Meeting the Challenges of Managing Large-Scale Scientific Workflows in Distributed Environments

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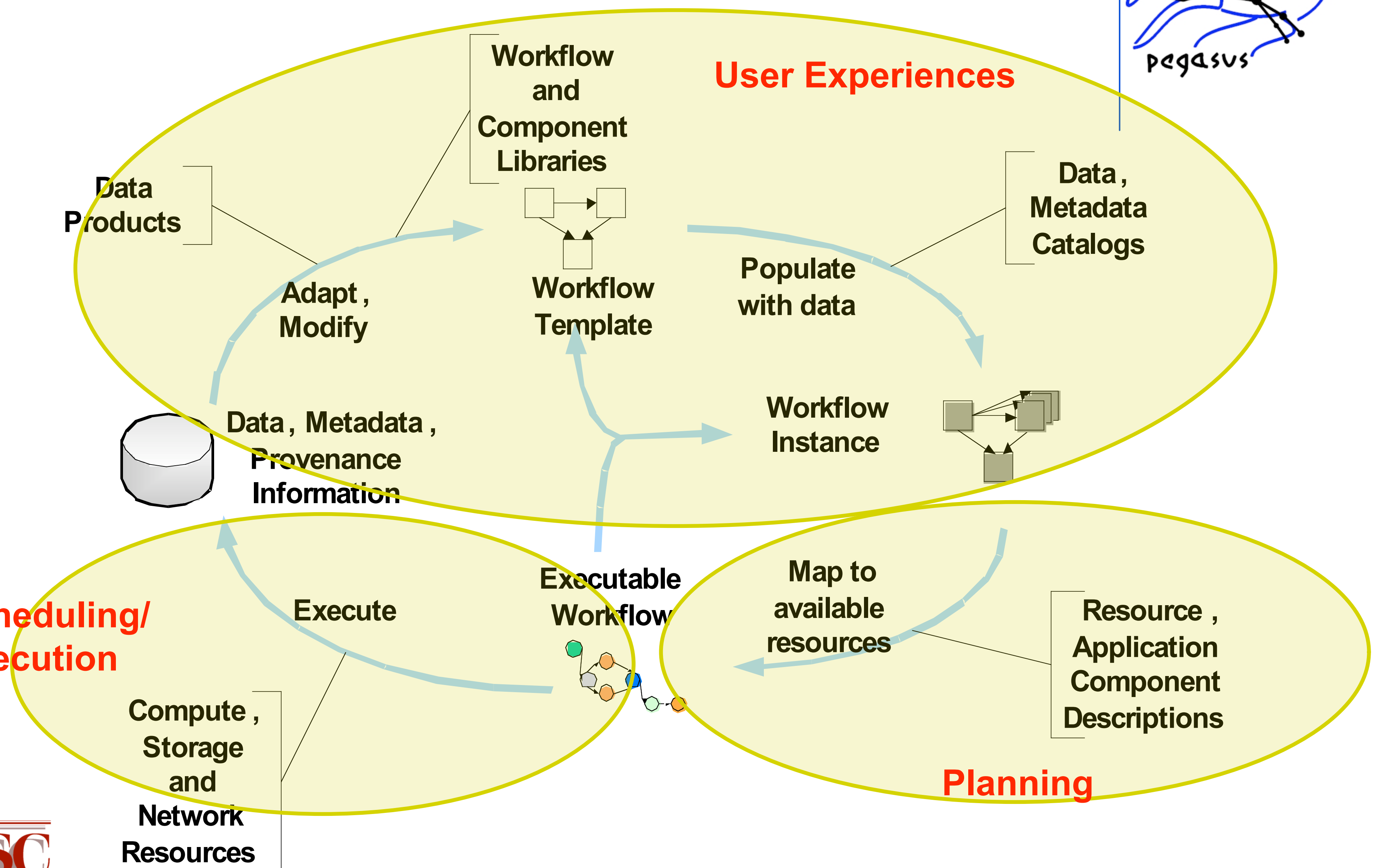
Scientific Workflows

- Current workflow approaches are exploring specific aspects of the problem:
  - Creation, reuse, provenance, performance, reliability
- New requirements are emerging
  - Streaming data, from batch to interactive steering, event-driven analysis, collaborative design of workflows
- Need to develop a science of workflows
  - A more comprehensive treatment of workflow lifecycle
  - Understand current and long-term requirements from science applications
    - reproducibility
  - Workflows as first-class citizens in CyberInfrastructure

