Stochastic Immersed Boundary Methods

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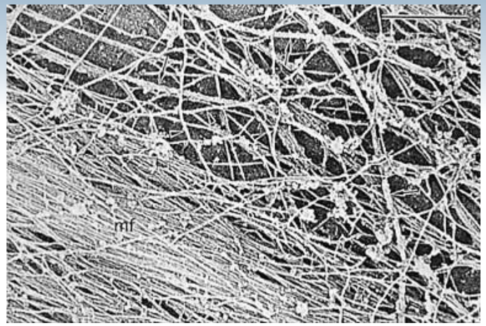
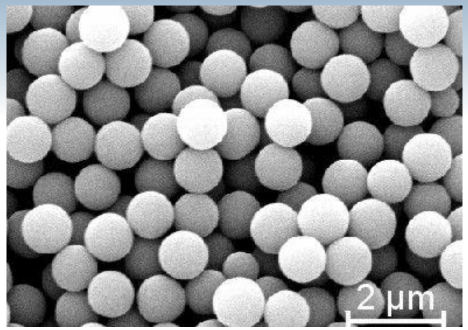
Stochastic Immersed Boundary Methods

Motivations

Motivations: Soft Materials, Complex Fluids, and Other Applications



Gels (Actin)

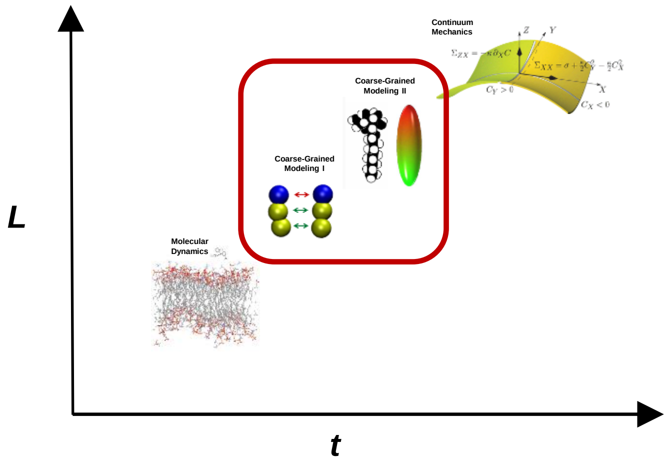


Colloids

Membranes (lipids)

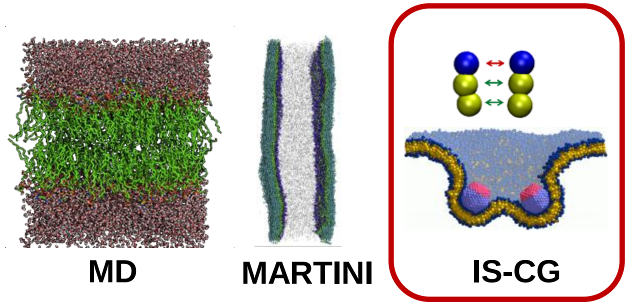
Soft Materials / Complex Fluids

- Microstructure interactions on the order of $K_B T$.
- Properties arise from balance of entropy-enthalpy.
- Solvent plays important role (interactions / dynamic responses).



Approaches

- Atomistic Molecular Dynamics.
- Continuum Mechanics.
- Coarse-Grained Particle Models (solvated or implicitly treated).
- Challenges from phenomena spanning wide temporal-spatial scales.

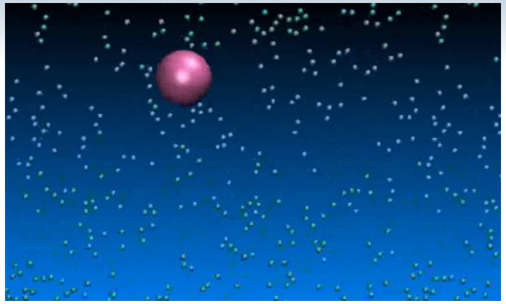


Marrink 2004 Deserno 2007

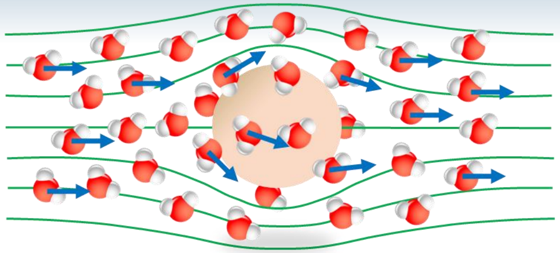
Simulation Aims

- Investigate how larger-scale mechanics arise from microstructure interactions / kinetics.
- Capture roles of solvent mediated interactions efficiently (i.e. continuum level).
- Resolve microstructure mechanics and dynamics.
- Computational efficiencies allow for accessing larger length and time-scales for investigating wider class of phenomena.

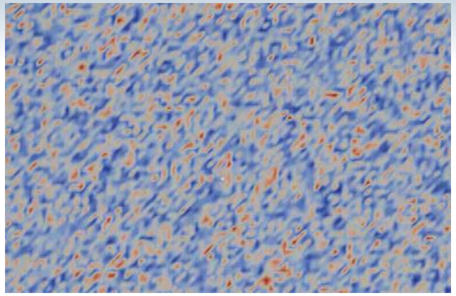
Fluctuating Hydrodynamics



Brownian Motion: Molecular Collisions



Hydrodynamics + Fluctuations



Continuum Gaussian Random Field

Landau-Lifschitz fluctuating hydrodynamics

$$\rho\left(\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + \mathbf{u}(\mathbf{x},t)\cdot\nabla\mathbf{u}(\mathbf{x},t)\right) = \mu\Delta\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \nabla\cdot\mathbf{\Sigma}(\mathbf{x},t).$$

$$\nabla\cdot\mathbf{u}(\mathbf{x},t) = 0.$$

$$\langle\Sigma_{ij}(\mathbf{x},t)\Sigma_{kl}(\mathbf{y},s)\rangle = 2\mu k_B T\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\delta(\mathbf{x}-\mathbf{y})\delta(t-s).$$

Landau ~1959

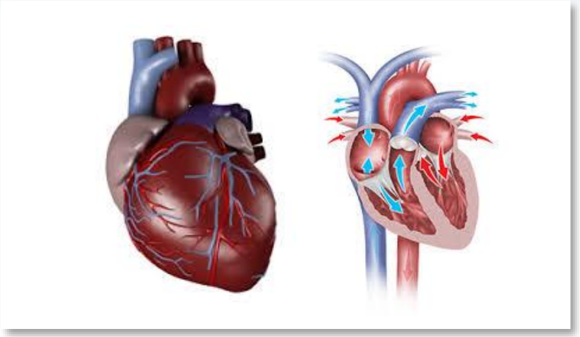
Fluctuations arise from spontaneous momentum transfer from molecular-level collisions.

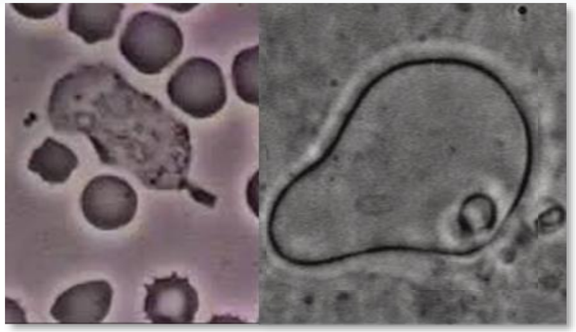
Stochastic model of thermal fluctuations captured through random stress Σ ~ Gaussian.

Challenges for analysis and numerical methods presented from the δ-correlation in space-time.

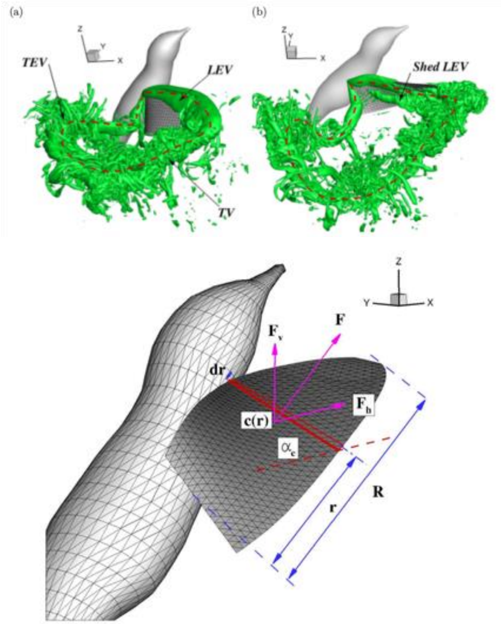
Fluid-structure interactions: How to incorporate tractably?

Fluid-Structure Interactions

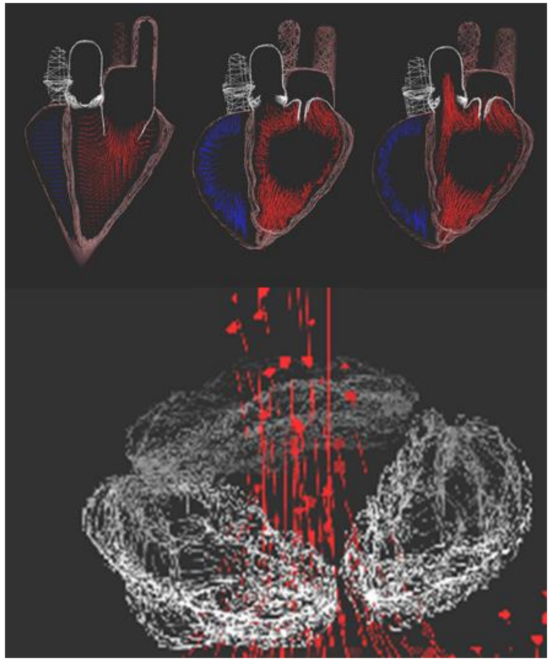




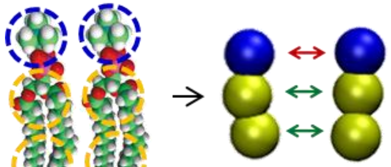
David Rogers



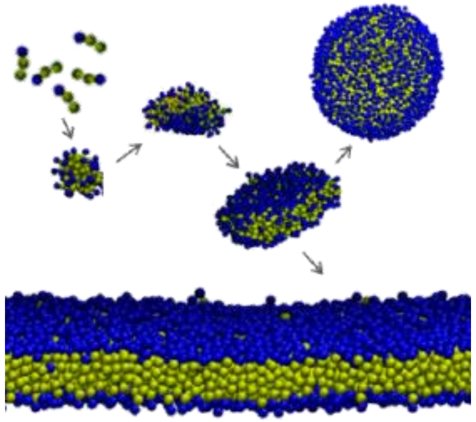
Song, J., Luo, H., Hedrick, T.L.



Peskin,C and McQueen, D. et al.
Griffith et al.



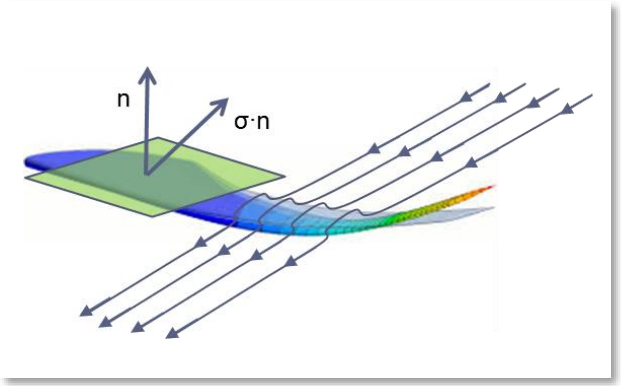
Deserno et al.

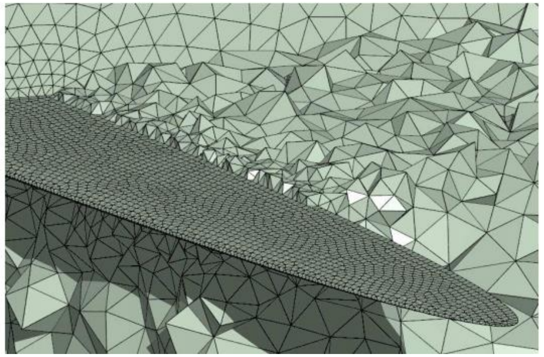


Atzberger, P.,Sigurdsson, J. et al.

