

Abstract Submitted
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Finite Element Discrete Variable Method for the Solution of the Time-Dependent Schroedinger Equation BARRY SCHNEIDER, Physics Division, National Science Foundation, LEE COLLINS, Theoretical Division, Los Alamos National Laboratory — We demonstrate how a discretization of the spatial Hamiltonian, using the finite element discrete variable representation, may be combined with the Lie-Trotter-Suzuki (LTS) approach to the time-propagation operator, to produce an extremely efficient algorithm for the solution of the time-dependent Schroedinger equation. The algorithm is explicit, unconditionally stable, scales linearly with the number of basis functions used for the spatial discretization and is easily parallelized. Calculations using a second and fourth order accurate version of LTS propagators will be compared on a few model problems for efficiency and accuracy.

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