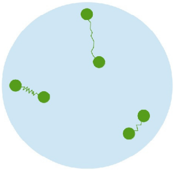
Multiscale method for viscoelastic polymeric flow

H. Mizerová, Bangwei She

Modelling

Dilute polymer solutions: a dumbbell model

- polymer molecules surrounded by Newtonian fluid
- no interactions between molecules
- polymer molecules modeled as dumbbells



A dumbbell model

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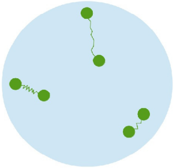

The Navier-Stokes equations

$$
\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla_x)\mathbf{u} &= 2\nu \mathbf{D}(\mathbf{u}) + \operatorname{div}_x \mathbf{T} - \nabla_x p && \text{in } (0, T) \times \Omega \\
\operatorname{div}_x \mathbf{u} &= 0 && \text{in } (0, T) \times \Omega \\
\mathbf{u} &= \mathbf{0} && \text{on } (0, T) \times \partial\Omega \\
\mathbf{u}(0) &= \mathbf{u}_0 && \text{in } \Omega
\end{aligned}
$$

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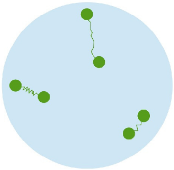

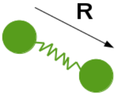

- the friction force from surrounding fluid
  $\mathbf{f} = \zeta(\dot{\mathbf{r}} - \mathbf{v}(\mathbf{r}, t))$
- the stochastic force due to the Brownian motion
  $\mathbf{B}_i = \sqrt{2kT\zeta} d\mathbf{W}_i/dt$
- the spring force $\mathbf{F}(\mathbf{R}) = \gamma_1(|\mathbf{R}|^2)\mathbf{R}$

$$-\zeta(\dot{\mathbf{r}}_1 - \mathbf{v}(\mathbf{r}_1, t)) + \mathbf{F}(\mathbf{R}) + \mathbf{B}_1 = 0,$$
$$-\zeta(\dot{\mathbf{r}}_2 - \mathbf{v}(\mathbf{r}_2, t)) - \mathbf{F}(\mathbf{R}) + \mathbf{B}_2 = 0.$$

$$\dot{\mathbf{R}} = \nabla\mathbf{v} \cdot \mathbf{R} - \frac{2}{\zeta}\mathbf{F}(\mathbf{R}) + \sqrt{\frac{4kT}{\zeta}} \frac{d\mathbf{W}_t}{dt}.$$

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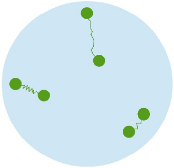

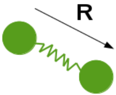

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The Fokker-Planck equation

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x)\psi - \frac{k\tau}{2\zeta}\Delta_x \psi = \mathrm{div}_R \Big(- \nabla_x \mathbf{u} \cdot \mathbf{R}\psi \Big) + \frac{2k\tau}{\zeta}\gamma_2(|\mathbf{R}|^2)\Delta_R\, \psi + \frac{2}{\zeta}\mathrm{div}_R \Big(\mathbf{F}(\mathbf{R})\psi \Big)$$

The Peterlin approximation

$$\frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla_x)\psi - \frac{k\tau}{2\zeta}\Delta_x \psi = \mathrm{div}_R \left(- \nabla_x \mathbf{u} \cdot \mathbf{R}\psi \right) + \frac{2k\tau}{\zeta}\gamma_2(|\mathbf{R}|^2)\Delta_R \psi + \frac{2}{\zeta}\mathrm{div}_R \left(\mathbf{F}(\mathbf{R})\psi \right)$$

- A. Peterlin: *Hydrodynamics of macromolecules in a velocity field with longitudinal gradient*, J. Polym. Sci. Pol. Lett. 4 (1966), pp. 287-291

