

The Collaboratory for Multi-scale Chemical Science (CMCS)

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Summary

The goal of the CMCS is to enhance chemical science research by breaking down the barriers to rapid sharing of validated information and by opening new paradigms for multi-scale science. To accomplish this CMCS is developing an adaptive informatics infrastructure and demonstrating proof-of-concept by publicly deploying an integrated set of key collaboration tools and chemistry-specific applications, data resources, and services. We have implemented a prototype of the Version 1 software, produced use-cases illuminating the central aspects of the project, and demonstrated these capabilities at SC2002.

The Collaboratory for Multi-scale Chemical Science (CMCS) is developing new infrastructure and data-sharing concepts and piloting them among a multi-disciplinary team of chemical scientists working to advance combustion science. The chemical scientists focus on different physical scales in the combustion problem and are geographically distributed. The physical scales range from the electronic structure of atoms and molecules to direct simulations of turbulent combustion phenomena that occur in engines or industrial processes. The proof-of-concept capabilities that CMCS is building are also applicable to many other research areas. These capabilities rely on a capable production network infrastructure that provides user-friendly data and security services, supported collaboration tools, and support for compute intensive applications.

A portal serves as the web interface for the adaptable informatics infrastructure being developed by the CMCS team. The data infrastructure takes advantage of a variety of standards and open-source information technologies to provide an unprecedented ability

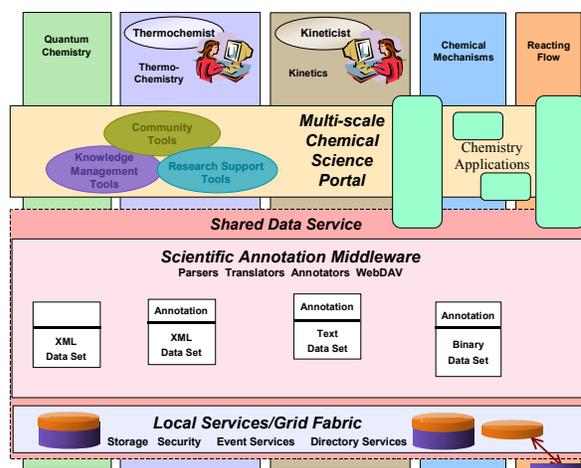


Figure 1. A diagram representing the major conceptual elements of the CMCS informatics infrastructure.

to share data, data pedigree, and project information within groups and across communities. The portal, which can easily be enhanced and customized through the inclusion of new 'portlets,' includes real-time collaboration capabilities, search and notification tools, and a pedigree browser. To support the chemistry community, the CMCS team has integrated a variety of powerful chemistry applications, data viewers, and data translators. Figure 1 shows how CMCS users interact primarily with the

top layer, the CMCS portal and chemistry applications. The applications can appear within the portal or provide their own user interfaces that interact directly with the underlying metadata/data and other CMCS services. The portal provides an array of functionality to support group and community processes, with an emphasis on simplifying the discovery and use of data. The shared data service, shown as the second layer, provides configurable capabilities for automating the generation of metadata, translating data between standard formats, and federating multiple data stores. At the lowest layer, the portal can take advantage of existing distributed services for security, event management, and data storage.

Data pedigree is at the heart of the CMCS project and is a key technology enabling new approaches to science. It allows researchers to categorize and trace scientific data across disciplines and scales and to identify the ultimate origin of scientific data. We have developed a DAV-aware pedigree browser (see lower screen shot in Fig. 2), which can easily display pedigree data (as well as annotations) and allows users to search, browse, and retrieve a data set's pedigree. Pedigree data and metadata are associated with CMCS resources by placing this information into the DAV properties of the data file in the CMCS data store. Pedigree data may also be an active link to a different, but associated, data resource.

Multiple science areas have made data available to the CMCS structure through program modification and data translators. These include data from NIST, NWChem, Ecce, GRI-Mech, Chemkin, and HCT. In addition, the first version of Active Thermochemical Tables (ATcT) has been developed in collaboration with the SciDAC CoG Kit project, with a Web portlet successfully integrated into CMCS. ATcT is a novel scien-

Figure 2. ATcT accessed from the CMCS portal.

The screenshot shows the ATcT web portlet within the CMCS portal. The portlet title is "ATcT" and it includes a search bar for chemical species. Below the search bar, a chemical reaction network is displayed for the methyl peroxy radical (CH₃OO). The network consists of the following nodes and connections:

- CH₃OO (top node, blue box)
- CH₃ and O₂ (middle nodes, red circles)
- CH₃O and O (bottom nodes, blue boxes)

Arrows indicate the reaction paths, with the number '1' on each arrow representing the stoichiometric coefficient. An orange arrow points from the "Active Tables" link in the CMCS portal sidebar to the ATcT portlet.

tific application, centered on a distinctively different paradigm of how to obtain reliable thermochemistry based on the thermochemical network approach. The ATcT Web portlet, shown in Figure 2, is available from a project team workspace in the CMCS Portal. The displayed portlet shows a network used to produce an optimized table of thermochemistry data for the methyl peroxy radical (important in low-temperature combustion).

In the coming year, CMCS will focus on continued chemical science application integration and pilot community involvement. These include connecting to SciDAC quantum chemistry projects, to PRiME (*Process Informatics Model*, an international collaboration on chemical mechanisms), and providing feature tracking for direct numerical simulations that serve the SciDAC reacting flow projects. (Other collaborations include SAM, CHEF, and CCTSS & SDM ISICs.)

For further information on this subject contact:

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