United Spaces for Distributed Science

News from the National Collaboratories and SciDAC Network Research Programs

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Scientific Discovery through Advan

Annual Meeting

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Napa, CA

OFFICE OF SCIENCE
U.S. DEPARTMENT of ENERGY

SciDAC—Goal Three

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Topics

- Collaboratory and Infrastructure Pilots
- Earth Systems Grid – Don Middleton
- Middleware Projects
- Network Research Projects

Collaboratory Pilots and Collaboratory Infrastructure

DOE Science Grid

National Fusion Collaboratory

Particle Physics Data Grid

Collaboratory for Multi-Scale Chemical Science

Earth System Grid - Middleton

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The DOE Science Grid

Computing and Data Infrastructure For Large-Scale Science

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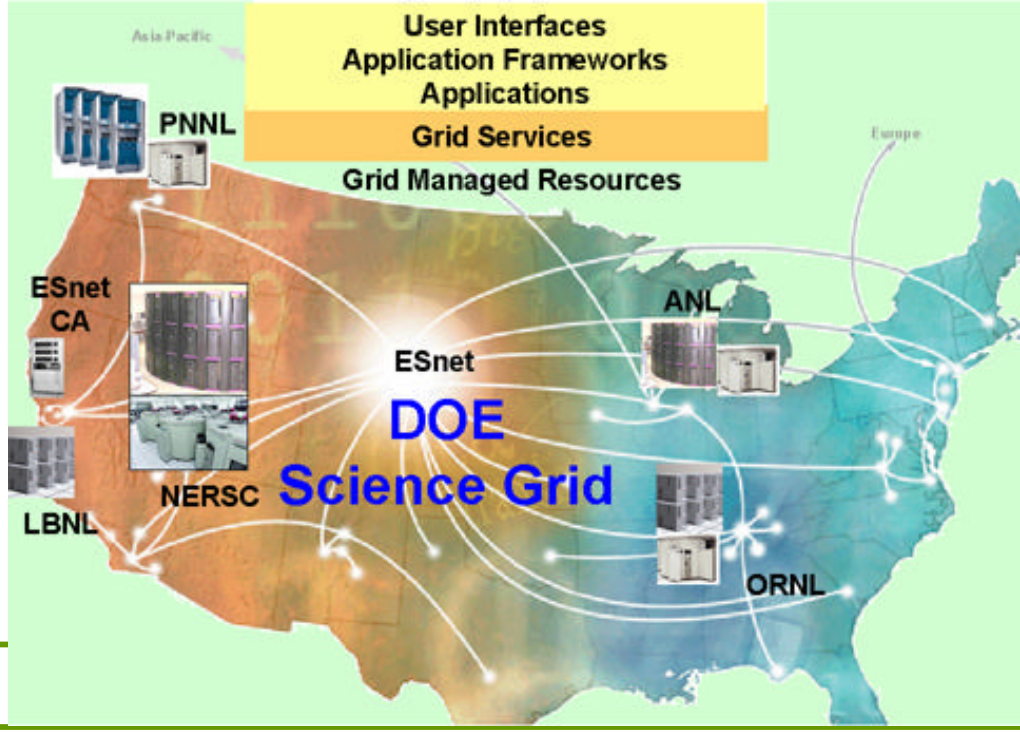


Objectives

- Grid technology dissemination to DOE science projects
- Middleware for uniform, secure, and highly capable access to large and small scale computing, data, and instrument systems, all of which are distributed across organizations
- Services supporting construction of application frameworks and science portals
- Persistent cyberinfrastructure for building and operating distributed applications (e.g. security services and resource access)
- Persistent resource infrastructure, e.g. NERSC on the Grid

Accomplishments

- Established effective inter-Lab coordination to build Science Grid and have resources committed to the Science Grid (e.g. PDSF at NERSC, Jazz cluster at ANL, Compact cluster at PNNL)
- Development of site firewall policy requirements for Grids
- Python wrapper for Globus – used for various monitoring applications
- Auditing and fault monitoring system
- Advances in Grid authorization - driven by HEP and Fusion
- ESnet DOEGrids CA project – a close collaboration w/ Science Grid
  - PKI authentication infrastructure supporting large-scale DOE science collaborations (HENP, Fusion, Science Grid)
  - Will sign subordinate CA certs (e.g. for Grid integration w/ Kerberos)
  - Provides a directory service for all certificates to support advanced authorization systems
  - Integrated policy with European Data Grid – HEP collaborators in US and Europe can now share resources, NERSC will accept EDG certs

Accomplishments (cont.)

