

UC Berkeley Results:

Brian Austin of The Lester group at U.C. Berkeley recently participated in IBM's fourth BGW days. The group's first aim was to exhibit the parallel scaling of its quantum Monte Carlo code, Zori, and to demonstrate Zori's particular suitability for the Blue Gene computer architecture.

Second, as part of a larger study of biological photoprotection, the allocated computer time would be used to forward calculation of the energy levels of the spheroidene molecule.

For simple test jobs using up to eight racks, Zori-computed energies agreed perfectly with single-processor runs. Wall time increased linearly with the number of processors at a rate of 7.5 sec/rack, though this number is certainly dependent on specific details of the job input.

This slowdown is dominated by the i/o overhead of reading initial walker configurations. The relative cost of this step will decrease for real calculations, which are much longer.

A 16-rack run was unsuccessful because Zori's load balancing routine exceeded BGW's memory limit by allocating an array that grew with the square of the number of processors. In response to this disappointing discovery, the routine has been rewritten to require only linear scaling memory.

The application to spheroidene could not be performed due, in part, to the parallel-scaling limitation described before, and more importantly, to problems with the HDF library, which prevented output in that format.

In circumstances less hurried than the brief BGW days, both of these difficulties can be overcome. Furthermore, neither issue represents a fundamental limitation of QMC, or Zori specifically, from using the maximum capacity of BGW, or future Blue Gene systems.