CFD : Approaches

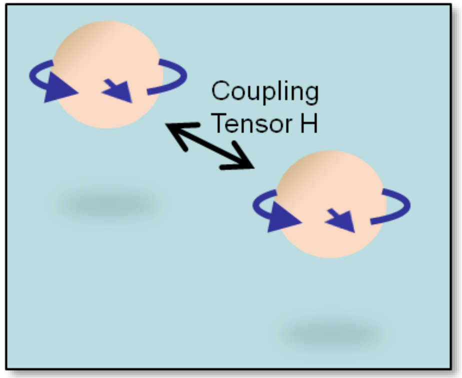
Boundary Coupling





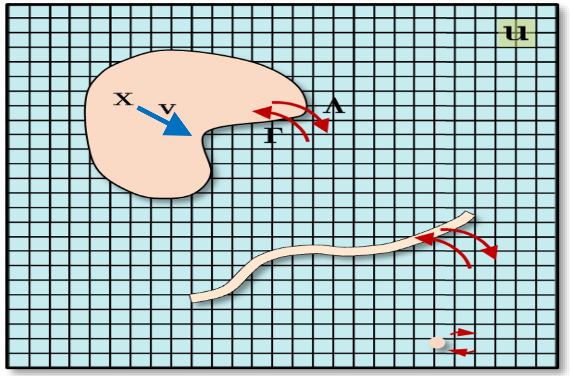
J. Peraire and P.-O. Persson

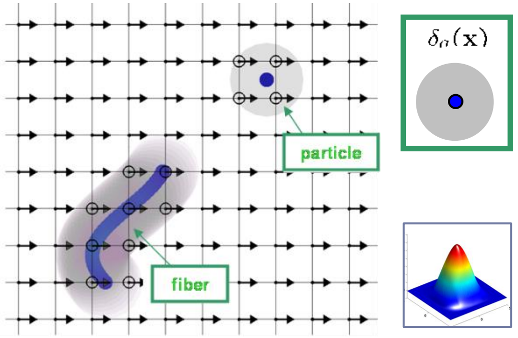
Coupling Tensor



Brady et al., G. Gompper et al.

IB Eulerian-Lagrangian





Atzberger, Peskin, Kramer 2007

Stochastic Immersed Boundary Methods

Background:
Statistical Mechanics
Stochastic Analysis

Background

Equilibrium Statistical Mechanics (Canonical Ensemble)

Consider a system with states X which have energy $E[X]$. At equilibrium in the NVT ensemble, the probability of observing state X is given by

$$\rho(X) = \frac{1}{Z}\exp\left[-\frac{E[X]}{k_B T}\right].$$

The Z is the *partition function* $Z = \int_\Omega \exp\left(-E/k_B T\right) dX$, k_B is Boltzmann's constant, T is temperature.

Fluctuation-Dissipation Principle

A spontaneous perturbation of the system due to fluctuations relaxes the same way as a small externally induced perturbation of the system.

Stochastic Differential Equations (SDEs) and Dynamics

The dynamics of many systems can be modeled using Stochastic Differential Equations (SDEs) of the general form

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

Here, we use Ito's interpretation with $a(x)$ giving the drift, b the covariance, and dW_t increments of the Weiner process.

Ito's Lemma

Consider the Stochastic Differential Equation (SDE)

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

with the change of variable $Y_t = f(X_t)$ with $f \in C^2(\Omega)$. The process Y_t satisfies the SDE given by

$$dY_t = \nabla f(X_t)dX_t + \frac{1}{2}dX_t^T\nabla^2 f(X_t)dX_t,$$

with conventions $[dW_t]_i[dW_t]_j = \delta_{ij}dt$ and $dtdt = 0 = dt[dW_t]_i$. More explicitly, we can express this as

$$dY_t = \left(\nabla f(X_t)a(X_t) + \frac{1}{2}\mathrm{Tr}\left[b(X_t)^T\nabla^2 f(X_t)b(X_t)\right]\right)dt + \nabla f(X_t)b(X_t)dW_t.$$

Fluctuation-Dissipation Principle and Ito's Lemma

Consider a system with energy $E[X] = \frac{1}{2}X^TC^{-1}X$ that has linear dynamics $dX_t = LX_tdt + QdW_t$. To obtain the equilibrium (steady-state) probability density $\rho(X) = (1/Z)\exp\left[-\frac{E[X]}{k_BT}\right]$ we must have that

$$QQ^T = -LC - C^TL^T.$$

Background

Fluctuation-Dissipation Principle and Ito's Lemma

Consider a system with energy $E[X] = \frac{1}{2}X^T C^{-1} X$ that has linear dynamics $dX_t = LX_t dt + QdW_t$. To obtain the equilibrium (steady-state) probability density $\rho(X) = (1/Z)\exp\left[-\frac{E[X]}{k_B T}\right]$ we must have that

$$QQ^T = -LC - C^T L^T.$$

This follows since $C_t = \langle X_t X_t^T\rangle := \mathbb{E}\left[X_t X_t^T\right]$ satisfies by Ito's Lemma

$$\begin{aligned} dC_t &= \langle dX_t X_t^T\rangle + \langle X_t dX_t^T\rangle + \langle dX_t dX_t^T\rangle = \left(L\langle X_t X_t^T\rangle + \langle X_t X_t^T\rangle L^T + QQ^T\right) dt \\ &= \left(LC_t + C_t^T L^T + QQ^T\right) dt. \end{aligned}$$

At steady-state we have $dC_t \to 0$ and $C_t \to C_*$ which gives

$$0 = LC_* + C_*^T L^T + QQ^T.$$

Consequence for modeling: If we know the equilibrium fluctuations have covariance structure C then the fluctuation-dissipation principle can be used to determine Q for how to thermally force the system.

Stochastic Eulerian Lagrangian Methods (SELMs) for Fluid-Structure Interactions

Fluid Equations

$$\begin{aligned}\rho\frac{\partial \mathbf{u}}{\partial t} &= \mathcal{L}\mathbf{u} + \Lambda[\Upsilon(\mathbf{v} - \Gamma\mathbf{u})] + \lambda + \mathbf{f}_{\mathrm{thm}} \\ \nabla\cdot\mathbf{u} &= 0\end{aligned}$$

Microstructure Equations

$$\begin{aligned}\frac{d\mathbf{X}}{dt} &= \mathbf{v} \\ m\frac{d\mathbf{v}}{dt} &= -\Upsilon\left(\mathbf{v} - \Gamma\mathbf{u}\right) - \nabla_{\mathbf{X}}\Phi[\mathbf{X}] + \zeta + \mathbf{F}_{\mathrm{thm}}\end{aligned}$$

Energy and Dissipation

$$E[u,v,X] = \frac{1}{2}\rho\int_{\Omega}\|u(x)\|^2dx + \frac{1}{2}m\|v\|^2 + \Phi(X)$$

$$\rho(\,\cdot\,) = (1/Z)\exp\left[-\frac{E[\,\cdot\,]}{k_BT}\right]$$

$$L = \begin{bmatrix}\rho^{-1}(\mathcal{L} - \Lambda\Upsilon\Gamma) & \rho^{-1}\Lambda\Upsilon \\ m^{-1}\Upsilon\Gamma & -m^{-1}\Upsilon\end{bmatrix}$$

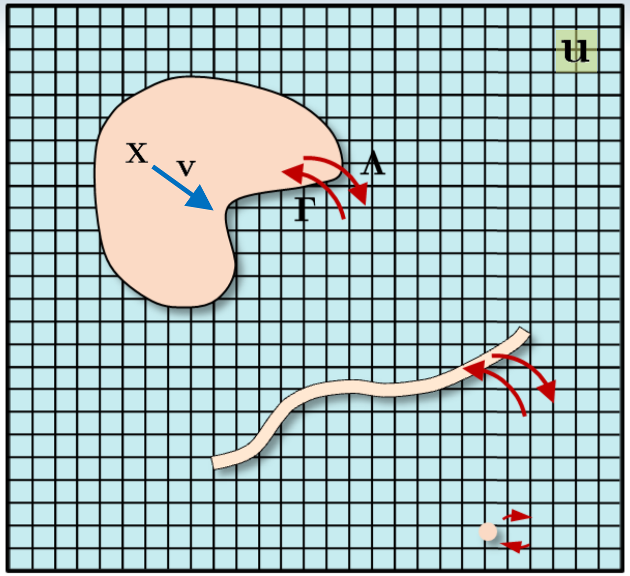
$$C = \begin{bmatrix}\rho^{-1}k_BT\delta(x-y) & 0 \\ 0 & m^{-1}k_BT\delta_{ij}\end{bmatrix}$$

$$QQ^T = -LC - C^TL^T$$

Thermal Fluctuations

$$\begin{aligned}\langle\mathbf{f}_{\mathrm{thm}}(s)\mathbf{f}_{\mathrm{thm}}^T(t)\rangle &= -\left(2k_BT\right)\left(\mathcal{L} - \Lambda\Upsilon\Gamma\right)\delta(t-s) \\ \langle\mathbf{F}_{\mathrm{thm}}(s)\mathbf{F}_{\mathrm{thm}}^T(t)\rangle &= \left(2k_BT\right)\Upsilon\,\delta(t-s) \\ \langle\mathbf{f}_{\mathrm{thm}}(s)\mathbf{F}_{\mathrm{thm}}^T(t)\rangle &= -\left(2k_BT\right)\Lambda\Upsilon\,\delta(t-s).\end{aligned}$$

Eulerian-Lagrangian Approach



Operators:

- $\mathcal{L} \longrightarrow$ Fluid dissipation (viscosity).
- $\Upsilon \longrightarrow$ Structure "slip" relative to local flow field.
- $\Gamma \longrightarrow$ Kinematic particle velocity for given flow.
- $\Lambda \longrightarrow$ Induced fluid force density from particle.

Notation:

- $\mathbf{u} = \mathbf{u}(\mathbf{x},t) \longrightarrow$ Fluid velocity.
- $\mathbf{X} = \mathbf{X}(\mathbf{q},t) \longrightarrow$ Structure configuration
- $\mathbf{v} = \mathbf{v}(\mathbf{q},t) \longrightarrow$ Structure velocity.

Peskin, Kramer, Atzberger 2007, Atzberger 2011

Coupling Operators

Fluid-Structure Interaction Models

Coupling Operators: Immersed Boundary Approach

Conservation of total momentum

$$\int_\Omega (\Lambda \mathbf{F})(\mathbf{x})d\mathbf{x} = \int_S \mathbf{F}(\mathbf{q})d\mathbf{q}$$

$\longrightarrow$ "integrates to one."

Conservation of energy

(overdamped limit)

$$E[\mathbf{u},\mathbf{X}] = \frac{1}{2}\int \rho|\mathbf{u}(\mathbf{y})|^2 d\mathbf{y} + \Phi(\mathbf{X})$$

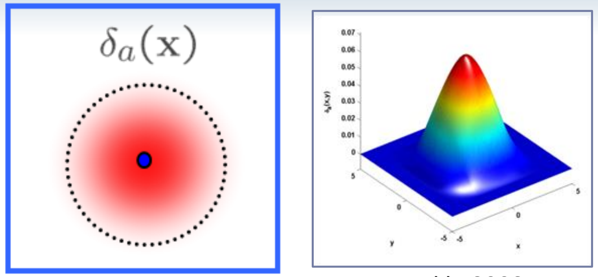
Adjoint condition

$$\int_S (\Gamma \mathbf{u})(\mathbf{q}) \cdot \mathbf{F}(\mathbf{q})d\mathbf{q} = \int_\Omega \mathbf{u}(\mathbf{x}) \cdot (\Lambda \mathbf{F})(\mathbf{x})d\mathbf{x}$$

$\longrightarrow \langle \Gamma \mathbf{u}, \mathbf{F}\rangle = \langle \mathbf{u}, \Lambda \mathbf{F}\rangle \longrightarrow$ "$\Gamma = \Lambda^T$"

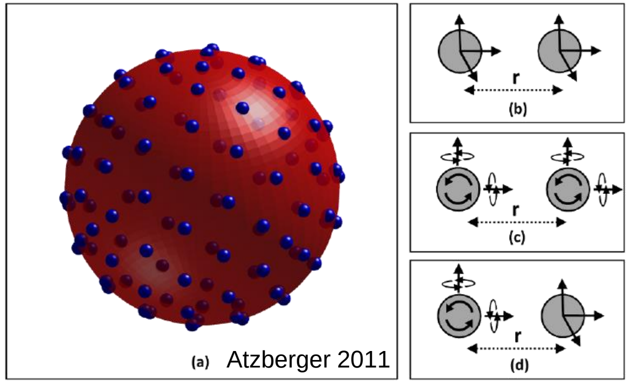
Non-dissipative coupling → requires operators be adjoints!

Useful for deriving operators modeling fluid-structure interactions.

