Collaboratory for Multi-scale Chemical Science
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Motivation for the Project

Progress on the many multi-scale problems in the chemical sciences is significantly hindered by the difficulties researchers working at each scale have in accessing and translating the best available information and methods from the other scales. Very often there are "gaps" between scales which cannot be bridged at present, often because there is an unresolved technical or mathematical issue in addition to the pervasive lack of translation software and problems with connecting the mismatched data models used at each scale. Problems are particularly severe for complex systems involving combustion and pyrolysis chemistry. For example, simulations used to design high-efficiency, low-emission homogeneous-charge compression-ignition (HCCI) engines typically contain thousands of different chemical species and reactions.

The engine designer running the macroscopic simulation is typically not an expert in chemistry – the macroscopic engine scale is quite complicated enough - so he or she needs all the important microscopic chemical details to be handled more or less automatically by software, and in a way that the chemistry models can be easily updated as additional information becomes available. All these microscopic chemistry details must be documented electronically in a way that is easy visible to the chemistry community, and these chemistry databases must be extensible, to make it practical to capture the benefits of the very large, but also very thinly spread (i.e. each chemist is expert in only a few types of molecules and reactions, under a limited range of conditions), expertise in the chemistry community. The numerical methods used by the engine designer were not designed to handle all this chemical detail, so intermediate pre-processing model-reduction software is needed to reduce the size of the chemical model. It is crucial that the approximation errors introduced in this step be properly controlled, so we do not lose significant accuracy in the final simulation results. Again, all the assumptions and calculations involved in this model-reduction process need to be documented, to facilitate future progress and to allow the engine model to be updated as more information on the combustion chemistry becomes available.

Overview of Progress

The CMCS team has pursued approaches for bridging many different scales, as well as computer science methods that enable cross-scale collaboration and data sharing. The complete team's final report is attached below.

Here we briefly summarize components of the overall CMCS team effort that were done primarily at MIT. The main MIT effort was to develop optimization-based methods for reducing large detailed chemical kinetic mechanisms (molecule scale), and to make it feasible for them to be used in simulations of larger scale phenomena (e.g. engine simulations and reacting-flow simulations). This required developing new numerical methods and new software packages. The new methods were demonstrated by

applications to HCCI engine simulations and to simulations of the flame structure in cylindrical burners.

The new numerical methods we developed (in collaboration with Prof. Paul Barton) for the first time allow solution of semi-infinite programs (optimization problems with an infinite set of constraints) to guaranteed global optimality, and allow one to find the globally optimal reduced model by reaction elimination. We were also able to develop a model reduction method which guaranteed that the reduced models would replicate the large detailed model to any user-desired accuracy over any user-specified range of reaction conditions. Perhaps most impressively, we were able to show that the new methods allow rigorous control of the error in reacting flow simulations caused by use of reduced chemistry models rather than the full detailed model. This error control is the key to guaranteeing accuracy as one connects across the scales. The new methods also include an interval-constrained reformulation of the reaction-elimination model-reduction problem which is particularly convenient for maintaining control of error in reacting-flow simulations.

The new methods for mechanism reduction and error control were implemented into a software package called RIOT, which is accessible by anyone via the Web using the CMCS cyberinfrastructure (KnECS).

The new methods were demonstrated on several different problems, most impressively in an HCCI engine simulation and in an adaptive-chemistry simulation of a burner flame, with on-the-fly mechanism reduction and rigorous error control.

The complete summary of work done by the team including publications and conference presentations is presented in the full report attached below, after a brief summary of major publications based on work done by team members at MIT.

Publications resulting from this grant based primarily on work done at MIT:

1) Binita Bhattacharjee, Douglas A. Schwer, Paul I. Barton, & William H. Green, "Optimally-Reduced Kinetic Models: Reaction Elimination in Large-Scale Kinetic Mechanisms", *Combustion & Flame* **135**, 191-208 (2003).
2) Pisi Lu, Binita Bhattacharjee, Paul I. Barton and William H. Green, "Reduced Models for Adaptive Chemistry Simulation of Reacting Flows", *Computational Fluid and Solid Mechanics: Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics*, ed. by K.J. Bathe (Elsevier, 2003).
3) Binita Bhattacharjee, William H. Green, Jr., and Paul I. Barton, "Interval Methods for Semi-Infinite Programs", *Computational Optimization and Applications* **30,** 63-93 (2005).
4) O.O. Oluwole and W.H. Green, “Rigorous Error Control in Reacting Flow Simulations Using Reduced Chemistry Models”, in *Computational Fluid and Solid Mechanics 2005* ed. by K.J. Bathe, pp. 787-791 (Elsevier, 2005).
5) K. Schuchardt, O. Oluwole, W. Pitz, L.A. Rahn, W.H. Green, D. Leahy, C. Pancerella, M. Sjoberg, J. Dec, “Development of the RIOT Web Service and Information Technologies to enable mechanism reduction for HCCI simulations.” *Journal of Physics: Conference Series* **16**:107-112 (2005).
6) B. Bhattacharjee, P. Lemonidis, W.H. Green and P.I. Barton "Global Solution of Semi-infinite Programs", *Mathematical Programming (Series B)* **103**(2), 283-307 (2005).

7) O.O. Oluwole, B. Bhattacharjee, J.E. Tolsma, P.I. Barton, W.H. Green, “Rigorous Valid Ranges for Optimally-Reduced Kinetic Models”, *Combustion and Flame* **146**, 348-365 (2006).
8) O.O. Oluwole, P.I. Barton, and W.H. Green, “Obtaining Accurate Solutions using Reduced Chemical Kinetic Models: A new Model Reduction method for models rigorously validated over ranges”, *Combustion Theory and Modelling* **11**(1), 127-146 (2007).

Collaboratory for Multi-scale Chemical Science (CMCS): Project Final Report

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1.0 Introduction

The CMCS project (http://cmcs.org/) was initiated in 2001 with a long-term vision of multi-scale science enabled by modern informatics and a commitment to realize this vision in support of combustion research. The vision was stated as "CMCS will enhance chemical science research by breaking down the barriers to rapid sharing of validated information and by opening new paradigms for multi-scale science."

