(Mostly) Monte Carlo Methods for Bridging Short and Long Time Scales in Decay of Metastable Phases

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Metastability: Physical Realizations

- Ferromagnets (Magnetic recording media)
- Ferroelectrics
- Crystalline phases (e.g., Diamond)
- Layered materials
- Protein folding
- Supercooled and superheated fluids
- High-energy physics and cosmology ("false vacuum")
- Event horizon of black holes

Methods Developed

- Constrained Transfer Matrix (CTM)
- n-fold Way: serial implementation
- n-fold Way: massively parallel implementation
- Monte Carlo with Absorbing Markov Chains (MCAMC)
- Random Walks in Slow Variables
- Projective Dynamics (PD)
  - Extrapolations in field
  - Extrapolations in system size
  - Forced escapes

Parallelization of n-fold Way

- Dynamics where discrete events are Poisson arrivals (anisotropic spin models, queuing systems) contain substantial amount of parallelism.
- Fast, scalable parallel computers available.

Difficulties:

- Traditional algorithms (Metropolis, Glauber, n-fold Way) attempt one local update at a time.
- Discrete events not globally synchronized.

However, these algorithms are *not inherently serial* (Lubachevsky, 1987).

Monte Carlo with

Absorbing Markov Chains (MCAMC)

Random walks in slow variables

Attempt to construct a random walk in one or more slow variables by projecting out the fast variables.

Typical choices of slow variables:
order parameter, energy.

Our first attempt:
Build the free-energy landscape in order-parameter space using Multicanonical method, and construct an approximate Markov process on this landscape.
(J. Lee, M. A. Novotny, and P. A. Rikvold, 1995.)

Better results:
Projective Dynamics (PD) method.
(M. Kolesik, M. A. Novotny, and P. A. Rikvold.)

Conclusions

Developed several algorithms for systems characterized by large free-energy barriers, enabling very large speed-ups compared to standard MC without changing the underlying dynamics.

Further work

- Phase transitions in electrochemical systems
- Grain growth (high q Potts model)
- Langevin dynamics for continuous spin systems
- Combinations with Molecular Dynamics
- Other coupled materials problems

Some relevant publications

- Constrained Transfer Matrix (CTM)
  - C. C. A. Günther, P. A. Rikvold, and M. A. Novotny, *Phys. Rev. Lett.* **71**, 3898–3901 (1993); *Physica A* **212**, 194–229 (1994).
- n-fold Way: serial implementation
  - A. B. Bortz, M. H. Kalos, and J. L. Lebowitz, *J. Comp. Phys.* **17**, 10 (1975).
  - M. A. Novotny, *Computers in Physics* **9** Jan./Feb., 46 (1995).
- n-fold Way: massively parallel implementation
  - G. Korniss, M. A. Novotny, and P. A. Rikvold, submitted to *J. Comp. Phys.* cond-mat/9812344.
- Monte Carlo with Absorbing Markov Chains (MCAMC)
  - M. A. Novotny, Phys. Rev. Lett. **74**, 1 (1995) and **75**, 1424E (1995).
- Random Walks in Slow Variables
  - J. Lee, M. A. Novotny, and P. A. Rikvold, *Phys. Rev. E* **52**, 356–372 (1995).

- Projective Dynamics (PD)
  - Extrapolations in field or system size
    - * M. Kolesik, M. A. Novotny, P. A. Rikvold, and D. M. Townsley, in *Computer Simulation Studies in Condensed Matter Physics X*, edited by D. P. Landau, K. K. Mon, and H. B. Schüttler, (Springer, Berlin, 1998), pp. 246–251.
    - * M. Kolesik, M. A. Novotny, and P. A. Rikvold, in *Microscopic Simulation of Interfacial Phenomena in Solids and Liquids*, edited by S. R. Phillpot, et al., *Mater. Res. Soc. Conf. Proc.* **492** (1998).
  - Forced escapes
    - * M. Kolesik, M. A. Novotny, and P. A. Rikvold, *Phys. Rev. Lett.* **80**, 3384–3387 (1998).
    - * M. A. Novotny, M. Kolesik, and P. A. Rikvold, *Computer Phys. Comm.* in press. cond-mat/9811039.