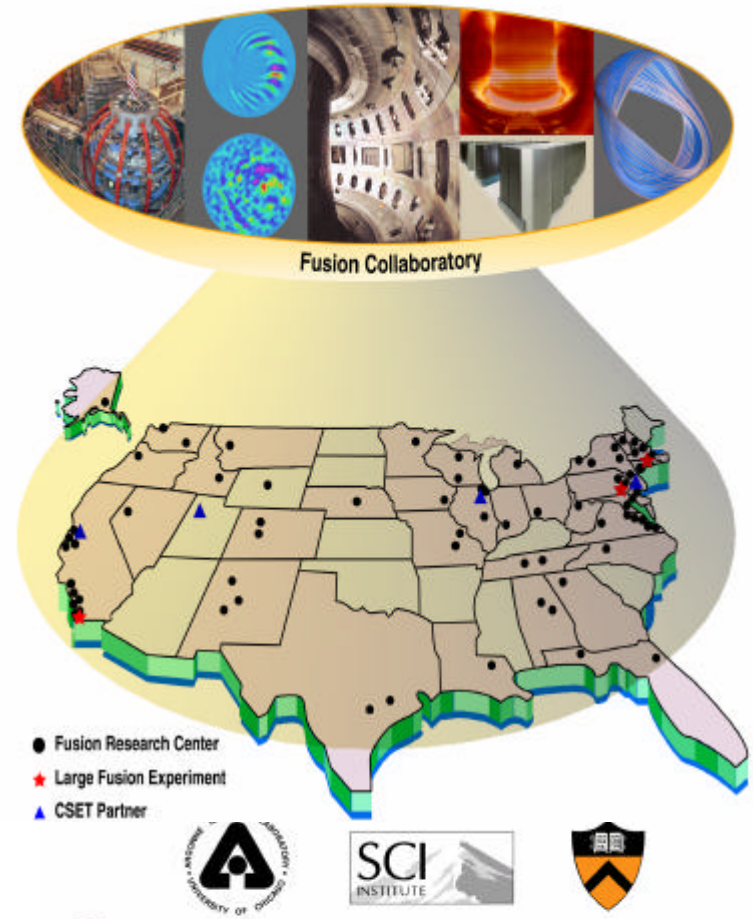
- NERSC
  - Risk mitigation plan for NERSC systems to be on the Grid
  - NERSC funded HPSS integration with Grid was tested and validated on the Science Grid
  - IBM collaboration for Globus on AIX/SP
  - A unified Grid authorization system based on LDAP server across all the production hosts
  - NERSC accounting system integrated with Grid ids
  - Working toward using Grid Security Infrastructure and certificates as a foundation for a single sign-on at NERSC

Available Software and Technology

- **DOEGrids CA is available to the DOE-related science community to issue PKI identity certificates for collaborations**
- **pyGlobus (Python callable Globus modules)**
  - **NetSaint Grid status monitoring**
  - **Grid administration tools**
- **Grid helpdesk software**
- **Grid auditing and fault monitoring (prototype)**

THE GOAL OF THE NFC IS TO ADVANCE SCIENTIFIC UNDERSTANDING & INNOVATION IN FUSION RESEARCH

Collaboratory is required to advance fusion science: geographically diverse community (37 states, 3 large experiments), leading to 1 worldwide experiment



