Speedy algorithms for lattice fields: status and unfinished (?) developments

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.....contain a brief review of the status of the topic and also devote a portion of time to speculation.....

my interpretation:

- a very subjective subset is reviewed
- some off-the-mainstream developments described
- some bias toward cluster methods

outline

- Speed of MC algorithms
- Scalar fields
- Gauge fields
- Fermions
- a page with references at the end
Speed of MC algorithms in equilibrium

equilibrate \longrightarrow (a_1, b_1, \ldots) \text{ update } (a_2, b_2, \ldots) \text{ update } \ldots \text{ update } (a_N, b_N, \ldots)

estimates \{a_i, b_i, \ldots\} \text{ of observables } A, B, \ldots \text{ separated by "update"}

\langle a_i \rangle = A, \ldots

autocorrelation function:

\Gamma_{AA}(t) = \langle (a_i - A)(a_{i+t} - A) \rangle, \ldots \quad \Gamma_{AB}(t) = \langle (a_i - A)(b_{i+t} - B) \rangle

- \langle \ldots \rangle \text{ dynamical average } (\leftrightarrow \text{ ensemble of MCs})
- \text{ coincides with statistical ('static') mean at equal MC time}

Standard estimator:

\bar{a} = \frac{1}{N} \sum_{i=1}^{N} a_i, \quad \langle (\bar{a} - A)^2 \rangle = \frac{V_A}{N/2\tau_{int,A}}

variance (static, independent of "update"):

V_A = \Gamma_{AA}(0) = \langle (a_i - A)^2 \rangle

integrated autocorrelation time (dynamical):

2\tau_{int,A} = \sum_{i=-\infty}^{t=+\infty} \frac{\Gamma_{AA}(t)}{\Gamma_{AA}(0)}

remarks:

- several definitions of \tau_{int,A} \text{ (agreeing when they are large)}
- \tau_{exp}: \text{ slowest mode for all observables (extremely hard to determine)}
- \Gamma, \tau_{int} \text{ have to be estimated numerically (construct estimators)}
- error of \tau_{int}: \leftrightarrow \text{ error of the error of observables}
- often estimate } f(A, B) \text{ by } f(\bar{a}, \bar{b}), \text{ errors from } \Gamma_{AA, AB, BB}
Critical slowing down

- $\tau_{\text{int}}$ (usually) diverge in the continuum limit $\xi = (am_{\text{phys}})^{-1} \rightarrow \infty$
  $$\tau_{\text{exp}} \propto \xi^z, \quad \tau_{\text{int, A}} \propto \xi^{z_A}$$

- $z, z_A$ close to 2 for standard local heatbath, Metropolis [referring to ‘sweeps’, i.e. cost(“update”) $\propto \#$ of lattice sites]

- QCD (Ukawa, lat2001): cost $\propto a^{-7}$, $z \sim 3$, large prefactor

- exponents $\leftrightarrow$ dynamical RG, universality classes of algorithms (?), not as well developed as the usual RG

practical upshot:

$\implies$ minimize $\tau_{\text{int, A}}$/ (exec. time of “update”) for optimally estimating $A$

Scalar fields and cluster algorithms

- ‘classical’ cluster algorithms for Ising, Potts and $O(n)$ $\sigma$-models

- for continuous $O(n)$ spins one practically or truely achieves $z_A = 0$

- $\xi \sim 100$ possible, $\tau_{\text{int}} \sim 1$, $O(\# \text{sites})$ ops. for independent config.

How?

$$Z = \int Ds(x) \ e^{-\beta H(s)}, \ s \in \mathbb{R}^n, \ |s| = 1$$

- for a given $\{s(x)\}$ parameterize a ‘target set’ $\{\tilde{s} = s_\perp + \sigma |s_\parallel|\}$ with respect to a random direction and an Ising field $\sigma(x) = \pm 1$

- $\tilde{H}(\sigma |s) = - \sum_{xy} J_{xy} \sigma(x)\sigma(y), \ J_{xy} = |s_\parallel(x)|s_\parallel(y)|$

- $J_{xy}$: no frustration, random bond ferromagnet

- update from initial $\sigma \equiv \text{sign}(s_\parallel)$ to new $\sigma(x)$ with any algo for $\tilde{H}$

