SU(3) equation of state on the lattice: status and new methods

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21st May 2018

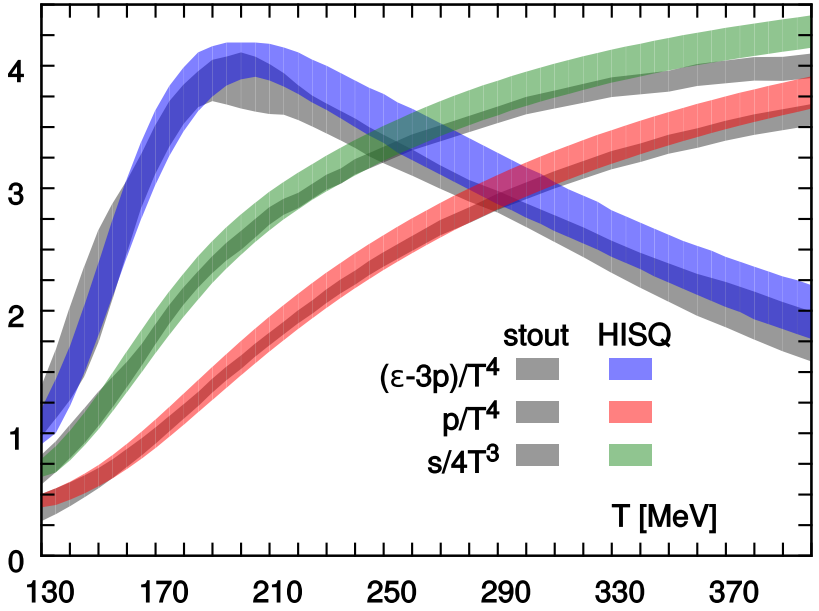
"16th International Conference on QCD in Extreme Conditions" – XQCD 2018

Frankfurt, Germany, 21-23 May 2018

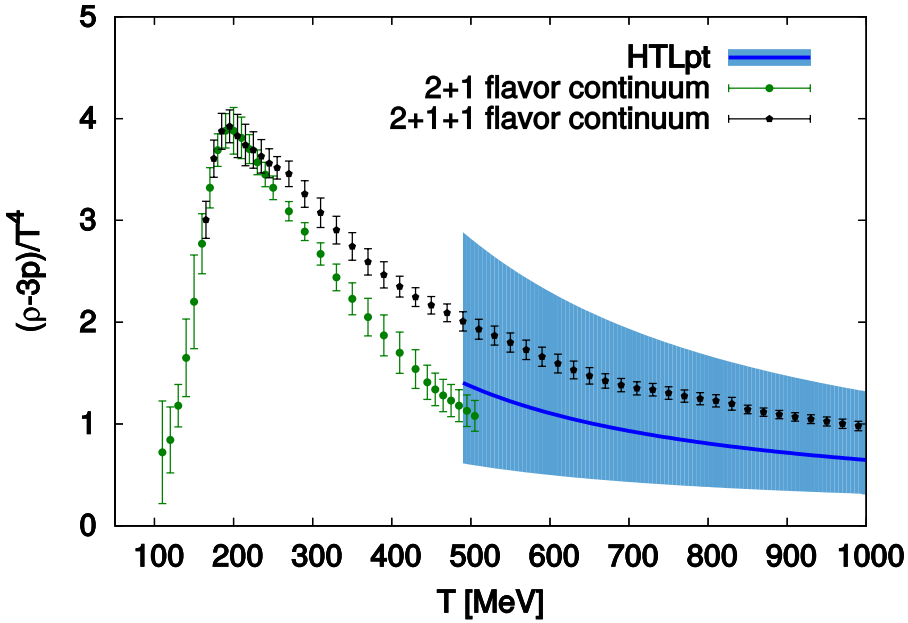
- The phase diagram of QCD displays a rich set of physically interesting phenomena, such as the deconfinement transition and the restoration of chiral symmetry, which are currently investigated experimentally (RHIC, LHC, FAIR, ...)

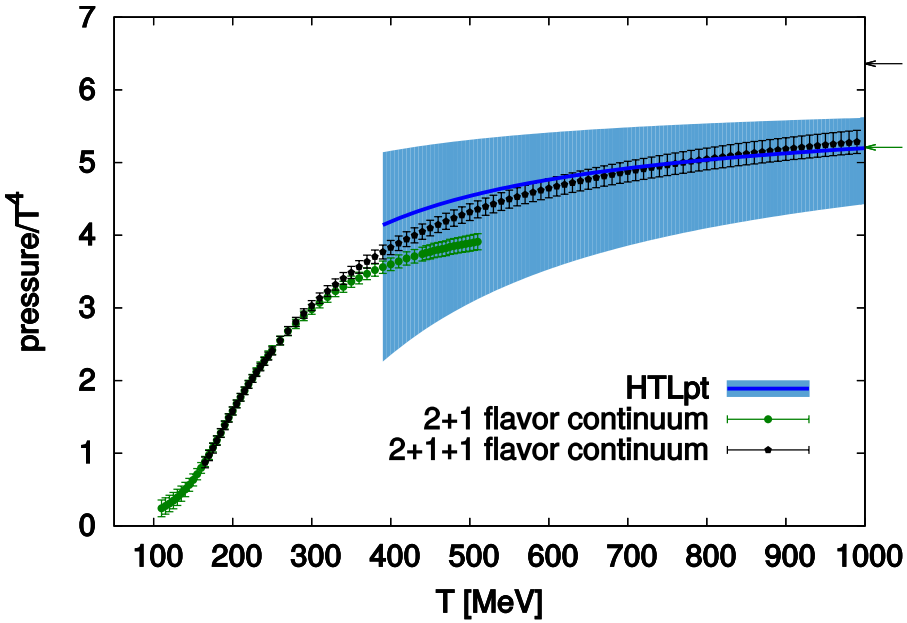
- The thermal properties of QCD and QCD-like theories in the high-temperature, $\mu = 0$ region are particularly well suited for being studied on the lattice, due to the *non-perturbative* nature of the deconfinement transition.

- Enormous progress in full-QCD lattice calculations for the **equation of state** has been made recently with staggered fermions: continuum results with $2+1$ dynamical flavours with HISQ **[HotQCD, 2014]** and stout **[Wuppertal-Budapest, 2014]** actions



More recent progress at even higher temperatures $2+1$ **[Bazavov et al., 2017]** and $2+1+1$ flavours **[Borsanyi et al., 2016]** (shown below)





Still, several challenges remain (such as a determination with Wilson fermions with comparable accuracy) and new, independent checks are required

$\rightarrow$ need for **new techniques**!

1. The equation of state on the lattice
   - ...using the integral method
   - ...with the gradient flow
   - ...in a moving frame

2. A non-equilibrium method for equilibrium thermodynamics
   - Jarzynski's equality

3. A comparison of results for the $\mathrm{SU}(3)$ e.o.s.

The integral method

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

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

A widely used technique to estimate it on the lattice is 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.

