Reduced basis methods for the Fokker–Planck equation in polymer fluid dynamics

Dr. David J. Knezevic (dknez@mit.edu), Prof. Tony Patera

- We are interested in simulating dilute polymeric fluids: often modeled as a suspension of non-interacting microscopic dumbbells in a Newtonian solvent
- Dumbbells: Two masses joined by a spring with Finitely Extensible Non-linear Elastic (FENE) force law $\underset{\sim}{F}(\underset{\sim}{q}) = \underset{\sim}{q}/(1 - |\underset{\sim}{q}|^2/b)$, where $\underset{\sim}{q} \in D = B(0, \sqrt{b}) \subset \mathbb{R}^d$, $d = 2$ or 3
- Fluid governed by coupled Stokes–Fokker–Planck system:

$$\mathrm{Re}\,\frac{\partial \underset{\sim}{u}}{\partial t} + \nabla_x p - (1-\beta)\Delta_x \underset{\sim}{u} = \frac{\beta}{\mathrm{Wi}}\frac{b+d+2}{b}\,\nabla_x \cdot \underset{\approx}{\tau}, \tag{1}$$

$$\nabla_x \cdot \underset{\sim}{u} = 0, \tag{2}$$

$$\underset{\approx}{\tau}(\underset{\sim}{x}, t) = \int_D \underset{\sim}{F}(\underset{\sim}{q}) \otimes \underset{\sim}{q}\, \psi(\underset{\sim}{x}, \underset{\sim}{q}, t)\, \mathrm{d}\underset{\sim}{q}. \tag{3}$$

  for $(\underset{\sim}{x}, t) \in \Omega \times (0, T]$ where the FP equation is:

$$\frac{\partial \psi}{\partial t} + \underset{\sim}{u} \cdot \nabla_x \psi + \nabla_q \cdot \left((\nabla_x \underset{\sim}{u})\ \underset{\sim}{q}\, \psi - \frac{1}{2\mathrm{Wi}} \underset{\sim}{F}(\underset{\sim}{q}) \psi \right) = \frac{1}{2\mathrm{Wi}}\, \Delta_q \psi \tag{4}$$

  for $(\underset{\sim}{x}, \underset{\sim}{q}, t) \in \Omega \times D \times (0, T]$
- High-dimensional FP equation is most computationally challenging part: posed in 6 spatial dimensions + time
- Working in Lagrangian coordinates, high-dimensional FP equation reduces to many-query problem: solve parabolic problem (with unbounded convection coefficient $\underset{\sim}{F}$) at each grid point in Ω
- For a given flow (i.e. for fixed Re, Wi, b, β, T), the family of FP equations are parameterized by $\underset{\sim}{x} \in \Omega \mapsto \underset{\approx}{\kappa}(t^k)$, hence we train the RB space using a training set $\Xi_{\mathrm{train}} = \{\underset{\sim}{x}^i \in \Omega, i = 1, \ldots, n_{\mathrm{train}}\}$ using a POD-greedy scheme
- We have developed offline-online decomposition for computing ψ and $\underset{\approx}{\tau}$, with rigorous error bounds with respect to the 'truth' finite element solution for isolated FP equation, e.g. the $\mathrm{C}^0(0, T; \mathrm{L}^2(D))$ bound for ψ is:

$$\Delta_N^{\hat{\psi},l}(\underset{\approx}{\kappa}) = \sqrt{\frac{m(e_N^0, e_N^0) + 2\mathrm{Wi}\Delta t \sum_{k=1}^{l} \varepsilon_N^2(t^k; \underset{\approx}{\kappa}) \prod_{j=1}^{k-1}(1 + \frac{1}{2\mathrm{Wi}}\sigma(\underset{\approx}{\kappa}^j)\Delta t)}{\prod_{j=1}^{l}(1 + \frac{1}{2\mathrm{Wi}}\sigma(\underset{\approx}{\kappa}^j)\Delta t)}},$$

- Each POD-Greedy step involves selecting the parameter $\underset{\sim}{x}^i \mapsto \underset{\approx}{\kappa}^i(t^k)$ in Ξ_{train} which maximizes the error bound, then perform a POD in time on the corresponding 'truth solution'
- This has enabled numerical methods with real-time response for the isolated FP equation
- Future work: numerical method with rigorous rigorous error bounds for the nonlinearly coupled Stokes–FP system using RB method for the FP equation