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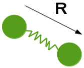
length of the spring is replaced by the average length

$$\gamma_i(|\mathbf{R}|^2) \mapsto \gamma_i(\langle|\mathbf{R}|^2\rangle) = \gamma_i(\mathrm{tr}\,\mathbf{C})$$



$$\mathrm{tr}\,\mathbf{C}(\psi) = \langle|\mathbf{R}|^2\rangle := \int_{\mathbb{R}^d} |\mathbf{R}|^2\psi(t,x,\mathbf{R})\,\mathrm{d}\mathbf{R}$$

$$\frac{\partial\psi}{\partial t} + (\mathbf{u}\cdot\nabla_x)\psi - \frac{k\tau}{2\zeta}\Delta_x\psi = \mathrm{div}_R\Big(-\nabla_x\mathbf{u}\cdot\mathbf{R}\psi\Big) = \frac{2k\tau}{\zeta}\gamma_2(\mathrm{tr}\,\mathbf{C})\Delta_R\,\psi + \frac{2}{\zeta}\mathrm{div}_R\Big(\gamma_1(\mathrm{tr}\,\mathbf{C})\mathbf{R}\psi\Big)$$

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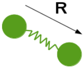

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Macroscopic closure of the Fokker-Planck equation

$$\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{C} - (\nabla\mathbf{u})\mathbf{C} - \mathbf{C}(\nabla\mathbf{u})^T = \frac{\gamma_2(\mathrm{tr}\,\mathbf{C})}{\lambda}\mathbf{I} - \frac{\gamma_1(\mathrm{tr}\,\mathbf{C})}{\lambda\gamma_{\mathbf{m}}}\mathbf{C} + \varepsilon\Delta\mathbf{C}$$

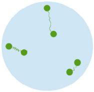
FENEP, Oldroyd-b

The Navier-Stokes-Fokker-Planck system

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla_x)\mathbf{u} = 2\nu \mathbf{D}(\mathbf{u}) + \mathrm{div}_x\, \mathbf{T} - \nabla_x p$$

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

$$\mathbf{T} = \gamma_3(\mathrm{tr}\, \mathbf{C}(\psi))\mathbf{C}(\psi) - \mathbf{I} \qquad \text{(Kramer's expression)}$$



Boundary and initial conditions: $\mathbf{u} = \mathbf{0}$ on $(0, T) \times \partial\Omega$, $\mathbf{u}(0) = \mathbf{u}_0$ in Ω

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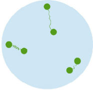

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$$\frac{\partial \psi}{\partial t} + (\mathbf{u}\cdot\nabla_x)\psi - \varepsilon\Delta_x\psi = \mathrm{div}_R\,(-\nabla_x\mathbf{u}\cdot\mathbf{R}\psi) + \frac{\gamma_2(\mathrm{tr}\,\mathbf{C})}{2\lambda}\Delta_R\,\psi + \frac{\gamma_1(\mathrm{tr}\,\mathbf{C})}{2\lambda\gamma_{\mathrm{M}}}\mathrm{div}_R\,(\mathbf{R}\psi)$$

Deborah number: $\lambda = \frac{\zeta}{4\gamma_{\mathrm{M}}}\frac{U_0}{L_0}$

$$\frac{\gamma_1(\mathrm{tr}\,\mathbf{C})}{\gamma_2(\mathrm{tr}\,\mathbf{C})} = \frac{\gamma_1(\mathrm{tr}\,\mathbf{C}_{\mathrm{M}})}{\gamma_2(\mathrm{tr}\,\mathbf{C}_{\mathrm{M}})} = \gamma_{\mathrm{M}}$$

center-of-mass diffusion: $\varepsilon = \left(\frac{l_0}{L_0}\right)^2 \frac{1}{8\lambda}$

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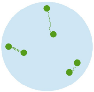

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Boundary/decay and initial conditions:

$$\psi \to 0 \qquad \text{on } (0, T] \times \Omega \text{ as } |\mathbf{R}| \mapsto \infty$$

$$\varepsilon \frac{\partial \psi}{\partial \mathbf{n}} = 0 \qquad \text{on } (0, T) \times \partial\Omega \times \mathbb{R}^d$$

$$\psi(0) = \psi_0 \qquad \text{on } \Omega \times \mathbb{R}^d$$

Existence of global weak solutions for Navier-Stokes-Fokker-Planck

* FENE: Barrett, Süli
* Hookean: Barrett, Süli
* Peterlin: P. Gwiazda, M. Lukáčová, H. Mizerová, A. Świerczewska-Gwiazda

Numerical Methods

Navier-Stokes: Characteristic FEM

$$\frac{Re}{\Delta t}(\mathbf{u}_h^{n+1}, \mathbf{v}_h) + 2\nu \left(D(\mathbf{u}_h^{n+1}), D(\mathbf{v}_h) \right) - (p_h^{n+1}, \nabla \cdot \mathbf{v}_h) - (\nabla \cdot \mathbf{u}_h^{n+1}, q_h)$$
$$+ s_h(p_h^{n+1}, q_h) = \frac{Re}{\Delta t}(\mathbf{u}_h^n \circ X, \mathbf{v}_h) - (\mathbf{T}_h^n, \nabla \mathbf{v}_h)$$

