Scalable GW-BSE code development

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Electronic excitations can play a significant role in designing new functional materials. Although density functional theory has been widely applied to study ground state properties of materials, it has showed limitations in describing excited states of electrons, such as band gaps and optical spectra. The GW-Bethe Salpeter Equation (GW-BSE) method is the fully *ab initio* method of choice for general materials problems involving one- and two-electron excitations. For large unit cells and/or nanoscale systems, the GW calculation is typically *extremely* expensive computationally and is the "show stopper". This is in part due to the computational load typically requiring enormous numbers of FFTs for plane wave bases; separately, the memory requirements for most GW algorithms can be daunting.

We describe our efforts to develop new algorithms that permit GW calculations to be performed on large-scale parallel computers efficiently. We will focus on the computation of the dielectric screening matrix which is one of the most expensive parts of a GW calculation. Our approach uses a real-space representation of the polarizability and avoids extensive use of FFTs, and we compare its behavior to the more conventional G-space GW approaches. Our GW software is in the process of being interfaced with the highly scalable Car-Parinello *ab initio* molecular dynamics simulation package "OpenAtom" [1]. We briefly describe how OpenAtom leverages the charm++ parallel libraries [2, 3] to achieve admirable parallel scaling on large problems as well as greatly reduce the complexity of the parallel code.

[1] `http://charm.cs.uiuc.edu/OpenAtom`

[2] E. Bohm, A. Bhatele, L. V. Kale, M. E. Tuckerman, S. Kumar, J. A. Gunnels and G. J. Martyna: "Fine grained parallelization of the Car-Parrinello ab initio MD method on Blue Gene/L" IBM J. RES. & DEV. VOL. 52 NO. 1/2, 2008.

[3] G. Martyna, E. Bohm, R. Venkataraman, L. Kale, and A. Bhatele: Chapter 5: OpenAtom: Ab-initio Molecular Dynamics for Petascale Platforms, BOOK: *Parallel Science and Engineering Applications: The Charm++ Approach*