

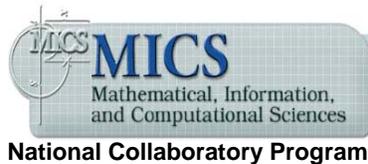


Overview of Collaboratory for Multi-scale Chemical Science (CMCS)

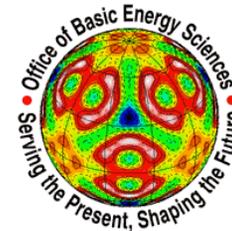


10th International Workshop on Premixed Turbulent Flames

August 12- 13, 2006
Hotel Mainzer Hof
Mainz, Germany



Larry A. Rahn
rahn@sandia.gov



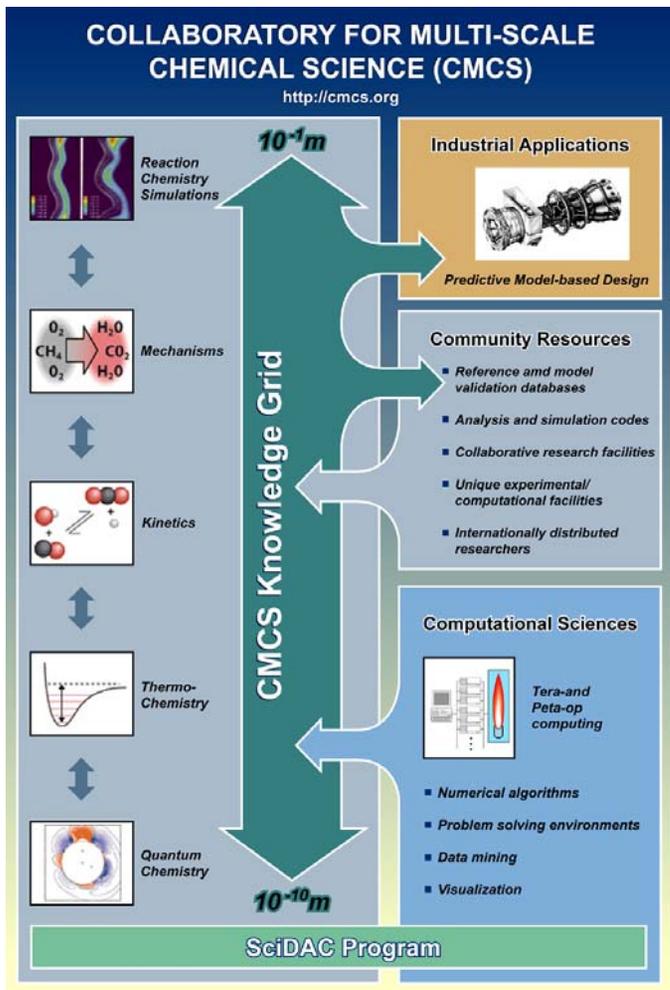
Combustion Research Facility, Sandia National Laboratories

CMCS Partner Institutions





Collaboratory for Multi-scale Chemical Science

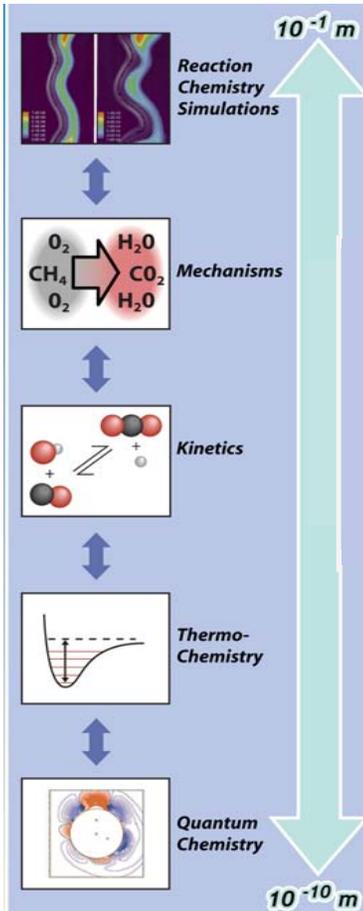


- A collaboration of 9 national labs and universities initiated in 2001
 - Chemical scientists spanning the scales from electronic structure of molecules to simulations of reacting flow
 - Computer and information scientists expert in emerging web-based technologies
- Funded by DOE/SC MICS office
 - Part of the National Collaboratory Program
 - Pilot project in DOE combustion research
 - Three year project, renewed in 2004 to 2006
- Target Chemical Science Community and BES SciDAC projects
- Broader, longer term goal to pilot concepts, software for Knowledge Grids





Multi-disciplinary CMCS Team



SNL - Larry Rahn*, Christine Yang, Carmen Pancerella, Wendy Doyle, Michael Chen, Jan Nobel

LANL- David Montoya*, Lili Xu

MIT - William H. Green, Jr.*, Luwi Oluwole, Jing Song

UCB - Michael Frenklach*, Zoran Djurisic

LLNL- William Pitz*

ANL - Branko Ruscic*, Al Wagner, Reinhardt Pinzon, Gregor von Laszewski, Deepti Kodeboyian

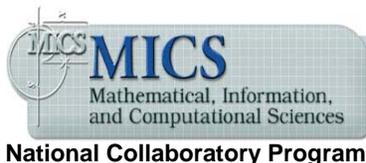
NCSA- James D. Myers*

NIST- Thomas C. Allison*

PNL - Brett Didier*, Karen Schuchardt, Todd Elsethagen, Jun Li, Lisong Sun, Vidhya Gurumoorthi, Jared Chase