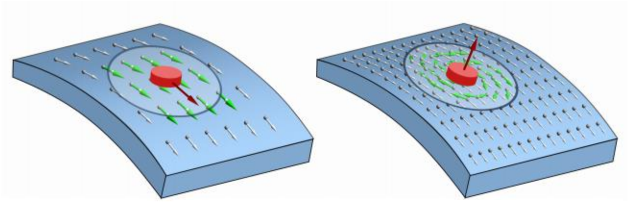


Peskin 2002

Peskin delta-function



Operators from Faxen Relations



2016 Atzberger & Sigurdsson

Surface operators from reference fields

Immersed Boundary Method Coupling and Rotne-Prager-Yamakawa Couplings

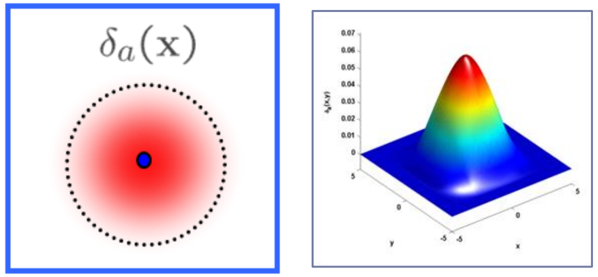
Coupling operators: Immersed Boundary Method

$$\Gamma[u] = \int \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t))\mathbf{u}(\mathbf{x},t)d\mathbf{x}$$

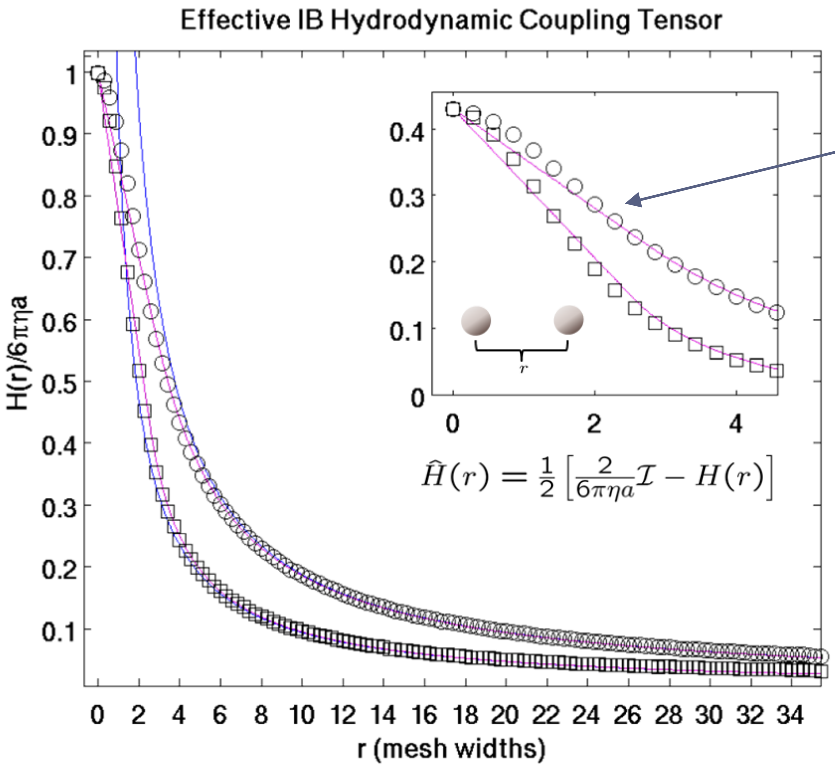
$$\Lambda[F] = \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t))\mathbf{F}$$

$$\text{“}\Gamma = \Lambda^T\text{”}$$

Peskin Delta-Function

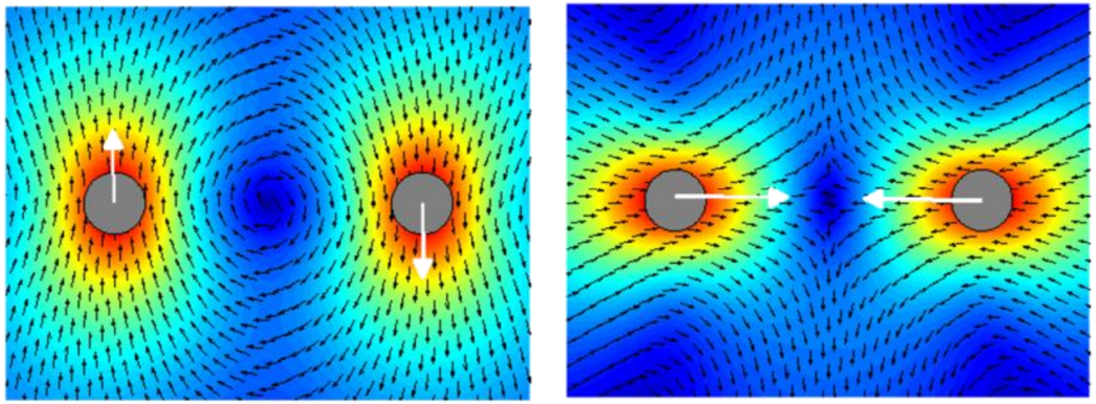


Peskin 2002



IB close to RPY

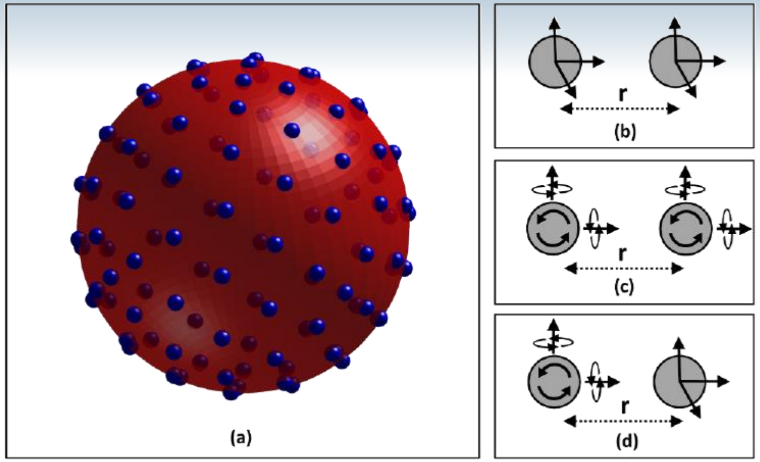
Hydrodynamic Coupling

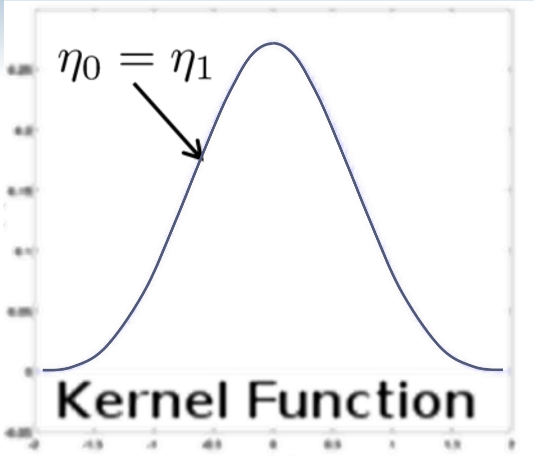


Atzberger 2011

RPY Tensor: Rotne & Prager 1969, Yamakawa 1970

Coupling Operators based on Faxen Relations





Adjoint condition

$$\int_{\mathcal{S}} (\Gamma \mathbf{u})(\mathbf{q}) \cdot \mathbf{F}(\mathbf{q}) d\mathbf{q} = \int_{\Omega} \mathbf{u}(\mathbf{x}) \cdot (\Lambda \mathbf{F})(\mathbf{x}) dx$$

$$\langle \Gamma \mathbf{u}, \mathbf{F} \rangle = \langle \mathbf{u}, \Lambda \mathbf{F} \rangle$$

$$\text{“}\Gamma = \Lambda^T\text{”}$$

Faxen Kinematic Relations→ Γ :

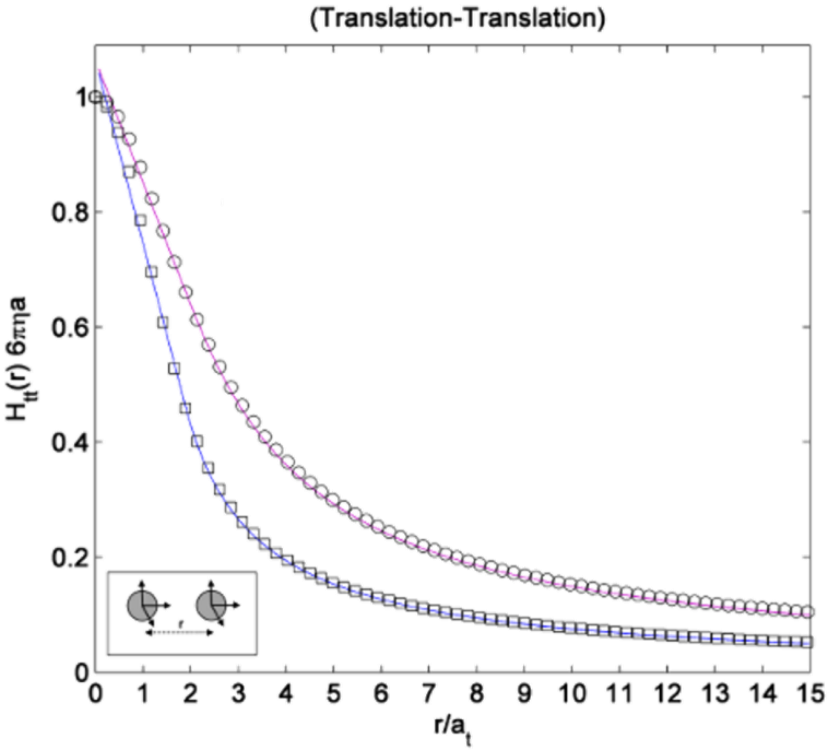
$$\Gamma_0 \mathbf{u} = \sum_{\mathbf{m}} \langle\ \eta_0(\mathbf{y}_{\mathbf{m}} - (\mathbf{X}_{\mathrm{cm}} + \mathbf{z}))\ \mathbf{u}_{\mathbf{m}}\ \rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \Delta x_{\mathbf{m}}^3$$

$$\Gamma_1 \mathbf{u} = \frac{3}{2R^2} \sum_{\mathbf{m}} \langle\ \eta_1(\mathbf{y}_{\mathbf{m}} - (\mathbf{X}_{\mathrm{cm}} + \mathbf{z}))\,(\mathbf{z} \times \mathbf{u}_{\mathbf{m}})\ \rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \Delta x_{\mathbf{m}}^3.$$

Adjoint Condition → Λ :

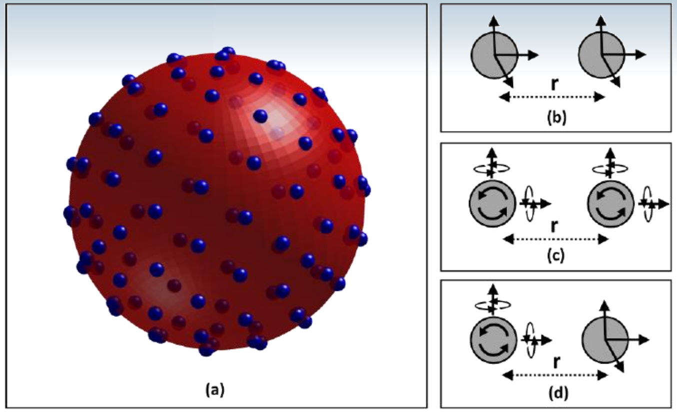
$$\Lambda_0(\mathbf{x}_{\mathbf{m}}) = \left(\langle\ \eta_0(\mathbf{x}_{\mathbf{m}} - (\mathbf{X}_{\mathrm{cm}} + \mathbf{z}))\ \rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \right) \mathbf{F}$$

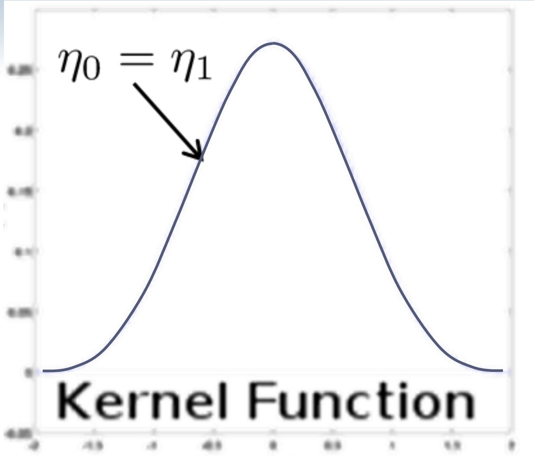
$$\Lambda_1(\mathbf{x}_{\mathbf{m}}) = -\frac{3}{2R^2} \left(\langle\ \mathbf{z} \eta_1(\mathbf{x}_{\mathbf{m}} - (\mathbf{X}_{\mathrm{cm}} + \mathbf{z}))\ \rangle_{\tilde{\mathcal{S}}, |\mathbf{z}|=R} \right) \times \mathbf{T}.$$



