Parallel tempering in pure gauge theory

Journal club - Lattice field theory - SS 2022

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Outline

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Why Parallel tempering?

- Introduced by Swendsen and Wang [1] in 1986.
- Used in Statistical Physics: e.g. Spin glass models [2].
- Aims to improve MC simulations:
  - Sampling at all parameter sets simultaneously.
  - Reduces autocorrelation.
- Suitable to explore critical points.

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Basics

- Numerical integration of expectation values

$$\langle f \rangle_\rho = \frac{\int_a^b \mathrm{d}x\, \rho(x) f(x)}{\int_a^b \mathrm{d}x\, \rho(x)} \equiv \int_a^b \mathrm{d}x\, T(x)$$

- Via uniform sampling:

$$\frac{1}{b-a}\langle f \rangle_\rho = \frac{1}{b-a}\int_a^b \mathrm{d}x\, T(x) = \langle T \rangle_{\rho_u} = \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} T(x_n)$$

with $\rho_u(x_n) = 1/(b-a)$.

- Lattice QCD: $\rho \rightarrow$ Boltzmann weight $e^{-S[U]}$
- **Importance sampling** Monte Carlo method:

$$\langle f \rangle_\rho = \frac{\int_a^b \mathrm{d}x\, \rho(x) f(x)}{\int_a^b \mathrm{d}x\, \rho(x)} \longleftrightarrow \langle \mathcal{O}[U] \rangle = \frac{\int \mathcal{D}[U]\, e^{-S[U]} \mathcal{O}[U]}{\int \mathcal{D}[U]\, e^{-S[U]}}$$

- Sample over

$$\mathrm{d}P(x) = \frac{\rho(x)\mathrm{d}x}{\int_a^b \mathrm{d}x\, \rho(x)} \longleftrightarrow \mathrm{d}P(U) = \frac{\mathcal{D}[U]\, e^{-S[U]}}{\int \mathcal{D}[U]\, e^{-S[U]}}$$

- Then

$$\langle f(x) \rangle_\rho = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(x_n) \longleftrightarrow \langle \mathcal{O}[U] \rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}[U_n]$$

Markov chain

- We need U_n distributed according to $\mathrm{d}P(U) \rightarrow$ **Markov chain**:

$$U_0 \longrightarrow U_1 \longrightarrow U_2 \longrightarrow \dots$$

- Transition probability:

$$P(U_n = U' | U_{n-1} = U) = T(U'|U)$$

- Satisfy obvious properties

$$0 \leq T(U'|U) \leq 1$$

$$\sum_{U'} T(U'|U) = 1$$

Equilibrium distribution

- Also the *balance equation*

$$\sum_U T(U'|U)P(U) = \sum_U T(U|U')P(U')$$

so

$$\sum_U T(U'|U)P(U) = P(U')$$

- $P(U)$ is a *fixed point* of the Markov chain:

$$P^{(0)} \xrightarrow{T} P^{(1)} \xrightarrow{T} P^{(2)} \xrightarrow{T} \ldots \xrightarrow{T} P$$

- Eventually get the equilibrium distribution.

Metropolis algorithm

- *Detailed balance condition*:

$$T(U'|U)P(U) = T(U|U')P(U')$$

- **Metropolis algorithm**: $T = T_0 T_A$ with T_0 *a priori selection probability* for candidate configuration U' and T_A the *acceptance probability*.

$$T_A(U'|U) = \min\left(1, \frac{T_0(U|U')e^{-S[U']}}{T_0(U'|U)e^{-S[U]}}\right) \overset{1}{=} \min\left(1, e^{-\Delta S}\right)$$

- *Sweep*: every time all links are visited.

