Suspensions of rod-like polymers

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5th International Symposium on Finite Volumes for Complex Applications
June 08-13, 2008
Aussois, France

Suspensions of rod-like molecules I

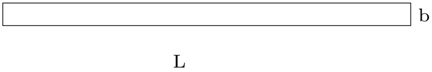
Content of the talk:

- A multiscale model for liquid suspensions of rod-like molecules
  - The coupled micro-macro system
  - Suspensions of rod-like molecules: The model
  - The Smoluchowski equation
- A characterisitc method for the 1D advection-diffusion equation
  - Derivation of method
  - Numerical results
  - Future Work

The molecules

<u>The molecules</u>

- rod-like
- non-deformable
- all of equal length L and width b, with $L \gg b$
- contained in an incompressible viscous fluid



Suspensions of rod-like molecules II

Suspensions of Molecules

- homogeneous concentration ν throughout the fluid
- Concentration Regime considered here:
  - Dilute concentrations, i.e. $\nu \ll L^{-d}$, where $d \in \{2, 3\}$ is the macroscopic space dimension.
  - $\rightarrow$ Molecules can rotate freely without mutual interaction

The coupled micro-macro model

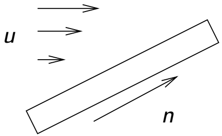
The coupled micro-macro model

- Shear forces from macroscopic velocity gradient change the orientation of the molecules $\longrightarrow$ Smoluchowski-equation
- Orientation of molecules influences macroscopic stress of fluid $\longrightarrow$ additional stress term σ.
- Macroscopic flow $\longrightarrow$ Stokes equation with this additional stress σ.

The coupled system of PDEs

Smoluchowski equation, stress, Stokes equation

$$\partial_t f + \nabla_x f \cdot u + \nabla_n \cdot (P_{n^\perp} \nabla_x u n) f - D_r \Delta_n f = 0$$
$$\int_{S^2} f \; dn = 1$$
$$f \geq 0$$
$$\int_{S^{d-1}} (3n \otimes n - id)\, f dn = \sigma$$
$$\nabla_x \cdot \big((\nabla_x u + \nabla_x^t u) - pid + \sigma \big) = 0$$
$$\nabla_x \cdot u = 0$$



$$P_{n^\perp} \nabla_x u\, n \;:=\; \nabla_x u\, n - (n \cdot \nabla_x u\, n)\, n$$

The Smoluchowski-equation I

Orientational distribution of molecules

- described by the Smoluchowski equation

$$\partial_t f + \underbrace{u \cdot \nabla_x f}_{(1)} + \underbrace{\nabla_n \cdot (P_{n^\perp} \nabla_x u n f)}_{(2)} = \underbrace{D_r \triangle_n f}_{(3)} . \tag{1}$$

Interpretation of terms

(1) $u \cdot \nabla_x f$	change of f due to macroscopic advection
(2) $\nabla_n \cdot (P_{n^\perp} \nabla_x u n f)$	rotational change due to macroscopic shear-forces
(3) $D_r \triangle_n f$	random change of orientation due to Brownian motion

The Smoluchowski equation II

Special case:

Consider spatially homogeneous solutions $f = f(t, n)$, $u = \kappa x$

$$\partial_t f + \nabla_n \cdot ((P_{n^\perp} \kappa n) f) = D_r \Delta_n f$$

Deborah number:

- $De := |\nabla_x u| / D_r$
  $\longrightarrow$ Meausures shear forces relative to rotational diffusion
- Analogy: Peclet-number $Pe = \frac{u_0 L}{D}$ for advection-diffusion
  $\longrightarrow$ measures advection relative to diffusion

Challenge for numerical simulation

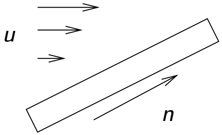
Demanding Simulation of coupled system due to

- high dimension of the system, in case $d = 3$
  - $d = 3$ macro space dimensions
  - $d - 1 = 2$ micro spacedimensions
  - $\Longrightarrow 3 + 2 = 5$ space dimensions for coupled system
- steep gradients that can occur in the solution of the Smoluchowski equation if Deborah-number De is large.
  - analogous: advection-dominated diffusion equations