- Diverse team
  - ANL: DSL & FL
  - GA: DIII–D Fusion Lab
  - LBNL: Distributed Systems
  - MIT: C–Mod Fusion Lab
  - Princeton Computer Science
  - PPPL: NSTX Fusion Lab
  - U. of Utah: Scientific Comp. & Imaging
- Objective is to advance fusion science
  - Experimental facilities
  - Integrate experiment, theory, modeling
  - Create a common toolkit for services

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FusionGRID www.fusiongrid.org

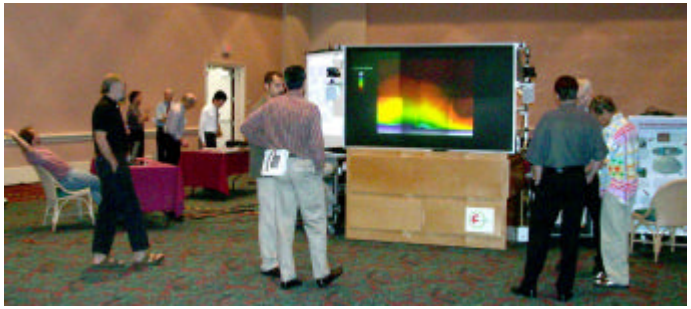
FIRST YEAR ACCOMPLISHMENTS OF THE NFC

Grid Computing

- FusionGrid created: MDSplus data system integrated with Globus GSI
- FusionGrid released with complete monitoring: TRANSP & GS2 fusion codes remotely accessible via Globus/Akenti and fine-grain authorization via GRAM
- FusionGrid used for scientific calculations presented at the APS/DPP Mtg
- Prototyped: between pulse pre-emptive scheduling, parallel MDSplus I/O

Visualization

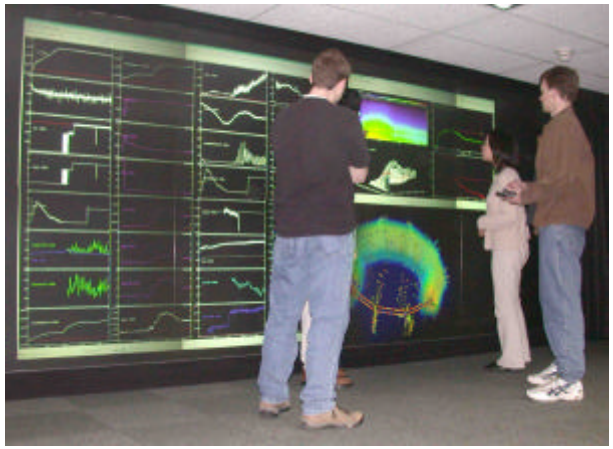
- SCIRun 3D visualization of NIMROD fusion data via MDSplus
- SCIRun visualizations used for scientific work presented at APS/DPP
- Access Grid functional on Tiled Wall as well as small scale system (PIG)
- Collaborative Visualization: Wall to wall/workstation (VNC, DMX), ELVis

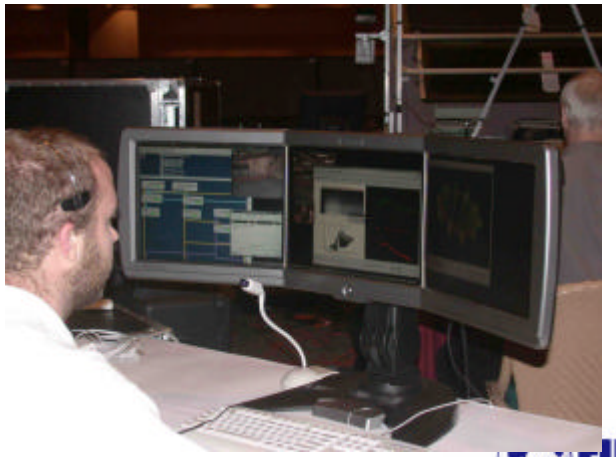


Culminated in a full demonstration at the Nov 2002 APS/DPP meeting attended by over 1000 fusion scientists

