Efficient simulation methods for quantum field theory and statistical physics models

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Oldenburg, 22.1.15

- common tasks in statistical physics and quantum field theory
- principles of Monte Carlo
- cluster and worm algorithms
- conclusions, outlook

Classical statistical physics

representative example:

$$\langle A \rangle = \frac{1}{Z} \sum_{\sigma} \mathrm{e}^{-\beta H[\sigma]} A[\sigma]$$

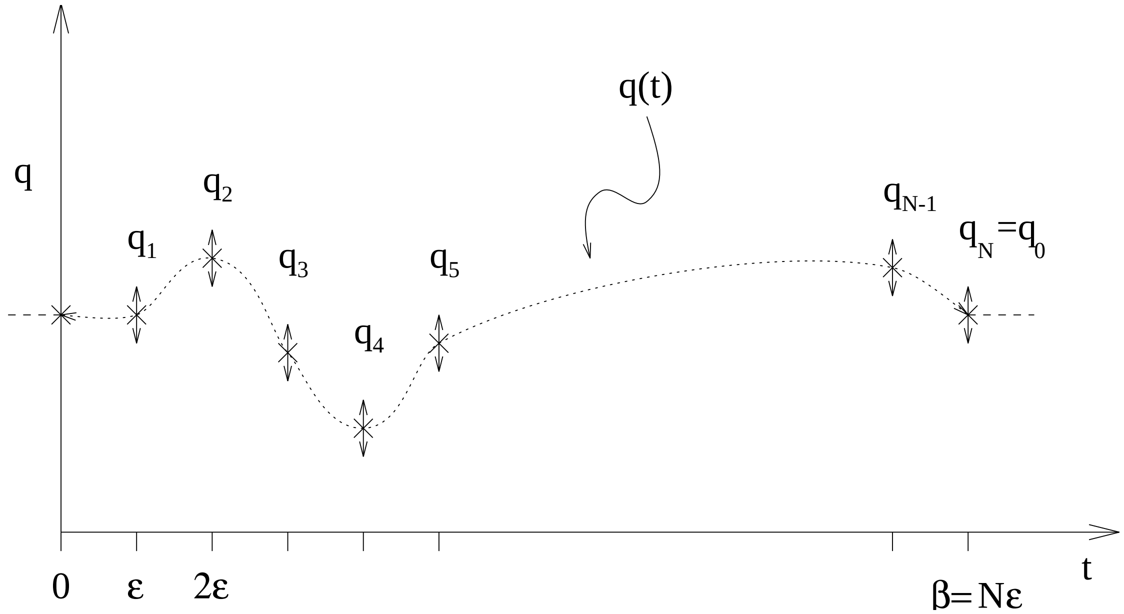
- $\sigma \equiv \{\sigma(x)\}$: (many!!) configurations on a lattice
  - $\sigma(x) = \pm 1$ (Ising), or $\sigma(x) \in S_{N-1}$ sphere, ...
- H: energy of a configuration, $\beta = (kT)^{-1}$
- A: observable, correlation, $A[\sigma] = \sigma(x)\sigma(y)$,...
- Z: normalization ($\langle 1 \rangle = 1$), partition function

$\Longrightarrow$ critical phenomena, phase transitions
universal critical exponents, direct links to condensed matter, ...

Lattice quantum field theory

Feynman path integral

$$\left\langle x \middle| \mathrm{e}^{-\frac{i}{\hbar} t \hat{H}} \middle| y \right\rangle = \int D[q(t)]_{(0,y)\to(t,x)}\, \mathrm{e}^{\frac{i}{\hbar} A[q]}, \quad \text{action}\, A = \int_0^t dt'\,(T - V)$$