*denotes Institutional Point of Contact

CMCS Development Partnerships

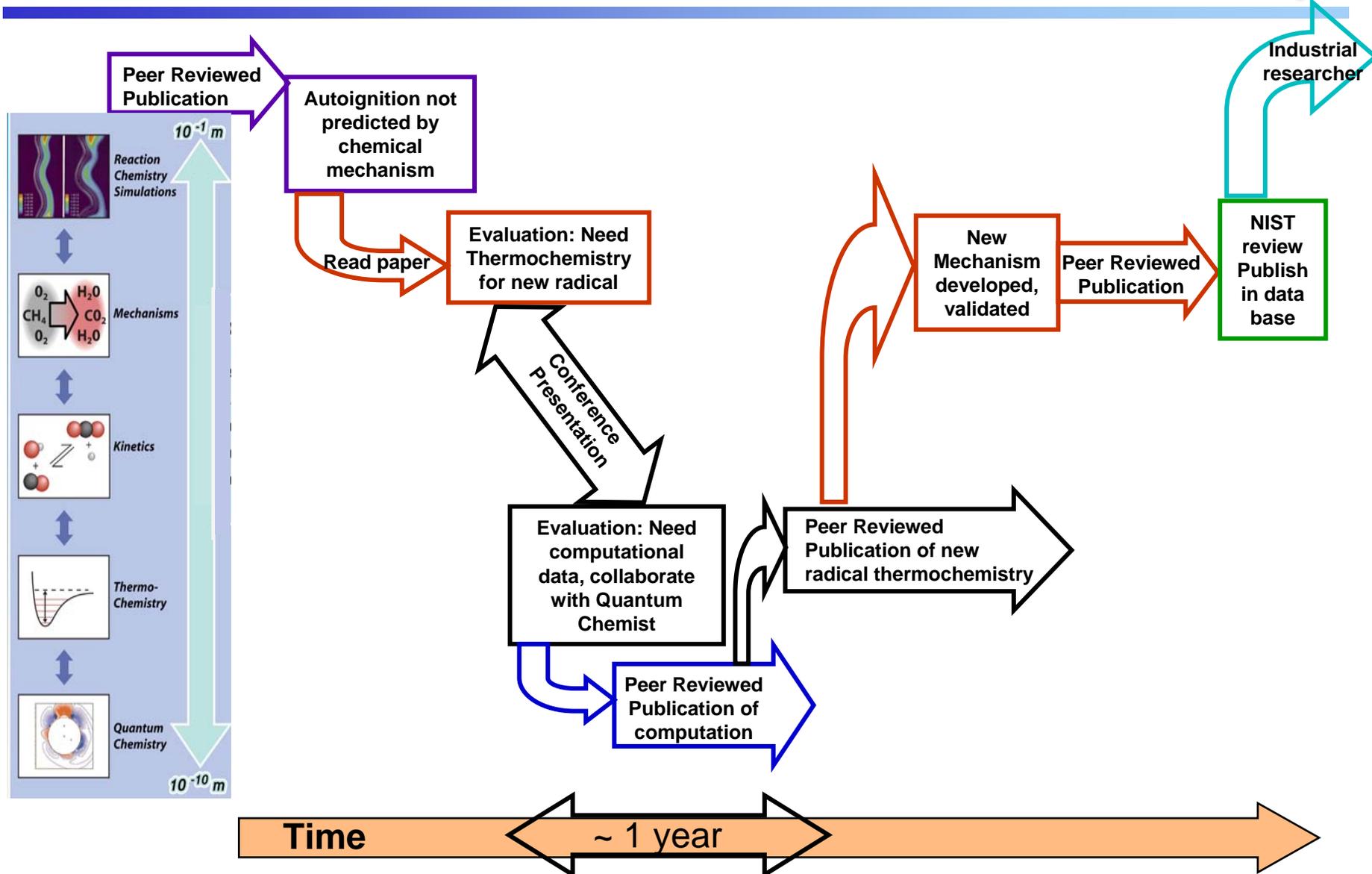


SAM



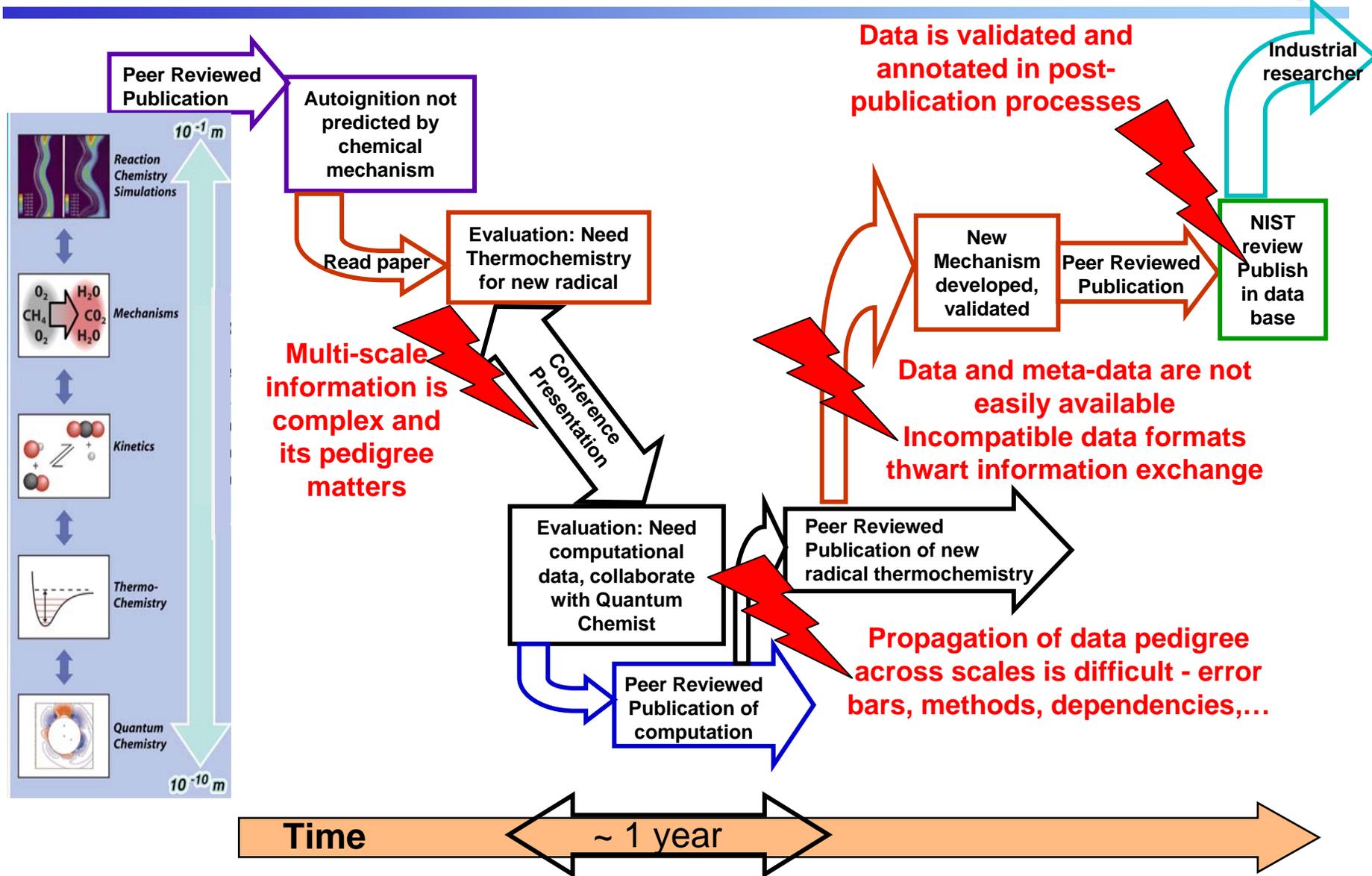


Challenge: Multi-scale science takes too long





Challenge: Multi-scale science sometimes does not happen



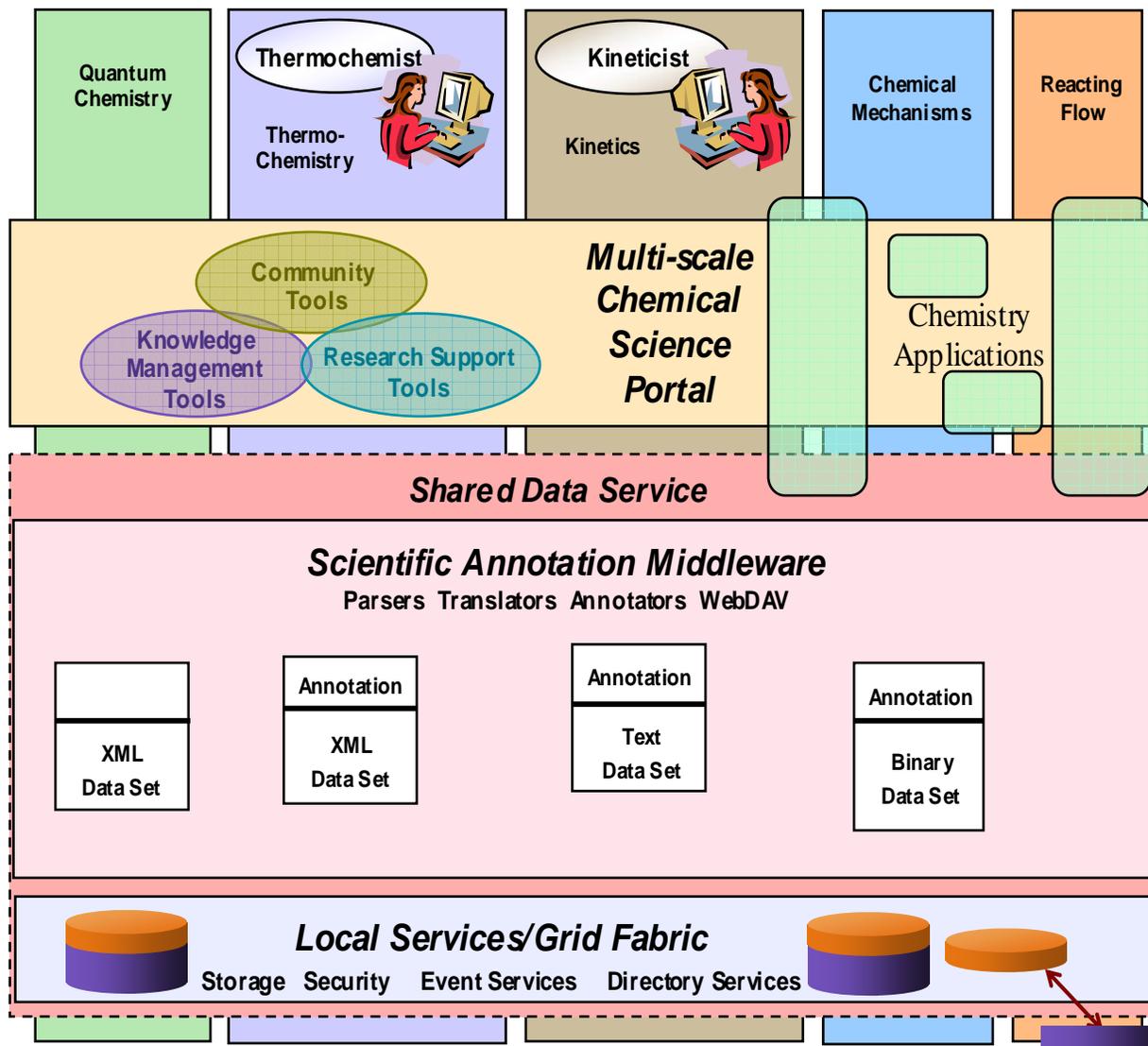


