Adaptive Finite Element Simulations for Kohn-Sham and Time Dependent Kohn-Sham Models

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In this talk, a general numerical framework of using adaptive finite element methods for solving Kohn-Sham and time dependent Kohn-Sham equations will be introduced. Numerical issues on discretization and solvers will be demonstrated in detail, as well as the mesh adaptive strategy and the error indicator used in our algorithm. A variety of numerical results would be given to verify the effectiveness of the algorithm. In particular, an application of our algorithm on a classical phenomenon in the quantum optics, i.e., high harmonic generation, will be illustrated.