



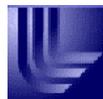
Portal

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CMCS Portal

- Goal: To create a dynamic and easily configurable web environment where users and scientists interact with colleagues to develop and manage data in focused areas as well as community interchange areas. Create ad-hoc or long term team efforts, community of interest interchange areas, ease of access to data management and translation capability, ease of integration of tools and data
- Team:
 - › David Montoya (lead)
 - › Karen Schuchardt
 - › Carmen Pancerella
 - › Sandra Bittner
 - › John Hewson
 - › Bill Pitz
 - › Yenling Ho
 - › Lili Xu
 - › Kathi Parker



Requirement Excerpt from CMCS Project Proposal



Requirements for the Collaboratory for Multi-scale Chemical Science (CMCS) project:

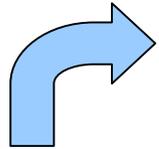
- A collaboration infrastructure is required to enable real-time and asynchronous collaborative development of standards for data and metadata description, inter-scale scientific communication, geographically distributed disciplinary collaboration, and project management.
- Tools now used to generate and analyze data at each scale must be modified to enable generation and storage of the required metadata in a format that allows interoperability with other tools and collaboratory functions, and must be made available for use by geographically distributed collaborators.
- Repositories are required to store chemical sciences data and metadata in a way that preserves data integrity and allows web access.
- New tools are required to search and query metadata, and to retrieve data across all scales, disciplines, and locations. These tools should be available via an integrated user-customizable interface or portal.

Driver for an environment to provide an infrastructure for data, tools and processes to be organized and interact –

