The equation of state with non-equilibrium methods

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in collaboration with

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Free-energy differences in LGTs

In lattice gauge theories the expectation values of a large set of physical quantities is *naturally* related to the computation (via Monte Carlo simulations) of free-energy differences (or, equivalently, of ratios of partition functions).

- the **pressure** ($\rightarrow$ equilibrium thermodynamics)
- but also: free-energy of interfaces, 't Hooft loops, magnetic susceptibility, entanglement entropy...

In general, the calculation of ΔF is a **computationally challenging** problem, since it usually cannot be performed directly.

- "integral method": computing first the *derivative* of the free energy with respect to some parameter, and then integrate
- reweighting ($\rightarrow$ snake algorithm)

Jarzynski's equality may provide a more efficient and intuitive method

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The Second Law of Thermodynamics

We start from Clausius inequality

$$\int_A^B \frac{\mathrm{d}Q}{T} \leq \Delta S$$

that for isothermal transformations becomes

$$\frac{Q}{T} \leq \Delta S$$

If we use

$$\begin{cases} Q = & \Delta E - W \quad \text{(First Law)} \\ F \stackrel{\text{def}}{=} & E - ST \end{cases}$$

the Second Law becomes

$$W \geq \Delta F$$

where the equality holds for reversible processes.

Moving from thermodynamics to **statistical mechanics** we know that the former relation (valid for a *macroscopic* system) becomes

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Jarzynski's equality

Let's consider a system with Hamiltonian H_λ (depending on some parameter $\lambda \to$ e.g. the coupling) with free energy $F(\lambda, T) = -\beta^{-1} \ln Z(\lambda, T)$.

We are interested in an evolution of the system driven during which **λ is changed** from an initial value λ_i to a final one λ_f.

We can state non-equilibrium equality **[C. Jarzynski, 1997]**

$$\left\langle \exp\left(-\frac{W(\lambda_i, \lambda_f)}{T}\right)\right\rangle = \exp\left(-\frac{F(\lambda_f) - F(\lambda_i)}{T}\right)$$

Jarzynski's equality relates the exponential statistical average of the work done on a system during a non-equilibrium process with the difference between the initial and the final free energy of the system.

This result can be derived for stochastic processes such as Markov chains and thus Monte Carlo simulations

The evolution is performed by changing continuously (as in real time experiments) or **discretely** (as in MC simulations) a chosen set of one or more parameters, such as the couplings of the system.

The initial state must be at equilibrium, but all the following ones do not!

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The initial state must be at equilibrium, but all the following ones do not!

It is instructive to see how this result is connected with the Second Law of Thermodynamics

Starting from Jarzynski's equality

$$\left\langle \exp\left(-\frac{W}{T}\right)\right\rangle = \exp\left(-\frac{\Delta F}{T}\right)$$

and using *Jensen's inequality*

$$\langle \exp x \rangle \geq \exp\langle x \rangle$$

(valid for averages on real x) we get

$$\exp\left(-\frac{\Delta F}{T}\right) = \left\langle \exp\left(-\frac{W}{T}\right)\right\rangle \geq \exp\left(-\frac{\langle W \rangle}{T}\right)$$

from which we have

$$\langle W \rangle \geq \Delta F$$

In this sense Jarzynski's relation can be seen as a **generalization** of the Second Law.

Jarzynski's equality in a Monte Carlo simulation

$$\left\langle \exp\left(-\frac{W(\lambda_0,\lambda_N)}{T}\right)\right\rangle = \exp\left(-\frac{\Delta F}{T}\right)$$

1. the non-equilibrium transformation begins by changing λ with some prescription (e.g. a linear one)

$$\lambda_0 \to \lambda_1 = \lambda_0 + \Delta\lambda$$

2. we compute the "work"

$$H_{\lambda_{n+1}}[\phi_n] - H_{\lambda_n}[\phi_n]$$

3. after each change, the system is updated using the new value → driving the system out of equilibrium!

