Tethered Monte Carlo: computing the effective potential without critical slowing down

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In collaboration with:
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Nuclear Physics B 807, 424-454 (2009)
arXiv:0806.0543
Aims

- All known Monte Carlo methods suffer critical or exponential slowing down when applied to important problems: Gauge theories, structural glasses, spin glasses, protein folding, …
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- Can we use external information (e.g. order parameter) to guide the simulations?
- We present here Tethered Monte Carlo, a general method to reconstruct the effective potential for the order parameter.
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We present here Tethered Monte Carlo, a general method to reconstruct the effective potential for the order parameter.

Even if we do not work in the canonical ensemble, canonical expectation values are recovered with high accuracy.
Main features

- **Tethered Ensemble**: original d.o.f. + Gaussian *magnetostat*:

- Related with Creutz microcanonical demon.
  - Continuous demons, coupled to \( m \) rather than to energy.
  - Extensive number of demons.
  - Demons integrated-out: \( \hat{m} \) is conserved globally, but not locally → Local algorithm without critical slowing down (for functions of \( m \)).

- Independent simulations at fixed \( \hat{m} \). Later, reconstruction of canonical effective potential \( \Omega_N \).

- Local algorithm (e.g. Metropolis) straightforward.

- Method demonstrated in the two dimensional Ising model.

- Currently implementing cluster methods: improved estimators promising.
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- Method demonstrated in the *two dimensional Ising model*.
- Currently implementing *cluster methods*: improved estimators promising.
Notations: $D = 2$ Ising model

- **Exact** results available even for *finite* lattices.
- Partition function and main observables:

\[
Z = \sum_{\{\sigma_x\}} e^{\beta \sum_{\langle x,y \rangle} \sigma_x \sigma_y + h \sum_x \sigma_x}, \quad \sigma_x = \pm 1,
\]

\[
U = Nu = - \sum_{\langle x,y \rangle} \sigma_x \sigma_y, \quad M = Nm = \sum_x \sigma_x.
\]

- Second order phase transition at $\beta_c = 0.440686 \ldots$
The Tethered Ensemble (I)

- Canonical pdf for order parameter \((h = 0)\),

\[
p_1(m) = \frac{1}{Z} \sum_{\{\sigma_x\}} \exp[-\beta U] \delta \left( m - \sum_i \frac{\sigma_i}{N} \right)
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- Extend configuration space with \(N\) decoupled Gaussian demons

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Z = \int_{-\infty}^{\infty} \prod_{i=1}^{N} d\eta_i \sum_{\{\sigma_x\}} \exp\left[-\beta U - \sum_i \eta_i^2 / 2\right], \quad R = Nr = \sum_i \eta_i^2 / 2.
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- \(r\) (almost) Gaussian distributed, \(r = \frac{1}{2} + \frac{\zeta}{\sqrt{N}}, \ |\zeta| \sim 1. \)
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- $r$ (almost) Gaussian distributed, $r = \frac{1}{2} + \frac{\xi}{\sqrt{N}}, |\xi| \sim 1$.

- Let $\hat{m} = m + r$. Its pdf is a convolution ($m$ and $r$ independent) $\rightarrow p(\hat{m} = m + \frac{1}{2})$ is a smoothing of $p_1(m)$. 
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- Let \( \hat{m} = m + r \). Its pdf is a convolution \((m \text{ and } r \text{ independent}) \rightarrow \)

\[
p(\hat{m} = m + \frac{1}{2}) \text{ is a smoothing of } p_1(m).
\]

- A smooth \( p(\hat{m}) \) has an effective potential \( \Omega_N(\hat{m}, \beta) \)

\[
p(\hat{m}) = \frac{1}{Z} \int_{-\infty}^{\infty} \prod_{i=1}^{N} d\eta_i \sum_{\{\sigma_x\}} e^{-\beta U - \sum_i \eta_i^2/2} \delta\left(\hat{m} - m - \sum_i \frac{\eta_i^2}{2N}\right) = e^{N\Omega_N(\hat{m}, \beta)}
\]
The tethered ensemble (II)

