

# DIRECT VALIDATION TECHNIQUE FOR NUMERICAL SIMULATIONS OF TIME-DEPENDENT HAMILTONIAN SYSTEMS

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## **Abstract:**

Computer simulations have become an indispensable tool for studies of the physics of dynamical systems. To achieve an appropriate level of confidence in the simulation results, accuracy assessments must be conceived as an integral part of the simulation strategies. A common indirect validation method is to cross-check the results of commensurable simulation codes against each other. Furthermore, the simulation results of particularly chosen scenarios may be compared against analytical models.

In this article, we present a "direct" technique for the error assessment of numerical simulations of time-dependent Hamiltonian systems. The method is based on an invariant  $I$  that has been shown to exist for  $n$ -degree-of-freedom Hamiltonian systems with general time-dependent potentials [1, 2]. Because of the generally limited accuracy of numerical methods, this invariant  $I$  can never be realized *strictly* in numerical simulations. The relative deviation of a numerically calculated "invariant"  $I(t)$  from the exact invariant  $I_0=I(0)$  may then be taken as the error estimation for the respective simulation. In this sense, the "direct" error assessment technique can be regarded as a generalization of a validation method that is applicable for autonomous (time-independent) Hamiltonian systems. For these cases, the Hamiltonian  $H$  itself represents an invariant.

Accordingly, the relative deviation of  $H(t)$  from  $H_0$  in the simulation is commonly used as an accuracy criterion. Our approach is applied to estimate the accuracy of a simulation of a three-dimensional system of Coulomb-interacting particles that are confined within a time-dependent quadratic external potential.