The resulting integrated capability was envisioned as a 'CMCS Knowledge Grid' as graphically depicted in Figure 1. For realistic fuels, the chemistry of combustion involves hundreds to thousands of chemical species participating in thousands of reactions. The structural and thermochemical properties of these species are determined from spectroscopic experiments and, increasingly, from computational quantum chemistry. These chemical reactions occur in an environment that is defined by both thermal conduction and radiation. Reaction rates as a function of temperature and pressure are determined experimentally and by a number of computational methods using detailed data from quantum chemistry computations. Collections of these properties and rates are assembled into chemical mechanisms to model chemical transformation associated with a whole

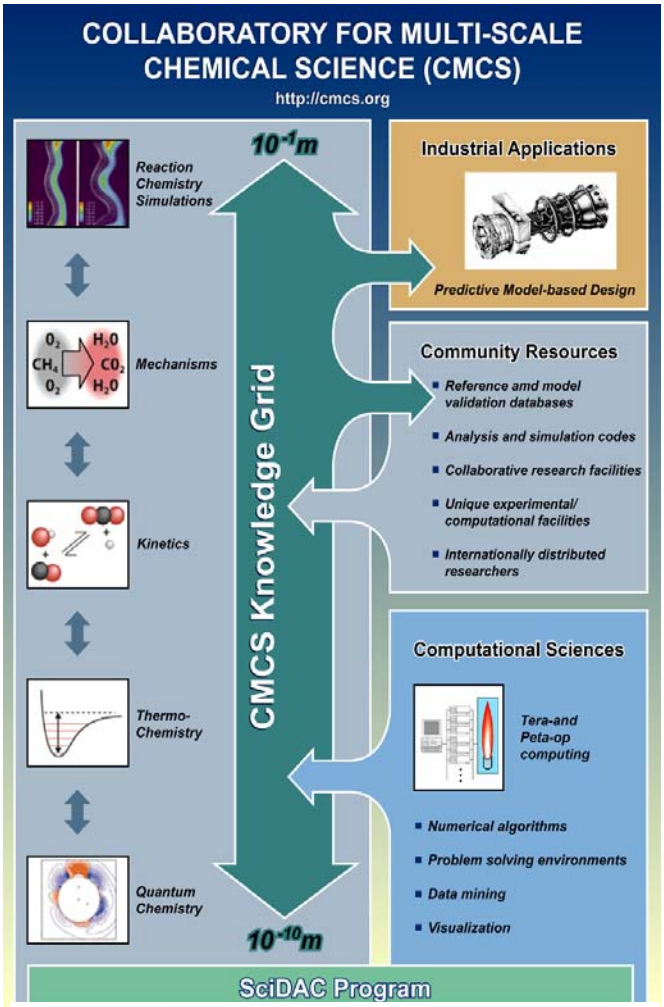

Figure 1. Predictive combustion modeling requires the integration of scientific knowledge over a large range of scales and an effective coupling among disciplines and community resources.

suite of reactions. These models (and often reduced forms of them) are used in detailed simulations that investigate the coupling of reaction chemistry to fluid dynamical processes. These interactions are then further modeled in codes that seek to provide predictive model-based design for combustion devices or systems.

Using such a knowledge grid, we envisioned diverse combustion research communities sharing data and analysis tools as they create verified, documented data sets and reference data. The grid would provide advanced provenance tracking, data interoperability, and multi-level application support and would facilitate collaboration among scientists and unique facilities. Thus the knowledge grid would couple scientists working across varying physical scales and disciplines in combustion research. Our vision was also that such a knowledge grid would not only facilitate interdisciplinary collaboration, but also enable scientists to move toward tackling data-intensive and multi-scale problems with systems science approaches. These approaches can enhance the discovery of knowledge gaps, clarify research priorities, and potentially accelerate scientific impact on industrial development and societal needs.

To enable this vision, the multi-disciplinary project team worked to develop a multi-scale informatics portal toolkit. The team also worked to integrate key chemistry resources, and to develop chemistry-specific informatics applications through an iterative development and deployment process. This process was driven by guiding use-cases and feedback from pilot user groups. This work has been communicated in numerous refereed publications [R1-R21], other publications [O1-O7], and conference presentations [P1-P27]. We found that the portal and underlying informatics toolkit developed in the CMCS project are general-purpose and useful to other science communities that have a need to develop and publish data, deploy science applications, and work together in both public and private groups. By separating the chemistry-specific applications from the infrastructure and making this collaborative science environment available to others, we have also sought to enable science projects in other disciplines. Thus, the resulting open source informatics toolkit, the Knowledge Environment for Collaborative Science (KnECS), has been separated from CMCS and licensed as open source software [A1]. KnECS has already been used by at least one other project [A2] in the development of a knowledge grid for their community. Our vision is that developers from an array of follow-on projects like CMCS will contribute enhancements to KnECS.

2.0 Significant accomplishments and scientific impact

Early in the CMCS project, the team focused on requirements definition, identifying detailed technical solutions, and on an iterative process of building prototypes for infrastructure and a few combustion applications. This process allowed iterative refinement of our vision and, most importantly, refinement of our scope. An iterative refinement process also allowed us to keep up with changes in both technology and the needs of our users. Necessarily, much of the emphasis was on getting an enabling infrastructure into place on which the team could explore actual science use cases and build application capabilities. The latter two years of project effort has thus been focused much more on developing and integrating a range of applications and data into a combustion knowledge grid while refining the infrastructure, interfaces, and enabling tools. Significant progress has been made in direct collaboration with application scientists to modify and integrate legacy codes, develop schema, transform data, develop new applications, and to understand how such new approaches can benefit science. With the breadth of disciplines, applications, and data required, it is clear that different styles of application integration and community interaction must be supported. In the remainder of this section, we summarize the project team's accomplishments, first in construction of the KnECS infrastructure, then highlighting a number of science capabilities and results. The latter accomplishments are ordered from the smaller scales to the larger scales (see Fig. 1), with the final one focused on the application of KnECS in other disciplines. We also learned how difficult some barriers are to overcome; these are assessed briefly in Section 3. The appendices contain publications associated with this project as well as other ancillary information.

2.1 Infrastructure and Tools

The Knowledge Environment for Collaborative Science (KnECS) KnECS defines a multilayer architecture as depicted in Figure 2. The primary user environment is a web portal based on the CompreHensive collaborativE Framework (CHEF) [A3] software which enhances standard portal technology with support for teams and community interaction tools such as chat and announcements. KnECS also leverages several middleware components. Of most significance is the Scientific Annotation Middleware (SAM) [R3], software for data and metadata services. SAM provides a range of capabilities for storing and retrieving data and metadata, searching, versioning, locking, and providing access control, as well as extensible mechanisms for extracting metadata from files, performing translations, and managing provenance and other data relationships. SAM is based on Apache Slide [A4] and implements the WebDAV protocol [A5].