$s_h(p, q) = -\delta \sum_\kappa h_\kappa^2 (\nabla p, \nabla q)_\kappa, \quad \mathbf{u}_h^n \circ X = ?$

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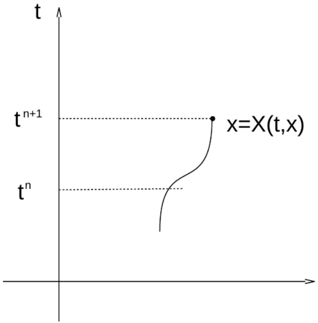
Characteristic method

Let X be the position of a particle,

$$\begin{cases} \frac{d}{dt}X = \mathbf{u}(X,t),\ \forall t\in[t^n, t^{n+1}], \\ X(t;x) = x. \end{cases}$$

Material derivative:
$\frac{D\phi}{Dt} = \frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi$
is discretized as
$\frac{D\phi}{Dt} \approx \frac{\phi - \phi(X(t-\Delta t;x), t-\Delta t)}{\Delta t}$



linear symmetric No CFL condition.

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Fokker-Planck

High dimension

unbounded domain

Multiscale simulation in whole space

$$\frac{\partial \psi}{\partial t} + (\mathbf{u}\cdot\nabla_x)\psi - \varepsilon\Delta_x\psi = \mathrm{div}_R\left(-\nabla_x\mathbf{u}\cdot\mathbf{R}\psi\right) + \frac{\gamma_2(\mathrm{tr}\,\mathbf{C})}{2\lambda}\Delta_R\,\psi + \frac{\gamma_1(\mathrm{tr}\,\mathbf{C})}{2\lambda\gamma_{\mathrm{M}}}\mathrm{div}_R\left(\mathbf{R}\psi\right)$$

→ **physical space:** $\frac{\partial \psi}{\partial t} + (\mathbf{u}\cdot\nabla_x)\psi - \varepsilon\Delta_x\psi = 0$

finite volume + upwind

finite element + characteristics

→ **configuration space:** $\frac{\partial \psi}{\partial t} + \mathrm{div}_R\left(\nabla_x\mathbf{u}\cdot\mathbf{R}\psi\right) - \frac{\gamma_2(\mathrm{tr}\,\mathbf{C})}{2\lambda}\Delta_R\,\psi - \frac{\gamma_1(\mathrm{tr}\,\mathbf{C})}{2\lambda\gamma_{\mathrm{M}}}\mathrm{div}_R\left(\mathbf{R}\psi\right) = 0$

3 angle-preserving transformations
+ spectral method

▶ H. Mizerová, B. She : *Multiscale simulation of the Fokker-Planck equation in the whole space*, in preparation.

Configuration space solver

1. transformation: Cartesian to polar coordinates

$$T_1 : \mathbb{R}^2 \longrightarrow [0, \infty) \times (-\pi, \pi], \qquad \mathbf{R} \longmapsto (\rho, \theta), \qquad \rho = \sqrt{R_1^2 + R_2^2}, \quad \theta = \arctan \frac{R_1}{R_2}$$

2. transformation: ***infinite plane to unit circle***

$$T_2 : [0, \infty) \times (-\pi, \pi] \longrightarrow [0, 1] \times (-\pi, \pi], \qquad (\rho, \theta) \longmapsto (r, \theta), \qquad r = \frac{1}{1 + \rho}$$

3. transformation: due to boundary conditions

$$T_3 : [0, 1] \times [-\pi, \pi) \longrightarrow [-1, 1] \times [-\pi, \pi), \qquad (r, \theta) \longmapsto (\eta, \theta), \qquad \eta = 2(1 - r)^2 - 1$$

- A. Lozinski, C. Chauvière : *A fast solver for Fokker-Planck equation applied to viscoelastic flows calculations: 2D FENE model*, J. Comput. Phys. 189 (2003), pp. 607–625

