Existence of global weak solutions to implicitly constituted kinetic models of incompressible homogeneous dilute polymers

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joint work with

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To Eitan Tadmor, on the occasion of his 60th birthday.
Viscoelastic fluids

Gareth McKinley’s Non-Newtonian Fluid Dynamics Group, MIT

Jonathan Rothstein’s Non-Newtonian Fluids Dynamics Lab, University of Massachusetts
Statement of the model

- $\Omega \subset \mathbb{R}^d$, $d = 2, 3$: bounded open Lipschitz domain,
- $T$: length of the time interval of interest, and
- $Q := \Omega \times (0, T)$: the associated space-time domain.
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Consider the following system of nonlinear PDEs:

\[
\rho (u_t + \text{div}(u \otimes u)) - \text{div} T = \rho f \quad \text{in } Q,
\]
\[
\text{div } u = 0 \quad \text{in } Q, \tag{1}
\]
\[
u(\cdot, 0) = u_0(\cdot) \quad \text{in } \Omega,
\]

and the boundary condition

\[
u = 0 \quad \text{on } \partial \Omega \times (0, T).
\]
We assume that the Cauchy stress $\mathbf{T}$ is decomposed as

$$\mathbf{T} = -p \mathbf{I} + \mathbf{S}_v + \mathbf{S}_e,$$

where

- $p : Q \to \mathbb{R}$ is the pressure;
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where

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- $\mathbf{S}_v : Q \to \mathbb{R}^{d \times d}_{sym}$ is the viscous part of the deviatoric stress;
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- $p : Q \to \mathbb{R}$ is the pressure;
- $\mathbf{S}_v : Q \to \mathbb{R}^{d \times d}_{sym}$ is the viscous part of the deviatoric stress;
- $\mathbf{S}_v$ and $\mathbf{D}(\mathbf{u}) := \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ are assumed to be related via a maximal monotone graph described by the implicit relation:

$$\mathbf{G}(\mathbf{S}_v, \mathbf{D}(\mathbf{u})) = 0,$$

where $\mathbf{G} : \mathbb{R}^{d \times d}_{sym} \times \mathbb{R}^{d \times d}_{sym} \to \mathbb{R}^{d \times d}_{sym}$ is a continuous mapping.

- $\mathbf{S}_e : Q \to \mathbb{R}^{d \times d}_{sym}$ is the elastic part of the deviatoric stress.
Examples of $G(S_v, D(u)) = 0$

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$$S_v = 2\hat{\mu}(|D(u)|^2, |S_v|^2)D(u);$$

- **Activated fluids**, such as Bingham and Herschel–Bulkley fluids:

$$|S_v| \leq \tau_* \Leftrightarrow D(u) = 0 \text{ and } |S_v| > \tau_* \Leftrightarrow S_v = \frac{\tau_*D(u)}{|D(u)|} + 2\nu(|D(u)|^2)D(u).$$
Examples of $G(S_v, D(u)) = 0$

- Newtonian (Navier–Stokes) fluids: $S_v = 2\mu_* D(u)$, with $\mu_* > 0$;
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$$|S_v| \leq \tau_* \iff D(u) = 0 \text{ and } |S_v| > \tau_* \iff S_v = \frac{\tau_* D(u)}{|D(u)|} + 2\nu(|D(u)|^2) D(u).$$

i.e. $2\nu(|D(u)|^2) (\tau_* + (|S_v| - \tau_*)_+) D(u) = (|S_v| - \tau_*)_+ S_v, \quad \tau_* > 0.$
Examples of $S_y(=\tau)$ vs. $D(u)(=\gamma)$
We identify the implicit relation (2) with a graph \( \mathcal{A} \subset \mathbb{R}_{sym}^{d \times d} \times \mathbb{R}_{sym}^{d \times d} \), i.e.,

\[
G(S, D) = 0 \iff (D, S) \in \mathcal{A}.
\]

We assume that, for some \( r \in (1, \infty) \), \( \mathcal{A} \) is a *maximal monotone r-graph*:

(A1) \( \mathcal{A} \) includes the origin; i.e., \((0, 0) \in \mathcal{A}\);

