

# Application of multilevel Monte Carlo to the simulation of dilute polymers

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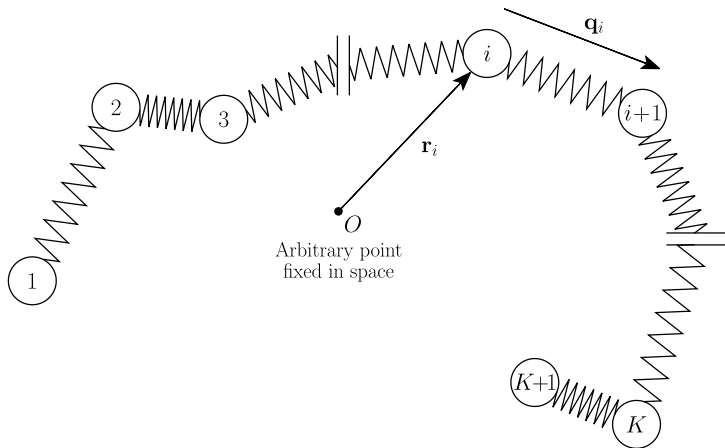
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# Outline

- 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:

elastic force + random force + viscous drag = 0

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

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

## Modelling

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

$$dr_i = (\kappa r_i - \nabla_{r_i} V(r)) dt + \sqrt{2} dW_i$$

where  $dW_i$  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  $i^{\text{th}}$  bond.

Hence,

$$dr_i = \left( \kappa r_i - \left( U'_{i-1}(\|q_{i-1}\|^2/2) q_{i-1} - U'_i(\|q_i\|^2/2) q_i \right) \right) dt + \sqrt{2} dW_i$$

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

$$dq_i = (\kappa q_i + U'_{i+1} q_{i+1} - 2 U'_i q_i + U'_{i-1} q_{i-1}) dt + \sqrt{2} (dW_{i+1} - dW_i)$$

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

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

## 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

$$dq^{(1)} = \left( \kappa q^{(0)} - D A(q^{(0)}) q^{(1)} \right) dt,$$

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

$$A_i(q_i^{(0)}) = U_i'(\|q_i^{(0)}\|^2/2) I + U_i''(\|q_i^{(0)}\|^2/2) q_i^{(0)}(q_i^{(0)})^T.$$

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

$$v^T A_i v = U_i' v^T v + U_i'' \left( (q_i^{(0)})^T v \right)^2 > 0,$$

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

$$dq^{(1)} = -D A(q^{(0)}) q^{(1)} dt.$$

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

$$dE = (q^{(1)})^T D^{-1} dq^{(1)} = -(q^{(1)})^T A(q^{(0)}) q^{(1)} dt$$

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

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

## 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:

$$\begin{aligned} q_{n+1}^{(0)} &= q_n^{(0)} - D \nabla V(q_n^{(0)}) h_n + \sqrt{2} L \Delta W_n \\ q_{n+1}^{(1)} &= q_n^{(1)} + \left( \kappa q_n^{(0)} - D A(q_n^{(0)}) q_n^{(1)} \right) h_n \end{aligned}$$

## 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  $i^{\text{th}}$  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  $\lim_{T \rightarrow \infty} \mathbb{E}[P(T)]$  where, in the nonlinear analysis,

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

or, using the linearisation approach,

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

We'll start by doing it for a fixed, large  $T$ , then address the challenge of letting  $T \rightarrow \infty$ .

# 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  $\varepsilon$ , 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

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

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.

