

Planning the SCEC Pathways: Pegasus at work on the Grid

Philip Maechling, Vipin Gupta, Thomas H. Jordan
Southern California Earthquake Center

Ewa Deelman, Yolanda Gil, Sridhar Gullapalli, Carl Kesselman, Jihie Kim, John McGee, Gaurang Mehta, Gurmeet Singh, Marc Spraragen, Mei-Hui Su, Karan Vahi
USC Information Sciences Institute

Maureen Dougherty, Brian Mendenhall, Garrick Staples
USC High Performance Computing and Communications

Planning the SCEC Pathways: Pegasus at work on the Grid

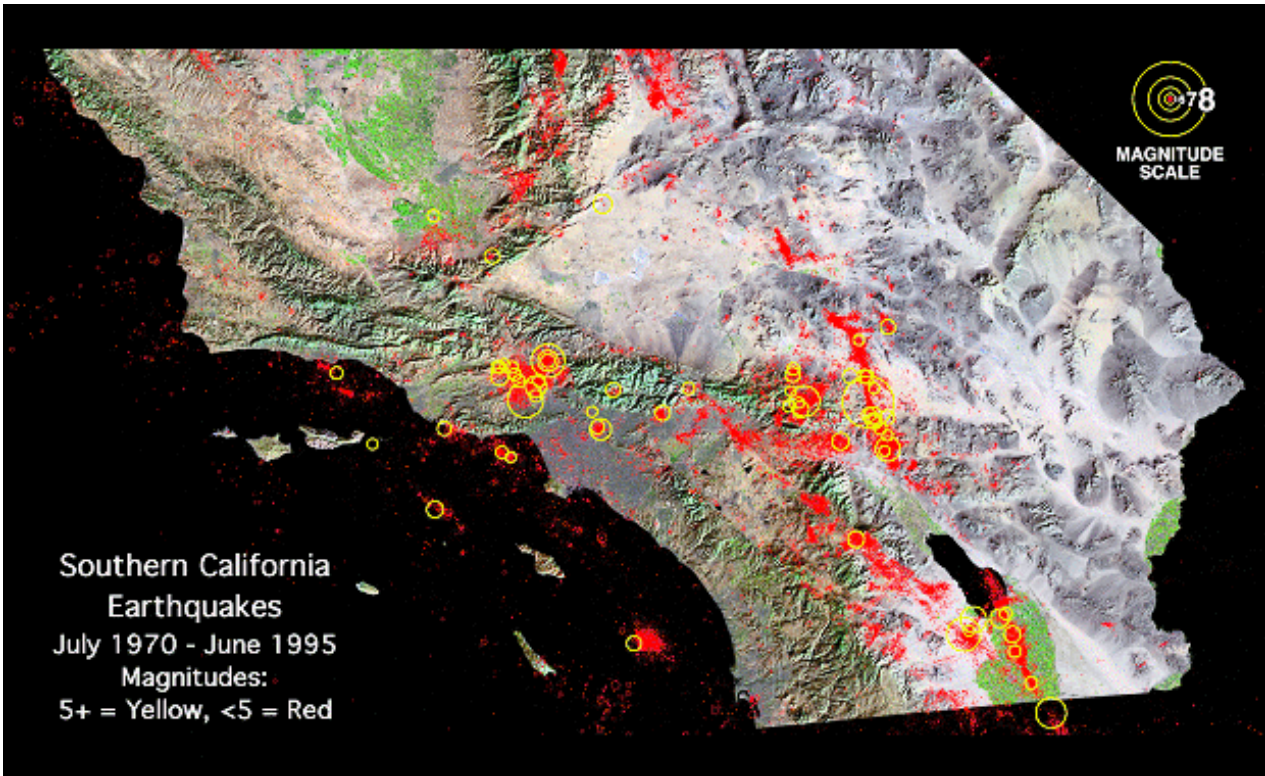
- Introduction to SCEC and SCEC/CME
- SCEC/CME System Challenges
- Initial SCEC/CME Workflow Approach
- Revised SCEC/CME Workflow Using NMI and Pegasus Tools
- SCEC/CME Workflow Innovations
- SCEC/CME Future Directions



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 \Rightarrow high risk
- Well established scientific and technical community
- Extensive research program coordinated by Southern California Earthquake Center (SCEC) under NSF and USGS sponsorship





