

# 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

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## 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:

$$\begin{aligned} \rho(\mathbf{u}_t + \operatorname{div}(\mathbf{u} \otimes \mathbf{u})) - \operatorname{div} \mathbf{T} &= \rho \mathbf{f} && \text{in } Q, \\ \operatorname{div} \mathbf{u} &= 0 && \text{in } Q, \\ \mathbf{u}(\cdot, 0) &= \mathbf{u}_0(\cdot) && \text{in } \Omega, \end{aligned} \tag{1}$$

and the boundary condition

$$\mathbf{u} = 0 \quad \text{on } \partial\Omega \times (0, T).$$

We assume that the *Cauchy stress*  $\mathbf{T}$  is decomposed as

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

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$\mathbf{S}_v$  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:

$$\mathbf{G}(\mathbf{S}_v, \mathbf{D}(\mathbf{u})) = \mathbf{0}, \quad (2)$$

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

- $\mathbf{S}_e : Q \rightarrow \mathbb{R}_{sym}^{d \times d}$  is the elastic part of the deviatoric stress.



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

- Newtonian (Navier–Stokes) fluids:  $\mathbf{S}_v = 2\mu_*\mathbf{D}(\mathbf{u})$ , with  $\mu_* > 0$ ;

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

$$|\mathbf{S}_v| \leq \tau_* \Leftrightarrow \mathbf{D}(\mathbf{u}) = \mathbf{0} \quad \text{and} \quad |\mathbf{S}_v| > \tau_* \Leftrightarrow \mathbf{S}_v = \frac{\tau_* \mathbf{D}(\mathbf{u})}{|\mathbf{D}(\mathbf{u})|} + 2\nu(|\mathbf{D}(\mathbf{u})|^2) \mathbf{D}(\mathbf{u}).$$

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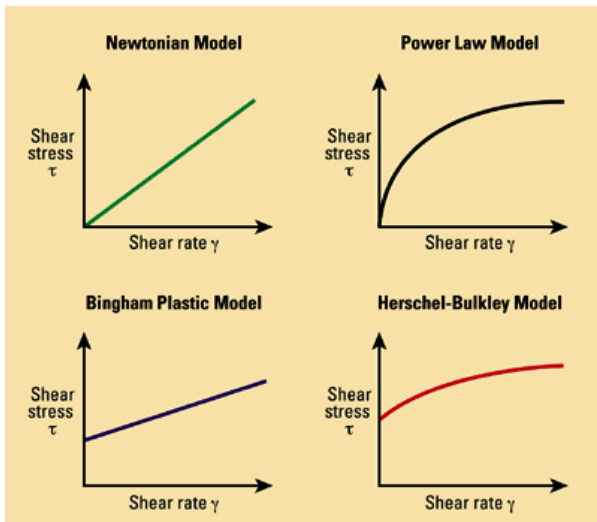
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$$\text{i.e.} \quad 2\nu(|\mathbf{D}(\mathbf{u})|^2)(\tau_* + (|\mathbf{S}_v| - \tau_*)_+)\mathbf{D}(\mathbf{u}) = (|\mathbf{S}_v| - \tau_*)_+\mathbf{S}_v, \quad \tau_* > 0.$$

# Examples of $\mathbf{S}_v(= \tau)$ vs. $\mathbf{D}(u)(= \gamma)$

## Rheological Models





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.,

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

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.,  $(\mathbf{0}, \mathbf{0}) \in \mathcal{A}$ ;

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








$$(\mathbf{S}_1 - \mathbf{S}_2) \cdot (\mathbf{D}_1 - \mathbf{D}_2) \geq 0 \text{ for all } (\mathbf{D}_1, \mathbf{S}_1), (\mathbf{D}_2, \mathbf{S}_2) \in \mathcal{A};$$

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

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

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

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

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## Definition of $\mathbf{S}_e$ : kinetic theory of polymers

Large number of internal degrees of freedom  $\longrightarrow$  statistical physics.