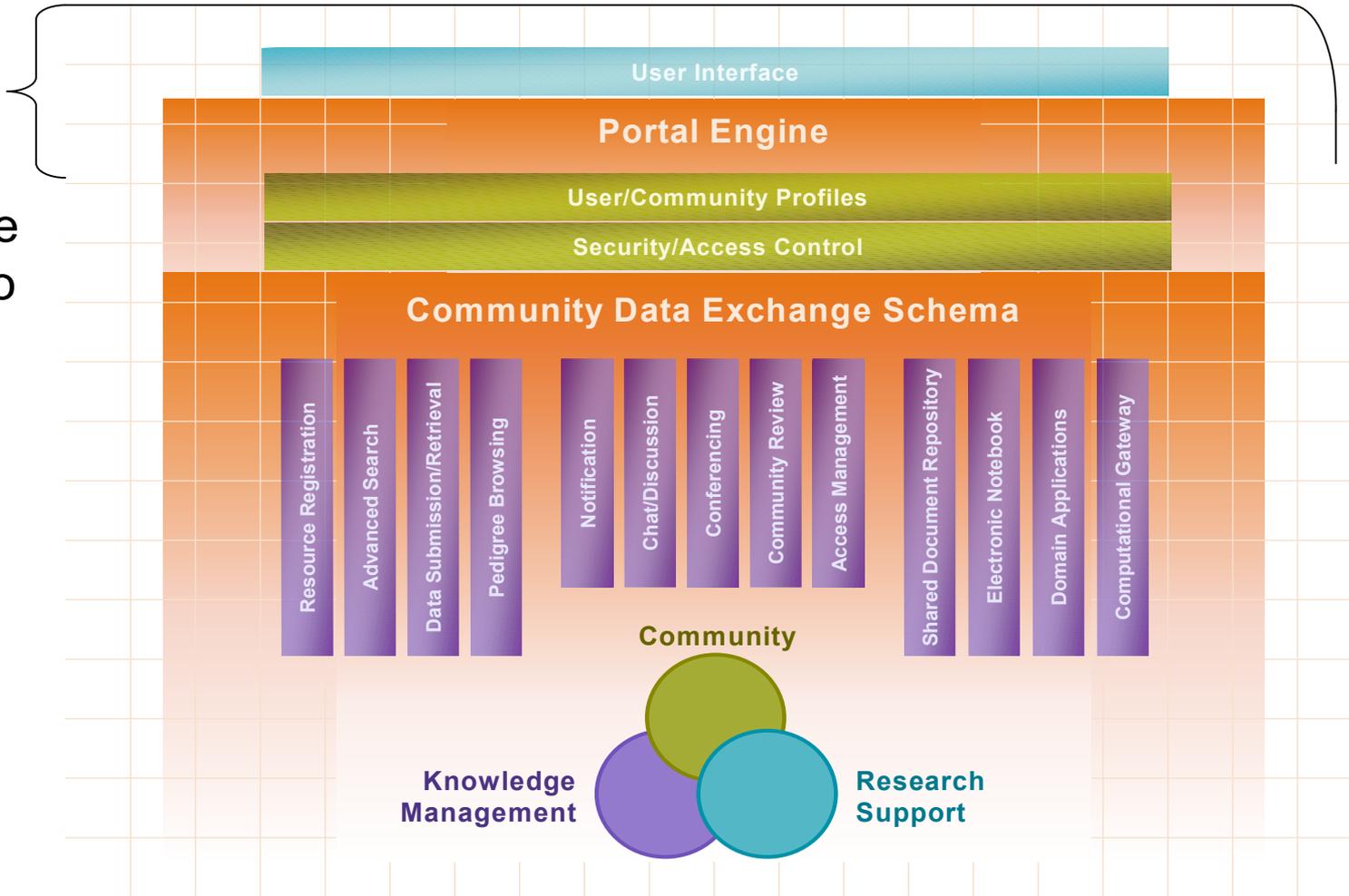
The Portal Framework



Portal in Relation to Other CMCS Areas

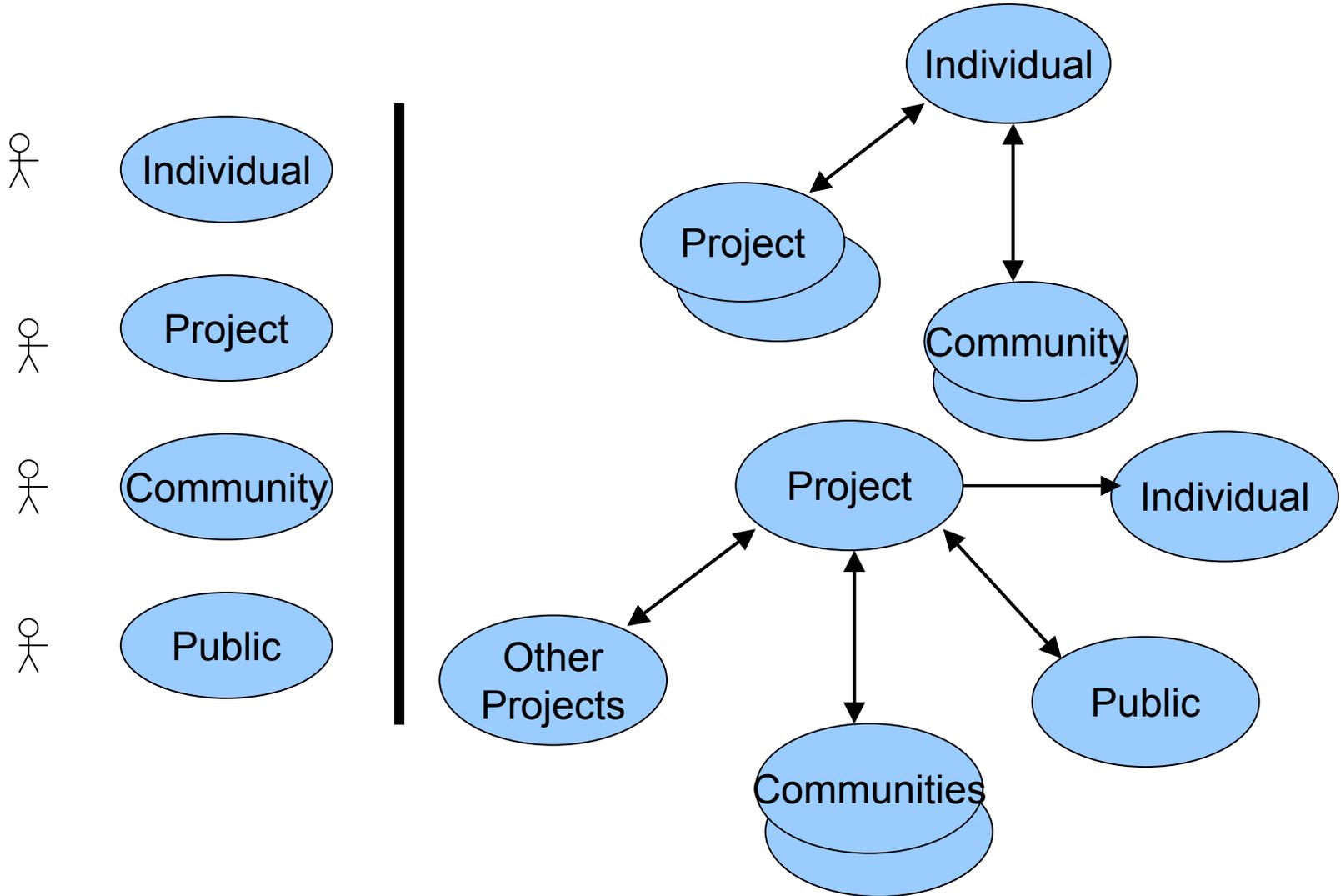


Provide flexible Environment to Support MCS Collaboratory functionality



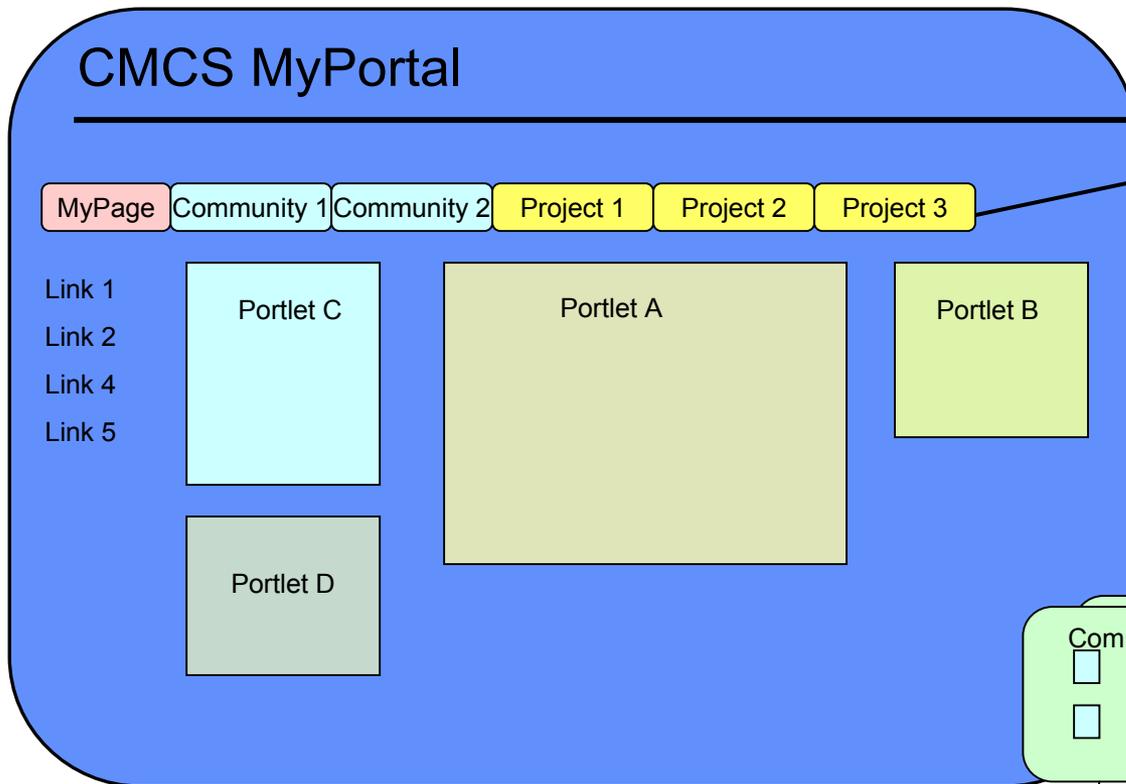


Facilitating Interaction