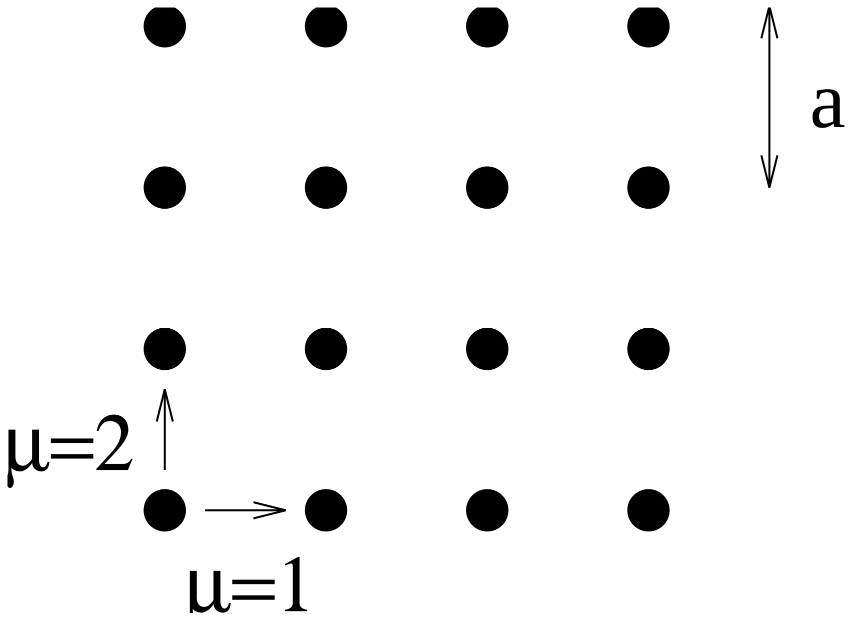
Similar:

$$\mathrm{tr}[\mathrm{e}^{-\beta \hat{H}}] = \int D[q(t)]_{\mathrm{closed}}\, \mathrm{e}^{-\frac{1}{\hbar} S[q]}, \quad \text{action}\, S = \int_0^t dt'\,(T + V) \geqslant 0$$

⇒can be generalized to fields:

$$\langle \varphi_\alpha(x)\varphi_\beta(y)\rangle = \frac{1}{Z}\int D[\varphi_\alpha(t,\vec{r}\,)]\,\varphi_\alpha(x)\varphi_\beta(y)\,\mathrm{e}^{-\frac{1}{\hbar}S[\varphi]}$$

- ∼canonical ensemble in classical statistical physics
- mean-values like $\langle \varphi_\alpha(x)\varphi_\beta(y)\rangle$ allow to extract properties of the excitations, e.g. particle masses, transition amplitudes...
- discretize, space-time lattice: $\int D\varphi \ldots = \prod_x \left(\int_{-\infty}^{\infty} d\varphi(x)\right)\ldots$
- example: $S = \int d^4x \left\{\frac{1}{2}(\partial_\mu\varphi)^2 + \frac{m^2}{2}\varphi^2 + \frac{\lambda}{24}\varphi^4\right\}$
  spin 0 relativistic boson, interaction strength λ



$$\int D\varphi \to \prod_x \int d\varphi(x)$$

$$\partial_\mu \varphi(x) \to \frac{\varphi(x+\hat{\mu}) - \varphi(x)}{a}$$

after reparametrization S (analogous to βH) reads:

$$S[\phi] = -\beta \sum_{\langle xy \rangle} \phi(x)\phi(y) + \sum_x \lambda(\phi^2(x) - 1)^2$$

- for $\lambda \to \infty$ only $|\phi| = 1$ contributes (Ising, $N-$vector model)
- particle physics (masses, scattering) $\leftrightarrow$
  universal correlations at critical point $\equiv$ continuum limit

Monte Carlo

task: $\langle A \rangle = \frac{1}{Z} \sum_\sigma \, \mathrm{e}^{-S[\sigma]} A[\sigma]$

