Overview of Reptation Quantum Monte Carlo

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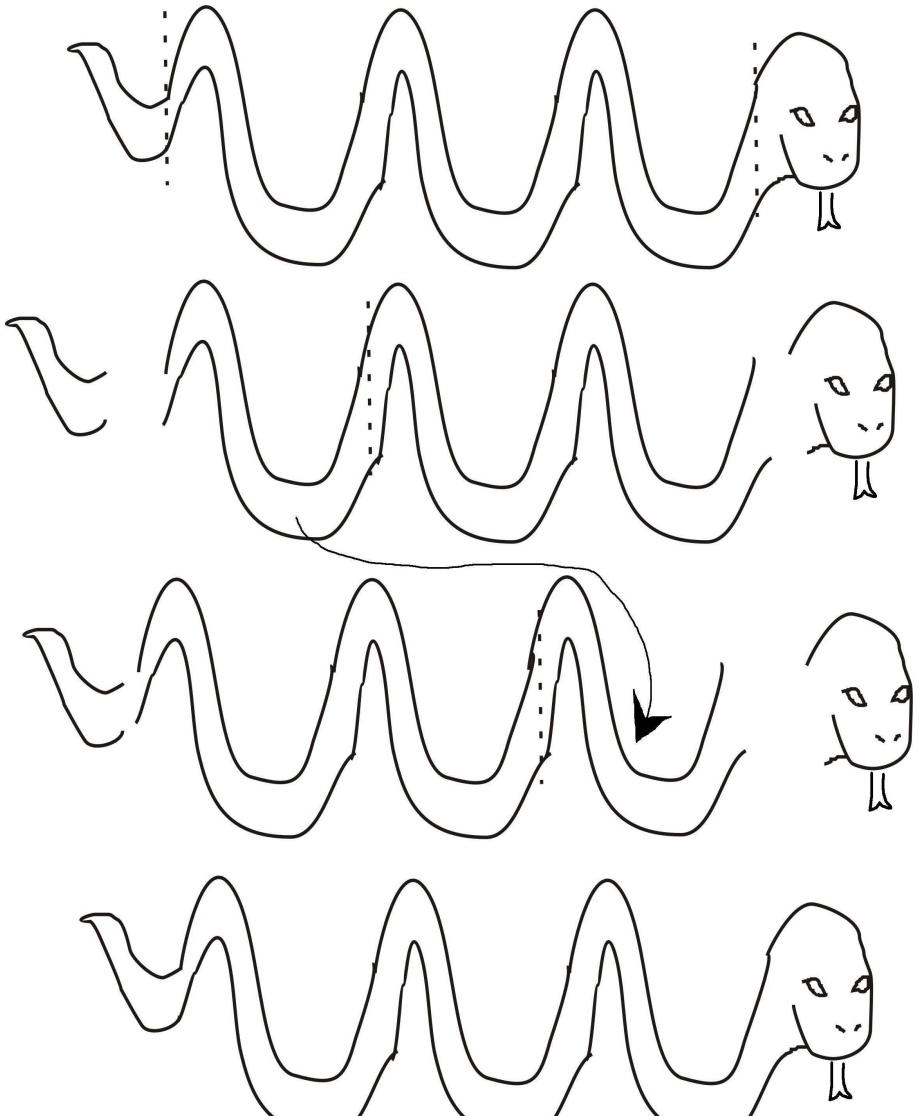
ESDG talk

Reptation: The action of creeping or crawling.

- *OED Online*

Physicists model of a snake



Introduction

- Quantum Monte Carlo is not all about Variational (VMC) and Diffusion Monte Carlo (DMC).

  Others exist, such as Auxiliary Field MC, Path Integral MC and Reptation QMC. They all have different strengths, weaknesses and purposes.
- Some of the problems that plague DMC
  - Time-step bias
  - Population control bias
  - Fixed-node approximation
  - Mixed estimators

  RQMC alleviates some of these, but not all.
- Some other advantages that RQMC provides
  - Imaginary-time correlations
  - Static response functions

Standard DMC and the mixed distribution

- In DMC, a random walk in configuration space generates a sequence of configurations $X = \{\mathbf{R}_0, \mathbf{R}_1, \ldots \mathbf{R}_M\}$. Statistics are collected *along the sequence*.
- Occasionally we have branching, which generates or destroys walkers.
- We use the importance sampled Green's function

$$\tilde{G}(\mathbf{R} \leftarrow \mathbf{R}', \tau) \approx G_{\mathrm{D}}(\mathbf{R} \leftarrow \mathbf{R}', \tau) G_{\mathrm{B}}(\mathbf{R} \leftarrow \mathbf{R}', \tau), \tag{1}$$

where

$$G_{\mathrm{D}}(\mathbf{R} \leftarrow \mathbf{R}', \tau) = \frac{1}{(2\pi\tau)^{3N/2}} \exp\left(-\frac{\left(\mathbf{R} - \mathbf{R}' - \tau \mathbf{V}(\mathbf{R}')\right)^2}{2\tau}\right) \tag{2}$$

is the drift-diffusion Green's function, and

$$G_{\mathrm{B}}(\mathbf{R} \leftarrow \mathbf{R}', \tau) = \exp\left(-\frac{\tau}{2}[E_L(\mathbf{R}) + E_L(\mathbf{R}') - 2E_T]\right) \tag{3}$$

is the branching Green's function.

