Separated representation approximation of a high-dimensional Fokker–Planck PDE for dilute polymers

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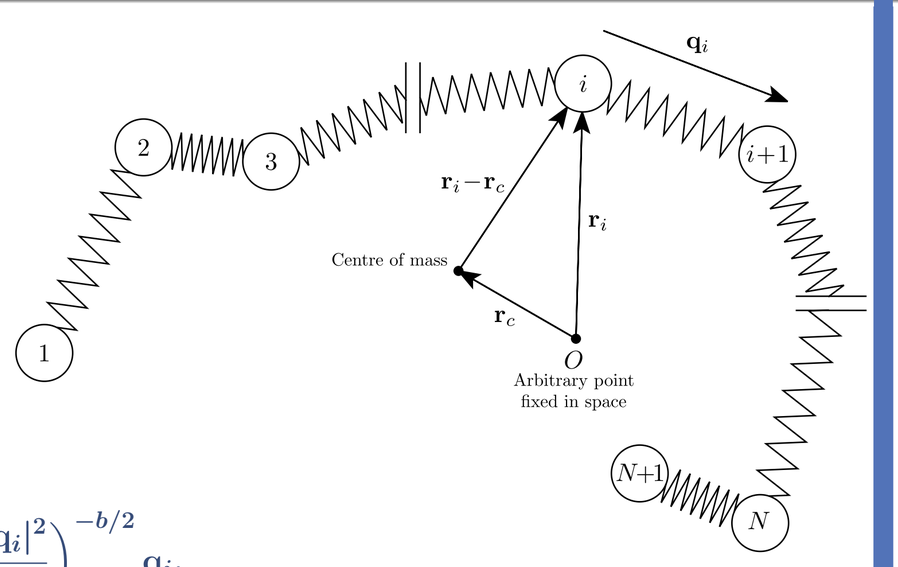
1. Polymer model

Our microscopic polymer model is the chain-like bead-spring *Rouse model*. Here, the state of a polymer macromolecule is described completely by its centre of mass and its N connector vectors $\mathbf{q}_i$. The force the i-th spring exerts on its neighbouring beads is, up to a change of sign,



$$U'(\tfrac{1}{2}|\mathbf{q}_i|^2)\mathbf{q}_i = \left(1 - \frac{|\mathbf{q}_i|^2}{b}\right)^{-b/2} \mathbf{q}_i,$$

where U is called the *FENE* potential. This force law is isotropic and nonlinear and, as it blows up when $|\mathbf{q}_i|^2 \to b_-$, each spring has a maximal extension $\sqrt{b}$; hence, the ensemble of connector vectors $\mathbf{q} = (\mathbf{q}_1, \cdots, \mathbf{q}_N)$ has to live in the Cartesian-product *configuration space* $D^N = D \times \cdots \times D$, where $D = B(0, \sqrt{b}) \subset \mathbb{R}^d$, $d = 2$ or 3.

2. Fokker–Planck equation

The *Fokker–Planck* equation we concern ourselves with appears when approximating the more complicated full Fokker–Planck equation which, in turn, arises from the polymer model described through statistical mechanics. It is defined on the configuration space $D^N \ni (\mathbf{q}_1, \ldots, \mathbf{q}_N) = \mathbf{q}$ and has the form

$$-\frac{1}{4\mathbf{Wi}} \sum_{i=1}^{N} \sum_{j=1}^{N} \nabla_{\mathbf{q}_i} \cdot \left[A_{ij} \left(U'(\tfrac{1}{2}|\mathbf{q}_j|^2)\mathbf{q}_j \psi + \nabla_{\mathbf{q}_j} \psi \right) \right] + \frac{1}{\Delta t} \psi = \hat{f},$$