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

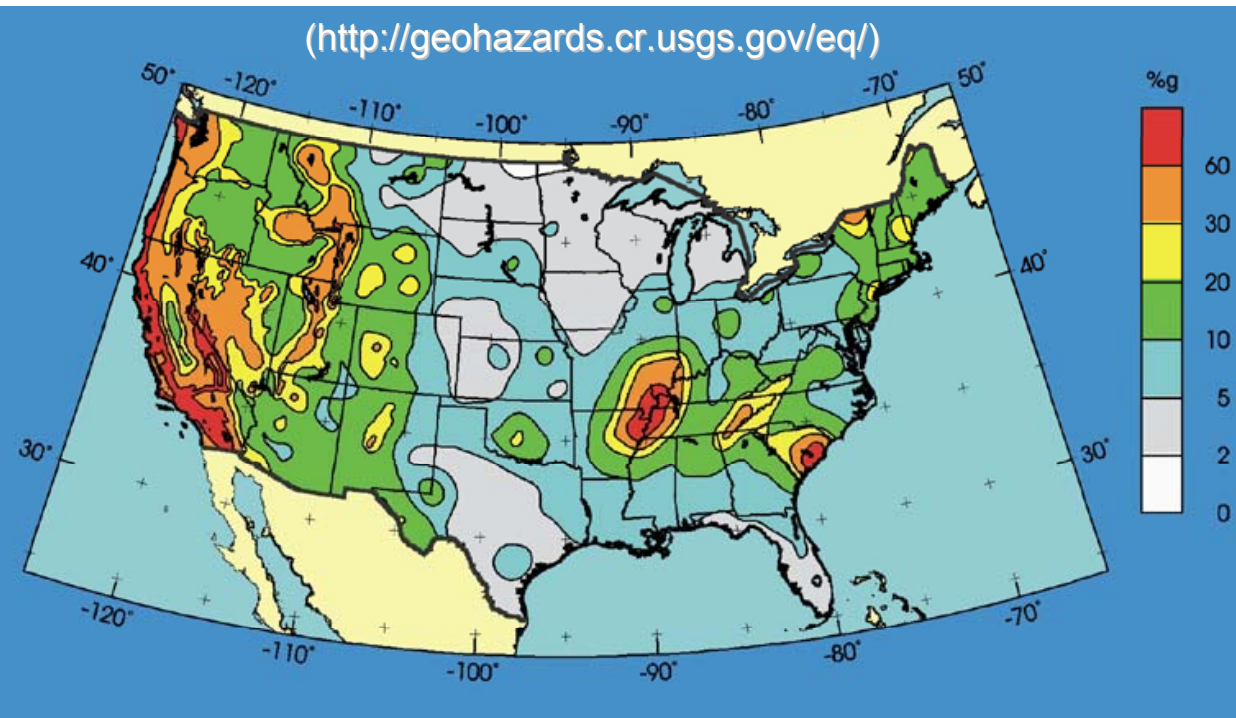


Seismic Hazard Analysis as a System-Level Earthquake Research Problem

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

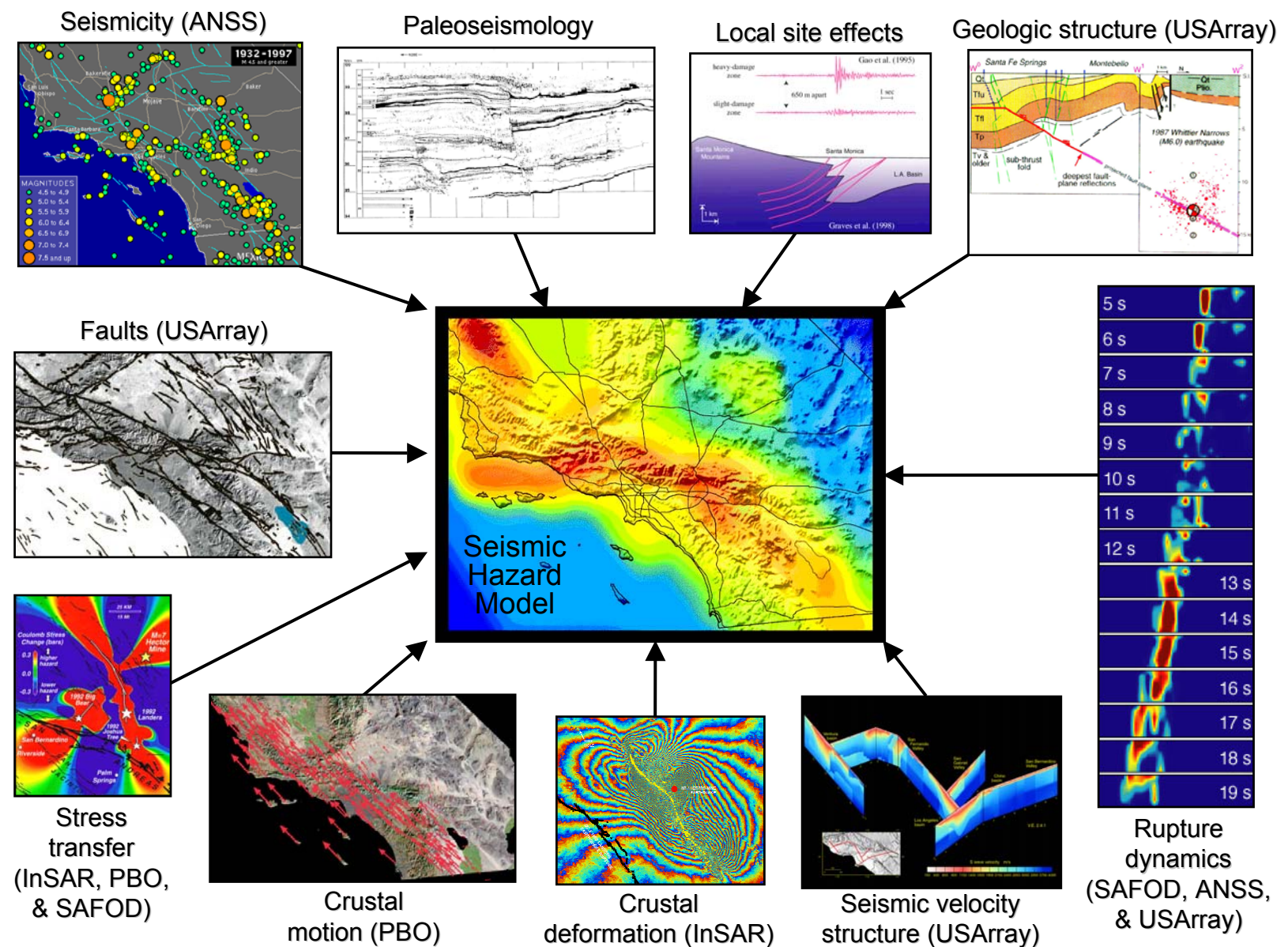
Example: National seismic hazard maps

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



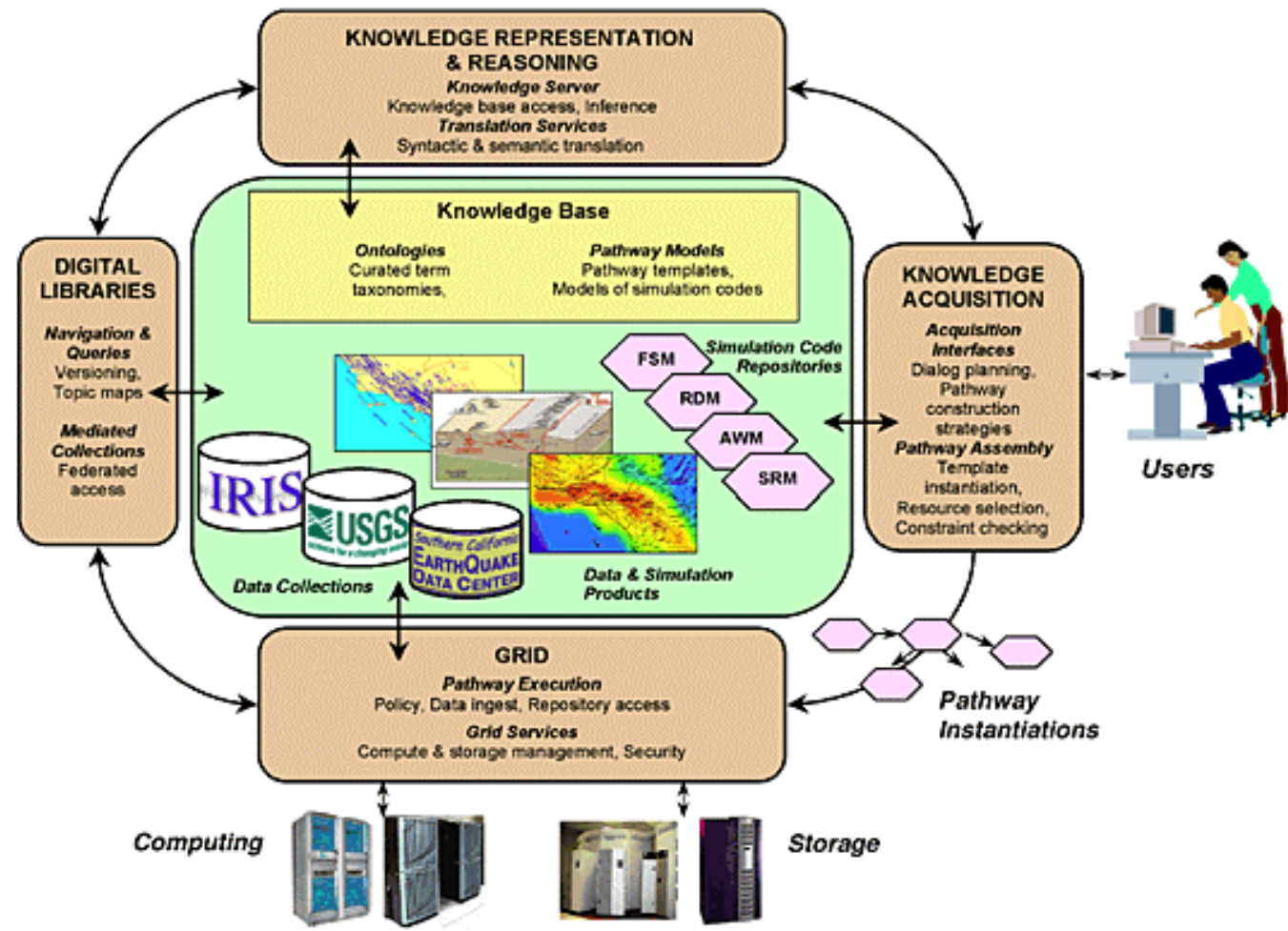


