Monte Carlo methods for massively parallel architectures

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September 29, 2017

While Moore's law of semiconductors has ensured for over forty years that the next generation of processors works significantly faster than the current one, for the last ten years or so *serial* code has not seen any speed-up from new hardware which, instead, achieves performance improvements only from packing more and more cores onto a single die. As a consequence, scientists working with computer simulations need to move away from intrinsically serial algorithms to find new approaches that can make good use of potentially millions of computational cores. Monte Carlo methods based on Markov chains are intrinsically serial and hence cannot be straightforwardly parallelized. For systems with short-range interactions, it it is possible to use domain decompositions to update several degrees of freedom simultaneously. A complementary approach simulates several chains in parallel, be it at different temperatures such as in replica-exchange Monte Carlo or at the same temperature by simply pooling the statistics from independent runs. I give an overview of parallel implementations of Monte Carlo methods in statistical physics and, in particular, focus on two especially promising approaches: the first is a parallel variant of the multicanonical simulation method that uses independent walkers to speed up the convergence and shows close to perfect scaling up to 10^5 threads. The second approach is a sequential Monte Carlo method known as population annealing, that simulates a large population of configurations at the same temperature and then uses resampling and successive cooling to propagate the population. This approach is particularly suitable for parallel computing, and I present an efficient GPU implementation. A number of improvements turn this approach into a fully adaptive algorithm for the simulation of systems with complex free-energy landscapes.

References

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