Numerical analysis for the BCF method in complex fluids simulations

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Joint work with Weinan E and Pingwen Zhang

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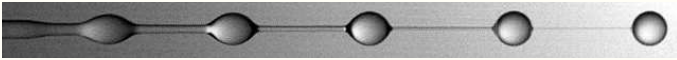
Outline

Introduction

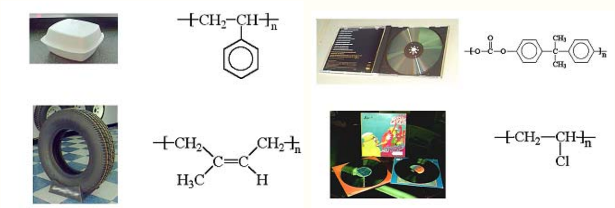
Numerical analysis

Polymeric fluids

- Complex fluids: viscoelastic fluids containing many macromolecules.



- Anomalous viscoelastic properties: shear shinning, shear thicking, tubeless siphon, Rod climbing, etc.
- Many industrial usage: liquid crystal displayer, synthesized products (CD, ...), plastics, ...



Mathematical models (solution case)

- Newtonian fluid (Linear constitutive relation)

$$\begin{cases} \boldsymbol{u}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p &= \nabla\cdot\tau, \\ \nabla\cdot\boldsymbol{u} &= 0, \end{cases}$$

where $\tau = \tau_s = \eta_s(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)$.

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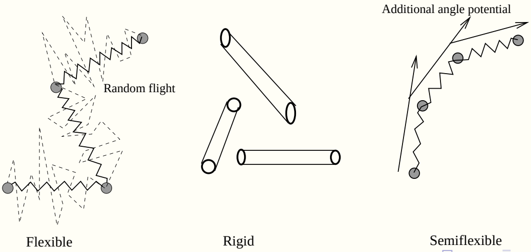
Coarse graining of polymers

- Molecular dynamics: limited space and time scales
- Macroscopic modelling: neglecting all of the molecular details
- Compromise: kinetic theory

  Bending persistence length: l_p

  Length of one single polymer: l



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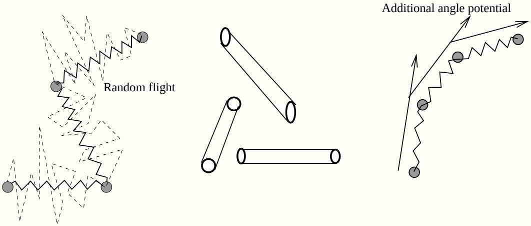

Flexible Rigid Semiflexible

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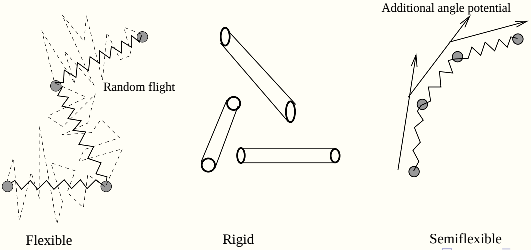

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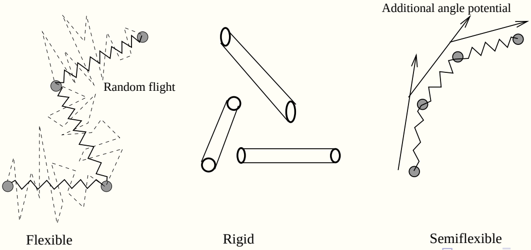

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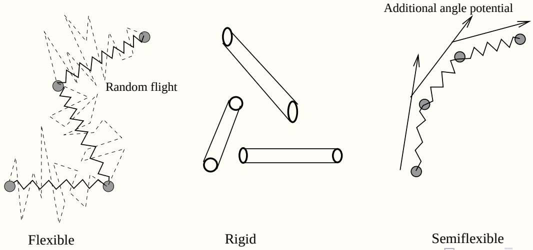

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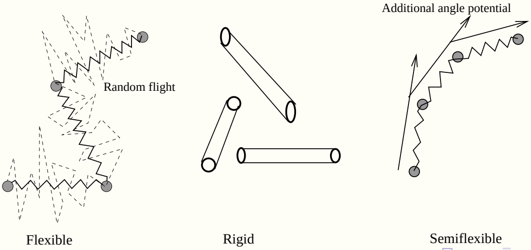

