Minimization of distance measures to efficiently capture the macroscale behavior of stochastic systems

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Multi scale models couple a global macroscopic equation with a local microscopic equation via averaging

$$
\begin{cases}
\dfrac{\mathrm{D}\,u}{\mathrm{D}\,t} & = \quad \mathcal{F}(\tau, u) \\[2em]
\tau(t) & = \quad \mathbb{E} g(X_t) \\[2em]
\mathrm{d}X_t & = \quad a(t, X_t, \nabla u)\,\mathrm{d}t + b(t, X_t)\,\mathrm{d}W_t
\end{cases}
\qquad
\begin{array}{l}
\boxed{\text{Macroscale}} \\[2em]
\boxed{\text{Coupling}} \\[2em]
\boxed{\text{Microscale}}
\end{array}
$$

Problem: the simulation is very expensive when scale separation is large ($\mathrm{d}t \ll \mathrm{D}\,t$)

Goal: accelerate the simulation of coupling variable

Closure approximation reduces a diffusion in configuration space to moment equations

$$\mathrm{d}X_t = a(X_t)\,\mathrm{d}t + b(X_t)\,\mathrm{d}W_t \quad \xrightarrow{\text{Restriction}} \quad \mathbf{M}(t) = \mathbb{E}\big[\mathbf{R}(X_t)\big]$$

Using Itô formula find equation for $\mathbf{M}$:

more complicated
moments appear

$$\mathrm{d}\mathbf{M} = \mathcal{H}(\mathbf{M})\,\mathrm{d}t \;+\; \mathcal{G}(\tilde{\mathbf{M}})\,\mathrm{d}t$$

and express coupling as algebraic function of this set of moments

$$\tau = \mathcal{T}(\mathbf{M}, \tilde{\mathbf{M}})$$

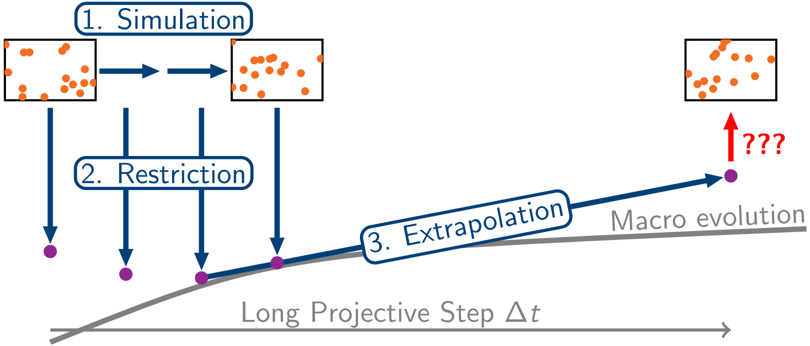
To avoid infinite hierarchies, approximate the more complicated moments in terms of the simpler ones.

Problem: closure is model dependent; we "forget" about microscopic model

Overview

- On-the-fly numerical closure and matching operator
- Minimum relative entropy moment matching
- Convergence of acceleration scheme with relative entropy
- Numerical example with polymeric fluids

Use **Coarse Projective Integration** to obtain closure on demand and accelerate macroscopic evolution



1. simulate ensemble of particles for short macro time
2. evaluate the values of coarse variables (by averaging)
3. extrapolate macro states forward in time
4. how to initiate the new microscopic state?

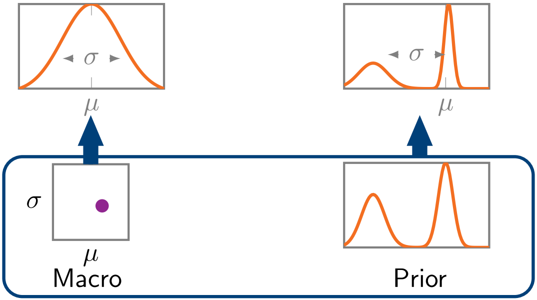
Matching – alternative for Lifting

Lifting

- Choses a distribution uniquely determined by current moments
- Introduces the modelling error

