National Science Foundation

Planning the SCEC Pathways: Pegasus at work on the Grid

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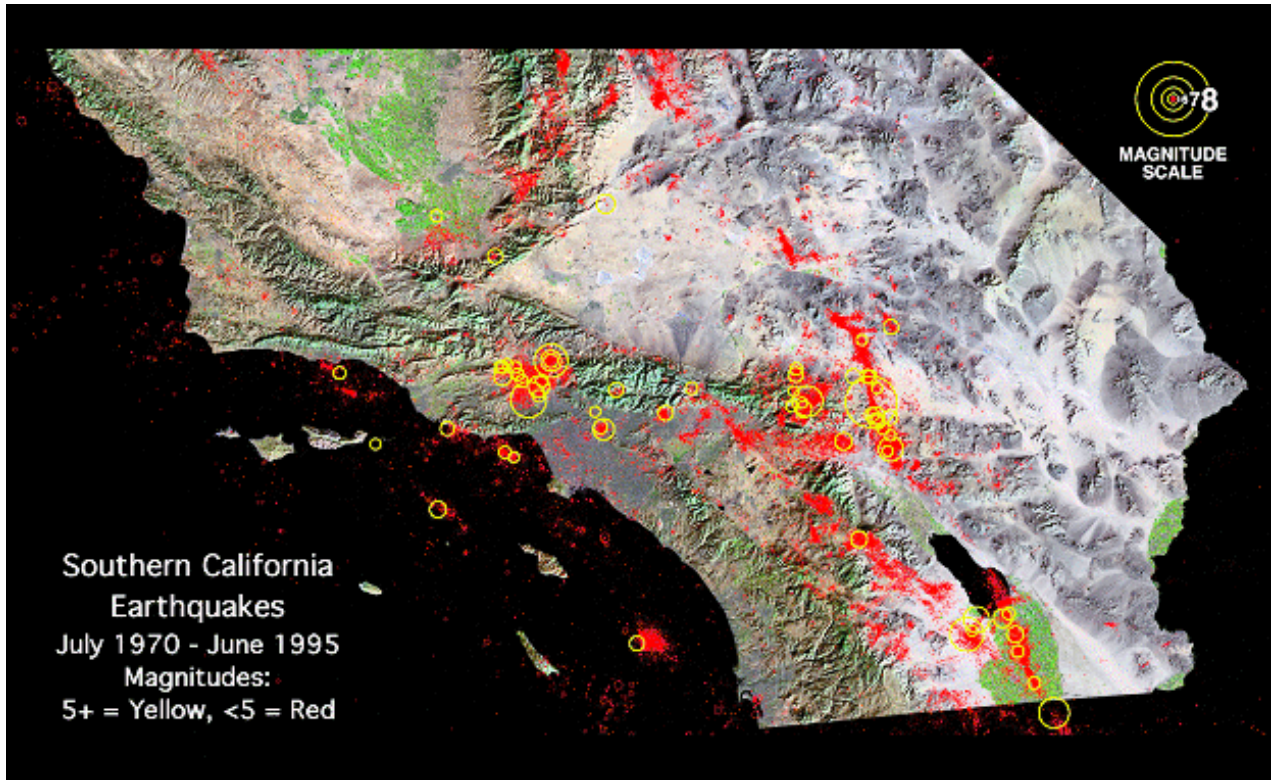
Planning the SCEC Pathways: Pegasus at work on the Grid

- Introduction to SCEC and SCEC/CME
- SCEC/CME System Challenges
- Initial SCEC/CME Workflow Approach
- Revised SCEC/CME Workflow Using NMI and Pegasus Tools
- SCEC/CME Workflow Innovations
- SCEC/CME Future Directions

Introduction to SCEC and SCEC/CME

Southern California: a Natural Laboratory for Earthquake Science

- Tectonic diversity
- Complex fault network
- High seismic activity
- Excellent geologic exposure
- Rich seismic and GPS data sources and catalogs
- Large urban population with densely built environment ⇒ high risk
- Well established scientific and technical community



- Extensive research program coordinated by Southern California Earthquake Center (SCEC) under NSF and USGS sponsorship

SCEC

an NSF+USGS center

Southern California Earthquake Center

Core Institutions

California Institute of Technology
Columbia University
Harvard University
Massachusetts Institute of Technology
San Diego State University
Stanford University
U.S. Geological Survey (3 offices)
University of California, Los Angeles
University of California, San Diego
University of California, Santa Barbara
University of Nevada, Reno
University of Southern California (lead)

- Consortium of 14 core institutions and 26 other participating organizations, founded as an NSF STC in 1991, and re-funded in 2001 for 5 additional years.
- Co-funded by NSF and USGS under the National Earthquake Hazards Reduction Program (NEHRP)
- Mission:
  - Gather all kinds of data on earthquakes in Southern California
  - Integrate information into a comprehensive, physics-based understanding of earthquake phenomena
  - Communicate understanding to end-users and the general public to increase earthquake awareness, reduce economic losses, and save lives

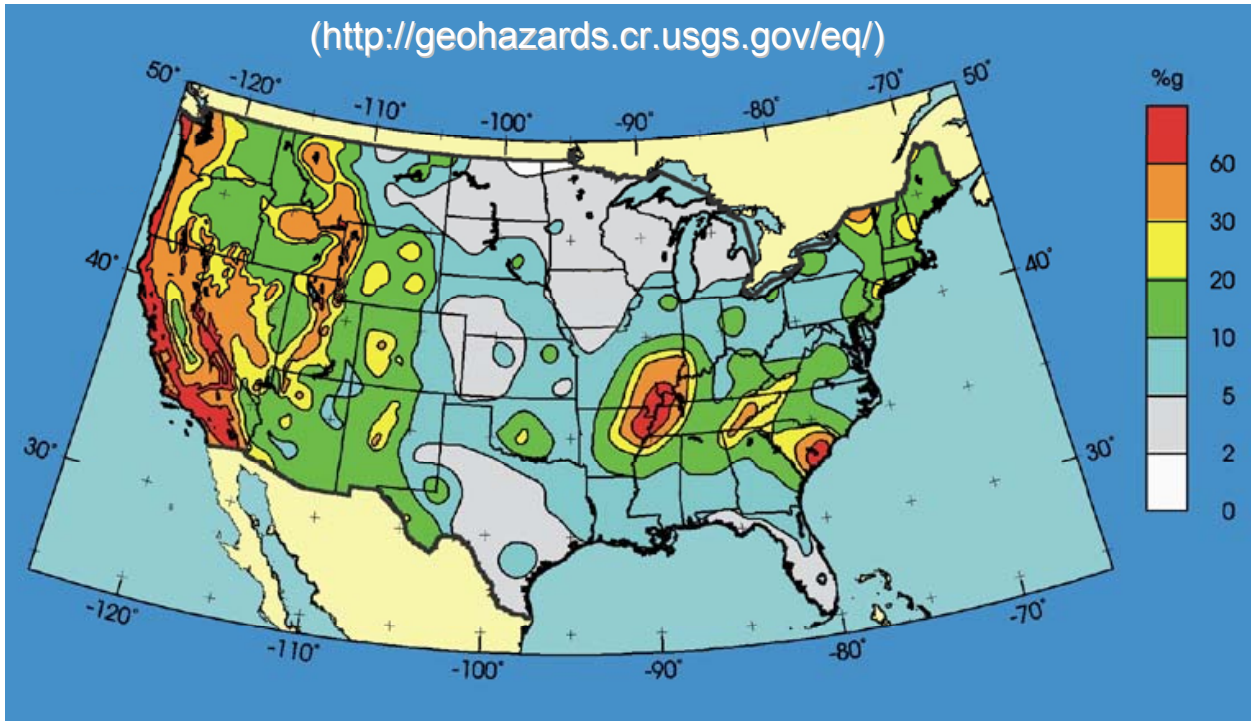
www.scec.org

Seismic Hazard Analysis as a System-Level Earthquake Research Problem

Definition: Specification of the maximum intensity of shaking expected at a site during a fixed time interval

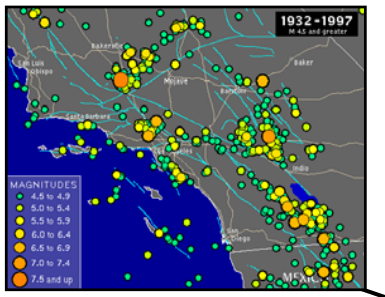
Example: National seismic hazard maps

- Intensity measure: peak ground acceleration (PGA)
- Interval: 50 years
- Probability of exceedance: 2%

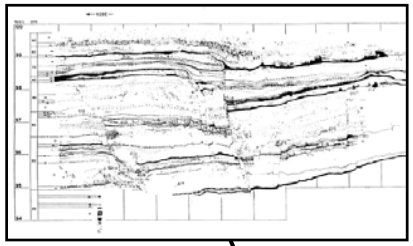


Seismic Hazard Analysis as a System-Level Problem

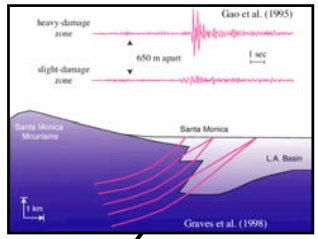
Seismicity (ANSS)



