

OpenMP and the Gaussian Quantum Chemistry Package

Experiences, Limitations and Future Prospects

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In 2003 a new version of the widely used Gaussian computational chemistry package was released. In contrast to previous releases that used a mixture of UNIX system calls, eg fork/exec, and vendor specific directives to achieve shared memory parallelism, the new code makes extensive use of OpenMP.

In this talk we will give a flavor of the sort of algorithms that are used in computational chemistry, and how they have been parallelized using OpenMP. Some contrast will be made between the use of OpenMP and the equivalent distributed memory parallel algorithms implemented using Linda. Use of shared counters to provide load balancing and the OpenMP "if" clause to switch between different parallel algorithms will be discussed. Experiments to optimize general global reduction operations and to determine the importance of data placement on NUMA architectures will be outlined. Performance results for a variety of platforms will be presented.