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Linear scaling techniques for the solution of the time-dependent Schrödinger equation[1]

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An efficient, accurate solution of the time-dependent linear/nonlinear Schrödinger equation (TDSE) is required for a wide variety of problems in physics and chemistry. These include the dynamics of atoms and molecules in intense/ultrashort external fields, time-dependent approaches to atomic collisions, the dynamics of ultracold media such as Bose-Einstein Condensates and plasmas, and the behavior of materials under extreme conditions. Various techniques have been developed for this purpose. We shall describe a new approach in which the Finite Element Discrete Variable Representation (FEDVR) is combined with the Real-Space Product (RSP) algorithm to generate a highly effective procedure (RSP-FEDVR) for solving the TDSE on supercomputers. Emphasis will be placed on the complete formalism and the implementation of parallelization within the Message-Passing-Interface (MPI) scheme on large, distributed-memory supercomputer clusters. Its superior performance will be illustrated by a number of three-/four-dimensional problems, in comparison to the conventional finite-difference (FD) methods.

[1]In collaboration with Barry I. Schneider (NSF) and Lee A. Collins (LANL).