

APPLIED MATHEMATICS COLLOQUIUM

DETERMINISTIC METHODS FOR SAMPLING THE CANONICAL ENSEMBLE

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ABSTRACT:

The Nose-Hoover thermostat is a deterministic dynamical system designed for sampling phase space integrals for the canonical ensemble (and can be modified for other ensembles). Newton's equations are modified by coupling an additional reservoir variable to the physical variables. The correct sampling of the phase space is dependent on the Nose-Hoover dynamics being ergodic. In joint work with Legoll and Moeckel, we have proven that the dynamics is not ergodic when the “mass” of the reservoir is large by demonstrating the existence of invariant tori that separate phase space into invariant regions. We will present numerical experiments that show that adding additional reservoir variables as proposed by Martyna, Klein, and Tuckerman can be consistent with ergodicity.

MONDAY, MAY 8, 2006
2:00 PM
Building 2, Room 135

*Reception at 3:00 PM in Room 2-349
(Applied Mathematics Common Room)*

Applied Math Colloquium: <http://www-math.mit.edu/amc/spring06>
Math Department: <http://www-math.mit.edu>



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