

Abstract Submitted  
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**Complex Kohn calculations on an overset grid** LOREN GREENMAN, University of California, Davis and Lawrence Berkeley National Lab, ROBERT LUCCHESI, Texas AM University, C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Lab — An implementation of the overset grid method for complex Kohn scattering calculations is presented, along with static exchange calculations of electron-molecule scattering for small molecules including methane. The overset grid method uses multiple numerical grids, for instance Finite Element Method - Discrete Variable Representation (FEM-DVR) grids, expanded radially around multiple centers (corresponding to the individual atoms in each molecule as well as the center-of-mass of the molecule). The use of this flexible grid allows the complex angular dependence of the wavefunctions near the atomic centers to be well-described, but also allows scattering wavefunctions that oscillate rapidly at large distances to be accurately represented. Additionally, due to the use of multiple grids (and also grid shells), the method is easily parallelizable. The method has been implemented in ePolyscat, a multipurpose suite of programs for general molecular scattering calculations. It is interfaced with a number of quantum chemistry programs (including MolPro, Gaussian, GAMESS, and Columbus), from which it can read molecular orbitals and wavefunctions obtained using standard computational chemistry methods. The preliminary static exchange calculations serve as a test of the applicability

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