# Multiscale sampling for Monte Carlo methods.

A.J. Chorin, O.H. Hald, P. Krause, P. Okunev, J. Weare
Lawrence Berkeley National Laboratory

**Summary: We have developed new multiscale Monte Carlo methods that preserve detailed balance exactly; we are applying them to various problems in physics.**

Monte Carlo methods solve problems through statistical sampling on the computer; the major factor that limits their usefulness is the phenomenon of "critical slowdown" which increases the effort required to produce independent samples just exactly in circumstances where Monte Carlo methods are most needed: when problems require the consideration of many coupled scales. Critical slowdown can be beaten by appropriate multiscale sampling schemes, yet such schemes are difficult to derive and implement.

As a byproduct of our work on the reduction of Hamiltonian systems by conditional expectations, we have succeeded in constructing a general and powerful multiscale sampling scheme. Its basis is the following beautiful theorem (Chorin, Hald, Kupferman 2002): Consider a frictionless mechanical system with many variables and random data; pick out a subset of variables, small enough so that computation is easy, and conditionally average the equations on the assumption that you know the values of the reduced set of variables. In this way you get a reduced set of equations. The theorem asserts that the new, reduced system is still frictionless, and the probabilities of the variables that one keeps in the new, smaller, system equal what they were in the full system with many more variables. This provides in principle a way to sample subsets of variables with no bias, and the problem is how to pick these subsets intelligently and then compute efficiently.

The general idea is to sample and average on multiple scales. Suppose there are only two scales: the real, physical, scale on which one models a physical (or economics) system, and a coarser scale in which one keeps only a subset of the variables- think of a detailed map and a map on a coarser scale where there fewer features are displayed. Sampling on the coarser scale is faster and cheaper, and, as long as one preserves probabilities as just described, perfectly accurate for the features that one has kept. Once this is done, one can go back to the finer scales and sample conditionally the features that are present there but not on the coarser scale, which also turns out to be inexpensive. The efficient version of this idea involves a large family of different scales.

* Telephone Number, E-mail address

The first step in using these ideas in computation was taken several years ago

(Chorin 2003), when we figured out how to use the Kadanoff expansion in successive linkages, well known in physics, as a numerical tool for evaluating conditional expectations efficiently. This does away with the need to calculate the cumbersome and expensive probability tables that appear in many block sampling algorithms and also suggests a good way to pick privileged variables for the successive coarsenings. The remaining problem was how to move samples from scale to scale without losing detailed balance, (roughly speaking, the issue is how to sample on several scales in such a way that the calculations remain self-consistent, and that all features of interest are taken into account once and only once). This has now been done by a mathematical argument based on a recurrence relation between successive conditional averages.

We now have what we feel is a unique computational tool. The first applications we are carrying out are: A calculation of exponents and an analysis of self-averaging in a short-range interaction spin glass model and a multiscale implementation of the particle Bayesian filter of Chorin and Krause (2004).

Spin glasses are of great interest both in physics and in neurology, and particle filters are have many applications in engineering as well as in meteorology and oceanography.

References:

A. Chorin, O. Hald, and R. Kupferman, Optimal prediction with memory. Physica D 166 (2002), pp. 239-257.

A. Chorin, Conditional expectations and renormalization. Multiscale Modeling and Simulation 1 (2003), pp. 105-118.

A. Chorin and P. Krause, Dimensional reduction for a Bayesian filter. Proc. Nat. Acad. Sci. USA 101 (2004), pp. 15013-15017.

A. Chorin and O. Hald, Stochastic Tools for Mathematics and Science. Springer-Verlag, New York (2005).

A. Chorin, New algorithms for multiscale sampling, with pplications to spin glasses, in preparation.

**For further information on this subject contact:**
Dr. Anil Deane, Program Manager
Mathematical, Information, and Computational Sciences Division
Office of Advanced Scientific Computing Research
Phone: 301-555-3691
Federal.M.Ployee@science.doe.gov

[*] Telephone Number, E-mail address