NFC'S TOOLS AND TECHNOLOGIES

- Secure MDSplus using Globus GSI available
  - Authentication and Authorization using DOE CA
- TRANSP available for worldwide usage on FusionGrid
  - Beowulf cluster, client application, complete job monitoring
  - Secure access by Globus GSI, Akenti, DOE Grids CA
- Personal Access Grid (PIG) software and spec's available
  - Installed at MIT and GA; PPPL has large AG node
- SCIRun for 3D visualization including MDSplus stored Fusion data
- Toolkits for sharing visualization wall to wall and on AG
  - Tiled walls at GA and PPPL





Particle Physics Data Grid Collaboratory Pilot

Computer Science Groups: Condor, Globus, SRM, SRB

Nuclear Physics Experiments: STAR, TJNAF

Lattice QCD: TJNF

High Energy Physics: ATLAS, BaBar, CMS, D0

PI's: Richard Mount, SLAC, Miron Livny, Wisconsin, Harvey Newman, Caltech

Steering Committee: John Huth, Harvard (ATLAS), Tim Adye, RAL (BaBar), Lothar Bauerdick, FNAL (CMS), Lee Lueking FNAL (D0), Chip Watson, TJNAF, Jerome Lauret, BNL (STAR), Miron Livny, Wisconsin (Condor), Jennifer Schopf, ANL (Globus), Ian Foster, ANL (Globus), Reagan Moore, SDSC (SRB), Arie Shoshani, LBNL (SRM)
Coordinators: Ruth Pordes, FNAL, Doug Olson, LBNL

Liaisons: Paul Avery (iVDGL), Larry Price (HICB), Mike Wilde(GriPhyN), Torre Wenaus, Ian Bird (LCG)

Program Managers: Mary Anne Scott (MICS), Irwin Gaines (HENP), Steve Steadman (NP)

Experiment data handling requirements:

- Petabytes of storage, Teraops of computing, Thousands of users,
- Hundreds of institutions, 10+ years of analysis ahead

Focus of PPDG:

- Vertical Integration of Grid technologies into Applications ongoing work
- Deployment, hardening and extensions of common Grid services and standards – data replication, storage and job management, monitoring and planning.
- Interdisciplinary teams of physicists, engineers and computer scientists
- Using and extending grid technologies ranging across architecture, integration, deployment and robustness
- Driven by demanding end-to-end applications of experimental physics
- Enabling new scales of research in experimental physics and experimental computer science

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PPDG Accomplishments

Application "Grids" with incremental capabilities

- **Data Replication for BaBar** - Terabyte stores replicated from California to France and England.
- **Replication and Storage Management for STAR** and **JLAB** - development and deployment of standard API and interoperable implementations.
- Production Simulation Grids for **ATLAS** and **CMS, STAR** distributed analysis jobs.
- **Data Transfer, Job and Information Management for D0** - GridFTP integrated with SAM; Condor-G job scheduler, MDS resource discovery all integrated with SAM.

Initial Security Infrastructure for Virtual Organizations

- **PKI certificate management**, policies and trust relationships (using DOE Science Grid and Globus)
- Authorization mechanisms – standard callouts for Local Center Authorization for Globus, EDG,
- Prototyping secure credential stores
- Engagement of site security teams.

Data and Storage Management

- Robust data transfer over heterogeneous networks using standard protocols: GridFTP, bbcp
- Distributed Data Replica management: SRB, SAM, SRM
- Common Storage Management interface and services across diverse implementations: SRM - HPSS, Jasmine, Enstore

Job Planning, Execution and Monitoring

- Job scheduling based on resource discovery and status - condor-g and extensions
- Retry and Fault Tolerance in response to error conditions - hardened gram, gass-cache, ftsh,
- Distributed monitoring infrastructure for resource discovery, resource and job information - MDS, Monalisa, Hawkeye

Prototypes and Evaluations

- Grid enabled physics analysis tools
- End to end troubleshooting and fault handling
- Cooperative Monitoring of Grid, Fabric, Applications

Technologies, Tools and Applications

Who uses what?