(A2) \( \mathcal{A} \) is a monotone graph; i.e.,

\[
(S_1 - S_2) \cdot (D_1 - D_2) \geq 0 \text{ for all } (D_1, S_1), (D_2, S_2) \in \mathcal{A};
\]

(A3) \( \mathcal{A} \) is a maximal monotone graph; i.e., for any \((D, S) \in \mathbb{R}_{sym}^{d \times d} \times \mathbb{R}_{sym}^{d \times d}\),

if \((\tilde{S} - S) \cdot (\tilde{D} - D) \geq 0 \text{ for all } (\tilde{D}, \tilde{S}) \in \mathcal{A}\), then \((D, S) \in \mathcal{A}\);

(A4) \( \mathcal{A} \) is an r-graph; i.e., there exist positive constants \( C_1, C_2 \) such that

\[
S \cdot D \geq C_1(|D|^r + |S|^{r'}) - C_2 \text{ for all } (D, S) \in \mathcal{A}.
\]


Definition of $S_e$: kinetic theory of polymers

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Let $D_i \subset \mathbb{R}^d$, $i = 1, \ldots, K$, be bounded open balls centred at $0$. 

Arbitrary point fixed in space
Definition of $S_e$: kinetic theory of polymers

Let $D_i \subset \mathbb{R}^d$, $i = 1, \ldots, K$, be bounded open balls centred at $0$.

Consider the Maxwellian $M(q) := M_1(q_1) \cdots M_K(q_K)$, with $q_i \in D_i$, where

$$M_i(q_i) := \frac{e^{-U_i(\frac{1}{2}|q_i|^2)}}{\int_{D_i} e^{-U_i(\frac{1}{2}|p_i|^2)} dp_i}, \quad i = 1, \ldots, K.$$
$S_e$ is defined by the *Kramers expression*:

$$S_e(x, t) := k_B T \sum_{i=1}^{K} \int_D M(q) \nabla q_i \hat{\psi}(x, q, t) \otimes q_i \, dq,$$

where $q = (q_1^T, \ldots, q_K^T)^T \in D_1 \times \cdots \times D_K =: D$ and

$$\hat{\psi} := \frac{\psi}{M}$$

is the normalized probability density function, that is the solution of a Fokker–Planck equation.
Fokker–Planck equation

The function $\hat{\psi} = \psi/M$ satisfies the Fokker–Planck equation:

$$(M\hat{\psi})_t + \text{div} (M\hat{\psi} u) + \text{div}_q (M\hat{\psi} (\nabla u) q) = \triangle (M\hat{\psi}) + \text{div}_q A (M \nabla_q \hat{\psi})$$

in $O \times (0, T)$, with $O := \Omega \times D$, subject to the boundary conditions:

$$M \nabla \hat{\psi} \cdot n = 0$$

on $\partial \Omega \times D \times (0, T)$,

$$(M\hat{\psi}(\nabla u)q_i - A_i (M \nabla_q \hat{\psi})) \cdot n_i = 0$$

on $\Omega \times \partial \bar{D}_i \times (0, T)$,

for all $i = 1, \ldots, K$, and the initial condition

$$\hat{\psi}(x, q, 0) = \hat{\psi}_0(x, q)$$

in $O$.

$A \in \mathbb{R}^{K \times K}_{\text{symm}}$: Rouse matrix (symmetric, positive definite).
Existence and equilibration of global weak solutions to kinetic models for dilute polymers I: Finitely extensible nonlinear bead-spring chains

Existence and equilibration of global weak solutions to kinetic models for dilute polymers II: Hookean-type bead-spring chains

Existence of global weak solutions to finitely extensible nonlinear bead-spring chain models for dilute polymers with variable density and viscosity


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Assumptions on the data

For the Maxwellian $M$ we assume that

$$M \in C_0(\overline{D}) \cap C_{\text{loc}}^{0,1}(D), \quad \text{and } M > 0 \text{ on } D. \quad (4)$$

For the initial velocity $u_0$ we assume that

$$u_0 \in L_{0,\text{div}}^2(\Omega). \quad (5)$$

For $\hat{\psi}_0 := \psi_0/M$ we assume, with $O := \Omega \times D$, that

$$\hat{\psi}_0 \geq 0 \; \text{a.e. in } O, \quad \hat{\psi}_0 \log \hat{\psi}_0 \in L_M^1(O), \quad (6)$$

and that the initial marginal probability density function

$$\int_D M(q) \hat{\psi}_0(\cdot, q) \, dq \in L^\infty(\Omega). \quad (7)$$
Theorem