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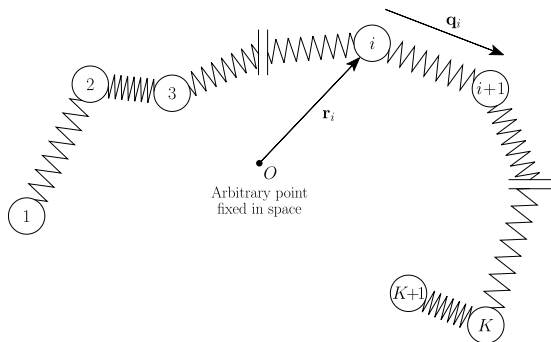
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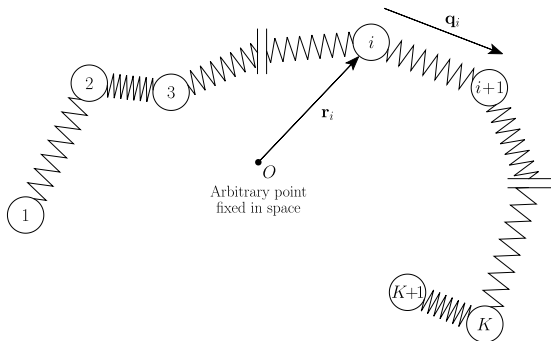
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Let  $D_i \subset \mathbb{R}^d$ ,  $i = 1, \dots, K$ , be bounded open balls centred at  $\mathbf{0}$ .

Consider the Maxwellian  $M(\mathbf{q}) := M_1(\mathbf{q}_1) \cdots M_K(\mathbf{q}_K)$ , with  $\mathbf{q}_i \in D_i$ , where

$$M_i(\mathbf{q}_i) := \frac{e^{-U_i(\frac{1}{2}|\mathbf{q}_i|^2)}}{\int_{D_i} e^{-U_i(\frac{1}{2}|\mathbf{p}_i|^2)} d\mathbf{p}_i}, \quad i = 1, \dots, K.$$

$\mathbf{S}_e$  is defined by the *Kramers expression*:

$$\mathbf{S}_e(x, t) := k_B \mathbb{T} \sum_{i=1}^K \int_D M(\mathbf{q}) \nabla_{\mathbf{q}_i} \hat{\Psi}(x, \mathbf{q}, t) \otimes \mathbf{q}_i d\mathbf{q},$$

where  $\mathbf{q} = (\mathbf{q}_1^T, \dots, \mathbf{q}_K^T)^T \in D_1 \times \dots \times D_K =: D$  and

$$\hat{\Psi} := \Psi / M$$

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

## Fokker–Planck equation

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

$$(M\widehat{\psi})_t + \operatorname{div}(M\widehat{\psi}\mathbf{u}) + \operatorname{div}_{\mathbf{q}}(M\widehat{\psi}(\nabla\mathbf{u})\mathbf{q}) = \Delta(M\widehat{\psi}) + \operatorname{div}_{\mathbf{q}}\mathbf{A}(M\nabla_{\mathbf{q}}\widehat{\psi}) \quad (3)$$

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

$$\begin{aligned} M\nabla\widehat{\psi} \cdot \mathbf{n} &= 0 && \text{on } \partial\Omega \times D \times (0, T), \\ (M\widehat{\psi}(\nabla\mathbf{u})\mathbf{q}_i - \mathbf{A}_i(M\nabla_{\mathbf{q}}\widehat{\psi})) \cdot \mathbf{n}_i &= 0 && \text{on } \Omega \times \partial\bar{D}_i \times (0, T), \end{aligned}$$

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

$$\widehat{\psi}(x, \mathbf{q}, 0) = \widehat{\psi}_0(x, \mathbf{q}) \quad \text{in } O.$$

$\mathbf{A} \in \mathbb{R}_{\text{symm}}^{K \times K}$ : *Rouse matrix* (symmetric, positive definite).