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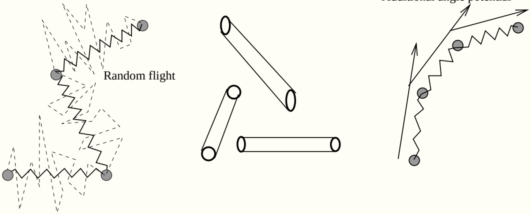

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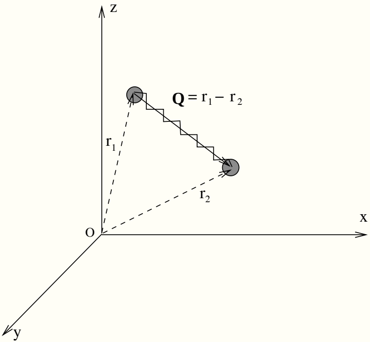
Simplest flexible polymers

- Dumbbell model



Dumbbell model (dilute limit)

- Stochastic differential equations (homogeneous approximation, mean position)

$$\begin{cases} d\boldsymbol{x} &= \boldsymbol{u}dt \\ d\boldsymbol{Q} &= (\kappa \boldsymbol{Q} - \frac{2}{\zeta}\boldsymbol{F}(\boldsymbol{Q}))dt + \sqrt{\frac{4k_B T}{\zeta}}d\boldsymbol{W} \end{cases}$$

- Kramers Expression: $\tau_p = -nk_B T\boldsymbol{I} + n\langle \boldsymbol{F}(\boldsymbol{Q}) \otimes \boldsymbol{Q}\rangle$
- Spring force

- A coupled deterministic-stochastic system ($\boldsymbol{u}$ and $\boldsymbol{Q}$).

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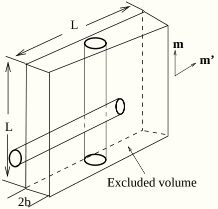
SDE for liquid crystal (high concentration case)

- Rod model for liquid crystals: an interacting particle system.



- The non-dimensionalized form for pdf ψ: (U is usually taken as mean field potential, $\mathcal{R} = \boldsymbol{m} \times \nabla_{\boldsymbol{m}}.$)

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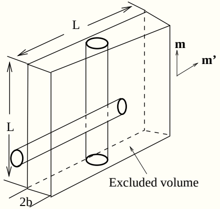

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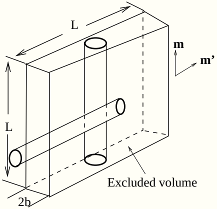

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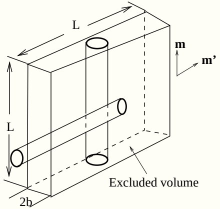

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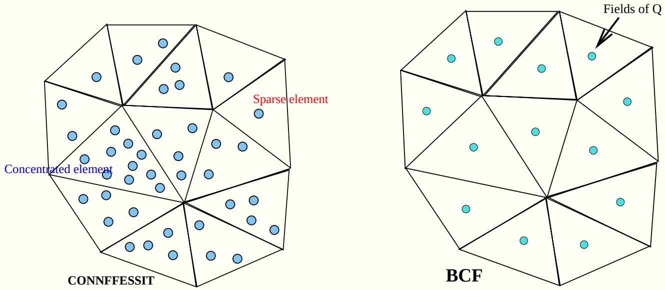

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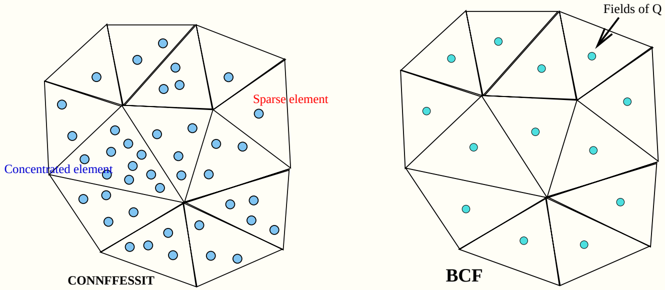

