Multilevel Monte Carlo for the simulation of dilute polymers

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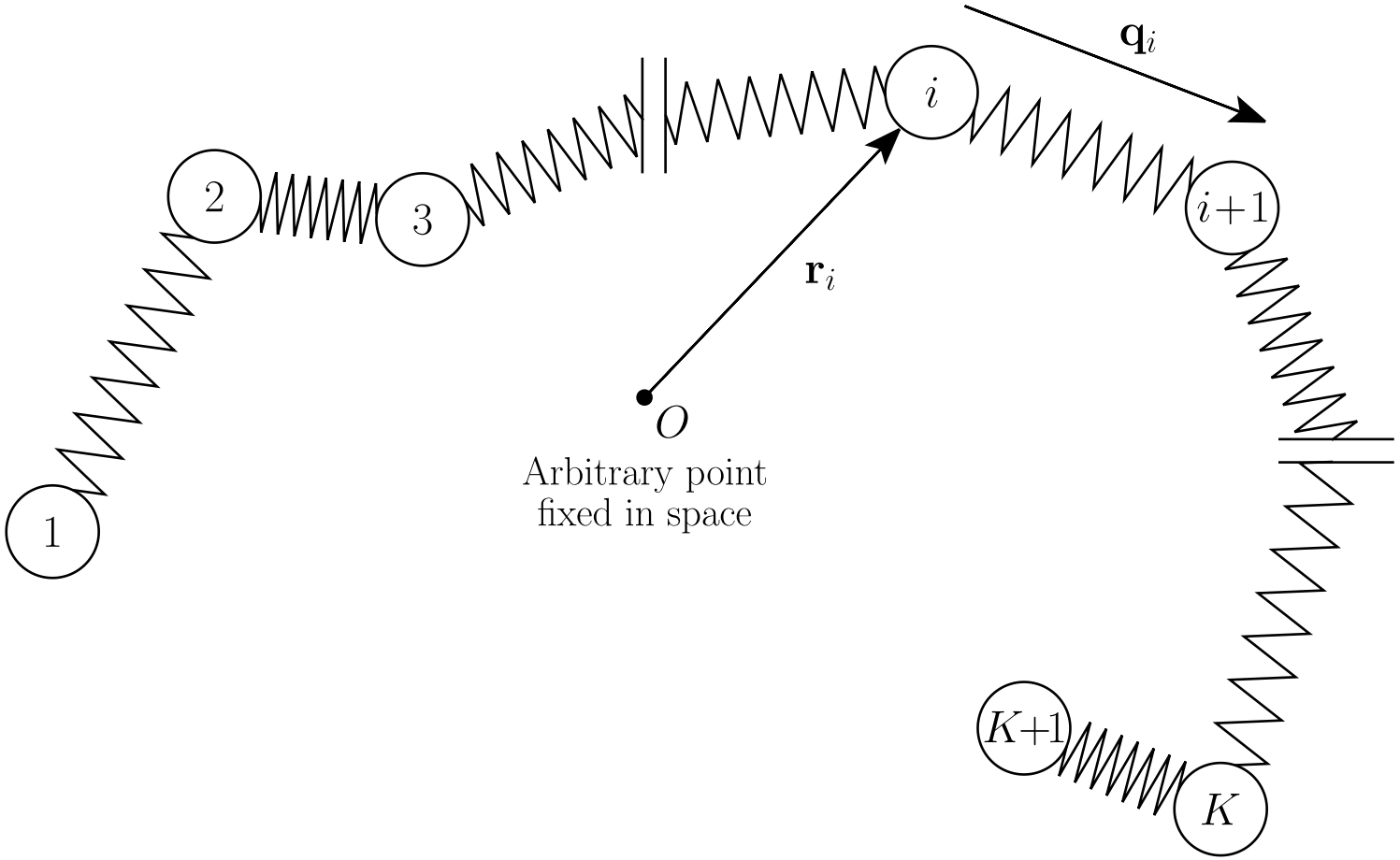
Outline

- mathematical modelling
- properties of the SDE
- numerical approximation
- multilevel Monte Carlo method
- adaptive time-stepping in MLMC
- MLMC for equilibrium distribution
- preliminary results
- conclusions

Modelling



- long-chain molecules in a fluid
- modelled as ball-and-spring systems, subject to random forcing
- K bonds, $K+1$ "balls", separation q_i will be key variable

