Lectures on Quantum Monte Carlo Methods

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Progression of Lectures

1 Stochastic Integration
2 Random Numbers
3 Classical Statistical Mechanical Simulations
4 Cluster algorithms for classical models
5 Quantum Monte Carlo
6 The continuum limit
7 Observables and Estimators
8 Finite-size scaling
9 More about the correlation length
10 Survey of other applications

10. Survey of other applications

Or, the many paths to insight.

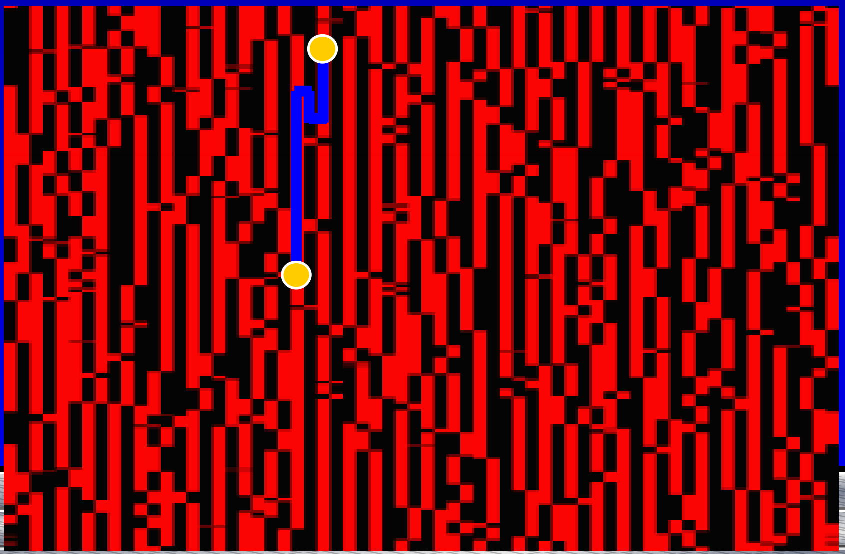
Exploring algorithm space

- Worm algorithms
- Cluster SSE
- Meron cluster algorithms
- Quantum link models

"Worm" algorithms also explore continuous configuration space

- Similar to CTCA, but "end-oriented"
  - ⇨During build, consider open ends of cluster:
    - » gives estimator for Green functions G(x,τ)
    - » motion of "kinks" likened to a worm

• Prokof'ev, Svistunov, Tupitsyn: "kink" and "antikink" are open ends of (unfinished) cluster; can accumulate statistics on Green functions