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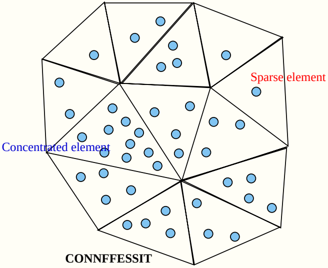

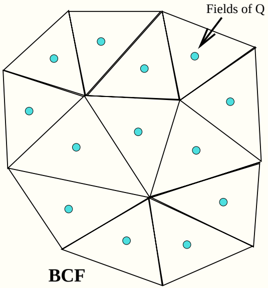

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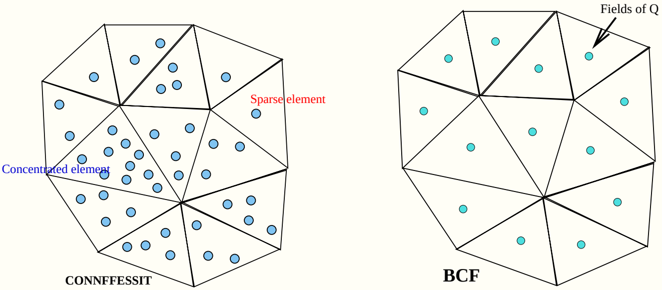

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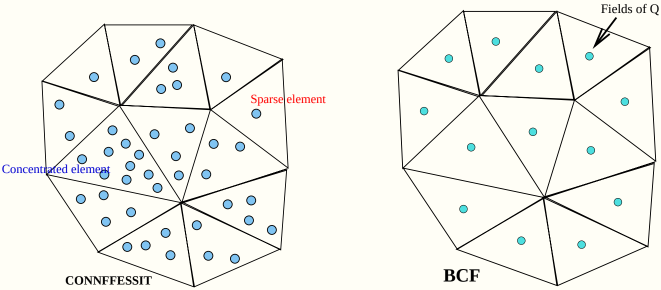

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An overview of the results for the BCF methods

- Well-posedness analysis
  - Hookean dumbbell under shear flow: Jourdain-Lelievre-Le Bris (2002)
  - FENE dumbbell under shear flow: Jourdain-Lelievre-Le Bris (2004)
  - General dumbbell model, high dim with polynomial growth: E-Li-Zhang (2004)
- Convergence analysis
  - Hookean dumbbell under shear flow: Jourdain-Lelievre-Le Bris, E-Li-Zhang (2002)
  - Rod-like model under shear flow: Li-Zhang-Zhou (2004)
  - High dimensional Hookean dumbbell model: Li-Zhang (2005)
  - Nonlinear dumbbell: Only partial results.

Simple SDE and discretization

- Simple SDE

$$dX_t = b(X_t)dt + dW_t$$

- Euler-Maruyama scheme

$$X_{n+1} = X_n + \Delta t b(X_n) + \Delta W_n$$

where ΔW_n are $i.i.d.$ $N(0, \Delta t)$ Gaussian R.V.s.

- Convergence result: Strong order 1. (Lipschitz continuity assumption)

$$\sup_n (\mathbb{E} E_n^2)^{\frac{1}{2}} \leq C \Delta t$$

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BCF scheme for Hookean dumbbell under shear flow

- Discretized equations (temporal and stochastic)

$$\begin{aligned} u^{n+1} - u^n &= u_{yy}^{n+1}\Delta t + \partial_y\Big(\langle P^n Q^n\rangle_N\Big)\Delta t, \\ P_i^{n+1} &= P_i^n + \left(u_y^{n+1} Q_i^n - \frac{P_i^n}{2}\right)\Delta t + dV_i^n, \\ Q_i^{n+1} &= Q_i^n - \frac{Q_i^n}{2}\Delta t + dW_i^n, \end{aligned}$$

where

$$\langle P^n Q^n\rangle_N \triangleq \frac{1}{N}\sum_{i=1}^{N} P_i^n Q_i^n.$$

- Remark: u^n are random variables, too!

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where

$$
\langle P^n Q^n \rangle_N \triangleq \frac{1}{N} \sum_{i=1}^{N} P_i^n Q_i^n .
$$

- Remark: u^n are random variables, too!