Seismic Hazard Analysis as a System-Level Problem



SCEC Community Modeling Environment

A collaboratory for system-level earthquake science





SCEC/CME System Challenges

SCEC/CME System Requirements

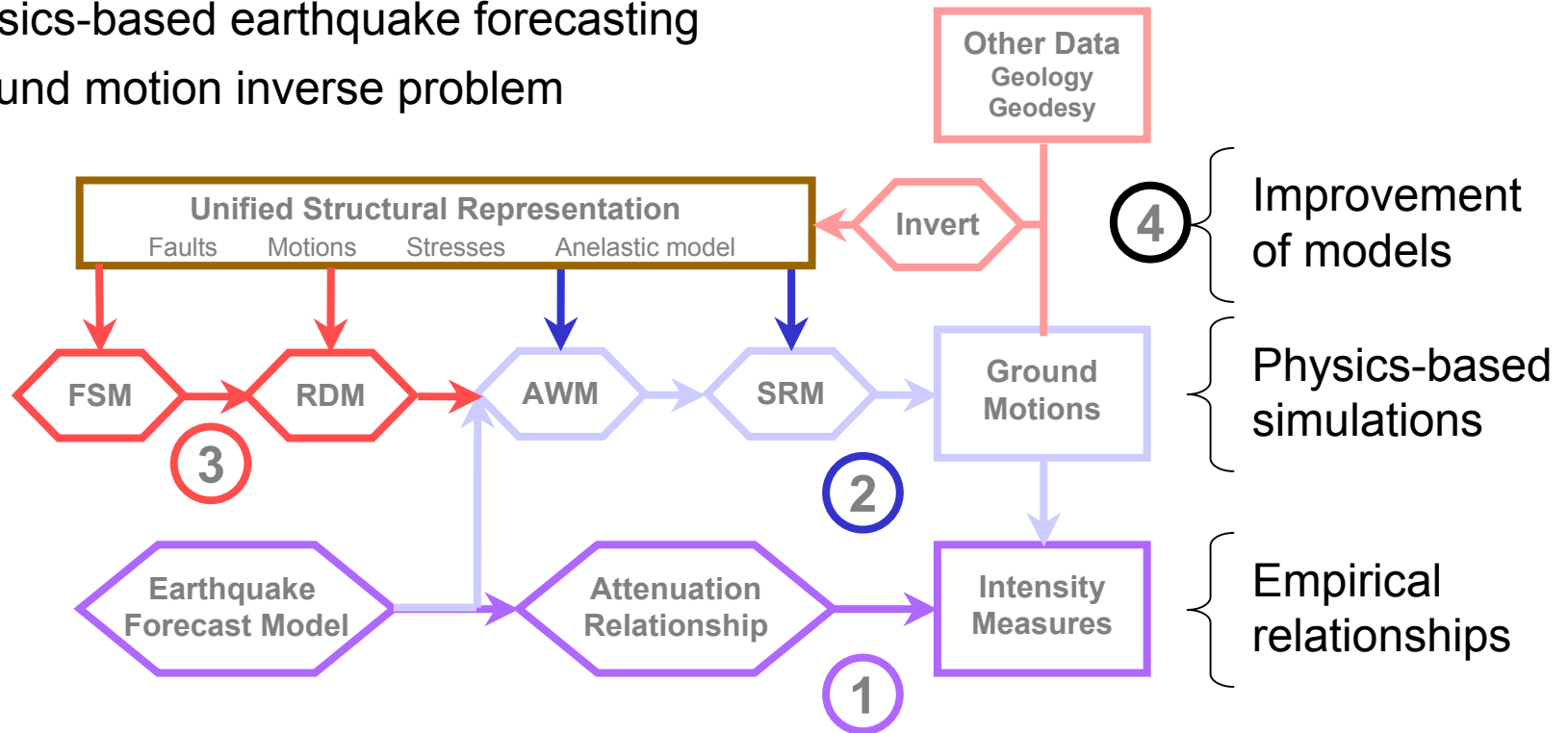
Develop an information infrastructure for system-level earthquake science to create a *SCEC collaboratory* that can:

- 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.