For $d \in \{2, 3\}$ let $D_i \subset \mathbb{R}^d$, $i = 1, \ldots, K$, be bounded open balls centred at the origin in $\mathbb{R}^d$, let $\Omega \subset \mathbb{R}^d$ be a bounded open Lipschitz domain and suppose $f \in L^{r'}(0, T; W_{0, \text{div}}^{1,r'}(\Omega))$, $r \in (1, \infty)$. Assume that $\mathcal{A}$, given by $\mathbf{G}$, is a maximal monotone $r$-graph satisfying (A1) – (A4), the Maxwellian $M : D \to \mathbb{R}$ satisfies (4), and $(u_0, \hat{\psi}_0)$ satisfy (5)–(7).

Then, there exist $(u, S_v, S_e, \hat{\psi})$ such that

$$u \in L^\infty(0, T; L_0^{2, \text{div}}(\Omega)^d) \cap L^r(0, T; W_0^{1,r}(\Omega)^d) \cap W^{1,r^*}(0, T; W_{0, \text{div}}^{1,r^*}(\Omega)),$$

$$S_v \in L^{r'}(0, T; L^{r'}(\Omega)^{d \times d}), \quad S_e \in L^2(0, T; L^2(\Omega)^{d \times d}),$$

$$\hat{\psi} \in L^\infty(Q; L_M^1(D)) \cap L^2(0, T; W_M^{1,1}(O)), \quad \hat{\psi} \geq 0 \text{ a.e. in } O \times (0, T),$$

$$M \hat{\psi} \in W^{1,1}(0, T; W^{-1,1}(O)), \quad \hat{\psi} \log \hat{\psi} \in L^\infty(0, T; L_M^1(O)),$$

where

$$r^* := \min \{r', 2, (1 + \frac{2}{d})r\} \quad \text{and} \quad r' := \frac{r}{r-1}.$$
Moreover, (1) is satisfied in the following sense:

\[
\int_0^T \langle u_t, w \rangle \, dt + \int_0^T \left( - (u \otimes u, \nabla w) + (S_v, \nabla w) \right) \, dt \\
= \int_0^T \left( - (S_e, \nabla w) + \langle f, w \rangle \right) \, dt \quad \text{for all } w \in L^\infty(0, T; W^{1,\infty,0}_{0,\text{div}}(\Omega)),
\]

where

\[
(S_v(x, t), D(u(x, t))) \in \mathcal{A} \quad \text{for a.e. } (x, t) \in Q,
\]

and \( S_e \) is given by the Kramers expression

\[
S_e(x, t) = k_B T \sum_{i=1}^K \int_D M \nabla q_i \hat{\psi}(x, q, t) \otimes q_i \, dq \quad \text{for a.e. } (x, t) \in Q.
\]
Theorem (Continued...)

In addition, the Fokker–Planck eqn (3) is satisfied in the following sense:

\[
\int_0^T \left[ \langle (M \hat{\psi})_t, \varphi \rangle - (M u \hat{\psi}, \nabla \varphi)_O - (M \hat{\psi}(\nabla u)q, \nabla q \varphi)_O \right] \, dt \\
+ \int_0^T \left[ (M \nabla \hat{\psi}, \nabla \varphi)_O + (M A \nabla q \hat{\psi}, \nabla q \varphi)_O \right] \, dt = 0
\]

for all \( \varphi \in L^\infty(0, T; W^{1,\infty}(O)) \),

and the initial data are attained strongly in \( L^2(\Omega)^d \times L^1_M(O) \), i.e.,

\[
\lim_{t \to 0^+} \| u(\cdot, t) - u_0(\cdot) \|_2^2 + \| \hat{\psi}(\cdot, t) - \hat{\psi}_0(\cdot) \|_{L^1_M(O)} = 0.
\]
Further, for \( t \in (0, T) \) the following energy inequality holds in a weak sense:

\[
\frac{d}{dt} \left( k \int_{O} M \hat{\psi} \log \hat{\psi} \, dx \, dq + \frac{1}{2} \| u \|_2^2 \right) + (S_v, D(u)) + 4k \left( M \nabla \sqrt{\hat{\psi}}, \nabla \sqrt{\hat{\psi}} \right)_O \\
+ 4k \left( MA \nabla_q \sqrt{\hat{\psi}}, \nabla_q \sqrt{\hat{\psi}} \right)_O \leq \langle f, u \rangle, \quad \text{with } k := k_B T.
\]
Proof