As illustrated, KnECS also includes middleware components that implement publish/subscribe messaging, authentication, and authorization. Authorization is managed via JAAS [A6] interfaces to support pluggable security. Mechanisms for integrating Fortran, C, or other computational codes are provided through synchronous and asynchronous web services. Grid services have been demonstrated via the Commodity Grid (CoG) toolkit [A7].

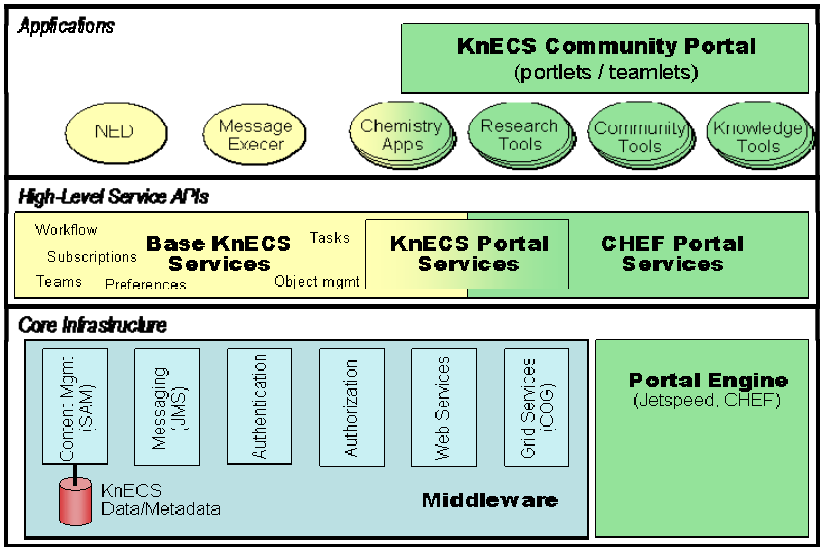

Figure 2. A schematic view of the KnECS multi-tier approach integrating data, applications, and informatics tools.

KnECS provides APIs for notification subscriptions, tasks, and other core portal objects such as users and teams. The Data Storage Interface (DSI) provides an easy to use API to the SAM data repository that hides the details of the data access protocol. Additional classes support the construction of structured metadata such as multi-valued container properties, as specified by RDF [A8], and XLinks [A9] for relationships.

KnECS maintains a separation of business logic from portal infrastructure so that non-portal applications that access KnECS APIs can be written. One such application, the Notification Email Daemon (NED), listens for events matching user or team notification subscriptions and sends immediate, daily or weekly digest email messages summarizing the events. This is typically used by teams as a light-weight method of keeping up to date on recent team activities.

KnECS includes several knowledge tools, the DataBrowser portlet being the primary example. The DataBrowser supports standard file and directory operations including single file and bulk upload, control over permissions, mouse-over preview of metadata, full metadata viewing and editing; data translation, and visualization. A lightweight file chooser was created from the DataBrowser code base to improve file selection interaction from other portlets. Furthermore, four additional tools are integrated to provide general knowledge management capabilities. A provenance graph tool displays data relationships. A search tool utilizing Lucene [A10] indexing of metadata properties, in conjunction with DASL [A11] queries, allows for data discovery. An annotation tool allows users to annotate data with text, sound, images, equations, or whiteboard drawings. A subscription tool allows users to set up individual and team notifications.

KnECS extends the CHEF team management portlet to automatically create both public and private workspaces on the data server upon team creation. Private workspaces are used to share and

perhaps develop data within a community while the public area can be used to publish verified reference data. Support for threaded, archived team email lists has been recently added as email remains a very popular way for teams to communicate.

2.2 Quantum Chemistry

CMCS accomplishments related to the quantum chemistry scale focused on the integration of Ecce [A12] and implementation of the Basis Set Exchange.

2.2.1 Ecce Integration

Ecce provides a suite of graphically rich tools that support setup, execution, analysis and management of quantum chemistry calculations using NWChem [A13], Gaussian [A14], and other codes which compute, from first principles, important properties such as minimum energy and vibrational frequencies. Ecce captures and saves, in their native formats, all the data (inputs, outputs, and setup parameters) as well as metadata to describe each calculation. Given that Ecce already uses WebDAV for its data and metadata management, we elected a lightweight integration where Ecce and SAM were made interoperable at the WebDAV protocol level. Ecce adopted the KnECS provenance strategy for fully describing relationships using XLink. Users can now directly use the KnECS SAM server for a calculation repository or export data to KnECS where portal tools can be used to share, discover, and visualize data or participate in community processing. Together, these are significant advancements towards our goal of multi-scale integration.

2.2.2 Basis Set Exchange

The Basis Set Exchange (BSE) was developed to help computational chemists use and share the basis sets that are used to expand the wave function. It was modeled after the EMSL tools, but leveraged KnECS infrastructure. The BSE is defining XML standards for various types of basis sets, adopting KnECS pedigree standards, and developing XSLT translators. A primary benefit of the KnECS infrastructure is the support for a community of basis set developers who can collectively contribute to and curate the data. Contributing data is a multi-step process and a navigation bar capability was developed to show the process visually as well as to support navigation. Curators can be notified when new data is contributed and access control lists (ACLs) control which community members can curate data. Finally, an XML-based generic logging capability was developed to track usage statistics with plans to develop summary statistics through translators. Statistic summaries can be readily tailored to sponsors, contributors, and users.

2.3 Thermochemical Science

The thermochemcial properties of the molecules and atoms involved in combustion (or any chemical reaction for that matter) provide fundamental information that is critical for predictive modeling. The historical dependence of this field on printed data tables of mostly independently determined values is being revolutionized by computational methods and systems science approaches. The CMCS team is proud to be a part of this emerging revolution, and sees it as an example of the impact that can be made in numerous related subdisciplines of combustion (and more generally, chemical and biochemical) science.

2.3.1 Active Thermochemical Tables (ATcT) Community Service

ATcT represent a synergism of breakthrough developments in the chemistry domain with those in collaborative computer and computational science in association with the CMCS. ATcT implements a Thermochemical Network (TN) concept that explicitly exposes the manifold of inherent interdependencies ignored in traditional approaches. This effort, led by Dr. Branko Ruscic of Argonne National Laboratory, is focused on improving the accuracy, reliability, and internal consistency of

thermochemical values that are fundamental to many areas of chemical science and industrial application. This work involves a growing number of collaborations, and an International Union of Pure and Applied Chemistry (IUPAC) community focused on the thermochemistry of radicals.