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More general transformation:

$$\eta = 1 - 2e^{-s\rho}, \quad \eta = \frac{\rho - s}{\rho + s}, \quad s > 0.$$

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Spectral method:

$$\psi(t,\mathbf{x},\eta,\theta) := (1-\eta)^s \phi(t,\mathbf{x},\eta,\theta)$$

$$\phi := \sum_{k=1}^{N_\eta} \sum_{z=0}^{N_\theta} \alpha_{zk} h_k(\eta) cos(2z\theta) + \sum_{k=1}^{N_\eta} \sum_{z=1}^{N_\theta} \beta_{zk} h_k(\eta) sin(2z\theta)$$

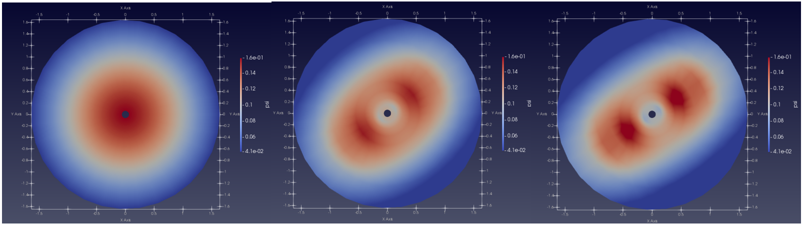
▶ A. Lozinski, C. Chauvière : *A fast solver for Fokker-Planck equation applied to viscoelastic flows calculations: 2D FENE model*, J. Comput. Phys. 189 (2003), pp. 607–625

Configuration space solver
Numerical test

$$\frac{\partial \psi}{\partial t} + \mathrm{div}_R\left(\nabla_x \mathbf{u} \cdot \mathbf{R}\psi\right) - \frac{1}{2\lambda}\Delta_R\,\psi - \frac{1}{2\lambda}\mathrm{div}_R\left(\mathbf{R}\psi\right) = 0, \qquad \lambda = 1$$

Shear flow: $\nabla \mathbf{u} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$

Initial value: $\psi_0 = \frac{1}{2\pi} \exp\left\{ \frac{-|\mathbf{R}|^2}{2} \right\}$



exact:	$C_{11} = 1 + 2\lambda^2$	$C_{12} = \lambda$	$C_{22} = 1$	$\int_{\mathbb{R}^d} \psi = 1$
numerical:	$C_{11} = 3.017$	$C_{12} = 1.004$	$C_{22} = 1.003$	$\int \psi = 1.025$

Weighted Hermite spectral

$$\tilde{H}_n(x) = \frac{\omega_\alpha^{-1}(x)}{\sqrt{2^n n!}} H_n(\alpha x), \quad \omega_\alpha(x) = e^{\alpha^2 x^2}, \quad H_n(x) = (-1)^n e^{x^2} \partial_x^n (e^{-x^2})$$

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Orthogonality

$$\int_{\mathbb{R}} \tilde{H}_m(x)\tilde{H}_n(x)\omega_\alpha(x)dx = \frac{\sqrt{\pi}}{\alpha}\delta_{m,n}$$

Derivatives

$$\begin{aligned}
\alpha x \tilde{H}_n(x) &= \sqrt{\frac{n+1}{2}}\tilde{H}_{n+1}(x) + \sqrt{\frac{n}{2}}\tilde{H}_{n-1}(x) \\
\partial_x \tilde{H}_n(x) &= -\alpha\sqrt{2(n+1)}\tilde{H}_{n+1}(x) \\
x\partial_x \tilde{H}_n(x) &= -\sqrt{(n+1)(n+2)}\tilde{H}_{n+2}(x) - (n+1)\tilde{H}_n(x) \\
\partial_x^2 \tilde{H}_n(x) &= 2\alpha^2\sqrt{(n+1)(n+2)}\tilde{H}_{n+2}(x)
\end{aligned}$$

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Let $\psi(t, \mathbf{x}, \mathbf{q}) = \sum_{m,n=0}^{N} \phi_{mn} \tilde{H}_m(r) \tilde{H}_n(s)$, $\mathbf{q} = (r, s)$.
Discretization of configuration space:
$r_i, i = 0, 1, \cdots, N$ are the roots of $H_{N+1}(r) = 0$.
Test with $\tilde{H}_z(r)\tilde{H}_k(s)\omega_\alpha(r)\omega_\alpha(s)$ and integrate over the whole space:

Weighted Hermite spectral

$$\tilde{H}_n(x) = \frac{\omega_\alpha^{-1}(x)}{\sqrt{2^n n!}} H_n(\alpha x), \quad \omega_\alpha(x) = e^{\alpha^2 x^2}, \quad H_n(x) = (-1)^n e^{x^2} \partial_x^n (e^{-x^2})$$