A new type of convergence

- Coupling issue

  The errors e^n are random variables!

$$\mathbb{E}\|e_y^{n+1}\|_{L_y^2}^2 \langle (\hat{Q}^n)^2 \rangle_N \neq \mathbb{E}\|e_y^{n+1}\|_{L_y^2}^2 \mathbb{E}\langle (\hat{Q}^n)^2 \rangle_N$$

  where $\hat{Q}^n$ satisfies

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$$\Delta t \langle (\hat{Q}^n)^2 \rangle_N \leq \frac{1}{2}$$

  after excluding a set $\mathcal{A}$ of exponentially small probability.

- Mean square convergence after excluding a set of exponentially small probability

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BCF for Liquid Crystal Polymers

- SDE form for Doi-Edwards model(shear flow, 1D)

$$\mathrm{d}\Theta_t = -\Big(a(\Theta_t, \mathcal{L}(\Theta_t)) + \partial_y u \sin^2 \Theta_t\Big)\mathrm{d}t + \mathrm{d}W_t,$$

$$\tau(y,t) = \mathbb{E}\left[\sin 2\Theta_t + a(\Theta_t, \mathcal{L}(\Theta_t)) \cos^2 \Theta_t + \partial_y u \sin^2 2\Theta_t\right],$$

where $a(\Theta_t, \mathcal{L}(\Theta_t)) = \int_{-\infty}^{+\infty} \sin 2(\Theta_t - \theta')\mathcal{L}(\Theta_t)(d\theta')$.

- Weakly interacting particle system after discretization.

$$\mathrm{d}\Theta_t = -a(\Theta_t, \mathcal{L}(\Theta_t))dt + \mathrm{d}W_t,$$

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$$\mathrm{d}\Theta_t^i = -\frac{1}{N}\sum_{j=1}^{N} \sin 2(\Theta_t^i - \Theta_t^j)dt + \mathrm{d}W_t^i,$$

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Convergence analysis for Liquid Crystal Polymers

- Convergence result (without excluding the small set)

$$\mathbb{E}\Big|\mathbb{E}f(\Theta_t) - \frac{1}{N}\sum_{j=1}^{N} f(\Theta_t^j)\Big|^2 \leq \frac{C}{N}$$

  This mean square convergence is due to the boundedness of $\sin$ function, which is quite special for this problem.

- Techniques (A.-S. Sznitman, LNM 1464 (1991))

  Wasserstein metric for iterative convergence.

  Centering for mean square convergence.

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High-D convergence analysis for dumbbell model

Define the error

$$\boldsymbol{E}^n := \boldsymbol{Q}^n - \hat{\boldsymbol{Q}}^n$$

only with time discretization, then $\boldsymbol{E}^n$ satisfies

$$\frac{1}{\Delta t}(\boldsymbol{E}^{n+1} - \boldsymbol{E}^n) + \boldsymbol{u}^n \cdot \nabla \boldsymbol{E}^{n+1} + \boldsymbol{e}^n \cdot \nabla \hat{\boldsymbol{Q}}^{n+1} = \kappa^n \boldsymbol{E}^{n+1} + \nabla \boldsymbol{e}^n \hat{\boldsymbol{Q}}^{n+1} - \boldsymbol{E}^n.$$

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$$\int_D \boldsymbol{u}^n \cdot \nabla \boldsymbol{E}^{n+1} \cdot \boldsymbol{E}^{n+1} d\boldsymbol{x} = 0$$

- In order to estimate $\int_D \boldsymbol{e}^n \cdot \nabla \hat{\boldsymbol{Q}}^{n+1} \cdot \boldsymbol{E}^{n+1} d\boldsymbol{x}$, one needs

$$\|\langle |\nabla \hat{\boldsymbol{Q}}^{n+1}|^2 \rangle_N \|_{L^\infty} \preceq Const.$$

Difficult! L^2-type estimate $\|\langle |\nabla \hat{\boldsymbol{Q}}^{n+1}|^2 \rangle_N \|_{L^2} \preceq Const.$ is easy. But it can't be transfered back to L^∞ norm.

