Chemistry performance at the Petascale: done! What’s next?

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Summary

- We have run computational chemistry calculations at the Petascale level of performance (1.39 PetaFLOP/s)
- Results of this large-scale simulations provided results that address important scientific problems (e.g. the structure of water).
- Chemistry software designed from the ground up to be scalable can survive hardware changes over an extended period of time (NWChem was first designed in 1993).
- Success of a computational project is not just based on good software practices, but also upon continuous progress in terms of theory, method development, and algorithmic implementation.

Scientific impact

- Objective: Modeling the properties of liquid water
- Highly accurate CCSD(T) study of the electronic properties of (H2O)24 represents a definitive scientific study
- Scientific results that
  1. Will be used by the scientific community at large as reference
  2. Cannot be obtained on commodity HW, truly require Petascale HW

Approaches to Large Scale Parallelization

- The one-sided nature of Global Arrays makes the entire resource of the Petascale machine available to a single calculation
- This is in contrast with other programming modules that resort to make use of more elaborate techniques (e.g. processor groups type parallelism) in order to achieve large scale parallelism.

Structural families of (H2O)17

Benchmark for perturbative Triples correction of CCSD(T)

Jaguarpf specifications

- 2.3-petaflop Cray XT5
- Cray's Seastar2+ network
- 224K AMD Opteron 2.6GHz cores
- 300 TB RAM
- 10 PB Lustre Filesystem

Chemistry Exascale Co-design Center

- Co-design approach to Computational chemistry to tackle the challenges of the Exascale Architectures and deliver a completely new generation of codes in chemistry and materials science
- Cooperative effort with a team made of applications scientists, computer scientists and applied mathematicians
- Development predictive tools for the electronic structure of molecules, solids and interfaces, incorporating environmental effects and dynamics
- Application to grand-challenge problems in energy conversion and storage
- Establishment of a practical path for computation at the exascale with emphasis on both high-productivity and portable high-performance
- Integrated approach to deal with the complexity of the Exascale HW (e.g. Fault-Tolerance, memory hierarchies, multi-core) and development of new programming models applied to algorithmic implementations with high level of concurrency
- Development of reduced-scaling and fast algorithms and the many-body methods of materials science, to facilitate the composition of multi-physics applications, and to exploit advanced autotuning and code-generation/ transformation

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