where $\psi = \psi(\mathbf{q})$ is the dependent variable, $\mathbf{Wi}$ is a positive parameter and $(A_{ij})_{i,j=1}^N$ a symmetric and positive definite matrix.
On introducing the (full) *Maxwellian* $\mathbf{M}\colon D^N \to \mathbb{R}$ and the *partial Maxwellian* $M\colon D \to \mathbb{R}$ via

$$\mathbf{M}(\mathbf{q}) := \exp\left[-\sum_{i=1}^{N} U(\tfrac{1}{2}|\mathbf{q}_i|^2) \right] = \prod_{i=1}^{N} M(\mathbf{q}_i)$$

we can write

$$\mathbf{M} \nabla_{\mathbf{q}_j} \left(\frac{\psi}{\mathbf{M}} \right) = U'(\tfrac{1}{2}|\mathbf{q}_j|^2)\mathbf{q}_j \psi + \nabla_{\mathbf{q}_j} \psi.$$

Using this identity and testing the Fokker–Planck equation with $\varphi/\mathbf{M}$ we obtain the variational problem

$$\text{(P)} \quad a(\psi, \varphi) = \sum_{i,j=1}^{N} \frac{A_{ij}}{4\mathbf{Wi}} \int_{D^N} \nabla_{\mathbf{q}_j} \left(\frac{\psi}{\mathbf{M}} \right) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\varphi}{\mathbf{M}} \right) \mathbf{M} \, \mathrm{d}\mathbf{q} + \frac{1}{\Delta t} \int_{D^N} \frac{\psi \varphi}{\mathbf{M}} \, \mathrm{d}\mathbf{q} = f(\varphi)$$

and find that it is naturally associated with the functional space $\mathbf{H}(D^N; \mathbf{M})$. This is an elliptic equation with degenerate coefficients defined on a $d\,N$-dimensional space.

The full Fokker–Planck is defined on time, physical space and configuration space. It has the form

$$0 = \underbrace{\frac{\partial \psi}{\partial t}}_{\text{discretised}} + \underbrace{\nabla_{\mathbf{x}} \cdot (\mathbf{u}\psi) - \frac{(N+1)^{-1}}{4\mathbf{Wi}} \varepsilon \Delta_{\mathbf{x}} \psi}_{\text{split away}}$$
$$+ \sum_{i=1}^{N} \nabla_{\mathbf{q}_i} \cdot \left[(\underbrace{\nabla_{\mathbf{x}} \mathbf{u}) \mathbf{q}_i \psi}_{\text{treated explicitly}} - \sum_{j=1}^{N} \frac{A_{ij}}{4\mathbf{Wi}} \left(U'(\tfrac{1}{2}|\mathbf{q}_j|^2)\mathbf{q}_j \psi + \nabla_{\mathbf{q}_j} \psi \right) \right]$$

where ε is a positive parameter and the text under each brace explains how this equation reduces to our time- and physical space-independent Fokker Planck equation.
When coupled with the Navier–Stokes and Kramers equations, the full Fokker–Planck equation gives a multiscale description of the flow of a dilute polymeric solution in an incompressible solvent. In particular, $\psi = \psi(t, \mathbf{x}, \mathbf{q})$ is, at each time and at each point of physical space, a probability density function for the configuration of a chain and $\mathbf{u} = \mathbf{u}(\mathbf{x})$ is the macroscopic velocity of the solvent.

3. Separated representation

The symmetry of the problem (P) allows for the characterisation

$$\psi = \arg\min \left\{ \frac{1}{2} a(\varphi, \varphi) - f(\varphi) \colon \varphi \in \mathbf{H}(D^N; \mathbf{M}) \right\}$$

which can be approximated using a standard Galerkin method; i.e., replacing $\mathbf{H}(D^N; \mathbf{M})$ by some finite dimensional subspace of itself. The problem with this is that the high dimensionality of D^N makes standard discretisations prohibitively expensive.
The *separated representation strategy* is based on replacing $\mathbf{H}(D^N; \mathbf{M})$ by its subset

