

Monte Karlo simulacije u statističkoj fizici. Metropolisov algoritam primenjen na mnogo putanja.

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Departman za fiziku
Univerzitet u Novom Sadu

Seminar Departmana za fiziku

Novi Sad, 04.11.2016.

Pregled predavanja

1 Uvod

2 Metropolisov rad

3 Naš rad

Multipath Metropolis Simulation: an Application to the Classical Heisenberg Model



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Multipath Metropolis simulation: An application to the classical Heisenberg model



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Motivacija

- MCMC - Markov chain Monte Carlo - nastao u Los Alamosu.

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- Stan Ulam - pasijans.

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- Stan Ulam - pasijans.
- -Nojman, Fermi, Metropolis.

Naziv dobio po kazinu u Las Vegasu gde je Ulamov otac ostavio poprilično novca.

Pregled predavanja

- 1 Uvod
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Impakt

- Metropolis, Rosenbluth, Teller, Teller, Equation of State Calculations by Fast Computing Machines (1953)

Impakt

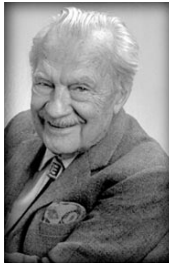
- Metropolis, Rosenbluth, Teller, Teller, Equation of State Calculations by Fast Computing Machines (1953)
- Do danas citiran 32747 puta. Izvor google scholar.

Po prvom autoru rada dobio naziv Metropolisov algoritam.

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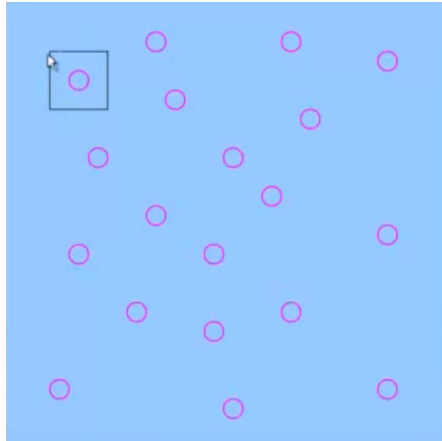
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Multipath Metropolis Simulation: an Application to the Classical Heisenberg Model



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- 2. Ako je promena energije $\Delta E > 0$ prihvatimo izmenu sa verovatnoćom $\exp(-\frac{\Delta E}{k_B T})$.

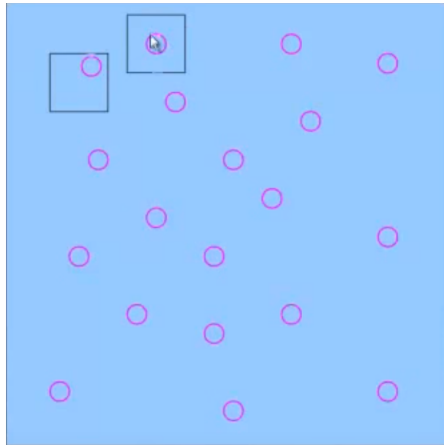
Impakt

- Metropolisov algoritam
- 1. Ako je promena energija $\Delta E < 0$ prihvatimo izmenu u konfiguraciji.
- 2. Ako je promena energije $\Delta E > 0$ prihvatimo izmenu sa verovatnoćom $\exp(-\frac{\Delta E}{k_B T})$.
- Uvodimo slučajan broj ξ između 0 i 1 i ako je $\xi < \exp(-\frac{\Delta E}{k_B T})$ konfiguracija se prihvata (molekul se pomeri unutar kvadrata). Ako ne vraćamo molekul u prvobitan položaj.