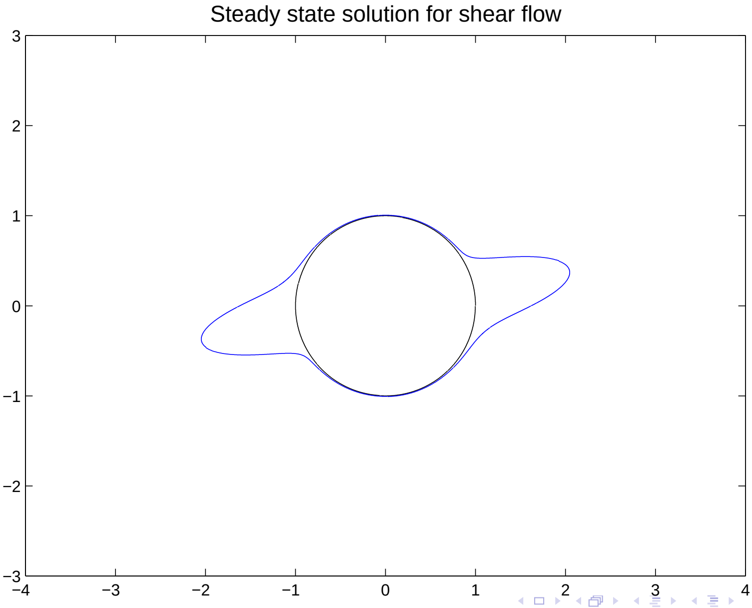
Spatially homogeneous Smoluchowski equation

Consider for dimension $d = 2$

- spatially homogeneous initial values $f(x, n, 0) = f(n, 0)$
- steady macroscopic shear flow $u = \kappa x_2 \Rightarrow \nabla_x u = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$
- $\Rightarrow u \cdot \nabla_x f = 0$
- homogeneous solution $f(x, n, t) = f(n, t)$
- Smoluchowski equation becomes
  - $\partial_t f + \partial_x(\sin^2(x) f) = D_r \, \partial_{xx} f \rightarrow$ advection-diffusion eq. on S^1
  - $\Longrightarrow$ Solution becomes steady in finite time.



Solution for shear flow - plot over S^1



The numerical method for advection-diffusion

So we now consider periodic advection-diffusion equation

$$\begin{aligned} \partial_t f + \partial_x (Vf) &= D \, \partial_{xx} f \\ f(x,0) &= f(x+2\pi,0) \end{aligned}$$

<u>Notation</u>

- x HERE is PREVIOUS n (for convenience)
- $V = V(x) =$ advection velocity
- $D = const =$ diffusion coefficient

The numerical method for advection-diffusion

Method proposed here

Characteristics-based finite volume method of ELLAM type. Properties

- Third order accuracy in space by use of 3rd-order B-splines (novel approach for FV-ELLAM-type methods)
- Second order accuracy in time
- Unconditional stability
  - large t-steps possible (no CFL restriction)
- Use of any adaptive mesh possible which satisfies
  - $\Delta x_i < \Delta x_{i-1} + \Delta x_{i+1} \quad \forall i$
    $\rightarrow$ satisfied by all grids of practical interest since many
    - vary only monotonously over three grid cells, or
    - vary only very little over three grid cells.
- accurate for large *De* (and large *Pe*).

Derivation of Numerical Method I

$$\partial_t f + \partial_x (Vf) = D\,\partial_{xx} f \tag{2}$$

Let

$$0 = x_0 < x_1 < \cdots < x_M = 2\pi$$

be the grid.
Define the characteristics of the hyperbolic part of (2) as solutions of ODE

$$\frac{dx(t)}{dt} = V(x(t)) \tag{3}$$

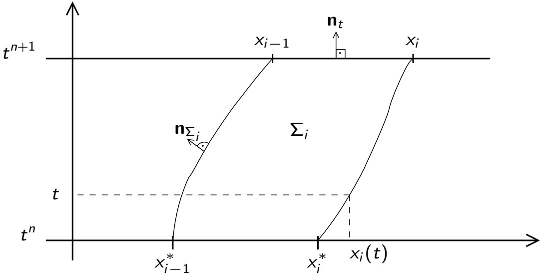
Derivation of Numerical Method II

Denote by Σ_i the space-time domain bounded by

- the characteristics $x_{i-1}(t), x_i(t)$ and
- the t-levels $t^n < t^{n+1}$

Define test-functions w_i of t-step $t^n \longrightarrow t^{n+1}$ by

$$w_i(x,t) = \begin{cases} 1, & \text{if } (x,t) \in \Sigma_i \\ 0, & \text{else.} \end{cases}$$



Derivation of Numerical Method III

Now

- multiply advection-diffusion equation (2) by w_i
- integrate over $\mathbb{R} \times \mathbb{R}_{>0}$.
- use partial integration

to obtain

$$
\begin{aligned}
&\int_{x_{i-1}}^{x_i} f(x, t^{n+1})\, dx - \int_{x_{i-1}^*}^{x_i^*} f(x, t^n)\, dx \\
&+ \int_{t^n}^{t^{n+1}} D\, \partial_x f(x_{i-1}(t), t)\, dt - \int_{t^n}^{t^{n+1}} D\, \partial_x f(x_i(t), t)\, dt = 0,
\end{aligned}
\tag{4}
$$

where $x_j^* = x_j(t^n)$.