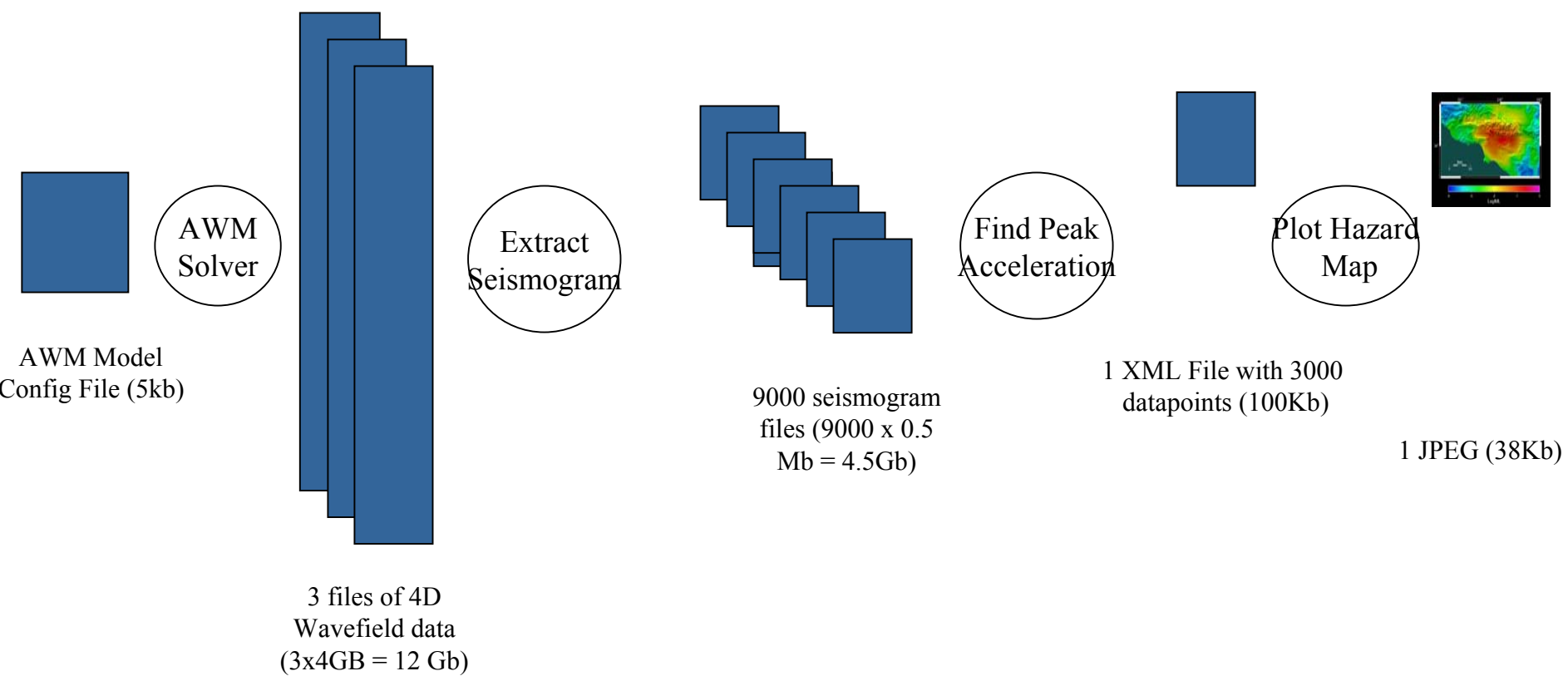
Initial SCEC/CME Workflow Approach





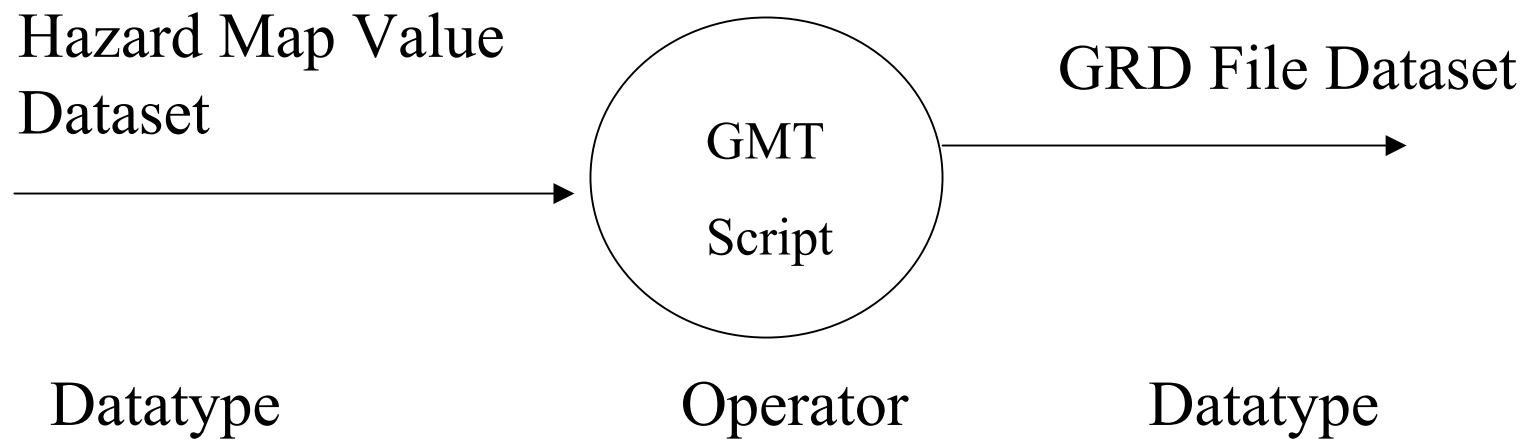
SCEC/CME Workflow Example

Example of SCEC/CME Computational Pathway:



Computational Step Concept

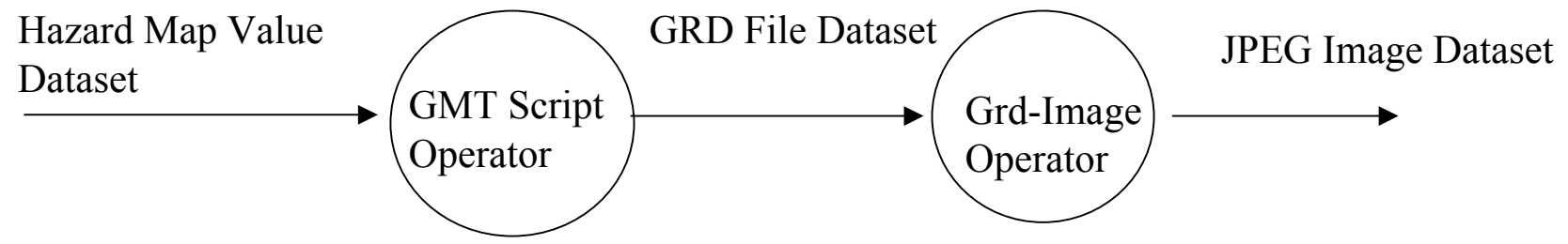
Computational Step modeled like a dataflow diagram:
Datatype inputs, transforming program, datatypes outputs



- 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



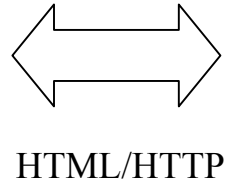
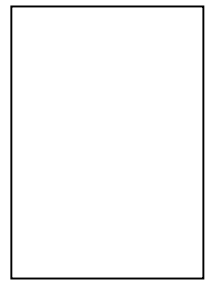


SCEC/CME Application Architecture

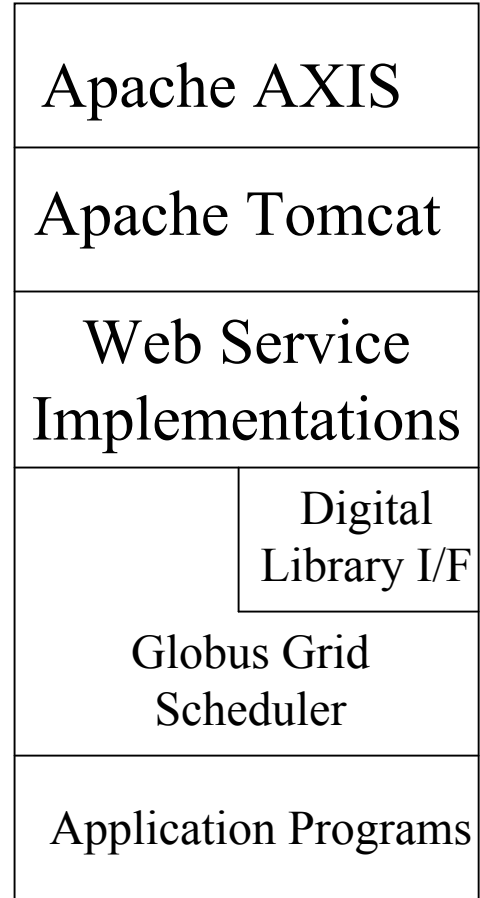
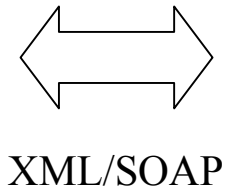
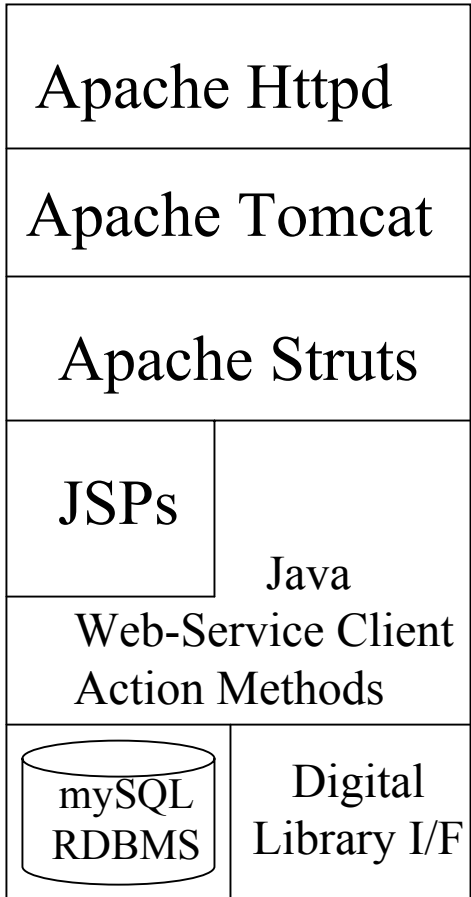
Users Computer