Multipath Metropolis Simulation: an Application to the Classical Heisenberg Model



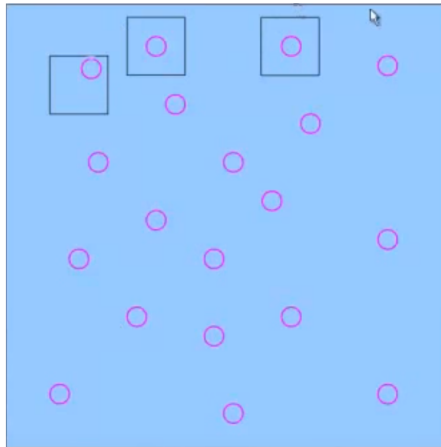
Multipath Metropolis Simulation: an Application to the Classical Heisenberg Model



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Pol Štern i Nikolas Metropolis igraju šah protiv Maniac-a

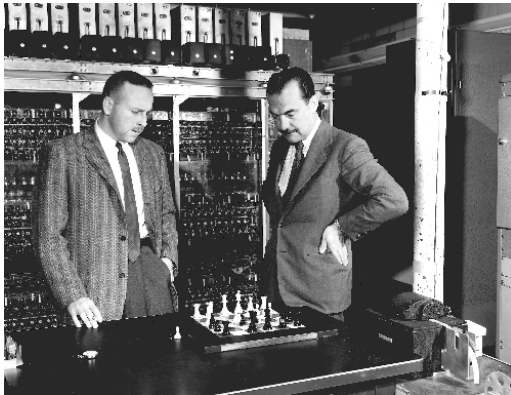
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-

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Markovljevi lanci

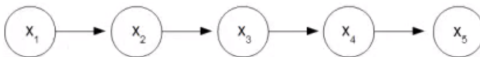
- Markovljevi lanci

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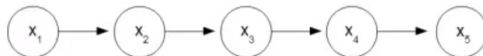
Markovljevi lanci

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- $p(x_5 | x_4, x_3, x_3, x_1) = p(x_5 | x_4)$

Gospodin Tompkins

- Usnijmo fiziku

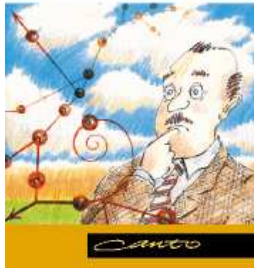
Gospodin Tompkins

- Usnijmo fiziku
- Avanture gospodina Tompkinsa.

Gospodin Tompkins

- Usnijmo fiziku
- Avanture gospodina Tompkinsa.

Mr Tompkins
in Paperback
GEORGE GAMOW



Kristali

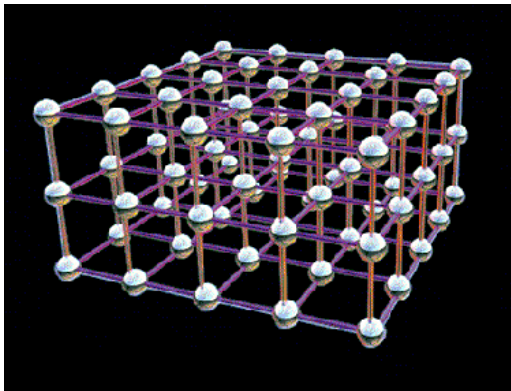
- Kristali

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Markovljevi lanci

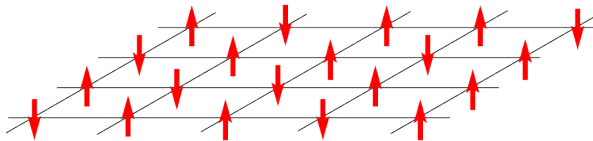
- 2d Izingov model

Markovljevi lanci

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-

Markovljevi lanci

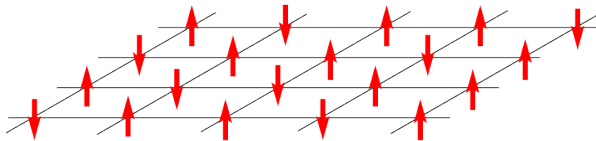
- 2d Izingov model



2-D Ising Model

Markovljevi lanci

- 2d Izingov model



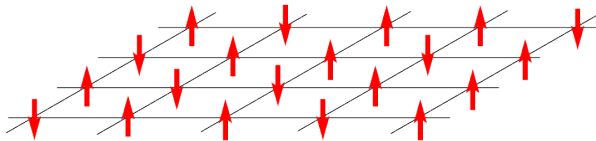
2-D Ising Model

- Hamiltonova funkcija (feromagnet)

