Optimized statistical ensembles
for slowly equilibrating classical and quantum systems

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Many interesting phenomena in complex many-body systems arise only in the presence of

- multiple energy scales
- complex energy landscapes
- slow equilibration

Motivation
Random walk in temperature space increases equilibration.
Simulation of Markov chains

Monte Carlo, parallel tempering, replica exchange molecular dynamics

- Sample configurations in **phase space**

\[ C_1 \rightarrow C_2 \rightarrow \ldots \rightarrow C_i \rightarrow C_{i+1} \rightarrow \ldots \]

**Metropolis algorithm (1953)**

- **Propose** a (small) **change** to a configuration

\[ c_i \rightarrow c_j \]

- **Accept/reject** the update with probability

\[ p_{acc} = \min \left( 1, \frac{w(c_j)}{w(c_i)} \right) \]

How do we choose these weights?
Sample configurations in **phase space**

\[ c_1 \rightarrow c_2 \rightarrow \ldots \rightarrow c_i \rightarrow c_{i+1} \rightarrow \ldots \]

Project onto random walk in **energy space**

\[ E_1 \rightarrow E_2 \rightarrow \ldots \rightarrow E_i \rightarrow E_{i+1} \rightarrow \ldots \]

We define a **statistical ensemble**

\[ w(c_i) = w(E_i) = \exp(-\beta E_i) \]

\[ p_{acc}(E_1 \rightarrow E_2) = \min \left( 1, \frac{w(E_2)}{w(E_1)} \right) = \min \left( 1, \exp(-\beta \Delta E) \right) \]
Statistical ensembles

- Sample configurations in **phase space**
  \[ C_1 \rightarrow C_2 \rightarrow \ldots \rightarrow C_i \rightarrow C_{i+1} \rightarrow \ldots \]

- Project onto random walk in **energy space**
  \[ E_1 \rightarrow E_2 \rightarrow \ldots \rightarrow E_i \rightarrow E_{i+1} \rightarrow \ldots \]

- **Phase space:** The simulated system does a biased, but **Markovian** random walk.

- **Energy space:** The projected random walk is **non-Markovian**, as memory is stored in the system’s configuration.
Extended ensemble simulations

- Broaden the sampled energy space, e.g. by sampling a flat histogram.

\[
\begin{align*}
    w(E) &= \exp(-\beta E) \\
    w(E) &= 1/g(E)
\end{align*}
\]

\[ n_w(E) = w(E) g(E) \]

Multicanonical simulations, Berg & Neuhaus
Wang-Landau algorithm
How well does this work?

The energy range scales like \( N \).

\[ E \sim N \]

The round-trip time should scale like \( N^2 \).

\[ \tau \sim N^2 \]

Flat-histogram sampling

\[ \tau \sim N^{2+z} \]

Critical slowing down.

The fully frustrated Ising model

\[ z = 0.9 \]

ferromagnetic Ising model

\[ z = 0.4 \]
The problem: local diffusivity not constant

\[ D(E, t_D) = \langle [E(t) - E(t + t_D)]^2 \rangle / t_D \]

- The **local diffusivity** is NOT independent of the energy.
Optimizing the ensemble

Measure the **current** in the energy interval

\[ j = D(E) \cdot n_w(E) \cdot \frac{df}{dE} \]

Determine the **local diffusivity**.

**Maximize** current by varying histogram/ensemble.

Optimizing the ensemble (cont’d)

**Optimal histogram** turns out to be

\[ n_{w}^{(opt)}(E) \propto \frac{1}{\sqrt{D(E)}} \]

**Ensemble optimization algorithm**

**Feedback** the local diffusivity

\[ w'(E) \propto w(E) \cdot \sqrt{\frac{df}{dE}} \cdot \frac{1}{n_w(E)} \]

optimized ensemble

and **iterate** feedback until convergence.

• Feedback reallocates resources towards the critical energy.
Performance of optimized ensemble

The round-trip times scale like $O\left([N \log N]^2\right)$. 

speedup $\sim 100$
Example

Folding of a (small) protein

ST, M. Troyer, U.H.E. Hansmann
A small protein: HP-36

The chicken villin headpiece

folding time: 4.3 microseconds
Parallel tempering


Simulate **multiple replicas** of the system at various temperatures.

Single replica performs **random walk** in temperature space.

\[ p(E_i, T_i \to E_{i+1}, T_{i+1}) = \min(1, \exp(\Delta \beta \Delta E)) \]

How do we choose the temperature points?
Ensemble optimization

Feedback algorithm

Measure **local diffusivity** $D(T)$ of current in temperature space.

**Optimal choice** of temperatures

$$\eta_{\text{opt}}(T) \sim \frac{1}{\sqrt{D(T)}}$$

density of $T$-points

**Iterate** feedback of diffusivity.
Random walk in temperature

- Multiple temperature scales are revealed by the local diffusivity.
Feedback reallocates resources towards the relevant temperature scales.
Example

Strong first-order transitions

B. Bauer, E. Gull, ST, M. Troyer, and D.A. Huse
The large-$Q$ Potts model

$Q = 250$

Energy $E / 2N$

Optimized histogram

Canonical histogram

Droplet formation

Droplet stripe transition

Droplet stripe transition
Example

Quantum systems

S. Wessel, N. Stoop, E. Gull, ST, M. Troyer
Quantum systems

Reconsider the high-temperature series expansion

\[ Z = \text{Tr} \ e^{-\beta H} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \text{Tr} \ (-H)^n = \sum_{n=0}^{\infty} g(n) \beta^n \]

coefficients

“density of states”

We can define a broad-histogram ensemble in the expansion order.


Stochastic series expansion (SSE) samples these coefficients

\[ n \to 0 \quad \text{high temperatures} \]

\[ \langle n \rangle \propto \beta N \]

\[ n \to \infty \quad \text{low temperatures} \]
Examples

**Thermal first-order transition**

hard-core bosons with next-nearest neighbor repulsion

\[ H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) + V_2 \sum_{\langle\langle i,k \rangle\rangle} n_i n_k - \mu \sum_i n_i \]

\[ \Lambda = 20 L^2 \]

**Spin-flop transition**

spin-1/2 XXZ model in a magnetic field

\[ H = J \sum_{\langle i,j \rangle} \left[ S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z \right] - h \sum_i S_i^z \]

\[ \Lambda_{\delta h} = 500 \]
Summary

Metropolis cycle

- configuration
- suggest an update
- accept/reject an update

- non-local update schemes: loops, worms, ...
- unconventional statistical ensembles

- improve sampling efficiency & overcome entropic barriers


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