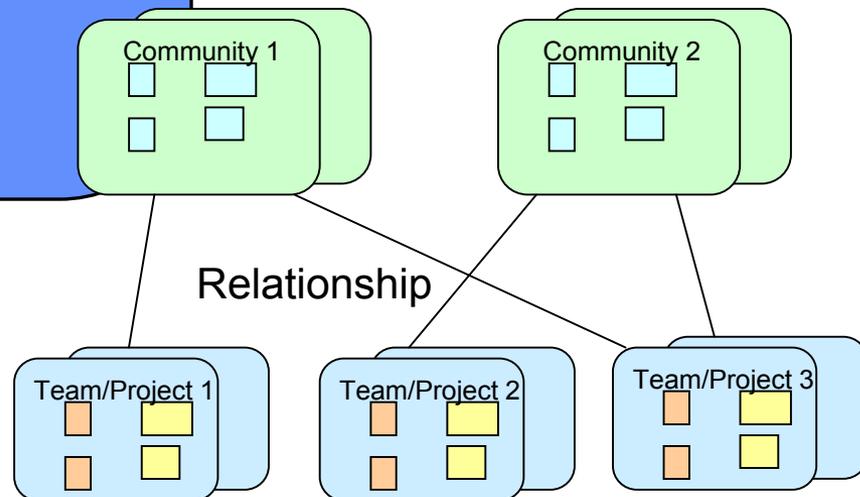
Portal Relationships for a User



Tabs that take you to other Portals that you are interested In or are a member of

Portlets can be selected to go in this section that may include tools, apps, data access, news, collaboration, etc.