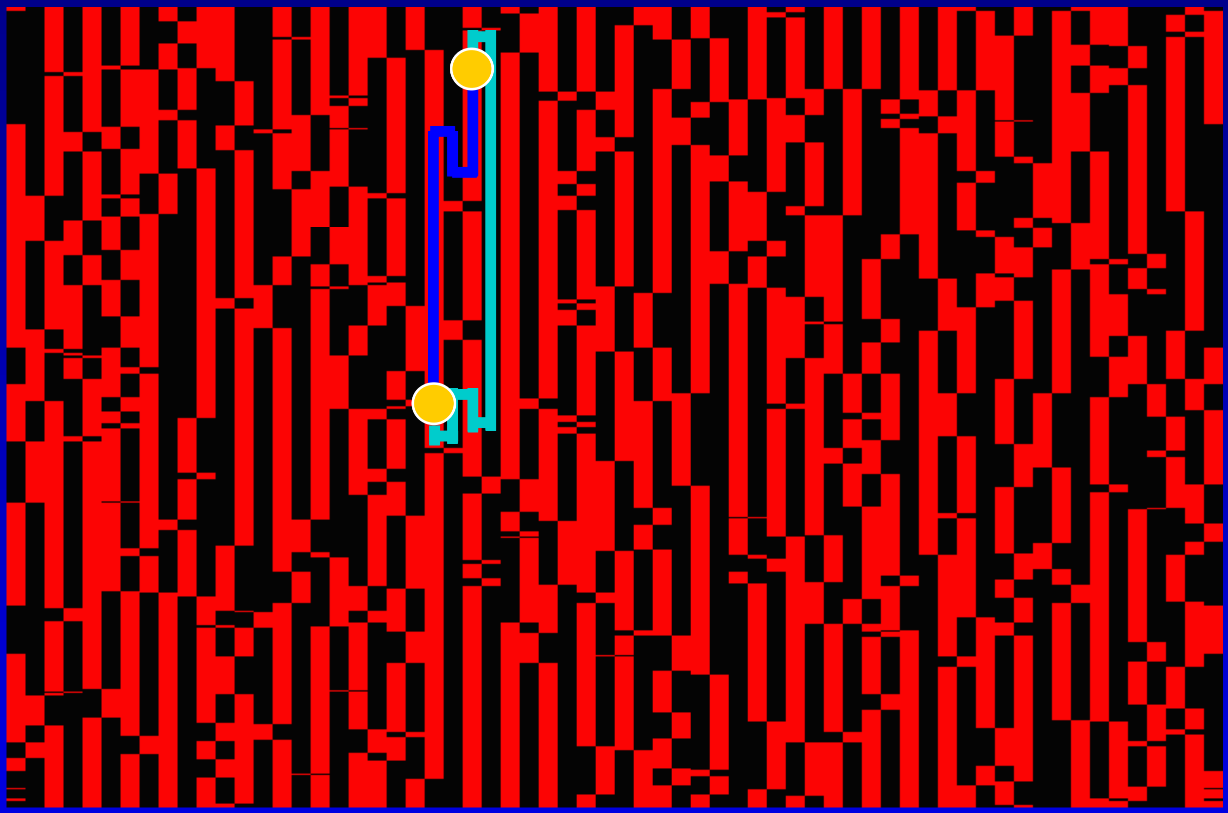


cf. cond-mat/9703200

In CTCA language:

- Non-diagonal operators cannot be sampled directly in our ensemble
  - ⇨e.g. $G_{S^1}(r,\tau) = \left\langle S_x^1 S_y^1 \right\rangle$: $S_x^1 S_y^1 \exp(-\beta H)$ doesn't contribute to Z
- But if we imagine building a cluster
  - ⇨then cutting it in two places x and y,
  - ⇨then flipping half the cluster,
  - ⇨this contributes to the Green function...
- Consistent with TACF estimator

Cluster-cutting enables estimate of off-diagonal operators



Worm idea applicable to all cluster observables

- Brower, Chandrasekharan, & Wiese (1998)
  - ⇨showed why cluster properties (e.g. cluster size distribution) are basis-independent
  - ⇨showed how to rewrite path integral in terms of "quantum clusters"
  - ⇨generalize PST idea to show how any operator can be measured in cluster ensemble

cf. cond-mat/9801003

Worm idea expands scope of loop cluster algorithm

- Enables *local* cluster move to include complete Hamiltonian, e.g. magnetic field
  - ⇨ no overall accept/reject step
  - ⇨ but possible long wait for worms to rejoin
    - » needed for measuring diagonal operators, e.g. energy
- Generalize to gauge theories, e.g. finding Wilson loop expectations with QLM
- Sandvik: worm SSE?

Stochastic Series Expansion (SSE) also operates in continuous time

- Generalization of Handscomb's method:
  - ⇨ AFHM: Write $H = -\frac{1}{2}\sum_{b=1}^{2N}\left[H_{1,b} - H_{2,b}\right] + \frac{N}{2}$

$$H_{1,b} = 2\left[\tfrac{1}{4} - S^z_{i(b)} S^z_{j(b)}\right] \ \text{i.e. diagonal} \qquad \begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$$

$$H_{2,b} = S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)} \ \text{i.e. off-diagonal} \qquad \begin{bmatrix} & 1 \\ 1 & \end{bmatrix}$$