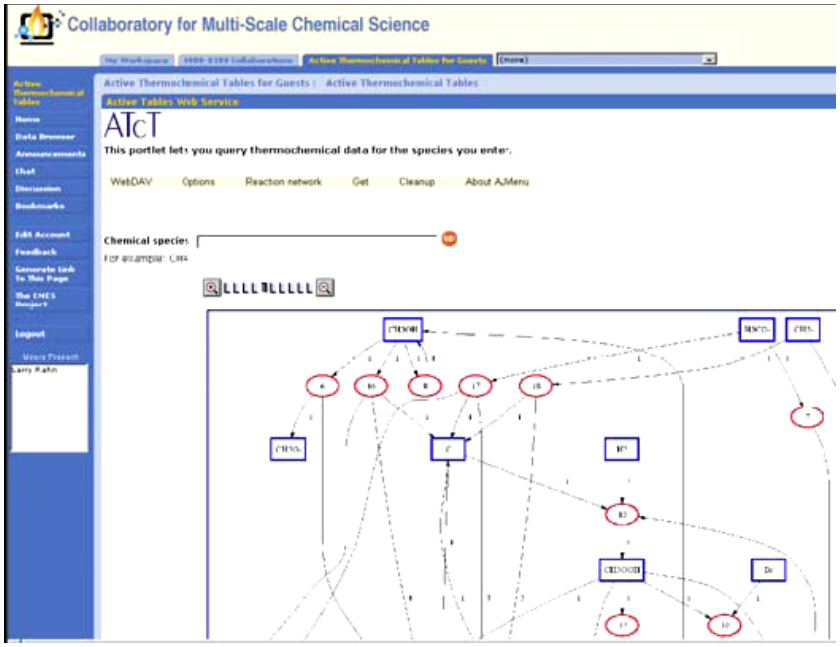

Figure 3. An ATcT thermochemcial network displayed in the CMCS Portal.

Many of the advantages of the ATcT approach stem from its use of the TN that explicitly exposes the manifold of inherent interdependencies among thermochemical properties and the experiments and computations from which they are derived. Thus, ATcT provides quick and painless propagation of new knowledge to update all affected thermochemical values. We have designed and implemented an ATcT community service that can expose the ATcT functionality as part of the CMCS portal. The service is reusing design principles and technologies pioneered by the Java CoG Kit. Crucial collaborative capabilities are derived from the CMCS portal, which makes the ATcT application and associated data broadly available to collaborators and supports data evaluation and other community processes. The ATcT interface in the CMCS Portal with a visualization of a TN is shown in Figure 3. An important capability deriving from the systems approach of ATcT allows researchers to discover 'weak links' in the TN. Such 'weak links' point scientists to new experimental or theoretical determinations will significantly improve the TN.

Utilizing the ATcT approach, new thermochemistry has been developed numerous molecular and some atomic species that have often motivated further work or new collaborations. A direct consequence of new results for the HO_2 radical, for example, was the implication that the accepted reverse kinetic rate constant of the famous Howard reaction ($HO_2 + NO \rightarrow OH + NO_2$) must be wrong by a factor of nearly 2. In order to verify this explicitly, new kinetic measurements were undertaken in collaboration with J. Michael (ANL), which proved exactly the ATcT prediction. Two papers on this subject have just appeared. [R18, R19] The HO_2 development also leveraged from the concomitant ATcT improvements in the NOx thermochemistry (also very relevant both in combustion and atmospheric chemistry), which in turn was made possible by the ATcT discovery of a 'weak link' in the network of values in related NOx compounds. The "weak link" discovery triggered new ATcT-related photoionization measurements of the threshold for formation of N+ from N2, conducted recently at the Advanced Light Source in Berkeley in collaboration with C.-Y. Ng (UC Davis). The direct measurements have been recently published,[R11] and a description of the resulting improvements to NOx thermochemistry is in preparation. The HO2 development is also part of a larger project that is developing definitive thermochemistry of H_NO_M species, including OH. A paper on this topic is also currently in preparation. ATcT also played a crucial role in developing a new electronic structure method (W4, which aims at consistent sub-kJ/mol accuracy) by the group of J. M. L. Martin (Weizmann), where ATcT provided the needed benchmarks and feedback as to which corrections are necessary in the method's formulation.[R20] Also, the first paper in the series of papers addressing the ATcT development on the topic of thermochemistry of carbon, which was another ATcT "weak link"

discovery, addressed by a collaborative effort with A. G. Csaszar (Eotvos, Budapest) and J. F. Stanton (UT Austin), has been recently submitted for publication.[R21] In addition, ATcT has been used to update - to the extent possible - the largest thermochemical database of polynomials currently in existence (A. Bucat, Technion), resulting in a joint report.[O7]

2.3.2 Group Additivity Thermodynamic Properties (GATP)

Chemists often need thermodynamic properties for chemical species when no experimental or theoretical determinations exist. GATP [P6] is a relatively new effort within CMCS that provides these estimates, particularly for larger molecules where more accurate approaches are not available. GATP uses an internal additivity database and the connectivity of the species to compute thermodynamic properties. A CMCS portlet provides an interface to the Java-based GATP code and provides access to computed properties, via XSLT translations, in a tabular or polynomial fit form commonly used by legacy combustion, atmospheric and chemical-engineering codes. Ultimately, the GATP additivity database will be available for community contribution and curation processes. Easy access to GATP, shared GATP results, and its additivity database allows scientists to address problems which involve chemical species with unknown thermochemical properties.

2.4 Kinetics and Kinetic Mechanisms

Chemical kinetics mechanisms are used to simulate the chemistry in combustion, the atmosphere, and chemical engineering processes. Scientists and engineers need to discover chemical kinetic mechanisms for a particular fuel or reactant, understand the range of their applicability, and access the data in a format suitable for their application. Accomplishing this requires the ability to search, view provenance and examine the sources for the detailed rate constants and thermodynamic parameters; to record comments on the performance and applicability of the mechanisms under various use cases; and to access conversion software that translate chemical kinetic mechanisms among various combustion and atmospheric modeling formats. The Large Mechanisms group has used the CMCS portal to develop schemas and translators to facilitate the accurate use of currently available chemical mechanisms and is providing documentation and validation data that will speed the development of new or improved mechanisms. A related capability is the Range Identification and Optimization Tool described below. Also included below is a summary of accomplishments from the PrIMe development group.