Atzberger 2011

Coupling Operators based on Faxen Relations





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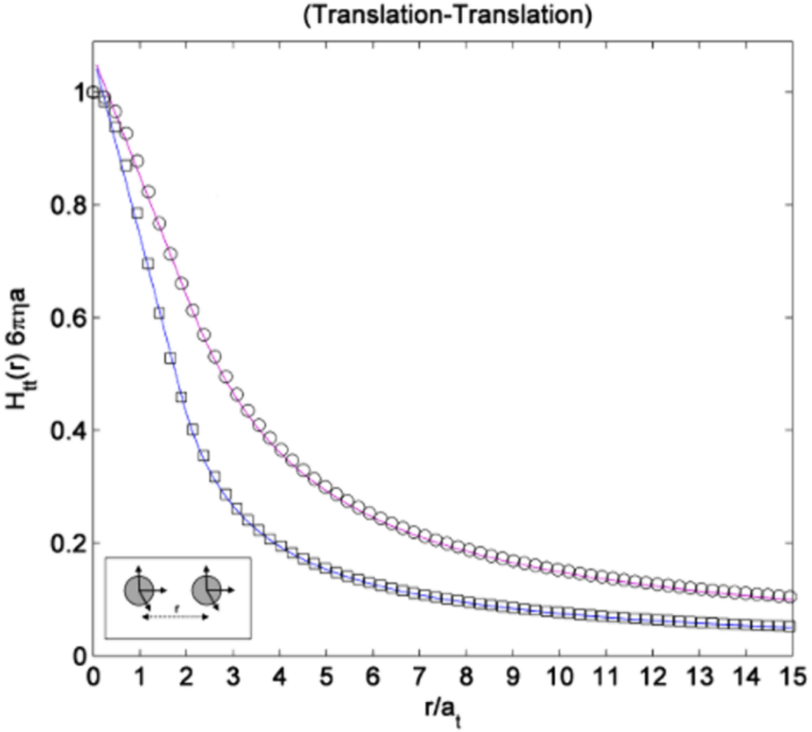
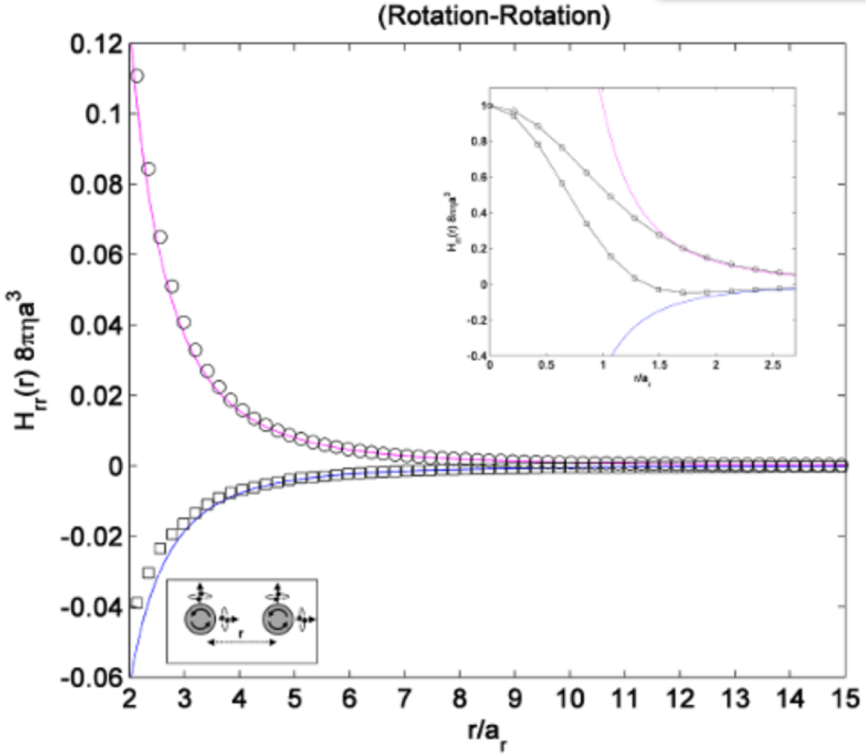
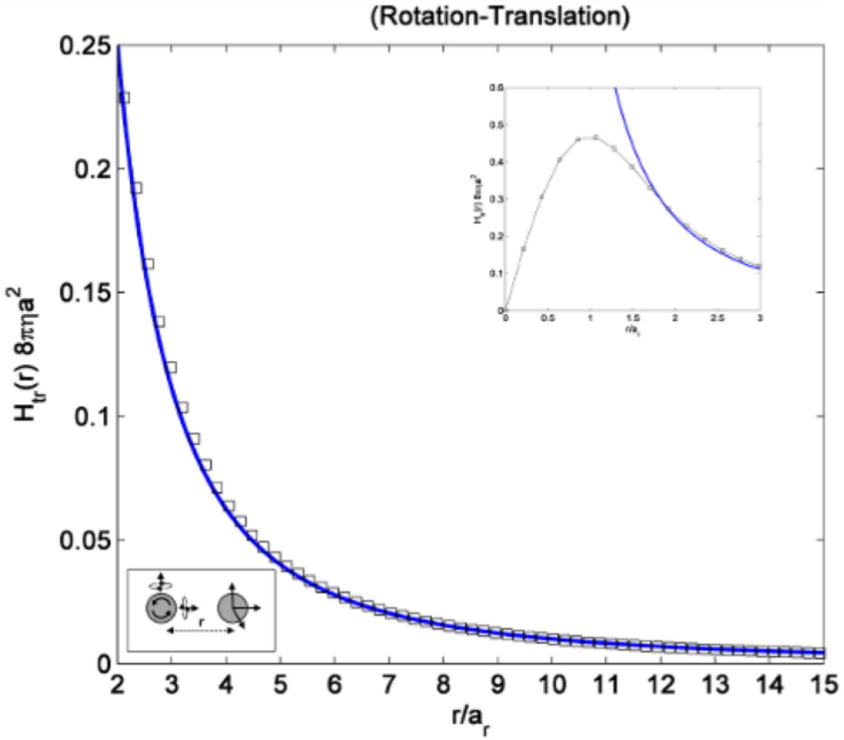
$$\langle \Gamma \mathbf{u}, \mathbf{F} \rangle = \langle \mathbf{u}, \Lambda \mathbf{F} \rangle$$

$$\text{“}\Gamma = \Lambda^T\text{”}$$







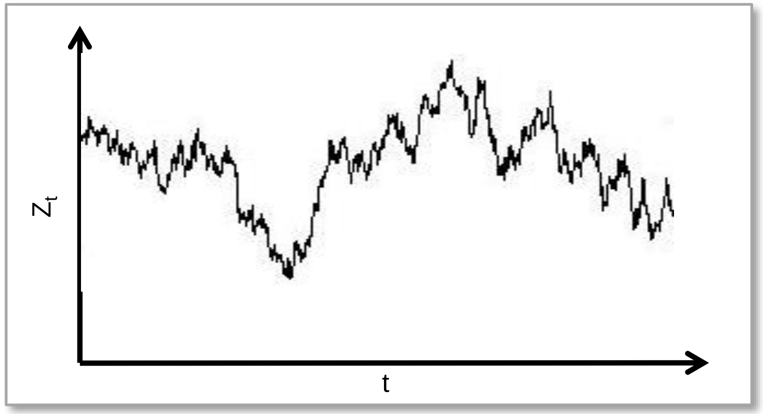
Excellent agreement for r > 2a ! Atzberger 2011

Fluid-Structure Interactions Subject to Thermal Fluctuations

A Few Physical Regimes

Time-Scales of Dynamics and Numerical Stiffness

Time-scales	
Fluid Modes	Particle Diffusion
$\tau_\lambda = \frac{\rho}{4\pi^2\mu}\lambda^2$	$\tau_{\text{diff}}(a) \approx \frac{a^2}{D_a}$
λ = 10nm : τ = 10^{-3}ns	$\tau_{\text{diff}}(1\text{nm}) \approx 10^0\text{ns}$
λ = 1000nm : τ = 10ns	$\tau_{\text{diff}}(10\text{nm}) \approx 10^3\text{ns}$



Stiffness

Thermal fluctuations excite all fluid modes.

For regime I formulation (additional sources):

- microstructure inertia
- fluid-structure slip $-\Upsilon\left(\mathbf{v} - \Gamma\mathbf{u}\right)$

Elasticity of microstructures.

Equilibration time-scales of system vary over wide range.

Approaches

- Perturbation analysis of SPDEs : reduced descriptions.
- Develop stiff stochastic time-step integrators.

Model Reduction for Stochastic Systems

Stochastic differential equation:

$$d\mathbf{Z}(t) = \mathbf{a}(\mathbf{Z}(t))dt + \mathbf{b}(\mathbf{Z}(t))d\mathbf{W}_t \longrightarrow \mathcal{A}_\epsilon = \mathrm{a}\cdot\frac{\partial}{\partial \mathrm{z}} + \frac{1}{2}\mathrm{b}\mathrm{b}^T : \frac{\partial^2}{\partial \mathrm{z}^2}$$

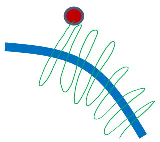
Backward-Kolomogorov PDE:

$$\frac{\partial u}{\partial t} = \mathcal{A}_\epsilon u, \quad u(x,0) = f(x) \longrightarrow u(x,t) = E^{x,0}\left[f(X_t)\right]$$

Perturbation Analysis:

$$u(\mathbf{z},t) = u_0(\mathbf{z},t) + u_1(\mathbf{z},t)\epsilon + u_2(\mathbf{z},t)\epsilon^2 \cdots + u_n(\mathbf{z},t)\epsilon^n + \cdots$$

Split operator into "slow" and "fast" parts: $z = (z_S, z_f)$ **invariant distribution**



$$\mathcal{A}_\epsilon = L_{slow} + L_{fast} \longrightarrow L_{fast} = \frac{1}{\epsilon}\left(L_2 + \epsilon\tilde{L}_2\right), \qquad L_2^*\Psi = 0, \ \int \Psi d\mathbf{z}_f = 1$$

average drift part — remainder

$$\longrightarrow L_{slow} = \bar{L}_1 + L_1 \longrightarrow \bar{L}_1 = \int \Psi(\mathbf{z}_f|\mathbf{z}_s)L_{slow}d\mathbf{z}_f, \quad L_1 = L_{slow} - \bar{L}_1$$

$$\mathcal{A}_\epsilon = \bar{L}_1 + \epsilon L_\epsilon, \ L_\epsilon = \frac{1}{\epsilon}\left(L_1 + \tilde{L}_2\right) + \frac{1}{\epsilon^2}L_2$$

$\epsilon \to 0$: compare orders

$$\mathcal{A} = \bar{L}_1 + \epsilon\bar{L}_0$$ leading order dynamics. $$\bar{L}_0 = -\int \Psi\left(L_1 + \tilde{L}_2\right)L_2^{-1}L_1 d\mathbf{z}_f$$

Reduced dynamics:

$$\mathcal{A} = \tilde{\mathrm{a}}\cdot\frac{\partial}{\partial \mathrm{z}} + \frac{1}{2}\tilde{\mathrm{b}}\tilde{\mathrm{b}}^T : \frac{\partial^2}{\partial \mathrm{z}^2} \longrightarrow d\tilde{\mathbf{Z}}_t = \tilde{\mathbf{a}}(\tilde{\mathbf{Z}}_t)dt + \tilde{\mathbf{b}}(\tilde{\mathbf{Z}}_t)d\tilde{\mathbf{W}}_t$$

Atzberger & Tabak 2015

Summary of Regimes for SELMs

Stochastic Eulerian Lagrangian Methods (SELMs)

Fluid dynamics:

$$\begin{aligned}\rho\frac{\partial \mathbf{u}}{\partial t} &= \mu\Delta\mathbf{u} - \nabla p + \Lambda[\Upsilon(\mathbf{v} - \Gamma\mathbf{u})] + \mathbf{f}_{\text{thm}} \\ \nabla\cdot\mathbf{u} &= 0\end{aligned}$$

Structure dynamics:

$$\begin{aligned}\frac{d\mathbf{X}}{dt} &= \mathbf{v} \\ m\frac{d\mathbf{v}}{dt} &= -\Upsilon(\mathbf{v} - \Gamma\mathbf{u}) - \nabla_{\mathbf{X}}\Phi[\mathbf{X}] + \zeta + \mathbf{F}_{\text{thm}}\end{aligned}$$

Thermal Fluctuations

$$\begin{aligned}\langle \mathbf{f}_{\text{thm}}(s)\mathbf{f}_{\text{thm}}^T(t)\rangle &= -(2k_BT)(\mu\Delta - \Lambda\Upsilon\Gamma)\,\delta(t-s) \\ \langle \mathbf{F}_{\text{thm}}(s)\mathbf{F}_{\text{thm}}^T(t)\rangle &= (2k_BT)\,\Upsilon\,\delta(t-s) \\ \langle \mathbf{f}_{\text{thm}}(s)\mathbf{F}_{\text{thm}}^T(t)\rangle &= -(2k_BT)\,\Lambda\Upsilon\,\delta(t-s).\end{aligned}$$

Microstructure density matched with fluid

$m \ll \rho\ell^3$

Fluid-structure dynamics:

$$\begin{aligned}\frac{d\mathbf{p}}{dt} &= \rho^{-1}\mathcal{L}\mathbf{p} + \Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\cdot\Lambda)\,k_BT + \lambda + \mathbf{g}_{\text{thm}} \\ \frac{d\mathbf{X}}{dt} &= \rho^{-1}\Gamma\mathbf{p} + \Upsilon^{-1}[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + \zeta + \mathbf{G}_{\text{thm}}. \\ \nabla_{\mathbf{X}}\cdot\Lambda &= \text{Tr}[\nabla_{\mathbf{X}}\Lambda]\end{aligned}$$

Phase space compressibility (p,X).

Thermal Fluctuations:

$$\begin{aligned}\langle \mathbf{g}_{\text{thm}}(s)\mathbf{g}_{\text{thm}}^T(t)\rangle &= -(2k_BT)\,\mathcal{L}\,\delta(t-s) \\ \langle \mathbf{G}_{\text{thm}}(s)\mathbf{G}_{\text{thm}}^T(t)\rangle &= (2k_BT)\,\Upsilon^{-1}\,\delta(t-s) \\ \langle \mathbf{g}_{\text{thm}}(s)\mathbf{G}_{\text{thm}}^T(t)\rangle &= 0.\end{aligned}$$

- Structure momentum no longer tracked.
- Removes a source of stiffness.
- Non-conjugate Hamiltonian formulation yields metric-factor in phase-space.