$$[\phi_n] \xrightarrow{\lambda_{n+1}} [\phi_{n+1}]$$

4. the **total work** $W(\lambda_0, \lambda_N)$ made on the system to change λ using **N steps** is

$$W(\lambda_0,\lambda_N) = \sum_{n=0}^{N-1}\left(H_{\lambda_{n+1}}[\phi_n] - H_{\lambda_n}[\phi_n]\right)$$

5. at the end, we create a new initial state ϕ_0 and we repeat this transformation for **n_r realizations**

The $\langle \dots \rangle$ indicates that we have to take the **average on all possible realizations** of the transformation
→ it must be repeated several times to obtain **convergence** to the correct answer!

We can check the convergence by looking for discrepancies between the 'direct' ($\lambda_i \to \lambda_f$) and 'reverse' ($\lambda_f \to \lambda_i$) transformations

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The equation of state with non-equilibrium methods

Pressure on the lattice

The thermal properties of QCD and QCD-like theories are particularly well suited for being studied on the lattice, due to *non-perturbative* nature of the deconfinement transition.

The **pressure** p in the thermodynamic limit equals the opposite of the **free energy density**

$$p \simeq -f = \frac{T}{V} \log Z(T, V)$$

On the lattice, the temperature T is the inverse of the temporal extent,

$$T = \frac{1}{L_t} = \frac{1}{a(\beta_g) N_t}$$

and it can be controlled by the inverse coupling β_g.

Jarzynski's relation gives us a **direct** method to compute the pressure: we can change temperature T (by controlling β_g) in a non-equilibrium transformation!

Pressure with Jarzynski's relation

If we focus on the $\mathrm{SU}(N)$ pure gauge theories, the dynamics of the theory on the lattice can be described by the Wilson action

$$S_W = -\frac{\beta_g}{N} \sum_x \sum_{0 \leq \mu < \nu \leq 3} \mathrm{Re\ Tr} U_{\mu\nu}(x)$$

If we use Jarzynski's equality the **difference in pressure** between two temperatures T and T_0 is

$$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = \left(\frac{N_t}{N_s}\right)^3 \log \langle e^{-W_{\mathrm{SU}(N_c)}} \rangle$$

with $W_{SU(N_c)}$ being the *"total work"* made on the system between T_0 and T:

$$W_{\mathrm{SU}(N_c)} = \sum_{n=0}^{N-1} \left[S_W(\beta_g^{(n+1)}, \hat{U}) - S_W(\beta_g^{(n)}, \hat{U}) \right]$$

Trace of the energy-momentum tensor, energy density and entropy density are obtained by

$$\frac{\Delta}{T^4} = T \frac{\partial}{\partial T} \left(\frac{p}{T^4} \right) \qquad \epsilon = \Delta + 3p \qquad s = \frac{\Delta + 4p}{T}$$

A test for the $\mathrm{SU}(2)$ pressure in the proximity of the deconfining transition yielded excellent results **[Caselle et al.,2016]**.

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The $\mathrm{SU}(3)$ equation of state

The equation of state of the $\mathrm{SU}(3)$ Yang-Mills theory has been determined in the last few years using different methods.

- using a variant of the integral method **[Borsànyi et al., 2012]**

  $\rightarrow$ the primary observable is the **trace of the energy-momentum tensor**

