JÜLICH FORSCHUNGSZENTRUM

Optimized parallel tempering Monte Carlo

September 27, 2010 | Marco Müller

Overview

1. Introduction
   - The Ising Model
   - Fundamental Quantities in Statistical Physics
2. Monte Carlo Methods
   - Simple sampling
   - Importance sampling
   - Metropolis-Algorithm
   - Parallel Tempering
3. Results

Motivation

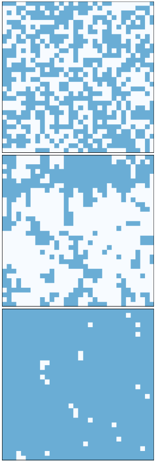
- (classical) Thermodynamics is well understood, lacks details
  - Out-of-equilibrium physics, structure formation?
  - Phase transitions?
  - Systems with $\approx 10^{23}$ particles
  - Known dynamics, but impractical to trace all particles

- Statistical Mechanics: approach by statistical methods

Ising Model

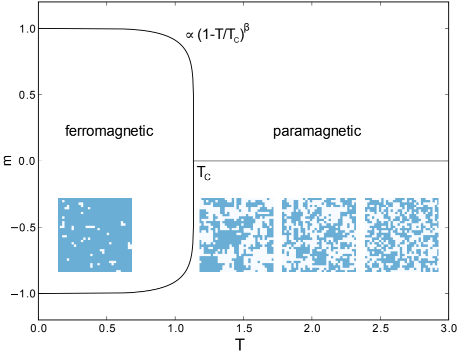
$$\mathcal{H} = -J \sum_{\langle i,k \rangle} \delta_{s_i s_k} \qquad s_i \in \{0, 1\}$$

- Many elementary magnets interacting with a coupling constant J
- Every magnet can be "up" or "down"
- Solved in 1d by [Ising, 1925]
- 2d-regular lattices:
  - Exact solution by [Onsager, 1944]
  - Exact calculation of the density of states *finite and periodic* regular lattices by [Beale, 1996]



Phase transition

- Continuous phase transition at Curie-temperature T_c, classification by critical exponents



- Ferromagnetic: m is preserved after an external field was removed
- Paramagnetic: $m = 0$, an external field is reinforced

Fundamental quantities

- Probability of finding a microstate with energy E_i for a system in a heat bath with temperature T:

$$\mathcal{P}^B(E_i) \propto e^{-\frac{E_i}{k_B T}} \qquad \beta := \frac{1}{k_B T}$$

- (canonical) partition function:

$$\mathcal{Z} = \sum_{\{\text{all states}\}} e^{-\beta E_i} = \sum_i \Omega(E_i) e^{-\beta E_i}$$

$\Omega(E_i) \ldots$ density of states with energy E_i

Exact enumeration

$$\mathcal{Z} = \sum_{\{\text{all states}\}} e^{-\beta E_i}$$

- Estimate for the 2d Ising magnet:

lattice size: $L \times L = 10 \times 10$
number of states: $2^{L \times L} \approx 10^{30}$
fast computer: $10^{-9}s/\text{spin-flip} \cdot 100\,\text{spins}$
$10^{-7}s/\text{configuration}$

$$\approx 10^{23}s \approx 10^{15}y \gg 10^{10}y \quad \text{age of the universe}$$

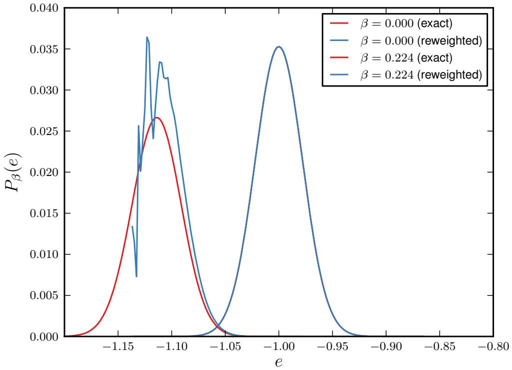
Better method?

Simple Sampling

while *not enough statistics* **do**
    for *every spin in the system* **do**
        draw a random number $r \in [0, 1)$;
        if $r < 0.5$ **then**
            set spin 0
        else
            set spin 1
        end
    end
    measure energy;
end

- $\mathcal{P}^B(E_i) = \frac{1}{\mathcal{Z}} e^{-\beta E_i}$
- Samples the disordered states $\beta = 0 \quad (T \to \infty)$

Simple Sampling (10^{11} samples)



$$\mathcal{Z} = \sum_i \Omega(E_i) e^{-\beta E_i}$$

Simple Sampling

```
while not enough statistics do
    for every spin in the system do
        draw a random number r∈ [0, 1);
        if r<0.5 then
            set spin 0
        else
            set spin 1
        end
    end
    measure energy;
end
```