	Atlas	BaBar	CMS	D0	STAR	TJNAF	TJNAF-LQCD
Globus GridFTP	x	bbcp	x	x	x	x	
Globus MDS	x		x	x			
Globus GSI	x	x	x (+KCA)	x (+KCA)	x	x	Java
Condor-G/GRAM	x/VDT	x/EDG	x/VDT	x			
SRM			x	x	x	x	
SRB		x	x				
Distributed Data Mgt.	MAGDA	Bbserver++	MOP	SAM	x	x	x
Analysis prototypes		JAS	Caigee Clarens	root/sam			
Automated Data Replication	x	x		x	x	x	x
Applications Grid	p	p/EDG	x	x/sam			
DOE SG Certs	x	x	x	x	x	x	x

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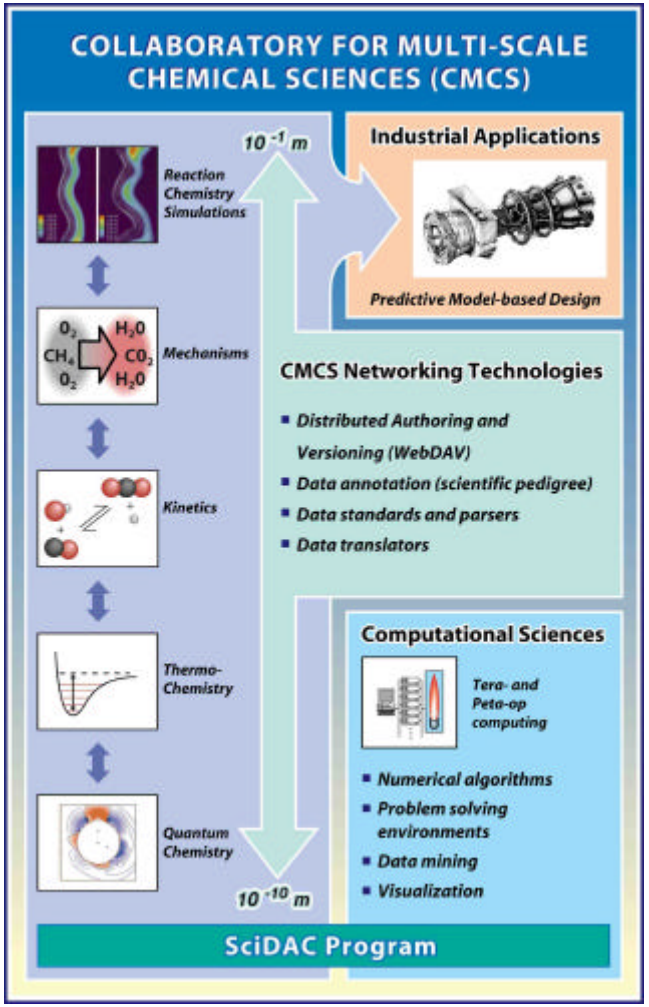
Collaboratory for Multi-scale Chemical Sciences (CMCS)



- A collaboration of eight national labs and universities
- Objectives
  - Architect and build an adaptive informatics infrastructure enabling multi-scale science
    - XML Data/metadata services
    - Chemical Sciences Portal
  - Pilot project within combustion community
    - Rapid exchange of multi-scale data/pedigree
    - Integrate Chemical Science applications
  - Demonstrate the power of adaptive infra-structure as CMCS evolves, and to new areas
  - Gain adoption/continued support by science community participation
  - Document success & continuation path