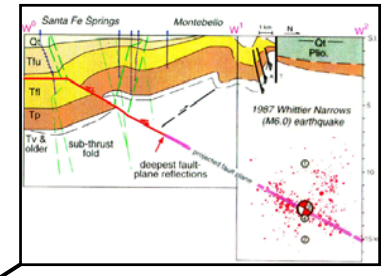
Paleoseismology



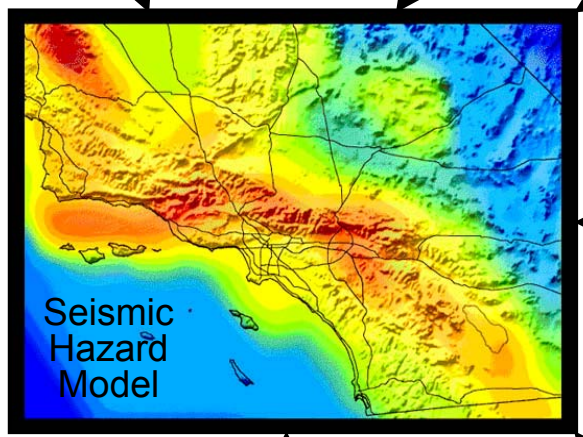
Local site effects

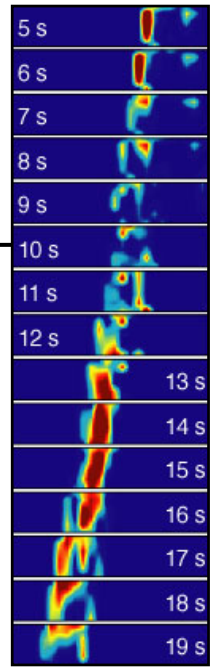


Geologic structure (USArray)

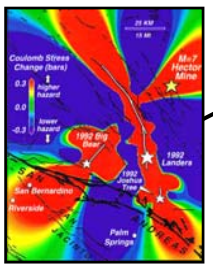


Faults (USArray)

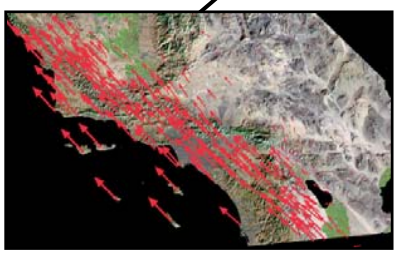




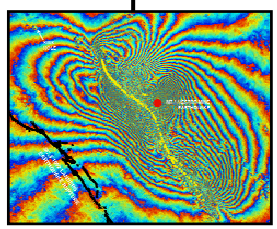
Rupture dynamics (SAFOD, ANSS, & USArray)



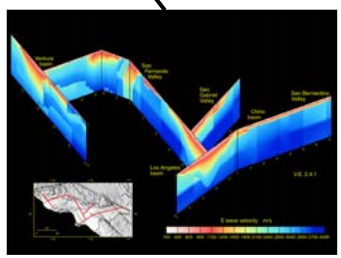
Stress transfer (InSAR, PBO, & SAFOD)



Crustal motion (PBO)

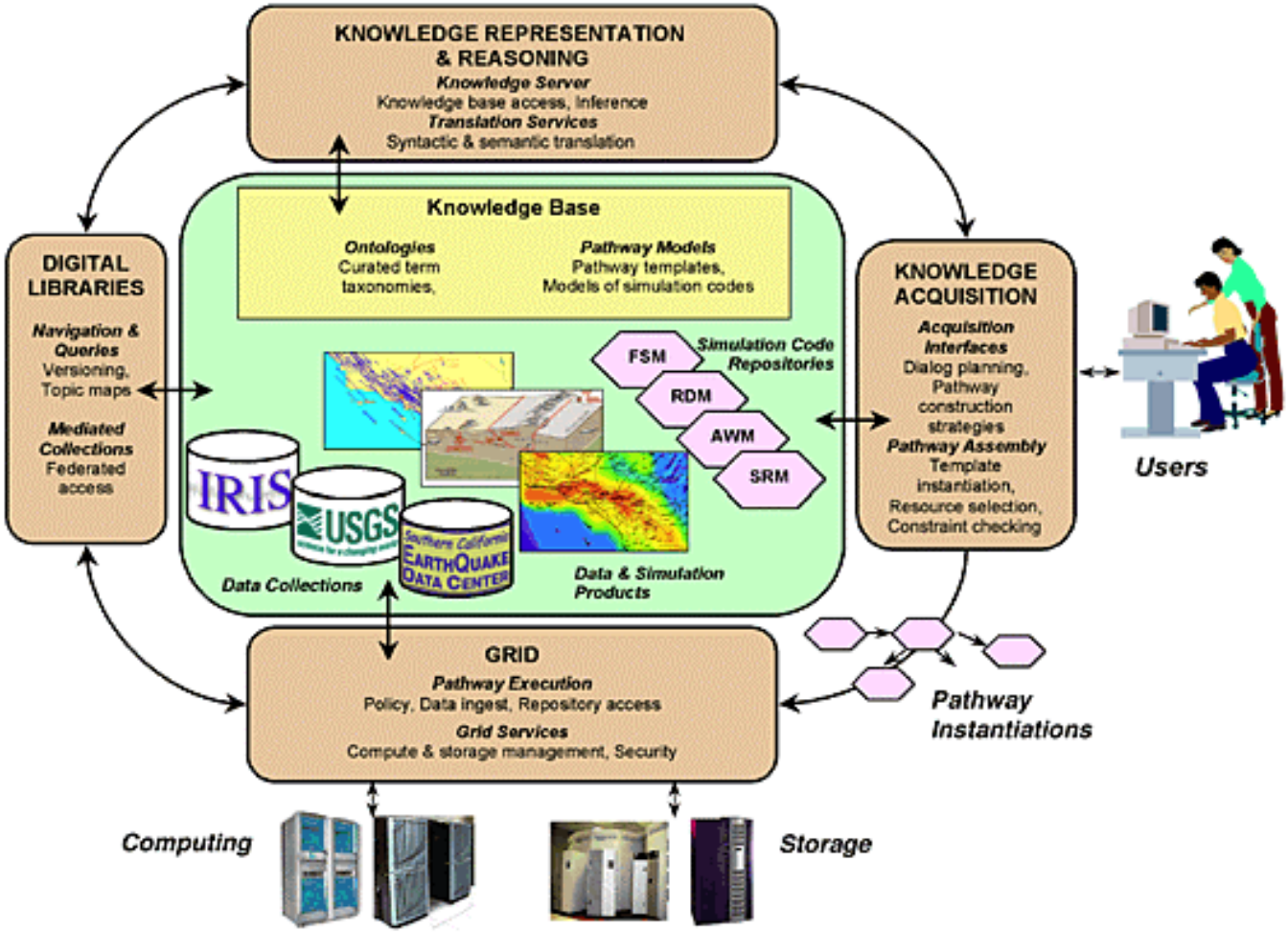


Crustal deformation (InSAR)



Seismic velocity structure (USArray)

SCEC Community Modeling Environment
A collaboratory for system-level earthquake science