$$\bigotimes_{i=1}^{N} \mathbf{H}(D; M) := \left\{ \bigotimes_{i=1}^{N} r^{(i)} \colon r^{(i)} \in \mathbf{H}(D; M) \right\}$$

where we denote by $\bigotimes_{i=1}^N r^{(i)}$ that function defined on D^N which maps $\mathbf{q}$ to $\prod_{i=1}^N r^{(i)}(\mathbf{q}_i)$—thus, for example, $\mathbf{M} = \bigotimes_{i=1}^N M$.
It is important to distinguish between the set $\bigotimes_{i=1}^N \mathbf{H}(D; M)$ from the $\mathbf{H}(D^N; \mathbf{M})$-closure of its span as the notation we use for the former is often used for the latter.

The function space associated to (P) is

$$\mathbf{H}(D^N; \mathbf{M}) = \{ \varphi \in \mathbf{L}^2_{1/\mathbf{M}}(D^N) \colon \nabla_{\mathbf{q}_i}(\varphi/\mathbf{M}) \in [\mathbf{L}^2_{\mathbf{M}}(D^N)]^d, 1 \le i \le N \}.$$

The space $\mathbf{H}(D^N; \mathbf{M})$, although exotic-looking, is isometrically isomorphic to the *weighted Sobolev space* $\mathbf{H}^1_{\mathbf{M}}(D^N)$ via the relation $\varphi \in \mathbf{H}^1_{\mathbf{M}}(D^N) \to \mathbf{M}\varphi \in \mathbf{H}(D^N; \mathbf{M})$. It is, then, a separable Hilbert space. We also need the space

$$\mathbf{H}(D; M) = \{ \varphi \in \mathbf{L}^2_{1/M}(D) \colon \nabla(\varphi/M) \in [\mathbf{L}^2_M(D)]^d \}$$

which is simply $\mathbf{H}(D^N; \mathbf{M})$ in the special case $N = 1$ and is thus isometrically isomorphic to the weighted Sobolev space $\mathbf{H}^1_M(D)$.
Basic results concerning $\mathbf{H}(D^N; \mathbf{M})$—namely, the compact embedding of $\mathbf{H}(D^N; \mathbf{M})$ into $\mathbf{L}^2_{1/\mathbf{M}}(D^N)$ and the density of $\mathbf{C}^\infty_0(D^N)$ in $\mathbf{H}(D^N; \mathbf{M})$—are attainable by exploiting the Cartesian-product structure of D^N and the tensor-product structure of $\mathbf{M}$. In general D^N is merely a Lipschitz domain which precludes the use of standard techniques.

4. A greedy algorithm

We can't expect

$$\psi_1 = \arg\min \left\{ \frac{1}{2} a(\varphi, \varphi) - f(\varphi) \colon \varphi \in \bigotimes_{i=1}^{N} \mathbf{H}(D; M) \right\}$$

to be a good approximation to ψ in general. Thus, we define

$$\hat{\psi}_2 = \arg\min \left\{ \frac{1}{2} a(\varphi, \varphi) - f(\varphi) - a(\psi_1, \varphi) \colon \varphi \in \bigotimes_{i=1}^{N} \mathbf{H}(D; M) \right\}$$

whence $\psi_1 + \hat{\psi}_2$ approximates ψ better. Then we define ψ_2 as the Galerkin projection of the problem (P) on the finite-dimensional space $\mathbf{span}\{\psi_1, \hat{\psi}_2\}$. We encode the iteration of this procedure in the

Orthogonal Greedy Algorithm

0. Let $f_0 := f \in \mathbf{H}(D^N; \mathbf{M})'$.
1. For $n \ge 1$ do:
   - 1.1 Let $\hat{\psi}_n := \arg\min \left\{ \frac{1}{2} a(\varphi, \varphi) - f_{n-1}(\varphi) \colon \varphi \in \bigotimes_{i=1}^{N} \mathbf{H}(D; M) \right\}$.
   - 1.2 Let $\psi_n := \arg\min \left\{ \frac{1}{2} a(\varphi, \varphi) - f(\varphi) \colon \varphi \in \mathbf{span}\{\hat{\psi}_1, \ldots, \hat{\psi}_n\} \right\}$.
   - 1.3 Let $f_n := f - a(\psi_n, \cdot)$.
   - 1.4 If $\|f_n\|_{\mathbf{H}(D^N;\mathbf{M})'} \ge$ TOL, then proceed to iteration $n+1$; else, stop.