An additive renormalization in the form of a subtraction of $T = 0$ plaquette expectation values is required for each β

$$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = 6{N_t}^4 \int_{\beta(T_0)}^{\beta(T)} \mathrm{d}\beta' \; (\langle U_\mathrm{p} \rangle_T - \langle U_\mathrm{p} \rangle_0)$$

and so the primary observable is the **trace of the energy momentum tensor** $\Delta = T_{\mu\mu}$

$$\frac{\Delta(T)}{T^4} = -N_t^4 \frac{\partial \beta}{\partial \log a} \left[6 \left(\langle U_\mathrm{p} \rangle_T - \langle U_\mathrm{p} \rangle_0\right)\right]$$

Thermodynamics from the gradient flow

Yang-Mills gradient flow **[Luscher, 2010], [Naranayan and Neuberger,2006]**

Small-t expansion relates non-zero t observables with the renormalized observables of the original theory **[Luscher and Weisz,2011]**

$$\tilde{O}(t,x) \underset{t\to 0}{\longrightarrow} \sum_i c_i(t) O_i^R(x)$$

In the case of the energy-momentum tensor (see also **[Del Debbio,Patella and Rago,2017]**), one can build **[Suzuki, 2013]**

$$T_{\mu\nu}(x,t) = \frac{1}{\alpha_{\tilde{U}}(t)} \tilde{U}_{\mu\nu}(t,x) + \frac{\delta_{\mu\nu}}{4\alpha_{\tilde{E}}(t)} \left(\tilde{E}(t,x) - \langle \tilde{E}(t,x) \rangle_0 \right)$$

where $\tilde{E}(t,x)$ and $\tilde{U}_{\mu\nu}(t,x)$ are dimension-4 gauge invariant operators.
From the $t \to 0$ extrapolation

$$T^R_{\mu\nu} = \lim_{t\to 0} T_{\mu\nu}(x,t)$$

one can extract, for example

$$\epsilon = -\langle T^R_{00}(x) \rangle \qquad p = \frac{1}{3} \sum_{i=1}^{3} \langle T^R_{ii}(x) \rangle$$

Double extrapolation (in a and t) is required.
First study with Wilson fermions available **[Taniguchi et al.,2017]**

Thermodynamics in a moving frame

Main idea: in relativistic thermal theories the entropy is proportional to the total momentum of the system as measured by a moving reference system

- shifted boundary conditions are imposed:

$$U_\mu(L_t, \vec{x}) = U_\mu(0, \vec{x} - L_t\vec{\xi})$$

- the temperature of the system is now given by

$$T = \frac{1}{L_t\sqrt{1+\vec{\xi}^2}}$$

- in this context new Ward identities can be derived (see also work on the renormalization of the energy-momentum tensor **[Giusti and Pepe,2015]**)

In particular one can extract the **entropy density** $s(T)$ **[Giusti and Meyer,2013]**

$$s(T) = -\frac{L_t(1+\vec{\xi}^2)^{\frac{3}{2}}}{\xi_k}\langle T_{0k}\rangle_{\vec{\xi}} Z_T$$

where Z_T is a renormalization constant that has to be computed separately

$$Z_T(g_0^2) = -\frac{\Delta f}{\Delta\xi_k}\frac{1}{\langle T_{0k}\rangle_{\vec{\xi}}}$$

opening the possibility for a study of the e.o.s. **[Giusti and Pepe, 2014]**

An implementation to fermionic degrees of freedom is ongoing **[Dalla Brida et al., 2017]**.

A non-equilibrium method for equilibrium thermodynamics

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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Let's consider a system with Hamiltonian H_λ parametrized by λ. Its partition function is

$$Z_\lambda(T) = \int \mathrm{d}\Gamma e^{-\beta H_\lambda(\Gamma)}$$

and the free energy is

$$F_\lambda(T) = -\beta^{-1} \ln Z_\lambda(T)$$

Now we are interested in letting the system evolve in time by varying the parameter λ between two values.
The crucial quantity is the **work** performed on the system

$$W = \int_{t_i}^{t_f} \mathrm{d}t \dot{\lambda} \frac{\partial H_\lambda}{\partial \lambda}$$

(this is not arbitrary: $\dot{H} = \dot{\lambda} \frac{\partial H}{\partial \lambda} + \dot{\Gamma} \frac{\partial H}{\partial \Gamma}$ can be identified with the First Law of Thermodynamics)

This is repeated in order to have an **ensemble** of realizations of this process: for each of them W is computed separately.

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Jarzynski's equality

Now we can precisely state the non-equilibrium equality [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.

At the beginning of each transformation the system must be at equilibrium.

In each step of the process the value of λ is changed and the system is brought **out of equilibrium**.

Moreover: using *Jensen's inequality*

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

(valid for averages on real x) we get

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

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

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Pressure with Jarzynski's relation

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

The **difference of 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 *"work"* made on the system:

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

here S_W is the standard Wilson action and $\hat{U}$ is a configuration of $\mathrm{SU}(N_c)$ variables on the links of the lattice.

A comparison of results for the $\mathrm{SU}(3)$ e.o.s.

Equilibrium thermodynamics in Yang-Mills theories

For YM thermodynamics highly precise determinations are relatively easy and available at high temperatures

$\rightarrow$ precision studies can be performed and compared with other theoretical tools

- *low-temperature phase* ($T < T_c$) $\rightarrow$ description in terms of a gas of massive, non-interacting hadrons $\rightarrow$ HRG model in QCD

  even more dramatic for pure Yang-Mills theories - lattice data in the confining region have been compared in detail with the prediction of a glueball gas with an Hagedorn spectrum **[Meyer, 2009; Borsányi et al., 2012; Caselle et al., 2015, Alba et al., 2016]**

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SU(3) equation of state: status report

A high-precision determination of the SU(3) Yang-Mills e.o.s. is an excellent benchmark for the **efficiency** and the **correctness** of any new technique

→ it has been determined in the last few years using **markedly different methods**

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

  → primary observable: **trace of the energy-momentum tensor**, up to $1000\,T_c$

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

  → primary observable: **entropy density**, up to $230\,T_c$

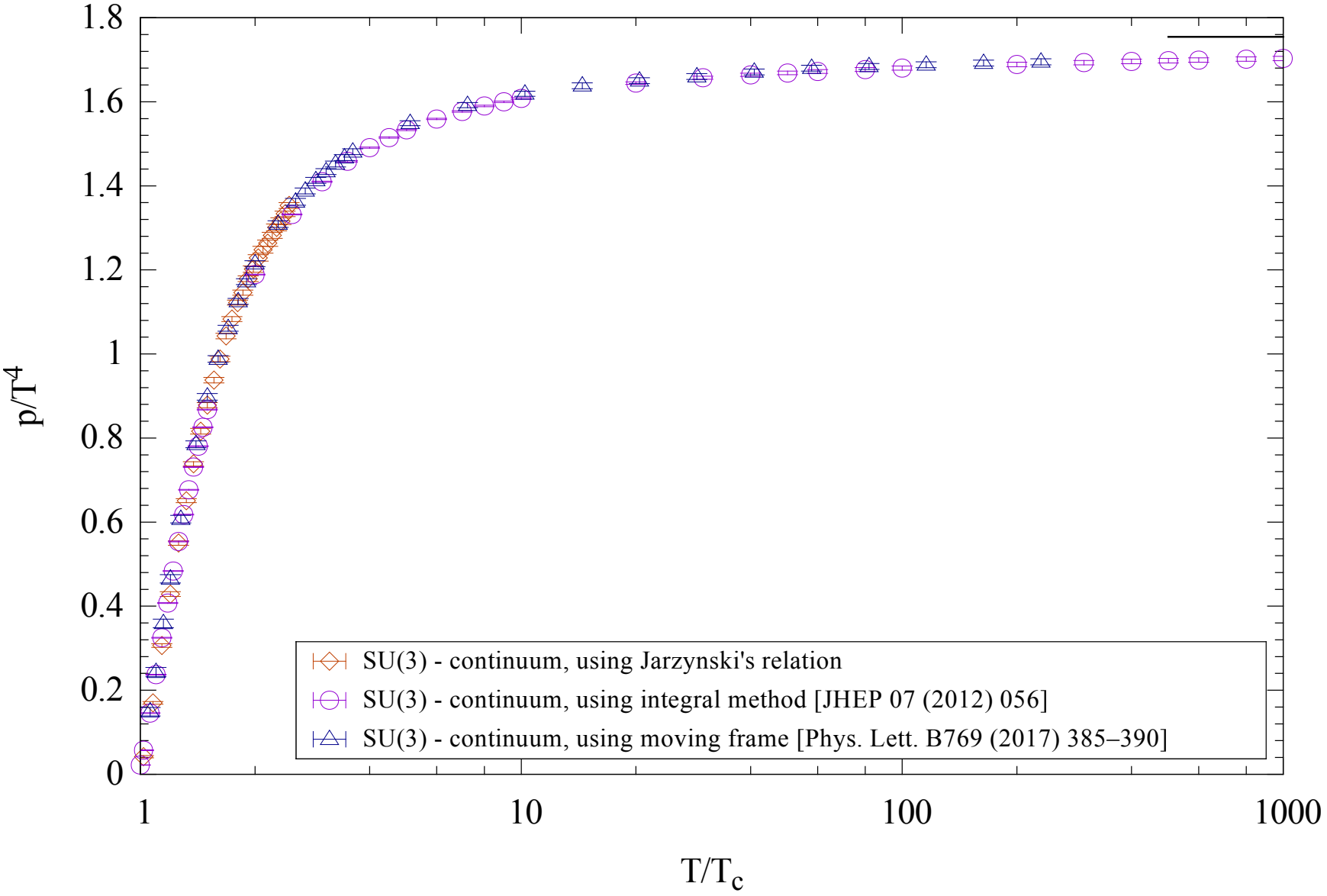
- using the gradient flow **[Kitazawa et al., 2016]**