SCEC/CME System Challenges

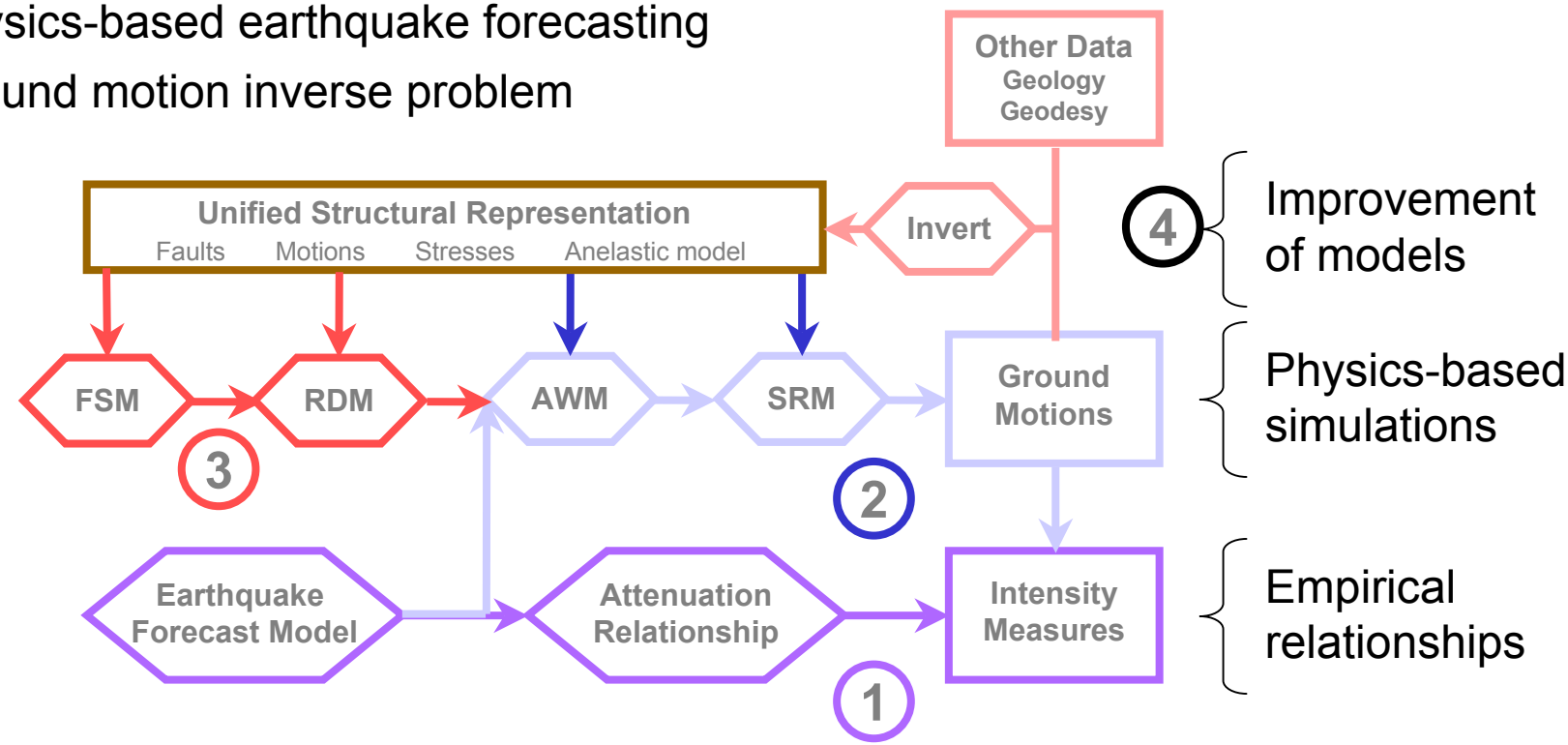
SCEC/CME System Requirements

Develop an information infrastructure for system-level earthquake science to create a *SCEC collaboratory* that can:

- Capture and manipulate the knowledge that will permit a variety of users with different levels of sophistication to configure complex computational pathways.
- Enable execution of physics-based simulations and data inversions that incorporate advances in fault-system dynamics, rupture dynamics, wave propagation, and non-linear site response.
- Manage large, distributed collections of simulation results, as well as the large sets of geologic, geodetic and seismologic data required to validate the simulations and constrain parameter values.
- Provide access to SHA products and methodologies to end-users outside of the SCEC community, including practicing engineers, emergency managers, decision-makers, and the general public.

SCEC Computational Pathways

1. Standardized Seismic Hazard Analysis
2. Ground motion simulation
3. Physics-based earthquake forecasting
4. Ground motion inverse problem



FSM = Fault System Model

RDM = Rupture Dynamics Model

AWP = Anelastic Wave Propagation

SRM = Site Response Model

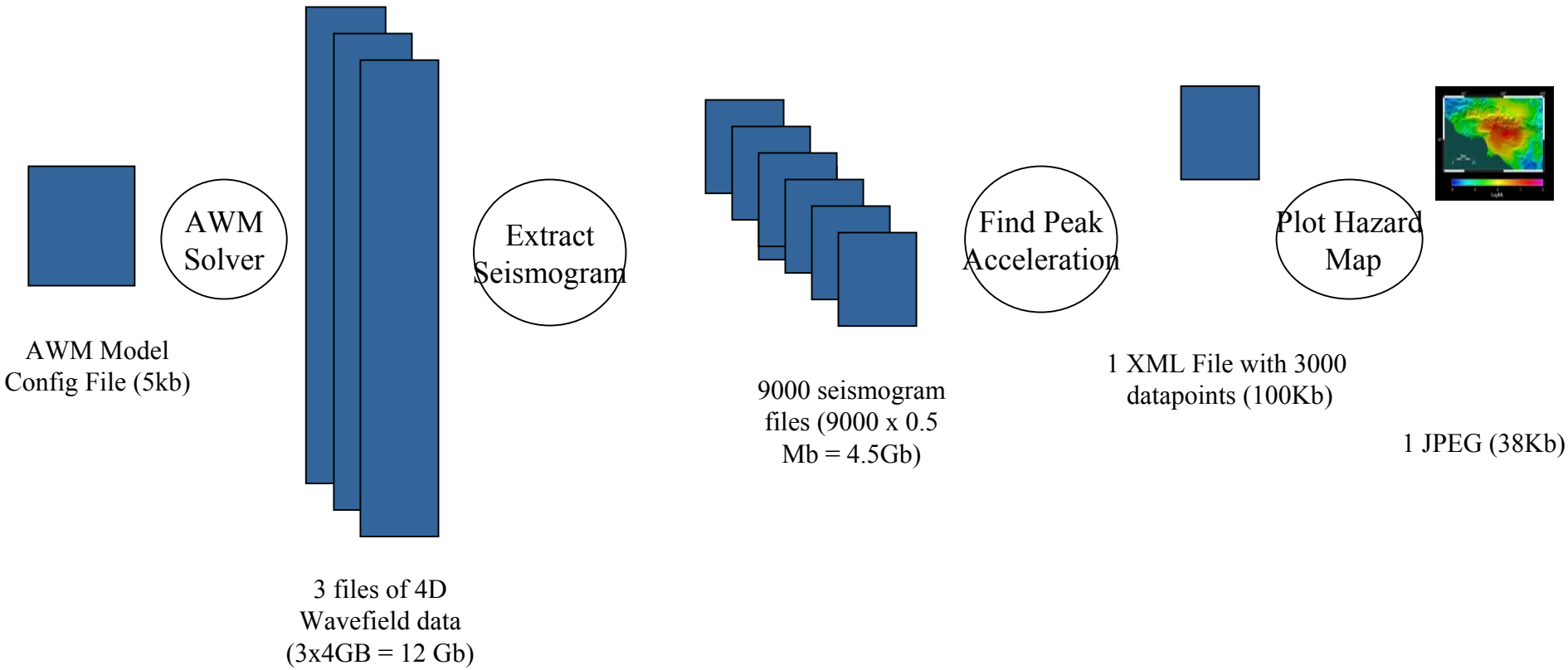
SCEC/CME System IT Challenges

- Scientific workflows must be created from heterogeneous library of geophysical programs and utilities.
- Workflow authoring system must support wide range of workflow authors, very naïve to very sophisticated.
- Data Management issues include scale (size and number) and difficulty of describing simulation data (metadata).
- Simulation data products must be distributed to users, well described, long lived, accessible, and citable.

Initial SCEC/CME Workflow Approach

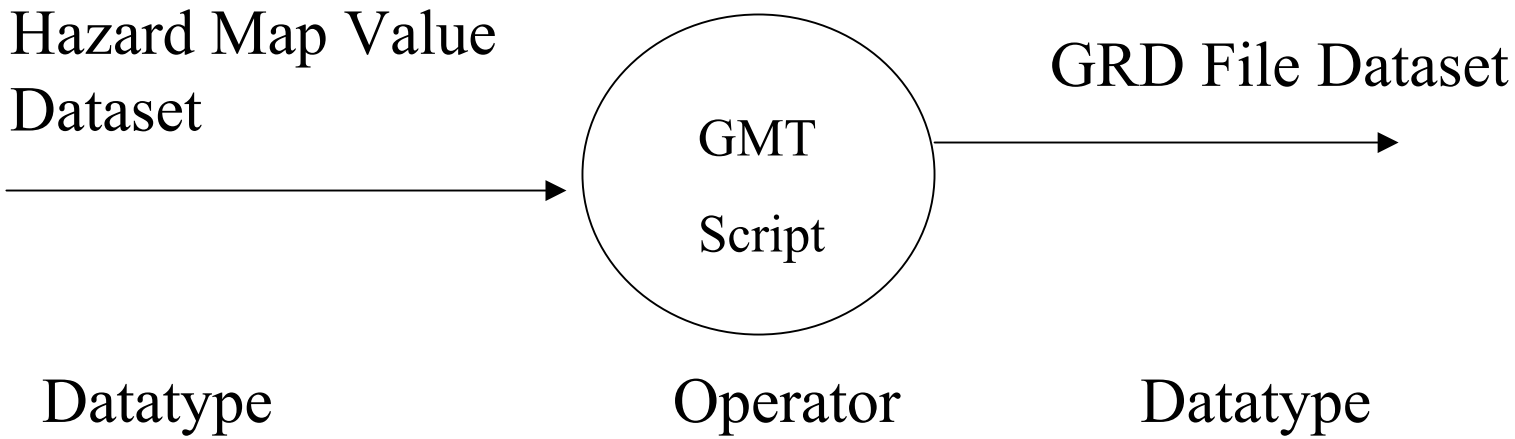
SCEC/CME Workflow Example

Example of SCEC/CME Computational Pathway:



Computational Step Concept

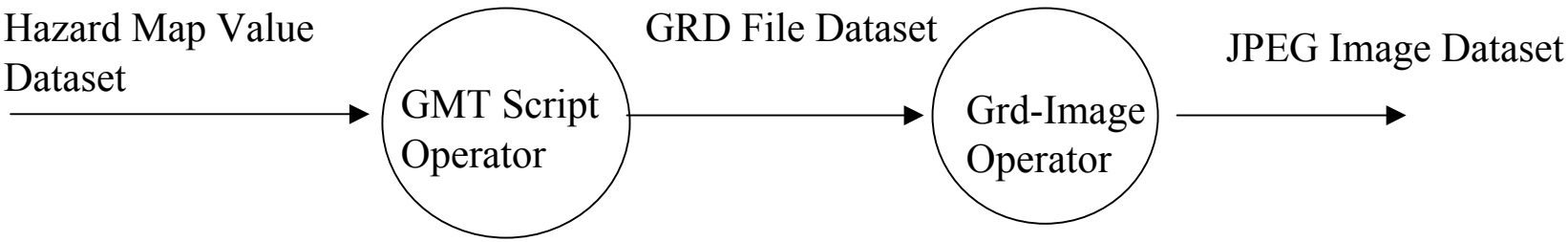
Computational Step modeled like a dataflow diagram:
Datatype inputs, transforming program, datatypes outputs



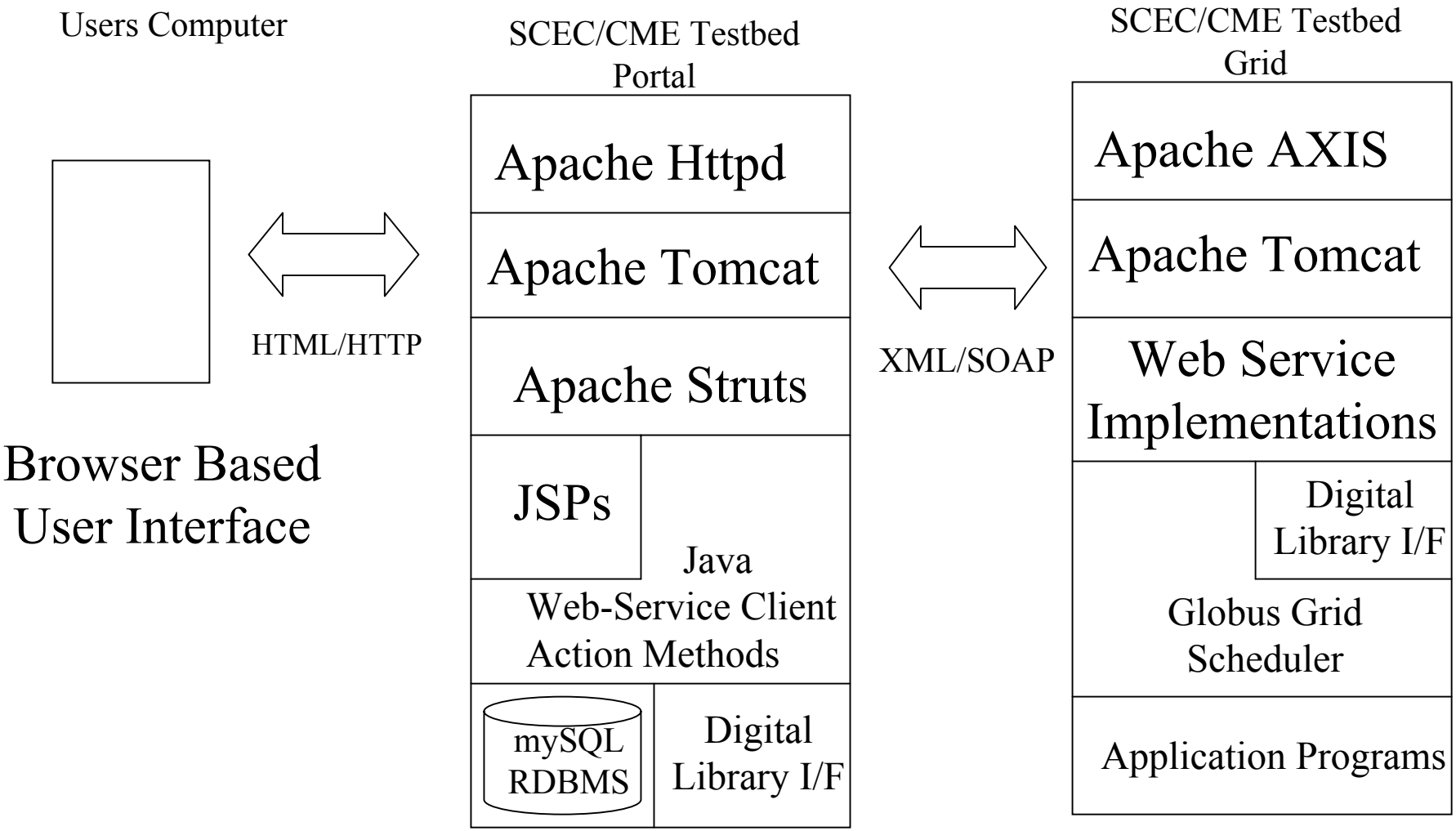
Data Type – Data formatted for use by a computational programs.
Dataset – an instance of a datatype accessible with a URL.
Operator – Inputs datatypes input and outputs datatype

Computational Pathway Concept

A Computational Pathway is series of Computational steps connected together



SCEC/CME Application Architecture



Issues with Initial SCEC/CME Workflow Implementation

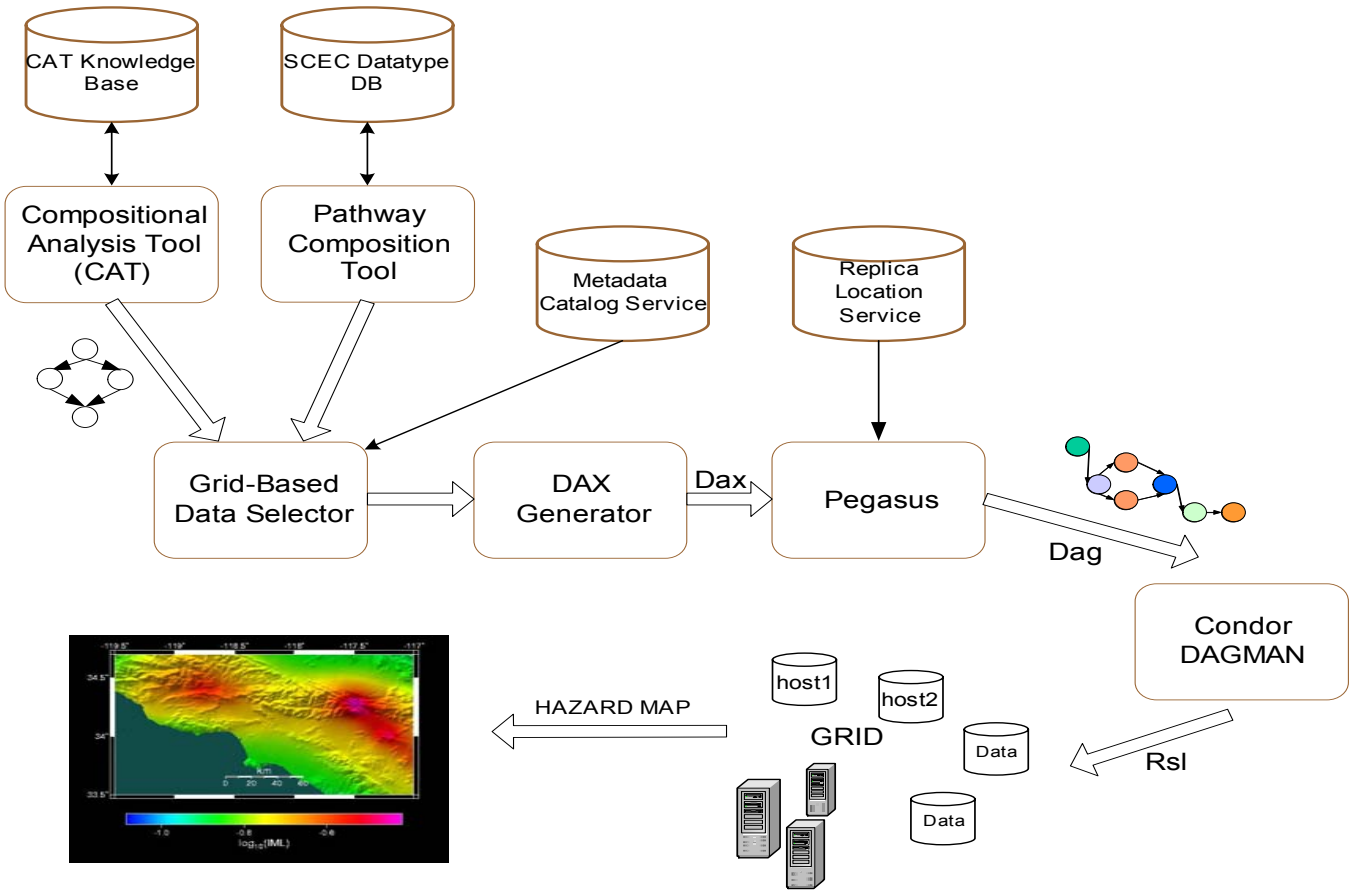
- Only Web Services were supported as predicates (transformations).
- Each Pathway was run using a different workflow application program.
- Computing resources were directly specified in job submission application programs.
- Non-secure web portal.