Simple Sampling

```
while true do
    for every spin in the system do
        draw a random number r∈ [0, 1);
        if r<0.5 then
            set spin 0
        else
            set spin 1
        end
    end
    measure energy;
end
```

Importance Sampling

- Need for suitable algorithm to draw configurations according to their Boltzmann weight $\mathcal{P}^B$
- Set up a Markov chain

$$\ldots \xrightarrow{p_{ij}} \{s_j\} \xrightarrow{p_{jk}} \{s_k\} \xrightarrow{p_{kl}} \ldots$$

- Allows to calculate expectation values as mean over a finite chain of length N

$$\langle \mathcal{O} \rangle = \sum_{\{s_i\}} \mathcal{O}(\{s_i\})\mathcal{P}^B \approx \frac{1}{N} \sum_{j=1}^{N} \mathcal{O}(\{s_i\}_j)$$

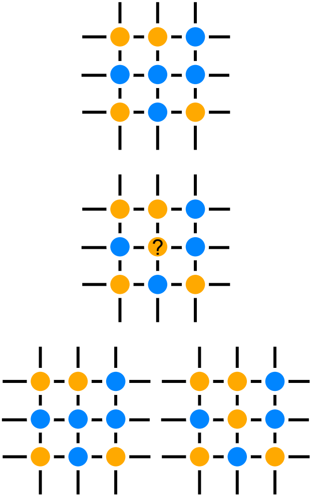
Metropolis Algorithm

- Update scheme for every system that allows the calculation of the energy of a state (discrete or continuous, short-range and long-range interactions, (off-)lattice, ...)
- Proposed by [Metropolis et al., 1953]

$$p_{ij} = \begin{cases} 1 & E_j < E_i \\ e^{-\beta(E_j - E_i)} & E_j \geq E_i \end{cases}$$

Metropolis Algorithm for spin models

initialize (system, initial state, geometry...);
while *not having enough measurements* **do**
  choose a spin;
  choose a new value for that spin;
  draw a random number r $\in (0, 1]$;
  if $r < p_{ij}^{metr}$ **then**
    accept new state;
  else
    reject new state;
  end
  if *system in equilibrium;*
  then
    measure observables;
  end
end



Parallel Tempering

- Problem: Application of Metropolis method extremely inefficient for systems exhibiting a particularly complex transition behaviour (e.g. spin glasses, proteins,. . .)
- Improvements: cluster updates
- Generalized methods:
  - multicanonical sampling
    [Berg and Neuhaus, 1991]
  - Wang-Landau method
    [Wang and Landau, 2001]
  - parallel tempering
    [Swendsen and Wang, 1986], [Geyer, 1991], [Hukushima and Nemoto, 1996]

Parallel Tempering

- Basic idea: after local updates, update full configuration

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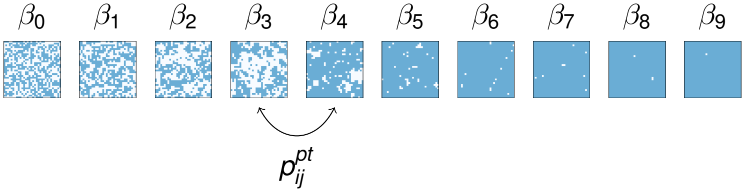

- Metropolis criterion: valid updates with probability

$$p_{ij}^{pt} = \min(1, e^{\Delta}) \qquad \Delta = (\beta_j - \beta_i)\left[E_j - E_i\right]$$

Parallel Tempering

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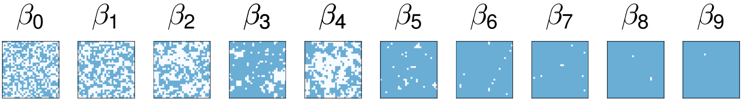
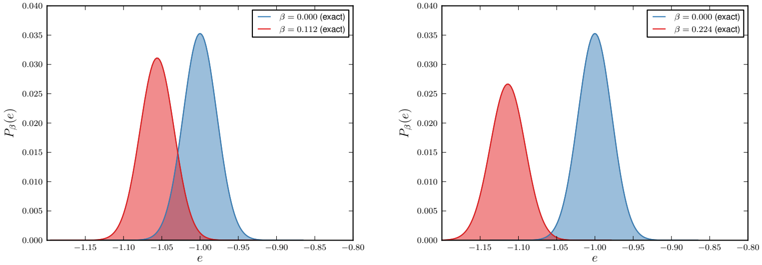


- Metropolis criterion: valid updates with probability

$$p_{ij}^{pt} = \min(1, e^{\Delta}) \qquad \Delta = (\beta_j - \beta_i)\,[E_j - E_i]$$