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Essential ingredient 1: Explicit solution for Q

- SPDE for $\boldsymbol{Q}$

$$d\boldsymbol{Q} + \boldsymbol{u} \cdot \nabla \boldsymbol{Q} = (\kappa \boldsymbol{Q} - \boldsymbol{Q})dt + d\boldsymbol{W}$$

- Introduce flow map

$$\frac{d\boldsymbol{x}(\alpha, t)}{dt} = \boldsymbol{u}(\boldsymbol{x}(\alpha, t), t), \qquad \boldsymbol{x}(\alpha, 0) = \alpha.$$

and deformation tensor

$$F(\alpha, t) = \frac{\partial \boldsymbol{x}}{\partial \alpha}, \quad \text{i.e.} \quad F_{ij} = \frac{\partial x_i}{\partial \alpha_j}$$

- Explicit solution in Lagrangian coordinates

$$\boldsymbol{Q}(\alpha, t) = e^{-t} F(\alpha, t) \boldsymbol{Q}_0(\alpha) + F(\alpha, t) \cdot \int_0^t e^{s-t} F^{-1}(\alpha, s) \cdot d\boldsymbol{W}_s.$$

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Essential ingredient 2: Strang's trick for estimating L_h^∞ norm

- Inverse inequality under spatial discretization

$$\|\boldsymbol{u}^n\|_{L_h^\infty} \le h^{-\frac{d}{2}}\|\boldsymbol{u}^n\|_{L_h^2}, \quad \|\tilde{\boldsymbol{Q}}^n\|_{L_h^\infty} \le h^{-\frac{d}{2}}\|\tilde{\boldsymbol{Q}}^n\|_{L_h^2}$$

- Continuation technique

$$\begin{aligned} \|\boldsymbol{u}_h^n\|_{L_h^\infty} &\le \|\boldsymbol{u}_h^n - \boldsymbol{u}^n\|_{L_h^\infty} + \|\boldsymbol{u}^n\|_{L_h^\infty} \\ &\le \|\boldsymbol{e}^n\|_{L_h^\infty} + \|\boldsymbol{u}\|_{C^0(D\times[0,T])} \\ &\le h^{-\frac{d}{2}}\|\boldsymbol{e}^n\|_{L_h^2} + \|\boldsymbol{u}\|_{C^0(D\times[0,T])} \\ &\le Ch^{p-\frac{d}{2}} + \|\boldsymbol{u}\|_{C^0(D\times[0,T])} \end{aligned}$$

If $p > \frac{d}{2}$, $\|\boldsymbol{u}_h^n\|_{L_h^\infty}$ is bounded.

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A stronger convergence result for high dimensional Hookean dumbbell model

- Final convergence result

$$\|\boldsymbol{e}^{\cdot,n+1}\|_{L_h^2}^2 + \left\langle \|\boldsymbol{E}^{\cdot,\cdot,n+1}\|_{L_h^2}^2 \right\rangle_N \preceq C(\delta t^2 + h^4 + \frac{1}{N^{1-\epsilon}})$$

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Nonlinear dumbbells: shear flow (decoupled case)

- Difficulties: non-Lipschitz property of the force $\boldsymbol{F}$

$$d\boldsymbol{Q}_t = \Big(\kappa \cdot \boldsymbol{Q}_t - \boldsymbol{F}(\boldsymbol{Q})\Big)dt + d\boldsymbol{W}_t$$

- One sided Lipschitz condition!

$$(\boldsymbol{F}(\boldsymbol{a}) - \boldsymbol{F}(\boldsymbol{b}), \boldsymbol{a} - \boldsymbol{b}) \geq 0 \quad \forall \boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^m.$$

- For FENE dumbbell model (implicit method)

$$\begin{aligned} P^{n+1} &= P^n + \Big(u_y(t_{n+1})Q^n - \frac{1}{2}\frac{P^{n+1}}{1 - (\boldsymbol{Q}^{n+1})^2/b}\Big)\Delta t + dV^n, \\ Q^{n+1} &= Q^n - \frac{1}{2}\frac{Q^{n+1}}{1 - (\boldsymbol{Q}^{n+1})^2/b}\Delta t + dW^n, \end{aligned}$$

A cubic equation for $\boldsymbol{Q}^{n+1}$, explicit unique solution in $[0, \sqrt{b})$.

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  How to construct explicit schemes?
- Direct discretization

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Nonlinear dumbbells: shear flow (coupled case)

Not available now!

Reference: review paper by Li-Zhang, Comm. Math. Sci. 5 (2007), 1-51.

Thank you!