Revised SCEC/CME Workflow Using NMI and Pegasus Tools

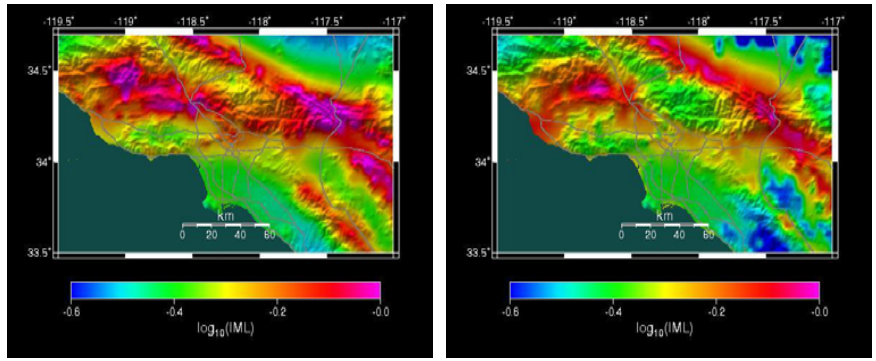
Revised SCEC/CME Workflow Approach

- NMI Portal tools (CHEF) and Proxy management tools (MyProxy) used for secure grid-computing.
- Grid-based computational infrastructure using Globus, Chimera, Pegasus.
- System supports high throughput, high performance, and storage oriented SCEC/CME Workflows
- Replica Location Service (RLS), and Metadata Catalog System (MCS) tools for file management.
- SCEC Data Discovery system based on Metadata Catalog System Metadata search capabilities.

Elements of SCEC/CME Workflow System



Probabilistic Hazard Map Calculations



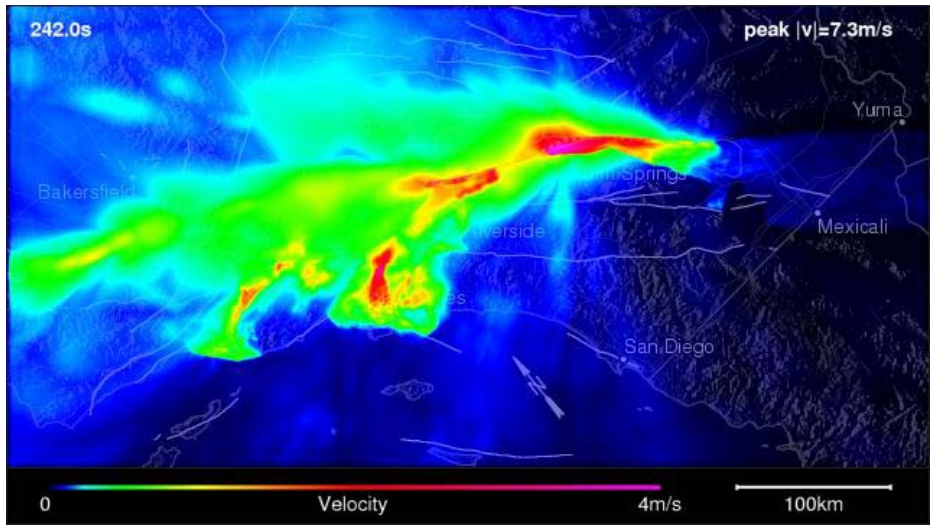
Software Description:

- Java code
- Many very similar calculations are performed for a large number of points (e.g. 10,000 points/map).
- The results of one calculation do not effect the results for other points.
- An output file is created for each point.

Computing Approach:

- This high throughput application is well suited for submission to a Condor Pool.
- This workflow uses a 100+ node Condor Pool at USC.

Anelastic Waveform Modeling



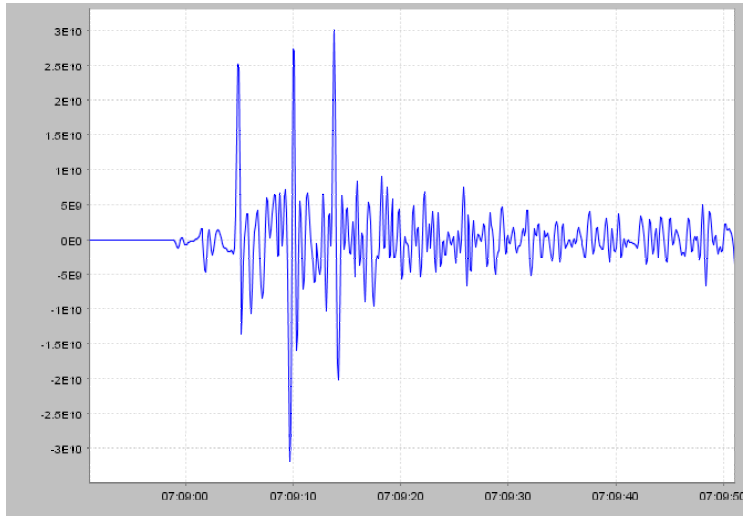
Software Description:

- Fortran-based MPI code
- These programs are Finite Difference and Finite Element wave propagation simulations.
- These simulations produce very large 4D output files (GB – TB)

Computing Approach:

- Code is run on USC High Performance Linux Cluster and Teragrid sites.
- This workflow uses Pegasus to help link preprocessing, simulation, and post-processing.

Calculation of Synthetic Waveforms using Green's Tensors



Software Description:

- Mixed Fortran and C code.
- A 27 TB dataset, created by running Pathway 2 simulations is used to generate synthetic seismograms.
- Synthetic seismograms are calculated for earthquakes specified in the Caltech Focal Mechanism Catalog.

Computing Approach:

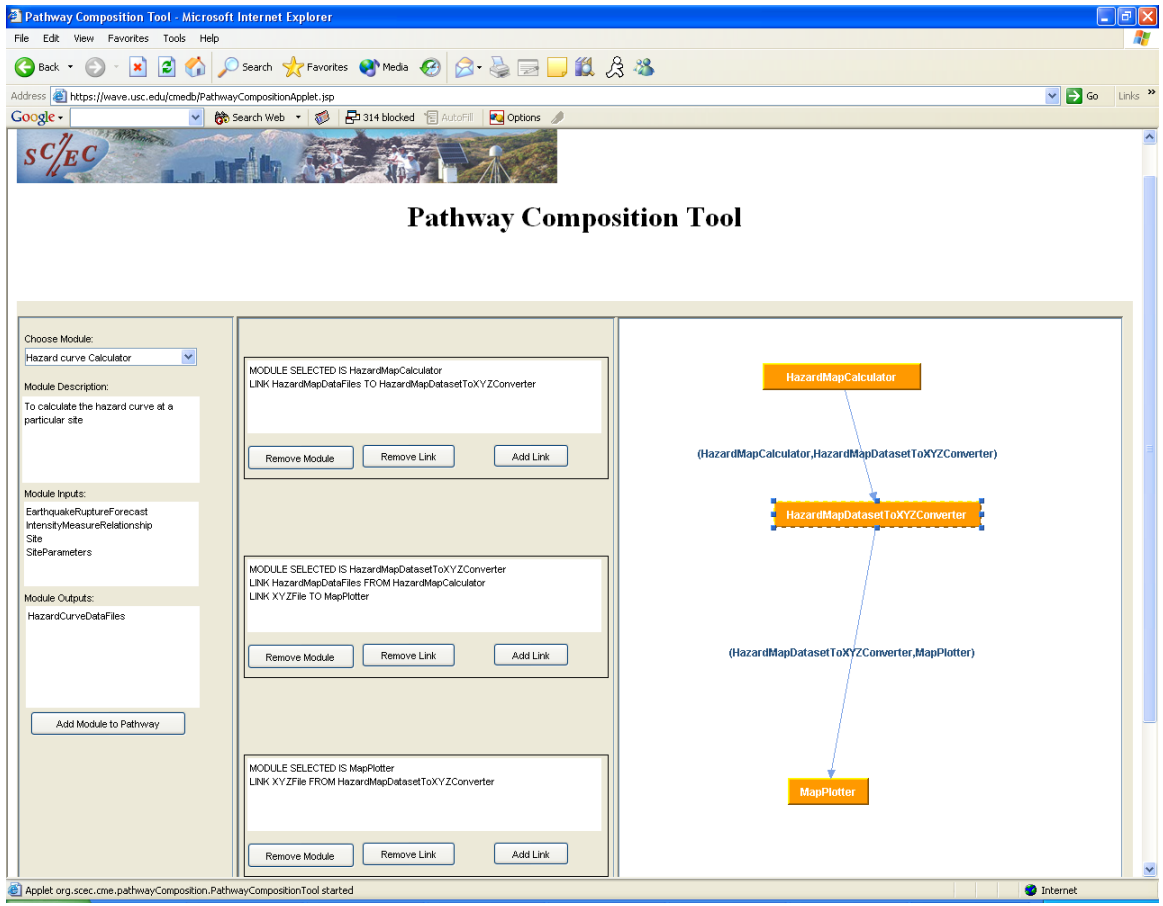
- The SCEC application program performs partial file reads on files in an SRB managed file system at SDSC so there is no need to copy the entire file from SDSC to USC.