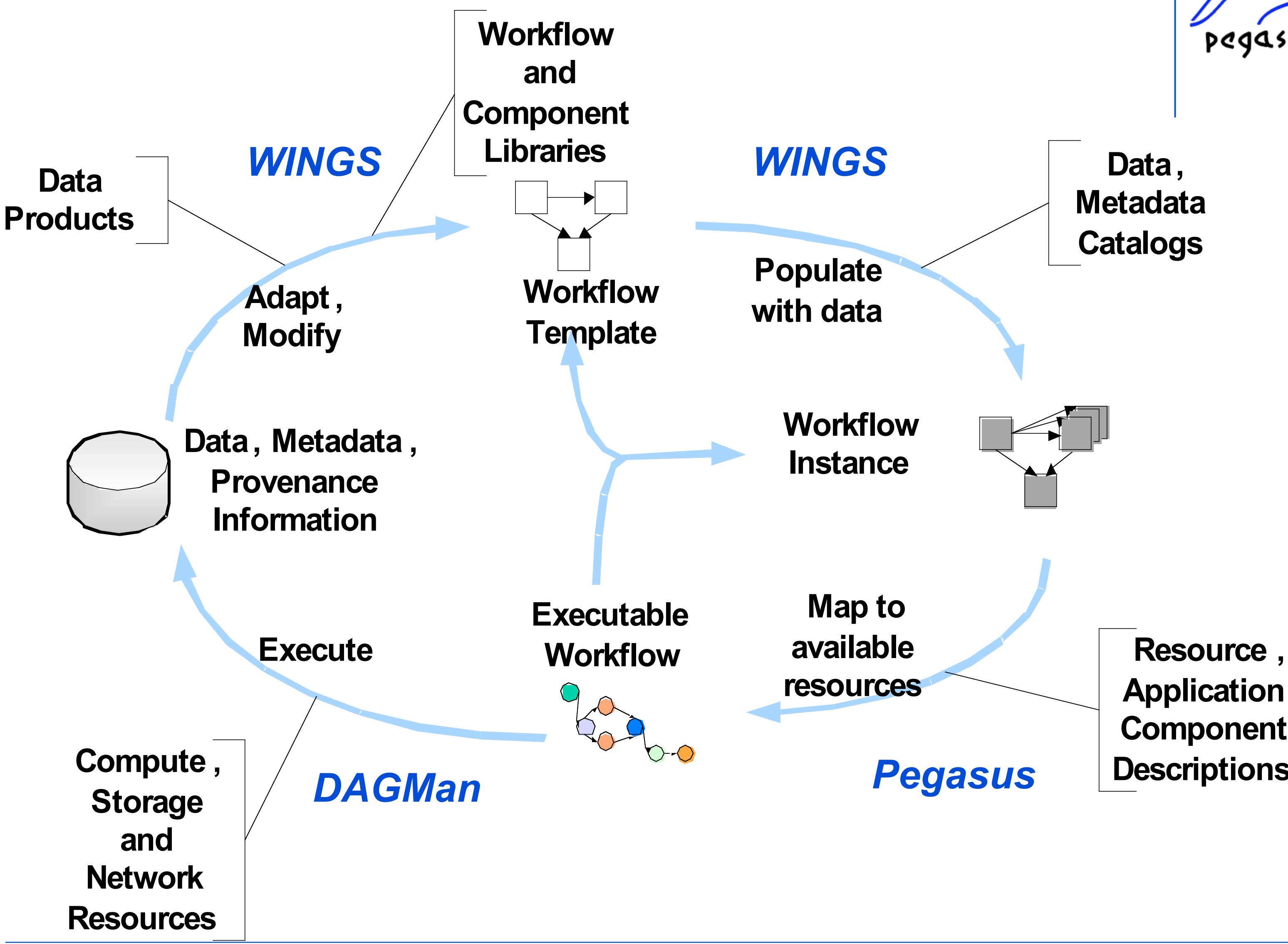
Workflow Lifecycle



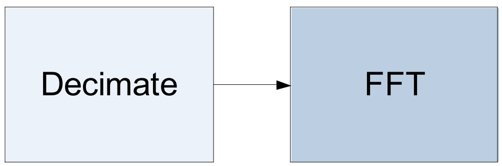
Outline

- Rendering the workflow lifecycle
  - Wings/Pegasus/DAGMan
- Challenges across the various aspects of workflow management
  - User experiences
  - Planning/Mapping
  - Execution
- Workflows-what are they good for?
- Research issues
- Conclusions

