# An Improved Dynamical Formulation for Constant Temperature and Pressure Dynamics, with Application to Particle Fluid Models

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## Abstract

A new fully dynamical scheme for constant temperature and pressure simulation of particle systems, based on a modification of the Nosé thermostat. A mechanical formulation for simultaneous control of temperature and pressure is also presented. This approach simplifies the construction of symplectic methods while providing a more intuitive perspective on the nature of controlled variable molecular dynamics. Moreover, the described method is Gallilean-invariant, hence angular momentum preserving, and the per-timestep simulation costs are similar to the per-timestep costs of microcanonical $(N, V, E)$ simulation. The scheme is suited to molecular simulation and to large scale particle models of fluids such as smooth particle hydrodynamics and dissipative particle models.

V.N. Alexandrov et al. (Eds.): ICCS 2001, LNCS 2074, p. 1069, 2001.