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Efficient Parallel Tempering with Multiple Gaussian Modified Ensembles

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We present some aspects of multiple Gaussian modified ensemble simulations (MGME) for the efficient Monte Carlo studies of temperature driven first order phase transitions.

It is a matter of fact, that most of nature's phase transitions are of discontinuous i.e., first order nature. In first order phase transitions one finds mixed phases, which for *finite sized* systems have finite and possibly small probability to be found in experiments as well as in computer simulations. Also frequent experimentation with nano-devices, as well as with soft matter like proteins, highlights the need for understanding the thermodynamics of finite sized systems[1]. These systems often are made from mixed phases, inhomogeneous in nature, one example being the aggregation of protein look alike molecules in a box, or the simple nucleation of droplets.

In this short note we turn to one of the simplest $2d$ spin models with a mixed phase, namely the $2d$ Potts model at a number of spin states $Q = 20$ and $Q = 256$, which both display strong first order behaviour. The $2d$ Potts model is a perfect testing ground for algorithmic developments as due to Baxter's and others work many observables at the first order phase transition are exactly known. MGME Monte Carlo simulations[2] are designed to calculate the density of states $g(E)$, that is the number of configurations at energy values E, for all values of the energy E.

The idea of MGME simulations consists in writing the partition function as a product

$$Z = \prod_{i=1}^{N_{rep}} Z_i \tag{1}$$

of $i = 1, ..., N_{rep}$ partition functions Z_i in such a way, that the normalised probability distribution functions $PDF_i(E)$ in the energy E of the replicas fulfil

$$0.63 \approx \sum_E \min[PDF_i(E), PDF_{i+1}(E)]. \tag{2}$$

Of course this overlap criterium is taken in-between all neigbouring factors i and $i + 1$ of the product form Z, which then ensures a broad sampling of all energy values on the interval $-2V, ..., 0$, where the Potts energy is $E = -\sum_{nn} \delta_{q_i,q_j}$ and V is the volume. Quite naturally also, one will distribute the various partition functions Z_i on the nodes of a parallel computer, and, utilising local spin updates, as well as parallel tempering swaps[3] in-between neighbouring partition functions Z_i and Z_{+1}, one will record the multi-histogram $\mathrm{MHIST}(E)$, for the probability of energy E occurring in Z. The multi-histogram $\mathrm{MHIST}(E)$ is then used to determine a stochastic estimate of $g(E)$. Modifications using Bennett's method[4] will be included into a forthcoming publication. The peculiar choice of the constant 0.63 in eq.(2) yields swap acceptance rates $P_{acc} \approx 0.5$ for unimodular, that is almost Gaussian PDF's.

In detail we factorise Z into $Z = Z_{\mathrm{lowT}} \times Z_{\mathrm{MGME}} \times Z_{\mathrm{highT}}$, where the first and third factors take care of broad histogram sampling in low and high temperature phases. Z_{MGME} covers the mixed phase at β_T for energy values $e_o V \leq E \leq e_d V$. For $Q = 20$ we have the energy density values $e_d = -0.62652917$ and $e_o = -1.82068443$, while $\beta_T = \ln[1 + \sqrt{Q}]$ generally. All of these three partition functions are itself products of Z_i functions and with $\beta = 1/T$ we write

$$Z_{\mathrm{lowT}} = \prod_i^{N_1} Z_{\mathrm{lowT,i}} \quad ; \quad Z_{\mathrm{lowT,i}} = \sum_{conf.} e^{-\beta_i E} \, \Theta(\frac{e_o + e_d}{2} - e) \tag{3}$$

$$Z_{\mathrm{MGME}} = \prod_i^{N_2} Z_{\mathrm{MGME,i}} \quad ; \quad Z_{\mathrm{MGME,i}} = \sum_{conf.} e^{-\beta_T E - [(E - E_0^i)/\Delta E_0]^2} \tag{4}$$

$$Z_{\mathrm{highT}} = \prod_i^{N_3} Z_{\mathrm{highT,i}} \quad ; \quad Z_{\mathrm{highT,i}} = \sum_{conf.} e^{-\beta_i E} \, \Theta(e - \frac{e_o + e_d}{2}) \tag{5}$$

with $N_{rep} = N_1 + N_2 + N_3$ and Θ denotes the Heaviside step function.

One important measure of computational efficiency in broad histogram sampling methods is the ergodicity time scale τ_{erg}[6,7], sometimes also called tunnelling autocorrelation time, for the completion - in the mean - of one single "tunnelling event" from the low to

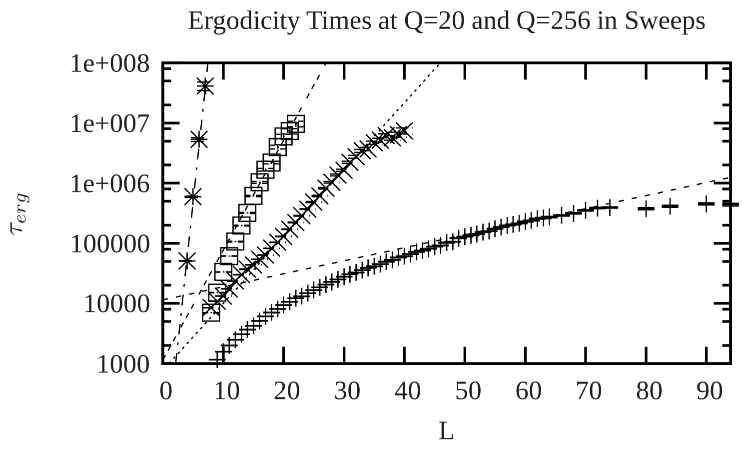

Figure 1. Parallel tempering ergodicity times τ_{erg} for $Q = 256$ (stars) and $Q = 20$ (squares) Potts models *without* MGME improvement. With MGME simulation we obtain the two data sets with small slopes for $Q = 256$ (large crosses) and $Q = 20$ (somewhat smaller crosses). All straight lines have slopes that can be calculated from the free energy of a classical lens shaped droplet at the droplet/strip transition on lattices with p.b.c.[5].

high - or high to low - temperature regions in phase space. We display our final τ_{erg} results from high statistics simulations, at about 1 Giga-Sweeps for each data point - and in a logarithmic scale, in the $Q = 20$ and $Q = 256$ Potts models in Fig.1. The figure contains four data sets. Two of these, the ones with the largest slopes in the figure, correspond to parallel tempering simulations at $Q = 256$ and $Q = 20$ *without* MGME improvement. They exhibit an asymptotic, that is large system size L, supercritical slowing down with τ_{erg} diverging as

$$\tau_{erg} \propto e^{+\ 1.1346\ 2\ L\ \sigma}. \tag{6}$$

The quantity σ hereby denotes the known planar interface tension in-between ordered and disordered phases at β_T in the Potts model. It is clear from these data, why standard parallel tempering at first order phase transitions does not yield useful information. However *with* MGME improvement, see the two data sets with small slopes in the figure, one finds residual supercritical slowing with τ_{erg} diverging as

$$\tau_{erg} \propto e^{+\ (1.1346-1)\ 2\ L\ \sigma}, \tag{7}$$

and thus:

- MGME simulations for first order phase transition studies have a similar level of computational efficiency as Wang Landau[8] and multicanonical ensemble simulations[9].

In conclusion, we think that MGME simulations are useful for the study of mixed phases of finite sized thermodynamics systems.

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