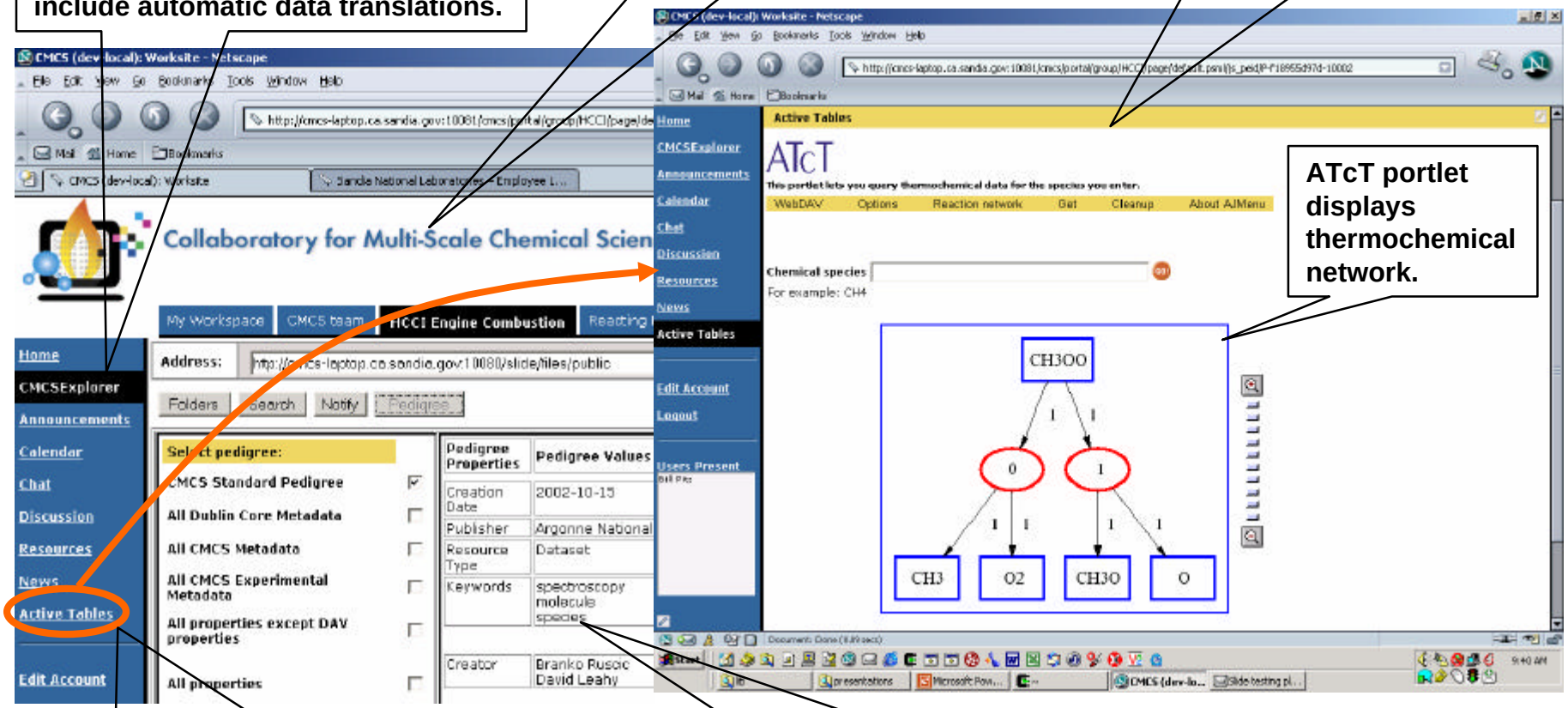
MICS Mathematical, Information, and Computational Sciences · Sandia National Laboratories · Pacific Northwest National Laboratory (Operated by Battelle for the U.S. Department of Energy) · Argonne National Laboratory · Los Alamos National Laboratory · NIST National Institute of Standards and Technology · MIT Massachusetts Institute of Technology · Berkeley University of California · U.S. Department of Energy National Collaboratories

CMCS Prototype Demonstrates Portal, Data Pedigree, Application Integration

CMCS Explorer Portlet provides rich interface to multi-scale data/metadata and services that include automatic data translations.

CMCS Portal environment, a CHEF Jetspeed collaboration

Thermochemical Active Tables (ATcT) and webservice a CoG Kit collaboration.