Modelling

- FENE (finitely extensible nonlinear elastic) model limits extension of molecular bonds
- motion of "balls" given by force balance:

$$\text{elastic force} + \text{random force} + \text{viscous drag} = 0$$

$$-\nabla V \quad + \quad R \quad - \quad k\,(\dot{r}_i - v(r_i)) \quad = \quad 0$$

where V is the elastic potential, and v is the velocity of the fluid

- shifting to a moving frame of reference, a local Taylor series expansion gives

$$v(x) \approx \kappa\, x$$

where κ is the local rate-of-strain tensor $\partial v/\partial x$

Modelling

This modelling leads to the following SDE for i^{th} "ball":

$$\mathrm{d}r_i = \left(\kappa\, r_i - \nabla_{r_i} V(r)\right)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_i$$

where $\mathrm{d}W_i$ is the Brownian forcing, assumed to be independent of the forcing of the others, and

$$V(r) = \sum_{i=1}^{K} U_i(\|q_i\|^2/2)$$

with U_i being the elastic potential for the i^{th} bond.

Hence,

$$\mathrm{d}r_i = \left(\kappa\, r_i - \left(U_{i-1}'\left(\|q_{i-1}\|^2/2\right)\, q_{i-1} - U_i'\left(\|q_i\|^2/2\right)\, q_i\right)\right)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_i$$

if we define $q_0 \equiv q_{K+1} \equiv 0$ to account for non-existent bonds on either end.

Modelling

Hence, the system of coupled SDEs for the bond vectors is

$$\mathrm{d}q_i = \left(\kappa\, q_i + U'_{i+1} q_{i+1} - 2\, U'_i q_i + U'_{i-1} q_{i-1}\right)\,\mathrm{d}t + \sqrt{2}\,\left(\mathrm{d}W_{i+1} - \mathrm{d}W_i\right)$$

which can be written collectively as

$$\mathrm{d}q = (K\, q - D\,\nabla V)\,\mathrm{d}t + \sqrt{2}\; L\;\mathrm{d}W$$

where $V(q) \equiv \sum_i U_i(\|q_i\|^2/2)$, and K, L and D are of the form

$$K = \begin{pmatrix} \kappa & & \\ & \kappa & \\ & & \kappa \end{pmatrix}, \qquad L = \begin{pmatrix} -I & I & \\ & -I & I \\ & & -I & I \end{pmatrix},$$

$$D = \begin{pmatrix} 2I & -I & \\ -I & 2I & -I \\ & -I & 2I \end{pmatrix} = L\,L^T.$$

Invariant distribution

The Fokker-Planck PDE for the probability density function $p(q,t)$ is

$$\frac{\partial p}{\partial t} = \nabla \cdot \Big((D\,\nabla V - K\,q)\,p + D\,\nabla p \Big),$$

so when $K=0$ the invariant (or equilibrium) distribution is

$$p_\infty(q) = C\,\exp(-V(q)).$$

In the particular case of the FENE model, we have

$$U_i(s) = -\beta\,\log(1-2s),$$

and therefore the invariant distribution for $K=0$ is

$$p_\infty(q) = C\,\prod_i (1-\|q_i\|^2)^\beta.$$

Contraction property

If κ is not too large, can prove the following result:

If two paths $q^{(1)}$, $q^{(2)}$ have

- different initial conditions
- same driving Brownian motion W_t

then

$$\left\| q^{(1)}(t) - q^{(2)}(t) \right\| \quad \longrightarrow \quad 0$$

exponentially as $t \to 0$.

Numerical approximation

The nonlinear SDE is approximated as

$$q_{n+1} = q_n + (K\, q_n - D\, \nabla V(q_n))\, h_n + \sqrt{2}\; L\; \Delta W_n$$

using an adaptive timestep h_n, and independent Brownian increments ΔW_n which can be expressed as

$$\Delta W_n = \sqrt{h_n}\; Z_n$$

where Z_n are vectors of independent $N(0,1)$ random variables.

Adaptive timestep

With the FENE model, no bond length can exceed 1 – numerical approximation should share this property.

Try to ensure this through the restrictions:

$$\begin{aligned} h_n \, U_i'(\|q_{i,n}\|^2/2) \, \|q_{i,n}\| &\leq 1 - \|q_{i,n}\| \\ 5\sqrt{2\,h_n} &\leq 1 - \|q_{i,n}\| \end{aligned}$$

where $q_{i,n}$ is the i^{th} bond vector at timestep n.