J.W. Barrett & E. Süli (M3AS, 21 (2011), 1211–1289):

Existence and equilibration of global weak solutions to kinetic models for dilute polymers I: Finitely extensible nonlinear bead-spring chains



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M. Bulíček, J. Málek & E. Süli (Communications in PDE, 38 (2013), 882–924):

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

DOI: 10.1080/03605302.2012.742104

## Assumptions on the data

For the Maxwellian  $M$  we assume that

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

For the initial velocity  $\mathbf{u}_0$  we assume that

$$\mathbf{u}_0 \in L_{0,\text{div}}^2(\Omega). \quad (5)$$

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

$$\int_D M(\mathbf{q}) \hat{\Psi}_0(\cdot, \mathbf{q}) \, d\mathbf{q} \in L^\infty(\Omega). \quad (7)$$

## Theorem

For  $d \in \{2, 3\}$  let  $D_i \subset \mathbb{R}^d$ ,  $i = 1, \dots, K$ , 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  $\mathbf{f} \in L^{r'}(0, T; W_{0, \text{div}}^{-1, r'}(\Omega))$ ,  $r \in (1, \infty)$ . Assume that  $\mathcal{A}$ , given by  $\mathbf{G}$ , is a maximal monotone  $r$ -graph satisfying **(A1)** – **(A4)**, the Maxwellian  $M : D \rightarrow \mathbb{R}$  satisfies (4), and  $(\mathbf{u}_0, \widehat{\psi}_0)$  satisfy (5)–(7).

Then, there exist  $(\mathbf{u}, \mathbf{S}_v, \mathbf{S}_e, \widehat{\psi})$  such that

$$\begin{aligned} \mathbf{u} &\in L^\infty(0, T; L_{0, \text{div}}^2(\Omega)^d) \cap L^r(0, T; W_0^{1, r}(\Omega)^d) \cap W^{1, r^*}(0, T; W_{0, \text{div}}^{-1, r^*}(\Omega)), \\ \mathbf{S}_v &\in L^{r'}(0, T; L^{r'}(\Omega)^{d \times d}), \quad \mathbf{S}_e \in L^2(0, T; L^2(\Omega)^{d \times d}), \\ \widehat{\psi} &\in L^\infty(Q; L_M^1(D)) \cap L^2(0, T; W_M^{1, 1}(O)), \quad \widehat{\psi} \geq 0 \text{ a.e. in } O \times (0, T), \\ M\widehat{\psi} &\in W^{1, 1}(0, T; W^{-1, 1}(O)), \quad \widehat{\psi} \log \widehat{\psi} \in L^\infty(0, T; L_M^1(O)), \end{aligned}$$

where

$$r^* := \min \left\{ r', 2, \left(1 + \frac{2}{d}\right)r \right\} \quad \text{and} \quad r' := \frac{r}{r-1}.$$

## Theorem (Continued...)

Moreover, (1) is satisfied in the following sense:

$$\begin{aligned} \int_0^T \langle \mathbf{u}_t, \mathbf{w} \rangle dt + \int_0^T (-(\mathbf{u} \otimes \mathbf{u}, \nabla \mathbf{w}) + (\mathbf{S}_v, \nabla \mathbf{w})) dt \\ = \int_0^T (-(\mathbf{S}_e, \nabla \mathbf{w}) + \langle \mathbf{f}, \mathbf{w} \rangle) dt \quad \text{for all } \mathbf{w} \in L^\infty(0, T; W_{0, \text{div}}^{1, \infty}(\Omega)), \end{aligned}$$

where

$$(\mathbf{S}_v(x, t), \mathbf{D}(\mathbf{u}(x, t))) \in \mathcal{A} \quad \text{for a.e. } (x, t) \in Q,$$

and  $\mathbf{S}_e$  is given by the Kramers expression

$$\mathbf{S}_e(x, t) = k_B \mathbb{T} \sum_{i=1}^K \int_D M \nabla_{\mathbf{q}_i} \widehat{\Psi}(x, \mathbf{q}, t) \otimes \mathbf{q}_i d\mathbf{q} \quad \text{for a.e. } (x, t) \in Q.$$

## Theorem (Continued...)

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

$$\begin{aligned} & \int_0^T [\langle (M\widehat{\Psi})_t, \varphi \rangle - (M\mathbf{u}\widehat{\Psi}, \nabla\varphi)_O - (M\widehat{\Psi}(\nabla\mathbf{u})\mathbf{q}, \nabla_q\varphi)_O] dt \\ & + \int_0^T [(M\nabla\widehat{\Psi}, \nabla\varphi)_O + (M\mathbf{A}\nabla_q\widehat{\Psi}, \nabla_q\varphi)_O] dt = 0 \\ & \text{for all } \varphi \in L^\infty(0, T; W^{1, \infty}(O)), \end{aligned}$$