- powerful with Swendsen-Wang or Single cluster algorithm for $\sigma$
Trivial identity: on each link write
\[ e^{\beta J \sigma \sigma'} = e^{-\beta J} \sum_{b=\text{off}, \text{on}} [\delta_{b,\text{off}} + (e^{2\beta J} - 1)\delta_{b,\text{on}} \delta_{\sigma, \sigma'}] \]

proof: consider \( \sigma \sigma' = + \) and \( \sigma \sigma' = - \)
- additional ('redundant') bond-variables \( \{b_{xy}\} \)
- throw new bonds for given spins (trivial)
- determine (bond-)percolation clusters (clever)
- throw new spins for given bonds (trivial)

Why is it so efficient? improved estimator identity:
\[ \langle s(x) \cdot s(y) \rangle = \left( (\text{smooth}) \times \Theta(x, y) \right)_{b, s}, \quad \Theta(x, y) = \begin{cases} 1 & \text{if } x, y \in \text{one cluster} \\ 0 & \text{else} \end{cases} \]
- cluster size automatically chained to the correlation length

Disappointment of the 90's: no analogous successful algorithms for gauge theories, not even for other \( \sigma \)-models: \( \text{RP}(n), \text{CP}(n), \text{SU}(n) \times \text{SU}(n) \)

Why is this so?
- Ising embeddings possible, but \( J_{xy} \) in \( \tilde{H} \) found frustrated
- cluster update still possible, but clusters too large
  \( \rightarrow \) cluster flips \( \approx \) global symmetry move, not dynamically relevant
- no improved estimator identity

Sokal et al. (heuristic) codimension-one 'no-go' argument:
- think of smooth classical \( s(x) \)
- clusters break, where \( \beta J_{xy} \ll 1 \Rightarrow s_{\parallel}(x) \approx 0 \) (\( s \) unchanged by flip)
- this is 1 real condition for \( x \rightarrow \) clusters isolated by \( d-1 \) dimensional hypersurfaces
- other embeddings: > 1 conditions, no isolation of clusters
- no-go theorem: embedded Ising spins \( \leftrightarrow \) involutory isometry of spin manifold; exists with \( \text{dim} = d-1 \) fixed point only for sphere \( \leftrightarrow \) \( O(n) \)
Interesting way out: make (extreme!) use of the freedom in formulation/discretization in view of available algorithms

**Cluster updates for ‘quantum’ models**

- $d$-dimensional Hamiltonian operator, Trotter-Suzuki formula, $H \rightarrow D = d + 1$ imaginary time path integral ($\sim$ euclidean FT)
- prototype: quantum Heisenberg model, $d = 1$

\[
H = J \sum_x \vec{S}_x \cdot \vec{S}_{x+a}, \quad [S_x^k, S_y^l] = \delta_{xy} \delta^{klm} S_x^m
\]

\[
Z = \text{Tr} e^{-\beta H} \approx \text{Tr} (e^{-\epsilon H_2} e^{-\epsilon H_1})^N
\]

with $\epsilon = \beta / N$, $H = H_1 + H_2$, 1, 2 $\leftrightarrow$ even/odd links
intermediate states: $S_x^3 |s\rangle = s_x |s\rangle$, $s_x = \pm \frac{1}{2}$

$$Z = \sum_{\{s(t,x) = \pm \frac{1}{2}\}} A[s]$$

- $A$ is made of many factors $\langle s'| e^{-\varepsilon H_1} |s\rangle$ and $\langle s'| e^{-\varepsilon H_2} |s\rangle$
- classical form, $D = 2$, here $A \geq 0$ ($= 0$ for many configs)
- connecting sites with $s(t,x) = + \frac{1}{2}$ $\leftrightarrow$ ‘worldlines’

![Diagram](attachment:image.png)

picture: Troyer et al, physics/0306128

- hard for local algorithms, but:
- nonlocal loop-cluster algorithm (Evertz, Lana, Marcu) works extremely well, global changes of worldlines
  - additional bond-type variables stochastically chosen
  - closed loops identified ($\leftrightarrow$ cluster search)
  - flip $s$-variables along loops
- high precision results for (anti)ferromagnet and other models

particular application (Wiese et al.):
- cluster simulations of $D = 2$ CP($n$) models:
  - devise a $d = 2$ quantum spin system with SSB of SU($n$) to U($n - 1$) with Goldstone bosons $\simeq$ SU($n$)/U($n - 1$) = CP($n - 1$)
  - on a strip geometry: no real SSB but very small mass $\rightarrow$ effectively $d = 1$ or $D = 2$ for the classical model (dimensional reduction)
• CP(n − 1) model emerges as effective theory (χPT)
• universality check: same finite size scaling as conventional discretization, also the O(3) has been simulated in this way
to some degree, the ‘quantum model’ approach extends to fermions:
see below
construction of gauge theories from ‘quantum link models’ also investigated