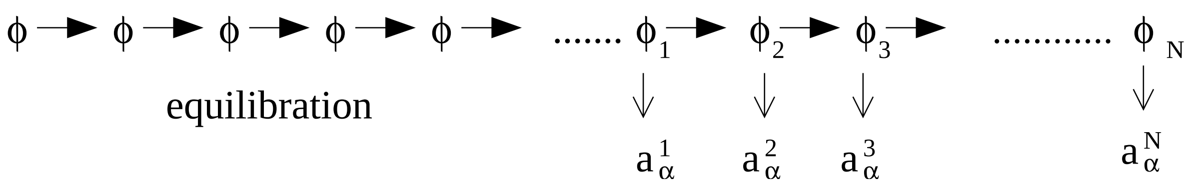
principle idea:

- generate independent random configurations $\sigma_1, \sigma_2, \ldots, \sigma_n$ with the normalized probability $P[\sigma] = \mathrm{e}^{-S[\sigma]}/Z$
- then approximate:

$$\langle A \rangle = \frac{1}{n} \sum_{i=1}^{n} A[\sigma_i] + \mathrm{O}(n^{-1/2})$$

- unfortunately there is no efficient way to generate such σ_i

Markov chain instead:



- $\phi_i \rightarrow \phi_{i+1}$: one step of MC algorithm [iterate!]
- transition probability matrix $\mathcal{M}(\phi \rightarrow \phi')$
- can be designed such that late members of the sequence are distributed with the desired $P[\phi]$
- problem: usually ϕ_i, ϕ_{i+1} differ only little (statist. dependent)

$$\Longrightarrow \text{error}(\langle A \rangle)^2 = \frac{v(A)}{n/2\tau}$$

- variance $v(A)$ independent of $\mathcal{M}$
- $n/2\tau$ = number of effectively independent samples
- at critical points: τ *diverges!* $\propto \xi^z$, often $z \approx 2$
- ξ: correlation length (QFT: ξ=phys. scale/lattice spacing)

algo-designers: get small τ for given CPU effort, dream: $z \approx 0$

Standard local Monte Carlo

usual procedure:

- run through all sites x
- propose a change $\sigma(x) \to \sigma'(x)$ at x only (other $\sigma(y)$ frozen)
- accept new config. with $p = \min(1, \mathrm{e}^{-S'+S})$, else keep old one
- CPU complexity $\propto$ volume (number of sites)

$\rightarrow$ universally applicable

$\rightarrow$ dynamical exponents $z \approx 2$

heuristic explanation:

- re-arrangements of size ξ needed for independent sample
- built from local steps (size one) by diffusion (random walk)
- ξ^2 steps needed
- $\Rightarrow$ collective changes of size ξ desirable, but not easy

Cluster algorithms

naive ideas, like 'propose spin-flip on blocks' (+ sample $e^{-S[\sigma]}$!) never work (zero acceptance), but Swendsen and Wang (1987):

- construct 'auxiliary' percolation clusters for flip

Ising ($\sigma \in \{+1, -1\}$):

$$Z = \sum_{\sigma} \prod_{\langle x\,y \rangle} e^{\beta[\sigma(x)\sigma(y)-1]}$$

on each bond:

$$e^{\beta[\sigma(x)\sigma(y)-1]} = \begin{cases} 1 & \text{if} \quad \sigma(x)=\sigma(y) \\ e^{-2\beta} & \text{else} \end{cases} = e^{-2\beta} + \delta_{\sigma(x),\sigma(y)}(1-e^{-2\beta})$$

