Development of a Scalable Algorithm to Solve the Schrödinger Equation for Applications in Quantum Chemistry

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The whole of chemistry can be described by the solutions of the Schrödinger equation, but very few analytic solutions exist, and only for very simple systems, therefore solutions for larger applications must be approximated numerically. Such numerical solutions are currently used for studying various chemical and biological processes, such as protein folding, drug development, and Alzheimer's research, but are very costly and slow. Being a diffusion partial differential equation, the eigenfunctions of the time independent Schrödinger equation can be solved by either implicit or explicit Finite Difference Time Domain (FDTD) schemes that are commonly used for Maxwell’s equations. An imaginary time transformation is used for this project to cause the higher energy frequencies to decay exponentially leaving the ground state eigenfunction. Throughout the process the wave function is normalized every time step, and is also orthogonalized with respect to the lower energy orbitals to calculate the excited states of the electrons. These functions are implemented as OpenCL kernels to be executed on a GPU. Various physical properties are then calculated, including the ionization energy (by integrating <psi|H|psi>), interatomic potentials (by integrating forces on protons from electron density w.r.t. displacement), binding energies, and bond lengths. The forces can be integrated by a symplectic integrator w.r.t. time to calculate atomic trajectories used in molecular dynamics simulations.

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