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Improving Statistical Components of Multi-scale Simulation Schemes

Peter Kramer
Jim Berger, Susie Bayarri, Murali Haran, John Harlim, Emily Kang, Hans Künsch, Sorin Mitran
Interaction of Deterministic and Stochastic Models
and
Numerical Methods for Stochastic Systems Working Groups

Rensselaer Polytechnic Institute
and Statistics and Mathematical Sciences Institute

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Challenges of Multiscale Computation

Not computationally feasible to adequately resolve equations in climate models

- spatial resolution in global models ranges from 25 km to 100 km
- equations technically require cm resolution (but standard large eddy simulation may be OK at 100 m)
- clouds are most important underresolved structure in atmosphere
  - precipitation and condensation affect heat flux and convection

Parameterization and Superparameterization

Care most about the large scale dynamics, so how about projecting equations onto resolvable scales?

- Nonlinearity implies unresolved scales affect dynamics of resolved scales

How to handle these unclosed terms?

- Ignore: disastrously wrong
- Parameterization: Approximations in terms of resolvable variables
- Superparameterization: Run selective "microscale" simulations, sample statistics to estimate terms

Example: Fluid Dynamics

Equations for continuum fluid density $\rho(\mathbf{x}, t)$ and momentum $\rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t)$:

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \boldsymbol{\nabla} \cdot (\mathbf{u}(\mathbf{x}, t)\rho(\mathbf{x}, t)) = 0,$$

$$\frac{\partial(\rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t))}{\partial t} + \boldsymbol{\nabla} \cdot (\rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t) \otimes \mathbf{u}(\mathbf{x}, t)) = -\boldsymbol{\nabla} \cdot \tau(\mathbf{x}, t),$$

which is not quite closed because of stress tensor τ.

- Could extend further to energy dynamics

Example: Fluid Dynamics

Equations for continuum fluid density $\rho(\mathbf{x}, t)$ and momentum $\rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t)$:

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$$\frac{\partial(\rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t))}{\partial t} + \boldsymbol{\nabla} \cdot (\rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t) \otimes \mathbf{u}(\mathbf{x}, t)) = -\boldsymbol{\nabla} \cdot \tau(\mathbf{x}, t),$$

which is not quite closed because of stress tensor τ.

For simple fluid, standard (Cauchy) parameterization works:

$$\tau(\mathbf{x}, t) = -\mu \boldsymbol{\nabla} \mathbf{u}(\mathbf{x}, t)$$

where μ is constant dynamic viscosity.

Example: Fluid Dynamics

Equations for continuum fluid density $\rho(\mathbf{x},t)$ and momentum $\rho(\mathbf{x},t)\mathbf{u}(\mathbf{x},t)$:

$$\frac{\partial \rho(\mathbf{x},t)}{\partial t} + \boldsymbol{\nabla}\cdot(\mathbf{u}(\mathbf{x},t)\rho(\mathbf{x},t)) = 0,$$

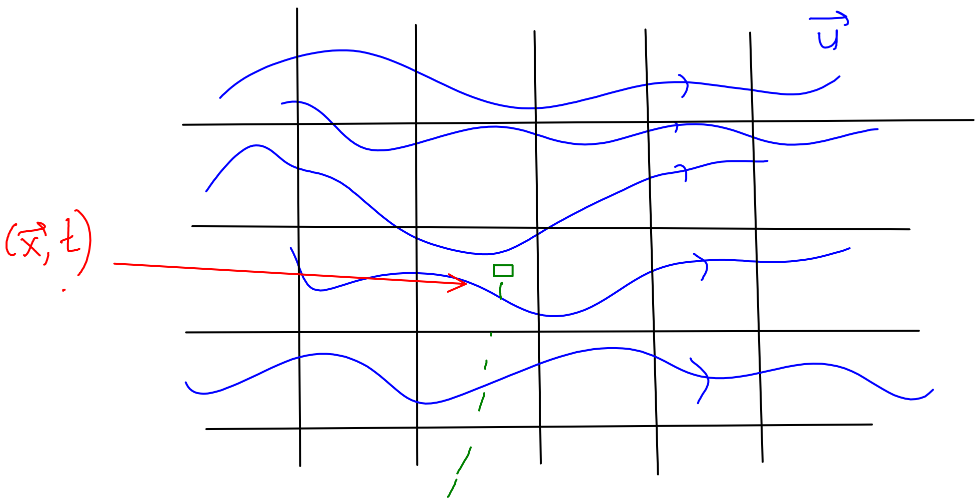
$$\frac{\partial(\rho(\mathbf{x},t)\mathbf{u}(\mathbf{x},t))}{\partial t} + \boldsymbol{\nabla}\cdot(\rho(\mathbf{x},t)\mathbf{u}(\mathbf{x},t)\otimes\mathbf{u}(\mathbf{x},t)) = -\boldsymbol{\nabla}\cdot\tau(\mathbf{x},t),$$