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

$$\lim_{t \rightarrow 0_+} \|\mathbf{u}(\cdot, t) - \mathbf{u}_0(\cdot)\|_2^2 + \|\widehat{\Psi}(\cdot, t) - \widehat{\Psi}_0(\cdot)\|_{L^1_M(O)} = 0.$$

## Theorem (Continued...)

Further, for  $t \in (0, T)$  the following energy inequality holds in a weak sense:

$$\begin{aligned} \frac{d}{dt} \left( k \int_O M \widehat{\psi} \log \widehat{\psi} \, dx \, d\mathbf{q} + \frac{1}{2} \|\mathbf{u}\|_2^2 \right) + (\mathbf{S}_v, \mathbf{D}(\mathbf{u})) + 4k \left( M \nabla \sqrt{\widehat{\psi}}, \nabla \sqrt{\widehat{\psi}} \right)_O \\ + 4k \left( M \mathbf{A} \nabla_{\mathbf{q}} \sqrt{\widehat{\psi}}, \nabla_{\mathbf{q}} \sqrt{\widehat{\psi}} \right)_O \leq \langle \mathbf{f}, \mathbf{u} \rangle, \quad \text{with } k := k_B T. \end{aligned}$$

# 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 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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  - ▶ Murat–Tartar Div–Curl lemma;
  - ▶ Uniform interior estimates on  $\Omega \times D \times (0, T)$ , obtained by function space interpolation from the energy inequality.

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

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

$$\lim_{t \rightarrow 0_+} \|\mathbf{u}(\cdot, t) - \mathbf{u}_0(\cdot)\|_2^2 + \|\widehat{\Psi}(\cdot, t) - \widehat{\Psi}_0(\cdot)\|_{L_M^1(O)} = 0.$$

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

$$\lim_{\ell \rightarrow \infty} \int_Q |(\mathbf{S}_v^\ell - \mathbf{S}^*(\mathbf{D}(\mathbf{u}))) \cdot \mathbf{D}(\mathbf{u}^\ell - \mathbf{u})|^\alpha \, dx dt = 0 \quad \forall \alpha \in (0, 1).$$

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

Thus, for a subsequence,

$$(\mathbf{S}_v^\ell - \mathbf{S}^*(\mathbf{D}(\mathbf{u}))) \cdot \mathbf{D}(\mathbf{u}^\ell - \mathbf{u}) \rightarrow 0 \quad \text{almost everywhere in } Q.$$

Moreover, using the energy inequality, we see that

$$\int_Q |(\mathbf{S}_v^\ell - \mathbf{S}^*(\mathbf{D}(\mathbf{u}))) \cdot \mathbf{D}(\mathbf{u}^\ell - \mathbf{u})| \, dx dt \leq C.$$

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

$$\lim_{k \rightarrow \infty} |Q \setminus Q_k| \rightarrow 0$$

and such that for any  $k$  there is a subsequence such that

$$(\mathbf{S}_v^\ell - \mathbf{S}^*(\mathbf{D}(\mathbf{u}))) \cdot \mathbf{D}(\mathbf{u}^\ell - \mathbf{u}) \quad \text{converges weakly in } L^1(Q_k).$$



By Vitali's theorem we then deduce that

$$(\mathbf{S}_v^\ell - \mathbf{S}^*(\mathbf{D}(\mathbf{u}))) \cdot \mathbf{D}(\mathbf{u}^\ell - \mathbf{u}) \rightarrow 0 \quad \text{strongly in } L^1(Q_k).$$

The weak convergence of  $(\mathbf{S}_v^\ell)$  to  $\mathbf{S}_v$  and  $(\mathbf{D}(\mathbf{u}^\ell))$  to  $\mathbf{D}(\mathbf{u})$  implies that

$$\lim_{\ell \rightarrow \infty} (\mathbf{S}_v^\ell, \mathbf{D}(\mathbf{u}^\ell))_{Q_k} = (\mathbf{S}_v, \mathbf{D}(\mathbf{u}))_{Q_k}.$$

The assumption that  $\mathcal{A}$  is a maximal monotone  $r$ -graph then implies that

$$(\mathbf{S}_v, \mathbf{D}(\mathbf{u})) \in \mathcal{A} \quad \text{a.e. in } Q_k, k = 1, 2, \dots$$

Finally, by a diagonal procedure and  $\lim_{k \rightarrow \infty} |Q \setminus Q_k| \rightarrow 0$  we deduce that

$$(\mathbf{S}_v, \mathbf{D}(\mathbf{u})) \in \mathcal{A} \quad \text{a.e. in } Q = \Omega \times (0, T).$$



## Open problems

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

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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 & Süli (Journal of Differential Equations, 2012).