SCEC/CME Testbed Portal

SCEC/CME Testbed Grid



Browser Based User Interface



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

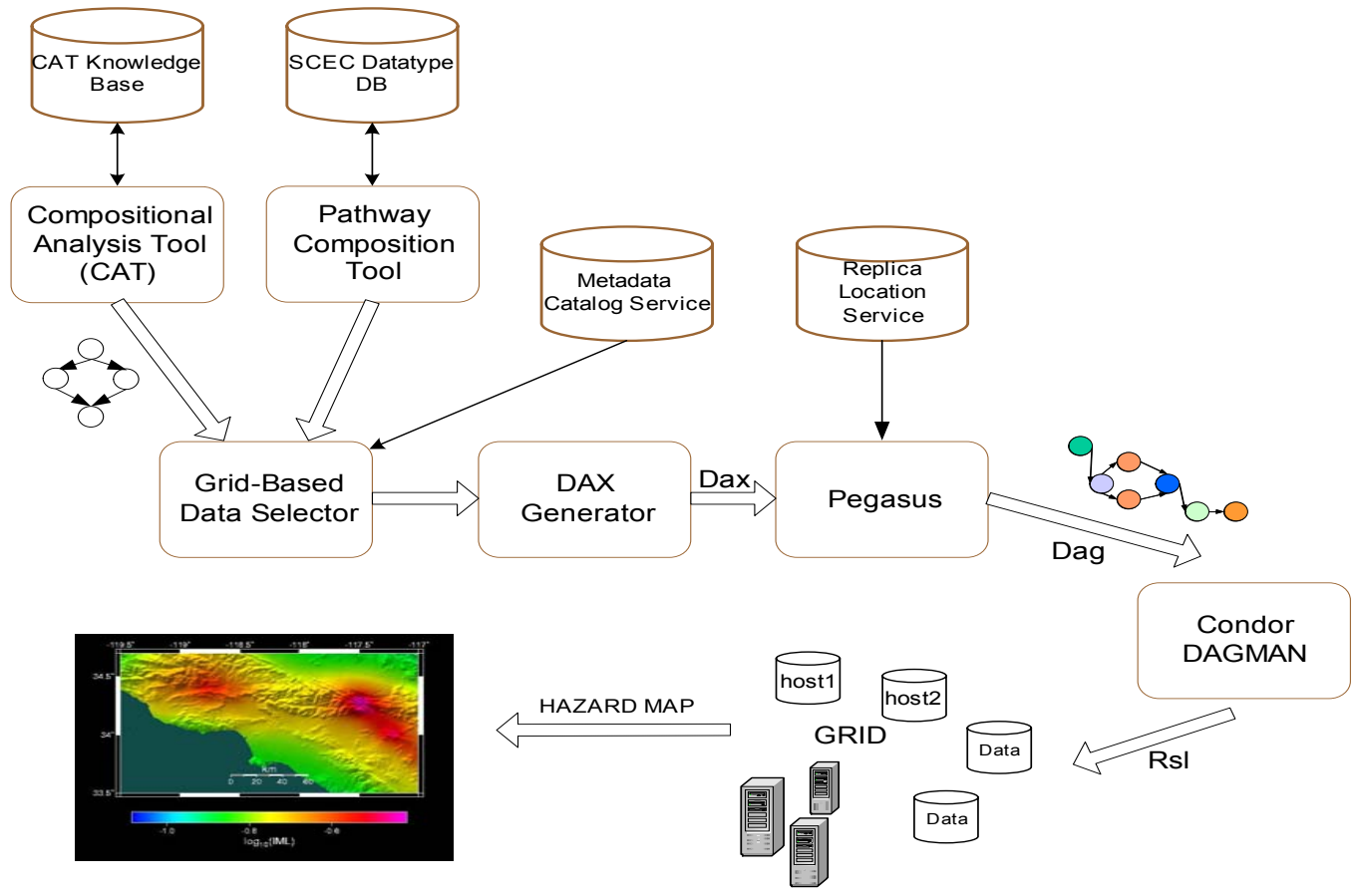


Revised SCEC/CME Workflow Approach

- 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.



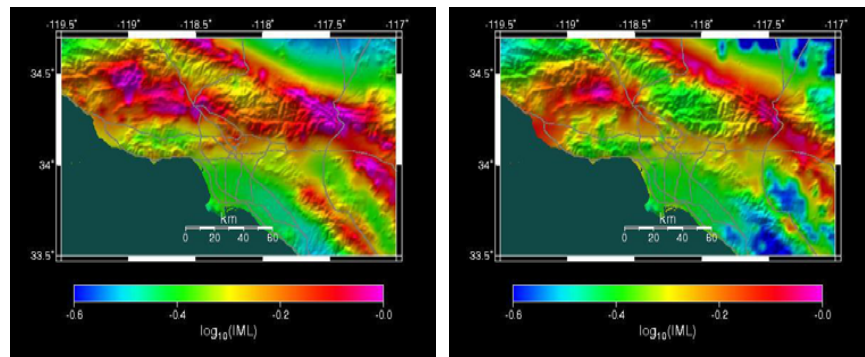
Elements of SCEC/CME Workflow System



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.