Let $\psi(t, \mathbf{x}, \mathbf{q}) = \sum_{m,n=0}^{N} \phi_{mn} \tilde{H}_m(r) \tilde{H}_n(s)$, $\mathbf{q} = (r, s)$.
Discretization of configuration space:
$r_i, i = 0, 1, \cdots, N$ are the roots of $H_{N+1}(r) = 0$.
Test with $\tilde{H}_z(r)\tilde{H}_k(s)\omega_\alpha(r)\omega_\alpha(s)$ and integrate over the whole space:

$$\frac{\partial \phi_{zk}}{\partial t} = \mathcal{L}(\phi_{zk}),$$

where

$$\begin{aligned}\mathcal{L}(\phi_{zk}) = {} & \phi_{z-2,k}(2\alpha^2\gamma_2 - A_{11})\sqrt{z(z-1)} + \phi_{z-1,k-1}(-A_{12} - A_{21})\sqrt{zk} \\ & + \phi_{z-1,k+1}(-A_{12})\sqrt{z(k+1)} + \phi_{z,k-2}(2\alpha^2\gamma_2 - A_{22})\sqrt{k(k-1)} \\ & + \phi_{z,k}(-A_{11}z - A_{22}k) + \phi_{z+1,k-1}(-A_{12})\sqrt{(z+1)k},\end{aligned}$$

and $A_{ij} = \gamma_1 \mathbf{I} - \nabla_x \mathbf{u}, \quad \psi_{z,k} \equiv 0$, for $m, n < 0$ or $> N$.

$$\frac{\phi_{zk}^{*} - \phi_{zk}^{n}}{\Delta t} = \mathcal{L}(\phi_{zk}^{*}), \quad (1)$$

$$\left(\frac{\phi_{zk}^{n+1} - \phi_{zk}^{*} \circ X^{n}}{\Delta t}, q_h\right) + \varepsilon\left(\nabla_x \phi_{zk}, \nabla_x q_h\right) = 0, \quad (2)$$

Lemma

If the probability distribution function is initially independent of the physical potion $\mathbf{x}$*, i.e.* $\psi(0, \mathbf{x}, \mathbf{q}) = \psi_0(\mathbf{q})$*, then we have*

$$\phi_{00}(t^n, \mathbf{x}) \equiv \phi_{00}(0, \mathbf{x}).$$

Step 1. from (1)

$$\phi_{00}^{*} - \phi_{00}^{n} = 0.$$

Step 2, if $\phi_{00}^{n}(\mathbf{x})$ is independent of $\mathbf{x}$, then $\phi_{zk}^{*} \circ \mathbf{X}^{n} = \phi_{zk}^{*}$ is a constant in the physical space, which results in $\phi_{00}^{n+1} = \phi_{00}^{*} = \phi_{00}^{n}$ from (2) .

Lemma (Mohammadi & Borzi, Int. J. Uncertain. Quantif. 2015)

$$\int_{\mathbb{R}} \tilde{H}_n(x)dx = 0, \;\; for\ n \geq 1.$$

If n is odd, the result is obvious as $\tilde{H}_n(-x) = (-1)^n \tilde{H}_n(x)$.

If n is even

$$\begin{aligned}\int_{\mathbb{R}} \tilde{H}_n(x)dx &= \frac{1}{\sqrt{2^n n!}} \int_{\mathbb{R}} H_n(\alpha x) e^{-\alpha^2 x^2} dx = \frac{1}{\alpha} \frac{1}{\sqrt{2^n n!}} \int_{\mathbb{R}} H_n(r) e^{-r^2} dr \\ &= \frac{2}{\alpha\sqrt{2^n n!}} \int_0^{\infty} H_n(r) e^{-r^2} dr = \frac{2}{\alpha\sqrt{2^n n!}} \lim_{x\to\infty} \int_0^{x} H_n(r) e^{-r^2} dr \\ &= \frac{2}{\alpha\sqrt{2^n n!}} \lim_{x\to\infty} \left(H_{n-1}(0) - e^{-x^2} H_{n-1}(x) \right) \\ &= 0.\end{aligned}$$

Lemma

If the probability distribution function is initially independent of the physical potion $\mathbf{x}$*, i.e.* $\psi(0, \mathbf{x}, \mathbf{q}) = \psi_0(\mathbf{q})$*, then we have the conservation of mass*

