Quantum Chemistry and the Common Component Architecture (CCA)

CCA Overview:
- The CCA Forum provides a specification and software tools for the development of high-performance components.
- Components are self-contained blocks of functionality that can be composed into larger applications.
- A component architecture specifies a framework for composition of components into applications.
- Key CCA benefits:
  - Programming language interoperability via scientific interface
  - Dynamic executability
  - Facilitates collaboration among domain scientists, mathematicians, and computer scientists.

Quantum Chemistry Scientific Application Partnership:
- Contributes to interoperating mechanism among several leading high-performance QD codes (NWChem, GAMESS, and MPQC).
- CCA_chem.generic package defines several interfaces for QC calculations:
  - Molecule, Model, GaussianBeats, IntegralEvaluator
- Every package implements these interfaces to create its own components... facilitates sharing capabilities among chemists and the wider scientific community.

CQoS in Quantum Chemistry: Motivation and Approach

Motivation:
- QCSAP Challenges: How, during runtime, can we make the best choices for reliability, accuracy, and performance of interoperable quantum chemistry components?
  - When several QC components provide the same functionality, what criteria should be employed to select one implementation for a particular application instance and computational environment?
  - How do we incorporate the most appropriate externally developed components (e.g., which algorithms to employ from numerical optimization components)?

CQoS Approaches:
- Overall: Develop infrastructure for dynamic component adaptability, i.e., composing, substituting, and reconfiguring running CCA component applications in response to changing conditions.
  - Performance, accuracy, mathematical consistency, reliability, etc.
- Approach: Develop CQoS tools for:
  - Control: Interpretation and execution of control laws to modify an application’s behavior.
  - CQoS database component: Manage interactions with performance and runtime databases to facilitate analysis and decision-making.

CQoS Infrastructure and Preliminary Results for Quantum Chemistry

CQoS Database Usage in Quantum Chemistry:
- We collected data about all functions provided to database components.
- Database calls are identified in the CQoS GUI to capture various database calls.
- CQoS runs on a variety of architectures.

CQoS Analysis Using PerfExplorer and PerfDMEM

Preliminary performance evaluation of QC packages to learn effective configurations.

Sample Results for GAMESS
- 126 executions on 3 configurations...