- using a moving frame **[L. Giusti and M. Pepe, 2016]**

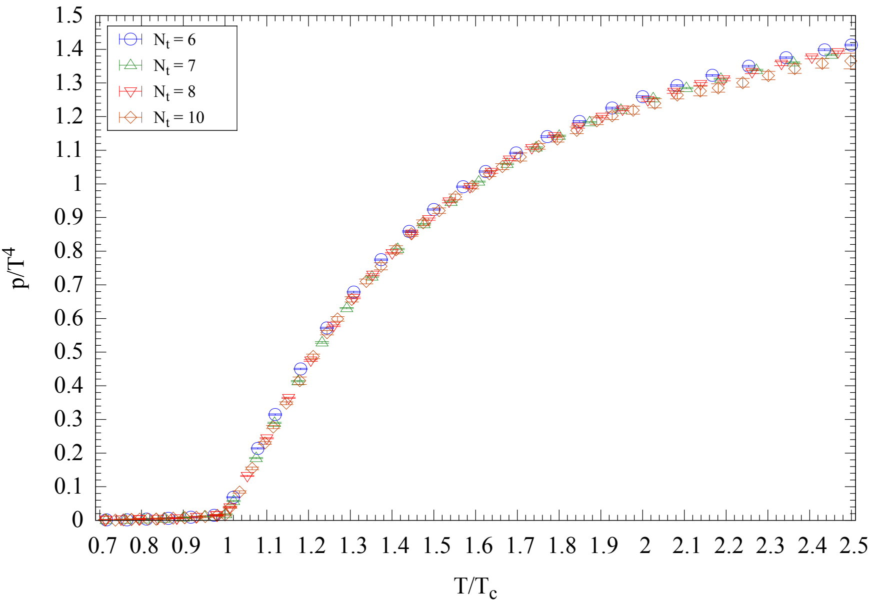
  $\rightarrow$ the primary observable is the **entropy density** (extracted from the spacetime components of the energy-momentum tensor)

  $\rightarrow$ see talk by Mattia Dalla Brida in the afternoon (17:40)

- using the gradient flow **[Kitazawa et al., 2016]**

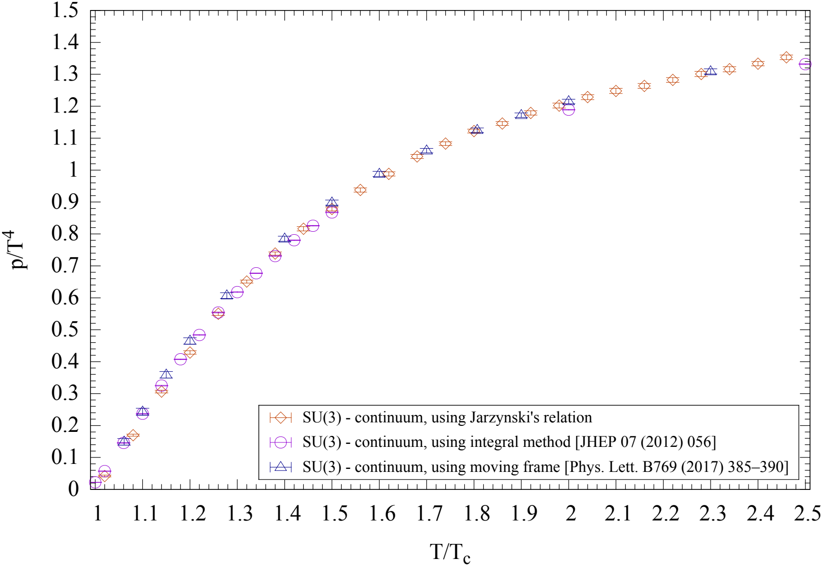
An high-precision determination of the $\mathrm{SU}(3)$ e.o.s. is an excellent benchmark for the **efficiency** of a technique based on non-equilibrium transformations.

SU(3) pressure across the deconfinement transition, for different values of N_t, with Jarzynski's equality

