Application of multilevel Monte Carlo to 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:

\[-\nabla V + R - k \left( \dot{r}_i - v(r_i) \right) = 0\]

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

\[v(x) \approx \kappa \cdot x\]

where \( \kappa \) is the local rate-of-strain tensor \( \partial v / \partial x \)
Modelling

This modelling leads to the following SDE for $i^{th}$ “ball”:

$$\text{d}r_i = (\kappa r_i - \nabla r_i V(r)) \, \text{d}t + \sqrt{2} \, \text{d}W_i$$

where $\text{d}W_i$ 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,

$$\text{d}r_i = \left(\kappa r_i - \left(U'_{i-1} (\|q_{i-1}\|^2/2) \, q_{i-1} - U'_i (\|q_i\|^2/2) \, q_i\right)\right) \, \text{d}t + \sqrt{2} \, \text{d}W_i$$

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

\[ dq_i = (\kappa q_i + U'_{i+1}q_{i+1} - 2 U'_iq_i + U'_{i-1}q_{i-1}) \, dt + \sqrt{2} (dW_{i+1} - dW_i) \]

which can be written collectively as

\[ dq = (\kappa q - D \nabla V) \, dt + \sqrt{2} \, L \, dW \]

where

\[ V(q) \equiv \sum_i U_i(\|q_i\|^2/2), \]

and \( L \) and \( D \) are of the form

\[
L = \begin{pmatrix}
-I & I & & \\
-I & -I & I & \\
& -I & -I & I
\end{pmatrix}, \quad
D = \begin{pmatrix}
2I & -I & \\
-I & 2I & -I & \\
& -I & 2I
\end{pmatrix} = LL^T.
\]
Invariant distribution

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

$$\frac{\partial p}{\partial t} = \nabla \cdot \left( (D \nabla V - \kappa q) p + D \nabla p \right),$$

so when $\kappa = 0$ 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 $\kappa = 0$ is

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

The nonlinear system of SDEs is

\[ dq = (\kappa q - D \nabla V) \, dt + \sqrt{2} L \, dW \]

If \( \kappa \) is small, then we can replace it by \( \varepsilon \kappa \), with \( \kappa = O(1) \) and \( \varepsilon \ll 1 \), and perform an asymptotic expansion

\[ q = q^{(0)} + \varepsilon q^{(1)} + O(\varepsilon^2), \]

and match up corresponding powers of \( \varepsilon \).

The \( O(1) \) terms give the nonlinear equation

\[ dq^{(0)} = -D \nabla V(q^{(0)}) \, dt + \sqrt{2} L \, dW. \]
Linear perturbation analysis

The $O(\varepsilon)$ terms give the linear perturbation equation

$$
\text{d}q^{(1)} = \left( \kappa q^{(0)} - D A(q^{(0)}) q^{(1)} \right) \text{d}t,
$$

where $A$ is a block-diagonal matrix with the $i^{th}$ block being

$$
A_i(q^{(0)}_i) = U'_i(\|q^{(0)}_i\|^2/2) \ I + U''_i(\|q^{(0)}_i\|^2/2) \ q^{(0)}_i(q^{(0)}_i)^T.
$$

Note that $A_i$ is symmetric, and if we assume that $U'_i \geq 0$ and $U''_i \geq 0$ then for any vector $v \neq 0$ we have

$$
v^T A_i v = U'_i v^T v + U''_i \left( (q^{(0)}_i)^T v \right)^2 > 0,
$$

so the $A_i$, and hence also $A$, are positive-definite.
Linear perturbation analysis

When $\kappa = 0$, the linearised equation for the perturbation $q^{(1)}$ is

$$d q^{(1)} = - D A(q^{(0)}) q^{(1)} \, dt.$$

If we define the energy as $E = \frac{1}{2} (q^{(1)})^T D^{-1} q^{(1)}$, then

$$d E = (q^{(1)})^T D^{-1} \, dq^{(1)} = - (q^{(1)})^T A(q^{(0)}) \, q^{(1)} \, dt$$

and since $A$ is symmetric positive-definite, it follows that the energy decreases over time, and so $q^{(1)} \to 0$ as $t \to \infty$.

Similarly, can prove that if $q_a^{(0)}$, $q_b^{(0)}$ are driven by the same Brownian path from different initial data, then $q_a^{(0)} - q_b^{(0)} \to 0$ as $t \to \infty$. 
Numerical approximation

The nonlinear SDE is approximated as

\[ q_{n+1} = q_n + (\kappa q_n - D \nabla V(q_n)) h_n + \sqrt{2} L \Delta W_n \]

using an adaptive timestep \( h_n \), and independent Brownian increments \( \Delta W_n \) 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.

For the asymptotic analysis, the approximations are:

\[ q_{n+1}^{(0)} = q_n^{(0)} - D \nabla V(q_n^{(0)}) h_n + \sqrt{2} L \Delta W_n \]
\[ q_{n+1}^{(1)} = q_n^{(1)} + \left( \kappa q_n^{(0)} - D A(q_n^{(0)}) q_n^{(1)} \right) h_n \]
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:

\[
    h_n U'_i(\|q_{i,n}\|^2/2) \|q_{i,n}\| \leq 1 - \|q_{i,n}\|
\]

\[
    5\sqrt{2} h_n \leq 1 - \|q_{i,n}\|
\]

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 \( \lim_{T \to \infty} \mathbb{E}[P(T)] \) where, in the nonlinear analysis,

\[
P(T) \equiv U'(\|q\|^2 / 2) q q^T \bigg|_{t=T}
\]

or, using the linearisation approach,

\[
P(T) \equiv U'(\|q(0)\|^2 / 2) \left( q^{(0)} (q^{(1)})^T + q^{(1)} (q^{(0)})^T \right) \\
+ ((q^{(0)})^T q^{(1)}) U''(\|q^{(0)}\|^2 / 2) q^{(0)} (q^{(0)})^T \bigg|_{t=T}
\]

We’ll start by doing it for a fixed, large \( T \), then address the challenge of letting \( T \to \infty \).
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

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

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
Given a desired RMS accuracy $\varepsilon$, 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

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

and for Milstein approximation (as used here) usually achieve $\varepsilon$ 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

\[ P^{(n)}_{\ell} - P^{(n)}_{\ell-1} \]

in

\[ N_{\ell}^{-1} \sum_{n=1}^{N_{\ell}} \left( P^{(n)}_{\ell} - P^{(n)}_{\ell-1} \right) \]

Strong convergence of the numerical approximation ensures that \( P^{(n)}_{\ell} - P^{(n)}_{\ell-1} \) is small, so has a small variance, \( O(h^2_{\ell}) \), 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 $\ell$ use

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

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

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

which can be re-expressed as

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

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

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

$$\left\| X_0^f - X_0^c \right\| \sim \exp(-cM_{\ell-1})$$
Multilevel Monte Carlo simulation

Back to our polymer application, instead of estimating

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

we use the same idea and estimate

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

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

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

$$\lim_{T \to \infty} \mathbb{E} \left[ q^{(0)}_T q^{(0)}_0 \bigg| t=T \right]$$

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

\[ \mathbb{N}_l \]

level \( l \)

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MLMC for polymer dynamics
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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.

- Future research will also investigate nonlinear / linearised treatments (e.g. does linearised provide sufficient accuracy? or is linearised a good control variate for nonlinear?)
References


Chang-han Rhee and Peter W. Glynn. “Exact estimation for the equilibrium of Markov chains”, draft paper, 2014

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

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