CMCS integrates capabilities into an adaptable infrastructure



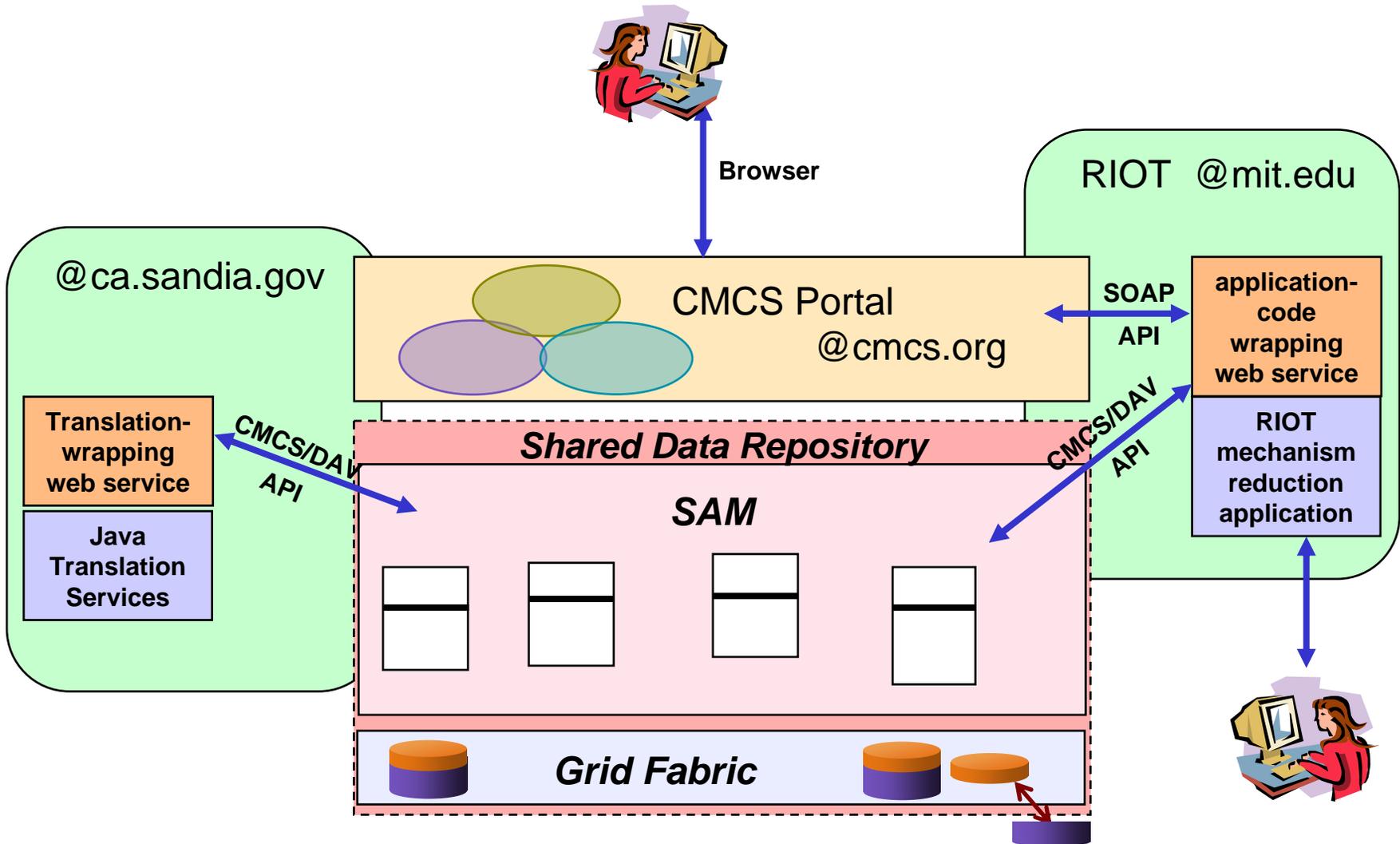
Infrastructure Capabilities

- Collaboration
- Data/metadata management
- Annotation
- Translation
- Visualization
- Notification
- Web service integration
- Search
- Security