This could be the environment for a user. The user has a page configured for their Own use and has included portals for two Communities and is a member of three Project teams.





Use

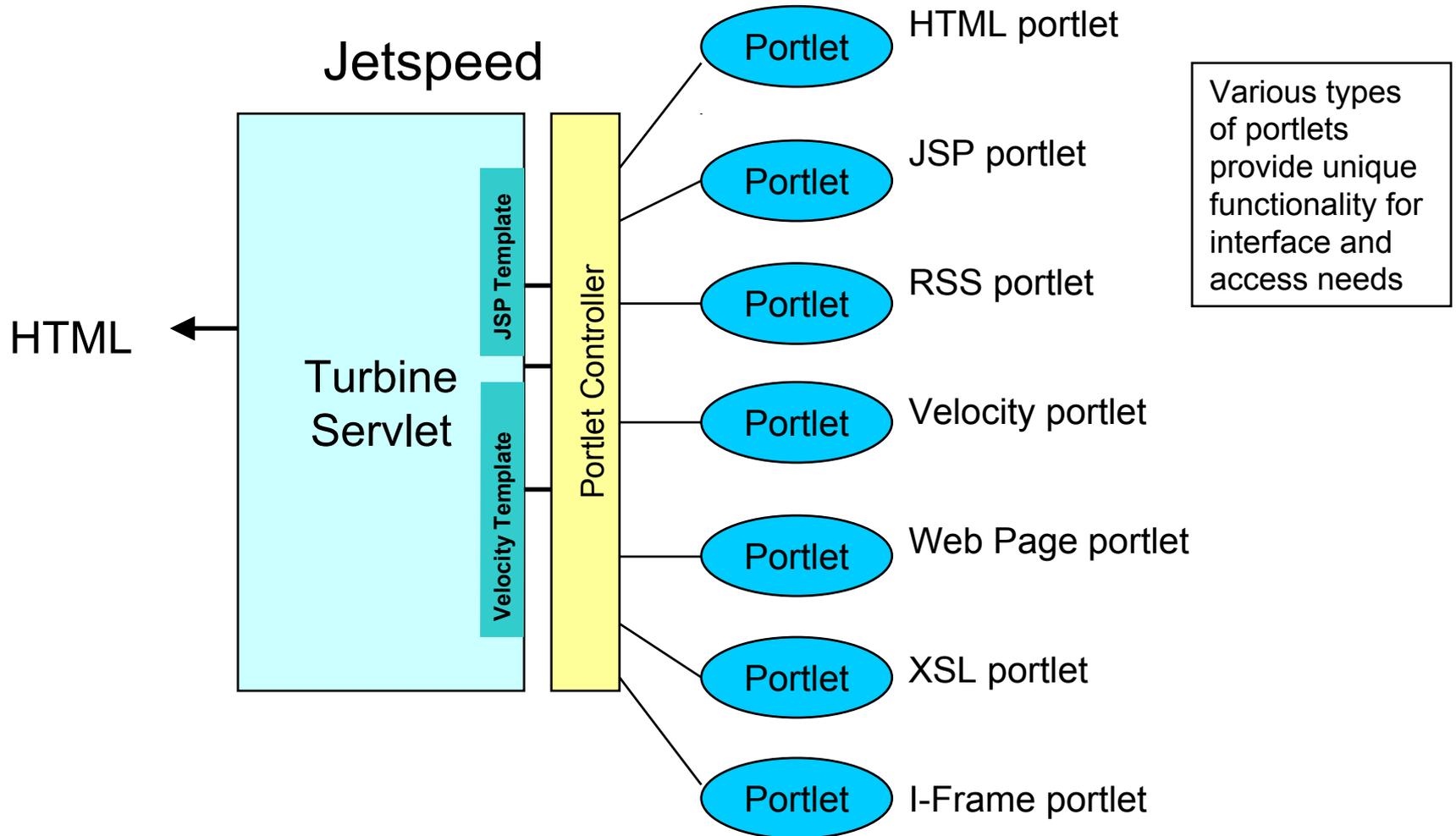


Why is this not just another web page?