STEP 1. Truncate $\hat{\psi}$ in the Kramers expression and in the drag term in the FP equation by replacing $\hat{\psi}$ with $T_\ell(\hat{\psi})$, preserving the energy inequality.
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STEP 2. We form a Galerkin approximation of the velocity and the probability density function, resulting in a system of ODEs in $t$. 

STEP 3. The sequence of Galerkin approximations satisfies an energy inequality, uniformly in the number of Galerkin basis functions and the truncation parameter $\ell$.

STEP 4. We extract weakly (and weak*) convergent subsequences, and pass to the limits in the Galerkin approximations.

STEP 5. We require strongly convergent sequences for passage to limit in $\ell$ in the various nonlinear terms. This is the most difficult step to realize.
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$$+ 4k \left( M A \nabla_{q} \sqrt{\hat{\psi}^{\ell}}, \nabla_{q} \sqrt{\hat{\psi}^{\ell}} \right)_{O} \leq \langle f, u^{\ell} \rangle,$$

with $k := k_{B} T$. 

Velocity: strong convergence immediate by Aubin–Lions–Simon compactness theorem.

Probability density function: (much more difficult)

▶ Vitali’s convergence theorem (a.e. convergence + $L^{1}$ equi-integrability);

▶ Weak lower semicontinuity of convex functions (Feireisl & Novotný);

▶ Murat–Tartar Div–Curl lemma;

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  - Uniform interior estimates on $\Omega \times D \times (0, T)$, obtained by function space interpolation from the energy inequality.
STEP 6. Identification of $S_e$: the sequence of truncated Kramers expressions $S^\ell_e$ converges to $S_e$ strongly in $L^q(0, T; L^q(\Omega)^{d\times d})$, $q \in [1, 2)$. 

STEP 7. The initial data are attained strongly in $L^2(\Omega)^{d\times d}\times L^1(M(\Omega))$, i.e.,

$$\lim_{t \to 0^+} \|u(\cdot, t) - u_0(\cdot)\|_2 + \|\hat{\psi}(\cdot, t) - \hat{\psi}_0(\cdot)\|_{L^1(M(\Omega))} = 0.$$ 

STEP 8. Identification of $S_v$: by a parabolic Acerbi–Fusco type Lipschitz-truncation of Diening, Ružička & Wolf (2010) and STEP 6:

$$\lim_{\ell \to \infty} \int_Q \left| \left( S^\ell_v - S^*\left( D(\cdot, u) \right) \right) \cdot D(\cdot, u - u_\ell) \right|^\alpha \, dx \, dt = 0 \quad \forall \alpha \in (0, 1).$$

$S^*_v$ is a measurable selection such that for any $D$ we have $(S^*_v(D), D) \in A$. 

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STEP 6. Identification of $S_e$: the sequence of truncated Kramers expressions $S^e_\ell$ converges to $S_e$ strongly in $L^q(0, T; L^q(\Omega)^{d \times d})$, $q \in [1, 2)$.

STEP 7. The initial data are attained strongly in $L^2(\Omega)^d \times L^1_M(O)$, i.e.,

$$\lim_{t \to 0^+} \|u(\cdot, t) - u_0(\cdot)\|_2^2 + \|\hat{\psi}(\cdot, t) - \hat{\psi}_0(\cdot)\|_{L^1_M(O)} = 0.$$
STEP 6. **Identification of $S_e$:** the sequence of truncated Kramers expressions $S^\ell_e$ converges to $S_e$ strongly in $L^q(0,T;L^q(\Omega)^{d\times d})$, $q \in [1,2)$. 