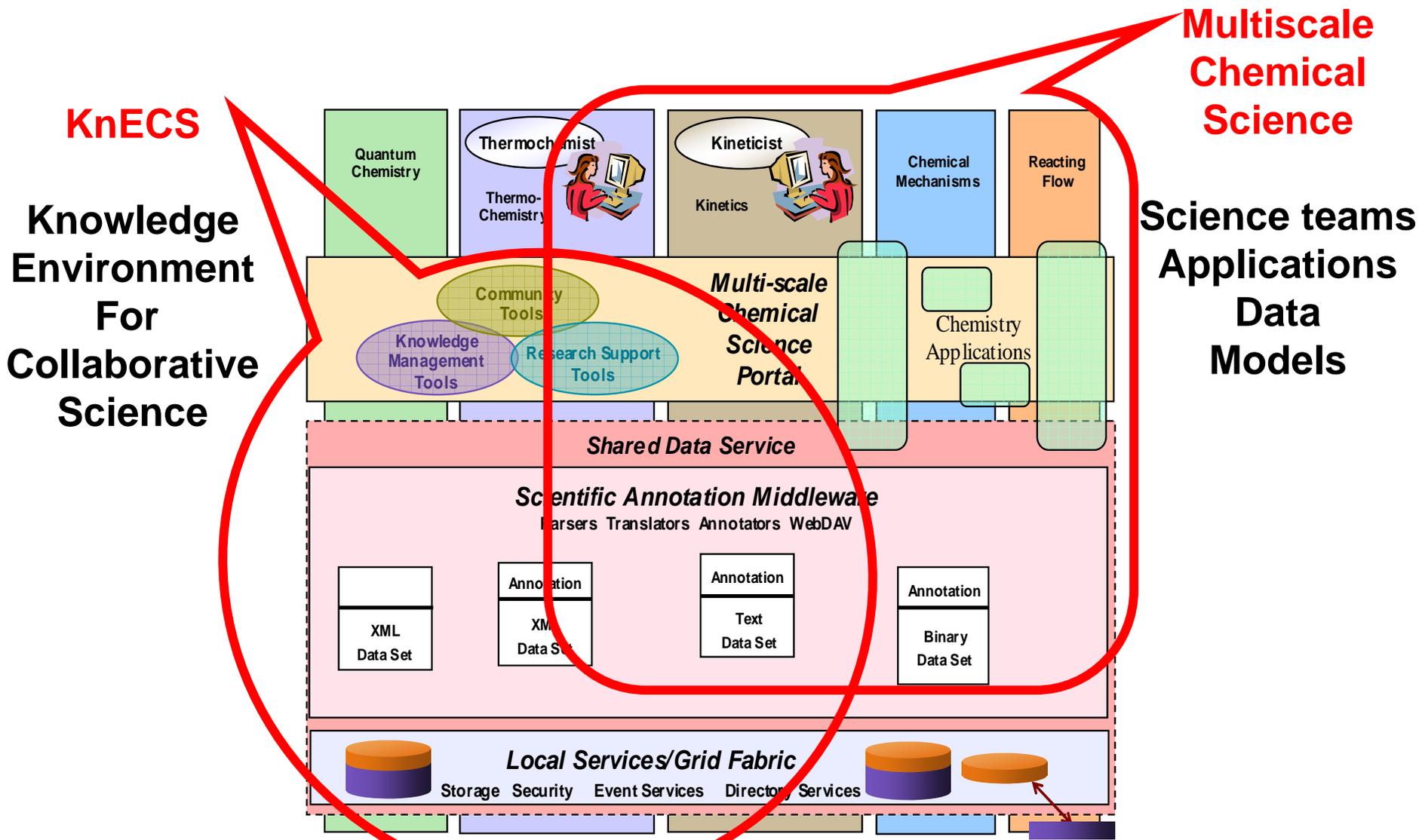


Applications like RIOT are enabled by CMCS infrastructure



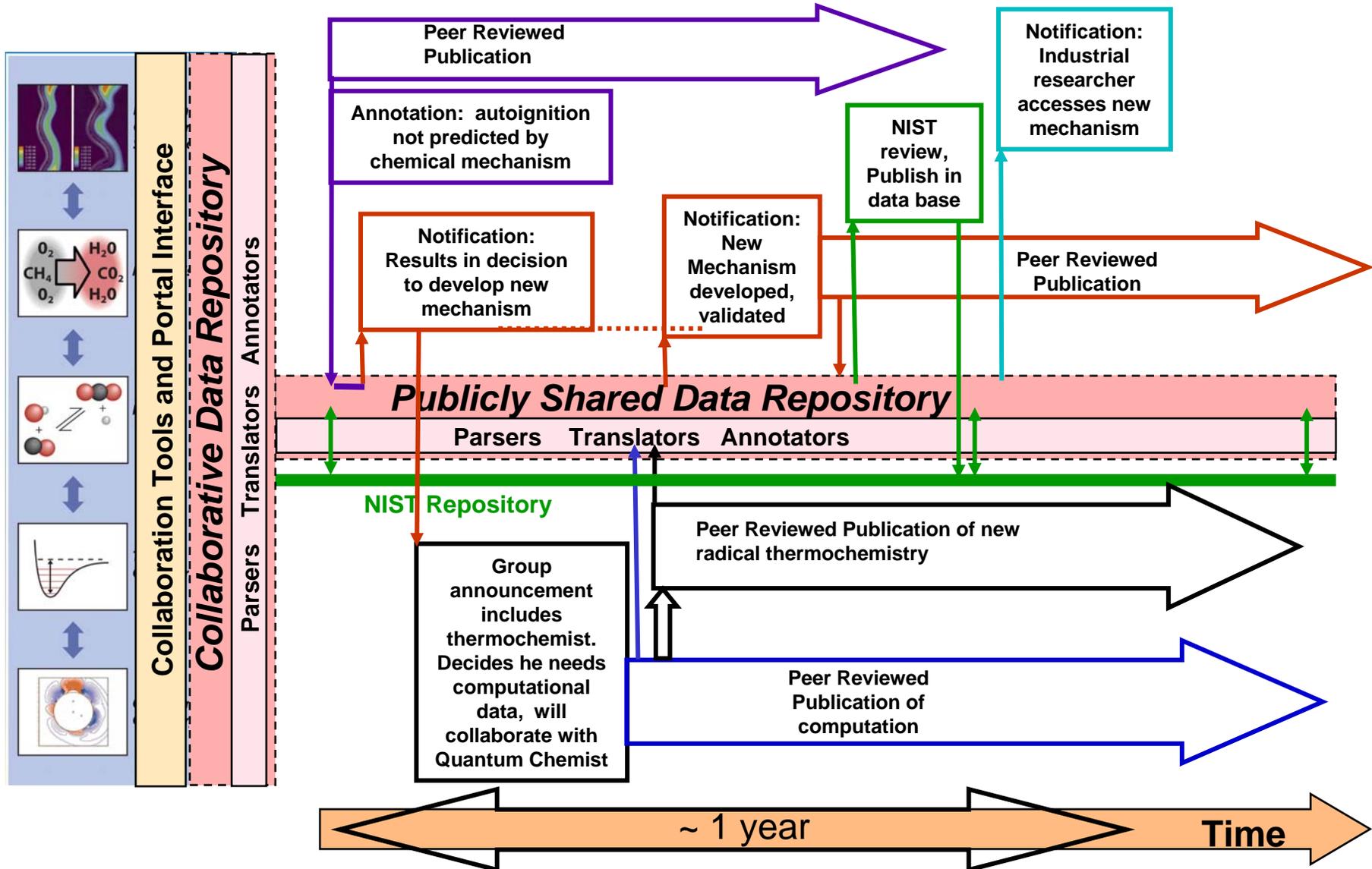


CMCS integrates infrastructure and science in a systems approach





Shared repository & tools enable timely & new multiscale science

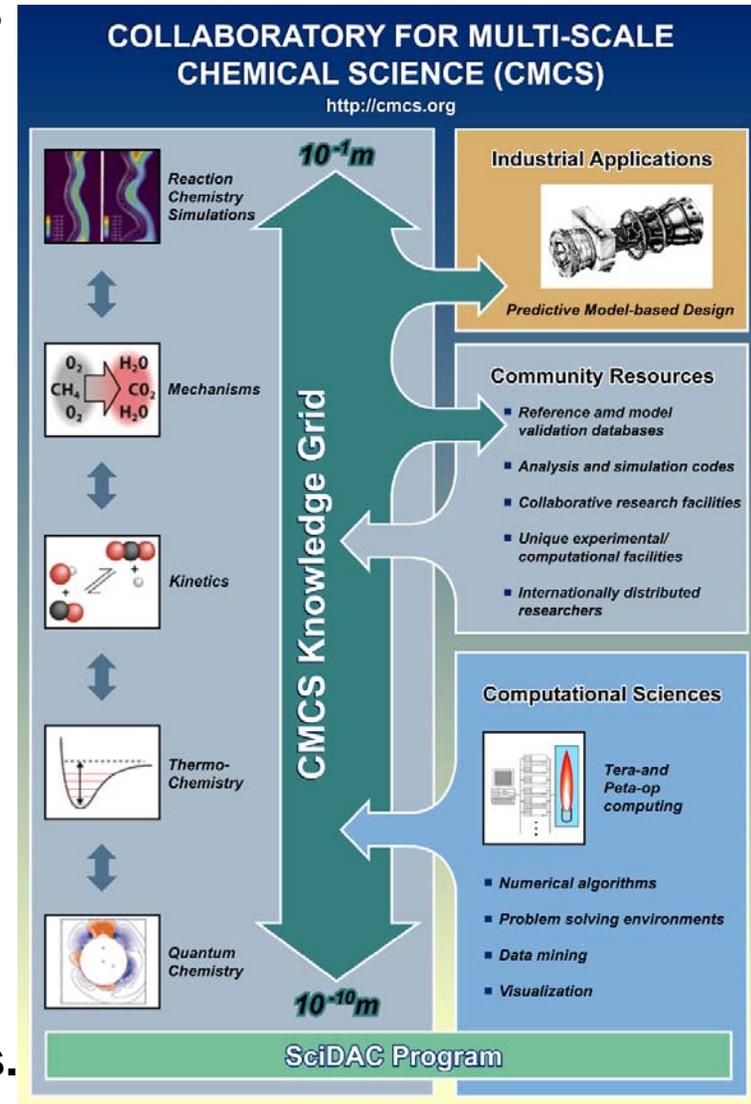




CMCS-Enabled Science Demonstrates that a 'New Paradigm' is Within Reach



- Enabling rapid formation of collaborations sharing validated data across scales to speed and improve science...
 - Integrates collaboration and data sharing tools into a Web-based Data Portal
 - Enables interoperability with new XML, annotation, and metadata standards and technology
- Facilitating new science with 'systems approach' to developing and using multi-scale data...
 - Enables direct interaction with Web-store, Portal-based GUI's, pedigree tracking
 - Data accessibility and 'Weak links' in systems approach drive new science
- Pilot communities are exploring 'systems approach' to multi-scale science, curating data for publication, and testing new ideas.





CMCS Production Data Portal is Serving Pilot Groups



CMCS Data Portal Capabilities

- Collaboration
- Data/metadata management
- Annotation
- Translation
- Visualization
- Notification
- Application integration via web services & API
- Search
- Security

The screenshot shows the CMCS Data Portal interface in a web browser. The main content area displays a file browser for the path `/sam/files/public/electronic_structure/Ecce/`. A table lists data sets with columns for 'Data Set', 'Author', 'Created', 'Modified', and 'Size'. The table contains entries for G3MP2-B3LYP-CH3OO- and G3MP2-B3LYP-CH3OOH. A search results page for 'ATcT' is also visible, showing a search box and a 'SAM ELN List' section.

The pop-up window shows a pedigree diagram for a data object named 'CH3queryResult.xml'. The diagram illustrates relationships between various data sources and the resulting object. The sources include 'SpeciesDictionary', 'NASA7ElementsLexicon', 'SpeciesCookbook', and 'NetworkEncyclopedia'. The relationships are labeled with terms like 'references', 'hasinputs', and 'ispartofproject'. The resulting object is shown as 'methyloperoxyNotes (0.001)' with a 'Simple View (text/html)' option.

The data portal user interface as it appears in a web browser. The lower box shows the pop-up visualization of the pedigree and other data relationships for a particular data object resulting from a search.