Microstructure-fluid no-slip coupling (S-Immersed-Boundary)

$\Upsilon \to \infty$

Fluid-Structure Equations:

$$\begin{aligned}\frac{d\mathbf{p}}{dt} &= \rho^{-1}\mathcal{L}\mathbf{p} + \Lambda[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\cdot\Lambda)\,k_BT + \lambda + \mathbf{g}_{\text{thm}} \\ \frac{d\mathbf{X}}{dt} &= \rho^{-1}\Gamma\mathbf{p}\end{aligned}$$

Thermal Fluctuations:

$$\langle \mathbf{g}_{\text{thm}}(s)\mathbf{g}_{\text{thm}}^T(t)\rangle = -(2k_BT)\,\mathcal{L}\,\delta(t-s).$$

- Structure dynamics no-longer inertial.
- Removes additional sources of stiffness.
- Regime of the Stochastic Immersed Boundary Method.
- Phase-space metric reflected in the drift term.

Microstructure-fluid stress balance

$\mu \to \infty$

Fluid-Structure Equations:

$$\begin{aligned}\frac{d\mathbf{X}}{dt} &= H_{\text{SELM}}[-\nabla_{\mathbf{X}}\Phi(\mathbf{X})] + (\nabla_{\mathbf{X}}\cdot H_{\text{SELM}})k_BT + \mathbf{h}_{\text{thm}} \\ H_{\text{SELM}} &= \Gamma(-\wp\mathcal{L})^{-1}\Lambda\end{aligned}$$

Thermal Fluctuations:

$$\langle \mathbf{h}_{\text{thm}}(s)\mathbf{h}_{\text{thm}}^T(t)\rangle = (2k_BT)\,H_{\text{SELM}}\,\delta(t-s).$$

- Fluid momentum no longer tracked.
- Balance of hydrodynamic stresses with elastic stresses.
- Removes additional sources of stiffness.
- Regime of the Stokesian-Brownian Dynamics (Brady 1980, McCammond 1980's).
- Phase-space metric reflected in the drift term.

Atzberger & Tabak 2015

Spatial and Temporal Discretizations

Fluctuation-Dissipation Balance

Stochastic Immersed Boundary Method

Fluid-structure equations

Fluid:

$$\rho\frac{D\mathbf{u}(\mathbf{x},t)}{Dt} = \mu\Delta\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \mathbf{F}_{\mathrm{prt}}(\mathbf{x},t)$$

$$\nabla\cdot\mathbf{u}(\mathbf{x},t) = 0.$$

Microstructure:

$$\frac{d\mathbf{X}^{[j]}(t)}{dt} = \int \delta_a(\mathbf{x}-\mathbf{X}^{[j]}(t))\mathbf{u}(\mathbf{x},t)d\mathbf{x}$$

$$\mathbf{F}_{\mathrm{ptr}}(\mathbf{x},t) = \sum_{j=1}^{M}\mathbf{F}^{[j]}\delta_a\left(\mathbf{x}-\mathbf{X}^{[j]}(t)\right)$$

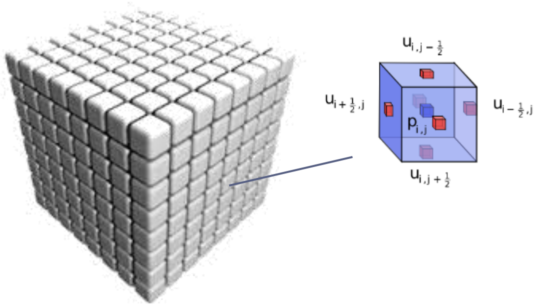
Thermal fluctuations

$$\mathbf{F}_{\mathrm{thm}}(\mathbf{x},t) = \mathbf{F}_{\mathrm{drift}}(\mathbf{x},t) + \mathbf{F}_{\mathrm{stoch}}(\mathbf{x},t) \sim \mathrm{Gaussian}$$

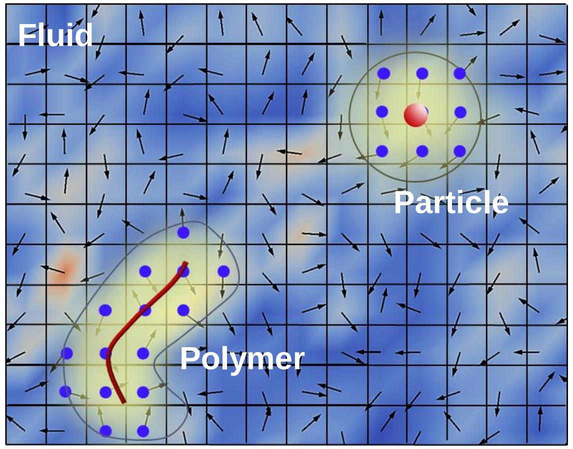
$$\langle\mathbf{F}_{\mathrm{stoch}}(\mathbf{x},t)\mathbf{F}_{\mathrm{stoch}}^{T}(\mathbf{y},s)\rangle = -2k_BT\mu\Delta\delta(\mathbf{x}-\mathbf{y})\delta(t-s)$$

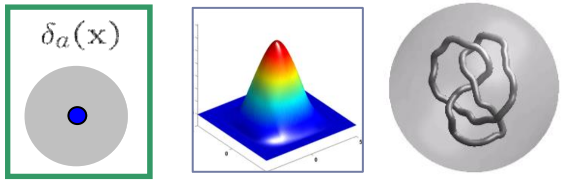
$$\mathbf{F}_{\mathrm{drift}} = -k_BT\sum_{j=1}^{M}\nabla_{\mathbf{X}^{[j]}}\delta_a(\mathbf{x}-\mathbf{X}^{[j]}(t))$$

Numerical Discretization



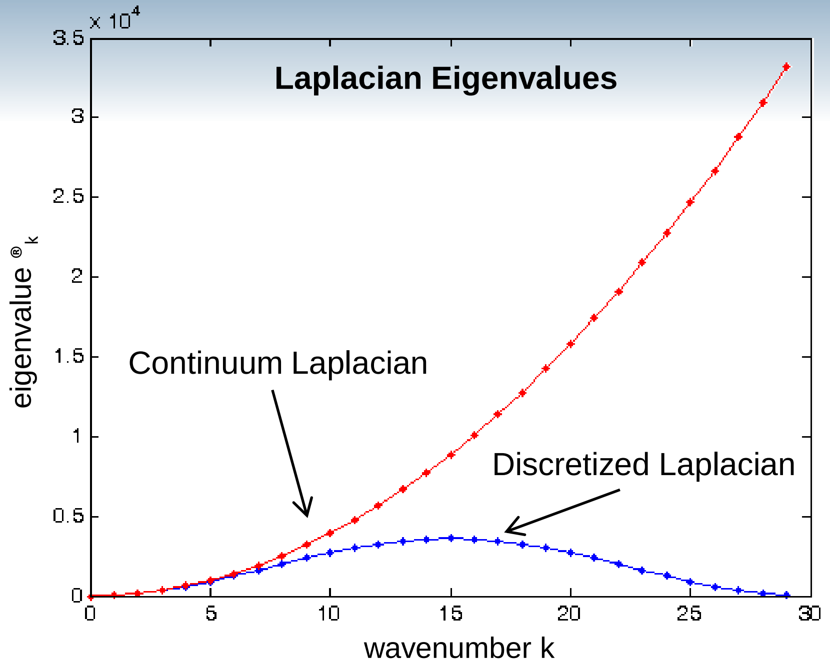
Fluid-Structure Coupling

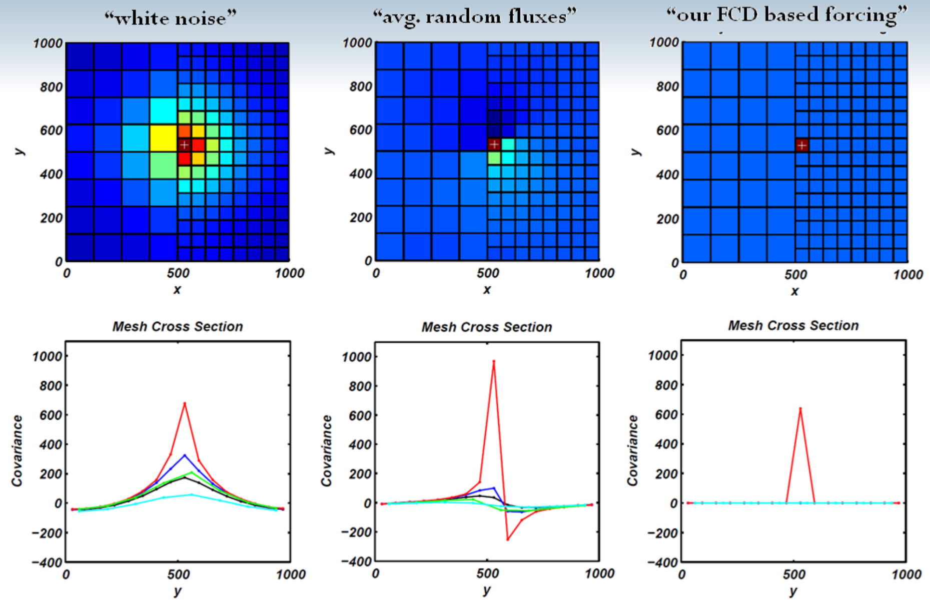




Peskin 1972, Atzberger, Peskin, Kramer 2007, Atzberger, Tabak 2015

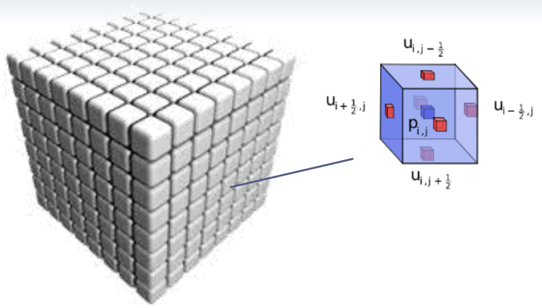
Numerical Methods and Spatial Discretization



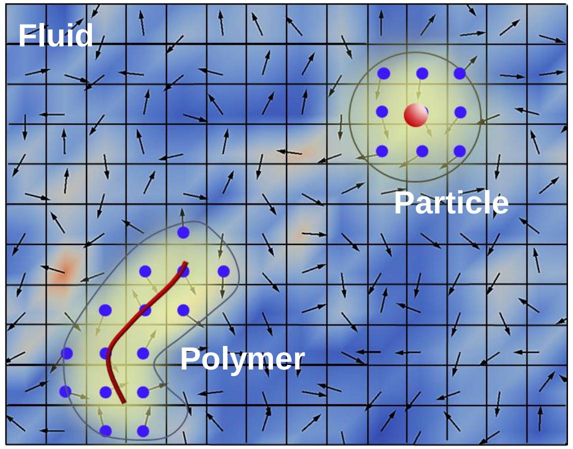


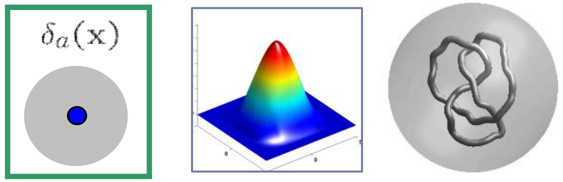
Atzberger 2010

Numerical Discretization



Fluid-Structure Coupling





Peskin 1972, Atzberger, Peskin, Kramer 2007, Atzberger, Tabak 2015

Dissipation rates not the same for continuum and discrete system.

Thermal forcing should be based on the spatial discretization method.

Fluctuation-dissipation-based discretizations

$$\mathbf{L}\mathbf{u} \leftarrow \Delta\mathbf{u} \qquad [Lu]_i^{(\ell)} = \sum_k \frac{u_{i+e_k}^{(\ell)} - 2u_i^{(\ell)} + u_{i-e_k}^{(\ell)}}{\Delta x^2}$$

$$E[u] = \frac{1}{2}\rho\sum_i u_i^2 \Delta x^3 \qquad \rho(u) = (1/Z)\exp\left[\frac{E[u]}{k_B T}\right]$$

$$C_{ij} \leftarrow \frac{k_B T}{\rho \Delta x^3}\delta_{ij}$$

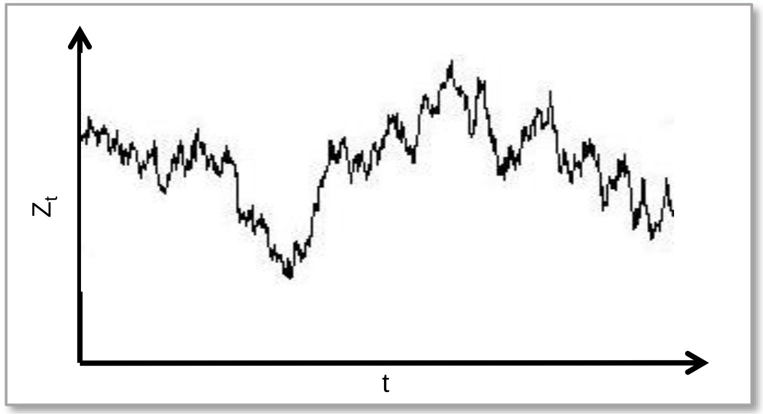
$$\langle \mathbf{f}_{\mathrm{thm}}(s)\mathbf{f}_{\mathrm{thm}}^T(t)\rangle = -\left(LC + CL^T\right)\delta(t-s)$$

Papers on methods for:

- **Finite Difference Methods** (Peskin, Kramer, Atzberger 2007).
- **Adaptive Meshes** (Atzberger 2010).
- **Finite Element Methods** (Plunkett, Pazner, Atzberger 2014, 2019).
- **Meshless Methods** (Gross, Atzberger 2020).