The algorithm generates approximations to ψ in the SVD-resembling form

$$\psi \approx \psi_n = \sum_{k=1}^{n} \alpha_k^{(n)} \hat{\psi}_k = \sum_{k=1}^{n} \alpha_k^{(n)} \bigotimes_{i=1}^{N} r_k^{(i)}.$$

The attractiveness of this algorithm is that the *enrichment step* (step 1.1) lends itself naturally to an alternating direction procedure where the factors $r_n^{(i)}$ that make up $\hat{\psi}_n$ are optimised one at a time, assuming the others constant. If the right-hand side functional f has tensor-product structure (which is often the case) the tensor-product structure of the Maxwellian ensures that the resulting subiterations are equivalent to a d-dimensional PDE.

5. Theorem

1. *The algorithm is well-defined.* This means, essentially, that there exists a minimiser in the enrichment step (step 1.1) of the algorithm.
2. *The method converges.* Given that at each iterate we get true solutions to both minimisation problems, this method is guaranteed to converge.
3. *If the solution ψ of* (P) *lives in*

$$\mathbf{H}^{d+1,\mathrm{mix}}(D^N; \mathbf{M}) = \Big\{ \varphi \in \mathbf{L}^2_{1/\mathbf{M}}(D^N) \colon \partial_\alpha(\varphi/\mathbf{M}) \in \mathbf{L}^2_{\mathbf{M}}(D^N), \ \max_{1 \le i \le N} |\alpha_i| \le d+1 \Big\}$$

and if the (ordered) eigenvalues $\boldsymbol{\lambda}_m$ of the problem (EV) *distribute asymptotically like $m^{2/d}$ there holds*

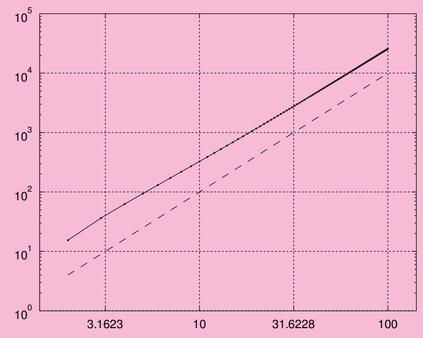
$$\|\psi - \psi_n\|_{\mathbf{H}(D;M)} \le C n^{-1/2}.$$

Here, the multi-index $\boldsymbol{\alpha}$ is assumed to be the concatenation of N d-dimensional multi-indices $\boldsymbol{\alpha}_i$.

The asymptotic distribution of the eigenvalues of the problem

$$\text{(EV)} \qquad \langle e, \varphi \rangle_{\mathbf{H}(D^N;\mathbf{M})} = \lambda \langle e, \varphi \rangle_{\mathbf{L}^2_{1/\mathbf{M}}(D^N)}$$

over $\mathbf{H}(D^N; \mathbf{M})$ is important because, if shown to be proportional to $m^{2/d}$, a characterisation of the space of fast convergence of the algorithm in terms of mixed regularity the solution ψ of (P) will exist. The plot to the right shows (a linear rescaling) of the computed first 99 eigenvalues of (EV) when $b = 3.1416$ (continuous line with dots) and the function m^2 in logarithmic scale. This suggests that in the (non-physical) case $d = 1$, the asymptotic distribution of eigenvalues is proportional to $m^{2/d}$.



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