



The University of Chicago
Departments of Computer Science,
Mathematics, and Statistics

Scientific and Statistical Computing Seminar

BENEDICT LEIMKUHNER

Department of Mathematics
University of Edinburgh

Thermostats for Flexible Control of a Molecular Ensemble

FRIDAY, October 28, 2011, at 3:30 PM

133 Eckhart Hall, 5734 S. University Avenue (unless announced otherwise).

ABSTRACT

Molecular systems are subject to uncertainty in the initial data, chaotic internal mixing, and unresolved interactions with an environment. For these reasons a statistical perspective is normally taken with respect to molecular dynamics: trajectories are tools for computing averages with respect to some statistical ensemble (defined by a suitable phase space density). I will discuss models for computing statistics in a generalized canonical ensemble, where the density is a smooth function of the energy of the restricted system (an equilibrium state). A stochastic-dynamic "thermostat" (actually a wide family of methods) can be used to define a restricted resolved dynamics modelling the system's embedding within the larger energetic bath, which leaves the desired target distribution invariant. The advantage of these techniques is that they provide an elegant control of the desired distribution: a small perturbation is often all that is needed to achieve correct sampling, and the perturbations can be introduced in restricted phase space directions. Although the thermostat method does not provide a proper dynamical closure, it is very straightforward to implement in a wide range of situations. Under certain assumptions, these methods can be shown to be ergodic, meaning that almost every extended dynamics trajectory samples the equilibrium measure. The strength of perturbation to the internal dynamics can be quantified and controlled in some cases. I will mention several examples to illustrate the power and flexibility of this approach, including methods for maintaining a target ensemble in systems with stiff restraining potentials and in systems subject to driving thermal perturbations (external heating).

Organizers:

Lek-Heng Lim, Department of Statistics, lekheng@galton.uchicago.edu,
Ridgway Scott, Departments of Computer Science and Mathematics, ridg@cs.uchicago.edu,
Jonathan Weare, Department of Mathematics. weare@math.uchicago.edu.
SSC Seminar URL: <http://sites.google.com/site/uchicagoss/>

If you wish to subscribe to our email list, please visit the following website:
<https://lists.uchicago.edu/web/arc/statseminars>.