  → primary observables: **components of $T_{\mu\nu}$**

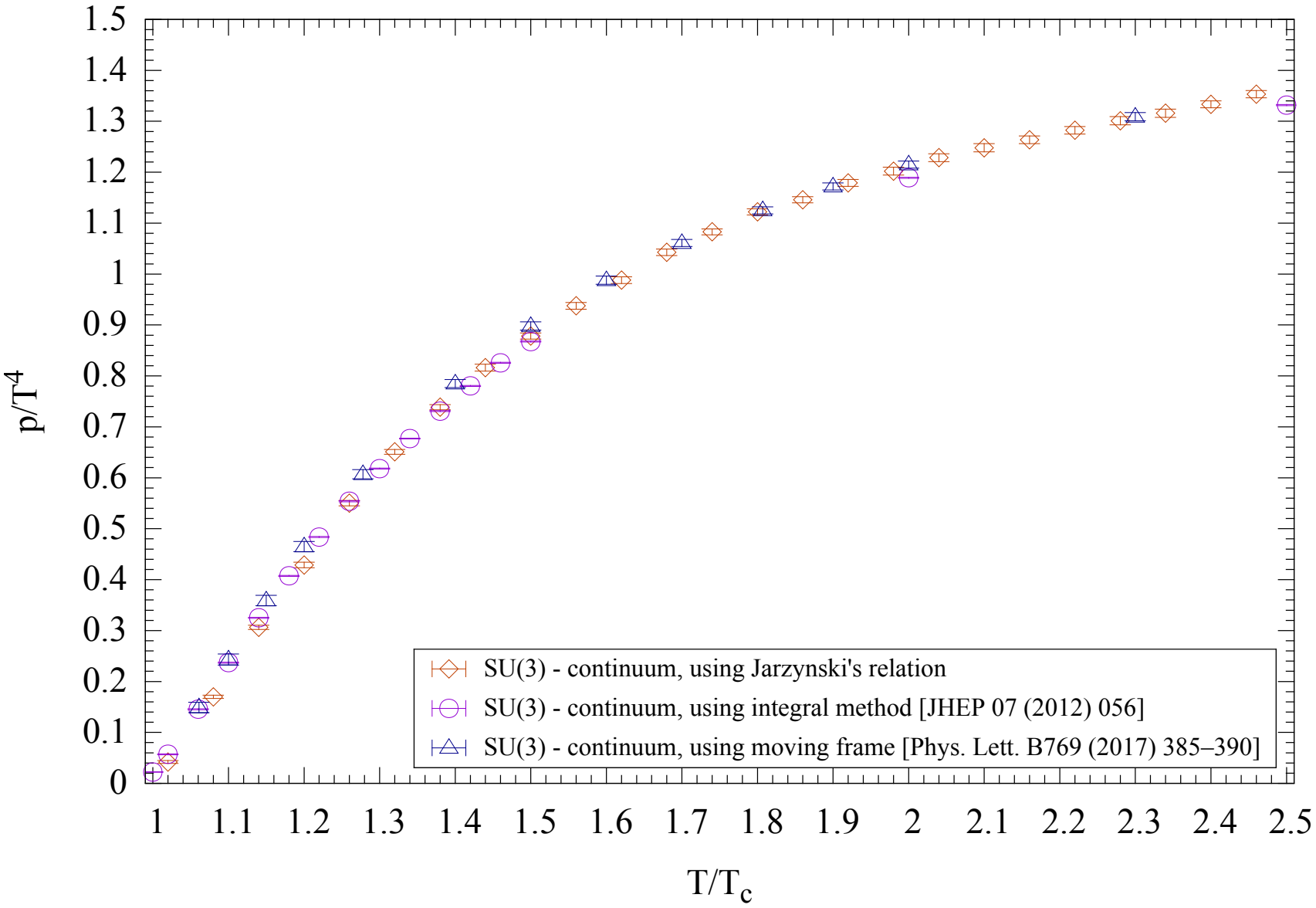
- using Jarzynski's equality **[M. Caselle,A.N.,M. Panero, 2018]**