Markovljevi lanci

- 2d Izingov model

-



2-D Ising Model

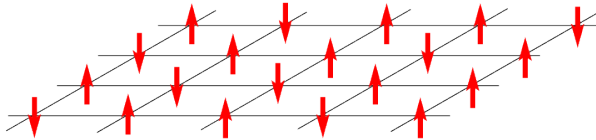
- Hamiltonova funkcija (feromagnet)

- $$H = E = -\frac{J}{2} \sum_{\vec{n}, \vec{\lambda}} S_{\vec{n}} S_{\vec{n}+\vec{\lambda}}$$

Markovljevi lanci

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2-D Ising Model

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- $$H = E = -\frac{J}{2} \sum_{\vec{n}, \vec{\lambda}} S_{\vec{n}} S_{\vec{n}+\vec{\lambda}}$$

- $S_{\vec{n}} = \pm 1$

Markovljevi lanci

- 2 čvora (2 spina)

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Markovljevi lanci

- 2 čvora (2 spina)



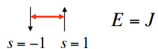


Diagram showing two spins, $s = -1$ and $s = 1$, with arrows pointing in opposite directions (antiparallel). A red double-headed arrow connects the two spins, indicating an interaction energy $E = J$.

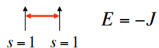


Diagram showing two spins, $s = 1$ and $s = 1$, with arrows pointing in the same direction (parallel). A red double-headed arrow connects the two spins, indicating an interaction energy $E = -J$.



Markovljevi lanci

- 2 čvora (2 spina)





$$s = -1 \quad s = 1 \quad E = J$$



$$s = 1 \quad s = 1 \quad E = -J$$

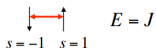


- prvi slučaj: $E = -J \cdot 1 \cdot (-1) = J$

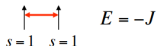
Markovljevi lanci

- 2 čvora (2 spina)





$$s = -1 \quad s = 1 \quad E = J$$



$$s = 1 \quad s = 1 \quad E = -J$$



- prvi slučaj: $E = -J \cdot 1 \cdot (-1) = J$
- drugi slučaj: $E = -J \cdot 1 \cdot 1 = -J$

Markovljevi lanci

- Beskonačna rešetka

Markovljevi lanci

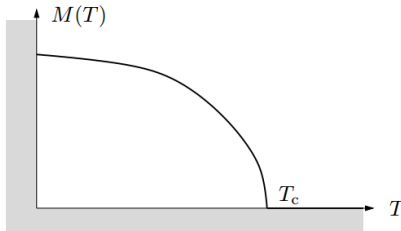
- Beskonačna rešetka
- Kritična temperatura za 2d Izing na kvadratnoj rešetki $\frac{k_B T_c}{J} = 2.269$

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Markovljevi lanci

- Ciklični granični uslovi
Slika preuzeta iz master rada Miloša Adamovića

Markovljevi lanci

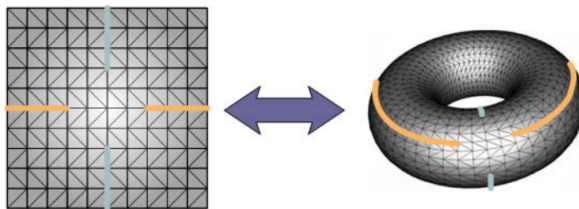
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-

Markovljevi lanci

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-



Impakt

- Monte Karlo srednja vrednost

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- $\langle A \rangle = \frac{1}{N} \sum_{i=1}^N A_i$