They can be combined to give

$$h_n = \frac{\min_i (1 - \|q_{i,n}\|)^2}{\max(2\beta, 50)}$$

This sets an upper bound on the timestep – smaller values need to be chosen for accuracy.

Clamping

Even so, it is possible for the discrete approximation to cross the boundary $\|q_i\| = 1$.

This is avoided through "clamping" by setting

$$q_{i,n+1}^{clamped} := \frac{1-\delta}{\|q_{i,n+1}\|}\, q_{i,n+1}$$

if $\|q_{i,n+1}\| > 1-\delta$, where $\delta \ll 1$ (typically 10^{-5}).

We believe that the additional weak error due to clamping is negligible.

Objective

Our objective is to numerically estimate $\lim_{T\to\infty} \mathbb{E}\left[P(T)\right]$ where

$$P(T) \;\equiv\; U'(\|q\|^2/2)\, q\, q^T \Big|_{t=T}$$

This corresponds to the stress exerted by the molecule on the fluid. In the future this will be applied to the fluid in a coupled simulation.

We start with a computation for a fixed, large T, then address the challenge of letting $T \to \infty$.

Monte Carlo simulation

The standard Monte Carlo approach would be to perform N independent path simulations and use the estimate

$$N^{-1} \sum_{n=1}^{N} P^{(n)}$$

However, to get good accuracy we would need to use very small timesteps and lots of paths, so the cost would be high.

Multilevel Monte Carlo simulation

Instead, MLMC uses a sequence of levels with differing accuracies / costs, and relies on the telescoping summation

$$\mathbb{E}[P_L] = \mathbb{E}[P_0] + \sum_{\ell=1}^{L} \mathbb{E}[P_\ell - P_{\ell-1}]$$

so we can use the estimator

$$N_0^{-1} \sum_{n=1}^{N_0} P_0^{(n)} \;+\; \sum_{\ell=1}^{L} \left\{ N_\ell^{-1} \sum_{n=1}^{N_\ell} \left(P_\ell^{(n)} - P_{\ell-1}^{(n)} \right) \right\}$$

with independent estimation for each level

Multilevel Monte Carlo simulation

Given a desired RMS accuracy ε, MLMC algorithm/theory tells us

- how many levels to use, to ensure that weak error due to discretisation is less than $\varepsilon/\sqrt{2}$
- how many samples to use on each level, to ensure that overall the statistical error is less than $\varepsilon/\sqrt{2}$

In standard SDE applications, use geometric sequence of levels with

$$h_\ell = 2^{-\ell}\, h_0$$

and for Milstein approximation (as used here) usually achieve ε accuracy at $O(\varepsilon^{-2})$ total cost, instead of $O(\varepsilon^{-3})$ with standard Monte Carlo method

Multilevel Monte Carlo simulation

Key point is using the same Brownian motion for each sample

$$P_\ell^{(n)} - P_{\ell-1}^{(n)}$$

in

$$N_\ell^{-1} \sum_{n=1}^{N_\ell} \left(P_\ell^{(n)} - P_{\ell-1}^{(n)} \right)$$

Strong convergence of the numerical approximation ensures that $P_\ell^{(n)} - P_{\ell-1}^{(n)}$ is small, so has a small variance, $O(h_\ell^2)$, and hence few samples are needed on finest levels.

With uniform timesteps, Brownian increments for coarse path are obtained by summing increments for fine path.

Potential problem: how does it work with adaptive time-stepping?

Multilevel Monte Carlo simulation

Actually, surprisingly easy, based on prior work with Chris Lester, Ruth Baker & Kit Yates (2014) for continuous-time Markov chains.