  → primary observable: **pressure**

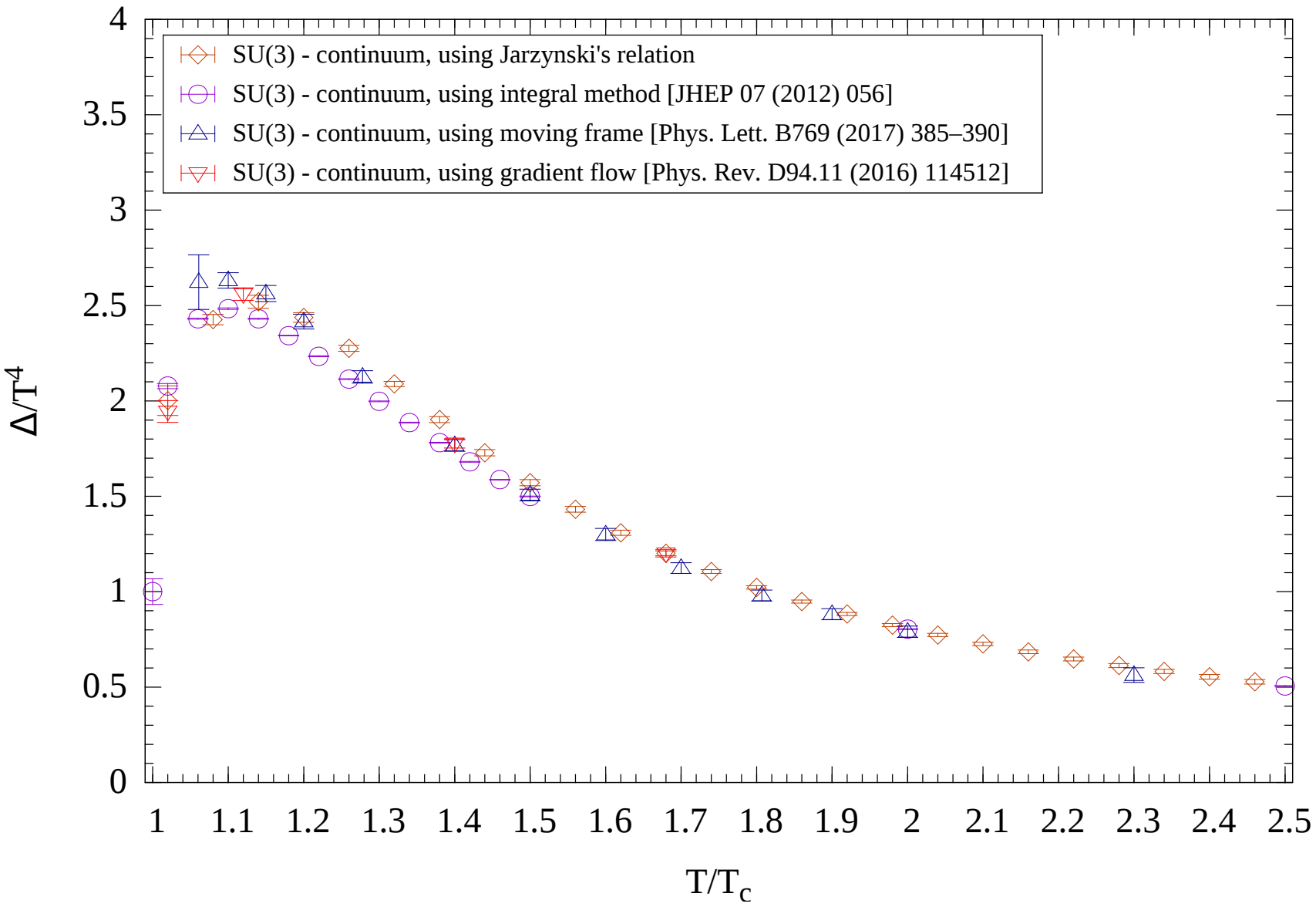
SU(3) pressure



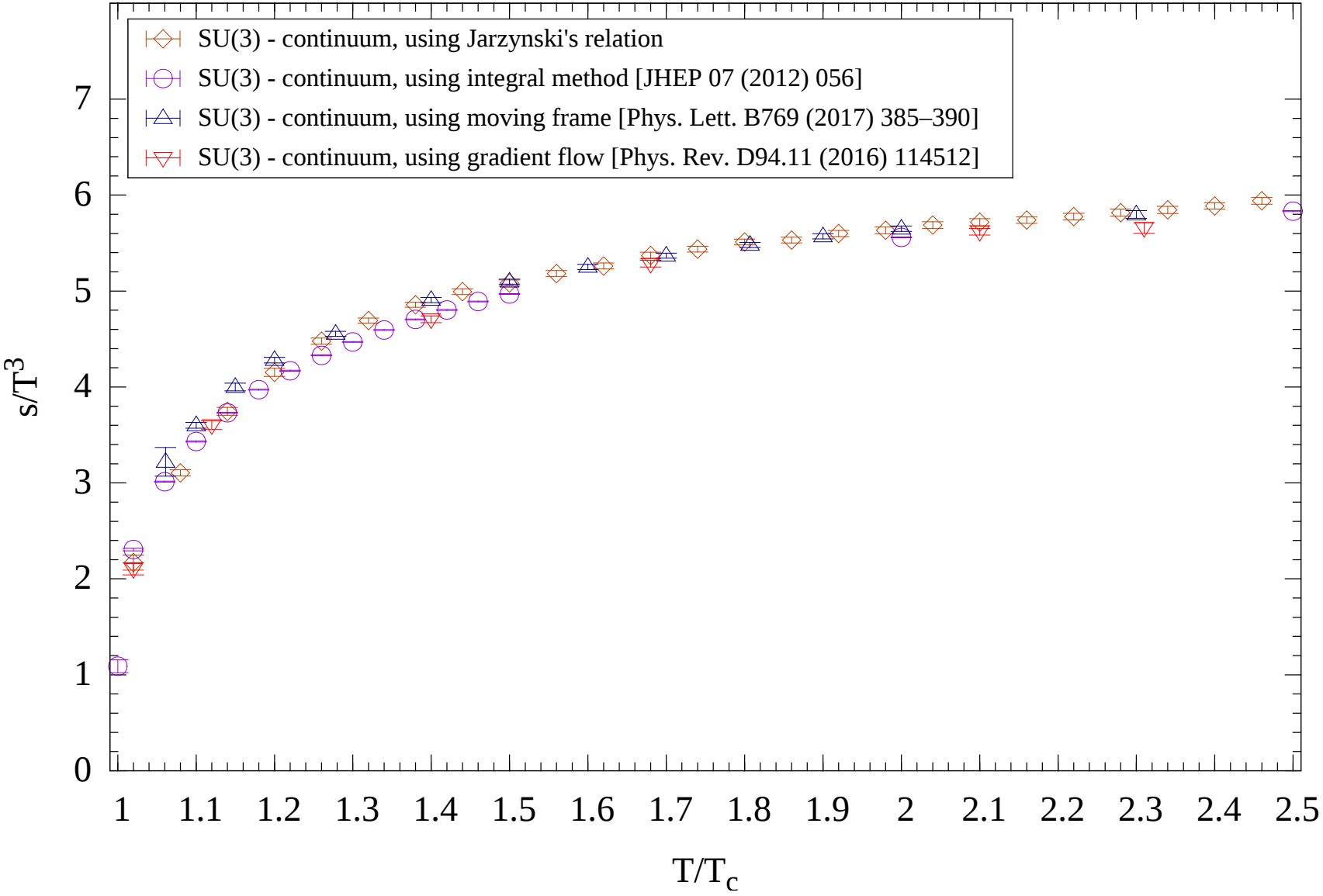
SU(3) pressure



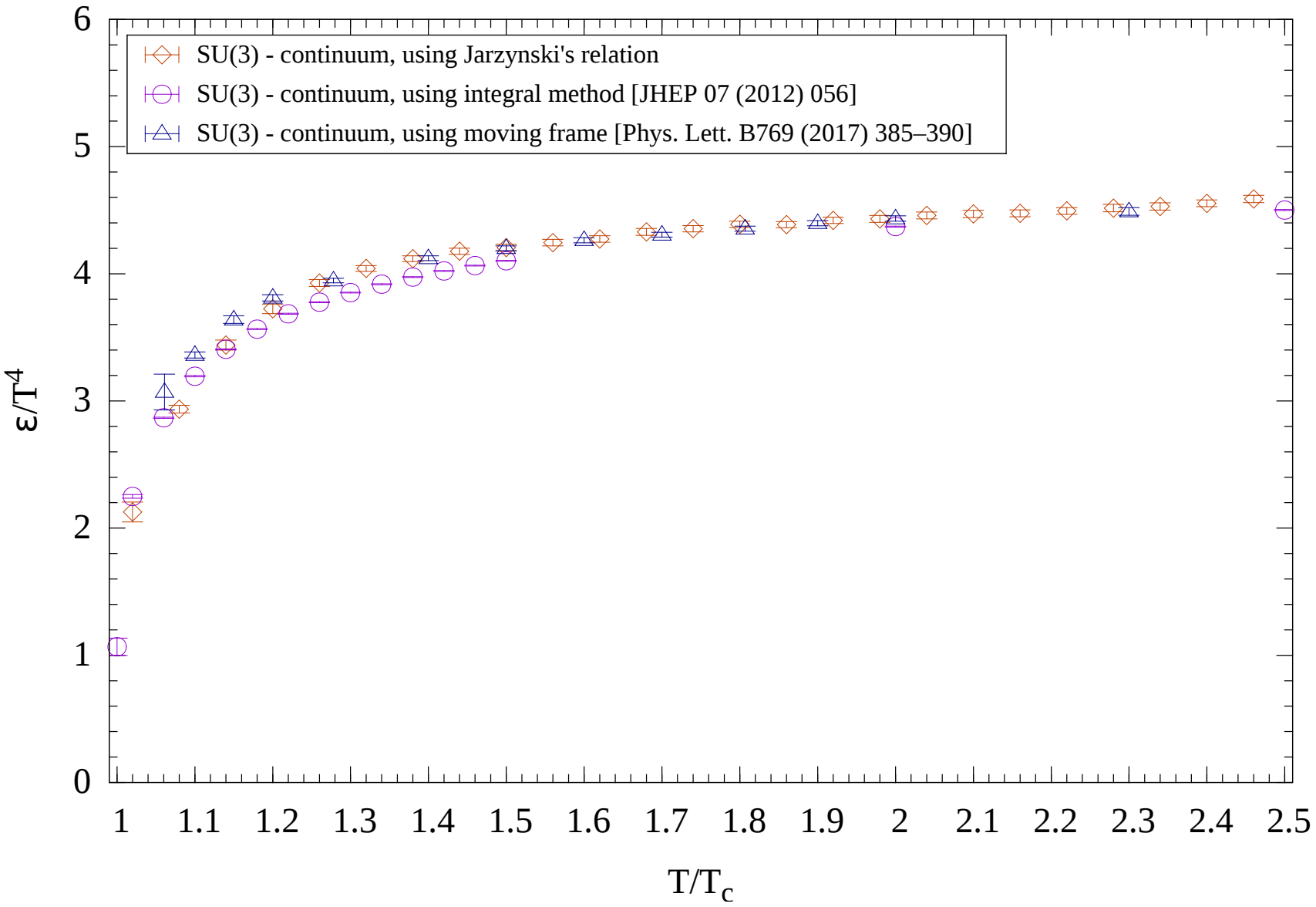
SU(3) trace anomaly



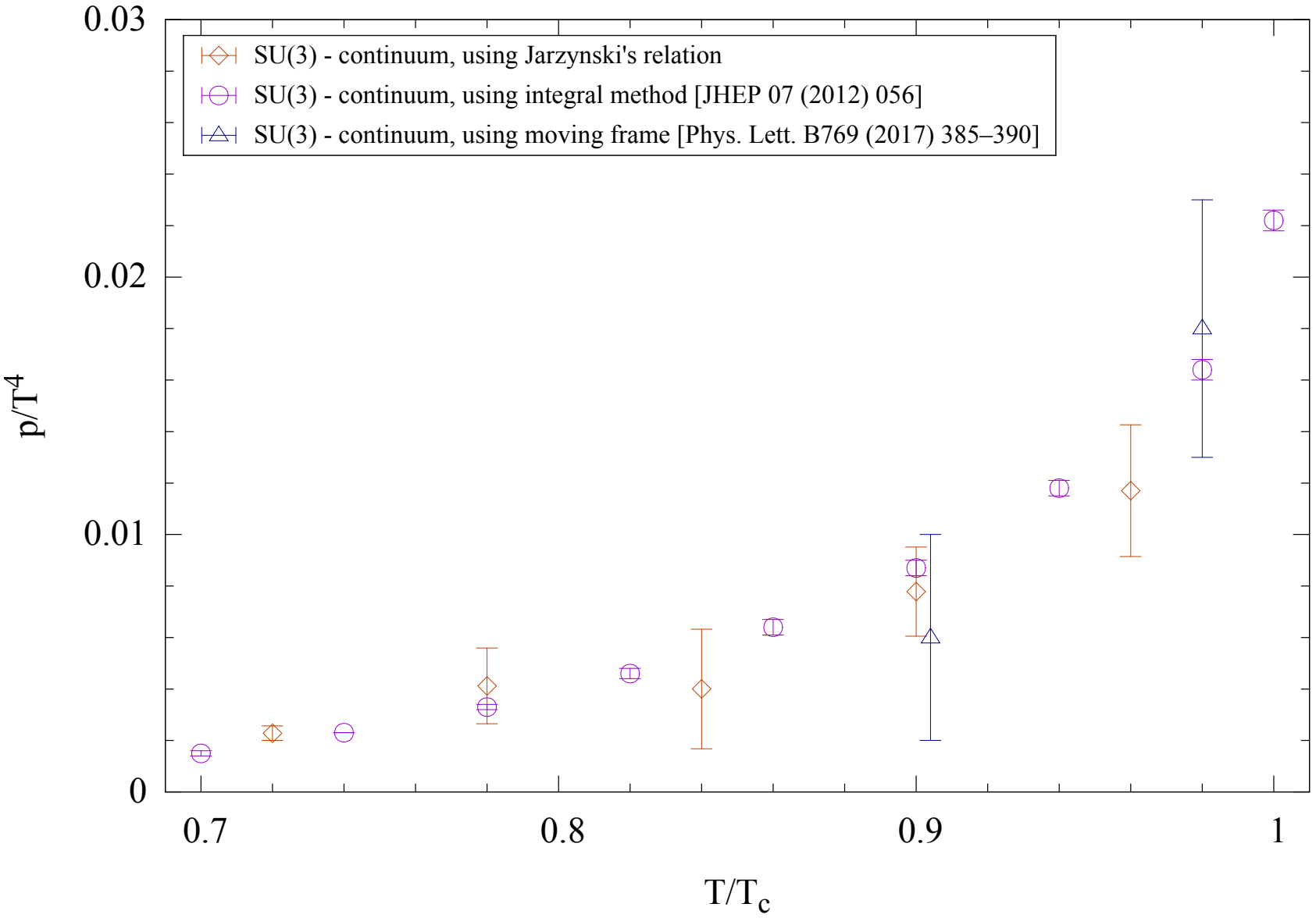
SU(3) entropy density



SU(3) energy density



SU(3) pressure - confining phase



Conclusions

- Several methods are able to determine with high accuracy the equation of state in the $\mathrm{SU}(3)$ pure gauge theory: general agreement in the continuum limit between different calculations is found...
- ...despite different "primary" observables are calculated and the renormalization is performed in completely different ways

- still, non-negligible discrepancies persist, especially in the $[1.1\,T_c, 2.5\,T_c]$ range
- possibly the results of a combination of factors:
  - uncertainty on T_c and on the scale setting should be assessed($\rightarrow$ horizontal error bars?)
  - cutoff effects (especially just above T_c)
  - the way "secondary" observables are calculated (by integration or derivation) has some degree of arbitrariness

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Thank you for the attention!