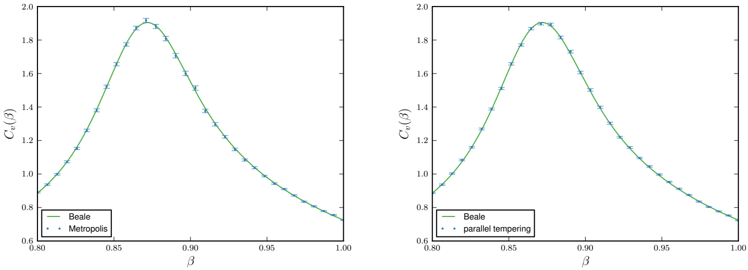
Parallel Implementation

- Exchange inverse temperatures instead of configurations
- Master-slave vs. exchange by each process
- Update attempts only on (β-)adjacent systems



First Results

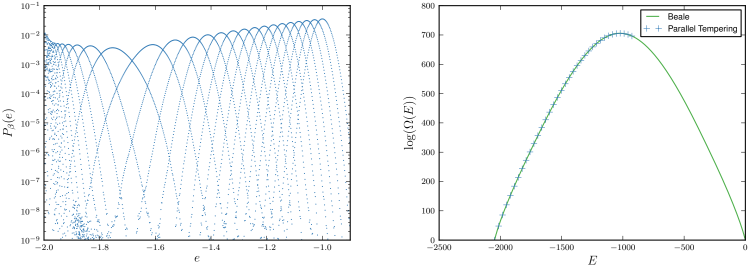
- Verification by Jackknifing time series



Specific heat near the critical point of the 2d-Potts-Model, simulated using the Metropolis algorithm (left) and parallel tempering (right) with the following parameters: $q = 2$, grid dimensions = 32×32, number of energies = 2^{17}, number of jackknife blocks = 2^9

First Results

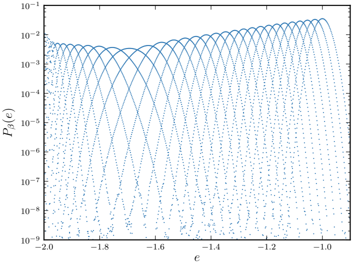
- Verification with histogram-reweighting

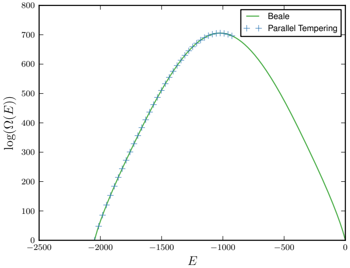


Single histograms for 32 inverse temperatures (left) and density of states after Ferrenberg-Swendsen reweighting (right); parameters: $q = 2$, grid dimensions = 32×32, number of energies = 2^{20}, number of jackknife blocks = 2^{12}

Optimizations – β-Distribution

- Choosing the inverse temperatures:
  - with constant spacing
  - with constant overlap of the histograms





Single histograms for 32 inverse temperatures (left) and density of states after Ferrenberg-Swendsen reweighting (right); parameters: $q = 2$, grid dimensions = 32×32, number of energies = 2^{20}, number of jackknife blocks = 2^{12}

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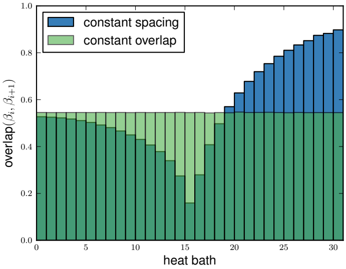

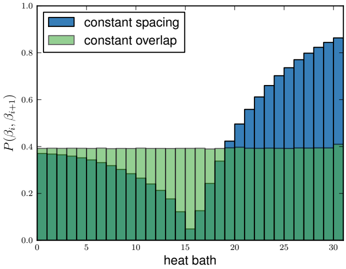

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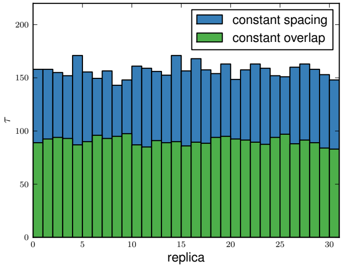
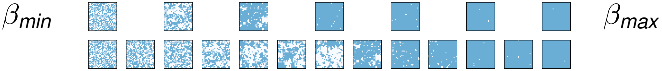


Achievements

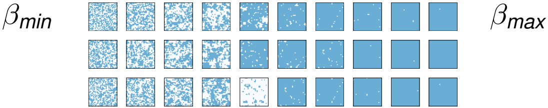
- Development of parallel tempering Monte Carlo simulation in C++ using MPI
- $\mathcal{H} = -\sum_{<i,j>} J_{ij}\delta_{s_i s_j} \qquad s_i \in \{0 \ldots q\}$
- Hypercubic lattice with arbitrary dimensions
- configuration file for simulation parameters
- Surrounding Python scripts for data analysis, histogram reweighting, plotting

Future Plans

- Refinement of the beta distribution



- Multiplexing



- Multithreading on shared memory (GPGPU)

Further reading I

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