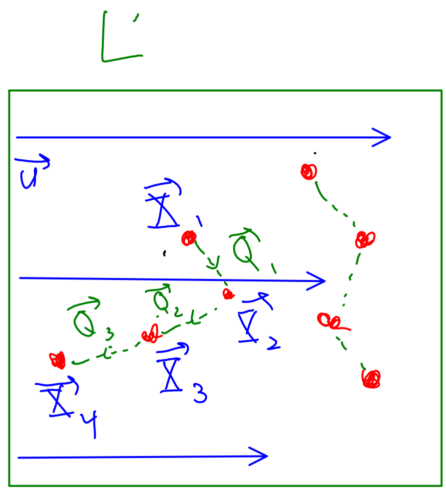
which is not quite closed because of stress tensor τ.

Complex fluid (immersed polymers, etc.)

- Standard Parameterization: Find more complex functional expression for $\tau = G(\mathbf{u})$ (Oldroyd-B, etc.).
- Superparameterization: Estimate τ for current macroscale fluid conditions by sampling simulations of immersed polymer dynamics

Macroscale fluid simulation





Microscale polymer simulation

Polymer chain dynamics

Overdamped dynamics for positions $\{\mathbf{X}_j(t)\}_{j=1}^N$:

$$\begin{aligned}
\gamma \mathrm{d}\mathbf{X}_1 &= \mathbf{F}(\mathbf{Q}_1)\,\mathrm{d}t + \mathbf{u}(\mathbf{X}_1(t),t)\,\mathrm{d}t \\
&\quad + \sqrt{2k_\mathrm{B}T\gamma}\,\mathrm{d}\mathbf{W}_1(t), \\
\gamma \mathrm{d}\mathbf{X}_k &= [\mathbf{F}(\mathbf{Q}_k) - \mathbf{F}(\mathbf{Q}_{k-1})]\,\mathrm{d}t + \mathbf{u}(\mathbf{X}_k(t),t)\,\mathrm{d}t \\
&\quad + \sqrt{2k_\mathrm{B}T\gamma}\,\mathrm{d}\mathbf{W}_k(t), 2 \le k \le M-1 \\
\gamma \mathrm{d}\mathbf{X}_M &= -\mathbf{F}(\mathbf{Q}_{M-1})\,\mathrm{d}t + \mathbf{u}(\mathbf{X}_{M-1}(t),t)\,\mathrm{d}t \\
&\quad + \sqrt{2k_\mathrm{B}T\gamma}\,\mathrm{d}\mathbf{W}_M(t),
\end{aligned}$$

with

- bond vectors $\mathbf{Q}_k \equiv \mathbf{X}_{k+1} - \mathbf{X}_k$
- monomer friction coefficient γ
- temperature T
- Boltzmann's constant k_B
- independent Brownian motions $\{\mathbf{W}_k(t)\}_{k=1}^M$

Polymer chain dynamics

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&\quad + \sqrt{2k_{\mathrm{B}}T\gamma}\,\mathrm{d}\mathbf{W}_M(t),
\end{aligned}$$

Bond force law examples:

- Linear (Rouse):

$$\mathbf{F}(\mathbf{Q}) = H\mathbf{Q}$$

- FENE:

$$\mathbf{F}(\mathbf{Q}) = \frac{H\mathbf{Q}}{1-(|\mathbf{Q}|/Q_0)^2}$$

Polymer chain dynamics

Overdamped dynamics for positions $\{\mathbf{X}_j(t)\}_{j=1}^{N}$:

$$\gamma \mathrm{d}\mathbf{X}_1 = \mathbf{F}(\mathbf{Q}_1)\,\mathrm{d}t + \mathbf{u}(\mathbf{X}_1(t),t)\,\mathrm{d}t + \sqrt{2k_\mathrm{B}T\gamma}\,\mathrm{d}\mathbf{W}_1(t),$$