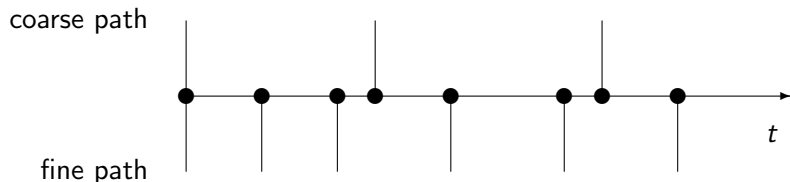
On level  $\ell$  use

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

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

# 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.

# Multilevel Monte Carlo simulation

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

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

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

which can be re-expressed as

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

and they use multilevel with  $M_\ell \rightarrow \infty$  as  $\ell \rightarrow \infty$  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

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

## Multilevel Monte Carlo simulation

Back to our polymer application, instead of estimating

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

we use the same idea and estimate

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

and use multilevel with  $h_\ell \rightarrow 0$ ,  $T_\ell \rightarrow \infty$  as  $\ell \rightarrow \infty$  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  $100\times$  speedup over MATLAB implementation

The latter handles polymers with up to 32 bonds

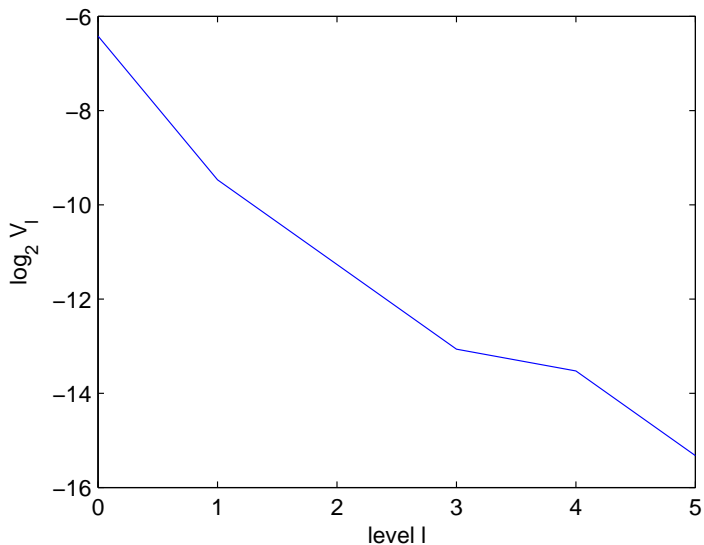
When there is a single bond, the code produces the correct value for

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

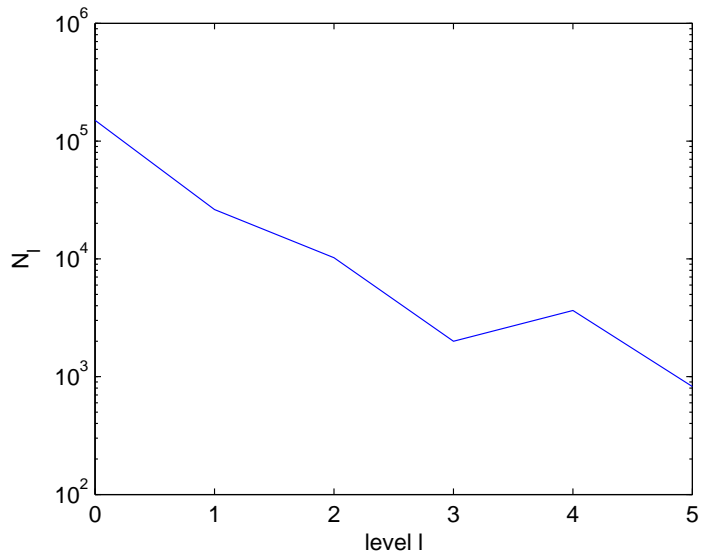
in comparison to the analytic value which can be deduced from the invariant distribution.



# Preliminary results



# 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
- 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

John W. Barrett and Endre Süli. “Existence of global weak solutions to some regularized kinetic models for dilute polymers”. *SIAM Multiscale Modelling and Simulation*, 6(2):506-546, 2007

M.B. Giles. “Multilevel Monte Carlo path simulation”, *Operations Research*, 56(3):607-617, 2008

M.B. Giles. “Multilevel Monte Carlo methods”, *Acta Numerica*, 2015

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

<http://people.maths.ox.ac.uk/gileesm/mlmc.html>

[http://people.maths.ox.ac.uk/gileesm/mlmc\\_community.html](http://people.maths.ox.ac.uk/gileesm/mlmc_community.html)