Impakt

- magnetizacija

$$\langle M \rangle = \frac{1}{N} \sum_{i=1}^N |M_i|$$

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- magnetizacija

$$\langle M \rangle = \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} |M_i|$$

- srednja energija

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Impakt

- magnetizacija

$$\langle M \rangle = \frac{1}{N} \sum_{i=1}^N |M_i|$$

- srednja energija

$$\langle H \rangle = \frac{1}{N} \sum_{i=1}^N H_i$$

- Binderovi kumulanti

$$U_L = 1 - \frac{1}{3} \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}$$

Markovljevi lanci

- Magnetizacija

Markovljevi lanci

- Magnetizacija
-

Markovljevi lanci

- Magnetizacija

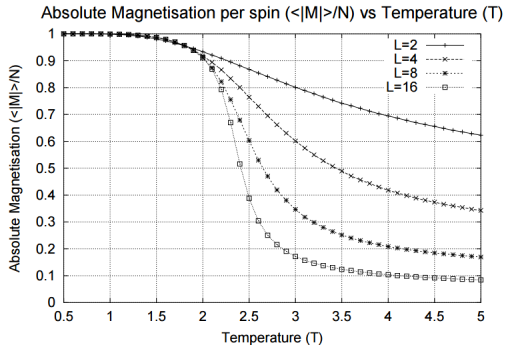


Figure 9: This plot shows the differing results of the Magnetization for varying lattice sizes, $L \times L$.



Markovljevi lanci

- Srednja energija

Markovljevi lanci

- Srednja energija
-

Markovljevi lanci

- Srednja energija

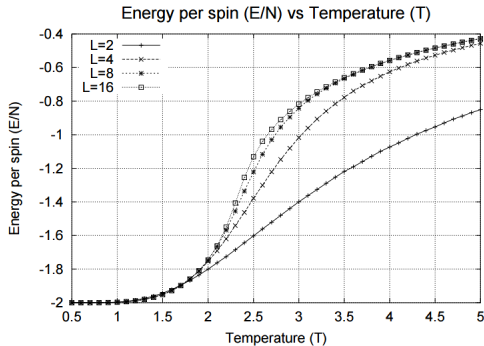


Figure 7: This plot shows the differing results of the Energy for varying lattice sizes, $L \times L$.



Problemi

- 1. zarobljavanje u neki minimum, koji nije globalni za datu temperaturu.

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Razvoj računarske industrije

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Razvoj računarske industrije

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Razvoj računarske industrije

-
- 3. paralelizacija procesa

Pregled predavanja

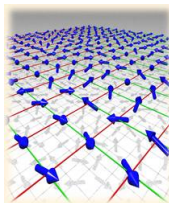
- 1 Uvod
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Klasični Hajzenbergov model

- Klasični Hajzenbergov model

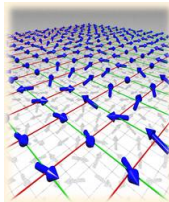
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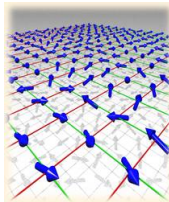
- Klasični Hajzenbergov model



- Kubna rešetka

Klasični Hajzenbergov model

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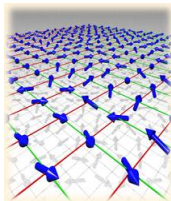
- Kubna rešetka
- Spinovi na čvorovima mogu da imaju proizvoljne orijentacije. Parametrizacija jediničnih vektora koji sede na čvorovima se vrši pomoću dva ugla θ i φ .