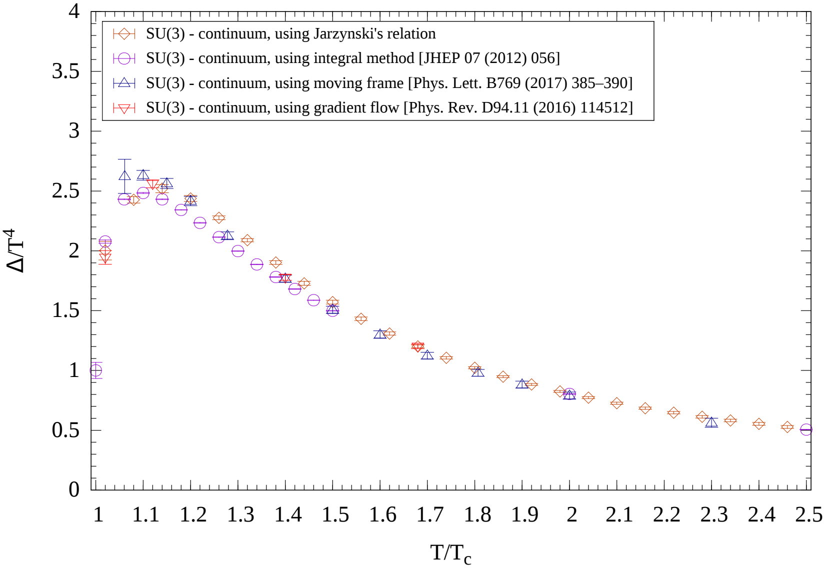


SU(3) pressure - continuum extrapolation

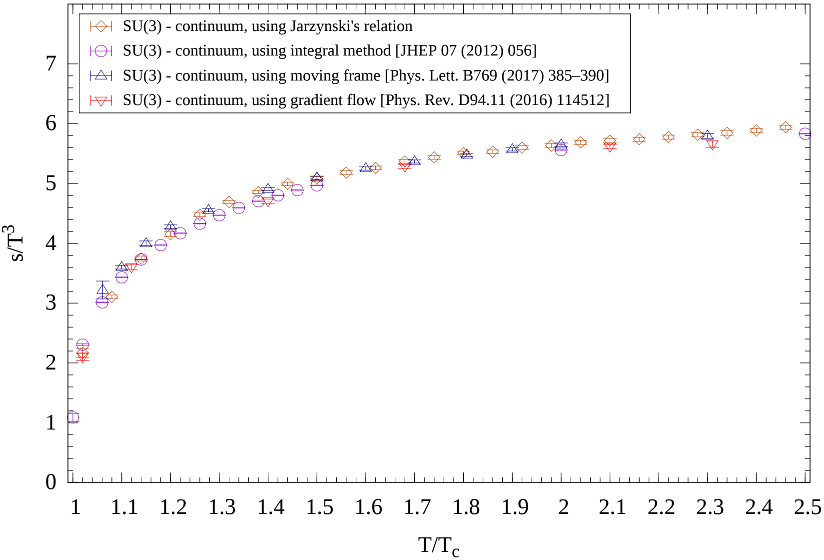
$\sim$ 700k configurations across all values of N_t were used in this region



SU(3) trace anomaly



SU(3) entropy density



Conclusions

Jarzynski's equality provides a new technique to compute **directly** the pressure on the lattice with Monte Carlo simulations.

- we can always verify the convergence of the method to the correct result by performing transformations in reverse and comparing the results
- with these checks we can look for systematic errors → especially useful close to the transition
- suitable choices of N and n_r provide high-precision results while keeping the expected discrepancies under control
- even with a limited amount of configurations it is possible to extract precise results

Why use it?

- very **efficient**: intuitively we are exploiting the autocorrelation, since the average is not taken across all configurations, but only on the different realizations
- to get more precise results we can not only increase n_r, but also N, i.e. we get closer to a **reversible transformation**

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Thank you for your attention!

Two special cases

Two insightful limits of Jarzynski's equality:

- the limit of $N \to \infty$: now the transformation is infinitely *slow* and the the system is always at equilibrium. The switching process is reversible: no energy is dissipated and thus

$$W = \Delta F$$

$\to$ this is the case of **thermodynamic integration** $\to$ a common way to estimate p on the lattice is by the "integral method" **[Engels et al., 1990]**

$$p(T) = \frac{1}{a^4} \frac{1}{N_t\, N_s^3} \int_0^{\beta_g(T)} d\beta_g' \frac{\partial \log Z}{\partial \beta_g'}$$

where the integrand is calculated from plaquette expectation values.

