

A Real-Time Adaptive Finite Element Method for Time-Dependent Kohn-Sham Equation

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In this talk, we will present an adaptive finite element method to solve the time-dependent Kohn-Sham equation in the time domain. The numerical method includes a Crank-Nicolson scheme for the temporal discretization, and a linear finite element method for the spatial discretization. To improve the simulation efficiency, the mesh adaptive methods are introduced in solving Kohn-Sham and time-dependent Kohn-Sham equations. The heuristic a posteriori error estimations for both equations are developed for the mesh local refinement and coarsening, respectively. We also developed an algebraic multigrid solver for the complex system derived from time-dependent Kohn-Sham equation, which works very well in the simulation. The effectiveness of our method is verified by numerical simulations for both linear and nonlinear phenomena.