

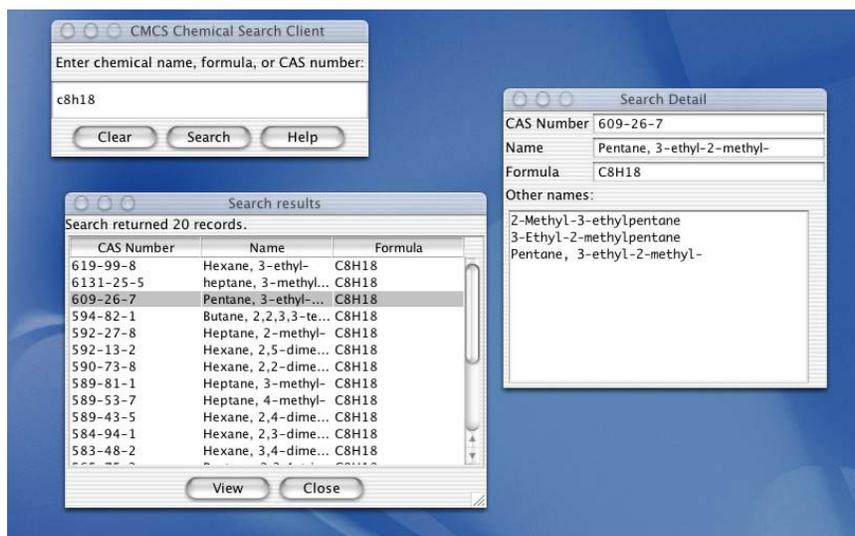
FY2002 Accomplishment

Collaboratory for Multi-Scale Chemical Sciences

(<http://cmcs.ca.sandia.gov/>)

One of the major bottlenecks in a multi-scale research enterprise is the passing of information from one level to the next in a consistent and validated manner. The vision of the Collaboratory for Multi-Scale Chemical Sciences (CMCS) is to bring together leaders in scientific research to develop an informatics-based approach to synthesizing multi-scale information to create knowledge in the chemical sciences. As part of this vision, the CMCS project will demonstrate that difficult multi-scale chemical science goals can be achieved more efficiently and under new paradigms. At a recent project workshop, several key capabilities toward eliminating this bottleneck were demonstrated. One demonstrated capability enables scientists to visualize networks of chemical reactions and to mathematically derive improved thermodynamic values from existing experimental data. Another new capability calculates thermochemical values based on data and metadata stored on a server. A search capability was demonstrated that searches the NIST WebBook database for chemical identifiers such as CAS number, formula and name.

A CMCS portal is being built to enable data-centric project- and community-level collaborations for chemical science researchers. The portal will provide data access, notification, data search, and data manipulation capabilities to chemical scientists. To enable chemistry communities to have knowledge of and access to the latest data available at any scale, a notification capability is essential. This capability to be notified of new data by email and/or to automatically invoke further processing has been demonstrated (for example converting a Janaf file to a NASA polynomial file). Another demonstrated capability was the extraction of metadata from binary files as the files were being added to the CMCS repository. This capability, enabled using the DOE-funded Scientific Annotation Middleware project, allows information from binary files to become searchable. A pedigree browsing capability, which allows scientists to search and examine author and data reproducibility information, was also demonstrated. The CMCS portal is built using the OpenSource JetSpeed portal (<http://jakarta.apache.org/jetspeed/>) and is leveraging work and collaborating with the University of Michigan for improving the usability of JetSpeed for scientific research.



Chemical Search Application. Image courtesy of Thomas Allison, NIST.