CMCS & ATcT are already changing the way thermochemical science is done



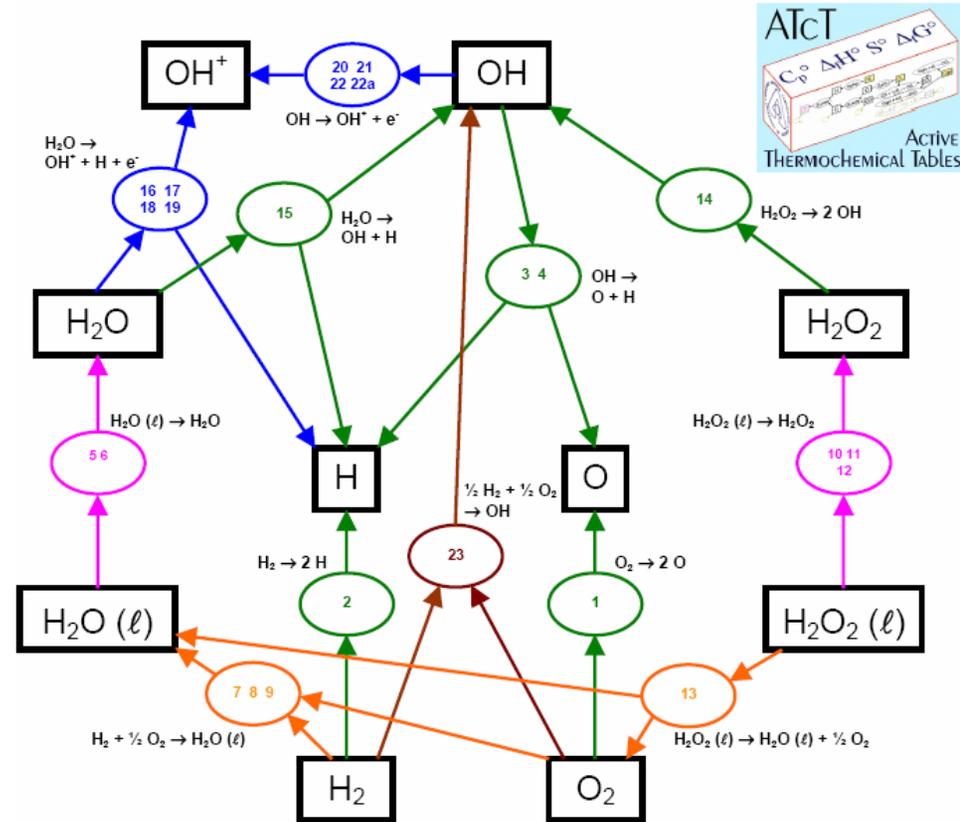
- The recent revision of the enthalpy of formation of hydroxyl (OH) has been confirmed and its uncertainty reduced by a factor of ~6.5.

B. Ruscic, A. F. Wagner, L. B. Harding, R. L. Asher, D. Feller, D. A. Dixon, K. A. Peterson, Y. Song, X. Qian, C.-Y. Ng, J. Liu, W. Chen, and D. W. Schwenke, *J. Phys. Chem. A* **106**, 2727 (2002)

B. Ruscic, R. E. Pinzon, M. L. Morton, G. von Laszewski, S. Bittner, S. G. Nijsure, K. A. Amin, M. Minkoff, and A. F. Wagner, *J. Phys. Chem. A* **108**, 9979 (2004).

- ATcT systems approach motivated new experiments by C.-Y. Ng, UC Davis that are improving N atom thermochemistry by >10.

- ATcT currently includes >2500 annotated scientific results. CMCS will facilitate publication and enable community participation in this database.



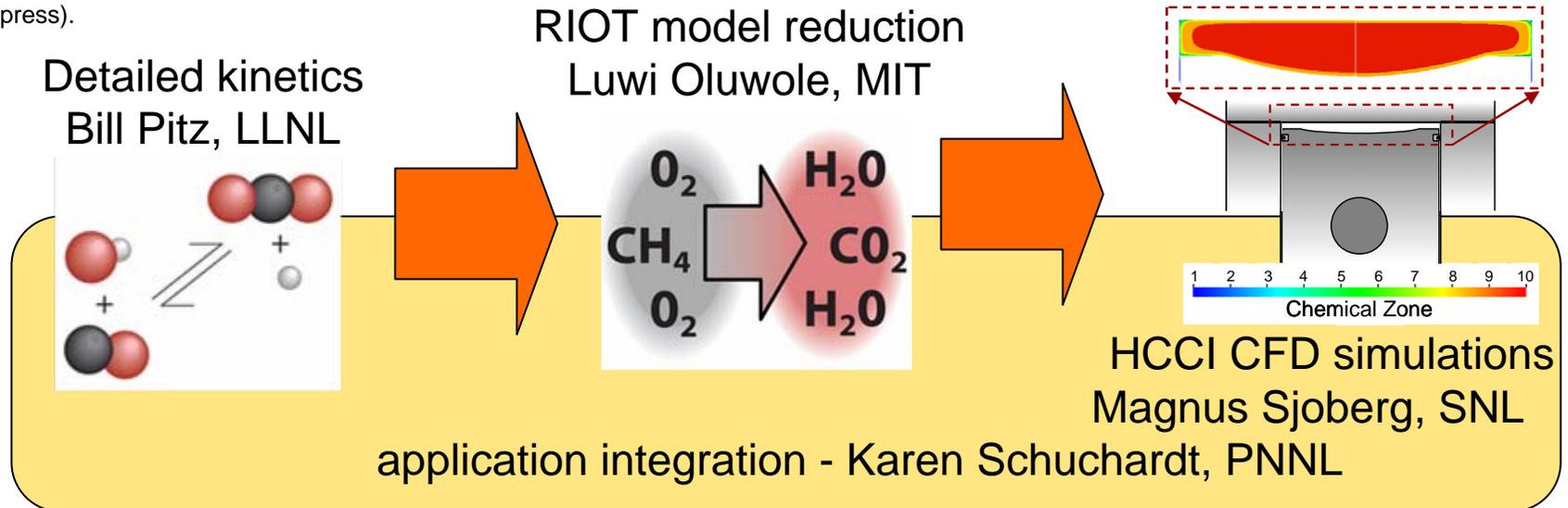
The Core (Argonne) Thermochemical Network, (C(A)TN) is the primary TN that enables ATcT. It includes >2500 results relating >500 species.

HCCI Engine Simulation: Example of Multi-scale Science

- The HCCI group is a cross-disciplinary team that is bringing detailed chemical kinetic models into improved simulations of ignition and pollutant formation in a Homogeneous Charge Ignition (HCCI) engine.
- Sharing of detailed kinetic models for fuels led by Bill Pitz using CMCS
- Range Identification and Optimization Tool (RIOT) for automates reduction of kinetic mechanisms to accurate sub-models needed to speed-up multi-zone calculation of combustion in HCCI engines.

B. Bhattacharjee, P. Lemonidis, W.H. Green, and P.I. Barton, "Global Solution of Semi-Infinite Programs", Math. Program. Ser. A (2005, in press).

O.O. Oluwole and W.H. Green, "Rigorous Error Control in Reacting Flow Simulations Using Reduced Chemistry Models", Computational Fluid and Solid Mechanics: Proceedings of the Third MIT Conference on Computational Fluid and Solid Mechanics, ed. by K.J. Bathe (Elsevier, 2005, in press).



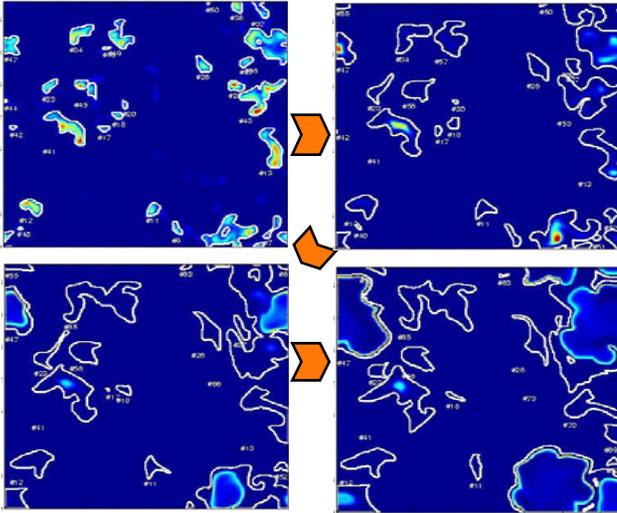


Other CMCS Chemical Science Communities

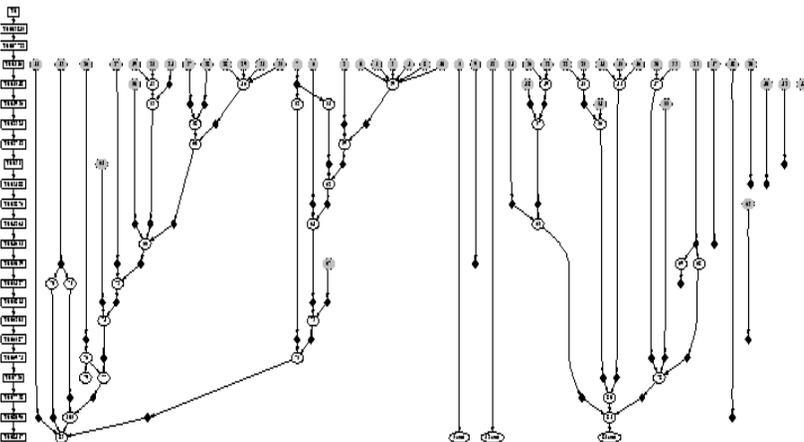


- Feature Tracking for CRF-led direct numerical simulations of combustion
 - Wendy Koegler collaborating with Habib Najm, Jackie Chen, Dave Leahy
- Premixed combustion community data – with Robert Cheng, LBNL
- Process Informatics Model (PrIME) establishing the NIST/PrIME Data Warehouse and building tools for dynamic model provision
 - Led by Michael Frenklach, UC Berkeley
 - Data Warehouse will launch with GRI-Mech Methane Mechanism, NIST Kinetics Database, and Leeds Methane Oxidation Mechanism
- Real Fuels research at NIST
- Publish data from low-pressure flame at ALS – Nils Hansen, CRF
- Publish quantum chemistry basis function data – led by PNNL
- CMCS collaborations with four NSF proposed chemical science cyberinfrastructure facilities – Purdue, Penn State, PrIME, U. Wiscon.