- the limit of $N = 1$: now the system is driven *instantly* to the final state and no updates are performed on the system after the parameter λ has been changed
$\to$ this is the **reweighting** technique.

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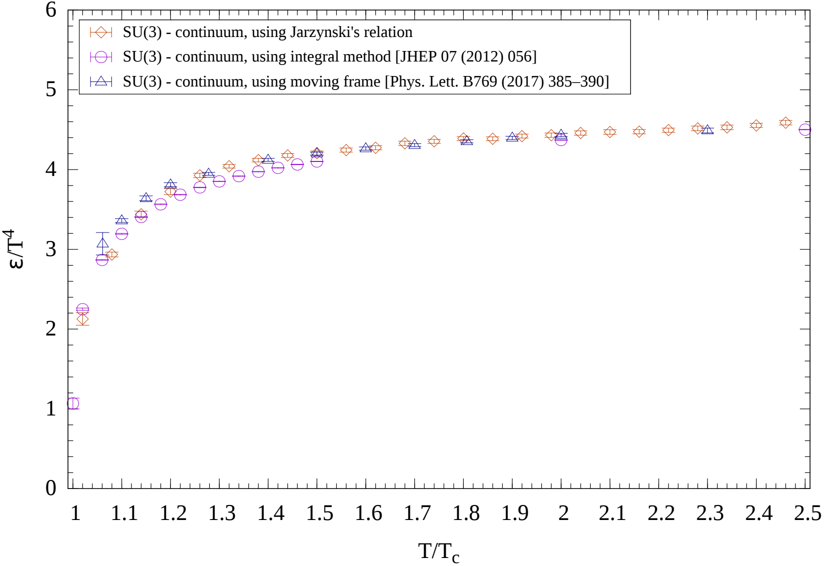
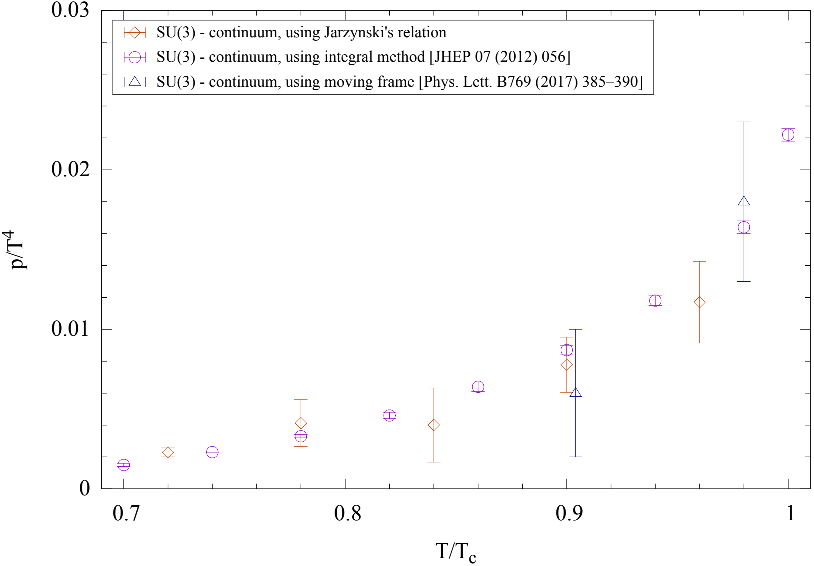
SU(3) energy density



SU(3) pressure - confining phase

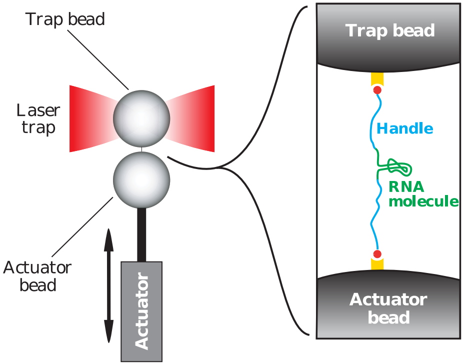


Applications beyond the equation of state

- In principle there are no obstructions to the derivation of numerical methods based on Jarzynski's relation for fermionic algorithms, opening the possibility for many potential applications in full QCD
- the free energy density in QCD with a **background magnetic field** B, to measure the magnetic susceptibility of the strongly-interacting matter.
- the **entanglement entropy** in $\mathrm{SU}(N_c)$ gauge theories
- studies involving the **Schrödinger functional**: Jarzynski's relation could be used to compute changes in the transition amplitude induced by a change in the parameters that specify the initial and final states on the boundaries.