2.4.1 Range Identification and Optimization Tool (RIOT)

For many years researchers have tried to predict how fuel changes will affect the performance of new engines on the drawing boards, but the many complicated details of combustion chemistry have made this difficult to impossible to accomplish. An automated method has been developed for extracting only the essential details from a complicated fuel chemistry mechanism, so they can be incorporated into efficient computer programs for the design of novel high-efficiency engines. The Range Identification and Optimization Tool (RIOT) has been developed to provide this reduction [R14]. It has been made available in the CMCS portal to facilitate setup, execution, and results analysis for scientists collaborating from other institutions and disciplines [O5]. The new mechanism-reduction method, developed by the CMCS, allows the user to control the error versus speed-up trade-off, and, in certain steady flame simulations, the user can even rigorously bound the error that will be introduced by neglecting the minor chemistry details. This sort of “coarse-graining with error control” makes it feasible to accurately predict the behavior of macroscopic devices based on first-principles models of the microscopic molecules reacting inside the engine, i.e. reliable multi-scale simulation. The CMCS portlet interface assists the user with specifying inputs to the RIOT code, generates the input file, ships the request to a web service interface to the code, and uploads and presents the results when the

reduction completes. Preliminary use of the RIOT/CMCS web service to build a reduced chemical reaction mechanism to model iso-octane HCCI yielded greater than a 20-fold improvement in computational efficiency while preserving the accuracy of the HCCI predictions.

2.4.2 Process Informatics Model (PrIMe):

PrIMe—Process Informatics Model (http://primekinetics.org)—is an international initiative fostering a new approach for developing predictive models of chemical reaction systems that is based on the scientific collaboratory paradigm and takes full advantage of existing and developing cyber infrastructure. The primary goals of PrIMe are collecting and storing data, validating the data and quantifying uncertainties, and assembling the data into predictive models with quantified uncertainties to meet specific user requirements. The principal components of PrIMe include: a data Depository, which is a repository of data provided by the community, a data Library for storage of evaluated data, and a set of computer-based tools to process data and to assemble data into predictive models. Two guiding principles of PrIMe are: open membership—any qualified individual can register to participate in the project; and open source—all submitted data, tools and models will be in the public domain. The PrIMe Initiative was officially launched on April 21-22, 2006. At the time of this writing, there are over 60 members registered.

Having members of PrIMe on the CMCS team provided numerous benefits to the CMCS project. PrIMe scientists participated in the development of the CMCS User Agreements, provided the initial CMCS demonstration projects of XML documents, participated in the design of various features of the CMCS portal, and developed the initial realistic WebDAV data collection for testing the CMCS software. Being in the vanguard of the project, PrIMe has developed XML standards for chemical elements, chemical species, chemical reactions, and experimental records, led in the development of WebDAV search capabilities, and introduced the CMCS team to the concept of data submission forms.

The PrIMe Warehouse is hosted by a Dell PowerEdge 800 computer, with 2.8 GHz Intel P4 CPU and 1 GB memory and 36 GB Ultra 320 SCSI hard disk rotating at 15000 rpm. The computer is running Microsoft Windows 2003 Server Standard Edition operating system. The web access to the PrIMe Warehouse is facilitated using operating system's built-in Internet Information Services 6 web server software with enabled WebDAV extensions compliant with RFC2518 Standard. To facilitate search, files are indexed upon depositing into the Warehouse, or when re-deposited after editing. Indexing is automatic, performed by operating system's built-in Indexing Services software. The search for XML files with criteria related to a particular node (for example, for all the species composed of four carbon atoms and less than seven hydrogen atoms), standard full-text indexing by Indexing Services is extended with an XML-specialized plug-in filter QLXFilter by QuiLogic Inc. Filtering criteria are designed by the PrIMe development team members, to make most of the XML nodes available for node-specific search requests. The search queries must adhere to MSSQL grammar. The XML interface to the search engine is accessible through an XML message compliant with WebDAV DASL standard (RFC proposal draft-reddy-dasl-protocol-04). Several client-side interfaces are commercially available for such a WebDAV search. The PrIMe development team created two custom interfaces for the PrIMe community, ASP-based form web page (available via publicly-accessed http://primekinetics.org) and Matlab-based graphical interface. For disaster recovery and historical purposes, the warehouse contents are regularly backed up.

The current collection is mostly based on data imported from NIST Kinetics Database, GRI-Mech 3.0 project data, and the experimental data from the Stanford University (the latter work co-funded by other sources, GCEP and NSF Chemistry Division). The Warehouse currently contains 87200 files in 18500 folders, consuming 342 MB of disk space.

With the current hardware and data collection, the performance is as follows. Newly deposited or edited XML files are indexed and available for search within 5 seconds of depositing. Searching the data, apparently regardless of search query complexity, generates response with a list of files satisfying

search criteria within typically 20 ms. Realistic response time to search query requested by a remote computer thus depends mostly on time for transfer of search results through the network between the PrIMe server and the remote user's computer. The time for WebDAV retrieval of a file from the Warehouse depends exclusively on the network traffic; retrieval time without the network overhead was too short for reliable measurement, typically shorter than 0.5 milliseconds.

The work will continue for another 12 months as a no-cost extension of the present grant to the University of California at Berkeley. This work will be devoted to completing the data management software and associated documentation. The data management software developed under this grant will be open-sourced and made available at souceforge.net at the time of completion. A complete final report will be prepared and submitted at the end of the extension period.

A team of PrIMe members (UC Berkeley, Stanford, MIT) received an NSF Chemistry Division award on Cyberinfrastructure. PrIMe became affiliated with the Center for Information Technology Research in the Interest of Society (CITRIS; http://citris-uc.org), and has already benefited from the support provided on web-site and hierarchical-group portal technologies.

