THE UNIVERSITY OF CHICAGO

Department of Statistics

**SPECIAL SEMINAR**

---


# GÁBOR CSÁNYI

Engineering Laboratory
University of Cambridge


## Numerically Integrating Exponential Probability Distributions: Partition Functions in Statistical Mechanics

**FRIDAY, October 4, 2013, at 12:00 PM**

Ryerson 276, 1100 E. 58th Street

## ABSTRACT


Key words: statistics and materials modelling, evidence integrals, Nested Sampling, partition function, hard spheres, Lennard-Jones clusters, first order phase transitions



A significant fraction of the compute cycles used by physicists, chemists and materials scientists is expended to sample the probability distribution proportional to $\exp[-\beta E(x)]$, where $\beta$ is the inverse temperature, $x$ describes the configuration of particles and $E(x)$ is the potential energy. In use are a wide range of ad-hoc techniques, each optimised to a particular situation, and include Markov Chain Monte Carlo with complicated moves, Hamiltonian dynamics, simulated annealing, replica exchange, etc. After recalling the connection to the evidence integral in Bayesian statistics, I will show how the application of Nested Sampling to compute the corresponding quantity in materials modelling—the partition function—has enabled the efficient and black-box computation of many thermodynamic quantities of interest. Heat capacity curves, phase transitions, phase diagrams, free energy profiles are all obtained without hassle, with the use of a few convergence parameters. While such an approach can often appear to cost more for the computation of a *particular* observable, the availability of very cheap and massively parallel computational resources heavily favours it against the traditional, more human intensive way of materials modelling. The exemplars are various systems using the Lennard-Jones interaction: mapping the hierarchical basin structure of clusters, and the temperature-pressure phase diagram of the extended system, including solid, liquid and gas phases.


---

For further information and inquiries about building access for persons with disabilities, please contact Dan Moreau at 773.702.8333 or send him an email at dmoreau@galton.uchicago.edu. If you wish to subscribe to our email list, please visit the following website: https://lists.uchicago.edu/web/arc/statseminars.