Pure gauge systems

standard (local) procedure Hybrid OverRelaxation
we discuss SU(2), ← SU(n) by Cabibbo-Marinari embedded SU(2)
take actions, for which the single link dependence is

\[ P(U) \propto \exp[\text{Re tr} (UM^\dagger)] = \exp[u^a m^a], \quad U = u^0 + u^k i \tau^k, \quad u^a u^a = 1 \]

• includes many actions (counterexample: adjoint, tr(\(U_{\text{plaq}}^{2}\))
• heatbath: new u with \(P(U)\)
• microcanonical/‘overrelaxation’: \(u = u_\parallel + u_\perp \rightarrow u_\parallel - u_\perp (\parallel, \perp \leftrightarrow m)\)
• HOR: 1 HB sweep followed by \(N_{OR}\) OR sweeps
• \(z \sim 1\) achievable, requires \(N_{OR} \propto \xi\) (similar \(\omega = 2 - \frac{c}{\xi}\) for ‘true’ OR)
• link order can be important, [loop-\(\mu\) [loop-x .......]] found ++
⇒ update time often negligible in quenched simulations

cluster algorithms for $\mathbb{Z}(2)$ gauge theories:

- throw bond on plaquettes

$$e^{\beta \sigma_1 \sigma_2 \sigma_3 \sigma_4} = e^{-\beta} \sum_{b=\text{off,on}} \left[ \delta_{b,\text{off}} + (e^{2\beta} - 1) \delta_{b,\text{on}} \delta_{\sigma_1 \sigma_2 \sigma_3 \sigma_4, 1} \right]$$

- find random new gauge field under constraint: $\sigma_{\text{plaqu}} = 1$ where $b=\text{on}$
  o this step is hard
  o efficient graph theoretical solution in $D=3$ (Ben-Av et al.)
  o linear algebra solution (Bunk), also for gauge-Higgs
  o $z \approx 0.5$

no embedding scheme for continuous variables, not even $3D$ U(1) model

- possible recent progress: ‘worm’ algorithms (Alet et al.), changing global flux loops

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**Dynamical fermions**

chiral invariant quarks: → talks by Tony Kennedy & Kostas Orginos

$$Z = \int D\bar{\psi} D\psi e^{-S_{\text{g}}(U) - a^4 \sum_x \bar{\psi} (\bar{\psi} + m) \psi}$$

**determinant methods** ($N_f$ degenerate flavors) use

$$\int D\bar{\psi} D\psi e^{-a^4 \sum_x \bar{\psi} (\bar{\psi} + m) \psi} = \det(\bar{\psi} + m)^{N_f}$$

**pseudofermionic methods** [take $N_f=2$, assume $\bar{\psi} = \gamma_5 \bar{\psi} \gamma_5$, set $Q = \gamma_5 (\bar{\psi} + m)$] use

$$\det(\bar{\psi} + m)^2 = \det(Q)^2 = \int D\varphi^\dagger D\varphi e^{-a^4 \sum_x \varphi^\dagger \varphi Q^{-2} \varphi}$$
standard workhorse: HMC ($a \equiv 1$)

$$\mathcal{H} = \frac{1}{2} \sum_{x \mu} \text{tr} \left[ \Pi^2_{\mu} \right] + S(U), \quad S(U) = S_G(U) + \sum_{x} \varphi^* Q^{-2} \varphi$$

- update $\varphi$ by global heatbath
- update $(\Pi, U)$ ‘almost microcanonically’ $\leftrightarrow$ discretized Hamilton eqs.
- accept step

general remarks:
- HMC is an exact algorithm including fermions
- HMC is a relatively slow algorithm in the pure gauge limit compared to HOR

plot: B. Gehrmann

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cost of algorithms at constant physics, $L \equiv L/a$
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recent improvements
A: momenta need not be exponentiated exactly (Lüscher)
B(essential): more than 1 pseudofermion (Hasenbusch)

- small \( m \to \) large condition number \( Q^{-2} \to \) large force \( \to \) only small \( \delta \tau \)
- factorization: \( \det(Q)^2 = \det(\tilde{Q}\tilde{Q}^\dagger) \times \det(Q(\tilde{Q}\tilde{Q}^\dagger)^{-1}Q) \)
- one pseudofermion for each \( \det \to \) smaller total force, larger \( \delta \tau \)