2.5 Reacting Flow Simulation and Experiment

2.5.1 Feature Tracking and FD Tools

A common and useful data analysis method, especially for time dependent simulation results, is to identify regions of interest and study their behavior over time. The process of finding coherent structures that persist over time, such as flames in combustion simulations and hurricanes in climate simulations, is called Feature Identification and Tracking. We have developed the Feature Detection & Tracking Library (FDTools), a serial framework to support the easy assembly of an extensible set of feature identification and tracking algorithms into a feature analysis pipeline. We used FastBit searching technology from the SciDAC Scientific Data Management Center to rapidly identify points satisfying user-specified conditions. We then group the points into regions, and compute the overlap among regions among consecutive time steps to identify the evolution of regions. One of the goals was to use features extracted from large-scale DNS (Direct Numerical Simulation) combustion data as searchable metadata at the CMCS Portal. FDTools was used to help discover new scientific knowledge in the combustion domain. In the study of autoignition, preignition kernels are generally identified as areas of high radical concentration. All autoignition sites start in preignition kernels, but not all preignition kernels ignite. FDTools was used to find, track, and examine the preignition kernels, and revealed that the kernels did not all ignite at the same time. By examining statistics of the features, the scientists were able determine a correlation between the dissipation rate and the fate of a preignition kernel.

During the course of implementation, it became obvious that a completely separate tool is not a good way to proceed. Any complicated analysis requires interpolation, derivatives and related functions and variables that are developed within the simulation code itself. Thus, while the concept was proven valuable, further development was deferred and ultimately submitted as part of proposal to the recent SciDAC 2 call.

2.5.2 Metadata Library for Premixed Turbulent Flame Experiments

The Premixed Turbulent Flame Working Group (http://purl.oclc.org/NET/preturb/) teamed up with CMCS to document and share information about their available data sets. These combustion scientists collect large data sets on measured velocities, temperatures and species concentrations in premixed, turbulent, laboratory-scale flames. Scientists need to store their important data, retrieve it, and share it with others. They also need to keep track of key information about the experimental data and computational results. The Premixed Turbulent Flame Working Group meets every two years to discuss their needs at the International Workshop on Premixed Turbulent Flames.

The Group meets in August of 2006 in Mainz, Germany to learn about and begin using new capabilities developed in collaboration with the CMCS team that enable the working-group scientists to upload MS Excel® data sheets that document their large datasets. During the upload, the KnECS infrastructure automatically converts the Excel® datasheet file into an XML file and an XSLT translator is invoked to extract metadata from the XML. This process is all done in the background. The critical metadata is then available which enables implementation of advanced search capabilities. This metadata

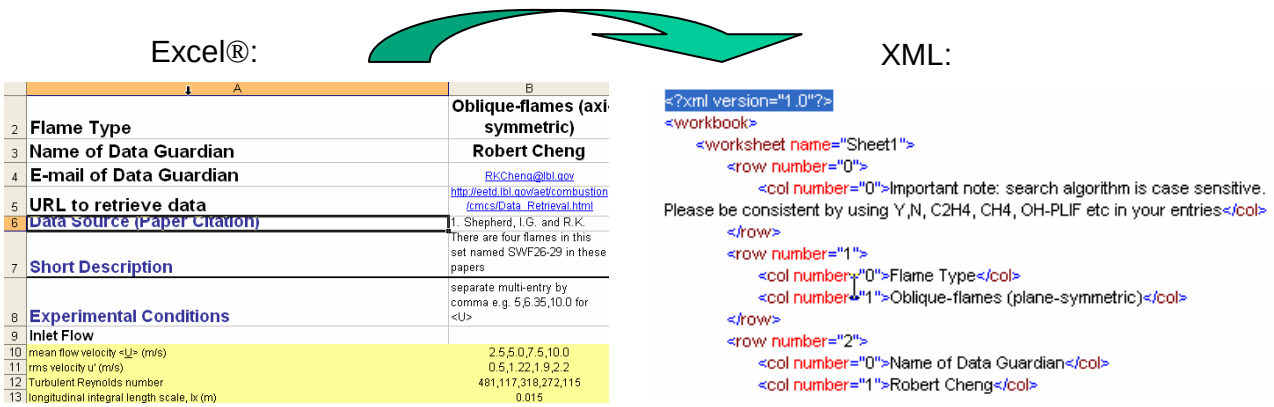

Figure 4. Illustration of the automatic extraction of metadata from and Excel® file.

includes experimental flow parameters such as equivalence ratio, inlet temperature, Karlovitz number, and fuel type. An advanced search form is made available that can easily be modified by user groups to meet their needs. Together, these capabilities and data enable scientists and engineers around the world to search on this metadata with a tailored search form in the portlet, allowing easy discovery and access to experimental datasheets of interest. The leaders of the Working Group anticipate that these capabilities will help resolve longstanding barriers to data sharing in this research community.

Figure 5. Premixed Turbulent group customizable search form.

2.5.3 Publication of Experimental Combustion Data Sets

A new approach for publication of combustion data that offers an interoperable format available from an easy to access, automatically updated web page has been prototyped for two international combustion science teams in collaboration with the CMCS. These teams, an international consortium for Synchrotron Photoionization Mass Spectrometry (PIMS) for investigation of combustion chemistry [A15], and the International Workshop on the Measurement and Computation of Turbulent Nonpremixed Flames (http://www.ca.sandia.gov/TNF/) are meeting in conjunction with the 31st International Symposium on Combustion during August, 2006 to present and discuss the new approach for data publication in their communities.

The publicly accessible publication web page features the ability to not only view and download the data in a translation back to the current text based, white-space delimited format, but also to view it in a tabular web view and/or in graphical plots. The web archive provides the option of browsing the data in a hierarchical folder structure as well as the ability to search and display the data based on key properties or metadata. Also, it is possible to simultaneously provide public access to multiple folders of data that are curated by different institutions. The new capabilities are built upon a data-sharing infrastructure developed by CMCS developers and are designed to meet the specific requirements for web-based publication by these communities. The implementation involves updating current data using a Java application designed to convert current text files into a semantic, self-descriptive XML format which contains added metadata. When such a formatted XML file is deposited into the archive, its contained metadata is automatically read and stored separately to enable rapid searches. From the archive, the XML file can then be viewed or downloaded in a variety of different forms, each associated with a (XSLT) translator offering a different viewable or downloadable format of the data. For example, one might translate the file into a graphical scatterplot view while another offers a downloadable text file in a newly defined format.