[1] If T_0 symmetric, $\Delta S = S[U'] - S[U]$

Correlation time

- Configurations generated from the same Markov chain are correlated.
- Estimation of the mean

$$\bar{\mathcal{O}} = \langle \mathcal{O} \rangle \pm \sqrt{\frac{2\tau_{\mathcal{O}} + 1}{N} \sigma^2(\mathcal{O})}$$

with τ the **(integrated) autocorrelation time**

$$\tau_{\mathcal{O}} = \sum_{t=1}^{\infty} C_{\mathcal{O}}(t)$$

and $C(t)$ the **correlation function**

$$C_{\mathcal{O}}(t) = C_{\mathcal{O}}(\mathcal{O}_i, \mathcal{O}_{i+t}) = \frac{1}{\sigma^2(\mathcal{O})} \langle (\mathcal{O}_i - \langle \mathcal{O}_i \rangle)(\mathcal{O}_{i+t} - \langle \mathcal{O}_{i+t} \rangle)$$

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General idea

- Usually physical simulations involve different parameters p_i:
  - Gauge coupling β.
  - Fermionic masses.
  - EM fields.
  - Chemical potentials.
  - ...
- Each set of parameter set have a sub-ensemble of configurations Γ_i and an action S_i.
- Close sub-ensembles in parameter space overlap.
- **Parallel tempering** allows to sample from all the sets of configurations the same time.

- Build a generalised Markov chain:

$$\Gamma_{\mathsf{PT}} = \prod_{i=1}^{N} \Gamma_i$$

- Equilibrates to

$$P^{\mathsf{eq}}_{\mathsf{PT}}[\{a_i\}] = \prod_i P^{\mathsf{eq}}_i(a_i) = \prod_i \frac{1}{Z_i} e^{-S_i(a_i)}$$

  with a_i configuration from Γ_i.

- Total partition function:

$$Z_{\mathsf{PT}} = \prod_i Z_i$$

Transitions

- Two types of transitions:
  - **Transitions within a sub-ensemble**: Using any Markovian updating procedure (e.g. Metropolis).
  - **Swapping updates of two sub-ensembles:** Mixes different ensemble spaces Γ_i and Γ_j. Propose to swap configurations $a \in \Gamma_i$ and $b \in \Gamma_j$ with probability $P_s(i,j)$.
- $P_s(i,j)$ has to satisfy detailed balance:

$$P_s(i,j)e^{-S_i(a)}e^{-S_j(b)} = P_s(j,i)e^{-S_i(b)}e^{-S_j(a)}$$

- Metropolis for swapping: $P_s(i,j) = \min(1, e^{-\Delta S})$ with

$$\Delta S = S_i(b) + S_j(a) - S_i(a) - S_j(b)$$

Algorithm

- Consider pure gauge case $\rightarrow$ only β matters.

Parallel tempering algorithm:

1. Initialise N streams separated by $\Delta\beta$. Usual Markovian process in each stream (HMC, local MC ...).
2. After some number of sweeps (e.g. 5), perform a swapping update between the streams.
3. Continue the individual Markov chains and repeat from 2.