Time-Scales of Dynamics and Numerical Stiffness

Time-scales	
Fluid Modes	Particle Diffusion
$\tau_\lambda = \frac{\rho}{4\pi^2\mu}\lambda^2$	$\tau_{\text{diff}}(a) \approx \frac{a^2}{D_a}$
λ = 10nm : τ = 10^{-3}ns	$\tau_{\text{diff}}(1\text{nm}) \approx 10^0\text{ns}$
λ = 1000nm : τ = 10ns	$\tau_{\text{diff}}(10\text{nm}) \approx 10^3\text{ns}$



Stiffness

Thermal fluctuations excite all fluid modes.

For regime I formulation (additional sources):

- microstructure inertia
- fluid-structure slip $-\Upsilon\left(\mathbf{v} - \Gamma\mathbf{u}\right)$

Elasticity of microstructures.

Equilibration time-scales of system vary over wide range.

Approaches

- Perturbation analysis of SPDEs : reduced descriptions.
- Develop stiff stochastic time-step integrators.

Stiff Time-step Integrator

Fluid equations

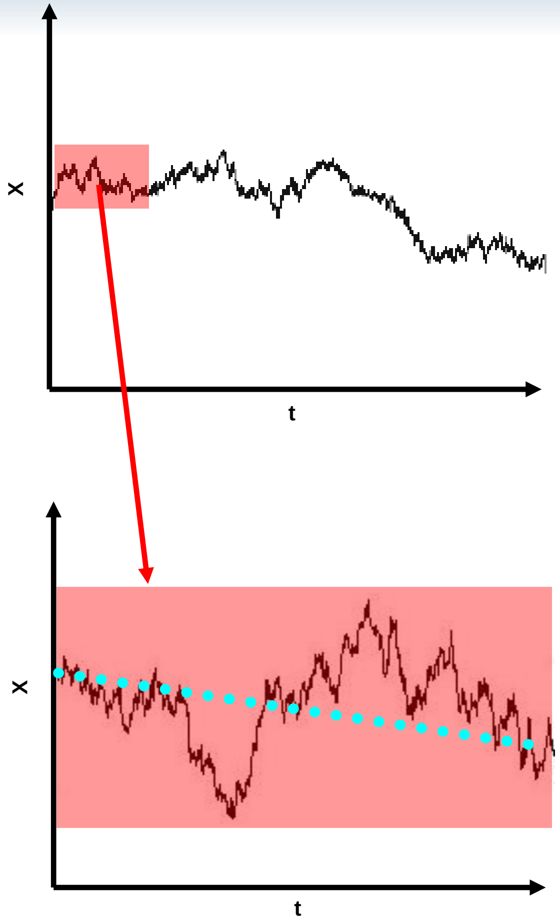
$$
\begin{aligned}
d\mathbf{u} &= \mathcal{L}\mathbf{u}\,dt && \text{(dissipation in fluid)}\\
&+ \rho^{-1}\mathbf{F}_{\text{prt}}\,dt && \text{(microstructure forces)}\\
&+ Q\,d\mathbf{B}_t && \text{(thermal force)}
\end{aligned}
$$

$$\nabla\cdot\mathbf{u} = 0 \qquad \text{(incompressibility)}$$

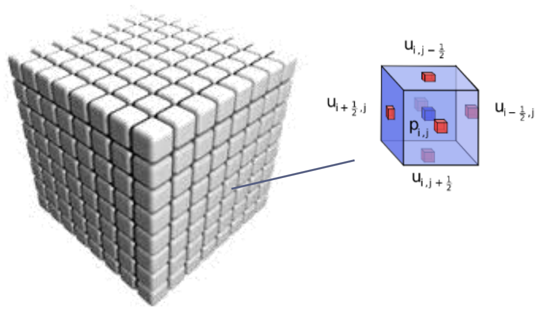
Structure equations

$$\frac{d\mathbf{X}^{[j]}(t)}{dt} = \int \delta_a(\mathbf{x}-\mathbf{X}^{[j]}(t))\,\mathbf{u}(\mathbf{x},t)\,d\mathbf{x}$$

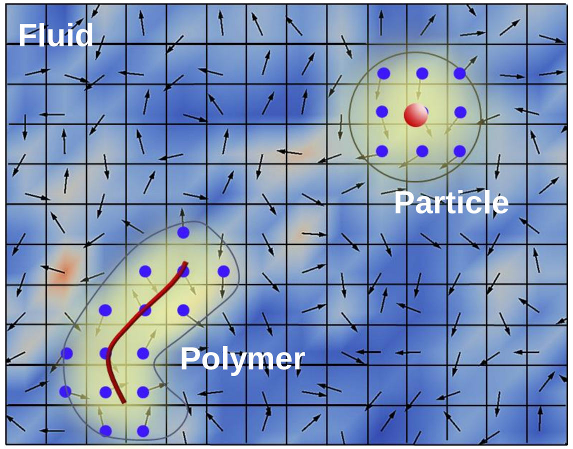
$$\mathbf{F}_{\text{prt}}(\mathbf{x},t) = \sum_{j=1}^{M} -\nabla_{\mathbf{X}^{[j]}} V(\{\mathbf{X}(t)\})\,\delta_a(\mathbf{x}-\mathbf{X}^{[j]}(t))$$



Numerical Discretization

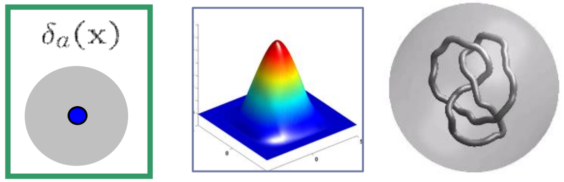


Fluid-Structure Coupling



Integration by exponential factor (ito calculus)

$$\mathbf{u}(t) = e^{t\mathcal{L}}\mathbf{u}(0) + \int_0^t e^{(t-s)\mathcal{L}}\rho^{-1}\mathbf{F}_{\text{prt}}(s)\,ds + \int_0^t e^{(t-s)\mathcal{L}}Q\,d\mathbf{B}_s = e^{t\mathcal{L}}\mathbf{u}(0) + \bar{\mathbf{I}}_{\text{prt}} + \bar{\mathbf{I}}_{\text{thm}}$$



Atzberger, Peskin, Kramer 2007

Stiff Time-step Integrator

Integration by exponential factor (ito calculus)

$$\mathbf{u}(t) \;=\; e^{t\mathcal{L}}\mathbf{u}(0) + \int_0^t e^{(t-s)\mathcal{L}}\rho^{-1}\mathbf{F}_{\text{prt}}(s)ds + \int_0^t e^{(t-s)\mathcal{L}} Q d\mathbf{B}_s \;=\; e^{t\mathcal{L}}\mathbf{u}(0) + \bar{\mathbf{I}}_{\text{prt}} + \bar{\mathbf{I}}_{\text{thm}}$$

Particle force

$$\mathbf{I}_{\text{prt}}(t) := \int_0^t e^{(t-s)\mathcal{L}}\rho^{-1}\mathbf{F}_{\text{prt}}(s)ds$$

Approximate by constant force

$$\mathbf{I}_{\text{prt}}(t) \approx -\rho^{-1}\mathcal{L}^{-1}\left[\mathcal{I} - e^{t\mathcal{L}}\right]\mathbf{F}_{\text{prt}}(0)$$

Thermal fluctuations

$$\mathbf{I}_{\text{thm}}(t) := \int_0^t e^{(t-s)\mathcal{L}} Q d\mathbf{B}_s$$

Ito calculus yields Gaussian with

$$\begin{aligned}\langle \mathbf{I}_{\text{thm}}(t)\rangle &= 0 \\ \langle \mathbf{I}_{\text{thm}}(t)\mathbf{I}_{\text{thm}}(t)^T\rangle &= \int_0^t e^{(t-s)\mathcal{L}} Q Q^T e^{(t-s)\mathcal{L}^T} ds := \Lambda(t)\end{aligned}$$

$$\Lambda_{\mathbf{k},\mathbf{k}}(t) = -\frac{1}{2\alpha_{\mathbf{k}}}\left[1 - e^{-2\alpha_{\mathbf{k}}\Delta t}\right] Q_{\mathbf{k},\mathbf{k}}^2$$

Atzberger, Peskin, Kramer 2007

Stiff Time-step Integrator

Integration by exponential factor (ito calculus)

$$\mathbf{u}(t) = e^{t\mathcal{L}}\mathbf{u}(0) + \int_0^t e^{(t-s)\mathcal{L}}\rho^{-1}\mathbf{F}_{\text{prt}}(s)ds + \int_0^t e^{(t-s)\mathcal{L}}Q d\mathbf{B}_s = e^{t\mathcal{L}}\mathbf{u}(0) + \bar{\mathbf{I}}_{\text{prt}} + \bar{\mathbf{I}}_{\text{thm}}$$

$$\mathbf{I}_{\text{prt}}(t) \approx -\rho^{-1}\mathcal{L}^{-1}\left[\mathcal{I} - e^{t\mathcal{L}}\right]\mathbf{F}_{\text{prt}}(0)$$

$$\Lambda_{\mathbf{k},\mathbf{k}}(t) = -\frac{1}{2\alpha_{\mathbf{k}}}\left[1 - e^{-2\alpha_{\mathbf{k}}\Delta t}\right]Q^2_{\mathbf{k},\mathbf{k}}$$

Fluid Integrator

$$\mathbf{u}^{n+1} = e^{\Delta t\mathcal{L}}\mathbf{u}^n + \mathcal{L}^{-1}\left[\mathcal{I} - e^{\Delta t\mathcal{L}}\right]\rho^{-1}\mathbf{F}^n_{\text{prt}} + \Gamma\xi^n$$

ξ is Gaussian with

$\langle\xi\rangle = 0$, $\langle\xi\xi^T\rangle = \mathcal{I}$

$\Lambda = \Gamma\Gamma^T$

Unconditionally stable for the fluid
Accuracy depends only on structure force approximation (otherwise exact).
Requires prior knowledge of Γ.
Method viable only if efficient to compute $e^{\Delta t\mathcal{L}}$.
Efficient for uniform meshes (FFTs).

Atzberger, Peskin, Kramer 2007

Stiff Time-step Integrator

Fluid equations

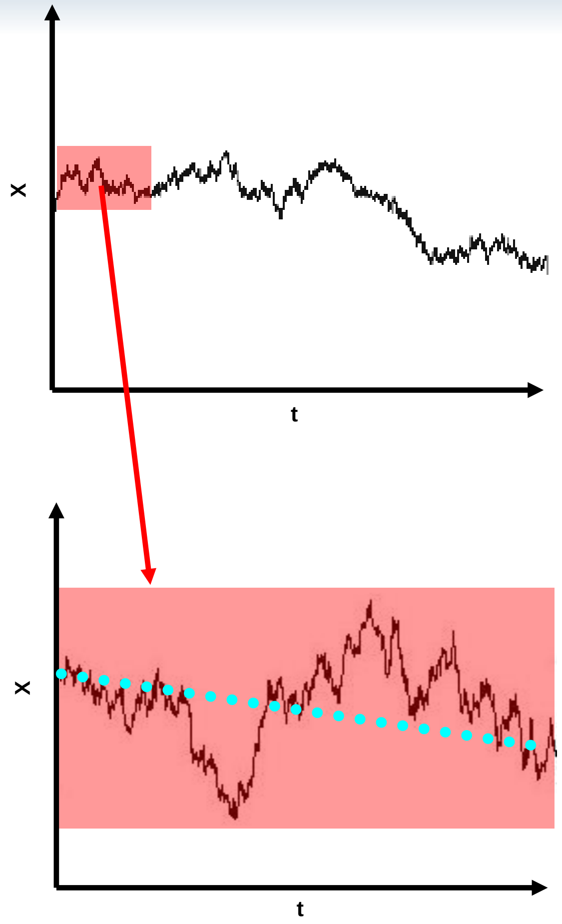
$$\begin{aligned} d\mathbf{u} &= \mathcal{L}\mathbf{u}dt && \text{(dissipation in fluid)} \\ &+ \rho^{-1}\mathbf{F}_{\text{prt}}dt && \text{(microstructure forces)} \\ &+ Q d\mathbf{B}_t && \text{(thermal force)} \end{aligned}$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{(incompressibility)}$$

Structure equations

$$\frac{d\mathbf{X}^{[j]}(t)}{dt} = \int \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t))\mathbf{u}(\mathbf{x},t)d\mathbf{x}$$

$$\mathbf{F}_{\text{prt}}(\mathbf{x},t) = \sum_{j=1}^{M} -\nabla_{\mathbf{X}^{[j]}} V(\{\mathbf{X}(t)\})\delta_a(\mathbf{x} - \mathbf{X}^{[j]}(t))$$