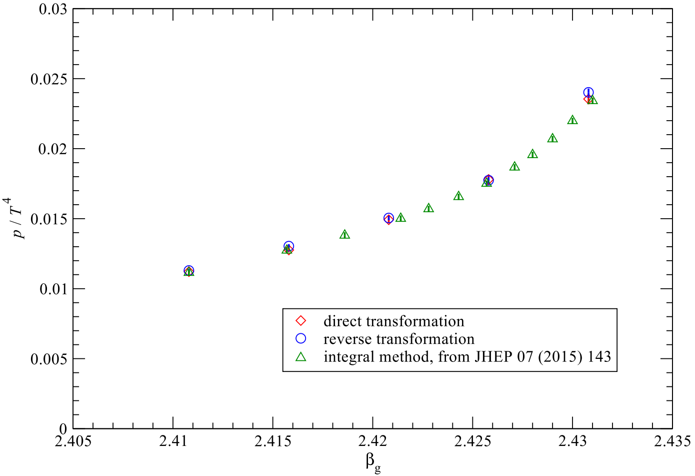
An experimental test of Jarzynski's equality was performed in 2002 by Liphardt *et al.* by mechanically stretching a single molecule of RNA between two conformations.

The irreversible work trajectories (via the non-equilibrium relation) provide the result obtained with reversible stretching.



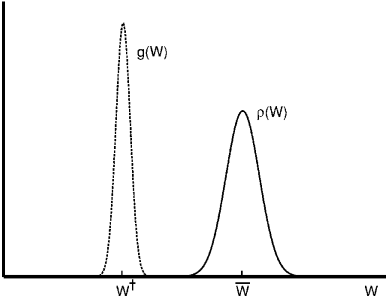
Preliminary results for the SU(2) model

Finite T simulations performed on $72^3 \times 6$ lattices. Temperature range is $\sim [0.9T_c, T_c]$.



Excellent agreement with integral method data [Caselle et al., 2015]

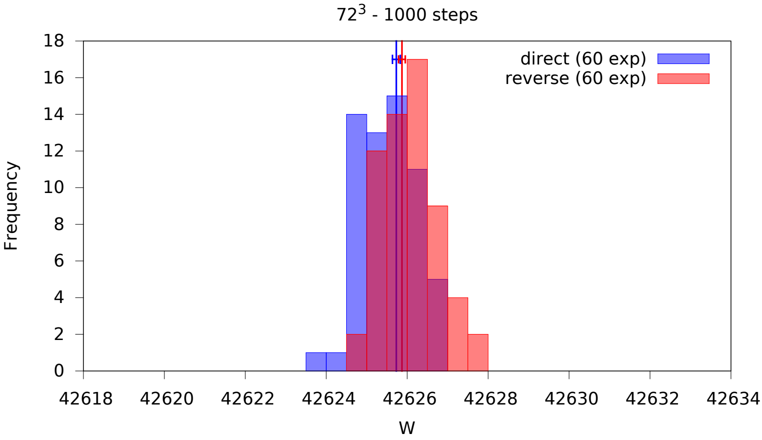
Dominant realizations



Picture taken from [Jarzynski (2006)]

The work is statistically distributed on $\rho(W)$; however the trials that dominate the exponential average are in the region where $g(W) = \rho(W)e^{-\beta W}$ has the peak.