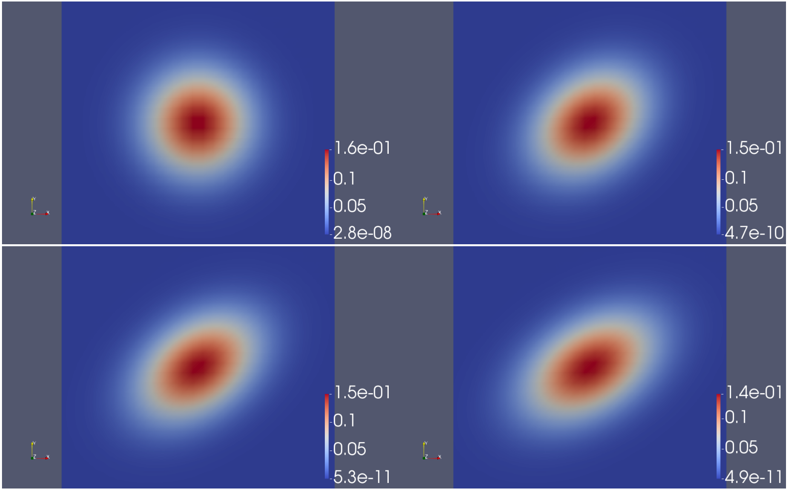
$$\int_{\mathbb{R}^2} \psi(t^n) = \int_{\mathbb{R}^2} \psi_0 = 1.$$

Application of the above lemmas:

$$\int_{\mathbb{R}^2} \psi(t^n) := \int_{\mathbb{R}^2} \sum_{i,j=0}^{N} \phi_{ij}(t^n) \tilde{H}_i(r) \tilde{H}_j(s) drds = \int_{\mathbb{R}^2} \phi_{00}(t^n) \tilde{H}_0(r) \tilde{H}_0(s) drds$$

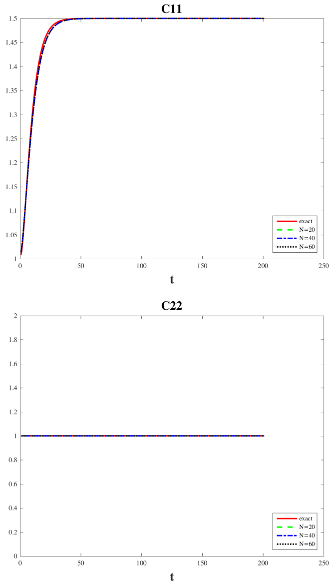
$$= \int_{\mathbb{R}^2} \phi_{00}(t^0) \tilde{H}_0(r) \tilde{H}_0(s) drds = \int_{\mathbb{R}^2} \sum_{i,j=0}^{N} \phi_{ij}(t^0) \tilde{H}_i(r) \tilde{H}_j(s) drds \; =: \int_{\mathbb{R}^2} \psi(t^0).$$

$\Delta t = 0.1$

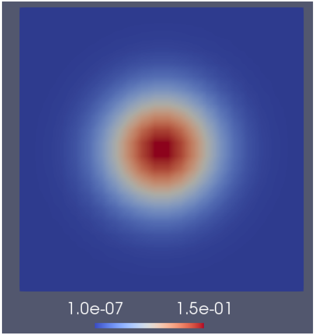


1.6e-01
0.1
0.05
2.8e-08
1.5e-01
0.1
0.05
4.7e-10
1.5e-01
0.1
0.05
5.3e-11
1.4e-01
0.1
0.05
4.9e-11