- This is a framework that is dynamic and configured.
- Users will be able to establish teams and configure their space to fit the work goals and the approach that they want to use
- Users will have access to data, research and expertise in focused (either specific project or community) areas of the portal and have the mechanism to search within and outside the portal – Data is currently being added to the DAV infrastructure. Other task teams are developing portlets to post and retrieve data in specific ways.
- Services will be established within the CMCS that the Portal will access to integrate tools to the data for the needs of the user
- Will not become static – the whole environment is managed, updated and grown by the user base not by administrators



Architecture and Components





Options for Portal Object Management



Portal objects include users, teams, defined portals, entities such as file collections, etc.. Almost anything within the environment that has multiples and needs to be managed.

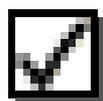
- WebDAV – Through API, store individual objects as files, use properties to link relationships, search, display list, Use sequential file numbering within a collection for creation.
- Relational Database – Such as MySQL or others. Create schema tables for relationships, contain link if files are created. Use sequential file numbering within a collection if multiple file are created.

With both performance, ease of use and extensibility are factors. Interaction with services developed also needs consideration

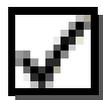


Portal Tasks

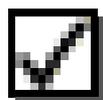
Q1/Q2
FY2002



Identified Apache Jetspeed as base for Portal Environment



Established a test environment on CMCS computing resources -CVS control and build process



Initial level of product capability understanding and trial applications -Base level of product tutorials



Established collaboration with University of Michigan CHEF project



Initial portlet development utilizing webDAV data access approach with velocity portlet



Team / Project prototype portal environment



Portal Tasks

Q3/Q4
FY2002



Document management portlet pointing to slide



Data view portlet pointing to slide / dav for management of data.



Design / definition of Portal Objects and their relationship rules -- Data management approach of objects established



Notification portlet integrated to all services



Integrate University of Michigan - CHEF chat tool



Integrate new jetspeed mechanisms for individually updatable page and others



Addition of integrated Tool portlets – graph, visualization, and other



Ability to select portal panes as portlets are now chosen.



User / portal profile communication to portlets



Current Portal Main



Jakarta Jetspeed Portal: Default Jetspeed page - Microsoft Internet Explorer

Address: <http://cmcs.ca.sandia.gov:8081/cmcs-test/index.jsp>

 **Collaboratory for Multi-Scale Chemical Science**

Username: Password:

[Create New Account](#) | [Login Help](#)

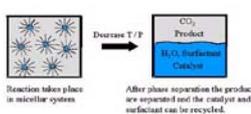
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Feature:

Phase Separable Homogeneous Catalysis in H₂O/CO₂ Micelles

LANL has developed a technique to perform biphasic homogeneous catalysis in H₂O/CO₂ micellar system which allows reaction with longer chain substrates. (Provisional Patent filed, Jacobson and Tumas) For more information contact [LANL Chemistry Division](#) or see the [Science information](#) pages.



Reaction takes place in micellar systems. After phase separation the products are separated and the catalyst and surfactant can be recycled.

CMCS Mission

To develop a pilot Collaboratory for the Multi-scale Chemical Sciences (CMCS) that will bring together leaders in scientific research and technological development across multiple DOE laboratories, other government laboratories and academic institutions to develop an informatics-based approach to synthesizing multi-scale information to create knowledge in the chemical sciences. The CMCS will use advanced collaboration and metadata-based data management technologies to develop an MCS (Multi-scale Chemical Sciences) portal providing community communications mechanisms and data search and annotation capabilities. The portal will also provide capabilities for defining and browsing cross-scale dependencies between data produced at one scale that is used as input for computations at the next. Notification mechanisms will make both researchers and their applications aware of updated values of relevant information such as reaction rates. The CMCS and its MCS portal will provide mechanisms to enhance the coordination of research efforts across related sub-disciplines in the chemical sciences, focusing research at one scale on obtaining or refining values critical in the next, reducing work performed using limited or outdated values, and enhancing the ability of the community to meet the national research challenges of DOE.

Working Groups

The CMCS development effort has been divided into three working groups and other focus areas to better approach the requirements needed for the effort. Plans and communication threads will be managed at this level and then coordinated through the CMCS management plan and the project technical leadership team. The areas are as follows:

- **Applications Development**
- **Infrastructure Development**
- **Portal Development**

CMCS News

GRI-Mech is an optimized detailed chemical reaction mechanism capable of the best representation of natural gas flames and ignition that we are able to provide at this time. Our ongoing program comprises development of extensions to include more chemistry,