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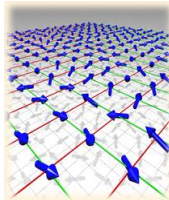
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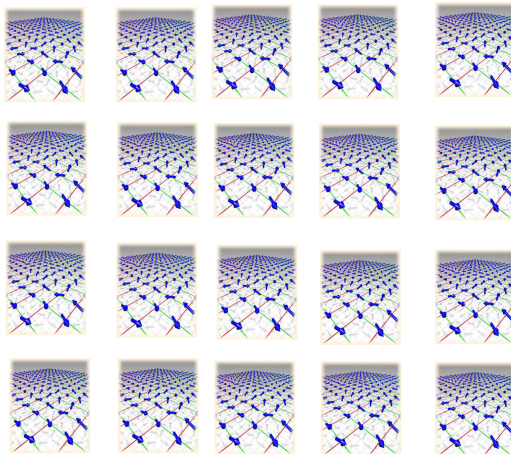
- $$H = -\frac{J}{2} \sum_{\vec{n}, \vec{\lambda}} \vec{S}_{\vec{n}} \cdot \vec{S}_{\vec{n}+\vec{\lambda}}$$

Klasični Hajzenbergov model

- Klasični Hajzenbergov model - Multipath

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- Klasični Hajzenbergov model - Multipath



Klasični Hajzenbergov model

- CESGA - Centro de Supercomputacion de Galicia

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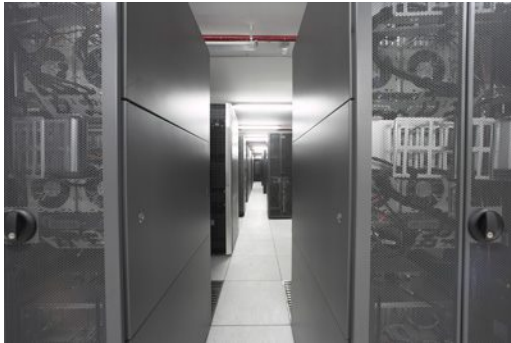


Klasični Hajzenbergov model

- CESGA - Centro de Supercomputacion de Galicia

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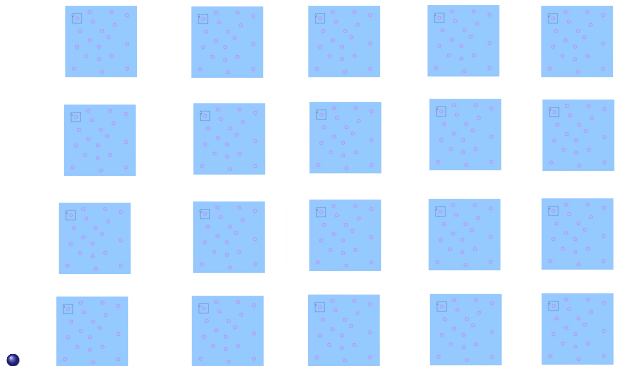


Klasični Hajzenbergov model

- Metropolisov sistem - Multipath

Klasični Hajzenbergov model

- Metropolisov sistem - Multipath

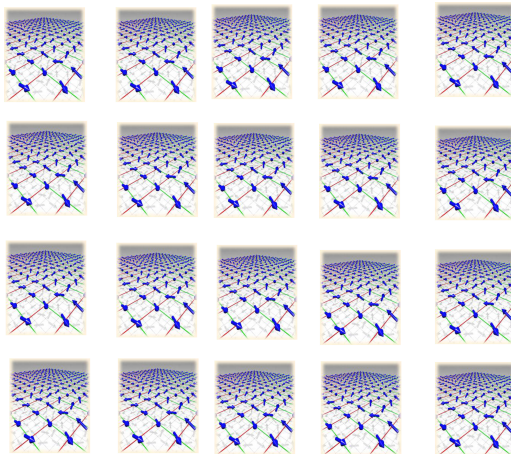


Klasični Hajzenbergov model

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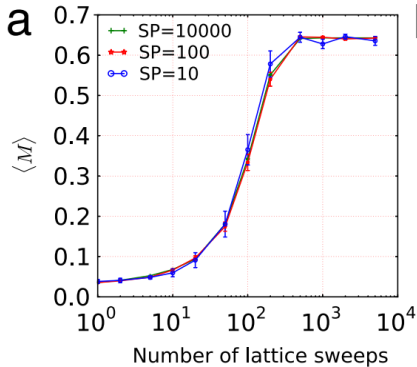