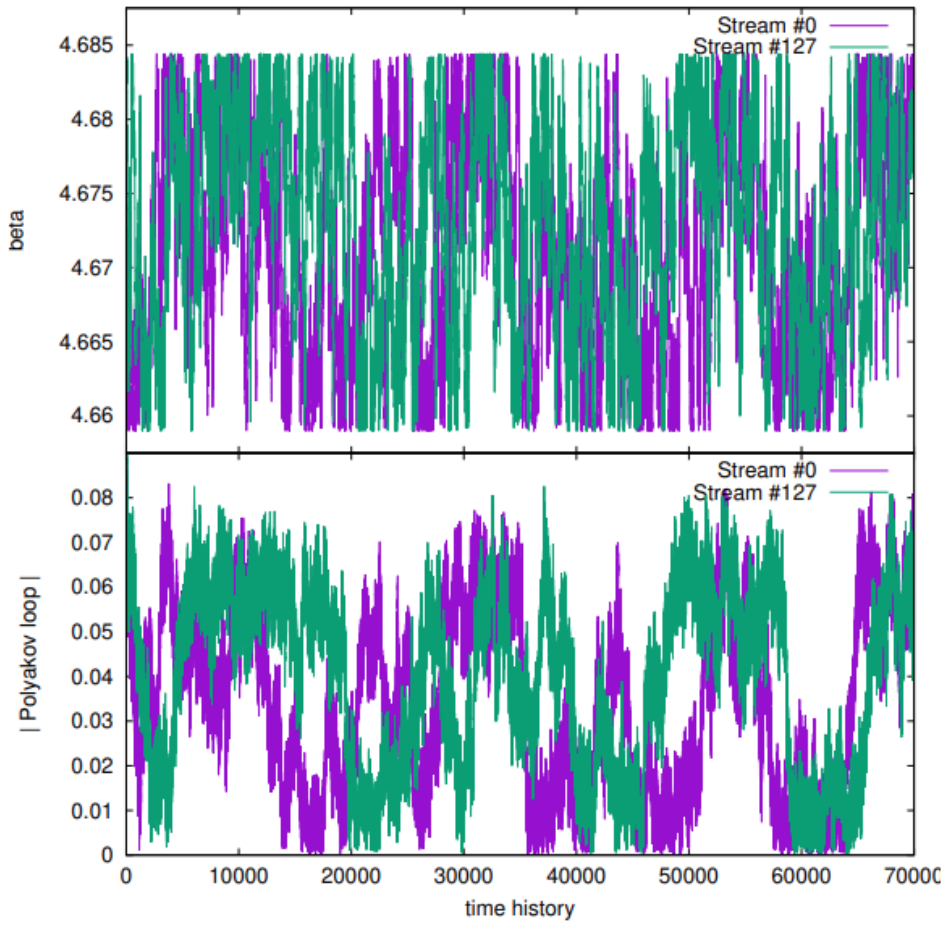

Figure: From [3]

Properties

- Random walk in parameter space.
- Smaller $\Delta\beta \rightarrow$ Bigger overlap between ensembles.
- Advantages:
  - Decrease autocorrelation in each ensemble.
    "Smaller computational cost".
- Disadvantages:
  - Samples from all parameter sets at the same time.
  - Introduces correlation between different ensembles.
  - $\Delta\beta$ should be small to maximise the overlap.
    Unsuitable for broad parameter spaces.

