset{\sim}{u}(t)\|^2 + \frac{\nu}{2}\int_0^t \|\underset{\approx}{\nabla}_x \underset{\sim}{u}(s)\|^2 \,\mathrm{d}s + \mu \int_{\Omega\times D} M \mathcal{F}(\widehat{\psi}(t)) \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x} \\
&\quad + 4\mu\varepsilon \int_0^t \int_{\Omega\times D} M\, |\underset{\sim}{\nabla}_x \sqrt{\widehat{\psi}}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\,\mathrm{d}s + \frac{a_0 \mu}{\lambda} \int_0^t \int_{\Omega\times D} M\, |\underset{\sim}{\nabla}_q \sqrt{\widehat{\psi}}|^2 \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\,\mathrm{d}s \\
&\quad \leq \|\underset{\sim}{u}^0\|^2 + \frac{1}{\nu}\int_0^t \|\underset{\sim}{f}(s)\|^2_{V'} \,\mathrm{d}s + \mu \int_{\Omega\times D} M \mathcal{F}(\widehat{\psi}^0) \,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x},
\end{aligned}
$$

with $\mathcal{F}(s) = s(\log s - 1) + 1$, $s \geq 0$.

Equilibration of global weak solutions

Theorem

Under the assumptions of the previous theorem and if M satisfies the Bakry–Émery condition: $\mathrm{Hess}(-\log M(\underset{\sim}{q})) \geq \kappa \mathrm{Id}$, *with* $\kappa > 0$; *then,*

$$\|\underset{\sim}{u}(T)\|^2 + \frac{\mu}{|\Omega|}\|\widehat{\psi}(T) - 1\|^2_{L^1_M(\Omega\times D)} \leq \mathrm{e}^{-\gamma_0 T}\left[\|\underset{\sim}{u}^0\|^2 + 2\mu\int_{\Omega\times D} M\mathcal{F}(\widehat{\psi}^0)\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\right] + \frac{1}{\nu}\int_0^T \|\underset{\sim}{f}\|^2_{V'}\,\mathrm{d}s, \ \ \forall T > 0,$$

where $\gamma_0 := \min\left(\frac{\nu}{C_{\mathrm{P}}^2}, \frac{\kappa a_0}{2\lambda}\right)$. *In particular if* $\underset{\sim}{f} \equiv 0$, *then*

$$\|\underset{\sim}{u}(T)\|^2 + \frac{\mu}{|\Omega|}\|\widehat{\psi}(T) - 1\|^2_{L^1_M(\Omega\times D)} \leq \mathrm{e}^{-\gamma_0 T}\left[\|\underset{\sim}{u}^0\|^2 + 2\mu\int_{\Omega\times D} M\mathcal{F}(\widehat{\psi}^0)\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}\underset{\sim}{x}\right].$$

Proof.

Again, very technical. Lower-semicontinuity argument based on:

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J.W. Barrett & E. Süli (Submitted to M3AS; March 2010)
http://arxiv.org/abs/1004.1432

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Again, very technical. Lower-semicontinuity argument based on:

- Logarithmic Sobolev inequality:

$$\int_D \widehat{\varphi}(\underset{\sim}{q}) \log \frac{\widehat{\varphi}(\underset{\sim}{q})}{\|\widehat{\varphi}\|_{L^1_M(D)}} M(\underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q} \leq \frac{2}{\kappa} \int_D \left| \underset{\sim}{\nabla}_q \sqrt{\widehat{\varphi}(\underset{\sim}{q})} \right|^2 M(\underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q},$$

  for all $\widehat{\varphi}$ such that $\widehat{\varphi} \geq 0$ on D and $\sqrt{\widehat{\varphi}} \in H^1_M(D)$.

  Arnold, Bartier & Dolbeault (2007)

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- Csiszár–Kullback inequality w.r.t. the Gibbs measure $\mathrm{d}\mu := M(\underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q}$:

$$\|\widehat{\psi}(\underset{\sim}{x}, \cdot, T) - 1\|_{L^1_M(D)} \leq \left[2 \int_D \mathcal{F}(\widehat{\psi}(\underset{\sim}{x}, \underset{\sim}{q}, T))\, M(\underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q} \right]^{\frac{1}{2}}.$$

□

J.W. Barrett & E. Süli (Submitted to M3AS; March 2010)
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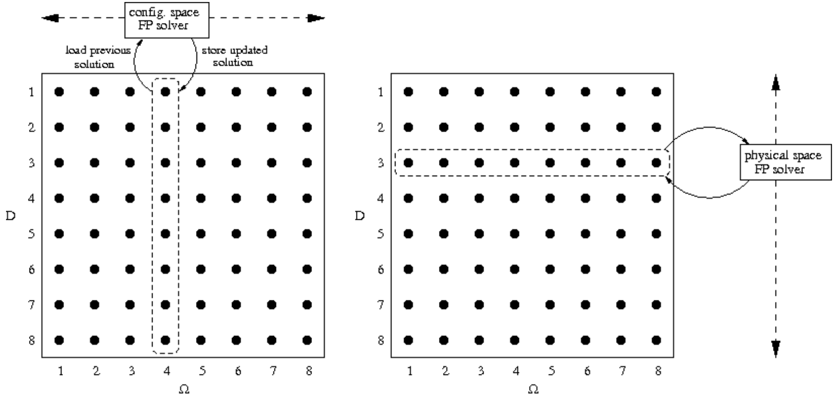
Heterogeneous ADI method for Fokker–Planck equation

- For single time step update, solve series of reduced-dimension problems – similar to alternating direction iteration (ADI).
- 3D dumbbell case: series of 3D solves, rather than one 6D solve.