$$\gamma \mathrm{d}\mathbf{X}_k = [\mathbf{F}(\mathbf{Q}_k) - \mathbf{F}(\mathbf{Q}_{k-1})]\,\mathrm{d}t + \mathbf{u}(\mathbf{X}_k(t),t)\,\mathrm{d}t + \sqrt{2k_\mathrm{B}T\gamma}\,\mathrm{d}\mathbf{W}_k(t), 2 \le k \le M-1$$

$$\gamma \mathrm{d}\mathbf{X}_M = -\mathbf{F}(\mathbf{Q}_{M-1})\,\mathrm{d}t + \mathbf{u}(\mathbf{X}_{M-1}(t),t)\,\mathrm{d}t + \sqrt{2k_\mathrm{B}T\gamma}\,\mathrm{d}\mathbf{W}_M(t),$$

Simplified Geometry Test Model

- Incompressible, constant density ρ
- Oscillating shear flow established by parallel oscillating walls

$$\mathbf{u}(\mathbf{x},t) = u(y,t)\hat{\mathbf{x}}$$

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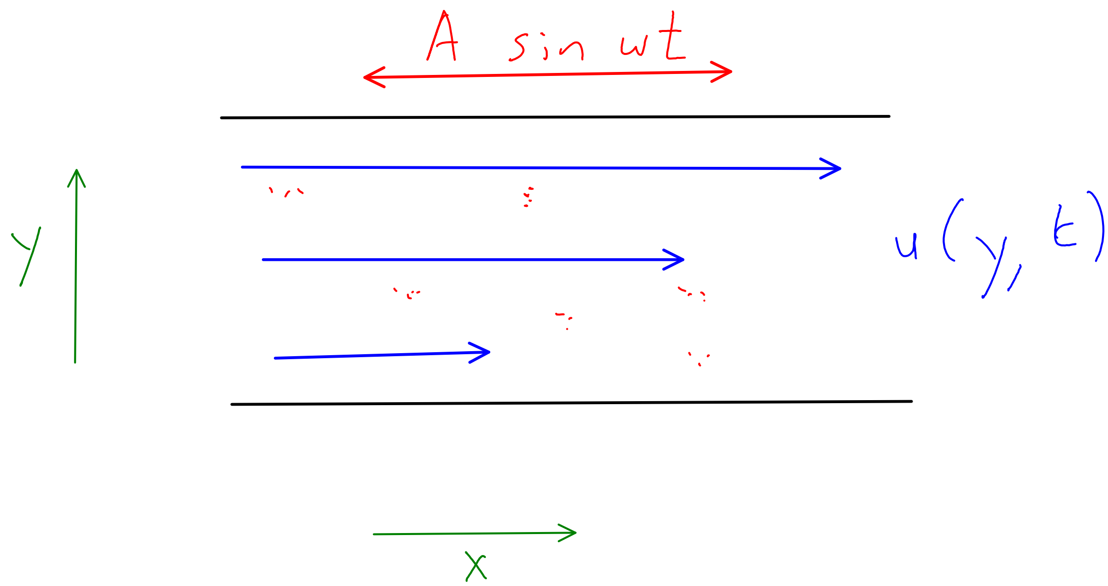

Interaction of Fluid and Polymer

Macroscopic affects microscopic:

- Fluid velocity gradient appears in equations for polymer dynamics
- Microscale statistics must be consistent with macroscopic constraints:

Microscopic affects macroscopic:

- Macroscopic stress on fluid at macroscale position $\mathbf{x}$ at time t obtained by statistical average $\langle\cdot\rangle$ of microscale polymer configuration:

$$\hat{\tau}_{xy} = -n\hat{\mathbf{y}} \cdot \left\langle \sum_{k=1}^{M-1} \mathbf{Q}_k \otimes \mathbf{F}(\mathbf{Q}_k) \right\rangle \cdot \hat{\mathbf{x}} + \eta \frac{\partial u}{\partial y},$$

- n is the number density of polymer chains, $\langle\cdot\rangle$ denotes statistical average.