Jarzynski's equality provides a solid framework 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 $\rightarrow$ 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**

- The equality requires no particular assumptions and holds under very general conditions: in our case (Markov chains) the detailed balance condition is sufficient

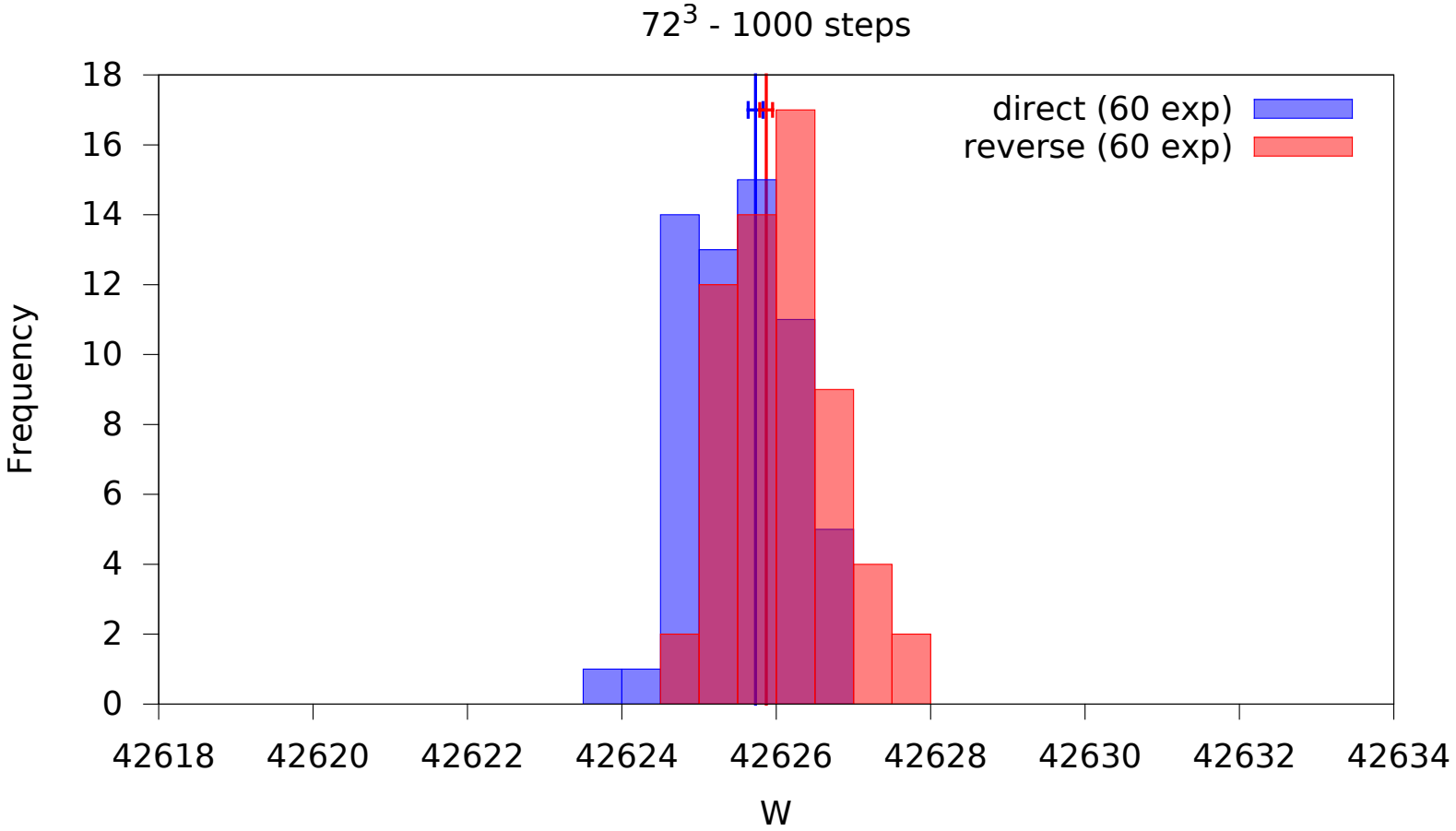
- in a Monte Carlo simulation we can control
  - N, the number of **steps** for each transformation between initial and final value of the parameter λ
  - n_r, the number of **"trials"**, i.e. realizations of the non-equilibrium transformation

- in general, a systematic **discrepancy** appears between 'direct' ($\lambda_i \to \lambda_f$) and 'reverse' ($\lambda_f \to \lambda_i$) transformations when n_r is finite. In practice, one has to choose a suitable combination of N and n_r in order to obtain convergence.