Autocorrelation

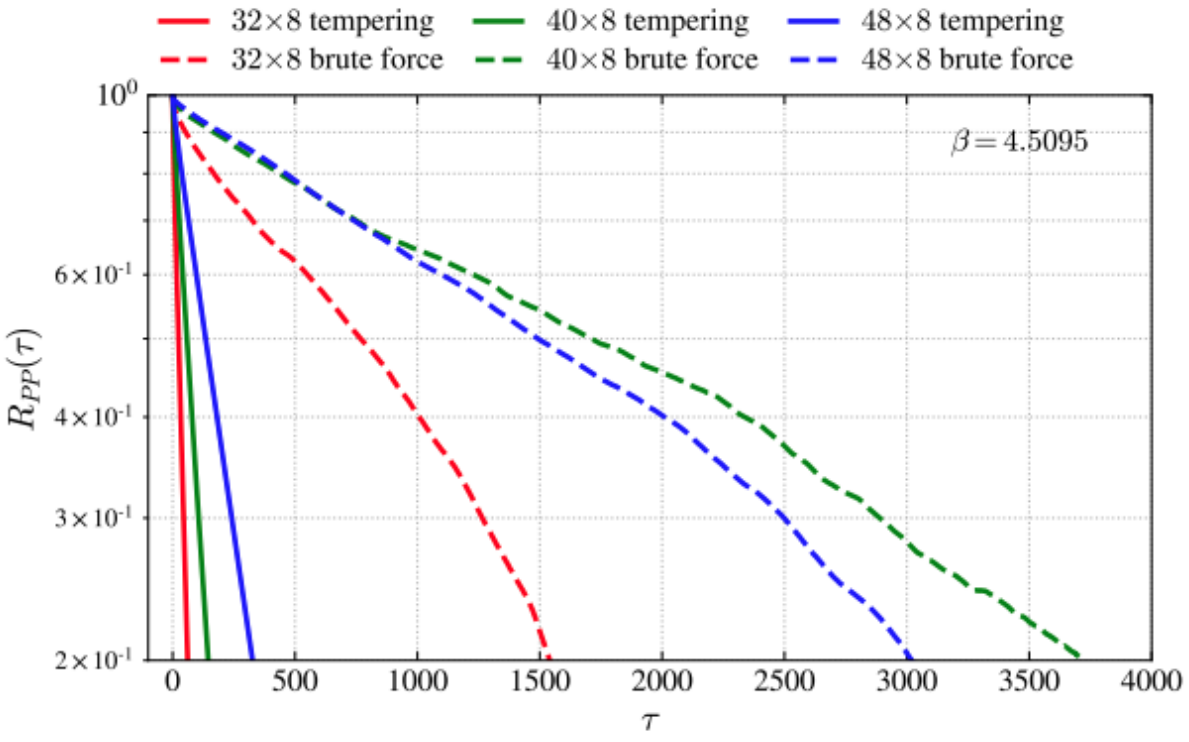

Figure: From [3]

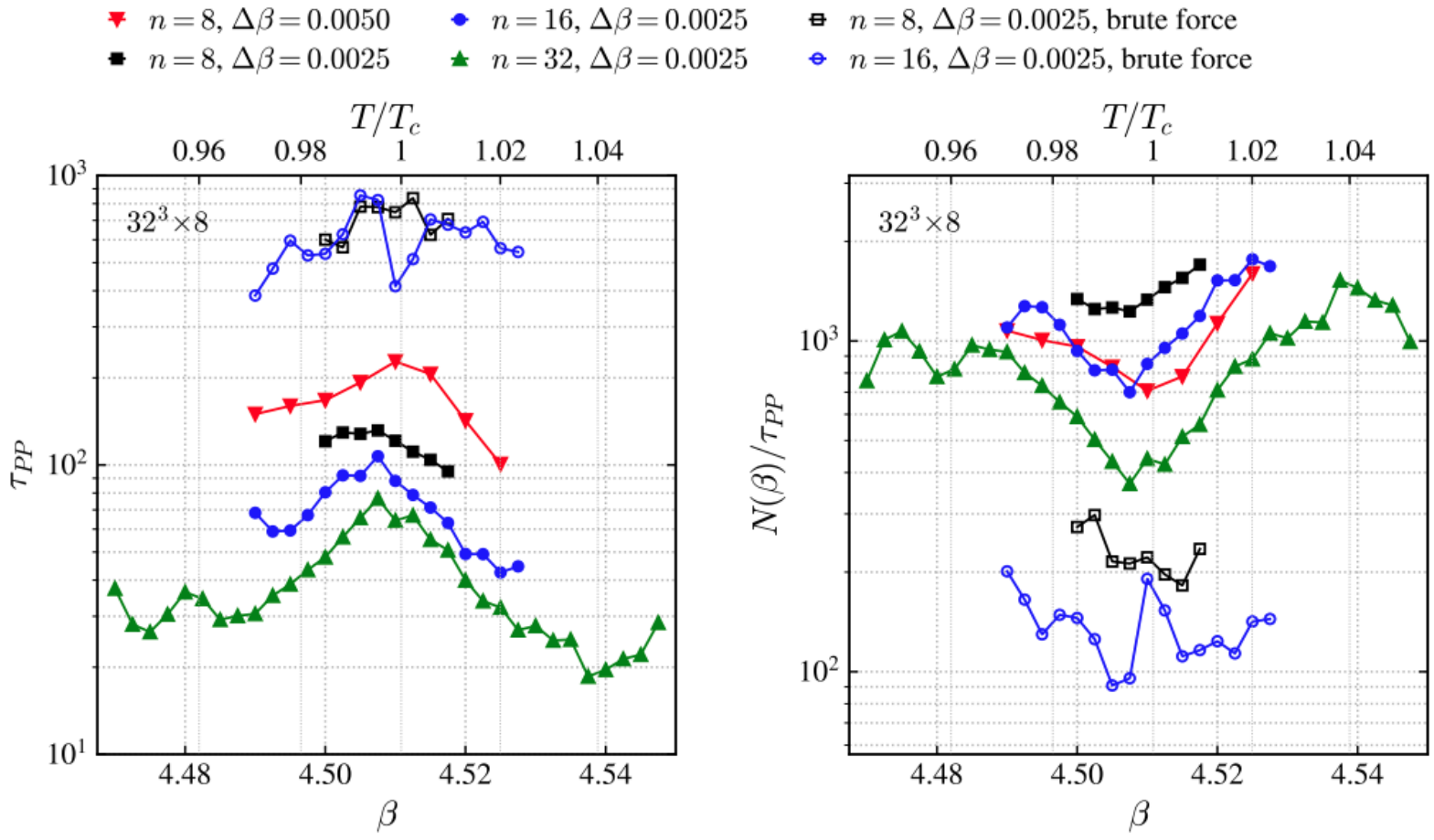

Figure: From [3]

