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Abstract

Effektiva lösningsmetoder för Schrödingerekvationen: en jämförelse

Solving the Schrödinger Equation efficiently: A comparison

Christoffer Zakrisson

In this paper the rate of convergence, speed of execution and symplectic properties of the time-integrators Leap-Frog (LF2), fourth order Runge-Kutta (RK4) and Crank-Nicholson (CN2) have been studied. This was done by solving the one-dimensional model for a particle in a box (Dirichlet-conditions). The results show that RK4 is the fastest in achieving higher tolerances, while CN2 is the fastest in achieving lower tolerances. Fourth order corrections of LF (LF4) and CN (CN4) were also studied, though these showed no improvements over LF2 and CN2. All methods were shown to exhibit symplectic behavior.

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ISSN: 1401-5757, TVE 13010 maj