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

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

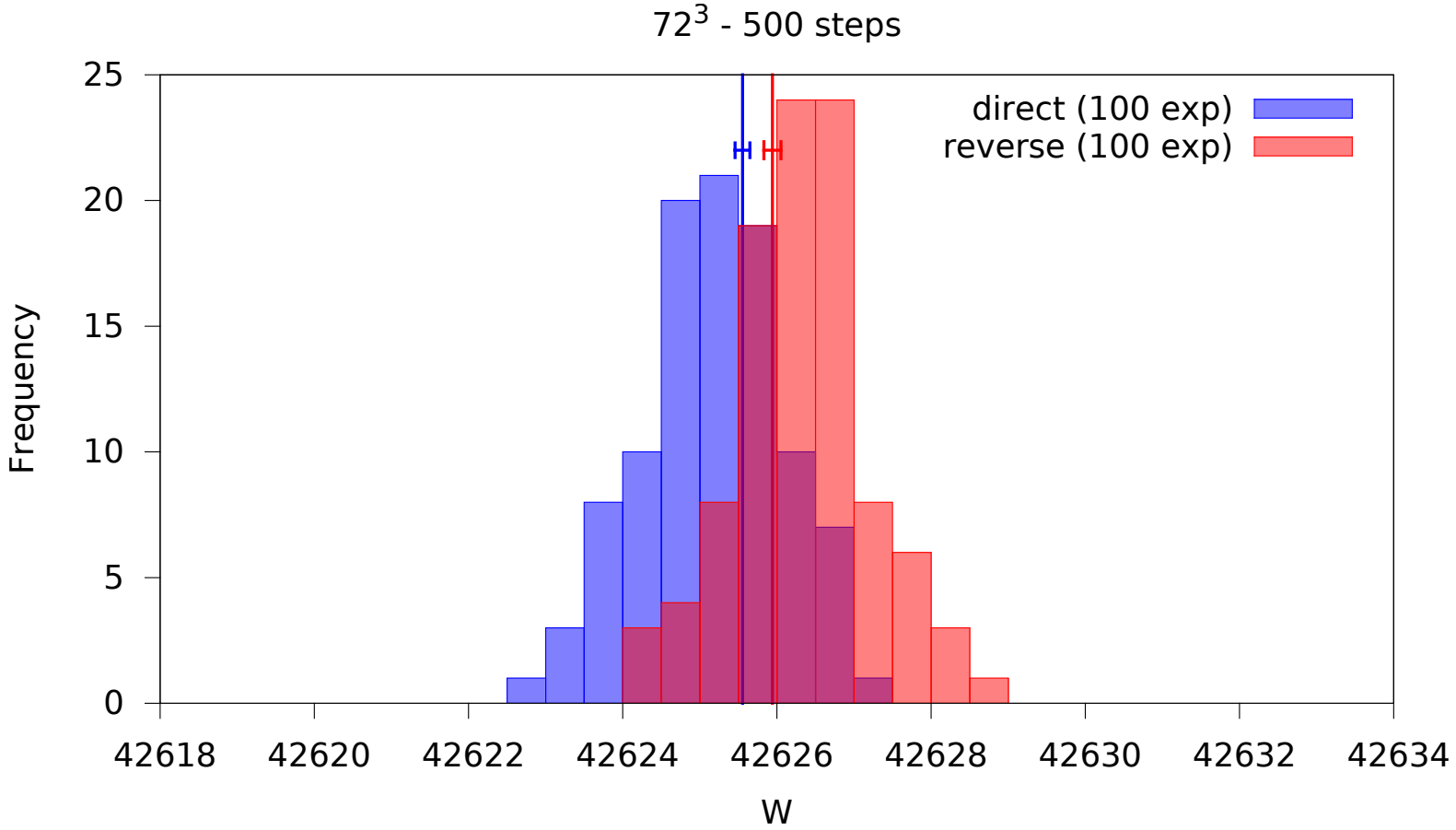
Work distributions



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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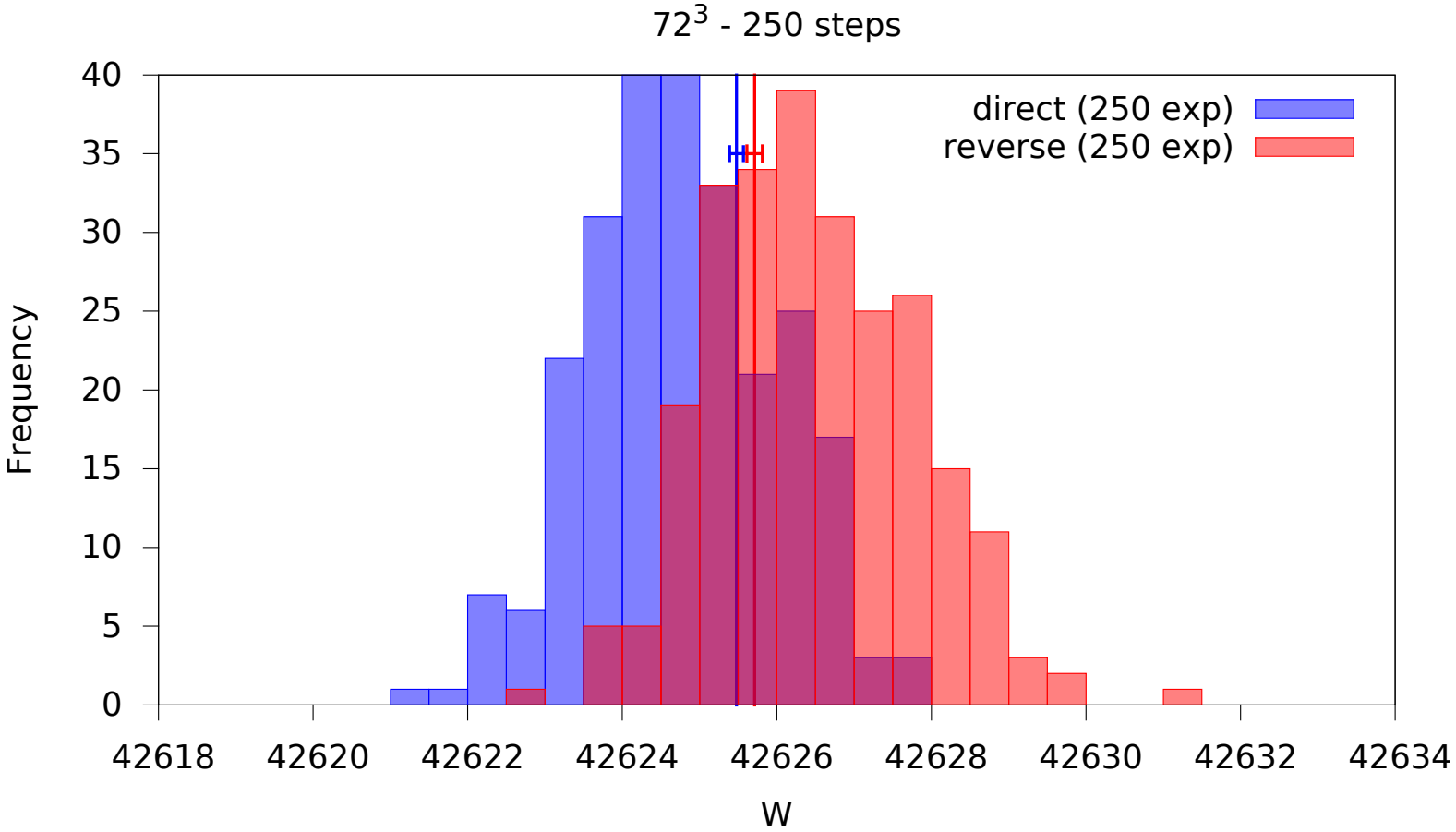

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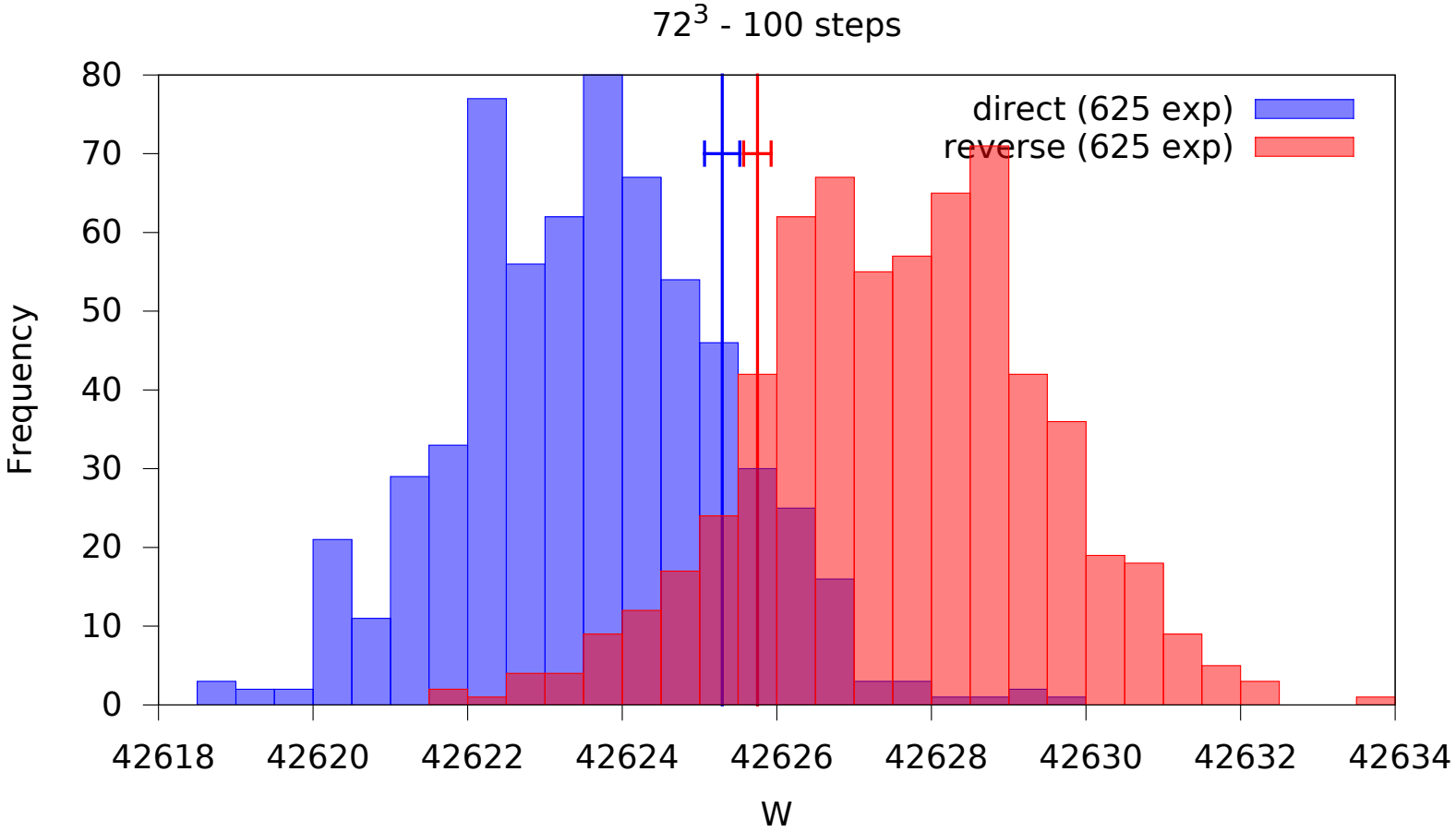