Macroscopic Constraints

Consistency of mass, momentum between microscale and macroscale easy to enforce:

$$\langle \mathbf{Q}_k \rangle = 0$$

But configuration tensor $\mathsf{A} = \langle \mathbf{Q} \otimes \mathbf{Q} \rangle$ in many cases evolves slowly, so included as macroscale variable, with dynamical equation:

$$\frac{\partial \mathsf{A}}{\partial t} = \frac{\partial u}{\partial y} [(\hat{\mathbf{x}} \otimes \hat{\mathbf{y}})\mathsf{A} + \mathsf{A}(\hat{\mathbf{x}} \otimes \hat{\mathbf{y}})] + 4k_{\mathsf{B}} T \gamma^{-1} \mathsf{I}$$
$$- 2\gamma^{-1} \frac{1}{M-1} \sum_{k=1}^{M-1} [\langle \mathbf{Q}_k \otimes \mathbf{F}(\mathbf{Q}_k) \rangle + \langle \mathbf{F}(\mathbf{Q}_k) \otimes \mathbf{Q}_k \rangle]$$

This again has an unclosed term depending on microscale configuration, and imposes a nontrivial constraint:

$$\frac{1}{M-1} \sum_{k=1}^{M-1} \langle \mathbf{Q}_k \otimes \mathbf{Q}_k \rangle = \mathsf{A}.$$

Mathematical Framework for Multiscale Computing (Vanden-Eijnden, E, Engquist)

Slow macroscale variables $\mathbf{Z}(t)$; fast microscale variables $\mathbf{Y}(t)$:

$$\mathrm{d}\mathbf{Z} = \mathbf{f}(\mathbf{Z},\mathbf{Y})\,\mathrm{d}t + \mathbf{\Gamma}(\mathbf{Z},\mathbf{Y})\,\mathrm{d}\mathbf{W}_Z(t), \tag{1}$$

$$\mathrm{d}\mathbf{Y} = \epsilon^{-1}\mathbf{g}(\mathbf{Z},\mathbf{Y})\,\mathrm{d}t + \epsilon^{-1/2}\mathbf{\Sigma}(\mathbf{Z},\mathbf{Y})\,\mathrm{d}\mathbf{W}_Y(t). \tag{2}$$

with small parameter $\epsilon \ll 1$. May also have some constraints $\mathbf{C}(\mathbf{Z},\mathbf{Y}) = \mathbf{0}$.

For small ϵ, dynamics of $\mathbf{Z}$ can be approximated:

$$\mathrm{d}\mathbf{Z} \approx \bar{\mathbf{f}}(\mathbf{Z})\,\mathrm{d}t + \bar{\mathbf{\Gamma}}(\mathbf{Z})\,\mathrm{d}\mathbf{W}_Z(t),$$

where $\bar{\mathbf{f}}$ and $\bar{\mathbf{\Gamma}}$ involve statistical averages over dynamics of $\mathbf{Y}$ under fixed value of $\mathbf{Z}$ (and the possible constraints). Usually not in explicitly useful form.

Mathematical Framework for Multiscale Computing (Vanden-Eijnden, E, Engquist)

Slow macroscale variables $\mathbf{Z}(t)$; fast microscale variables $\mathbf{Y}(t)$:

$$\mathrm{d}\mathbf{Z} = \mathbf{f}(\mathbf{Z},\mathbf{Y})\,\mathrm{d}t + \mathbf{\Gamma}(\mathbf{Z},\mathbf{Y})\,\mathrm{d}\mathbf{W}_Z(t), \quad (1)$$

$$\mathrm{d}\mathbf{Y} = \epsilon^{-1}\mathbf{g}(\mathbf{Z},\mathbf{Y})\,\mathrm{d}t + \epsilon^{-1/2}\mathbf{\Sigma}(\mathbf{Z},\mathbf{Y})\,\mathrm{d}\mathbf{W}_Y(t). \quad (2)$$

with small parameter $\epsilon \ll 1$. May also have some constraints $\mathbf{C}(\mathbf{Z},\mathbf{Y}) = \mathbf{0}$.

For small ϵ, dynamics of $\mathbf{Z}$ can be approximated:

$$\mathrm{d}\mathbf{Z} \approx \bar{\mathbf{f}}(\mathbf{Z})\,\mathrm{d}t + \bar{\mathbf{\Gamma}}(\mathbf{Z})\,\mathrm{d}\mathbf{W}_Z(t),$$

Parameterization: Make ansatz for structure of $\bar{\mathbf{f}}$ and $\bar{\mathbf{\Gamma}}$.

Superparameterization: Run simulations of $\mathbf{Y}$ (conditioned on $\mathbf{Z}$) as needed to evaluate $\bar{\mathbf{f}}(\mathbf{Z})$ and $\bar{\mathbf{\Gamma}}(\mathbf{Z})$.

