OPTIMIZATION AND PARALLELIZATION OF GAMESS ON DoD HIGH PERFORMANCE COMPUTING MACHINES

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The General Atomic and Molecular Electronic Structure System (GAMESS) code is a quantum chemistry code developed by the Gordon Research Group at the Department of Energy Ames Laboratory and Iowa State University.[a] It is employed in the first-principles modeling of complex molecular systems by using the density functional theory (DFT) method as well as a number of other post Hartree-Fock methods. Both DFT and time-dependent DFT (TDDFT) are of particular interest to the DoD computational biology, chemistry, and materials science community. Millions of CPU hours per year are expended by GAMESS calculations on DoD high performance computing systems. Therefore, any reduction in wall-clock time for these calculations will represent a significant saving in CPU hours. As part of this work, three areas for improvement were identified: (1) integration-grid replacement, (2) TDDFT parallelization, and (3) DFT and TDDFT code optimization. We summarize the work performed in these task areas and present the resulting speed-ups in wall-clock times. Our performance improvements are platform-independent and we anticipate the incorporation of these enhancements into the next official release of the GAMESS code.[b]

[a] M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. J. Su, T. L. Windus, M. Dupuis, and J. A. Montgomery, J. Comput. Chem. 14, 1347 (1993); http://www.msg.ameslab.gov/GAMESS/GAMESS.html.

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