

CCA Impacts in Computational Quantum Chemistry

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Summary

Within computational quantum chemistry, the Common Component Architecture (CCA) has enabled the standardization of interfaces and the interaction of several chemistry and mathematics packages as well as development groups. As a result, molecular geometry optimization now benefits from state-of-the-art numerical optimization methods. Recent accomplishments include improvements in parallel scalability and flexibility as well as the exploration of deeper integration within chemistry packages.

Historically lacking common interfaces, the computational quantum chemistry community has shared ideas but lacked collaborative software development. The Common Component Architecture (CCA) chemistry project within the SciDAC Center for Component Technology for Terascale Simulation Software (CCTSS) has demonstrated the potential impact that component-based software development holds for computational chemistry and the broader field of scientific simulation. Common interfaces and components now integrate several chemistry and numerical software packages, thereby increasing dynamic programming and parallel efficiency and providing a pathway for developing new methods and algorithms.

The discovery of molecular geometries corresponding to stable and reactive chemical species is a fundamental step in computational processes, including combustion modeling, catalyst design, and the simulation of biological processes (Figure 1). Classic optimization algorithms

suitable for geometry optimization have been implemented in widely used quantum chemistry (QC) packages, but subtle techniques and newer algorithms capable of improving efficiency and robustness are unlikely to be adopted directly due to limitations in manpower and mathematics expertise.

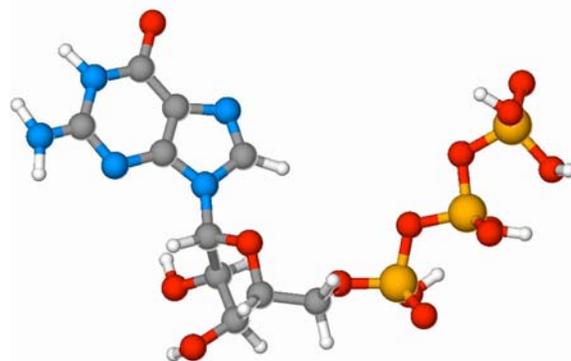


Figure 1. Guanosine Triphosphate in Minimal Energy Configuration

By adopting the methodology and tools of the CCA, a component architecture for molecular geometry optimization is now available, with the Toolkit for Advanced Optimization (TAO) providing a robust and efficient optimization solver component.

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The NWChem and MPQC packages provide interchangeable chemistry components that compute energies and energy derivatives, and the PETSc and Global Array (GA) packages provide linear algebra support. This collaborative effort enables chemists to leverage current research in numerical optimization without duplicating the efforts of experts in the field. Benchmarking of the component application demonstrates reductions in run times up to 43% compared to the stand-alone chemistry packages.

In recent work, NWChem developers have explored algorithms with multiple levels of dynamic parallelism using the CCA. One such algorithm is the determination of energy second derivatives through numerical differentiation of gradients, which may in turn be obtained from numerical differentiation of energies. At the top of the multilevel approach, a CCA driver, operating in the multiple program, multiple data (MPMD) paradigm, instantiates components to calculate gradients using processor subgroups. Each component then uses the GA framework in an MPMD fashion to compute energies using subsets of processors within its original subgroup. Each energy evaluation, itself, can utilize a number of processors in a single program, multiple data (SPMD) fashion, resulting in three levels of parallelism (Figure 2). Dynamic creation and management of subgroups, using the CCA and GA frameworks, has enabled the expression of multiple levels of parallelism, yielding a speedup in NWChem by a factor of ten.

Moving beyond simple *interchangeability* of quantum chemistry packages within larger simulations, recent work within MPQC has focused on lower level components that allow true *interoperation* of QC packages. While all QC codes calculate chemical properties based on electronic structure, the

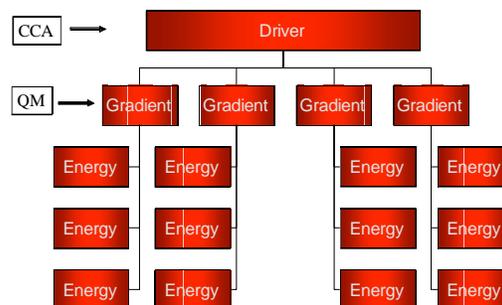


Figure 2: Example of subgroup use for numerical second derivative computations.

algorithms and molecular integrals available in each package differ. As the building blocks for new and exciting algorithms were not previously available to any single package, the adoption of molecular integral components using standard interfaces will allow new scientific capabilities. Prototype interfaces and implementations of molecular integral components have been developed, providing a path to new chemical understanding as well as a test bed for fine-grained component interactions.

With the recent addition of a third chemistry package, GAMESS, the CCA quantum chemistry project is becoming a powerful force in the field, encouraging a transition from numerous disparate packages into a community code base. Future plans include branching out from electronic structure capabilities, enabling the computation of classical molecular mechanics quantities, and developing interfaces and new capabilities with dynamic software. These additions will enable the exploration of reaction rates and dynamical properties in a manner that is currently unavailable.

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