Heterogeneous Multiscale Method

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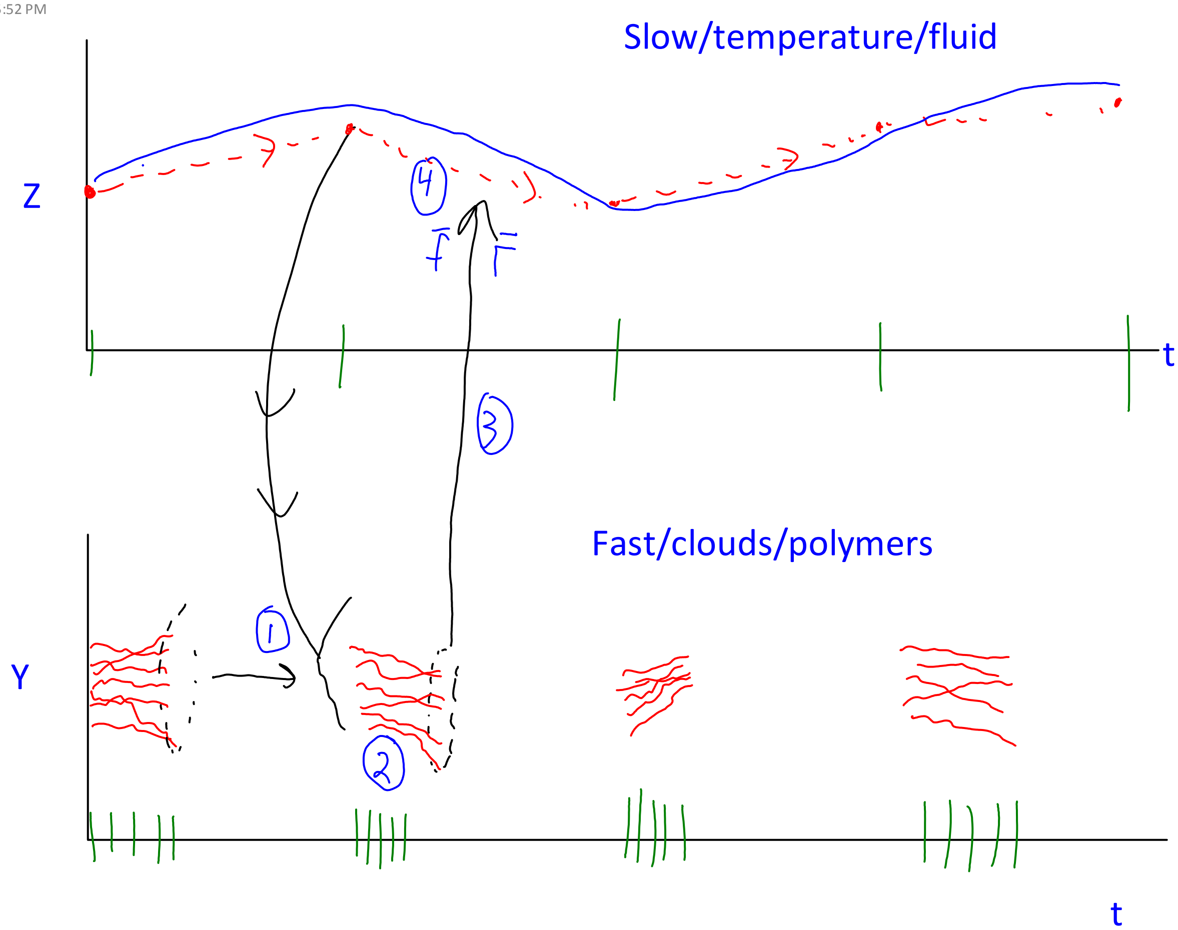

A time-parallel multiscale algorithm for non-equilibrated microscopic phenomena

Sorin Mitran

Applied Mathematics
University of North Carolina
Chapel Hill

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Laboratoire Jacques-Louis Lions
Paris 6