Matching

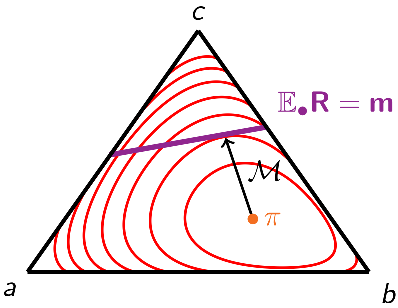
- Perturbes the prior distribution in a unique way to match current moments
- Follows the microscopic model



Minimise a "distance" to match

$$\underset{\text{extrapolated moments}}{\mathcal{M}(\mathbf{m}}, \underset{\text{prior distribution}}{\pi)} = \underset{\phi \in \mathrm{Prob}}{\operatorname{argmin}} \, \mathrm{dist}(\phi|\pi) \quad : \quad \underbrace{\mathbb{E}_\phi \mathbf{R} = \mathbf{m}}_{\text{finite set of linear constraints}}$$

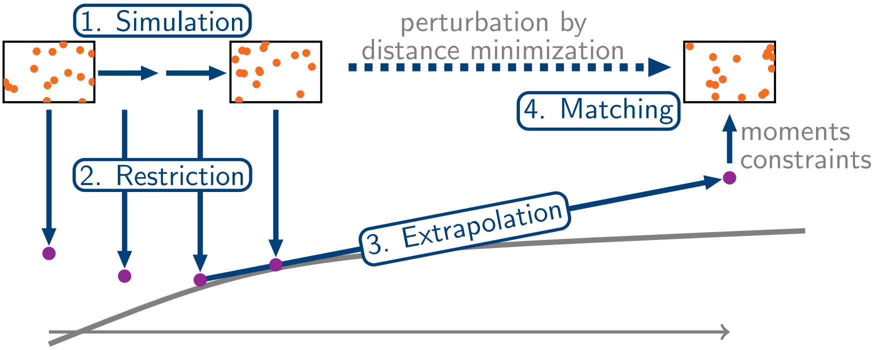
- dist introduces geometry on the space of all distributions
- matching is a *projection* in this geometry
- it may not be a metric (no symmetry, no triangle inequality)



Level sets of relative entropy distance from prior π on the three element alphabet $\{a, b, c\}$.

Overview

- On-the-fly numerical closure and matching operator



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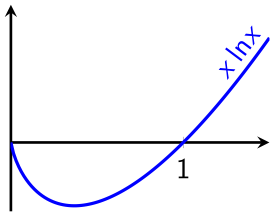
Principle of minimum relative entropy

For ϕ *absolutely continuous* w.r.t. π

$$\mathrm{dist}_{RE}(\phi|\pi) = \mathbb{E}_\phi\Big[\underbrace{\frac{\phi}{\pi}\ \ln\Big(\frac{\phi}{\pi}\Big)}_{\text{convex function bounded below}}\Big]$$



✓ $\mathcal{M}_{RE}(\mathbf{m}, \pi)$ is a convex minimisation problem.

- We have the uniqueness of solutions.
- The existence of solutions is related to the moment problem:
  When a given vector $\mathbf{m}$ corresponds to the average $\langle \mathbf{R} \rangle$ w.r.t. some probability distribution?

Computing the matching: dual formulation leads to a finite dimensional set of nonlinear equations

$$\boxed{\mathcal{M}_{RE}(\mathbf{m}, \pi) = \frac{1}{Z(\boldsymbol{\lambda}^*, \pi)} \exp\big(\boldsymbol{\lambda}^{*T} \mathbf{R}\big)\, \pi}$$

exponential family

where $\underset{\substack{\uparrow \\ \text{partition function}}}{Z}(\boldsymbol{\lambda}, \pi) = \mathbb{E}_\pi\big[\exp\big(\boldsymbol{\lambda}^T \mathbf{R}\big)\big]$ and $\boldsymbol{\lambda}^*$ satisfies

$$\nabla_{\boldsymbol{\lambda}} \ln Z(\boldsymbol{\lambda}^*, \pi) = \mathbf{m}.$$

dual problem

Computation with system of replicas $\{X_\pi^j\} \sim \pi \longleftarrow$ obtained from stochastic simulation