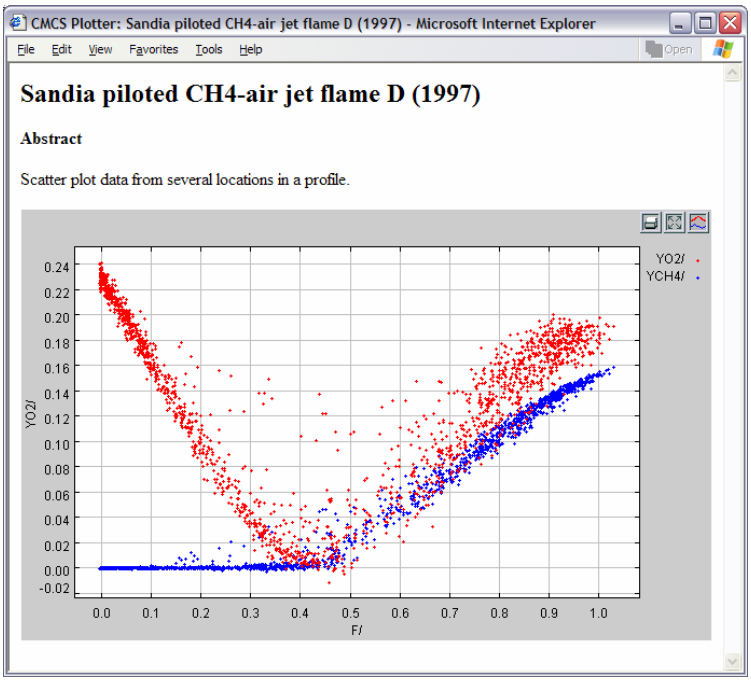

Figure 6. Example Scatterplot of Sandia Piloted CH_4-Air Jet Flame D.

The demonstration of this prototype enables, and challenges, these scientific communities to invest more in the curation and publication their data, and to work on new agreements for broader participation in data publication. The vision is for an archive where experimental, computation, and modeling data all exist in a form that is easily searched and displayed by a computer while being available in formats that are easily read by other software applications.

2.6 KnECS Implementations In Other Science Communities

CMCS is a unique example of how cyberinfrastructure can actively support research processes rather than just being a means to provide access to finished, 'text-book' information and services. Similar requirements for such a 'cyberenvironment' that provides end-to-end support for the research lifecycle exist in many fields. A current example of the implementation of KnECS for a different discipline is a project in which a group of biomedical scientists leading the development of new technique termed ‘MS3D’ are collaborating with researchers in CMCS to build the Collaboratory for MS3D (C-MS3D) [A2]. This is a multi-institution project with partners funded by the National Institutes of Health and the National Science Foundation.

This collaboration has greatly facilitated the new project, enabling deployment of a C-MS3D production portal and a development portal within the first 6 months. MS3D uses chemical crosslinking and mass spectrometry to probe the structure and dynamics of proteins, RNA, and macro-molecular complexes. The objective of this 5-year project is to broadly enable an emerging MS3D collaborative community as it develops new tools, analysis approaches, and data schema to integrate constraint data from chemical crosslinking and mass spectrometry with other information (including that

obtained from computation, NMR, EPR, FRET, X-Ray crystallography) to determine otherwise inaccessible macro-molecular structures.

The more general capabilities developed by CMCS have been made available to others as the Knowledge Environment for Collaborative Science (KnECS). KnECS is an open source portal and data management environment that can be customized with discipline-specific tools, data translators, and data viewers. The KnECS deployment process was revised by the CMCS team to support configuration of the portal for other projects such as C-MS3D. The C-MS3D team branded the portal to reflect the C-MS3D project identity. Using the development library for creating asynchronous web services in KnECS, the C-MS3D team integrated existing MS3D codes into the portal, making the latest tools accessible across the group. The project is using some of the translators, metadata extractors, and visualization tools developed by CMCS while developing others that are more specific to biology.

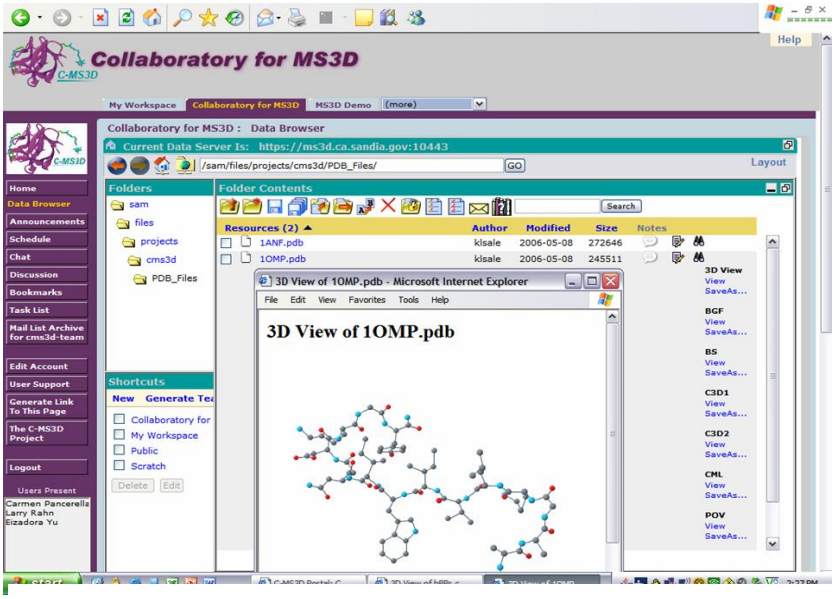

Figure 7. A screen shot of the C-MS3D Portal illustrating one of the many translations available for a Protein Data Base file.

3.0 Overall Assessment

As the discussion of the accomplishments and scientific impact presented in Section 2 above indicates, there are many successes that CMCS project team, collaborators, sponsors and stakeholders can claim. Still, this discussion is incomplete and, at best, only a summary. Futhermore, much of what has been accomplished is only a foothold into a new future of cyber enabled science that promises high returns for DOE mission science and high impact for national needs. This vision still faces many challenges, however. We summarize in this section some of the particular challenges that we faced, with the hope that our shared experiences may benefit future efforts.

3.1 Challenges

The CMCS project team has identified critical challenges facing developers of science applications using KnECS. Some are significant, and must be addressed if portal-based knowledge environments are to become ubiquitous in science. The technology must offer modularity that empowers application scientists, the flexibility and adaptability to integrate rapidly changing technologies, applications, and other data stores. We discuss these issues by theme.

3.1.1 Data Management Challenges

Performance: As data repositories grow in size, and multiple data repositories are used, data federation will be necessary. Performance issues associated with very large data sets must be addressed. Large data sets are also an issue for real time translation and XML description. The latter is addressed by emerging standards such as the Data Format Definition Language [A16] which has been recently implemented with open source from the Defuddle project [A17].