Impakt

- $L = 10, T = 1$

Impakt

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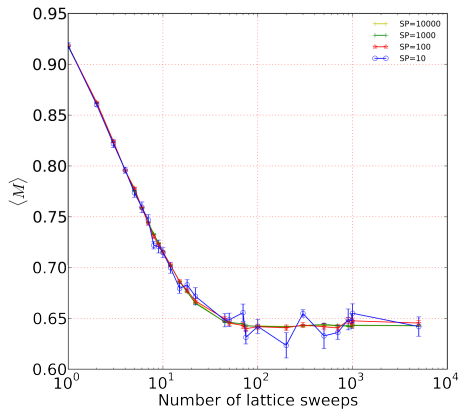


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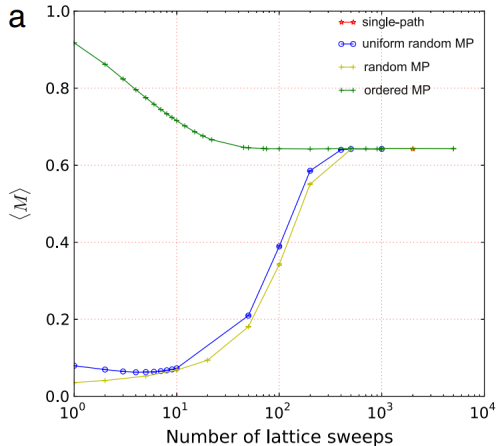


Impakt

- $L = 10, T = 1, \mathcal{N} = 10000$

Impakt

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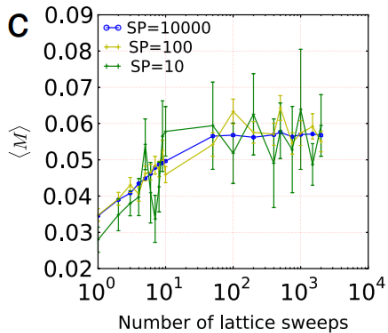
Impakt