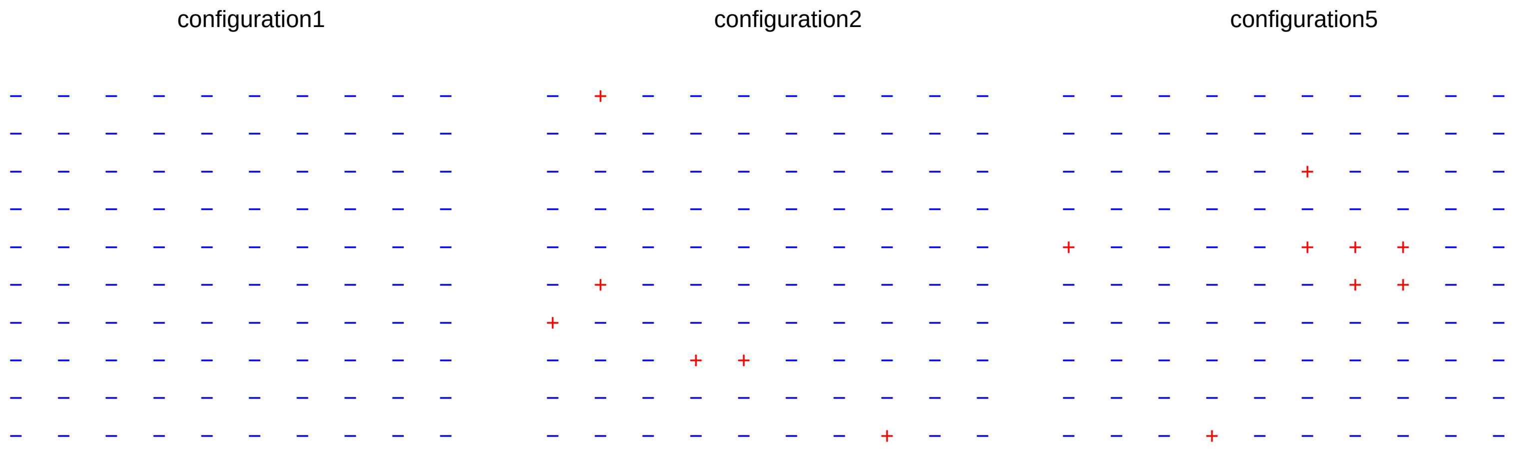
$\Rightarrow$ replace bonds stochastically by a superposition of

- no bond with probability $p = e^{-2\beta}$ (spins independent)
- rigid bond with probability $1-p$ (spins locked)

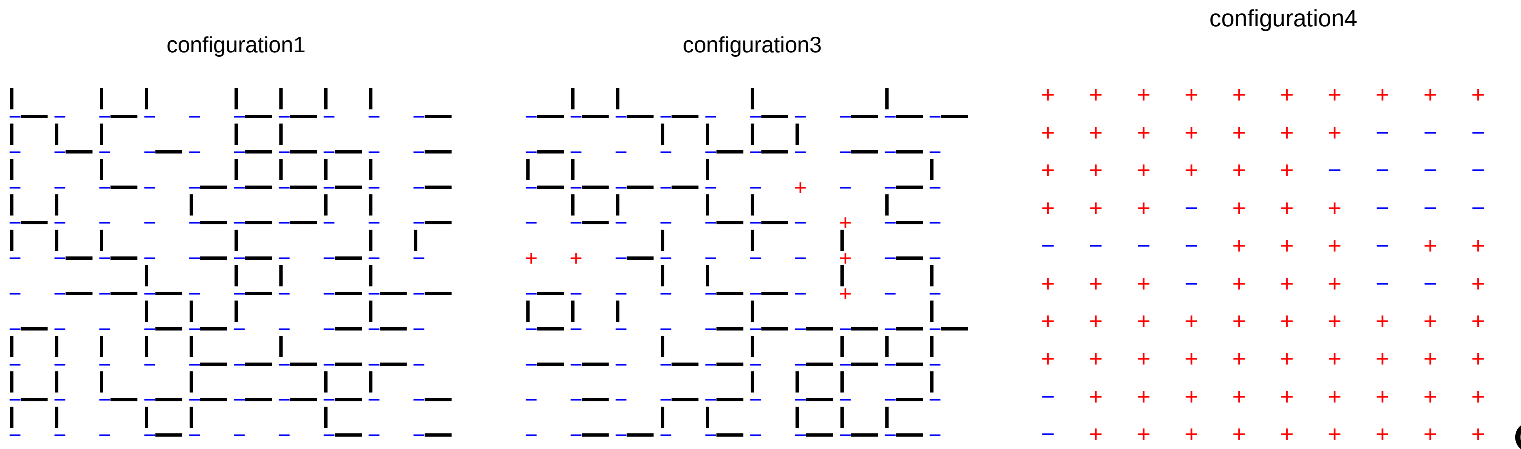
now spin-update (non-local):