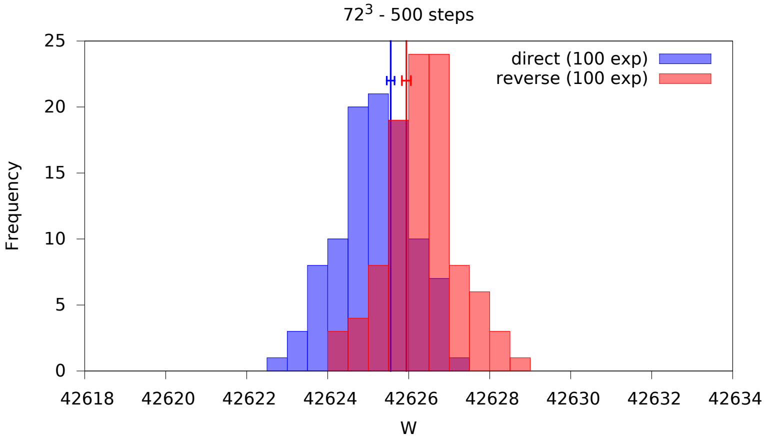
Work distributions



Total work W distributions for realizations of the transformation: $\beta = 2.4158 \leftrightarrow 2.4208$.

Vertical lines indicate the value of ΔF obtained from these trials.

Work distributions



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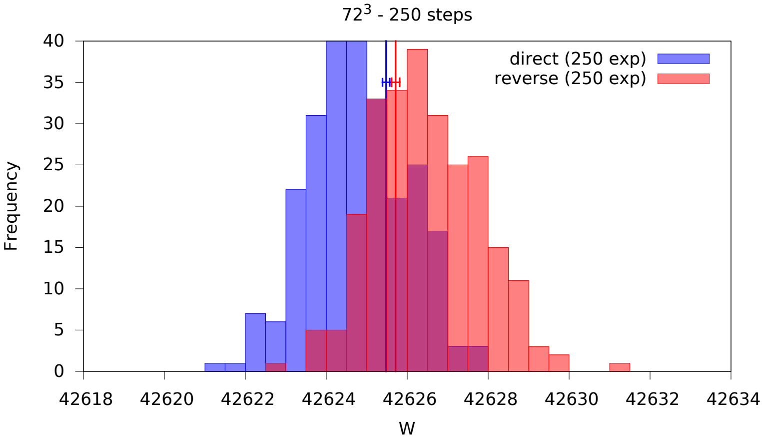

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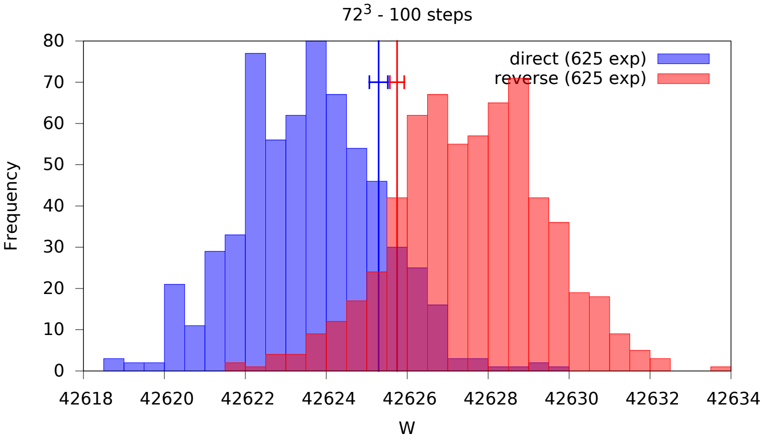

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Extended to non-isothermal transformations [Chatelain, 2007] (the temperature takes the role of λ)

$$\left\langle \exp\left(- \sum_{n=0}^{N-1} \left\{ \frac{H_{\lambda_{n+1}}[\phi_n]}{T_{n+1}} - \frac{H_{\lambda_n}[\phi_n]}{T_n} \right\} \right) \right\rangle = \frac{Z(\lambda_N, T_N)}{Z(\lambda_0, T_0)}$$