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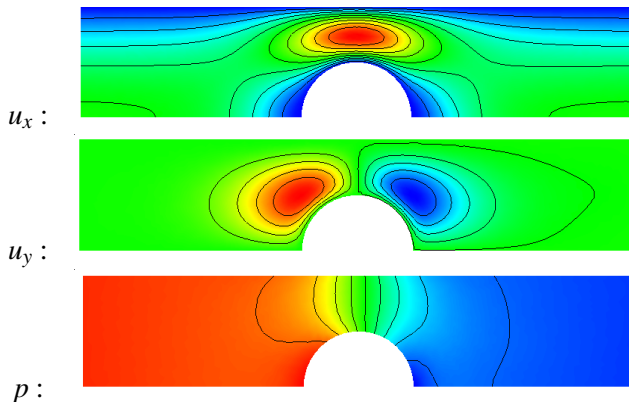
- ▶ Barrett & Süli (Journal of Differential Equations, 2012).
- The numerical analysis of implicitly constituted kinetic models of polymers is open.

### *Special cases:*

- ▶ Barrett & Süli (M2AN, 2012)
- ▶ Dienes, Kreuzer & Süli (SIAM J. Numer. Anal., 2013)
- ▶ Kreuzer & Süli (In preparation, 2014).

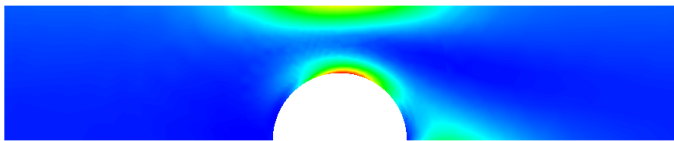
## 2D/4D: Flow around a cylinder

- 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):

