

## Abstract:

The Collaboratory for Multi-scale Chemical Science (CMCS) is developing a powerful informatics-based approach to synthesizing multi-scale information and supporting interconnected collaborations across scientific disciplines. An open source multi-scale informatics toolkit (the Knowledge Environment for Collaborative Science (KnECS)) has been developed by CMCS that addresses a number of issues core to the emerging concept of knowledge grids including the tracking of data provenance and the lightweight federation of data and application resources into cross-scale information flows. KnECS also includes a wide range of collaborative tools including chat, shared tasks lists, an electronic notebook, and email lists and archives, to which CMCS has added chemistry-specific analysis and visualization tools, within an overall portal-centric environment.

The CMCS portal is currently in use by a number of high-profile pilot groups and is playing a significant role in enabling their efforts. CMCS has pioneered the use of scientific content management, multiscale/multidisciplinary provenance tracking, and the idea of collaborative community data curation. However, in many ways, CMCS/KnECS is just an early example of a “Cyberenvironment” and there are complimentary capabilities and relevant technologies being explored in other communities. Looking at the capabilities currently available within CMCS, and extrapolating based on these other developments, it is possible to envision a very rich and very flexible model for cyber-enabled combustion research. This talk will provide an overview of CMCS and its potential directions. It will also include a brief discussion of design principles for cyberenvironments that capture lessons-learned on CMCS and in other projects in a way that can guide future efforts to develop persistent, pervasive, scalable environments for cyber-enabled science and engineering.