  - ⇨ expand exponential Z=exp(-βH) power series:

$$Z = \sum_{|\alpha\rangle} \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-1)^{n_2}\beta^n}{n!} \left\langle \alpha \left| \prod_{i=1}^{n} H_{a_i,b_i} \right| \alpha \right\rangle$$

SSE is built around the Taylor expansion of exp(-βH)

$$Z = \sum_{|\alpha\rangle} \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-1)^{n_2} \beta^n}{n!} \left\langle \alpha \left| \prod_{i=1}^{n} H_{a_i, b_i} \right| \alpha \right\rangle$$

trace

product of local operators

Sum over sequences S_n

Sum over lengths of sequences S_n

n_1=number of diagonal operators $H_{1,b}$ $a_i=1,2$

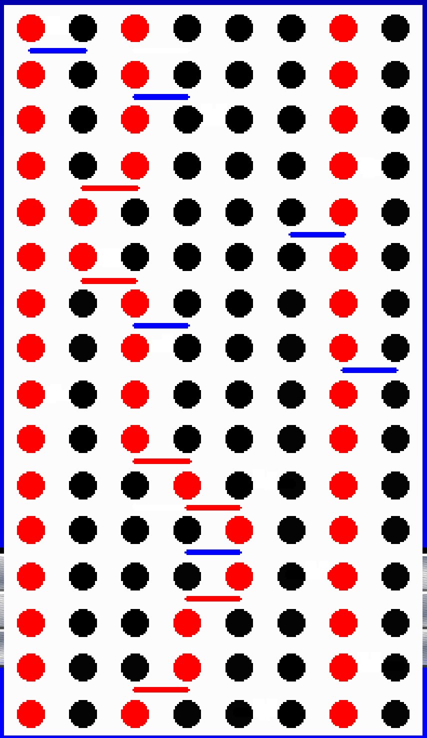
n_2=number of off-diagonal operators $H_{2,b}$ $b_i=1\ldots2N$

$n=n_1+n_2$

- Can show n_2 is always even, hence $(-1)^{n_2}$ superfluous

SSE configuration space bears superficial resemblance to DTCA

- terms in trace are essentially Gaussian distributed
- can neglect all terms $n > N_{cutoff}$
- insert identity operators to make all sequences the same length
- design updating rules to provide detailed balance



- still have spin sites
- still have “bonds”
- only one non-trivial operator per slice
- but “transitions” now indicate non-diagonal operators
- No Trotter error...

Stochastic Series Expansion (SSE) with cluster updates is competitive

- Initial applications used Metropolis updates
  - ⇨inefficient
  - ⇨not ergodic -- initial simulations studied zero magnetization sector only
- Sandvik (1999) introduced "operator-loop updates" (i.e. cluster SSE)
- Dorneich & Troyer (2001) document good performance of cluster SSE

cf. cond-mat/9902226, 0106471

Other problems: fermionic systems have notorious "sign problem"

- Fermionic interchange terms troublesome
  - ⇨alternating signs lead to large cancellations
  - ⇨small "signal" gets large relative errors
- Long-hoped-for improved estimator for sign solves only half the problem
  - ⇨Without improved estimator, $N_{MC} \propto \exp\left(2\beta V \Delta f_{fb}\right)$
  - ⇨With improved estimator, $N_{MC} \propto \exp\left(\beta V \Delta f_{fb}\right)$

Error ∝ exponential in βV

$Z_f = \sum_n \mathrm{Sign}[n] \exp(-S[n])$ fermionic action

$S[n]$ = bosonic action, $Z_b = \sum_n \exp(-S[n])$

$$\langle Q \rangle_f = \frac{1}{Z_f} \sum_n Q[n] \mathrm{Sign}[n] \exp(-S[n]) = \frac{\langle Q \,\mathrm{Sign} \rangle}{\langle \mathrm{Sign} \rangle}$$

Average sign $\langle \mathrm{Sign} \rangle = \frac{Z_f}{Z_b} = \exp\left(-\beta V \Delta f_{bf}\right)$