Geometric interpretation of Integral equation

$$\int_{x_{i-1}}^{x_i} f(x, t^{n+1})\,dx - \int_{x_{i-1}^*}^{x_i^*} f(x, t^n)\,dx$$
$$+ \int_{t^n}^{t^{n+1}} D\,\partial_x f(x_{i-1}(t), t)\,dt - \int_{t^n}^{t^{n+1}} D\,\partial_x f(x_i(t), t)\,dt = 0,$$

From t-step $t^n \rightarrow t^{n+1}$

- advection transports mass f contained in $[x_{i-1}^*, x_i^*]$ into $[x_{i-1}, x_i]$
- diffusion acts as flux across the characteristics

Derivation of Numerical Method IV

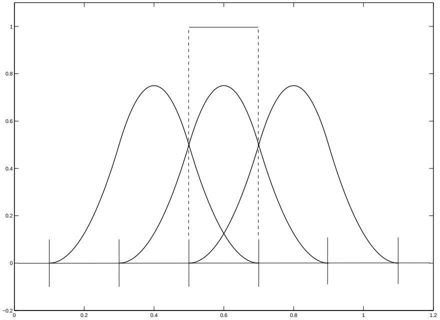
Using the trapezoid rule we get

$$
\begin{aligned}
&\int_{x_{i-1}}^{x_i} f(x,t^{n+1})dx + \frac{\Delta t}{2}\cdot D\,\partial_x f(x_{i-1},t^{n+1}) - \frac{\Delta t}{2}\cdot D\,\partial_x f(x_i,t^{n+1}) \\
= &\int_{x_{i-1}^*}^{x_i^*} f(x,t^n)\,dx \, - \frac{\Delta t}{2}\cdot D\,\partial_x f(x_{i-1}^*,t^n)\,dt \, + \frac{\Delta t}{2}\cdot D\,\partial_x f(x_i^*,t^n)
\end{aligned}
\tag{5}
$$

Derivation of numerical method V

Approximate f in (5) by piecewise quadratic spline using a B-spline basis.
$\Longrightarrow$

- all Integrals in (5) can be evaluated analytically
- (5) becomes linear system of N equations with tridiagonal structure.



The linear system of equations

Resulting linear system

- is strictly diagonal-dominant for all $D \geq 0$, if $\Delta x_i < \Delta x_{i-1} + \Delta x_{i+1}$ holds for all i.
- Then the linear system
  - is well conditioned and
  - can be solved iteratively or directly [Strikwerda 1989].

Simulation of Smoluchowski equation

Consider velocity gradient from a macroscopic elongational flow in 2D.

$$\nabla_x u = \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix}$$

Smoluchowski equation becomes

$$\partial_t f + \partial_x(-\frac{3}{2}\sin(2x)f) = D\,\partial_{xx} f$$

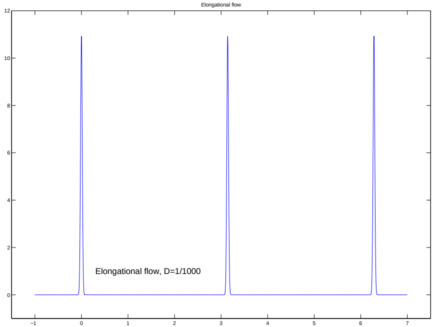
Steady state analytical solution:

$$f(x) = C\exp(-\frac{3}{2D}\sin^2 x),$$

with C obtained from

$$\int_0^{2\pi} f dx = 1 \quad \text{(density requirement)}$$

Solution for elongational flow



L^∞-error	Δx	Adaptive Grid	Wiggles
$2,6\%$	0.0123	No	Yes
$0,42\%$	0.05 (average)	Yes: $\frac{\Delta x_{\max}}{\Delta x_{\min}} = 20$	No

Future work

- comparison with other methods
- higher order in time discretisation
- extension to 2D
- .....