Integrate microstructure dynamics (ito calculus)

$$\mathbf{X}^{[j]}(t) = \mathbf{X}^{[j]}(0) + \int_0^t \int \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(s))\mathbf{u}(\mathbf{x},s)d\mathbf{x}ds \approx \mathbf{X}^{[j]}(0) + \int \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(0)) \int_0^t \mathbf{u}(\mathbf{x},s)dsd\mathbf{x}$$

Atzberger, Peskin, Kramer 2007

Stiff Time-step Integrator

Integrate structure dynamics (ito calculus)

$$\mathbf{X}^{[j]}(t) \approx \mathbf{X}^{[j]}(0) + \int \delta_a(\mathbf{x} - \mathbf{X}^{[j]}(0)) \int_0^t \mathbf{u}(\mathbf{x}, s)\,ds\,d\mathbf{x}$$

$$\longrightarrow \mathbf{X}^{[j],n+1} = \mathbf{X}^{[j],n} + \int \delta_a(\mathbf{x} - \mathbf{X}^{[j],n})\mathbf{I}_{\text{vel}}(\mathbf{x}, \Delta t)\,d\mathbf{x}$$

$$\mathbf{I}_{\text{vel}}(t) := \int_0^t \mathbf{u}(s)\,ds$$

Integrated fluctuating fluid velocity

$\mathbf{I}_{\text{vel}}(t)$ is a Gaussian with

$$\bar{\mathbf{I}}_{\text{vel}} := \langle \mathbf{I}_{\text{vel}}(t) \rangle = \int_0^t \langle \mathbf{u}(s) \rangle ds = -\mathcal{L}^{-1}\left[\mathcal{I} - e^{t\mathcal{L}}\right]\mathbf{u}(0) + -\mathcal{L}^{-1}\left[t + \mathcal{L}^{-1}\left[\mathcal{I} - e^{t\mathcal{L}}\right]\right]\mathbf{F}_{\text{prt}}(0)$$

$$\Phi := \left\langle \left(\mathbf{I}_{\text{vel}}(t) - \bar{\mathbf{I}}_{\text{vel}}(t)\right)\left(\mathbf{I}_{\text{vel}}^T(t) - \bar{\mathbf{I}}_{\text{vel}}^T(t)\right)\right\rangle = \int_0^t \int_0^t e^{r\mathcal{L}} C e^{s\mathcal{L}^T} dr\,ds + \int_0^t \int_0^t \int_0^{s \wedge r} e^{(r-w)\mathcal{L}} QQ^T e^{(s-w)\mathcal{L}^T} dw\,dr\,ds$$

$\mathbf{I}_{\text{vel}}(t)$ is correlated with $\mathbf{I}_{\text{thm}}(t)$

$$W := \left\langle \left(\mathbf{I}_{\text{vel}}(t) - \bar{\mathbf{I}}_{\text{vel}}(t)\right)\mathbf{I}_{\text{thm}}^T(t)\right\rangle = \mathcal{L}^{-1}\int_0^t e^{(t-w)\mathcal{L}} QQ^T e^{(t-w)\mathcal{L}^T} dw + \mathcal{L}^{-1} QQ^T \mathcal{L}^{-T}\left[\mathcal{I} - e^{t\mathcal{L}^T}\right]$$

Microstructure Integrator

$$\mathbf{X}^{[j],n+1} = \mathbf{X}^{[j],n} + \int \delta_a(\mathbf{x} - \mathbf{X}^{[j],n})\mathbf{I}_{\text{vel}}(\mathbf{x}, \Delta t)\,d\mathbf{x}$$

Stability depends now on structure forces.
Accuracy depends on

- fluid sampling approximation X(t) ~ X(0) and structure force approximation.

Method viable only if efficient to compute exponentials.
Efficient for uniform meshes (FFTs).

Atzberger, Peskin, Kramer 2007

Summary : Stiff Integrator for SIBM

Fluid Integrator

$$\mathbf{u}^{n+1} = e^{\Delta t\mathcal{L}}\mathbf{u}^n + \mathcal{L}^{-1}\left[\mathcal{I} - e^{\Delta t\mathcal{L}}\right]\rho^{-1}\mathbf{F}^n_{\text{prt}} + \Gamma\xi^n$$

ξ is Gaussian with

$$\langle\xi\rangle = 0, \quad \langle\xi\xi^T\rangle = \mathcal{I}$$

$$\Lambda = \Gamma\Gamma^T$$

Microstructure Integrator

$$\mathbf{X}^{[j],n+1} = \mathbf{X}^{[j],n} + \int \delta_a(\mathbf{x} - \mathbf{X}^{[j],n})\mathbf{I}_{\text{vel}}(\mathbf{x},\Delta t)d\mathbf{x}$$

$\mathbf{I}_{\text{vel}}(t)$ is a Gaussian with

$$\bar{\mathbf{I}}_{\text{vel}} := \langle\mathbf{I}_{\text{vel}}(t)\rangle = \int_0^t\langle\mathbf{u}(s)\rangle ds = -\mathcal{L}^{-1}\left[\mathcal{I} - e^{t\mathcal{L}}\right]\mathbf{u}(0) + -\mathcal{L}^{-1}\left[t + \mathcal{L}^{-1}\left[\mathcal{I} - e^{t\mathcal{L}}\right]\right]\mathbf{F}_{\text{prt}}(0)$$

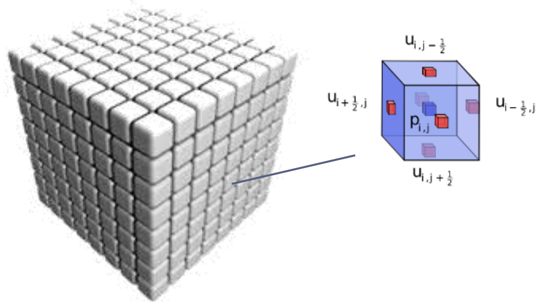
$$\Phi := \left\langle\left(\mathbf{I}_{\text{vel}}(t) - \bar{\mathbf{I}}_{\text{vel}}(t)\right)\left(\mathbf{I}^T_{\text{vel}}(t) - \bar{\mathbf{I}}^T_{\text{vel}}(t)\right)\right\rangle = \int_0^t\int_0^t e^{r\mathcal{L}}Ce^{s\mathcal{L}^T}drds + \int_0^t\int_0^t\int_0^{s\wedge r} e^{(r-w)\mathcal{L}}QQ^Te^{(s-w)\mathcal{L}^T}dwdrds$$

$\mathbf{I}_{\text{vel}}(t)$ is correlated with $\mathbf{I}_{\text{thm}}(t)$

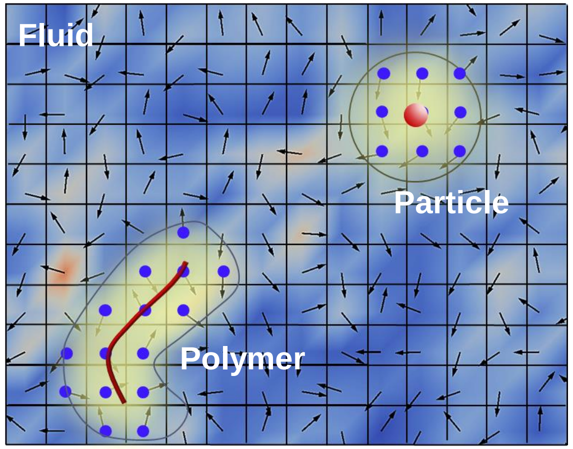
$$W := \left\langle\left(\mathbf{I}_{\text{vel}}(t) - \bar{\mathbf{I}}_{\text{vel}}(t)\right)\mathbf{I}^T_{\text{thm}}(t)\right\rangle = \mathcal{L}^{-1}\int_0^t e^{(t-w)\mathcal{L}}QQ^Te^{(t-w)\mathcal{L}^T}dw + \mathcal{L}^{-1}QQ^T\mathcal{L}^{-T}\left[\mathcal{I} - e^{t\mathcal{L}^T}\right]$$

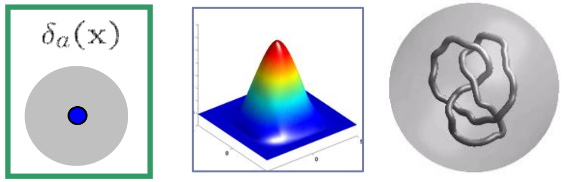
Method viable only if efficient to compute exponentials.
Viable for uniform meshes (FFTs).
Under-resolves fluid mode dynamics and fluctuations.
Time-step limited by structure's motions.

Numerical Discretization



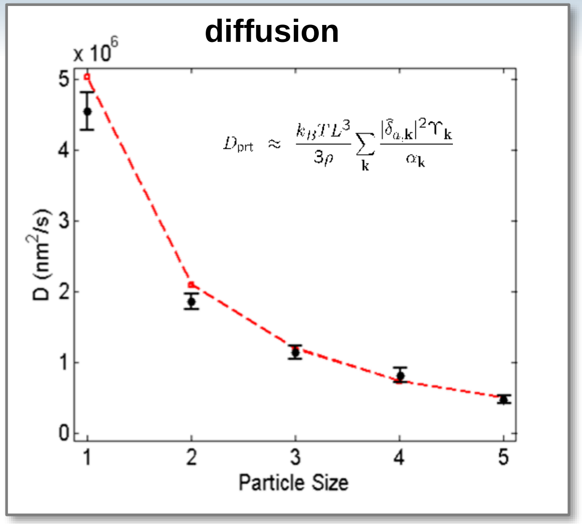
Fluid-Structure Coupling

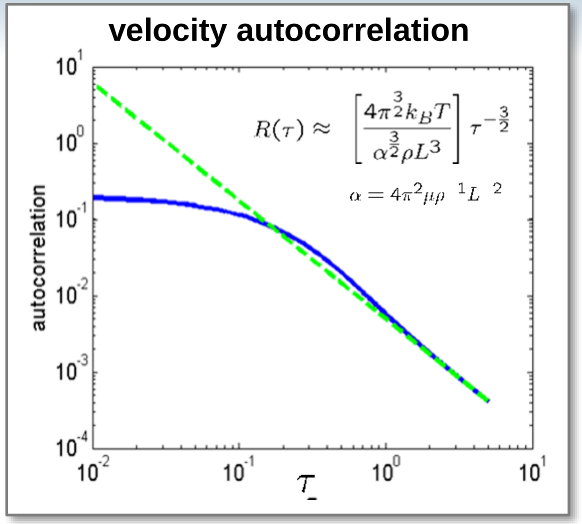


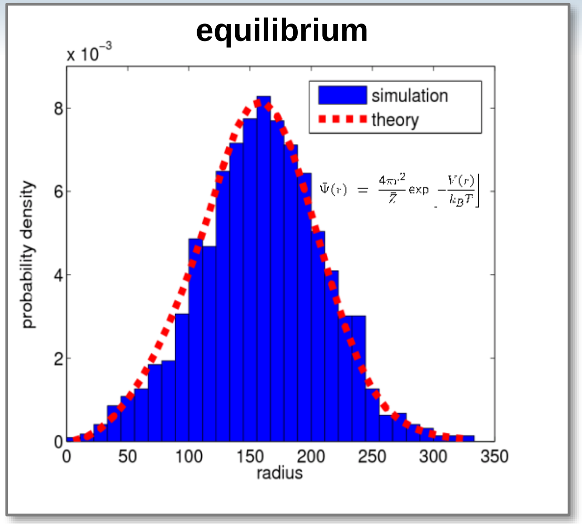


Atzberger, Peskin, Kramer 2007

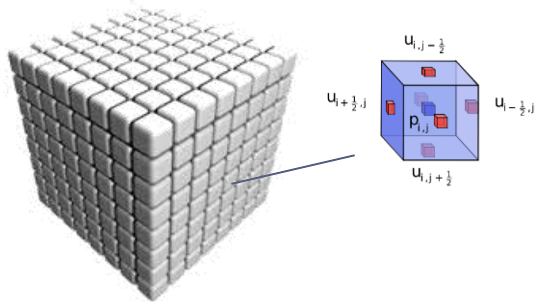
Validation of Numerical Methods for SIBM



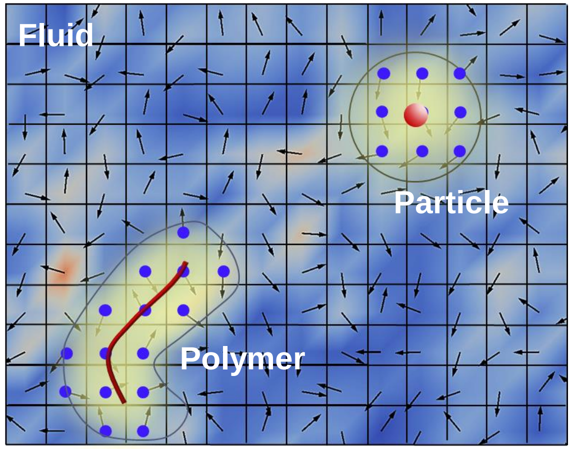


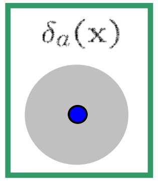


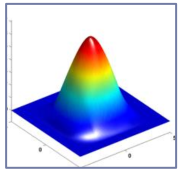
Numerical Discretization



Fluid-Structure Coupling







Validation

Diffusivity of under-resolved particles correct.