- $L = 10, T = 1.5$

Impakt

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•

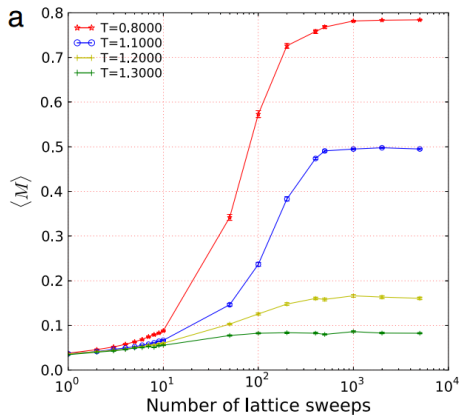


Impakt

- $\mathcal{N} = 1000$

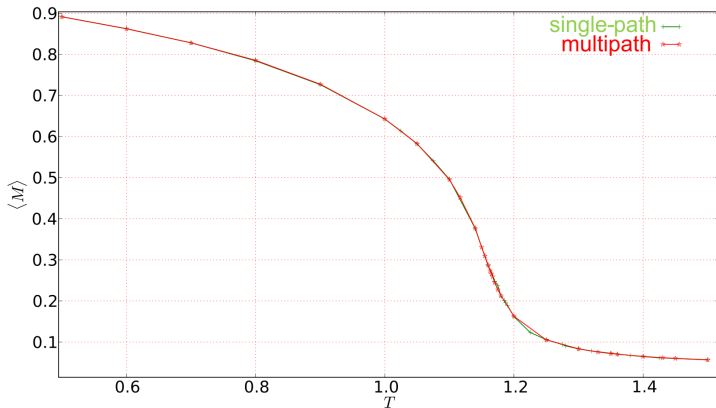
Impakt

• $\mathcal{N} = 1000$



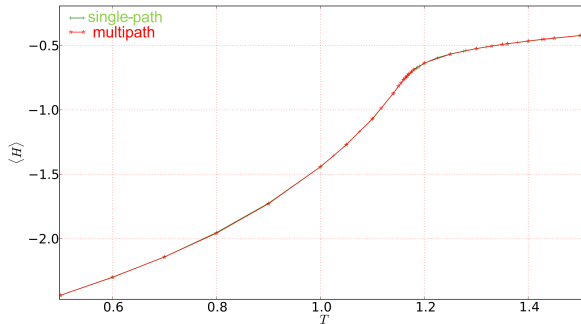
- $L = 10$, Multipath $LS = 10000$, $SP = 10000$, Singlepath
 $THERM = 2 \cdot 10^6$, $SO = 5 \cdot 10^5$

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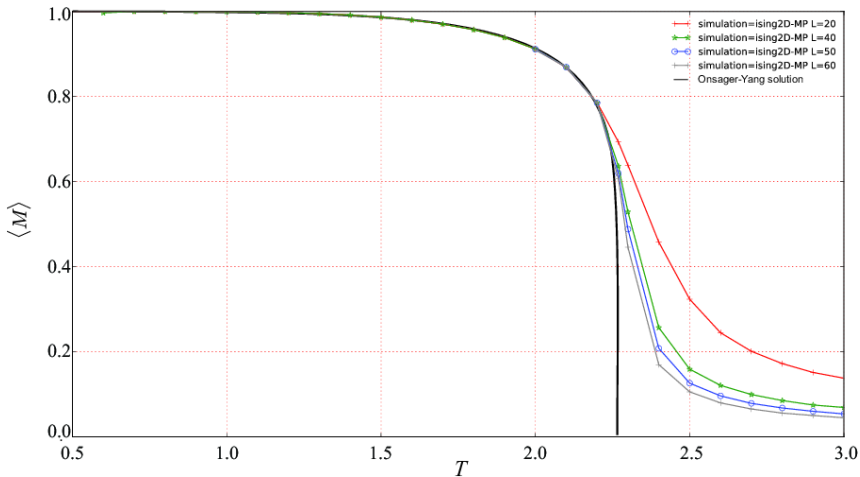


Impakt

- Izing multipath

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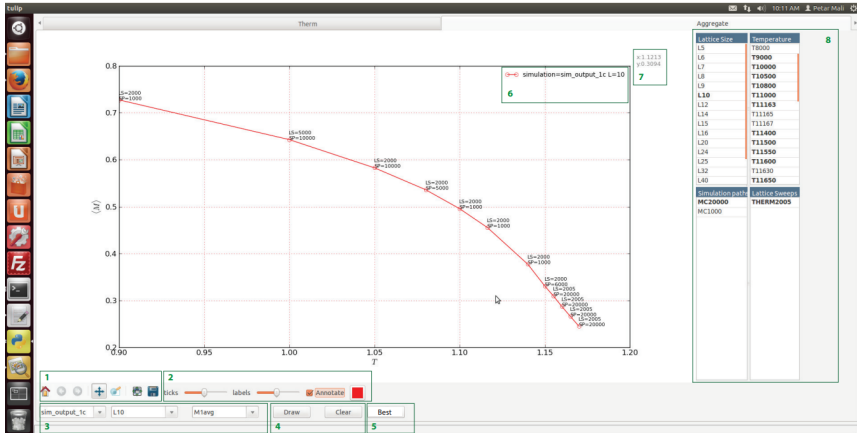


Impakt

- Tarin "Tulipko"

Impakt

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- Hvala na pažnji!