SCEC/CME Workflow Composition Process

- CAT (Compositional Analysis Tool) an ontology based workflow composition tool or PCT (Pathway Composition Tool) generate the application workflows template (using ontologies and data types).
- The Grid-Based Input Data selection component allows the user to select the input data necessary to populate the workflow template. The result in an abstract workflow that refers only to the logical application components and logical input data required for a pathway.
- The DAX generator translates the abstract workflow to a corresponding XML description (DAX).
- Pegasus takes in the DAX and generates the concrete workflow.
- Concrete Workflow identifies the resources that are used to run on the grid and refers to the physical locations of input data.
- Condor DAGMAN submits the workflow on the grid and tracks the execution of the workflow.
- Successful execution generates the final hazard map for the region.

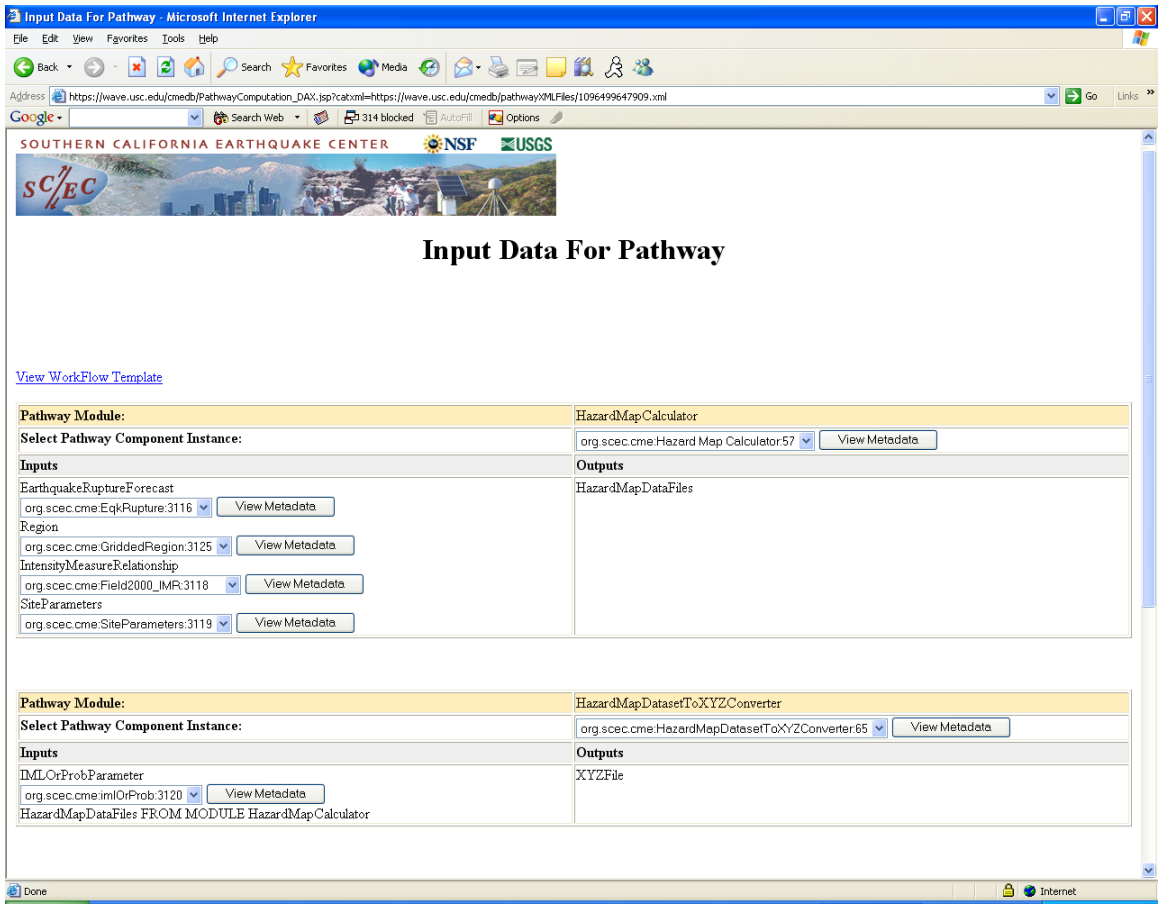
Compose Workflow Display

Choose transformations and connect them:



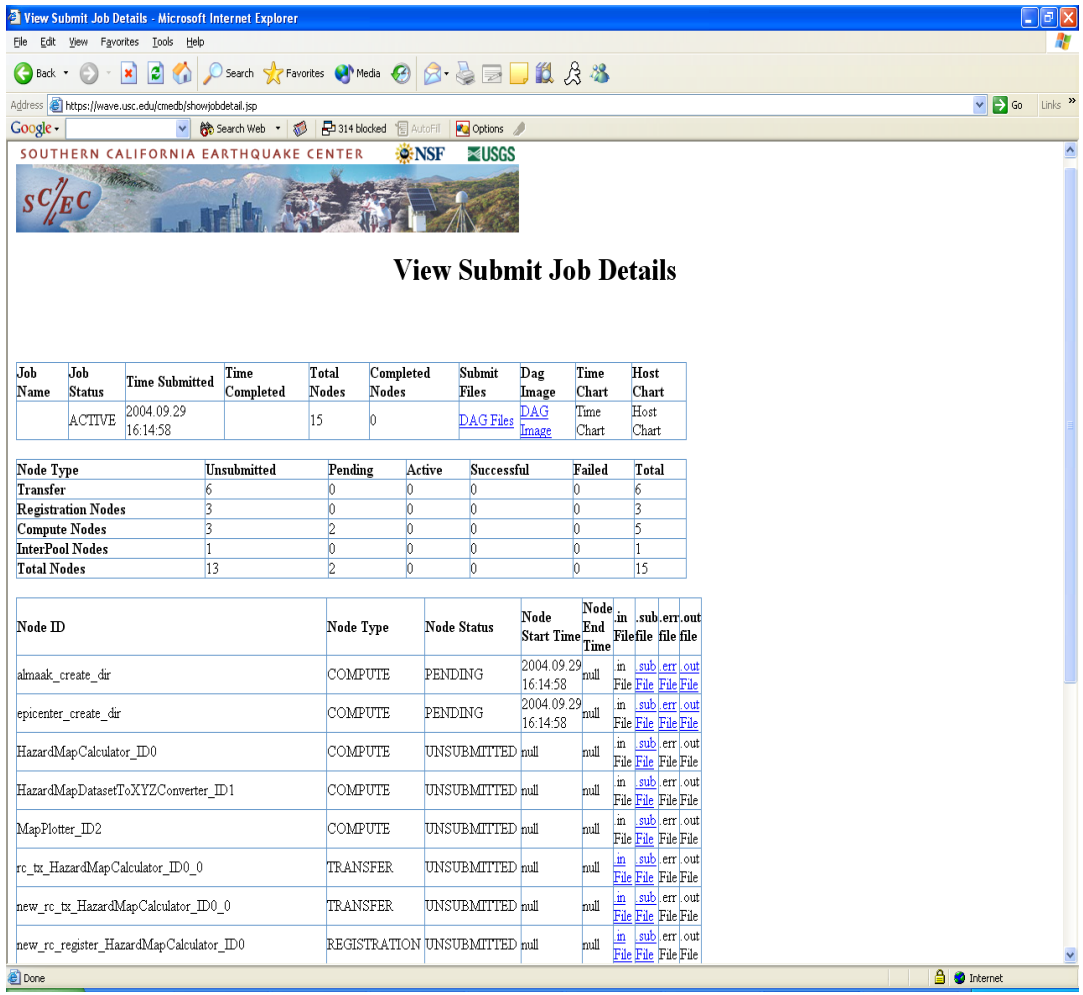
Select the specific files for input

Users views list of files that are registered into RLS. Metadata in MCS can also be viewed for each entry.