- MC estimates $Z(\boldsymbol{\lambda}, \pi) \approx \frac{1}{J} \sum_j \boldsymbol{\lambda}^T \mathbf{R}(X_j)$
- Newton-Raphson iteration to approximate $\boldsymbol{\lambda}^*$
- re-weighting $\big\{\big(w^j, X_\pi^j\big)\big\} \sim \mathcal{M}_{RE}(\mathbf{m}, \pi)$

$$w^j = \frac{1}{Z(\boldsymbol{\lambda}^*, \pi)} \exp\left(\boldsymbol{\lambda}^{*T} \mathbf{R}(X^j)\right)$$

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We are interested in approximating averages, thus we consider the weak error

$$\mathrm{Err}(L, \Delta t, \delta t) = \left| \mathbb{E} f(X_T) - \mathbb{E} f(Y_{N(\Delta t)}) \right|$$

Parameters

- $\Delta\tau$ $(\to 0)$ – microscopic time step
- Δt $(\to 0)$ – macroscopic time step
- $L = \dim \mathbf{R}$ $(\to +\infty)$ – number of moments for extrapolation

One-step increment operator

$$\mathcal{F}_{\Delta t}(Y) = \left\{ \mathsf{Match} \circ \mathsf{Extr}(\Delta t) \circ \mathsf{Res}(L) \circ \mathsf{Sim}(\Delta\tau) \right\} (\underset{\substack{\uparrow \\ \text{depends only on} \\ \text{the law of } Y}}{Y})$$

Iteration

$$Y_{N(\Delta t)} = \left(\mathcal{F}_{\Delta t} \right)^{N(\Delta t)} X_0$$

Local errors do not vanish as Δt goes to zero

$$\mathrm{LocErr}(\mathbf{R}, \Delta t) = \|\underset{\substack{\uparrow \\ \text{diffusion} \\ \text{semigroup}}}{\mathcal{S}_{\Delta t}}\pi - \mathcal{F}_{\Delta t}(\pi)\|_{TV} / \Delta t$$

From Pinsker's inequality:

$$\|\mathcal{S}_{\Delta t}\pi - \mathcal{F}_{\Delta t}(\pi)\|_{TV} \leq \sqrt{2\mathcal{I}\big(\mathcal{M}(\underset{\substack{\uparrow \\ \text{moments of} \\ \text{evolved prior}}}{\mathbf{m}_{\mathcal{S}_{\Delta t}\pi}}, \pi) \| \mathcal{S}_{\Delta t}\pi\big)} + \underbrace{\mathcal{O}_\pi\big((\Delta t)^2\big)}_{\substack{\text{error due to} \\ \text{extrapolation}}}$$

Relative entropy is a "square distance":

$$\mathcal{I}\big(\mathcal{M}(\mathbf{m}_{\mathcal{S}_{\Delta t}\pi}, \pi) \| \mathcal{S}_{\Delta t}\pi\big) = (\Delta t)^2 C\big(\underset{\substack{\uparrow \\ \text{semigroup} \\ \text{generator}}}{\mathbf{m}_{\mathcal{L}\pi}}, \mathbb{V}_\pi(\mathbf{R}), \mathbb{E}_\pi|\mathcal{L}\pi/\pi|^2\big) + \\ + \mathcal{O}_\pi\big((\Delta t)^3\big)$$

Propagation of local errors is controlled by norms of Lagrange multipliers

Lipschitz estimate for $\mathcal{F}_{\Delta t}$ with constant

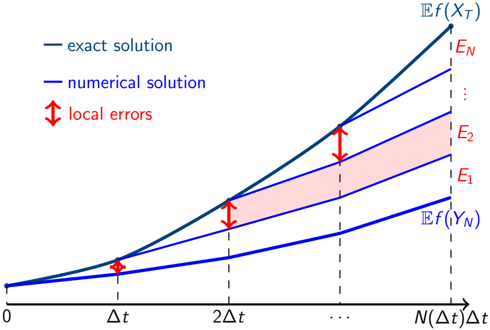
$$1 + L\Delta t$$

Uniform constant L

$$\Downarrow$$

Uniform boundedness of

$$\|(\mathcal{F}_{\Delta t})^{N(\Delta t)}(\cdot)\|_{TV}$$



Matching $\mathcal{M}(\mathbf{m}, \cdot)$ is TV-TV and weak*-weak* continuous.

