SCF and Integral Implementation in GAMESS

RHF SCF driver

This is the structure of the main SCF driver. There are essentially three major components:
1. Screening of integrals at shell level (not described at the point)
2. SCF iteration
3. Fock update

Update Fock matrix

The computed integrals are multiplied by electron density. The result is accumulated in the Fock matrix.

OpenMP SCF Algorithms

There are two major technical issues to threading GAMESS: making the code thread-safe since the use of compiler directives is vendor-specific, and adapting the core modules. In this work, we present three different ways to update the Fock matrix using OpenMP threads. The algorithms have been benchmarked on a cluster of 89 water molecules for the RHF SCF MVEST-3G iteration, in the screening of integrals, and for [ss|ss] integrals only. All benchmarking calculations are done on one BlueGene/Q node. For fair comparison, we varied the number of MPI ranks and used a number of threads on OpenMP. The minimum number of Fock matrix parallelization was determined to be 2 local and 2 threads, which effectively drove down the serial times. Moreover, OpenMP parallelization is done over N and index.

Results

All calculations have been done on a cluster of 89 water molecules in the MVEST-3G/SA level.

Conclusions

In this work, we have applied our initial code optimizations, and developed a thread-safe Rys quadrature integral code with parallelized Self-Consistent field method using OpenMP. We implemented and benchmarked three different hybrid-MPI/OpenMP algorithms. The results using the OpenMP algorithm was benchmarked against an MPI-only implementation on the IBM Blue Gene/Q supercomputer and was shown to be consistently faster by a factor of two.

Supercomputer Challenge

Wall-parallelized and scalable algorithms are required to efficiently use a supercomputer’s enormous number of cores, which is a challenge for quantum-chemistry codes such as GAMESS. To take full advantage of the hardware capabilities of Mira, our development plans include modifying the integral code and incorporating algorithmic improvements, such as the use of ensemble calculations. It is very important to parallelize code efficiently at both MPI and OpenMP levels.

Allocation Programs

Mira is primarily used by projects from DOE's INCITE and ALCC programs. The Innovative and Novel Computational Impact on Theory and Experiment (INCENTE) and ASCI Leadership Computing Challenge (ALCC) programs aim to coordinate scientific discoveries and technological innovations by awarding, on a competitive basis, time on DOE supercomputers to researchers with large-scale, computationally intensive projects that address "grand challenge" in science and engineering. In 2014, INCITE allocations at the ALCF amount to 3.16E+6 core-hours on Mira.

Library

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GAMESS (General Atomic and Molecular Electronic Structure System)

> Ab initio quantum chemistry package
> Generalized Hartree-Fock method

argonne/crt/np/bc.png

The Rys quadrature, one of the oldest and most popular two-electron integral schemes, is applicable to a shell quartet of arbitrary angular momentum. In this quadrature approach, a six-dimensional two-electron integral is computed by Gaussian quadrature over a Rys polynomial.

$$\int (\Psi | (-\nabla | \nabla) \Psi) = \sum_{\text{spatial Gaussians}} \int \Psi^* (-\nabla | \nabla) \Psi$$

where the number of roots, N, is related to the total quartet angular momentum L (i.e., the sum of the angular momenta of the four functions in the integral). A quadrature can be decomposed into the following steps:

1. Evaluate the exponents and weights of the Rys polynomial
2. Evaluate the three- and two-dimensional intermediate integrals
3. Combine the univariate and multidimensional Rys polynomials into the final six-dimensional contracted two-electron integral

$$\int (\Psi^* | (-\nabla | \nabla) \Psi) = \sum_{\text{spatial Gaussians}} \int \Psi^* (-\nabla | \nabla) \Psi$$

where the index i refers to a particular contraction. The roots and weights are typically found using piecewise polynomial fits, or more generally, using Shullenberger's (V.H. J. Quantum Chem., 48, 827 (1992)).

Platform

The Rys quadrature (computer (JUKL))

The structure of the Rys quadrature integral code is shown below. It is implemented using OpenMP. The method has been benchmarked against an IBM Blue Gene/Q supercomputer and was shown to be consistently faster by a factor of two.