Integrating demons out in the constrained (fixed $\hat{m}$) partition function $\to$ tethered expectation values:

$$\langle O \rangle_{\hat{m}, \beta} = \frac{\sum_{\{\sigma_x\}} O(\hat{m}; \{\sigma_x\}) \omega(\beta, \hat{m}, N; \{\sigma_x\})}{\sum_{\{\sigma_x\}} \omega(\beta, \hat{m}, N; \{\sigma_x\})},$$

The canonical $\Omega_N$ follows from Fluctuation-Dissipation

$$\hat{h}(\hat{m}; \{\sigma_x\}) = -\frac{1}{N} + \frac{N}{2} - \frac{1}{\hat{M} - \hat{m}} = \Rightarrow \langle \hat{h} \rangle_{\hat{m}, \beta} = \frac{\partial \Omega_N(\hat{m}, \beta)}{\partial \hat{m}}.$$
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- Integrating demons out in the \textit{constrained} (fixed \( \hat{m} \)) partition function \( \rightarrow \) tethered expectation values:

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\[
\omega(\beta, \hat{m}, N; \{\sigma_x\}) = e^{-\beta U + M - N \hat{m}} (\hat{m} - m)^{(N-2)/2} \theta(\hat{m} - m).
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- The *canonical* $\Omega_N$ follows from Fluctuation-Dissipation

\[
\hat{h}(\hat{m}; \{\sigma_x\}) = -1 + \frac{N/2 - 1}{\hat{M} - M} \quad \implies \quad \langle \hat{h} \rangle_{\hat{m}, \beta} = \frac{\partial \Omega_N(\hat{m}, \beta)}{\partial \hat{m}}.
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Numerical methods

Steps

1. Select a mesh of \( \hat{m} \) values.

\[
\exp[N \Omega_N(\beta, \hat{m})] \quad \text{Lineal scale}
\]

\[
\log \quad \text{Log scale}
\]

- Tethered: \( \langle u \rangle_{m, \beta} = -1.419 \)
- Exact: \( \langle u \rangle_{\beta, c} = -1.419 \)
Numerical methods

Steps

1. Select a mesh of $\hat{m}$ values.
2. Independent simulation for each $\hat{m}$. Get $\langle O \rangle_{\hat{m}, \beta}$.

Tethered: $\langle u \rangle_{\beta}^{c} = -1.41905$.
Exact: $\langle u \rangle_{\beta}^{c} = -1.419076 \ldots$
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3. $\langle O \rangle_{\hat{m},\beta}$ smooth functions of $\hat{m}$ → interpolate (e.g. spline).
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4. Numerical integration of $\langle \hat{h} \rangle_{\hat{m}, \beta}$ yields $\Omega_N(\hat{m}, \beta)$. 

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5. Reconstruct canonical \( \langle O \rangle_\beta \) from \( p(\hat{m}) \) and \( \langle O \rangle_{\hat{m},\beta} \).
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Tethered: $\langle u \rangle_{\beta}^{\text{c}} = -1.41905$.

Exact: $\langle u \rangle_{\beta}^{\text{c}} = -1.419076$.

Graphs showing $\exp[N \Omega_N(\beta, \hat{m})]$ in lineal and log scale for $L = 128$. Tethered averages and exact canonical value.
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Tethered: $\langle u \rangle_{\beta_c} = -1.41905(5)$
Exact: $\langle u \rangle_{\beta_c} = -1.419076 \ldots$
Autocorrelation times

- $\tau_{\text{int}}$: dramatic dependence on observable, and on $\hat{m}$.
- Functions of $m$ (e.g. $\hat{h}$): no measurable critical slowing down.
- Energy or propagator's Fourier transform ($\vec{k} \neq 0$)
  $\tau_{\text{int}}(\hat{m} = 0.5) \approx L^2$
- Worst case: $m \sim 0$ or $\hat{m} = \frac{1}{2}$.
Results at the critical point

- $\exp[N \Omega_N(\beta, \hat{m})]$
- $L = 16$
- $L = 32$
- $L = 64$
- $L = 128$

Parameters
- 51 points in $\hat{m}$ mesh for $L \leq 256$.
- 77 points in $\hat{m}$ mesh for $L \geq 512$.
- $10^7$ Metropolis sweeps per $\hat{m}$.
- Comparison with Ferdinand and Fisher's exact results for finite $L$.