- The walk is guided by a trial wavefunction. E.g. the drift vector is

$$\mathbf{V}(\mathbf{R}) = \Psi^{-1}\nabla\Psi. \tag{4}$$

- This generates a *mixed distribution*, $f(\mathbf{R}) = \Psi(\mathbf{R})\Phi_0(\mathbf{R})$, where $\Phi_0(\mathbf{R})$ is the ground state of the system. This means that except for an initial equilibration period, the elements in the sequence X are distributed according to f.
- Statistics collected for a local operator result in a *mixed estimate*. Crudely, we collect statistics using the sequence X as:

$$\bar{O} = \frac{1}{M}\sum_{i}^{M} O(\mathbf{R}_i) \approx \langle\Psi|\mathcal{O}|\Phi_0\rangle. \tag{5}$$

- If $\mathcal{O}$ doesn't commute with the Hamiltonian $\mathcal{H}$, then $\langle\Psi|\mathcal{O}|\Phi_0\rangle$ *does not* equal the ground state expectation value $\langle\Phi_0|\mathcal{O}|\Phi_0\rangle$.

Weighted DMC

- Branching can be replaced by allowing a walker to accumulate a weight. If the walker starts at $\mathbf{R}_0$, the total weight after m steps is

$$W_m = \prod_{i=1}^{m} G_{\mathrm{B}}(\mathbf{R}_i \leftarrow \mathbf{R}_{i-1}, \tau). \tag{6}$$

- The walker generates a sequence $X = \{\mathbf{R}_0, \mathbf{R}_1, \ldots \mathbf{R}_M\}$ of configurations over a total of M steps.
- Expectation value is now given by

$$\bar{O} = \frac{1}{M} \sum_{m=0}^{M} W_m \, O(\mathbf{R}_m) \approx \langle \Psi | \mathcal{O} | \Phi_0 \rangle \tag{7}$$

DMC to RQMC

- Call the sequence X with a fixed length M a *path*. Then the DMC *probability distribution of the path* is given by

$$P_{\mathrm{DMC}}(X) = \prod_{i=1}^{M} G_{\mathrm{D}}(\mathbf{R}_i \leftarrow \mathbf{R}_{i-1}, \tau)\Psi^2(\mathbf{R}_0). \tag{8}$$

- The *weight of the path* is simply $W(X) = W_M$.
- We can define a new probability distribution of path as

$$\pi(X) = P_{\mathrm{DMC}}(X)\, W(X). \tag{9}$$

- *The aim of RQMC is to generate a set of paths according to the distribution* $\pi(X)$.

Significance of RQMC path distribution

- **Key result**: *Configurations at the centre of the paths are distributed according to the true ground state!* (Not proved here, but not difficult.)

$$P(R_c) = \int d\mathbf{R}_0 \dots d\mathbf{R}_{c-1} d\mathbf{R}_{c+1} \dots d\mathbf{R}_M \pi(X) \approx \Phi_0^2(\mathbf{R}_c) \tag{10}$$

- Exact ground state expectation value of local operators (*pure estimators*)

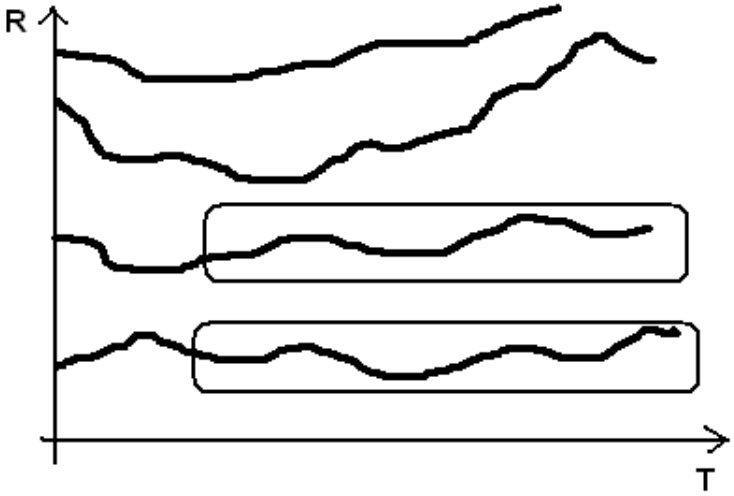
$$\langle \Phi_0 | \mathcal{O} | \Phi_0 \rangle \approx \int dX O(\mathbf{R}_c) \pi(X) \approx \frac{1}{N_p} \sum_{i=1}^{N_p} O(\mathbf{R}_c^i) \tag{11}$$

