Population annealing algorithm, its GPU implementation and its analysis

Lev Barash[1,2,3], *Martin Weigel*[4], *Michal Borovský*[5], *Wolfhard Janke*[6], *Lev Shchur*[1,2,3]

1) Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia
2) Science Center in Chernogolovka, 142432 Chernogolovka, Russia
3) National Research University Higher School of Economics, 101000 Moscow, Russia
4) Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, United Kingdom
5) P.J. Šafárik University, Park Angelinum 9, 040 01 Košice, Slovak Republic
6) Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, 04009 Leipzig, Germany

Population annealing is a promising recent approach for Monte Carlo simulations in statistical physics, in particular for the simulation of systems with complex free-energy landscapes. It is a hybrid method, combining importance sampling through Markov chains with elements of sequential Monte Carlo in the form of population control. While it appears to provide algorithmic capabilities for the simulation of such systems that are roughly comparable to those of more established approaches such as parallel tempering, it is intrinsically much more suitable for massively parallel computing.

Here, we present a highly optimized implementation of the population annealing algorithm on GPUs and obtain speed-ups of several orders of magnitude as compared to a serial implementation on CPUs. Our code includes implementations of some advanced algorithmic features that have only recently been suggested, such as the automatic adaptation of temperature steps and a multi-histogram analysis of the data at different temperatures.

We also present a detailed study of the statistical error and bias in the calculations, and of application of the algorithm to first- and second-order phase transitions.

[1] L.Yu. Barash, M. Weigel, M. Borovsky, W. Janke, L.N. Shchur, Computer Physics Communications 220, 341 (2017).

[2] L.Yu. Barash, M. Weigel, L. Shchur, W. Janke, Exploring first-order phase transitions with population annealing, Eur. Phys. J. Special Topics 226, 595 (2017).

[3] M. Borovský, M. Weigel, L.Yu. Barash, M. Žukovič, GPU-Accelerated Population Annealing Algorithm: Frustrated Ising Antiferromagnet on the Stacked Triangular Lattice, EPJ Web of Conferences 108, 02016 (2016).

Acknowledgments: This work was supported by the Russian Science Foundation (project nos. 14-21-00158)