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tP-CKM algorithm

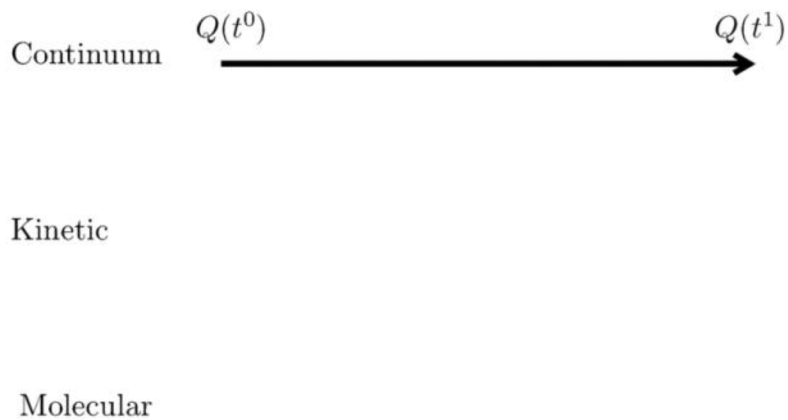
- Simultaneously solve
  - Continuum conservation equations (e.g. incompressible viscoelastic)
  - Kinetic equation for p.d.f. of micro-configuration
  - Stochastic equations for micro-configuration

Numerics

- Continuum solver
  - Finite volume
  - Time-samples kinetic solver to compute closure
- Kinetic solver
  - Grid-based for initial tests
  - Meshless particle-based (large-dimension configuration space)
  - Minimum-entropy modification of p.d.f. (continuum moments)
  - Optimal transport of p.d.f.'s
- Molecular solver
  - Stochastic differential equations on GPUs
  - Time-parallel kinetic-molecular interaction