Feature Tracking in Direct Numerical Simulations



Evolution of hydroperoxy, HO₂, features at different fractions of autoignition induction time.



'Feature Graph' of feature history and feature interactions.

● Accomplishments

- FDTOOLs modular framework
- Auto generation of feature graphs
- Feature XML Schema (v0.1)
- Autoignition feature data on CMCS DAV

● Issues

- Found that further development required direct integration with simulation code framework
- Wendy moved to a new position

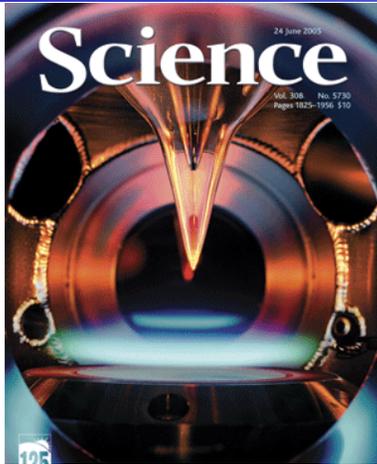
● Future

- Integrated with Ultra-scale computing vision in SciDAC2 proposals-
 - ✓ Parallelize framework
 - ✓ Mobile code for very large data

Wendy Kooger working with Jackie Chan and Habib Najaoui steering DNS simulations



Reacting Flow Data at CRF



Synchrotron Photoionization Mass Spectrometry for Investigation of Combustion Chemistry
Contact – Nils Hansen

- International Consortium for Synchrotron Photoionization Mass Spectrometry (PIM) for Investigation of Combustion Chemistry
 - International team taking data at chemistry beam line at LBL Advanced Light Source
 - Focus is on converting data to XML, adding metadata, sharing data and analysis tools, and publishing data and models for others to use.
 - Embarking on V2 schema, and prototype data publication



International Workshop on the Measurement and Computation of Turbulent Nonpremixed Flames

<http://www.ca.sandia.gov/TNF/>

Contact – Rob Barlow

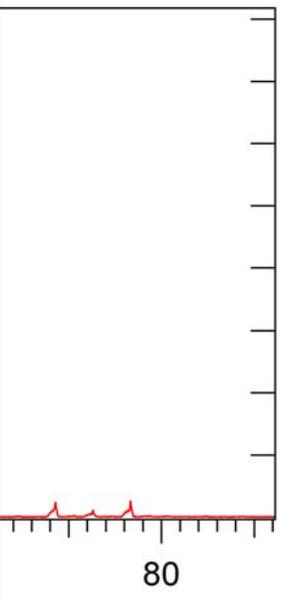
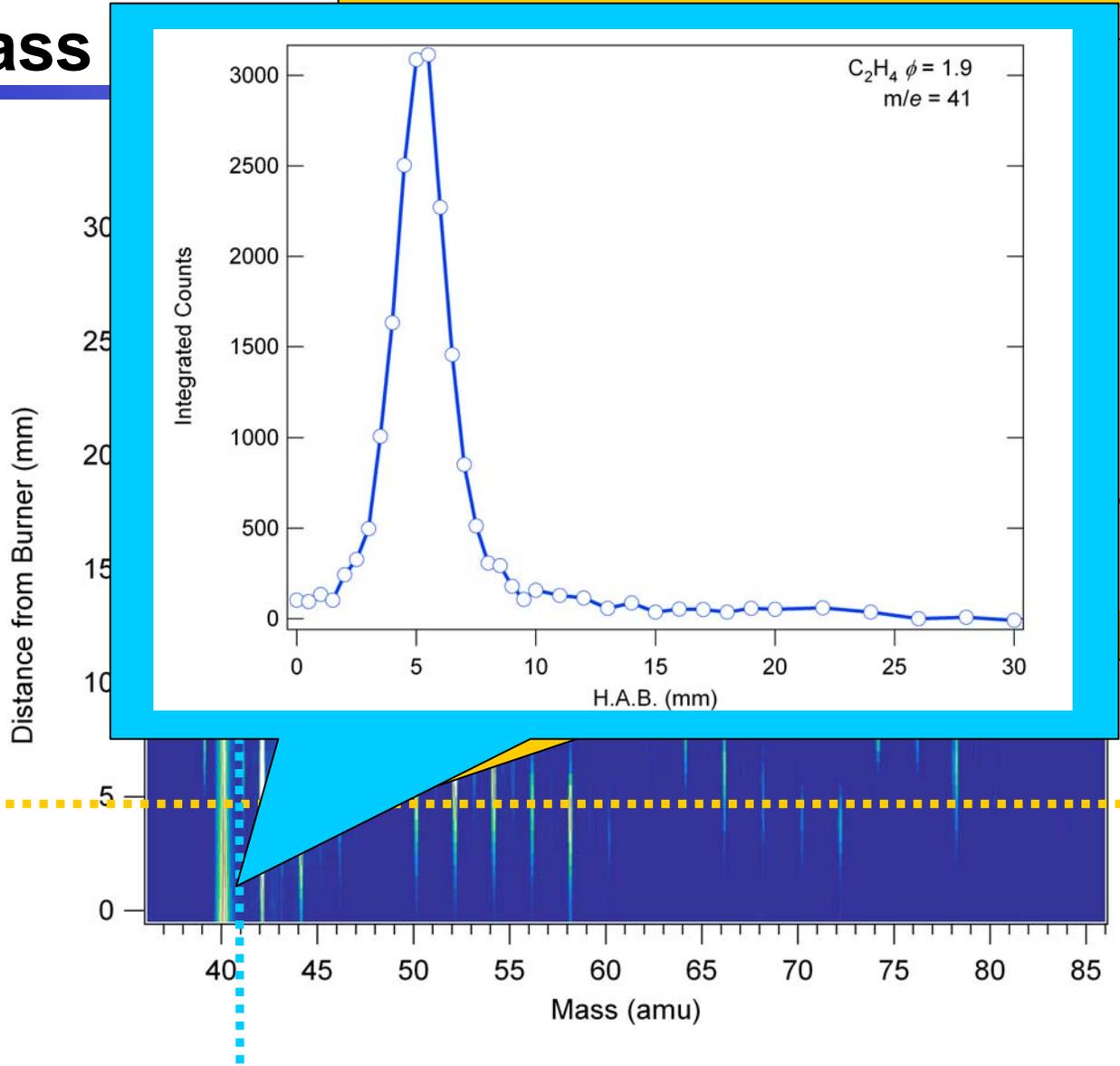
- International Workshop on the Measurement and Computation of Turbulent Nonpremixed Flames
 - About 80 scientists meeting bi-annually to compare experiments and models
 - Initial CMCS focus beginning with current zipped archival data available on web
 - Plan to move to new, larger and more complex data, and include modeling results



Burner Scan:

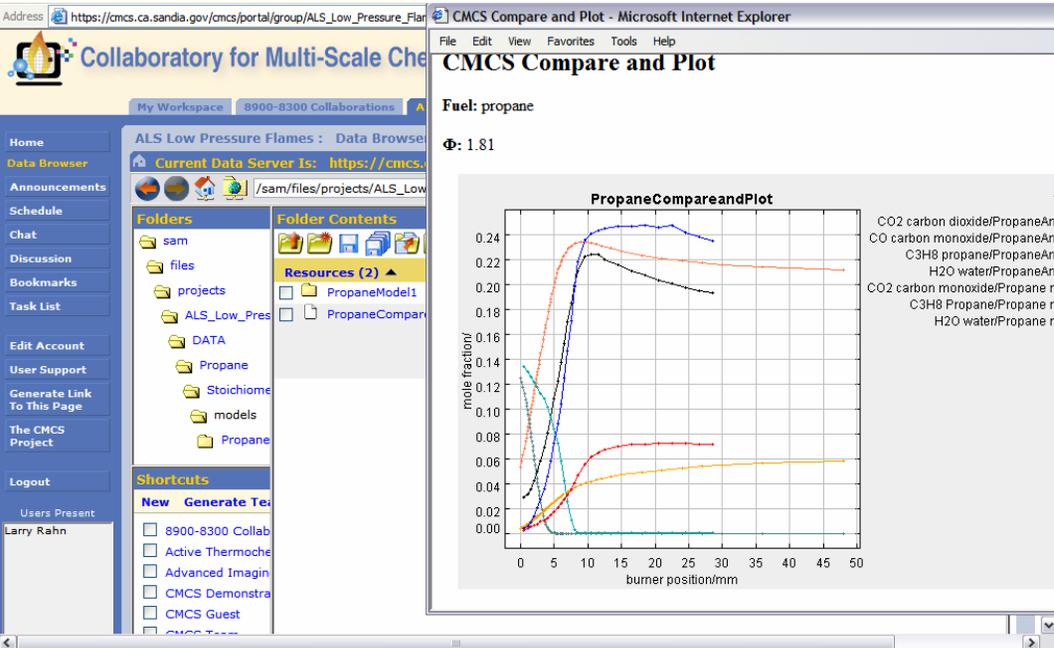


Mass





PIM Low-Pressure Flame Data



Plot translation allows visualization of experimental data and model results

Progress

- Java framework for data conversion of about 15 flame experiments so far
- Entering metadata from lab notebooks
- Translations for visualizing data and models

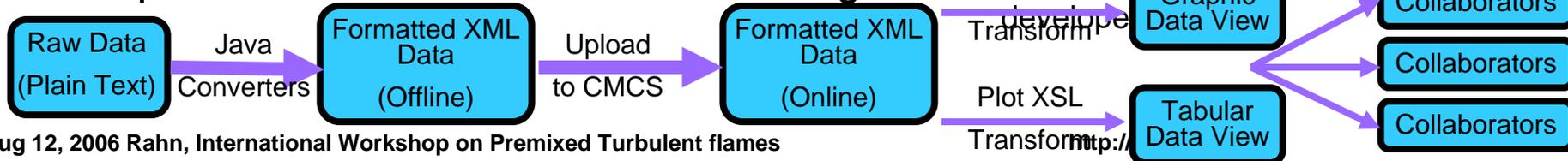
Issues

- V2 schema required to incorporate add'l metadata and facilitate publication
- Incorporation of models from others, analysis tools, maintaining links when data is reorganized
- Data publication links for all institutions, coupling to groups like PrIme
- Support (tools, people, standards) for data curation

Future

- Enable and document data analysis workflow

Rapid Data Conversion and Publishing





Evolution of CMCS Project Organization



Courier Content - Microsoft Internet Explorer

Address: https://cmcs-dev.ca.sandia.gov/cmcs/portal/user/anon/panel/Main/template/courier_content/js_peid/710

Public Data / Turbulent Nonpremixed Flames (TNF) / Piloted Jet Flames (Total 1 Entries)

Title: Flames CDEF: Sandia piloted CH4-air jet flames data

Type: Piloted **Fuel:** 25% CH4, 75% air **Location:** Sandia

Modified: 2006-08-02 23:10:16 GMT
Authors: Erwin Dunbar;

[View Details](#) [View File](#)

CMCS Portal: Welcome: Welcome: Public Data - Microsoft Internet Explorer

Collaboratory for Multi-Scale Chemical Science

Username: Password: [Login](#) [Create New Account](#)

Public Data

Current Data Server Is: <https://cmcs-dev.ca.sandia.gov:9443>

Path: /sam/files/public/TNF_Dev/DATA/pmCDEFarchivesXML

Resources (13)	Author	Modified	Size
Up to parent folder			
Group Files	cmcsroot	2006-08-02 23:05:04 GMT	0
images	cmcsroot	2006-08-02 17:14:21 GMT	0
pmC.scats	cmcsroot	2006-08-01 19:51:41 GMT	0
pmC.stat	cmcsroot	2006-08-01 19:53:32 GMT	0
pmD.scats	cmcsroot	2006-08-01 19:51:50 GMT	0
pmD.stat	cmcsroot	2006-08-01 19:53:49 GMT	0
pmE.scats	cmcsroot	2006-08-01 19:51:59 GMT	0
pmE.stat	cmcsroot	2006-08-01 19:54:07 GMT	0
pmF.scats	cmcsroot	2006-08-01 19:52:08 GMT	0
pmF.stat	cmcsroot	2006-08-01 19:54:24 GMT	0
Velocity Data	cmcsroot	2006-08-01 18:10:32 GMT	0

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CMCS v2.3rc1 | SAM v2.1.48B | CHEF v1.1.01 [build #307231] | Jetspeed v1.4b2[cvs08oct2002p]

Sandia Piloted Jet Flames CDEF

Authors: Robert Barlow; Jonathan Frank;
Date: 1997

Abstract: Sandia piloted flames CDEF. Contains experiment parameters and conditions. Notes: Temperatures in data files are from Rayleigh scattering measurements, except at x/d=1,2,3 which use Raman LIF

Organization Information:

Flame Type:	Piloted
Fuel:	25% CH4, 75% air
Location:	Sandia (Scalar), TU Darmstadt (Velocity)

Pilot Information:

Phi:	.77
Mixture:	C2H2; H2; air; CO2; N2;

Burner Dimensions:

Name:	Sydney Burner
Main Jet:	Inner Diameter: 7.2 mm
	Inner Diameter: 7.7 mm; Wall Thickness: 0.25 mm
Pilot Annulus:	Outer Diameter: 18.2
Burner Outer Wall Diameter:	Outer Wall Diameter: 18.9 mm; Wall Thickness: 0.35 mm
Wind Tunnel Exit:	30 cm x 30 cm

Scalar Boundary Conditions:

Coflow Velocity (Ucfl):	0.9 m/s (+/- 0.05) @ 291 K, 0.993 atm
Main Jet Kinematic Viscosity:	1.58e-05 m^2/s (from chemkin)
Visible Flame Length:	67d (48 cm)
Probe Volume:	0.75 mm^3

Hi Larry,

Dev side of CMCS came back up, so I was able to test s... Details page will work after talking with Mike about curren link.

If you have time, please check https://cmcs-dev.ca.sandia.gov/cmcs/portal/user/anon/js_peid/710/act/eventSubmit.do?openentry=null&entry=Turbulent Nonpremixed and View Conditions.

Have an excellent time in Europe, and it was great workin

-Erwin

Erwin "Dan" Dunbar, Student Intern, Chemical Sciences
Sandia National Labs eddunba@sandia.gov
MS 9051 Phone (925)294-3312

Thu 8/3/2006 11:45 AM 5 KB
Thu 8/3/2006 11:43 AM 32 KB
Thu 8/3/2006 11:28 AM 23 KB
Thu 8/3/2006 11:17 AM 11 KB
Thu 8/3/2006 10:51 AM 327...
Thu 8/3/2006 10:25 AM 8 KB
Thu 8/3/2006 10:04 AM 5 MB



cmcs.org - Welcome to the Collaboratory for Multi-scale Chemical Science - Microsoft Intern...

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites Recycle Mail Print Wordpad New Folder Favorites People

Address <http://cmcs.org/> Go Links



Collaboratory for Multi-Scale Chemical Science

Welcome to cmcs.org! This is the home page for CMCS, the Collaboratory for Multi-scale Chemical Science.

Start by selecting an area of interest...

- Go to [The CMCS Portal](#)
- Go to [Getting Started](#) to learn how to use the CMCS Portal
- Search CMCS [Public Data](#)
- Look at [Teams](#) to see collaborations and resources hosted within the CMCS Portal
- Learn more about the [CMCS Project](#)
- Involved in CMCS development? Go to [CMCS Developers](#) to learn about tools and resources for developers.

Internet



https://cmcs.ca.sandia.gov/cmcs/portal/user/anon/template/UserAgreement - Microsoft Int...

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Collaboratory for Multi-Scale Chemical Science

NOTICE TO USERS:

CMCS Content Provider Agreement version 1.0.1

This version was created on 2003-10-17.

Introduction

Welcome to the pilot Collaboratory for Multi-scale Chemical Sciences ("CMCS") Service. These Terms of Service govern the use of the CMCS Service as a Content Provider ("CP"). CMCS reserves the right to modify this agreement at any time without prior notice. CP will be given the opportunity to accept these modifications as a condition of continued use of the CMCS Service; if CP declines, CP's account will be terminated and CP's Content will be removed from the CMCS Service. CP use of the CMCS Service constitutes acceptance of these Terms of Service and creates a binding legal agreement, so please read them carefully.