**ALPHA** realization of this: \( Q \leftrightarrow \) Wilson/clover (even/odd), \( \tilde{Q} = Q - i \rho \)

\( \Rightarrow S_\varphi = \sum_x \varphi_1^\dagger(Q^2 + \rho^2)^{-1}\varphi_1 + \varphi_2^\dagger(Q^{-2} + \rho^{-2})\varphi_2 \)

so far: \( \rho \sim \) equal condition numbers, main cost: \( Q^{-2} \)
better: different step size for \( \varphi_1, \varphi_2 \) (QCDSF), smaller \( \rho \)
gains reported range form 2...6, only minor modification of code

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**No pseudofermion**

- want: \( \lim_{N_t \to 0} \) (myalgo) = HOR (not HMC)
- true for: (detailed bal.) proposal with HOR + accept with \( |\det Q|^2 \)
- improve: proposal need not take just \( S_G \to \) so-called UV-filtering
- problem: no fermion-guided proposal \( \to \) acceptance ok?
- probably in general no, but SF in (phys.) small volume?
- successful in 2-D Schwinger model (Knechtli, Wolff)
- any stochasticity in the Metropolis step for \( |\det Q|^2 \) costs acceptance, exact inequality, a few exact generalized eigenvalues can help

\[ Q^2(U_{\text{new}})\psi = \lambda Q^2(U_{\text{old}})\psi \]
No determinant

- Grassmann integral: finite sum of nonzero terms on any finite lattice
- can this be sampled directly? beware: minus-sign problem
- early example with recent progress: LQCD $\beta=0$

staggered fermions, gauge group $U(n)$:

$$Z = \int D\psi D\bar{\psi} DU e^{\sum_x \left( m_0 \bar{\psi}_x \psi_x + \sum_\mu \frac{g_\mu(x)}{2} \left[ \bar{\psi}(x) U_\mu(x) \psi(x + \mu) - \bar{\psi}(x + \mu) U_\mu^\dagger(x) \psi(x) \right] \right)}$$

integrate $U$ link by link ⇒ local model in $\bar{\psi}_x \psi(x)$ (‘ultralocal confinement’)
do Grassman integral site by site ⇒ discrete monomer-dimer representation:

$$Z = \sum_{\{k_\mu(x) = 0, \ldots, n\}} \prod_x \alpha_{k_\mu(x)} \prod_x \beta_{\sigma(x)} m^{\sigma(x)}$$

$\alpha_i$, $\beta_i$ known weights ($\geq 0$), $k_\mu(x)$ dimers on link $x\mu$
$\sigma(x) = n - \sum_\mu k_\mu(x) + k_\mu(x - \mu)$ monomers at site $x$,

text continues...
● overcome for a class of Hubbard-like models by the meron cluster technique (Chandrasekharan, Wiese)
  ○ combine analytically configurations → weights ≥ 0
  ○ modified importance sampling, reweighting
● only certain models, clever construction needed case by case
● warning: the generic ‘sign problem’ may NP-hard (Troyer, Wiese, cond-mat/0408370)

Conclusions

● classical cluster algorithms restricted to O(n) and discrete models
● progress via quantum models → think of non-standard discretizations
● steady progress for the ‘standard’ fermion method (via det, pseudofermions, HMC): optimized solvers, integration schemes, preconditioning, 2 (or more) pseudofermions, domain decomposition (Lüscher), ...
● break-through type gains???
● maybe we should keep looking for a representation of relativistic fermions as a weighted sum over configurations (other than the standard nonlocal ‘bosonization’) in connection with cluster-type algorithms
● clearly a long way to go for QCD
Some references

incomplete, reviews where available, add ‘and further references found there’ to each entry....
errors, autocorrelations: U. Wolff, hep-lat/0306017
review on classical cluster algorithms: F. Niedermayer, hep-lat/9704009
codim. one no-go theorem: S. Caracciolo et al., hep-lat/9205005
loop cluster algorithm: H.G. Evertz, cond-mat/9707221
CP(n) cluster simulation: B.B. Beard, U. Wiese, hep-lat/0406040
meron cluster algorithm: S. Chandrasekharan et al., cond-mat/0201360
quantum spin and fermion models: M. Troyer et al, physics/0306128,
2 pseudofermions: M. Hasenbusch, hep-lat/0107019, hep-lat/0310029
dimer models: D.H. Adams, S. Chandrasekharan, hep-lat/0303003