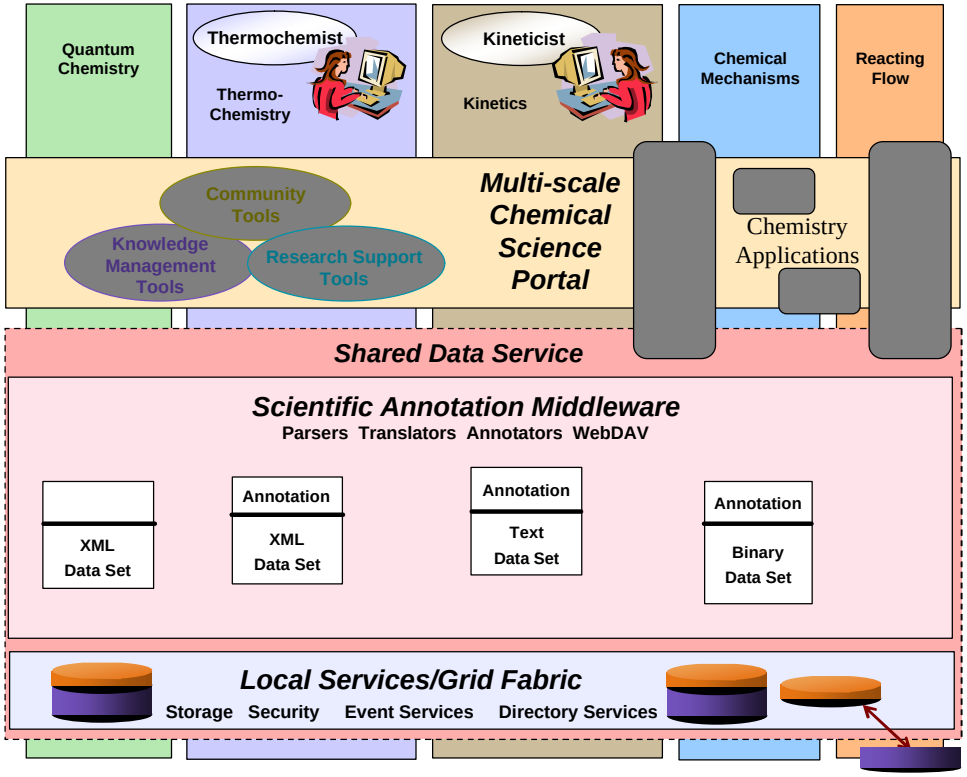
ATcT portlet displays thermochemical network.

ATcT Web service accessed from portlet in the HCCI Project Team workspace in the CMCS Portal

Pedigree of data viewed from CMCS Explorer with links and annotation enables 'Pedigree Browsing'.

CMCS Tools and Technologies

- CMCS Data/Metadata services
  - SAM translation, annotation
  - WebDAV implementation
  - Notification (JMS, NED)
  - Search
  - Pedigree browsing
  - Core XML schema
- Chemical Science Portal
  - Jetspeed (CHEF)
  - Explorer and application portlets
  - Community services
- Application Integration
  - Webservices
  - WebDAV API
  - Multi-scale data including NIST access



A diagram representing the major conceptual elements of the CMCS Informatics Infrastructure.

Interactions-Collaborations-Relationships

	National Fusion Collab.	Particle Physics Data Grid	DOE Science Grid	Earth System Grid	Collab for Multiscale Chemical Science
Intra-discipline	*Yes*	*Yes*	*Yes (inter-discipline)*	*Yes*	*Yes*
Intra-SciDAC projects	*Goal 1* *Goal 2* *Goal 3*	*Goal 2* *Goal 3*	*Goal 2* *Goal 3*	*Goal 1* *Goal 2* *Goal 3*	*Goal 1* *Goal 3*
Base projects	*Middleware and services*	*Middleware and sevices*	*Middleware and services* *Additional applications*	*Middleware and services*	*Middleware and services*
Interagency		*EU* *NSF (Trillium)*	*EU*	*UK* *NSF* *NASA*	

The Earth System Grid

http://www.earthsystemgrid.org

- *Enabling the simulation and data management team in organizing and managing terascale data*
- *Enabling the research community in analyzing and visualizing results*
- *Enabling broad multidisciplinary communities to easily discover and access simulation results*

PARTICIPANTS

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