Velocity auto-correlation has $t^{-3/2}$ tail (Adler & Wainright 1950),

Auto-correlation persists from hydrodynamic "memory."

Equilibrium configurations have Gibbs-Boltzmann statistics.

Approach can be extended to other coupling types, regimes, and numerical discretizations.

Atzberger, Peskin, Kramer 2007

Stochastic Immersed Boundary Methods

Simulations

Topology and Immersed Boundary Simulations

Topological Features

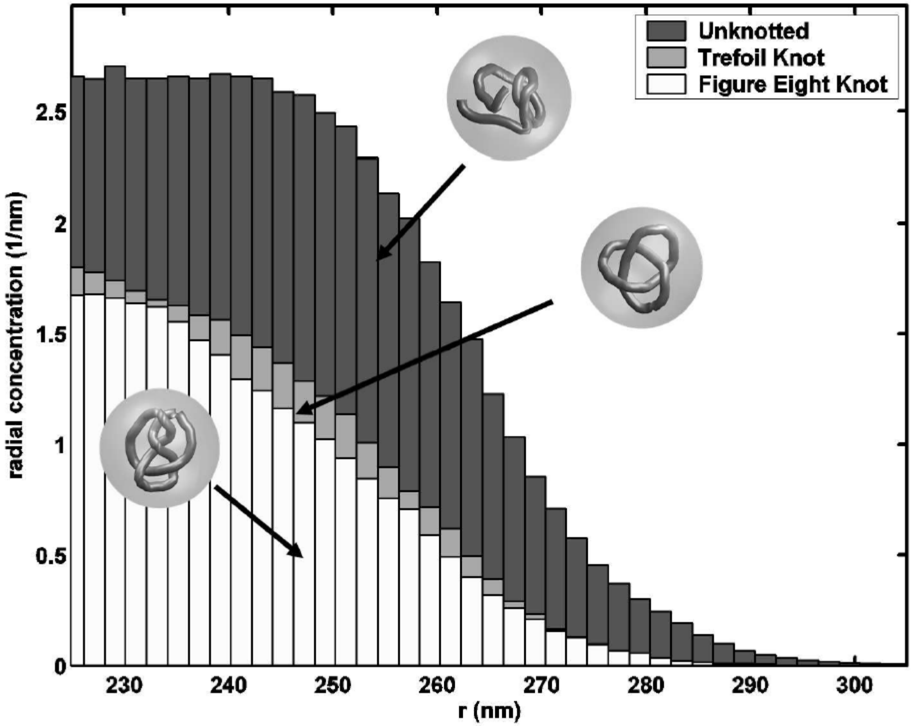
Structure motions reference a common continuum velocity field.

Solution map is homeomorphism.

Preserves topological invariants (up to numerical error)

Knotted structures remain knotted.

Simulation: Osmotic pressures of knotted polymers.



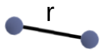
Knot Type	Osmotic Pressure $(\mathrm{amu}/\mathrm{nm}\cdot\mathrm{ns}^2)$
Unknotted	0.16
Trefoil Knot	0.0439
Figure Eight Knot	0.0392

Atzberger, Peskin, Kramer 2007

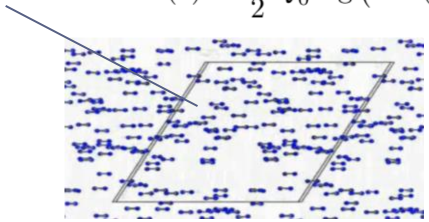
Rheological Properties and Microstructure Dynamics

Rheometry:

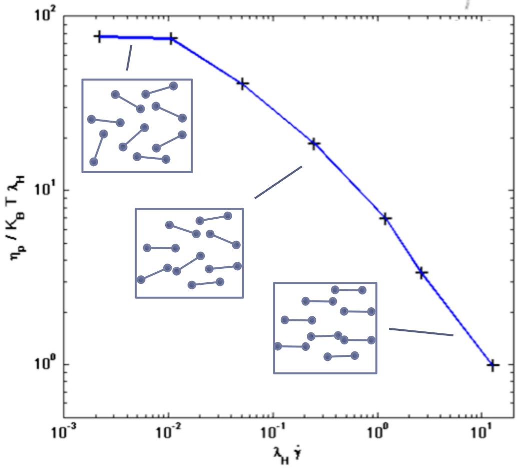
Polymeric Fluid (FENE)



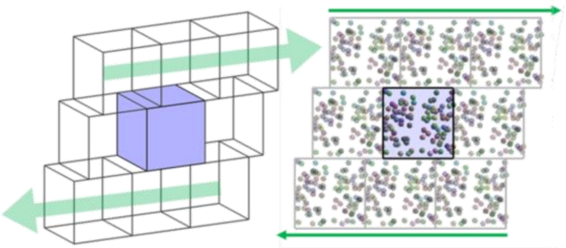
$$U(r) = \frac{K}{2} Q_0^2 \log\left(1 - (r/Q_0)^2\right)$$



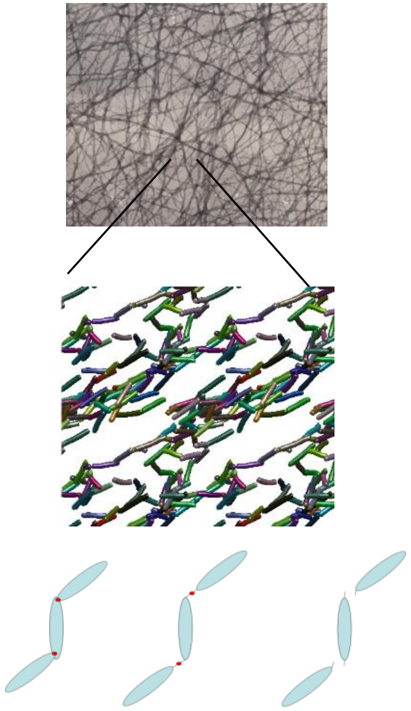
Shear Viscosity $\eta_p = \frac{\sigma^{(s,v)}}{\dot{\gamma}}$



Lees-Edwards Conditions:

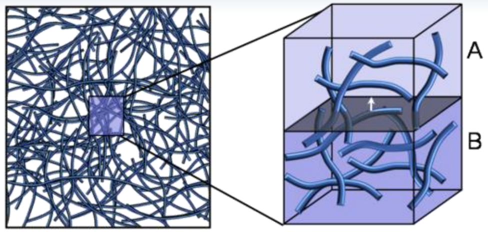


Polymeric Material

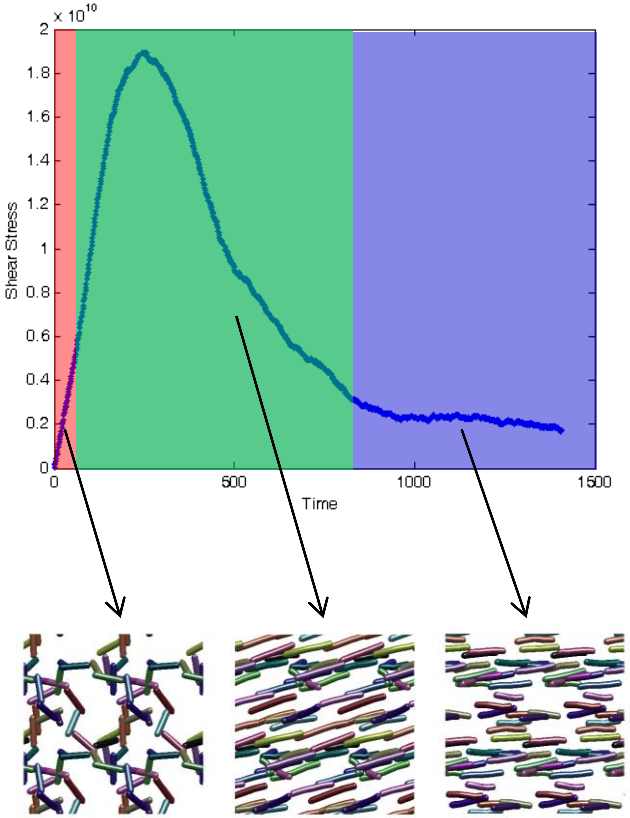


Atzberger 2013

Material Stress ← Forces

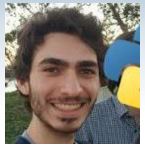


$$\sigma^{(n)}_{\ell,z} = \frac{1}{AL} \sum_{\mathbf{q}\in\mathcal{Q}_n} \sum_{j=1}^{n-1} \left\langle \mathbf{f}^{(\ell)}_{\mathbf{q},j} \cdot \left(\mathbf{x}^{*,(z)}_{q_n} - \mathbf{x}^{*,(z)}_{q_j}\right)\right\rangle$$



Conclusions

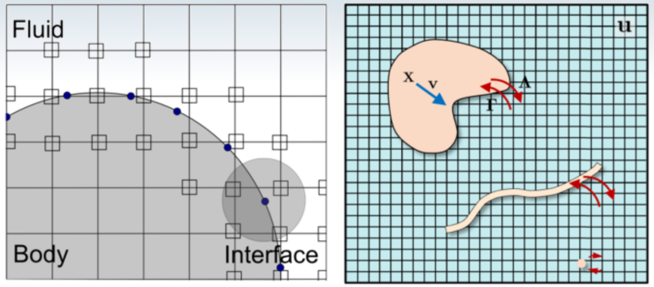

B. Gross


D. Rower

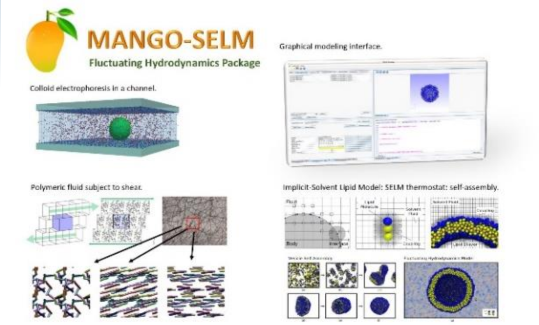

M. Padidar


J. Sigurdsson

UCSB Recent Student Collaborators



IB Eulerian-Lagrangian Methods



SELM Software

2016 Atzberger & Sigurdsson

Summary

Stochastic Immersed Boundary Methods *with numerical solvers preserving statistical mechanics properties.*

Applications *in soft materials, complex fluids, rheology, microfluidics, biophysics, lipid bilayer membranes.*

Surface Fluctuating Hydrodynamics for drift-diffusion dynamics of microstructures in membranes.

Software packages available for methods integrated with MD packages for simulating models (more on this later).

Mango-Selm package for Fluctuating Hydrodynamics
http://atzberger.org

Papers

A Stochastic Immersed Boundary Method for Fluid-Structure Dynamics at Microscopic Length Scales,
P.J. Atzberger, P.R. Kramer, and C.S. Peskin, J. Comp. Phys., Vol. 224, Iss. 2, (2007).

Stochastic Eulerian Lagrangian Methods for Fluid Structure Interactions with Thermal Fluctuations,
P.J. Atzberger, J. of Comp. Phys., 230, pp. 2821--2837, (2011).

Surface Fluctuating Hydrodynamics Methods for the Drift-Diffusion Dynamics of Particles and Microstructures within Curved Fluid Interfaces,
D. Rower, M. Padidar, and P. J. Atzberger, arXiv:1906.01146, (2019).

Meshfree Methods on Manifolds for Hydrodynamic Flows on Curved Surfaces: A Generalized Moving Least-Squares (GMLS) Approach,
Gross B. J., Kuberry P. A., Trask N., Atzberger P. J., J. Comp. Phys., 409, 15 May (2020).

UCSB Recent Student Collaborators

B. Gross, M. Padidar, D. Rower,
J. K. Sigurdsson.

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More information: http://atzberger.org/

Publications

A Stochastic Immersed Boundary Method for Fluid-Structure Dynamics at Microscopic Length Scales,
P.J. Atzberger, P.R. Kramer, and C.S. Peskin, J. Comp. Phys., Vol. 224, Iss. 2, (2007). http://dx.doi.org/10.1016/j.jcp.2006.11.015

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Gross B. J., Kuberry P. A., Trask N., Atzberger P. J., J. Comp. Phys., 409, 15 May (2020). https://doi.org/10.1016/j.jcp.2020.109340

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Spatially Adaptive Stochastic Methods for Fluid-Structure Interactions Subject to Thermal Fluctuations in Domains with Complex Geometries,
P. Plunkett, J. Hu, C. Siefert, P.J. Atzberger, Journal of Computational Physics, Vol. 277, 15 Nov. 2014, pg. 121--137, (2014).
http://dx.doi.org/10.1016/j.jcp.2014.07.051

Incorporating Shear into Stochastic Eulerian Lagrangian Methods for Rheological Studies of Complex Fluids and Soft Materials,
P.J. Atzberger, Physica D, Vol. 265, pg. 57–70, (2013). http://dx.doi.org/10.1016/j.physd.2013.09.002

For additional information: http://atzberger.org/