SCEC/CME Workflow Monitoring Display

- Uses Pegasus' portal solution for displaying job status
- Displays performance and status information about individual workflow tasks and entire workflows



Job Name	Job Status	Time Submitted	Time Completed	Total Nodes	Completed Nodes	Submit Files	Dag Image	Time Chart	Host Chart
	ACTIVE	2004.09.29 16:14:58		15	0	DAG Files	DAG Image	Time Chart	Host Chart

Node Type	Unsubmitted	Pending	Active	Successful	Failed	Total
Transfer	6	0	0	0	0	6
Registration Nodes	3	0	0	0	0	3
Compute Nodes	3	2	0	0	0	5
InterPool Nodes	1	0	0	0	0	1
Total Nodes	13	2	0	0	0	15

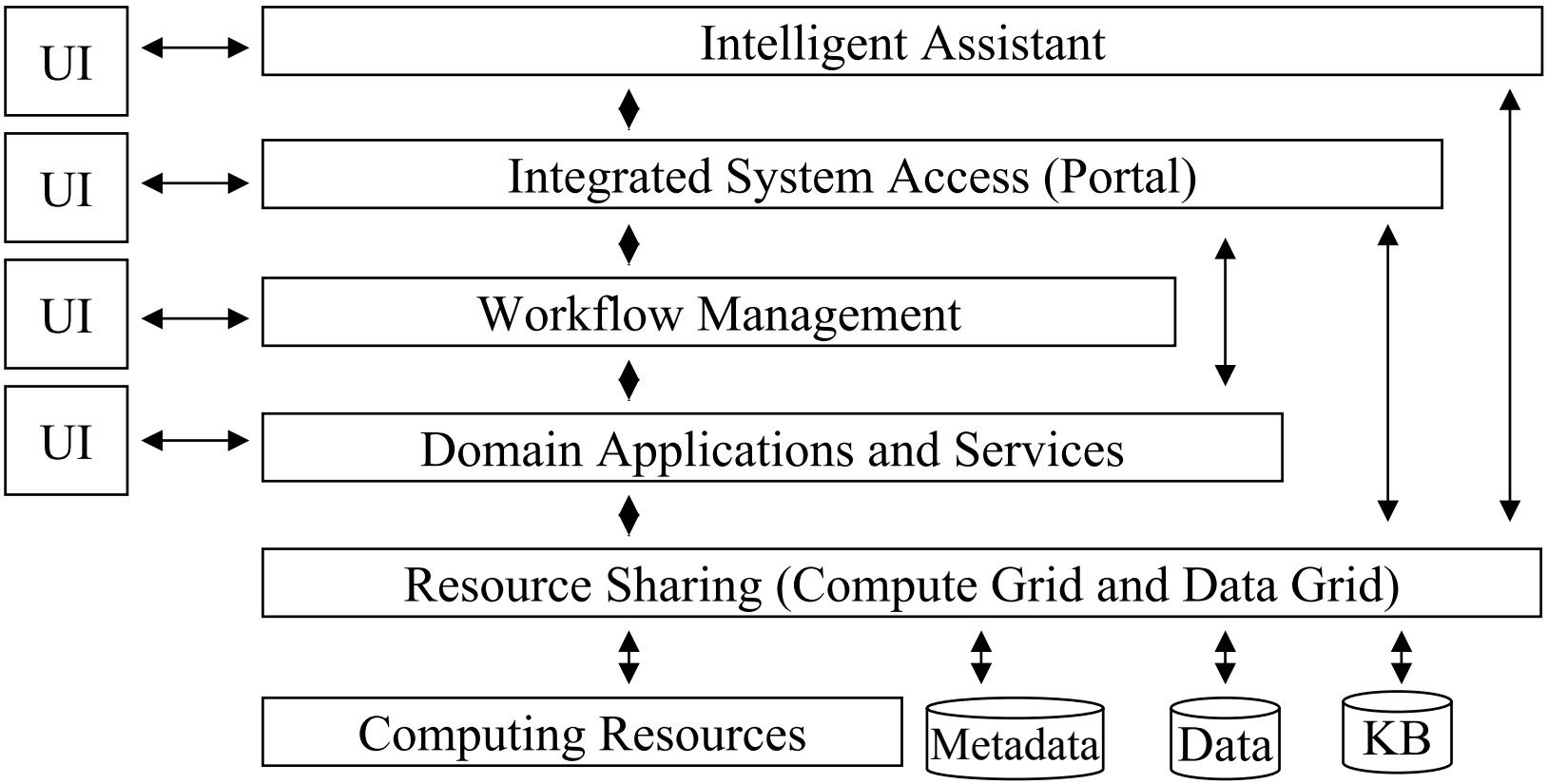
Node ID	Node Type	Node Status	Node Start Time	Node End Time	.in File	.sub file	.err file	.out file
almaak_create_dir	COMPUTE	PENDING	2004.09.29 16:14:58	null	.in File	.sub File	.err File	.out File
epicenter_create_dir	COMPUTE	PENDING	2004.09.29 16:14:58	null	.in File	.sub File	.err File	.out File
HazardMapCalculator_ID0	COMPUTE	UNSUBMITTED	null	null	.in File	.sub File	.err File	.out File
HazardMapDatasetToXYZConverter_ID1	COMPUTE	UNSUBMITTED	null	null	.in File	.sub File	.err File	.out File
MapPlotter_ID2	COMPUTE	UNSUBMITTED	null	null	.in File	.sub File	.err File	.out File
rc_tx_HazardMapCalculator_ID0_0	TRANSFER	UNSUBMITTED	null	null	.in File	.sub File	.err File	.out File
new_rc_tx_HazardMapCalculator_ID0_0	TRANSFER	UNSUBMITTED	null	null	.in File	.sub File	.err File	.out File
new_rc_register_HazardMapCalculator_ID0	REGISTRATION	UNSUBMITTED	null	null	.in File	.sub File	.err File	.out File

Benefits of Integrating SCEC Workflow with NMI Tools and Pegasus

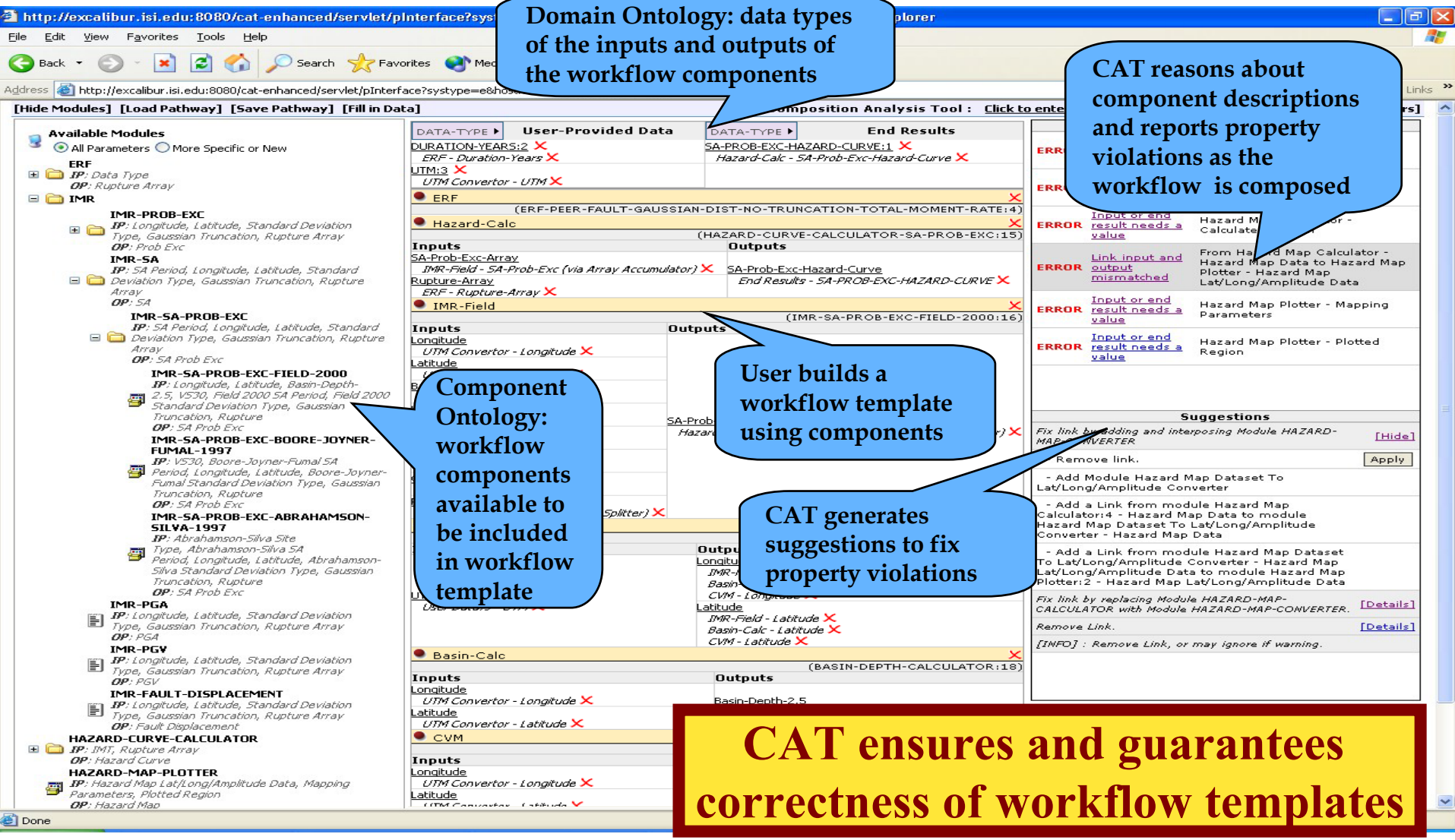
- Standardized secure job submission through portal using MyProxy.
- Grid-based connectivity with collaborators sites including USC,UCSB, PSC.
- Standardized Workflow construction using “workflow templates”.
- Optimized conversion of Condor DAG’s to RSL by Pegasus.
- Automatic data movements scripted by Pegasus.
- Integration with File and Metadata Management Tools (MCS and RLS).
- Automatic selection of computing resources from resource pool by Pegasus.
- Automatic parallelization of workflow by Pegasus in some case.
- Grid-based job monitoring tools using Pegasus.