We have bound: $L \leq F\big(\|\boldsymbol{\lambda}(\mathbf{m}, \pi)\|, \|\nabla_{\boldsymbol{\lambda}} A(\boldsymbol{\lambda}(\mathbf{m}, \pi), \pi)\|\big)$.

Uniform bounds follow from compactness (Prokhorov's theorem).

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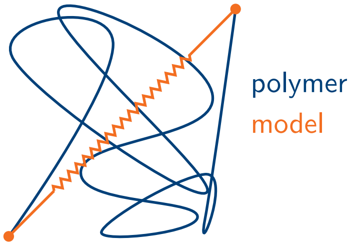
FENE dumbbells – the simplest non-linear kinetic model of dilute polymeric solutions

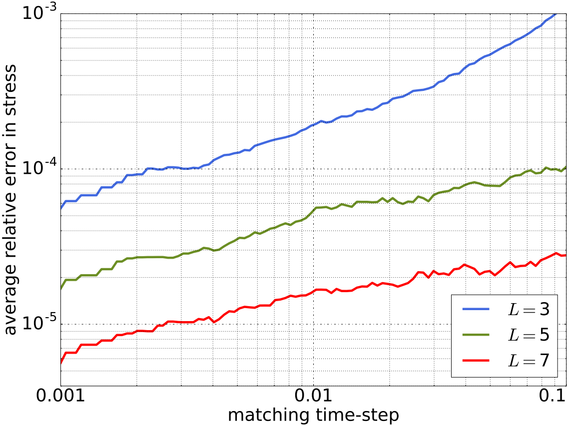
$$\mathrm{d}X = \Big[\underbrace{\kappa}_{\text{velocity gradient}} \cdot X - \frac{1}{2} \cdot \frac{X}{1 - |X|^2/\underbrace{b}_{\text{maximal polymer length}}}\Big]\,\mathrm{d}t + \frac{1}{\sqrt{2}}\,\mathrm{d}W, \quad |\underbrace{X}_{\text{connector vector}}|^2 < b$$

The most important observable is polymeric stress given by:

$$\tau_p = \mathbb{E}\Big[\frac{|X|^2}{1 - |X|^2/b}\Big].$$



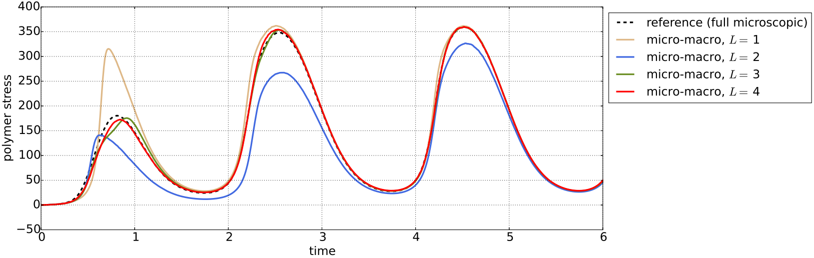
$\mathcal{M}_{RE}(\mathbf{m}_{\mathcal{S}_{\Delta t}\pi}, \pi)$ vs $\mathcal{S}_{\Delta t}\pi$ – error in stress



Relative entropy matching – long time evolution of stress

Time-dependent velocity field:

$$\kappa(t) = 2 \cdot (1.1 + \sin(\pi t)).$$



Extrapolation covers $\sim$ 70% – 75% of total time domain.

In a nutshell

Summary

- New micro-macro acceleration method to simulate expectations
- Distance minimisation to match the prior with extrapolated moments
- Proof of convergence and numerical results for nontrivial case

Joint work with

- Kristian Debrabant, IMADA – University of Southern Denmark
- Tony Lelièvre, CERMICS – Ecole des Ponts ParisTech
- Giovanni Samaey, Dept. of Computer Science – KU Leuven

Reference

- A micro-macro acceleration method for the Monte Carlo simulation of stochastic differential equations; arXiv:1511.06171