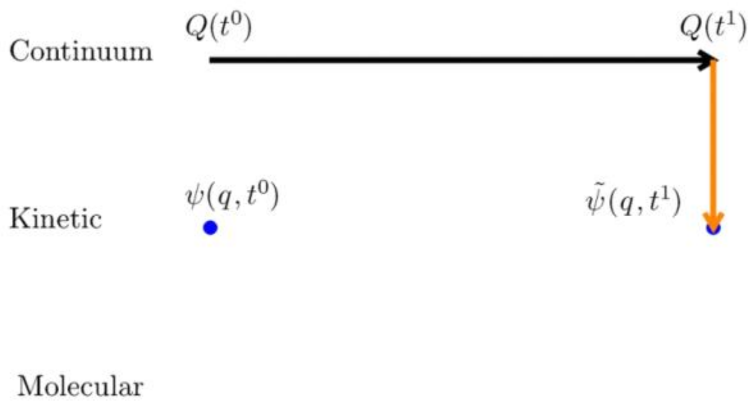
Time evolution

- Continuum predictor



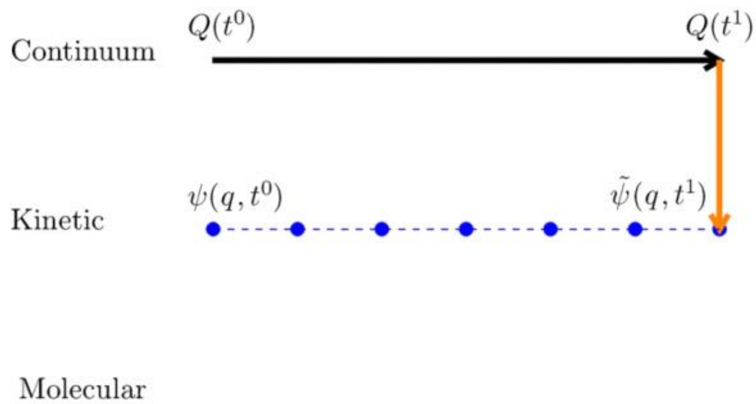
Time evolution

- Modify previous probability density



Time evolution

- Generate intermediate probability densities



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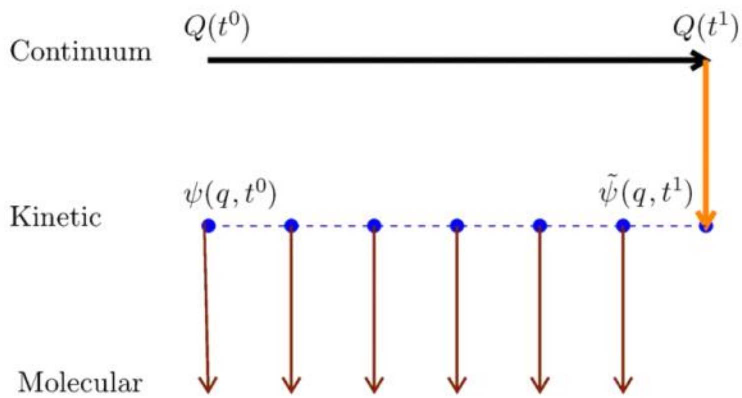
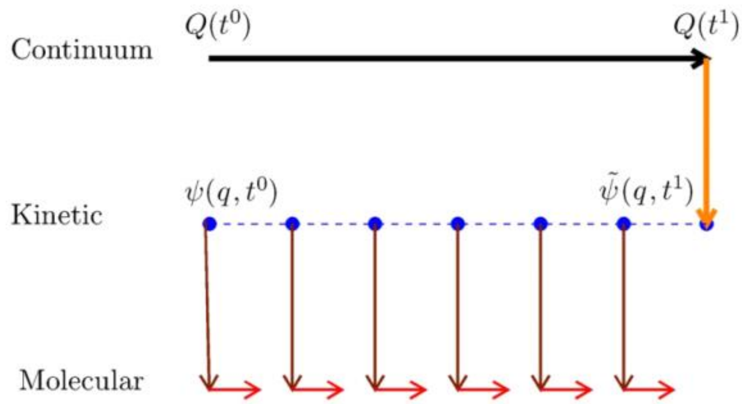
Time evolution

- Generate molecular ensembles



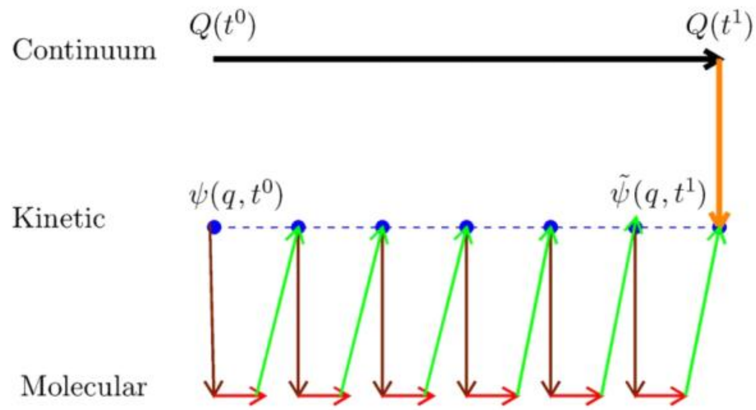
Time evolution

- Evolve stochastic differential equations (GPU)



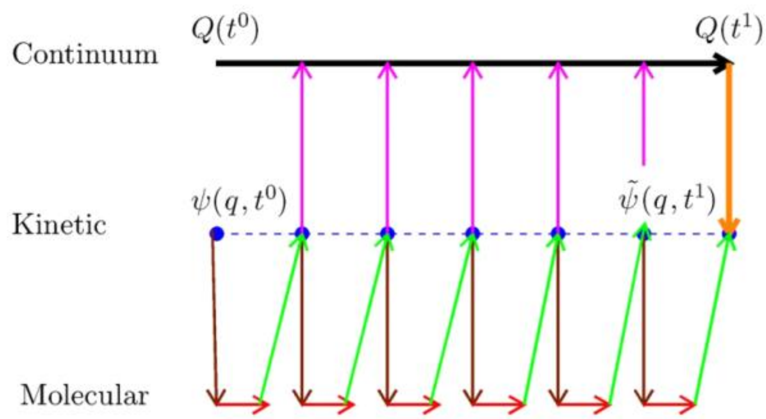
Time evolution

- Compare probability density estimates



Time evolution

- Update continuum viscoelastic stress



Initialization of Microscale Variables

Possible approaches

- Recycle end results from previous cycle
- Reinitialize from scratch by sampling from prescribed probability distribution depending on macroscale variables

Reinitialization:

- Typically not accurate guess so require longer microscale simulations to heal
- Problematic when microscale variable has slow relaxation

Recycling apparently more efficient but can violate constraints. Possible resolution:

- Project microscale samples onto constraint subspace (how?)
- Accept discrepancy; add compensatory forcing to dynamics
- Reweight the microscale samples (particle filtering)

Mesoscale Representation of PDF

Currently accomplished by expansion into radial basis functions

$$\tilde{\psi}_{\mathbf{Y}}(\mathbf{y}, t) \equiv \sum_{\ell=1}^{L} c_\ell(t) B\left(\|\mathbf{y} - \mathbf{y}^{(\ell)}\|\right)$$

where

- $\{\mathbf{y}^{(\ell)}\}_{\ell=1}^{L}$ are points interpolating between mean of $\tilde{\psi}(\mathbf{y}, t_0)$ at beginning of macro time step and mean of estimated $\tilde{\psi}(\mathbf{y}, t_1)$ at end of macro time step
  - uses Jordan-Kinderlehrer-Otto (JKO) gradient flow formalism for Fokker-Planck equation
- $B(y)$ is a radial basis function, taken as Gaussian

$$B(y) = \frac{\exp(-y^2/(2h^2))}{\sqrt{2\pi h^2}}$$

  with h a fixed parameter
- $c_\ell(t)$ are coefficients computed through JKO and spline interpolation

