



McGill Computational Science and Engineering Seminar



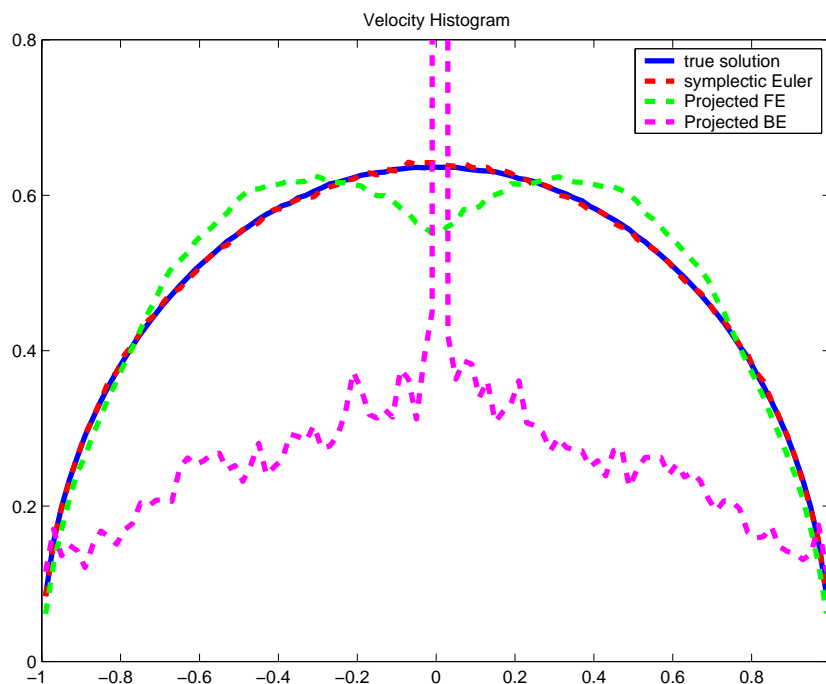
Friday Oct 5th at 14:30 in McConnell Engineering Bldg Room 103

Computing Statistics for Hamiltonian Systems

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SCCM, Stanford University

In molecular dynamics, researchers use computer simulations to determine macroscopic properties of materials. They describe the motion of a large group of atoms or molecules in the material with a system of Hamiltonian differential equations. They then numerically solve these equations over very long time intervals and extract statistical information about the system from the computed trajectories. Results of statistical mechanics then allow them to infer from this microscopic statistical information the properties of the material in bulk.

Since researchers need to solve the equations over long periods of time, most standard methods do not work because they do not conserve important quantities of the system, such as energy. In this talk we will consider two different numerical techniques for integrating Hamiltonian systems that do not suffer from this difficulty: symplectic methods and step-and-project methods. We will assess these two techniques by applying them to a simple Hamiltonian system and seeing how able they are to compute statistical information about the system. We will demonstrate the superiority of the symplectic methods and provide an explanation for the poor performance of step-and-project methods.



Coffee and desserts are served before the seminar at 14:00
in McConnell Engineering Building Room 321.