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Efficient Massively-Parallel Approach for Soving the Time-Dependent Schrodinger Equation B.I. SCHNEIDER, NSF, S.X. HU, L.A. COLLINS, LANL — A variety of problems in physics and chemistry require the solution of the time-dependent Schrödinger equation (TDSE), including atoms and molecules in oscillating electromagnetic fields, atomic collisions, ultracold systems, and materials subjected to external forces. We describe an approach in which the Finite Element Discrete Variable Representation (FEDVR) is combined with the Real-Space Product (RSP) algorithm to generate an efficient and highly accurate method for the solution of both the linear and nonlinear TDSE. The FEDVR provides a highly-accurate spatial representation using a minimum number of grid points (N) while the RSP algorithm propagates the wavefunction in O(N) operations per time step. Parallelization of the method is transparent and is implemented by distributing one or two spatial dimension across the available processors within the Message-Passing-Interface (MPI) scheme. The complete formalism and a number of three-dimensional (3D) examples are given.

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