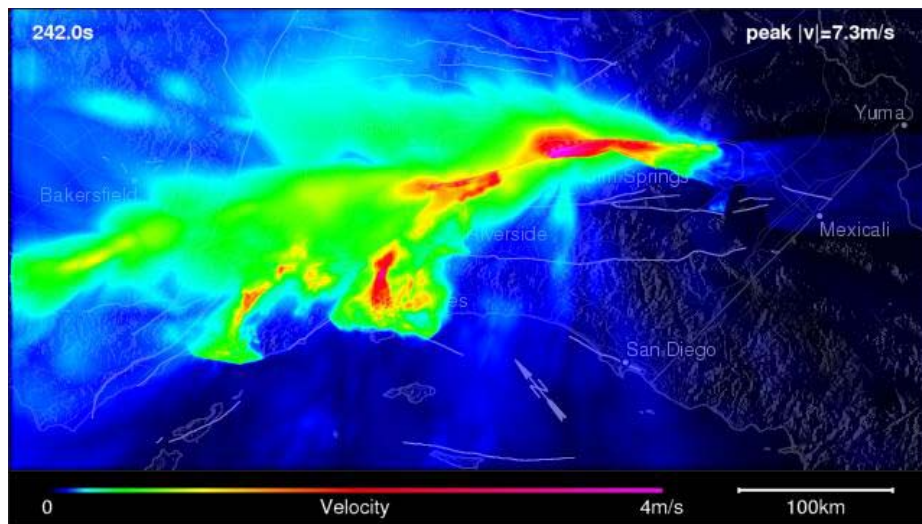
Computing Approach:

- 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)



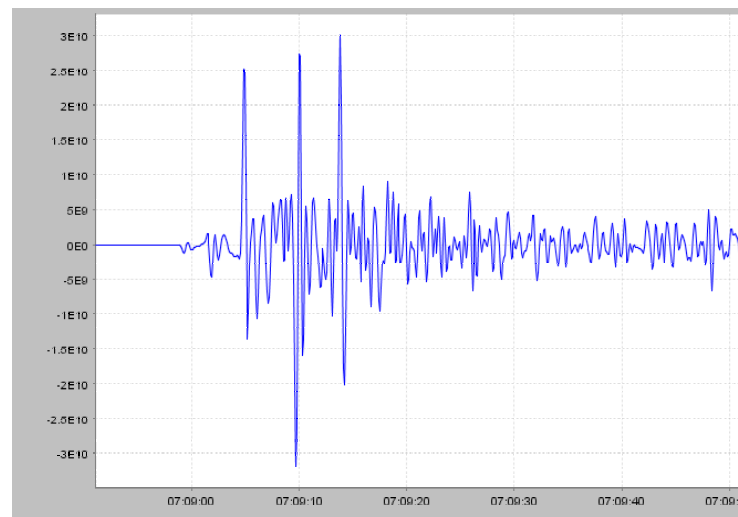
Computing Approach:

- 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:

The screenshot shows a web browser window titled "Pathway Composition Tool - Microsoft Internet Explorer". The address bar shows the URL: <https://wave.usc.edu/cmecdb/PathwayCompositionApplet.jsp>. The page features the SC/EC logo and the title "Pathway Composition Tool".

The interface is divided into several sections:

- Choose Module:** A dropdown menu is set to "HazardMap Calculator".
- Module Description:** "To calculate the hazard curve at a particular site".
- Module Inputs:** "EarthquakeRuptureForecast", "IntensityMeasureRelationship", "Site", "SiteParameters".
- Module Outputs:** "HazardCurveDataFiles".
- Add Module to Pathway:** A button at the bottom of the left sidebar.

The main workspace displays a workflow diagram with three modules connected by arrows:

- Module 1:** "HazardMapCalculator".
LINK: HazardMapDataFiles TO HazardMapDatasetToXYZConverter.
- Module 2:** "HazardMapDatasetToXYZConverter" (highlighted with a dashed orange border).
LINK: HazardMapDataFiles FROM HazardMapCalculator
LINK: XYZFile TO MapPlotter.
- Module 3:** "MapPlotter".

Connections are labeled with coordinates: "(HazardMapCalculator, HazardMapDatasetToXYZConverter)" and "(HazardMapDatasetToXYZConverter, MapPlotter)".

At the bottom of the browser window, the status bar shows "Applet.org_scec.cme.pathwayComposition.PathwayCompositionTool started" and "Internet".

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.

Input Data For Pathway

[View WorkFlow Template](#)

Pathway Module:	HazardMapCalculator
Select Pathway Component Instance:	org.sceec.cme.HazardMapCalculator:57 <input type="button" value="View Metadata"/>
Inputs	Outputs
EarthquakeRuptureForecast org.sceec.cme.EqkRupture:3116 <input type="button" value="View Metadata"/>	HazardMapDataFiles
Region org.sceec.cme.GriddedRegion:3125 <input type="button" value="View Metadata"/>	
IntensityMeasureRelationship org.sceec.cme.Field2000_IMR:3118 <input type="button" value="View Metadata"/>	
SiteParameters org.sceec.cme.SiteParameters:3119 <input type="button" value="View Metadata"/>	
Pathway Module:	HazardMapDatasetToXYZConverter
Select Pathway Component Instance:	org.sceec.cme.HazardMapDatasetToXYZConverter:65 <input type="button" value="View Metadata"/>
Inputs	Outputs
IMLOrProbParameter org.sceec.cme.imlOrProb:3120 <input type="button" value="View Metadata"/>	XYZFile
HazardMapDataFiles: FROM MODULE HazardMapCalculator	



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

View Submit Job Details - Microsoft Internet Explorer

Address: https://wave.usc.edu/cmedb/showjobdetail.jsp

SOUTHERN CALIFORNIA EARTHQUAKE CENTER NSF USGS

View Submit Job Details

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		File	File	File	File
epicenter_create_dir	COMPUTE	PENDING	2004.09.29 16:14:58		File	File	File	File
HazardMapCalculator_ID0	COMPUTE	UNSUBMITTED			File	File	File	File
HazardMapDatasetToXYZConverter_ID1	COMPUTE	UNSUBMITTED			File	File	File	File
MapPlotter_ID2	COMPUTE	UNSUBMITTED			File	File	File	File
rc_tx_HazardMapCalculator_ID0_0	TRANSFER	UNSUBMITTED			File	File	File	File
new_rc_tx_HazardMapCalculator_ID0_0	TRANSFER	UNSUBMITTED			File	File	File	File
new_rc_register_HazardMapCalculator_ID0	REGISTRATION	UNSUBMITTED			File	File	File	File