- Imaginary time correlations

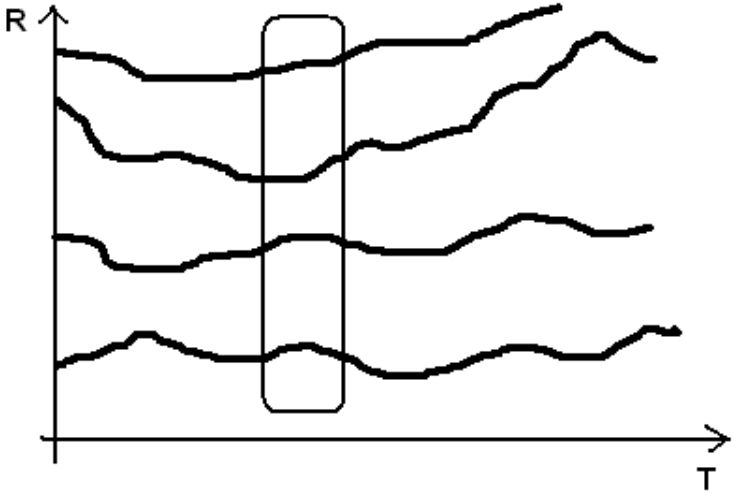
$$C_{\mathcal{O}}(n\tau) = \langle \Phi_0 | \mathcal{O}(n\tau) \mathcal{O}(0) | \Phi_0 \rangle \approx \int dX O(\mathbf{R}_{c+n}) O(\mathbf{R}_c) \pi(X) \tag{12}$$

Configuration sampling in DMC and RQMC

Major difference is whether configuration samples are taken *along* or *across* paths.



DMC



RQMC

Generating paths in RQMC

- Use the Metropolis algorithm to sample paths.
- Start with some path X.
- Suggest a new path X' using some transition matrix $T(X \to X')$.
- Accept or reject the new path with acceptance probablity

$$A = \min\left\{1, \frac{T(X' \to X)\pi(X')}{T(X \to X')\pi(X)}\right\}. \tag{13}$$

- Accumulate statistics using new path. Repeat.
- **Reptation**: *New path is suggested by removing some configurations at one end of the path and adding new configurations at other end.*
- Example:
  $X = \{\mathbf{R}_0, \mathbf{R}_1 \ldots \mathbf{R}_M\}$
  $X' = \{\mathbf{R}_1 \ldots \mathbf{R}_M, \mathbf{R}_{M+1}\}$

- The new configuration R_{M+1} is generated using the DMC drift-diffusion Green's function. Then

$$T(X \rightarrow X') = G_{\rm D}(\mathbf{R}_{M+1} \leftarrow \mathbf{R}_M, \tau) \tag{14}$$

- Acceptance probability greatly simplifies! Using $\pi(X) = P_{\rm DMC}(X)W(X)$, lot of terms cancel. End up with:

$$\begin{aligned} A &= \min\left\{1, \frac{G_{\rm B}(\mathbf{R}_{M+1} \leftarrow \mathbf{R}_M, \tau)}{G_{\rm B}(\mathbf{R}_0 \leftarrow \mathbf{R}_1, \tau)}\right\} \qquad (15) \\ &= \min\left\{1, \exp\left(-\frac{\tau}{2}[E_L(\mathbf{R}_{M+1}) + E_L(\mathbf{R}_M) - E_L(\mathbf{R}_1) - E_L(\mathbf{R}_0)]\right)\right\}, \end{aligned}$$

  where $E_L(\mathbf{R}) = \Psi^{-1}(\mathbf{R})\hat{H}(\mathbf{R})\Psi(\mathbf{R})$ is the *local energy*.

- Lots of other subtleties not even mentioned here, such as having to move path both backwards and forwards, symmetrizing Green's functions, taking multiple steps at a time etc. etc.

Conclusions

- RQMC is based on random walk in space of paths.
- Statistics are accumulated between paths.
- It allows the calculation of pure estimators, imaginary time correlations, static response functions etc. that DMC can't do or can only do with great difficulty.
- It eliminates population control bias.
- RQMC still suffers from time-step bias and fixed node approximation.
- Calculating total energy is slower than with DMC.
- One day it may well be an option in CASINO!