Lead developer of a Python code "PSCF Lead developer of a Python code "PSCF Postdoctoral Appointee Lemont, IL Authorized to work in the US for any employer Work Experience Lead developer of a Python code "PSCF Postdoctoral Appointee - Argonne, IL, US January 2014 to Present Argonne, IL Development, and code implementation of linear algebra methods tailored for large matrices with efficient parallelization. Analyzed the performance of an existing code and improved the strong scaling beyond 200,000 cores. This work was published on the cover of Journal of Computational Chemistry and highlighted on ALCF newsbytes. Improved the strong scaling of a popular ab initio molecular dynamics software "SIESTA" by integrating a novel eigensolver that we developed. Lead developer of a Python code "PSCF" that is based on empirical parameters and performs self-consistent optimizations for quantum chemistry. 1 Cython is used for computationally intensive parts of the code and loops are vectorized for performance. PSCF scales efficiently beyond 1,000 cores. Written successful proposals and awarded with more than 5 million computational hours. Postdoctoral Associate Massachusetts Institute of Technology - Cambridge, MA July 2012 to January 2014 Member of the development team of chemical kinetics and reaction mechanism generator software "RMG" written in Java and Python. Contributed to the coding, testing and bug-fixing efforts before the major release of the Java version and the parallelization of the Python version. Development of a "fit-for-purpose" model using lumping analysis, for predicting key quantities of a proprietary hydrotreater reactor as a part of an industrial project for BP. The reductions in the model can eliminate various feed characterization experiments and reduce capital costs significantly. Research Assistant University of Illinois at Urbana-Champaign - Urbana, IL August 2010 to May 2012 Invented a method (XVSCF) in quantum chemistry that is two orders of magnitude faster than its competitors. Lead developer of a modular Fortran code "MaVi" that can fit potential energy surfaces and solves partial differential equations for quantum chemistry applications. Research/Teaching Assistant University of Florida - Gainesville, FL August 2006 to July 2010 Established a general scheme by combining different methods in quantum chemistry to improve the accuracy of predictions. Developed and applied quantum chemistry methods for fast simulation of atomic systems. Given physics lectures for classes of more than 20

students coming from different backgrounds. Awards Graduate student fellowship by the University of Illinois at Urbana-Champaign in 2011 and 2012. Conference travel awards by the University of Florida in 2010 and by the University of Illinois at Urbana-Champaign in 2011 and 2012. First place in the poster presentation competition at the 18th conference on Current Trends in Computational Chemistry in Jackson, Mississippi in 2009. Comprehensive scholarship (covers tuition, accommodation, and monthly salary) during B.Sc. and M.Sc. studies at Bilkent University. Education Ph.D. in Chemical Physics University of Illinois at Urbana-Champaign - Urbana, IL 2012 B.Sc. in Sc & M.Sc Bilkent University - Ankara 2004 to 2006 Skills Python (9 years), C (3 years), Fortran (9 years) Additional Information Skills Programming: Python, Fortran, C, Java, cython, bash scripting Version control: git, svn Parallel computing: MPI, OpenMP, mpi4py, scoop, multiprocessing Debugging & profiling: gdb, gprof, Totalview, valgrind Documentation: Doxygen Software: MATLAB, Octave, Maple, Aspen Python modules: numpy, scipy, scikit-learn, numba, petsc4py, f2py, matplotlib Numerical libraries: PETSc, SLEPc, MUMPS, PT-Scotch, ParMETIS, Elemental, BLAS, LAPACK/ScaLAPACK Expert in computational chemistry, high-performance computing, quantum simulations. Author/coauthor of 17 journal articles and 2 book chapters. Total number of citations over 250 with an h-index of 11. Delivered invited talks at the universities, national labs and research companies.

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