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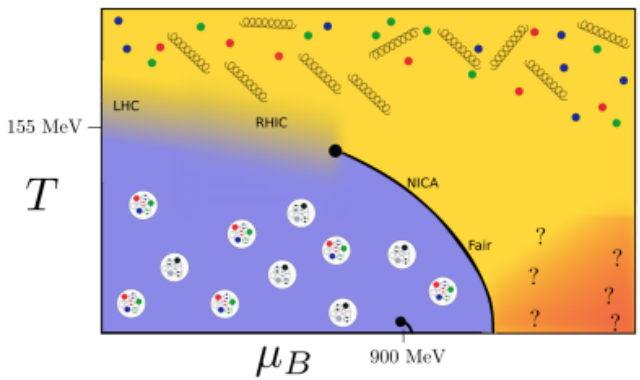
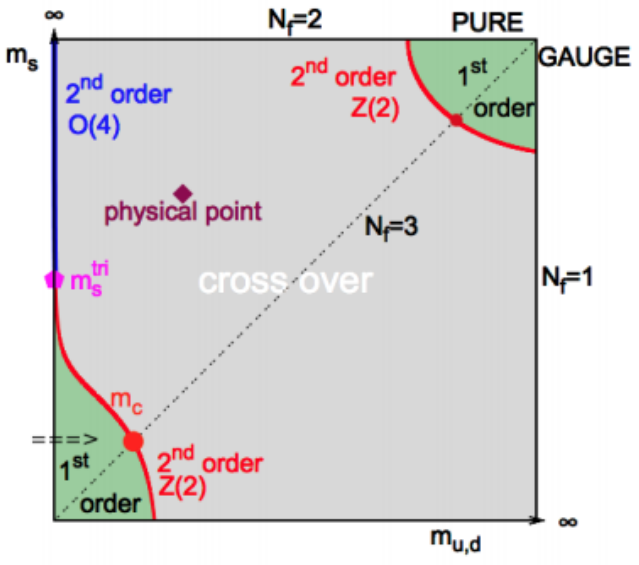
Columbia plot



(a) QCD phase diagram [4]



(b) Columbia plot [5]

First order phase transition

- Polyakov loop:

$$P = \frac{1}{N_s^3} \sum_{\vec{x}} \mathrm{Tr} \left[\prod_t U_4(\vec{x}, t) \right]$$

- Order parameter for confinement:
  - $\langle |P| \rangle = 0 \rightarrow$ confinement
  - $\langle |P| \rangle \neq 0 \rightarrow$ no confinement
- Polyakov loop susceptibility:

$$\chi = N_s^3 (\langle |P|^2 \rangle - \langle |P| \rangle^2)$$

- First order phase transition $\rightarrow \chi \sim V$

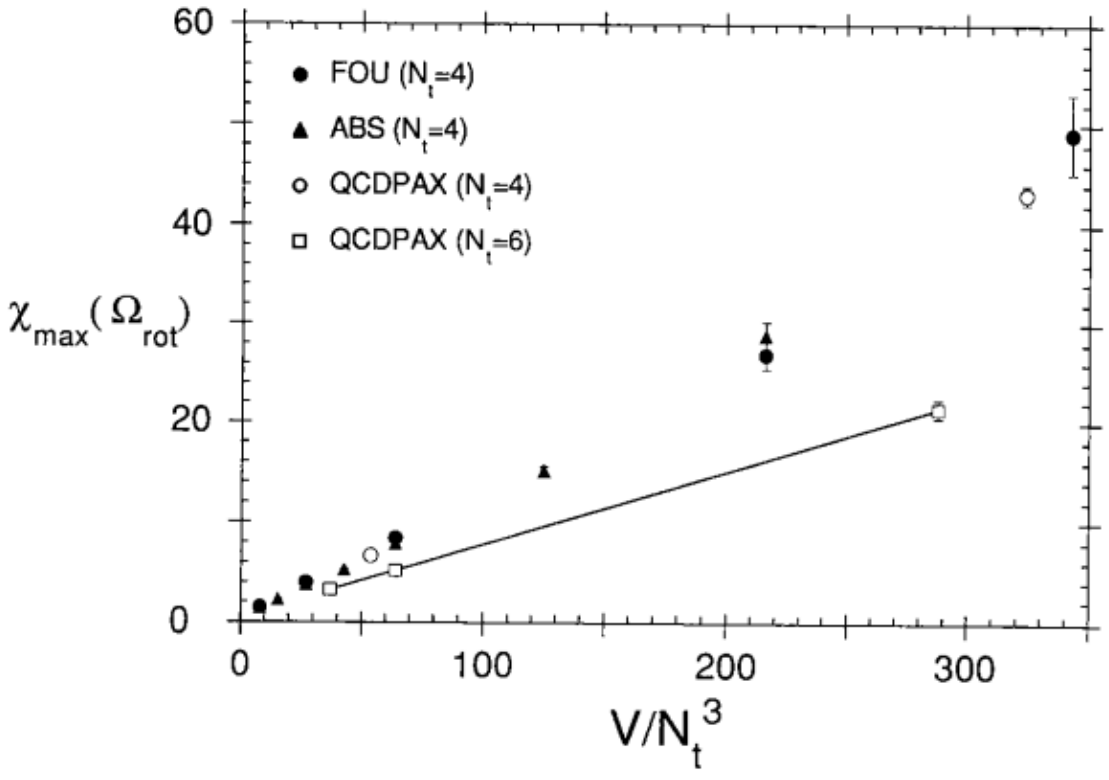


Figure: From [6]

Polyakov loop susceptibility

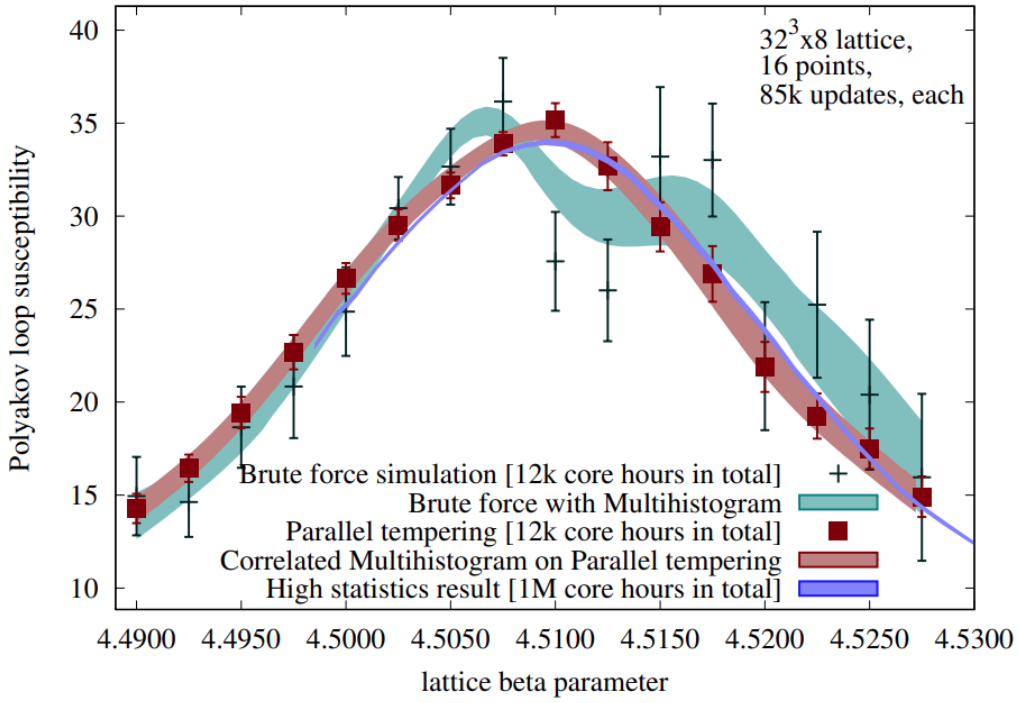


Figure: From [3]