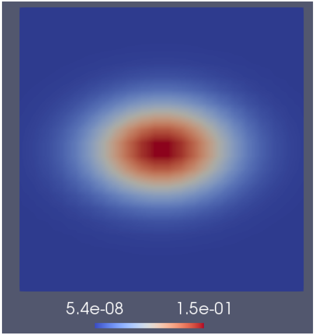
$\Delta t = 0.1$



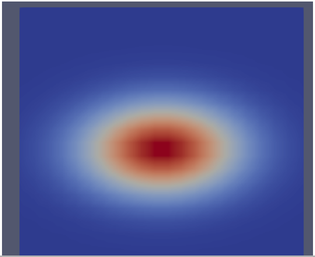
Extensional flow

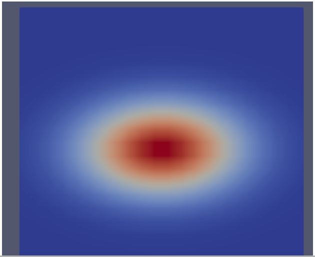


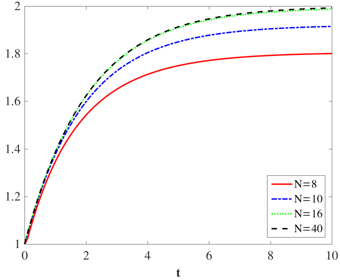
(a) t=0



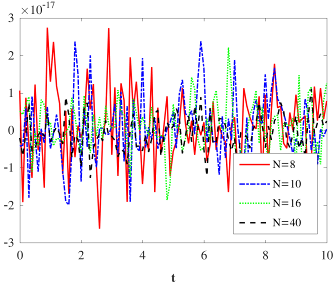
(b) t=1



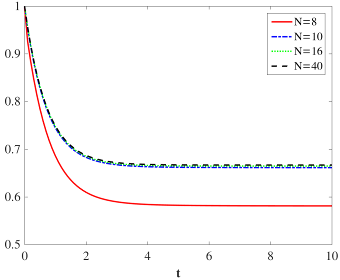


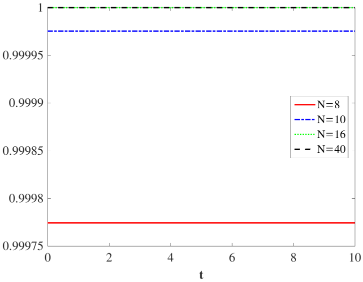

N=8
N=10
N=16
N=40
t

(a) C_{11}


×10^-17
N=8
N=10
N=16
N=40
t

(b) C_{12}


N=8
N=10
N=16
N=40
t


N=8
N=10
N=16
N=40
t

Steady state of extensional flow

$$\psi_{\text{ref}} = cM \exp(We\,\mathbf{q}^T \nabla_{\mathbf{x}} \mathbf{u} \mathbf{q}),$$

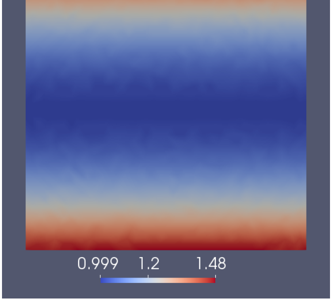
$$M = \frac{1}{2\pi} \exp(-\frac{1}{2}|\mathbf{q}|^2)$$

$$\mathbf{C}_{\text{ref}} = \text{diag}\{2, 2/3\}$$

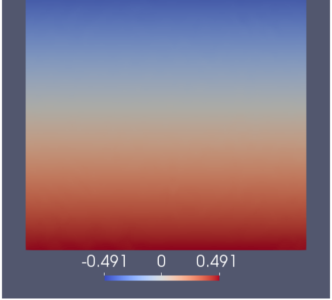
.

Table : Numerical error of planar extensional flow

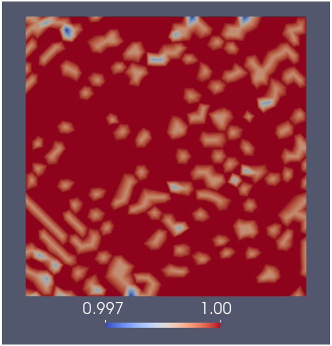
N	8	10	16	20	30
$\|\psi_h - \psi_{exact}\|_{L_2(\mathbb{D})}$	2.1e-02	1.3e-02	3.3e-03	1.3e-03	1.5e-04
$\|C_{11} - C_{11\,\text{ref}}\|$	1.9e-1	7.9e-2	5.5e-3	8.8e-4	6.2e-5
$\|C_{22} - C_{22\,\text{ref}}\|$	8.6e-2	5.5e-3	2.2e-3	7.0e-5	1.0e-6

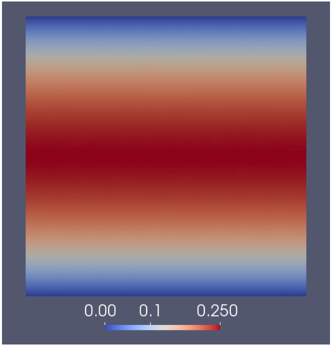


(a) C_{11}



(b) C_{12}





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Thank you for your attention!