Speeding up ChemApp by Parallelization

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Abstract

ChemApp is a thermochemical programming library which is widely used in universities, government laboratories, development departments and corporate research. It enables the user to perform complex thermochemical equilibrium calculations across a wide spectrum of applications for multi-component, multi-phase systems and the determination of associated energy balances. ChemApp consists of a library of subroutines for data handling and phase equilibrium calculation. It is available in object code for a wide variety of platforms and can be added as a module into virtually any application software. Major application areas are CFD (Computational Fluid Dynamics) and process simulation programs.

OpenMP is the current de facto programming model for parallel programming on shared memory multicore parallel computers. Further development of ChemApp currently involves making it OpenMP enhanced thereby optimizing its performance by enabling a significant reduction in computational time. A sample test case is presented and the obvious performance gains from the preliminary enhanced version of ChemApp are discussed.