- identify groups of locked spins (bond percolation clusters)
- assign random new ± 1 spin to each cluster as a whole

equilibration on 10^2 from $\sigma \equiv -1$ (unbroken phase):



local



cluster

formally:

$$Z = \sum_{b_{\langle xy \rangle}=0,1} \sum_{\sigma} \prod_{\langle xy \rangle} \left(p\delta_{b_{\langle xy \rangle},0} + (1-p)\delta_{b_{\langle xy \rangle},1}\delta_{\sigma(x),\sigma(y)} \right)$$

- alternate between b-updates and $\sigma -$ updates

one easily proves:

$$\langle \sigma(x)\sigma(y) \rangle = \langle \theta(x,y;b) \rangle \propto \mathrm{e}^{-|x-y|/\xi}$$

θ=cluster incidence function:

$$\theta(x,y;b) = \begin{cases} 1 & \text{if } x, y \text{ in one cluster defined by } \{b\} \\ 0 & \text{else} \end{cases}$$

- cluster (updates) have size ξ
- spontaneous magnetization $\Leftrightarrow$ percolation

$\Rightarrow$(almost) no more slowing down, $z = 0 \ldots 0.3$

single cluster variant (UW 1989):

- pick random x
- construct only one cluster attached to x
- flip all spins on this cluster

extension (UW 1989) N-vector model (spins $s(x) \in S_{N-1}$):

- pick a random direction $r \in S_{N-1}$
- decompose: $s(x) = \sigma(x) r |s_r(x)| + s_\perp(x)$
- cluster-update the embedded Ising signs $\sigma(x)$
- it has $\beta \to \beta_{\langle xy \rangle}$; but no problem!
- works even better: $z \approx 0$ (single cluster variant)

Worm algorithm

again explain for Ising, use on each bond $\left[\begin{pmatrix} c \\ s \\ t \end{pmatrix} = \begin{pmatrix} \cosh \\ \sinh \\ \tanh \end{pmatrix} (\beta) \right]$

$$e^{\beta\sigma(x)\sigma(y)} = c + s\sigma(x)\sigma(y) = c \sum_{k=0,1} t^k \, [\sigma(x)]^k [\sigma(y)]^k$$