Data Curation: Several applications require support for curation of reference data sets. However, the model(s) for what curation means is not yet well defined. Individual communities will

define curation mechanisms that meet their needs. We expect some common elements to span many data sets/communities. These include facilitating data entry (e.g. using schema driven forms), annotating data with curation provenance and status information and curator notes (though the schemas will vary), versioning of data sets, setting up automated validation steps (though the processes themselves will vary), and manual editing/correcting of data which could use generated forms for editing XML content. Curated data shares a common trait of an associated publication reference. Standards, tools and on-line access to a reference repository may be beneficial.

This area is also subject to cultural and policy issues, in that the time and skills required to curate scientific data sets are not yet highly valued in much of the scientific culture. For example, many sponsors of science do not value curated data enough provide a way for it to be included as a metric in scientific performance. Of course, this is related to one of the central issues the CMCS team has tackled, the fact that there are few ways to publish curated data where it can be referenced and reliably discovered, explored, downloaded, maintained, and archived.

3.1.2 Integration Challenges

Legacy Integration: As discussed in Section 3, many communities require integration of legacy codes. There are many possible models for integration including: direct process invocation, simple synchronous or asynchronous web services with or without load balancing or QOS support, grid services, and ultimately multiple processes connected via workflows. The application with which CMCS worked use several models: synchronous web services, asynchronous web service jobs and asynchronous grid tasks via the COG toolkit. However, more work is needed to create a simple API that can exploit different underlying implementations.

Portlet Integration: In general, developing complex applications in a portal environment is difficult. JSR168, the Java portlet API [A18], addresses a standard portlet specification; however, it does not make portlet development easier and does not address collaboration-style portlets, thus resulting in non-standard extensions.

Support for Different Granularities of Application Integration: From the diverse application areas discussed above in Section 2, it is clear that different styles of integration are required, so we have implemented several models. These range from simple file sharing, to loose integration of external tools, to portlet wrappers for computational codes, to applets or Java Web Start enabled applications. The model proposed by Web Services for Remote Portlets (WSRP) [A19] is a desirable alternative that addresses important intellectual property issues but robust implementations are needed. The choice of which to use depends on many factors including ownership, whether the software exists yet or not, the resources required, and the availability of skilled portlet developers. A community portal toolkit should support all of these models.

3.1.3 Reuse Challenges

Customization: When a new application is integrated into a portal, data input and conversion tools typically need to be customized to support this application. The development and deployment of data input forms and data converters should be easy. Furthermore, as new groups or communities form, each project and/or institution wants a unique workspace, so portal branding for projects and/or organizations must be easy and provide the appropriate level of identity for the community. While individual groups can brand their CMCS Portal view with a graphic, the reuse of the KnECS infrastructure by other disciplines (e.g., the biomedical community discussed in Sec/ 2.6) requires a careful identification and separation of all elements in the code base that contribute to branding. This was undertaken by the CMCS team as a part of our effort to make KnECS more usable (see Sec. 3.1.5 below.).

Even with customization, it is difficult for one infrastructure implementation to meet enough needs of some groups to be satisfactory. The reasons for this appear to be both technical (e.g., tradeoffs

of features versus performance) and sometimes cultural (e.g., disagreement on common features, issues over who is in control or hosting infrastructure, etc.). The technical issues support arguments for modularity, for the adoption of standards for interoperation of modules, and for the use of open source code bases. The cultural issues are discussed more in the following section.

3.1.4 Usage Challenges

Social and Intellectual Property Issues For Scientists: Though science collaboratories have been in existence for over fifteen years, there are still social and science issues impeding adoption. Preserving the ownership and controlling the use of data and tools is necessary in a scientific community. Once KnECS is adopted and deployed to a science community, that community must also adopt guidelines for data publication and address intellectual property issues surrounding contributed data and software tools. Many of these issues will be more easily resolved by adoption of policies and practices of example communities who have successfully established and use a common cyberenvironment. This is a significant impact that pilot efforts such as CMCS team can offer to the scientific community.

Need for an End-to-End Solution: Until the infrastructure, data, and applications that support collaborative science fits as an integral part of scientist's day-to-day work and a part of a 'full solution' for research, collaboration tools will always be in the background and used only occasionally. This was evidenced, for example, in our experience presenting computational tools via web portlets. In this case issues such as unique molecule identifiers, definition of the uncertainty in the results, documentation of the provenance of the results, and the capture all the data for inputs and outputs in user friendly ways were found to be barriers to adoption across disciplinary boundaries. It seems that this requires considerable flexibility (e.g., modularity, modes of access, etc.) and more standards to facilitate interoperability.

3.1.5 Open Source Challenges

Active Open Source Development Community: While the KnECS infrastructure has been licensed as open source, much work remains to organize and document it so that other communities can easily deploy and extend it to create their own knowledge grids. KnECS leverages many third party capabilities, such as SAM and CHEF, creating a challenging maintenance environment. An active community with long-term sustainability is required to convince scientists to build upon these capabilities. The CMCS project team is currently in the final stages of reorganizing the open source code base for release in a more usable form on SourceForge.net[A1].

3.1.6 Collaboration Challenges

Security and Group Management: As collaborative groups and communities form, there is a need for hierarchical groups, with flexible approaches to access control and privileges. Also, different communities have varying requirements on how teams should be formed and managed. The security access controls are intimately related to the group or file structure. From a scientific collaboration point of view, however, this mapping does not work well. Most scientists participate and share data in more than one collaborative group. Thus, different data may be contributed to more than one collaboration, each having a different control hierarchy. Fully enabling such mixed-mode collaborations requires a much more general way to manage security, membership, and hierarchy for overlapping collaborative groups.

3.2 Realization of the CMCS Vision

Many of the elements of the original CMCS vision were largely met. For example, pedigree browsing, data interoperability via XML technologies and automatic translations among schema,

integration of collaboration tools with data management and application sharing capabilities, and the stimulation of new approaches for science. Other aspects of our vision are clearly still more futuristic than accomplished; such as the formation of active, sustained interdisciplinary collaborations across all of the scales in combustion (see Fig. 1) or the use of CMCS as a route to 'publish' community curated data. Note that we made progress against these goals, but it will clearly take efforts that are sustained beyond the typical project life time to change the culture and practice of science. Perhaps it is just too early to make such judgments since there are continuing activities from related projects, and the fact that Sandia National Laboratories's Combustion Research Facility will continue to operate the CMCS production servers. It is clear, however, that continued support for research, development, and pilot activities is still a critical need if cyberenviornments are to be developed, deployed, and adopted for the benefit of DOE's science mission.

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