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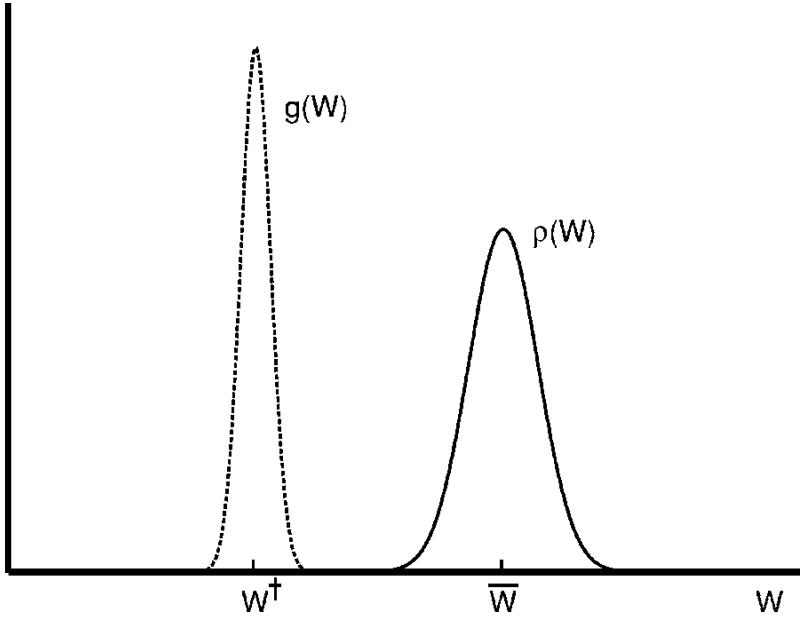
Dominant realizations



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.

Crooks fluctuation theorem

Crooks discovered in 1998 another relation deeply connected with Jarzynski's equality

$$\frac{P_F(W)}{P_R(-W)} = e^{\beta(W-\Delta F)}$$

The $P_{F,R}$ indicate the probability distribution of the work performed in the forward and reverse realizations of the transformation.

$W_d = W - \Delta F$ is the **dissipated** work.

Pressure renormalization

The pressure is normalized to the value of $p(T)$ at $T = 0$ in order to remove the contribution of the vacuum. Using the 'integral method' the pressure can be rewritten (relative to its $T = 0$ vacuum contribution) as

$$\frac{p(T)}{T^4} = -{N_t}^4 \int_0^\beta d\beta' \left[3(P_\sigma + P_\tau) - 6P_0\right]$$

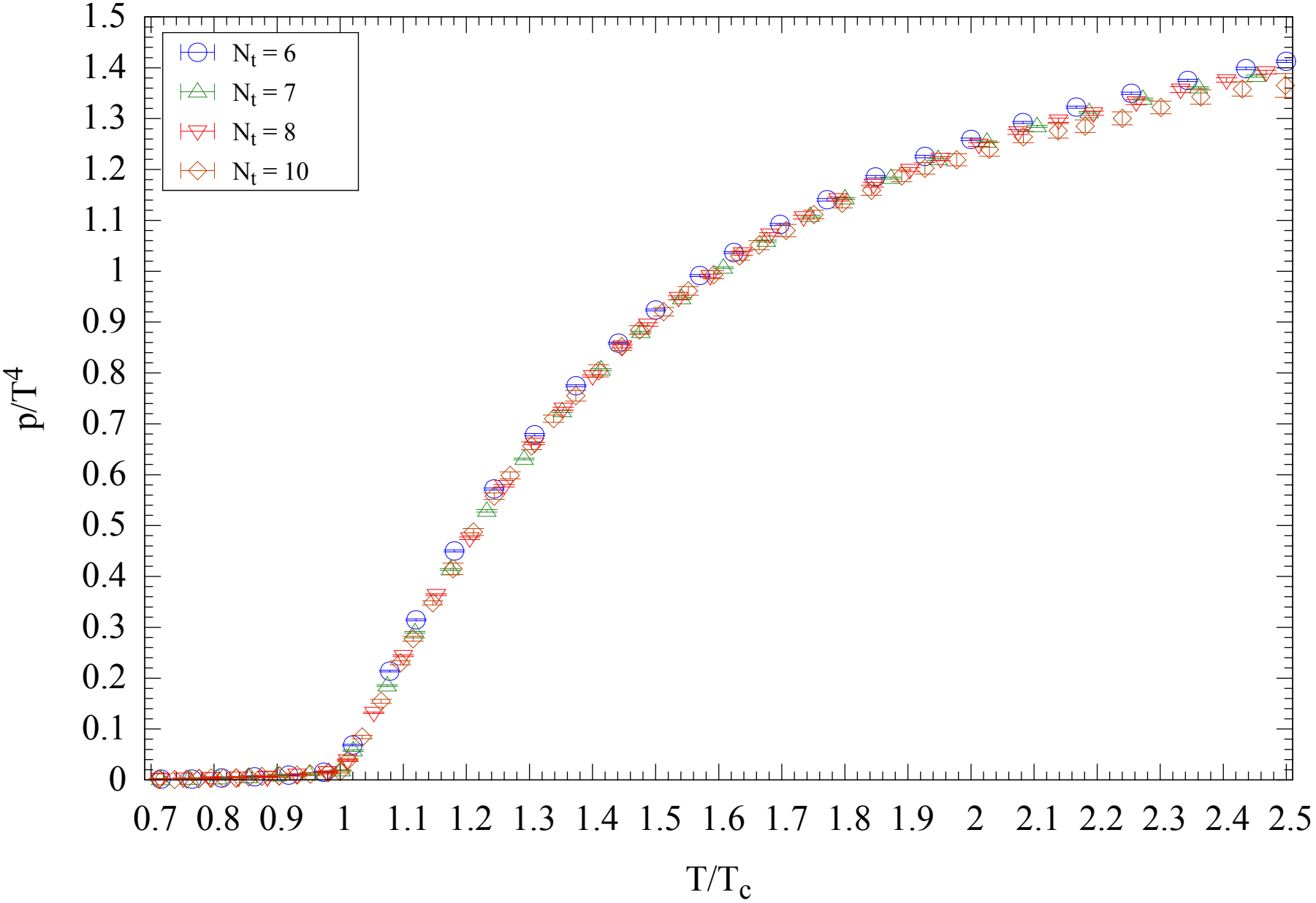
where P_σ and P_τ are the expectation values of spacelike and timelike plaquettes respectively and P_0 is the expectation value at zero T.

Using Jarzynski's relation one has to perform another transformation $\beta_i \to \beta_f$ but on a symmetric lattice, i.e. with lattice size $\widetilde{N}_s^4$ instead of $N_t \times N_s^3$. The finite temperature result is then normalized by removing the $T = 0$ contribution calculated this way.

$$\frac{p(T)}{T^4} = \frac{p(T_0)}{T_0^4} + \left(\frac{N_t}{N_s}\right)^3 \ln \frac{\left\langle \exp\left[-W_{\mathrm{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{N_t \times N_s^3}\right]\right\rangle}{\left\langle \exp\left[-W_{\mathrm{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{\widetilde{N}^4}\right]\right\rangle^\gamma}$$

with $\gamma = \left(N_s^3 \times N_0\right) / \widetilde{N}^4$.

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



Some potential applications beyond the e.o.s.

- 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.