Relative error $\frac{\Delta \mathrm{Sign}}{\langle \mathrm{Sign} \rangle} = \frac{\sqrt{\langle \mathrm{Sign}^2 \rangle - \langle \mathrm{Sign} \rangle^2}}{\sqrt{N} \langle \mathrm{Sign} \rangle} = \frac{\exp\left(\beta V \Delta f\right)}{\sqrt{N}}$

Improved estimator solves half the sign problem

If we can arrange perfect cancellation of most signs,

then $\text{Sign} = (+1-1=)0 \text{ or } 1,\ \text{so Sign}^2 = \text{Sign},\ \text{then}$

$$\text{Relative error } \frac{\Delta\text{Sign}}{\langle\text{Sign}\rangle} = \frac{\sqrt{\langle\text{Sign}\rangle - \langle\text{Sign}\rangle^2}}{\sqrt{N}\langle\text{Sign}\rangle} = \frac{\exp\left(\beta V \Delta f/2\right)}{\sqrt{N}}$$

Chandrasekharan & Wiese: Meron cluster algorithm

- "Meron" clusters = clusters that change the overall sign of a configuration when flipped
- Meron clusters provide improved estimator for Sign in some systems
- Key step: restrict configuration space to zero- and two-meron sectors
  - ⇨ reweighting & rejections equalize statistics
  - ⇨ eliminates other half of $\exp(\beta V \Delta f)$

cf. cond-mat/9902128

Gauge theories are current target of cluster algorithm research

- Quantum link models (QLM) for SU(2) and and U(1) written by Horn in 1981
- Rediscovered several times
  - ⇨Orland & Rohrlich (1990)
  - ⇨Chandrasekharan & Wiese (1997)
- Related to ordinary gauge theories via dimensional reduction

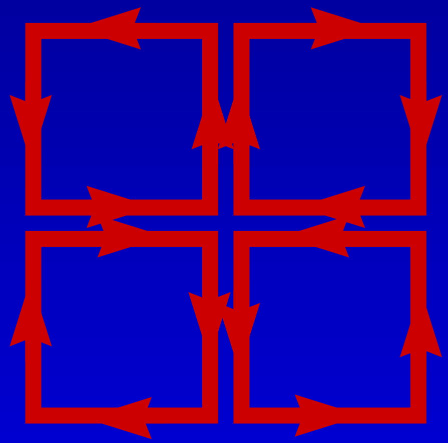
cf. hep-lat/9811025

Quantum link models are generalization of spin models

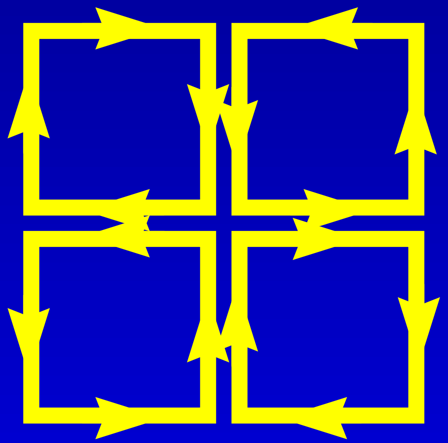
- Instead of integrating over classical field configurations…
  - ⇨replace classical vectors (e.g. gauge field link variables) by quantum spin operators
  - ⇨classical action is replaced by Hamiltonian
- Can be formulated in any representation, not just S=½
- $\xi >> 1 \Rightarrow$ dimensional reduction

Example program: U1samp.exe

- Presents U(1) gauge theory in 2+1 dimensions
- Flux direction color coding:



Red: CW even, CCW odd



Yellow: CCW even, CW odd

- Cluster builds in blue (oriented surface, light/dark blue)

Cluster algorithms are an exciting area of research

- Efficient CTCAs: zero systematic error
- Diverse offshoots
  - ⇨Worm algorithms
  - ⇨Cluster SSE
  - ⇨Gauge theories
- Provide context to solve long-standing problems, e.g. meron clusters for sign problem

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