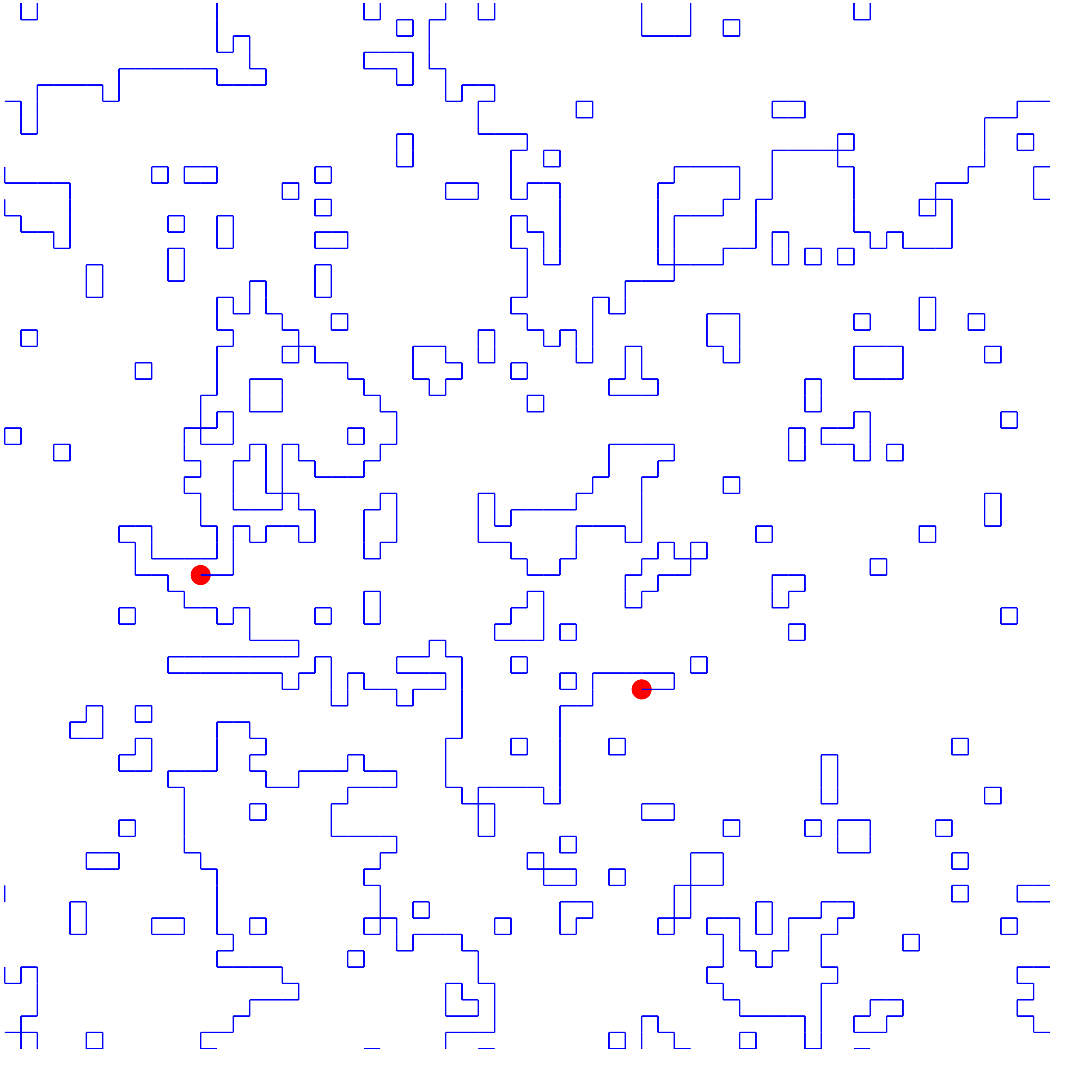
- use this on each bond, $k \to k_{\langle xy \rangle}$
- sum over spins, $\sum_{\sigma=\pm} \sigma^K = \begin{cases} 2 & \text{if} \quad K = \text{even} \\ 0 & \text{if} \quad K = \text{odd} \end{cases}$

$$\sum_{\sigma} e^{-S[\sigma]} \sigma(u)\sigma(v) \propto \sum_{k} t^{\sum_{\langle xy \rangle} k_{\langle xy \rangle}} \Delta(k; u, v)$$

- $\Delta = 1$ iff sites u, v surrounded by odd $\sum k$, other sites even
- reformulation: ‘all order strong coupling expansion’
- convergent: stochastic summation

$$\langle \sigma(x)\sigma(0) \rangle = \langle \delta_{x,u-v} \rangle$$

typical configuration:



Worm algorithm (Prokof'ev, Svistunov, 2001):

- propose move to nearest neighbor $u \to u'$
- with $k_{\langle uu' \rangle} \to 1 - k_{\langle uu' \rangle}$ ($\Rightarrow \Delta = 1$ preserved!)
- weight change $t^k \to t^{1-k}$ accept/reject

Monte Carlo sampling of all graphs in $\tanh(\beta)$ expansion

- almost no slowing down as $\beta \to \beta_c$
- $\delta_{x,u-v}$ is low noise estimator for correlation

successfully generalized to:

- N-vector model, CP(N) models,....

Summary, outlook

- cluster: practically independent sampling for N-vector and some other systems
- worm: reformulated version (all order s.c.) easier to sample; some observables well accessible. Covers more models than cluster
- unsolved (=only 'slow' standard methods available):
  - gauge fields
  - fermions in $D > 2$: quarks, Hubbard model,..
- algorithm research significant part of lattice field theory
- unfortunately more art than systematic
  - needs understanding of the physics
  - use freedom of universality