SCEC/CME Workflow Innovations

SCEC/CME Layered Software Architecture



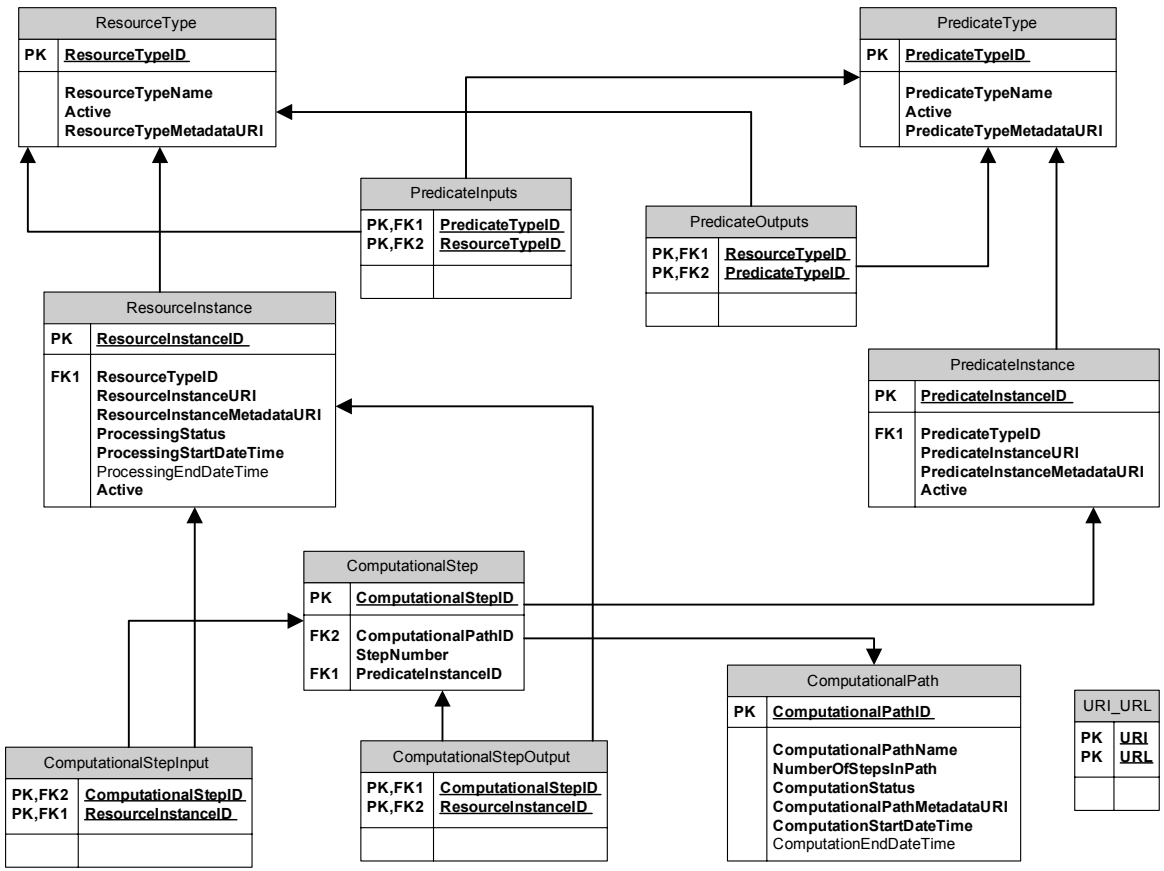
CAT: Intelligent Assistant for Workflow Composition



SCEC/CME Management of Pathways Using Data Types and Program Types

- SCEC/CME RDBMs contains lists of all known Datatypes and Operator types. (Note key concepts of Datatypes versus Datasets (Datasets are instances of data types that are accessible by a URL).
- SCEC/CME RDBMS contains information on what input and output datatypes are required by each Operator type.
- SCEC/CME RDBMS contains information about each dataset in the system.
- SCEC/CME RDBMCS contains information about metadata for each dataset in the system.
- SCEC/CME RDBMS information contains processing status information as computational steps are completed in a computational pathway calculation.

SCEC/CME RDBMS Schema

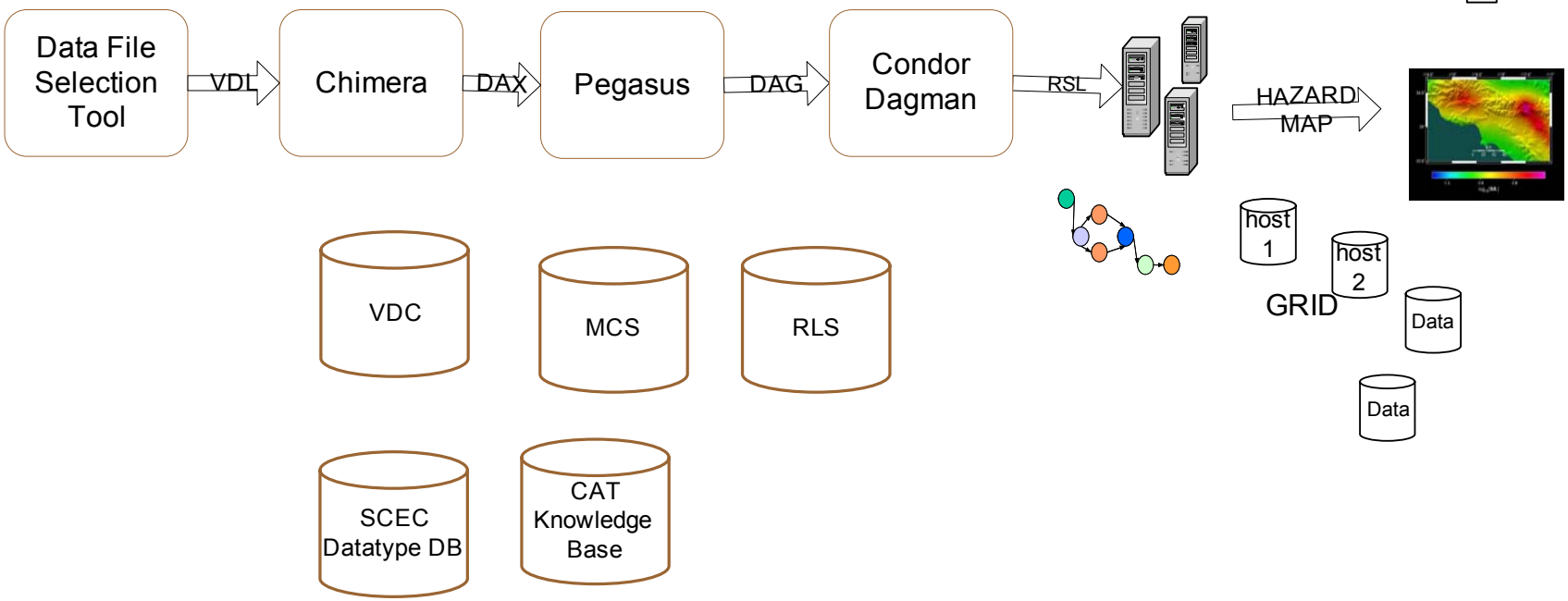


SCEC/CME Future Directions

SCEC/CME Creator to Consumer System

Intelligent Assistant Workflow Construction

Web-based, metadata-based, data discovery and distribution site.



Develop Complete Modeling Environment User Functionality

Capture Model Elements	**Find, Create, and Analyze Data**	**Construct and Execute Pathways**
Monitor Pathways And System SOH	**System and User Admin**	**Data Curation**

EXTERNAL USERS

Public Data Access

Public Utility Computing

National Science Foundation

Information about the relevant projects and software components

- SCEC/CME: www.scec.org/cme
- Pegasus: pegasus.isi.edu
- CAT: www.isi.edu/ikcap/cat/
- VDT: www.ivdgl.org
- Chimera: www.griphyn.org/chimera
- GriPhyN: www.griphyn.org
- Email: maechlin@usc.edu