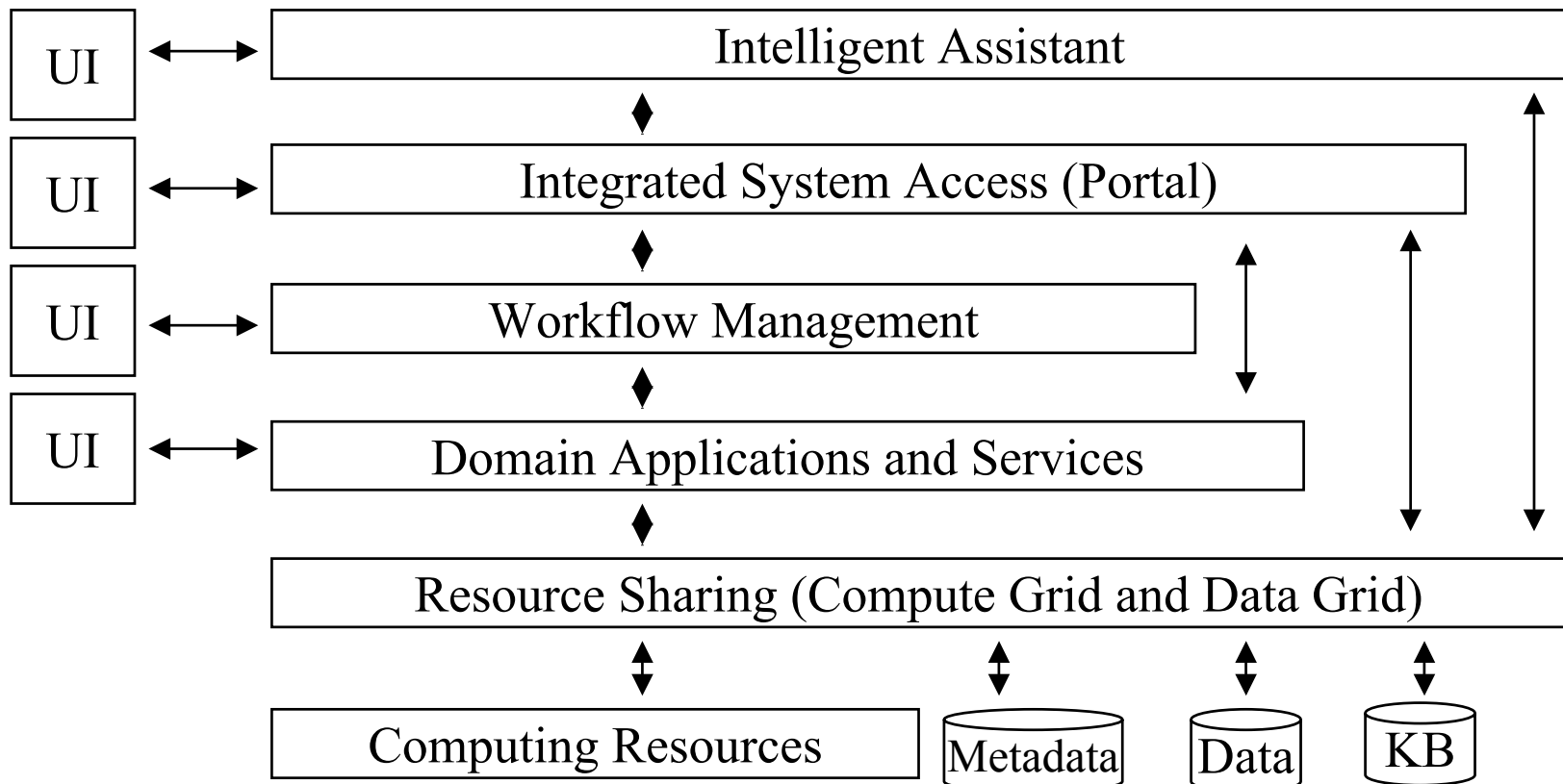
Benefits of Integrating SCEC Workflow with NMI Tools and Pegasus

- 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

<http://excalibur.isi.edu:8080/cat-enhanced/servlet/plInterface?sys...>

File Edit View Favorites Tools Help

Address <http://excalibur.isi.edu:8080/cat-enhanced/servlet/plInterface?sys...>

[Hide Modules] [Load Pathway] [Save Pathway] [Fill in Data]

Composition Analysis Tool: [Click to ente...](#)

Domain Ontology: data types of the inputs and outputs of the workflow components

CAT reasons about component descriptions and reports property violations as the workflow is composed

Component Ontology: workflow components available to be included in workflow template

User builds a workflow template using components

CAT generates suggestions to fix property violations

CAT ensures and guarantees correctness of workflow templates

Available Modules

- All Parameters More Specific or New
- ERF
 - IP: Data Type
 - OP: Rupture Array
- IMR
 - IMR-PROB-EXC
 - IP: Longitude, Latitude, Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: Prob Exc
 - IMR-SA
 - IP: SA Period, Longitude, Latitude, Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: SA
 - IMR-SA-PROB-EXC
 - IP: SA Period, Longitude, Latitude, Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: SA Prob Exc
 - IMR-SA-PROB-EXC-FIELD-2000
 - IP: Longitude, Latitude, Basin-Depth-2.5, VS30, Field 2000 SA Period, Field 2000 Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: SA Prob Exc
 - IMR-SA-PROB-EXC-BOORE-JOYNER-FUMAL-1997
 - IP: VS30, Boore-Joyner-Fumal SA Period, Longitude, Latitude, Boore-Joyner-Fumal Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: SA Prob Exc
 - IMR-SA-PROB-EXC-ABRAHAMSON-SILVA-1997
 - IP: Abrahamson-Silva Site Type, Abrahamson-Silva SA Period, Longitude, Latitude, Abrahamson-Silva Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: SA Prob Exc
 - IMR-PGA
 - IP: Longitude, Latitude, Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: PGA
 - IMR-PGV
 - IP: Longitude, Latitude, Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: PGV
 - IMR-FAULT-DISPLACEMENT
 - IP: Longitude, Latitude, Standard Deviation Type, Gaussian Truncation, Rupture Array
 - OP: Fault Displacement
- HAZARD-CURVE-CALCULATOR
 - IP: IMT, Rupture Array
 - OP: Hazard Curve
- HAZARD-MAP-PLOTTER
 - IP: Hazard Map Lat/Long/Amplitude Data, Mapping Parameters, Plotted Region
 - OP: Hazard Map

DATA-TYPE User-Provided Data

DURATION-YEARS:2 ✗
ERF - Duration-Years ✗
UTM:3 ✗
UTM Converter - UTM ✗

End Results

SA-PROB-EXC-HAZARD-CURVE:1 ✗
Hazard-Calc - SA-Prob-Exc-Hazard-Curve ✗

Inputs

SA-Prob-Exc-Array ✗
IMR-Field - SA-Prob-Exc (via Array Accumulator) ✗
Rupture-Array ✗
ERF - Rupture-Array ✗

Outputs

SA-Prob-Exc-Hazard-Curve ✗
End Results - SA-PROB-EXC-HAZARD-CURVE ✗

Inputs

Longitude ✗
UTM Converter - Longitude ✗
Latitude ✗

Outputs

SA-Prob-Exc-Hazard-Curve ✗

Inputs

Longitude ✗
UTM Converter - Longitude ✗
Latitude ✗

Outputs

Basin-Depth-2.5 ✗

Inputs

Longitude ✗
UTM Converter - Longitude ✗
Latitude ✗

Outputs

Basin-Depth-2.5

ERROR

Input or end result needs a value Hazard Map Calculator - Hazard Map Data to Hazard Map Plotter - Hazard Map Lat/Long/Amplitude Data

Link input and output mismatched From Hazard Map Calculator - Hazard Map Data to Hazard Map Plotter - Hazard Map Lat/Long/Amplitude Data

Input or end result needs a value Hazard Map Plotter - Mapping Parameters

Input or end result needs a value Hazard Map Plotter - Plotted Region

Suggestions

Fix link by adding and interposing Module HAZARD-MAP-CONVERTER. [Hide]

Remove link. [Apply]

- Add Module Hazard Map Dataset To Lat/Long/Amplitude Converter
- Add a Link from module Hazard Map Calculator:4 - Hazard Map Data to module Hazard Map Dataset To Lat/Long/Amplitude Converter - Hazard Map Data
- Add a Link from module Hazard Map Dataset To Lat/Long/Amplitude Converter - Hazard Map Lat/Long/Amplitude Data to module Hazard Map Plotter:2 - Hazard Map Lat/Long/Amplitude Data

Fix link by replacing Module HAZARD-MAP-CALCULATOR with Module HAZARD-MAP-CONVERTER. [Details]

Remove Link. [Details]