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STEP 8. **Identification of $S_v$:** by a parabolic Acerbi–Fusco type Lipschitz-truncation of Diening, Ružička & Wolf (2010) and STEP 6:

$$\lim_{\ell \to \infty} \int_{Q} \left| (S^\ell_v - S^*(D(u))) \cdot D(u^\ell - u) \right|^\alpha \, dx \, dt = 0 \quad \forall \alpha \in (0,1).$$

$S^*$ is a measurable selection such that for any $D$ we have $(S^*(D),D) \in \mathcal{A}$. 
Thus, for a subsequence,

\[(S_v^\ell - S^*(D(u))) \cdot D(u^\ell - u) \to 0 \quad \text{almost everywhere in } Q.\]

Moreover, using the energy inequality, we see that

\[
\int_Q \left| (S_v^\ell - S^*(D(u))) \cdot D(u^\ell - u) \right| \, dx \, dt \leq C.
\]

We apply Chacon’s Biting Lemma to find a nondecreasing countable sequence of measurable sets \(Q_1 \subset \cdots \subset Q_k \subset Q_{k+1} \subset \cdots \subset Q\) such that

\[
\lim_{k \to \infty} |Q \setminus Q_k| \to 0
\]

and such that for any \(k\) there is a subsequence such that

\[(S_v^\ell - S^*(D(u))) \cdot D(u^\ell - u) \text{ converges weakly in } L^1(Q_k).\]
By Vitali’s theorem we then deduce that
\[(S_v^\ell - S^*(D(u))) \cdot D(u^\ell - u) \to 0\] strongly in \(L^1(Q_k)\).

The weak convergence of \((S_v^\ell)\) to \(S_v\) and \((D(u^\ell))\) to \(D(u)\) implies that
\[\lim_{\ell \to \infty} (S_v^\ell, D(u^\ell))_{Q_k} = (S_v, D(u))_{Q_k}.\]

The assumption that \(\mathcal{A}\) is a maximal monotone \(r\)-graph then implies that
\[(S_v, D(u)) \in \mathcal{A} \quad \text{a.e. in } Q_k, \ k = 1, 2, \ldots.\]

Finally, by a diagonal procedure and \(\lim_{k \to \infty} |Q \setminus Q_k| \to 0\) we deduce that
\[(S_v, D(u)) \in \mathcal{A} \quad \text{a.e. in } Q = \Omega \times (0, T).\]
Open problems

- The extension of these results to implicitly constituted kinetic models with variable density, density-dependent viscosity and drag is open.

Special case:
- For Navier–Stokes–Fokker–Planck systems with variable density and density-dependent dynamic viscosity and drag the existence of global weak solutions was shown in Barrett & Suli (Journal of Differential Equations, 2012).

The numerical analysis of implicitly constituted kinetic models of polymers is open.

Special cases:
- Barrett & Suli (M2AN, 2012)
Open problems

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  **Special cases:**
  - Barrett & Süli (M2AN, 2012)
2D/4D: Flow around a cylinder

- Standard benchmark problem: flow around a cylinder
- Assume Stokes flow, parabolic inflow BCs on $u_x$, no-slip on stationary walls and cylinder
- Steady state solution (computed on 8 processors):
2D/4D: Flow around a cylinder: extra stress tensor

\((S_e)_{11}\):

\[(S_e)_{12}\]:

\[(S_e)_{22}\]:
2D/4D: Flow around a cylinder: probability density fn.

Figure: Configuration space cross-sections of $\psi$ for $x$ in $(r, \theta)$-coordinates: (a) wake of cylinder, and (b) between cylinder and wall.
2D/4D: Flow around a cylinder: probability density fn.
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 $\mathbf{q} = (q_1, q_2, q_3) \in D$ and 1800 3D solves per time-step in $\mathbf{x} = (x, y, z) \in \Omega$.
- Computed using 120 processors; 45s/time step; 10 time steps; $\Delta t = 0.05$; $\lambda = 0.5$. 
3D/6D: Flow past a ball in a channel: elastic part of the Cauchy stress

\[(S_e)_{11}, (S_e)_{12}, (S_e)_{13}, (S_e)_{22}, (S_e)_{23}, (S_e)_{33}\]
HAPPY BIRTHDAY, EITAN!