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Optimizing GW for Petascale HPC and Beyond[1] JACK DESLIPPE,
ANDREW CANNING, Lawrence Berkeley National Lab, YOUSEF SAAD, University of Minnesota, JAMES CHELIKOWSKY, University of Texas at Austin,
STEVEN LOUIE, University of California, Berkeley — The traditional GW-Bethe-Salpeter (BSE) approach has, in practice, been prohibitively expensive on systems with more than 50 atoms. We show that through a combination of methodological and algorithmic improvements, the standard GW-BSE approach can be applied to systems with hundreds of atoms. We will discuss the massively parallel GW-BSE implementation in the BerkeleyGW package (on-top of common DFT packages) including the importance of hybrid MPI-OpenMP parallelism, parallel IO and library performance. We will discuss optimization strategies for and performance on many-core architectures.

Jack Deslippe
Lawrence Berkeley National Lab

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