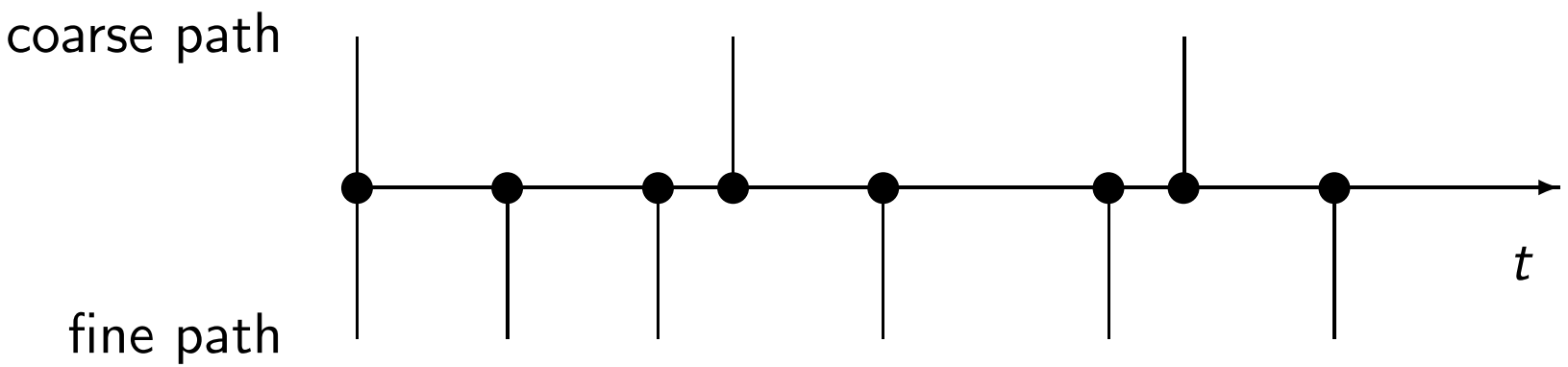
On level ℓ use

$$h_{\ell,n} = 2^{-\ell}\ \frac{\min_i(1-\|q_{i,n}\|)^2}{\max(2\beta, 50)}$$

Coarse and fine paths each compute their own adaptive timesteps independently – this ensures the telescoping sum works correctly

Multilevel Monte Carlo simulation

As time proceeds, Brownian increments are generated as needed at discretisation times which are a union of coarse and fine path times:



The fact that the timesteps are not nested is not a problem – strong convergence still ensures a strong coupling between the coarse and fine paths.

Multilevel Monte Carlo simulation

Final challenge: how to obtain expectation as $T \to \infty$?

Key idea here comes from Chang-han Rhee and Peter Glynn (2014) who consider contracting Markov chains:

$$X_0 = x, \quad X_{n+1} = \phi_n(X_n), \quad n \geq 0$$

where $\{\phi_n\}$ is a sequence of iid random functions such that

$$\sup_{x \neq y} \mathbb{E}\left[\left(\frac{d(\phi_n(x), \phi_n(y))}{d(x,y)}\right)^{2\gamma}\right] < 1$$

for some distance metric d, and some $\gamma \in (0,1)$.

Multilevel Monte Carlo simulation

They are interested in

$$\lim_{M\to\infty} \left\{ \mathbb{E}[f(X_M)] \mid X_0 = x \right\}$$

which can be re-expressed as

$$\lim_{M\to\infty} \left\{ \mathbb{E}[f(X_0)] \mid X_{-M} = x \right\}$$

and they use multilevel with $M_\ell \to \infty$ as $\ell \to \infty$ and same random ϕ_n for *coarse* and *fine* paths for $-M_{\ell-1} \le n < 0$.

This works because contraction property leads to effect of difference in values at $-M_{\ell-1}$ decaying exponentially, so

$$\left\| X_0^f - X_0^c \right\| \;\sim\; \exp(-c\, M_{\ell-1})$$

Multilevel Monte Carlo simulation

Back to our polymer application, instead of estimating

$$\lim_{T\to\infty} \Big\{ \mathbb{E}[P(q(T))] \mid q(0) = q_0 \Big\}$$

we use the same idea and estimate

$$\lim_{T\to\infty} \Big\{ \mathbb{E}[P(q(0))] \mid q(-T) = q_0 \Big\}$$

and use multilevel with $h_\ell \to 0$, $T_\ell \to \infty$ as $\ell \to \infty$ and the same Brownian motion $W(t)$ for coarse and fine paths for $-T_{\ell-1} < t < 0$.

This again works because of the contraction property which leads to effect of difference in q values at time $-T_{\ell-1}$ decaying exponentially, so

$$\Big\| q^f(0) - q^c(0) \Big\| \;=\; O(h_\ell) \;+\; O(\exp(-c\, T_{\ell-1}))$$

Implementation

Two versions of the MLMC algorithm have been implemented:

- MATLAB for development purposes
- CUDA C for execution on NVIDIA GPUs – offers 100× speedup over MATLAB implementation