Centers of Radial Basis Functions

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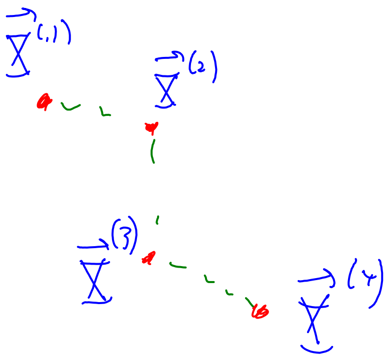
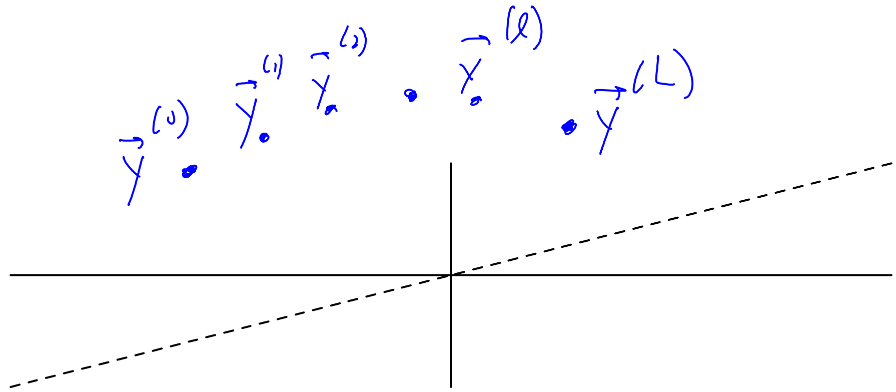


$$\vec{Y} = \begin{pmatrix} \vec{X}^{(1)} \\ \vec{X}^{(2)} \\ \vec{X}^{(3)} \\ \vec{X}^{(4)} \end{pmatrix}$$



Statistical Projection: Microscale $\rightarrow$ Mesoscale

From statistics of $\{\mathbf{Q}_k(t)\}_{k=1}^{M-1}$, want to estimate PDF. Currently, this is done (??) by projecting the microscale data onto the vector space spanned by the same radial basis functions as used to represent the mesoscale, to obtain PDF estimated by microscale data:

$$\hat{\psi}_{\mathbf{Y}}(\mathbf{y}, t) \equiv \sum_{\ell=1}^{L} \hat{c}_\ell(t) B\left(\|\mathbf{y} - \mathbf{y}^{(\ell)}\|\right)$$

- only $\{\hat{c}_\ell\}_{\ell=1}^{L}(t)$ depend on the data

Comparison of microscale and mesoscale data is done by appropriate vector space norm $\|\mathbf{c} - \hat{\mathbf{c}}\|$ with

$$\mathbf{c} = \{c_\ell\}_{\ell=1}^{L}, \qquad \hat{\mathbf{c}} = \{\hat{c}_\ell\}_{\ell=1}^{L}.$$

Statistical Projection: Microscale $\rightarrow$ Mesoscale

From statistics of $\{\mathbf{Q}_k(t)\}_{k=1}^{M-1}$, want to estimate PDF.
Possible areas for improvement:

- Account for how well microscale data is actually consistent with proposed mesoscale representation
- Better kernel estimation procedures for the high-dimensional PDF $\hat{\psi}$, allowing centers and widths to respond to data

Systematic Biases in Microscale-Mesoscale Comparisons

The microscale-mesoscale comparisons may not detect a small systematic error which accumulates.
Ideas:

- Statistical test for correlations in errors
- Estimate accumulated error through "vectorial" addition of errors at each time step
- Use mesoscale theory to estimate amplification and accumulation of error

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Work in Progress

Classical HMM:

- Initialization of microscale variables

tpCKM:

- Mesoscale representation frameworks
- Statistical projection of microscale variables onto mesoscale PDF
- Estimation of secular errors in microscale-mesoscale comparisons