Description of Service

The CMCS Service is controlled and operated by the M&O contractor operating Sandia National Laboratories ("SNL") herein after known as CMCS, for the purpose of supporting research in chemical science (the

I Agree I Disagree

Done Local intranet

https://cmcs.ca.sandia.gov/cmcs/portal/user/anon/page/default.psm1/template/...

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Address https://cmcs.ca.sandia.gov/cmcs/portal/user/anon/page/default.psm1/ter Go Links

Collaboratory for Multi-Scale Chemical Science

Create New Account

Required information:

Username:

Password:

Password: (confirm)

First Name

Last Name

Email:

I want to be notified when others request data that matches my expertise...

Create New Account Cancel

Done Local intranet



CMCS Portal: My Workspace: My Workspace: Home - Microsoft Internet Explorer

Address: https://cmcs.ca.sandia.gov/cmcs/portal

Collaboratory for Multi-Scale Chemical Science

My Workspace | 8900-8300 Collaborations | ALS Low Pressure Flames | (more)

Home

Data Browser

Data Requests

Schedule

Bookmarks

Teams

Rahn ELN#1

Edit Account

User Support

Generate Link To This Page

The CMCS Project

Logout

Users Present

Larry Rahn

My Workspace : Home

Message of the Day

Options...

The CMCS production server will be upgraded Thursday, July 6, 2006. The portal and data server will be offline during this time.
(CMCS Root - Jul 5, 2006 1:11 pm)

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CMCS v2.3rc1 | SAM v2.1.4b8 | CHEF v1.1.01 [build #307231] | Jetspeed v1.4b2[cvs08oct2002p]

CMCS Portal: My Workspace: My Workspace: Teams - Microsoft Internet Explorer

Address: https://cmcs.ca.sandia.gov/cmcs/portal/user/rahn/js_pane/600

Collaboratory for Multi-Scale Chemical Science

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Larry Rahn

My Workspace : Teams

Teams

New Team

Team Title (Team Id)	Description	Joinable?
20060301-Test Team	This team created as not joinable then changed to joinable.	✓
20060301-Test Team 2	This team created as joinable.	✓
8900-8300 Collaborations (8900-8300_Collaborations)	Information, etc. on collaborative projects including SciDAC and CMCS	✓
Active Thermochemical Tables for Guests	Test Run of Active Thermochemical Tables for Visitors	✓
Advanced Imaging Lab		
ALS Low Pressure Flames	Low pressure Flame Investigations applying VUV Photoionization Mass	✓

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https://cmcs.ca.sandia.gov/cmcs/portal/user/rahn/js_pane/700?action=Select&site=%7Eral

CMCS Portal: Premixed Turbulent Flames Working Group: Premixed Turbulent Flames Working Group: ...

File Edit View Favorites Tools Help

Address https://cmcs.ca.sandia.gov/cmcs/portal/group/Premixed_Turbulent_Working_Group

Collaboratory for Multi-Scale Chemical Science

My Workspace 8900-8300 Collaborations ALS Low Pressure Flames (more)

Premixed Turbulent Flames Working Group : Home

Experimental Database for Premixed

Welcome to your team workspace!

Recent Announcements

Recent Discussion Items

Recent Chat Messages

Team Members

Member	Email
Robert K Cheng (RKCheng)	RKCheng@lb
Fred Gouldin (Gouldin)	fcg2@cornell
Carmen Pancerella (carmen)	carmen@ca.:
Bill Pitz (pitz)	pitz1@lnl.go
Larry Rahn (rahn)	rahn@sandi:
Karen Schuchardt (karen)	Karen.Schud
jim driscoll (jamesfd)	jamesfd@um
vidhya gurumoorthi (vidhya)	vidhya.gurur

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CMCS v2.3rc1 | SAM v2.1.4b8 | CHEF v1.1.01 [build #307231] | Jetspeed v1.4b2[cvs08oct2002p]

CMCS Portal: Premixed Turbulent Flames Working Group: Premixed Turbulent Flames Working Group: ...

File Edit View Favorites Tools Help

Address https://cmcs.ca.sandia.gov/cmcs/portal/group/Premixed_Turbulent_Working_Group/js_pane/200

Collaboratory for Multi-Scale Chemical Science

My Workspace 8900-8300 Collaborations ALS Low Pressure Flames (more)

Premixed Turbulent Flames Working Group : Data Browser

Current Data Server Is: <https://cmcs.ca.sandia.gov:9443>

Path: /sam/files/projects/Premixed_Turbulent_Working_Group

Resources (8)	Author	Modified	Size	Notes
Up to parent folder				
10th International Workshop Presentations	pitz	2006-07-24 23:11:17 GMT	0	
Annotated templates	pitz	2006-04-10 18:22:36 GMT	0	
Envelope Flames Experimental Database	RKCheng	2006-03-06 19:14:00 GMT	0	
Excel test files	pitz	2006-06-13 21:01:15 GMT	0	
Oblique Flames Experimental Database	RKCheng	2006-02-06 19:17:50 GMT	0	
Templates	RKCheng	2006-03-07 18:09:35	0	

Mouse over a resource to see a synopsis of its metadata. Click on a resource's metadata icon for full metadata viewing/editing.

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CMCS Portal: Premixed Turbulent Flames Working Group: Premixed Turbulent Flames Working Group: ...

File Edit View Favorites Tools Help

Address https://cmcs.ca.sandia.gov/cmcs/portal/group/Premixed_Turbulent_Working_Group/js_pane/200

Collaboratory for Multi-Scale Chemical Science

My Workspace 8900-8300 Collaborations ALS Low Pressure Flames (more)

Premixed Turbulent Flames Working Group : Data Browser

Current Data Server Is: <https://cmcs.ca.sandia.gov:9443>

Path: / sam / files / projects / Premixed_Turbulent_Working_Group / Oblique Flames Experimental Database

Resources (3) ▲	Author	Modified	Size	Notes
Up to parent folder				
<input type="checkbox"/> LBNL_Plane-oblique_PNAS_set_1	pitz	2006-03-15 22:19:15 GMT	15474	
<input type="checkbox"/> LBNL_Plane-oblique_PNAS_set_1	pitz	2006-04-05 16:51:27 GMT	24576	
<input type="checkbox"/> LBNL_Plane-oblique_PNAS_set_1	carmen	2006-04-05 19:26:29 GMT	12913	

Mouse over a resource to see a synopsis of its metadata. Click on a resource's metadata icon for full metadata viewing/editing.

powered by Chef SCIENTIFIC ANNOTATION MIDDLEWARE Jetspeed

CMCS v2.3rc1 | SAM v2.1.4b8 | CHEF v1.1.0.1 [build #307231] | Jetspeed v1.4b2[cvs08oct2002p]

CMCS Portal: Premixed Turbulent Flames Working Group: Premixed Turbulent Flames Working Group: ...

File Edit View Favorites Tools Help

Address https://cmcs.ca.sandia.gov/cmcs/portal/group/Premixed_Turbulent_Working_Group/js_pane/200

Collaboratory for Multi-Scale Chemical Science

My Workspace 8900-8300 Collaborations ALS Low Pressure Flames (more)

Premixed Turbulent Flames Working Group : Data Browser

Current Data Server Is: <https://cmcs.ca.sandia.gov:9443>

Path: / sam / files / projects / Premixed_Turbulent_Working_Group / Oblique Flames Experimental Database

Resources (3) ▲	Author	Modified	Size	Notes
Up to parent folder				
<input type="checkbox"/> LBNL_Plane-oblique_PNAS_set_1	pitz	2006-03-15 22:19:15 GMT	15474	
<input checked="" type="checkbox"/> LBNL_Plane-oblique_PNAS_set_1	pitz	2006-04-05 16:51:27 GMT	24576	
<input type="checkbox"/> LBNL_Plane-oblique_PNAS_set_1	carmen	2006-04-05 19:26:29 GMT	12913	

Mouse over a resource to see a synopsis of its metadata. Click on a resource's metadata icon for full metadata viewing/editing.

XML View View SaveAs..

https://cmcs.ca.sandia.gov:9443/sam/translatedto/text/html/XML View/files/projects/Premixed_Tur - Microsoft ...

```

File Edit View Favorites Tools Help

<workbook>
<worksheet name="Sheet1">
  <row number="0">
    <col number="0">Important note: search algorithm is case sensitive. Please be consistent by
  </row>

  <row number="1">
    <col number="0">Flame Type</col>

    <col number="1">Oblique-flames (plane-symmetric)</col>
  </row>

  <row number="2">
    <col number="0">Name of Data Guardian</col>

    <col number="1">Robert Cheng</col>
  </row>

  <row number="3">
    <col number="0">E-mail of Data Guardian</col>

    <col number="1">RKCheng@lbl.gov</col>
  </row>

```