Volume dependence

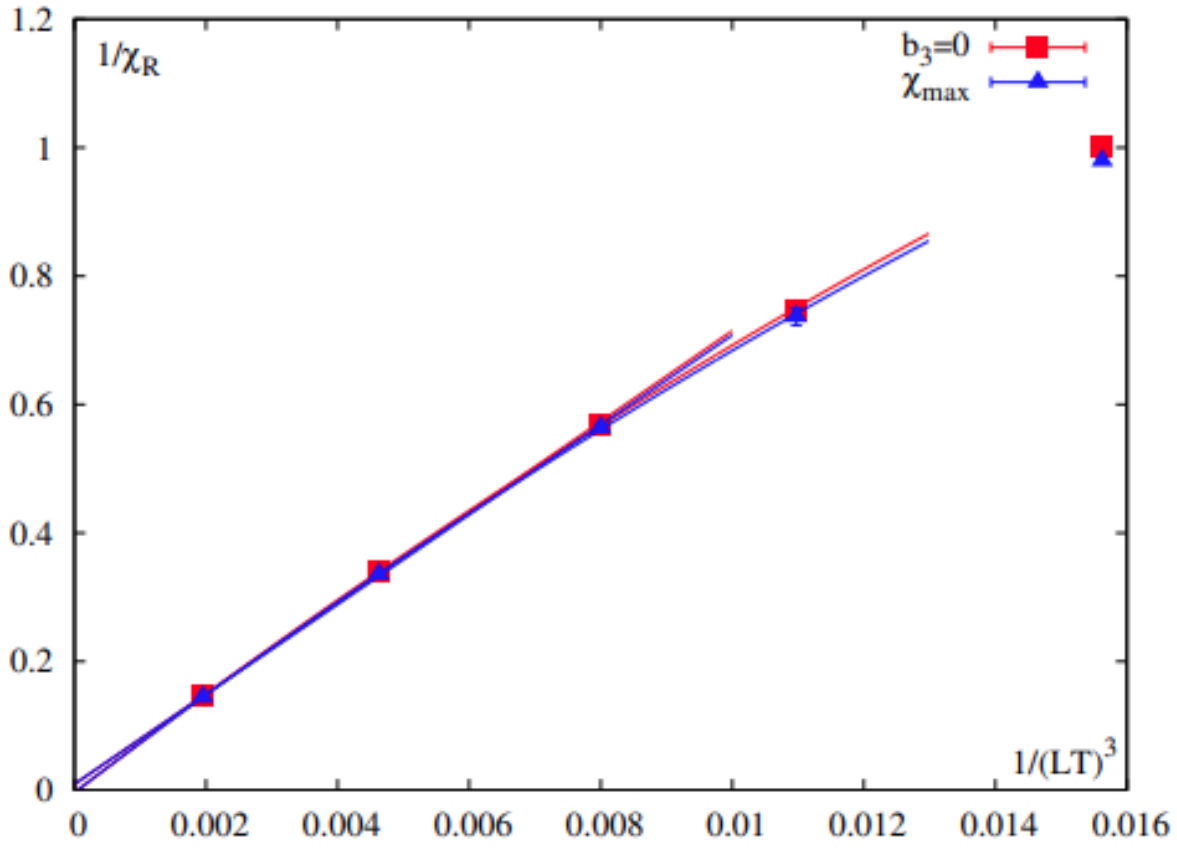


Figure: From [3]

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Conclusion

Parallel tempering:

- Reduces considerably autocorrelation time in each ensemble.
- Helps dealing with MC critical slowing down.
- Interesting tool for investigating critical points.
- Only feasible in small parameter space intervals.
- Full QCD: [7], [8], [9].

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