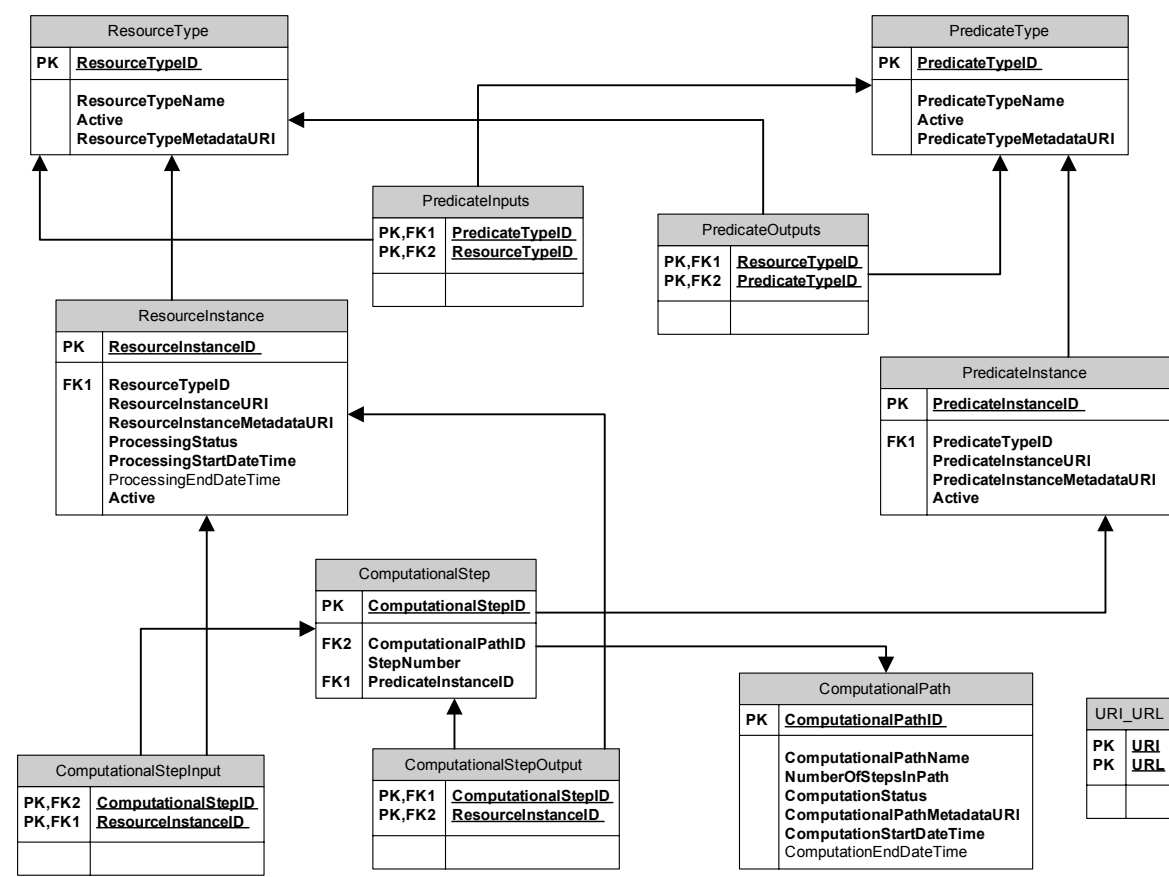
[INFO]: Remove Link, or may ignore if warning.

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

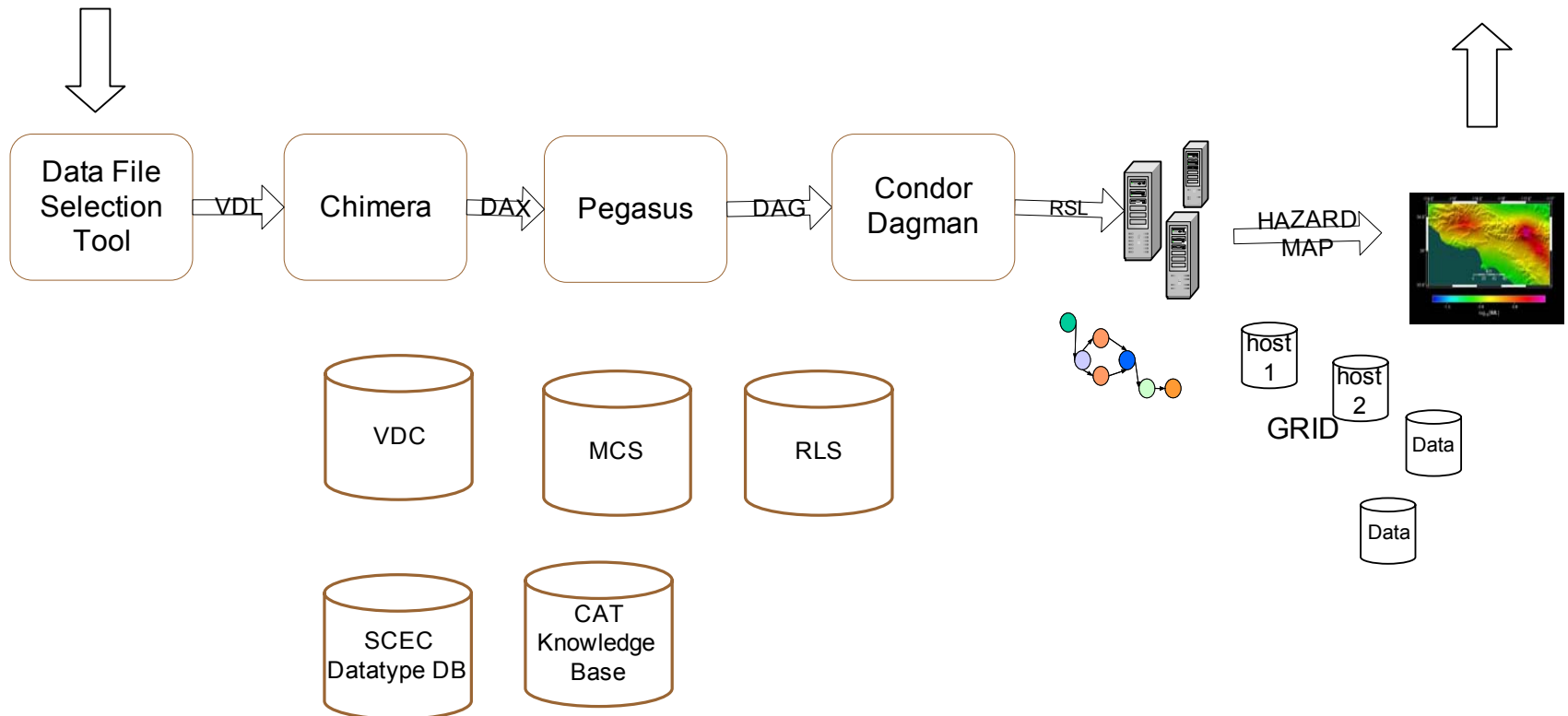
SCEC/CME Creator to Consumer System



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
----------------------------------------------------	--------------------------------------	--------------------------

E
X
T
E
R
N
A
L

U
S
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R
S

**Public
Data
Access**

**Public
Utility
Computing**

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