(a) (b)

Overall algorithm

1. Initialise: $\underset{\sim}{u}(\underset{\sim}{x},0) = \underset{\sim}{u}^0(\underset{\sim}{x})$, $\psi(\underset{\sim}{x},\underset{\sim}{q},0) = \psi^0(\underset{\sim}{x},\underset{\sim}{q})$, and $\underset{\approx}{\tau}(\underset{\sim}{x},0) := \underset{\approx}{0}$.

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6. Update $\underset{\sim}{u}$ using the updated stress field.
   Return to Step 3 and loop until the final time is reached or a termination condition, such as $\frac{\|\underset{\sim}{u}^{n+1} - \underset{\sim}{u}^n\|_\infty}{\Delta t} < \text{TOL}$, is met.

Numerical Results

- Algorithm implemented in C++ using open source finite element library, libMesh: `http://libmesh.sourceforge.net`
- Computations performed on *Lonestar*, a Linux cluster at the Texas Advanced Computing Centre (TACC): `http://www.tacc.utexas.edu`

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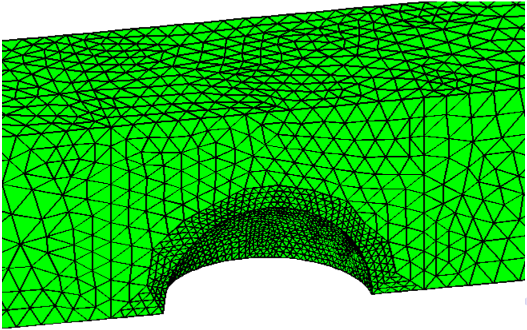
Lonestar has 5400 processors, 11 TB of memory,
peak performance 62 TFLOPS ($= 62 \times 10^{12}$ FLOPS/s).

D. Knezevic & E. Süli (M2AN, 2009)
Spectral Galerkin approximation of Fokker–Planck equations with unbounded drift

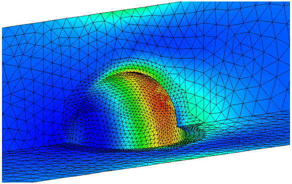
D. Knezevic & E. Süli (M2AN, 2009)
A heterogeneous alternating-direction method for a micro-macro dilute polymeric fluid model

3D/6D: Flow past a ball in a channel

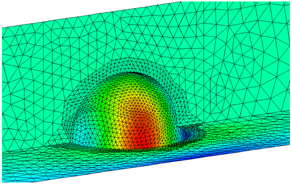
- Pressure-drop-driven flow past a ball in hexahedral channel.
- P_2/P_1 mixed FEM for (Navier–)Stokes equation on a mesh with 3045 tetrahedral elements and 51989 Gaussian quadrature points.
- Fokker–Planck equation solved using heterogenous ADI method in 6D domain $\Omega \times D$. 51989 3D solves per time step in $\underset{\sim}{q} = (q_1, q_2, q_3) \in D$ and 1800 3D solves per time-step in $\underset{\sim}{x} = (x, y, z) \in \Omega$.
- Computed using 120 processors; 45s/time step; 10 time steps; $\Delta t = 0.05$; $\lambda = \mathrm{Wi} = 0.5$.



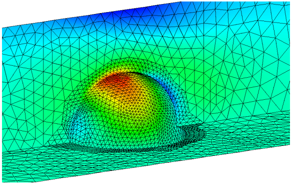
3D/6D: Flow past a ball in a channel: extra stress tensor



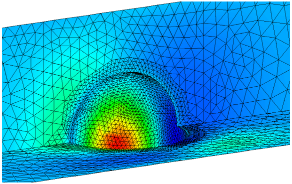
τ_{11}



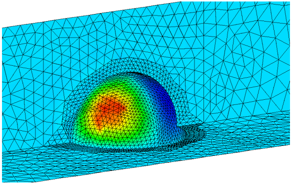
τ_{12}



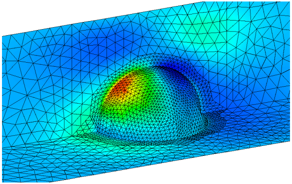
τ_{13}



τ_{22}



τ_{23}



τ_{33}

5. Conclusions

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   L. Figueroa & E. Süli (2010):
   Greedy algorithms for high-dimensional Fokker–Planck equations with unbounded drift

5. Conclusions

1. We showed the existence of global-in-time weak solutions to a general class of finitely extensible nonlinear bead-spring chain models for dilute polymers, and their exponential convergence to an equilibrium.

2. We have developed a numerical algorithm for the associated 6D Fokker–Planck equation coupled to the 3D Navier–Stokes equation.

   L. Figueroa & E. Süli (2010):
   Greedy algorithms for high-dimensional Fokker–Planck equations with unbounded drift

3. We have now also shown the existence of global-in-time weak solutions to a general class of kinetic models with Hookean springs:

   J.W. Barrett & E. Süli (2010, in preparation):
   Existence and equilibration of global weak solutions to Hookean bead-spring chain models