<table>
<thead>
<tr>
<th>$L$</th>
<th>Energy</th>
<th>Specific heat</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TMC</td>
<td>Exact</td>
</tr>
<tr>
<td>32</td>
<td>-1.43369(4)</td>
<td>-1.433659…</td>
</tr>
<tr>
<td>64</td>
<td>-1.42397(4)</td>
<td>-1.423938…</td>
</tr>
<tr>
<td>128</td>
<td>-1.41905(5)</td>
<td>-1.419076…</td>
</tr>
<tr>
<td>256</td>
<td>-1.41663(5)</td>
<td>-1.416645…</td>
</tr>
<tr>
<td>512</td>
<td>-1.41542(4)</td>
<td>-1.415429…</td>
</tr>
<tr>
<td>1024</td>
<td>-1.41489(5)</td>
<td>-1.414821…</td>
</tr>
</tbody>
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Results in an external field: magnetization $m(h)$

- No new simulations needed to obtain results in a field
- Just shift $\Omega_N(\hat{m}, \beta) \rightarrow \Omega_N(\hat{m}, \beta) - \hat{m}h$, and normalize $p(\hat{m}, \beta, h)$. 

![Graph showing magnetization $m(\beta)$ vs. field $h$ for different system sizes $L$.]
A funny way of computing the anomalous dimension

\[ p(\hat{m}, \beta_c, L) = \frac{1}{L^\beta} f \left( \frac{\beta}{\nu} (\hat{m} - \frac{1}{2}) \right) \]
A funny way of computing the anomalous dimension

- $p(\hat{m}, \beta_c, L) = L^{\frac{\beta}{\nu}} f \left( L^{\frac{\beta}{\nu}} (\hat{m} - \frac{1}{2}) \right)$

- $p(\hat{m})$ has two peaks at $m^{\pm} + \frac{1}{2}$:
  
  $m^{\pm} \propto L^{-\frac{\beta}{\nu}}$, $\eta = 2 - D + \frac{2\beta}{\nu}$
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Finding maxima numerically ill conditioned. Finding roots is OK:

\[ 0 = \langle \hat{h} \rangle^{\frac{1}{2} + m^\pm \beta_c} \]
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\[ m^\pm \propto L^{-\frac{\beta}{\nu}}, \eta = 2 - D + \frac{2\beta}{\nu} \]

Finding maxima numerically ill conditioned. Finding roots is OK:
\[ 0 = \langle \hat{h} \rangle^{\frac{1}{2}} + m^\pm, \beta_c \] (byproduct, simulation not optimized to this aim)

\[ m^\pm = L^{-\frac{1}{8}} [A + BL^{-\frac{7}{4}}], \chi^2/\text{dof} = 0.98/4^(-), 2.85/4^+(+) \]

<table>
<thead>
<tr>
<th>( L )</th>
<th>(-m^-_{\text{peak}})</th>
<th>( m^+_{\text{peak}})</th>
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<td>32</td>
<td>0.764 01(10)</td>
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<td>0.703 0(2)</td>
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We presented **Tethered Monte Carlo**, a general strategy to compute the *canonical* effective potential.

Observables that depend only on the order parameter, for instance $\hat{\mathbf{h}}$, do not suffer critical slowing down ($\hat{\mathbf{m}}$ is conserved only globally).

New opportunities: to compute anomalous dimension, just solve $0 = \langle \hat{h} \rangle \hat{m}$, $\beta_c$. No need to simulate the full $\hat{m}$ range.

Promising when suffering from large tunneling barriers associated to the order parameter: Random Field Ising Model, Diluted antiferromagnets on a field, Condensation transition, . . .
We presented Tethered Monte Carlo, a general strategy to compute the canonical effective potential. Metropolis simulation straightforward and no more costly than a canonical simulation (look-up-table).

Particularly efficient in the presence of a magnetic field, or in the broken symmetry, low temperature phase. Observables that depend only on the order parameter, for instance $\hat{h}$, do not suffer critical slowing down ($\hat{m}$ is conserved only globally).

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