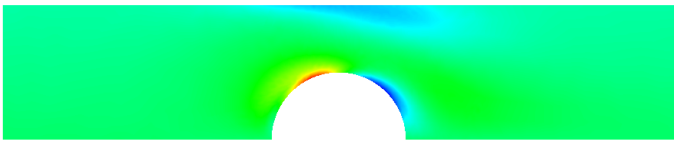


## 2D/4D: Flow around a cylinder: extra stress tensor

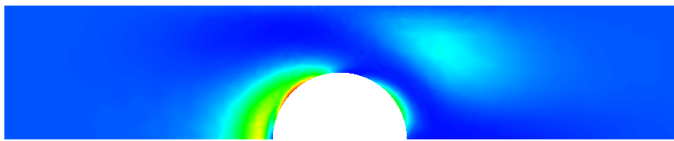
$(\mathbf{S}_e)_{11} :$



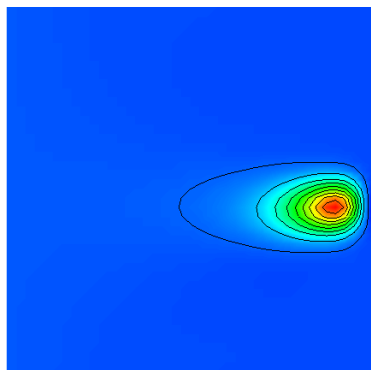
$(\mathbf{S}_e)_{12} :$



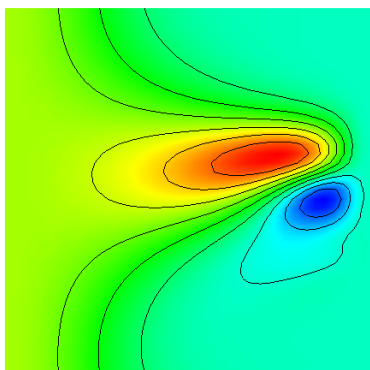
$(\mathbf{S}_e)_{22} :$



## 2D/4D: Flow around a cylinder: probability density fn.



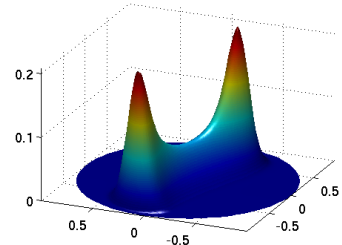
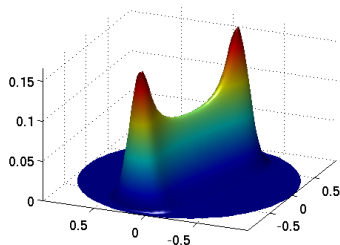
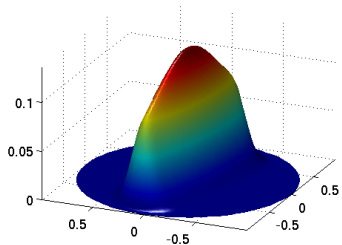
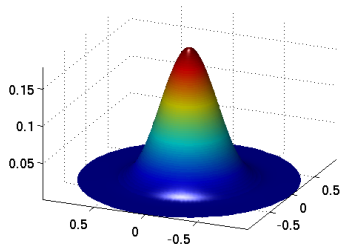
(a)



(b)

Figure : Configuration space cross-sections of  $\psi$  for  $x$  in  $(r, \theta)$ -coordinates: (a) wake of cylinder, and (b) between cylinder and wall.

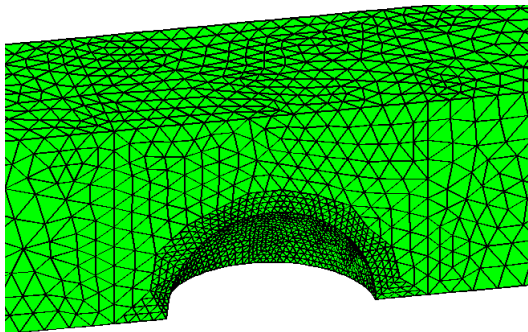
## 2D/4D: Flow around a cylinder: probability density fn.



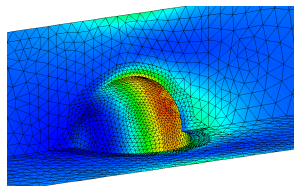


## 3D/6D: Flow past a ball in a channel

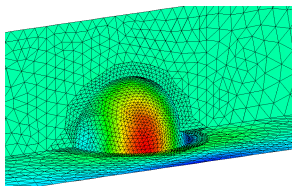
- Pressure-drop-driven flow past a ball in hexahedral channel.
- $P_2/P_1$  mixed FEM for (Navier–)Stokes equation on a mesh with 3045 tetrahedral elements and 51989 Gaussian quadrature points.
- Fokker–Planck equation solved using heterogenous ADI method in 6D domain  $\Omega \times D$ . 51989 3D solves 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;  $\Delta t = 0.05$ ;  $\lambda = 0.5$ .



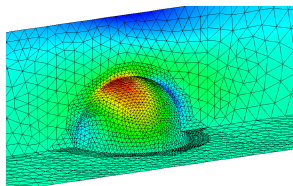
# 3D/6D: Flow past a ball in a channel: elastic part of the Cauchy stress



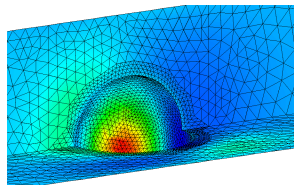
$(\mathbf{S}_e)_{11}$



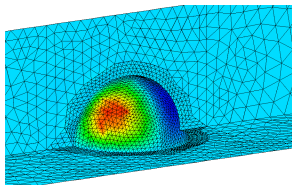
$(\mathbf{S}_e)_{12}$



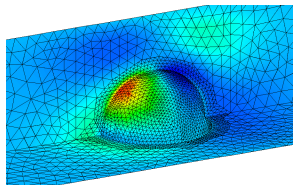
$(\mathbf{S}_e)_{13}$



$(\mathbf{S}_e)_{22}$



$(\mathbf{S}_e)_{23}$



$(\mathbf{S}_e)_{33}$



HAPPY BIRTHDAY, EITAN!