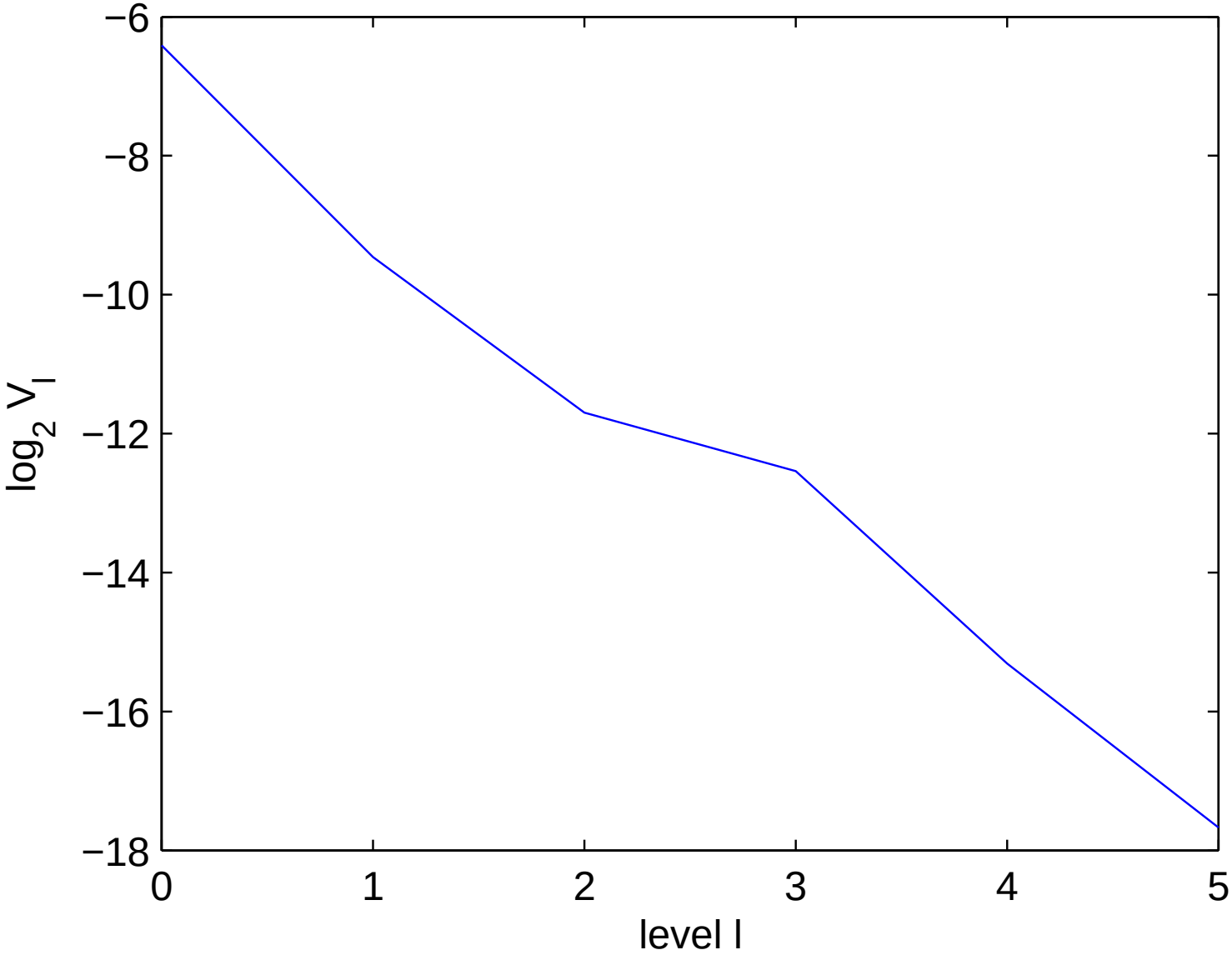
The latter handles polymers with up to 32 bonds

When there is a single bond, the code produces the correct value for

$$\lim_{T\to\infty} \mathbb{E}\left[q^{(0)\,T}\, q^{(0)} \,\Big|_{t=T}\right]$$

in comparison to the analytic value which can be deduced from the invariant distribution.

Preliminary results



Conclusions

- other research by Süli and Ye has used Fokker-Planck approach when there is just 1 bond, but SDE approach is only viable method when the number of bonds is large
- multilevel Monte Carlo greatly reduces the computational cost
- adaptive timestepping is necessary, and not difficult
- new idea due to Rhee and Glynn is crucial for estimating quantities associated with invariant distribution
- more validation required
- current research is investigating coupling to fluid calculation, and inclusion of history effects

References

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`http://people.maths.ox.ac.uk/gilesm/mlmc.html`

`http://people.maths.ox.ac.uk/gilesm/mlmc_community.html`