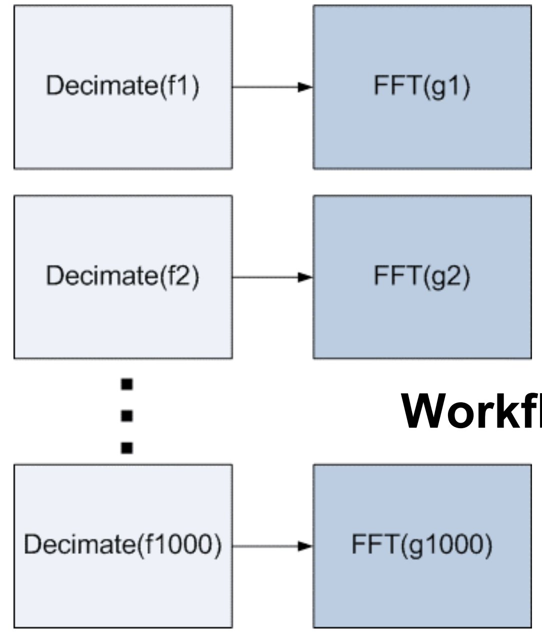
Workflow Lifecycle



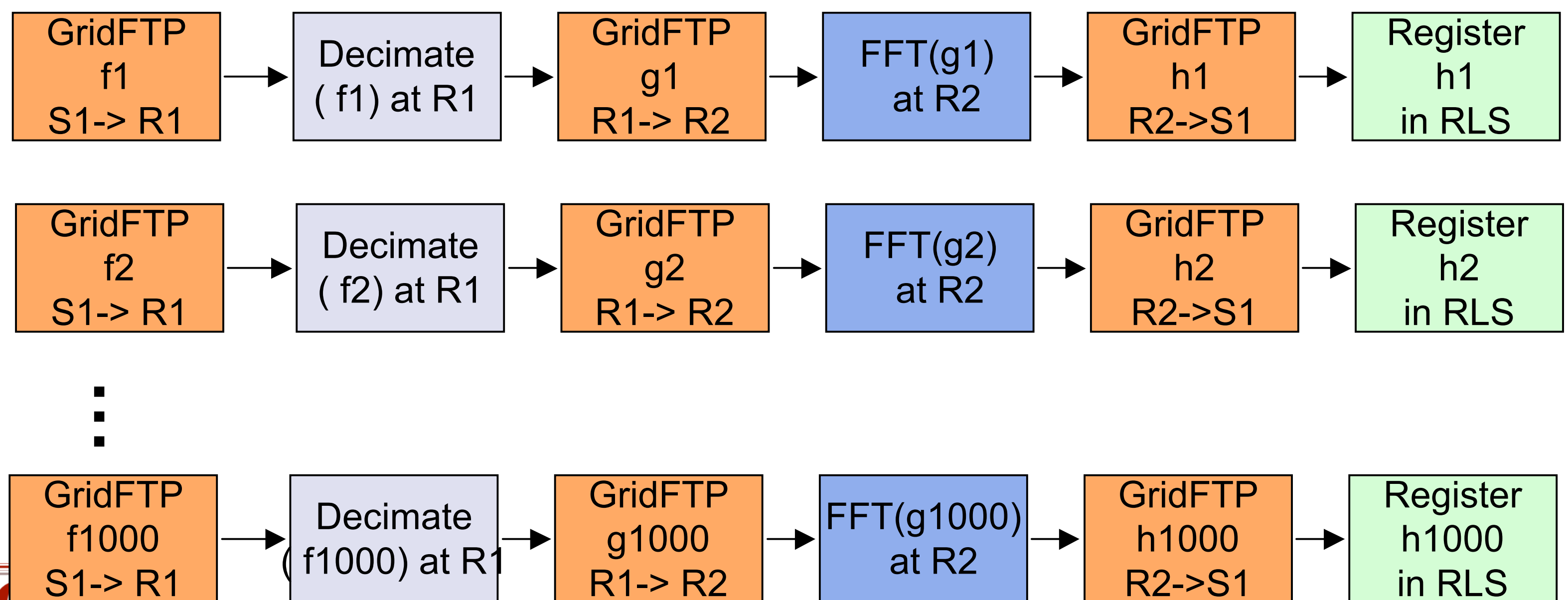
Workflow Entities



Workflow Template

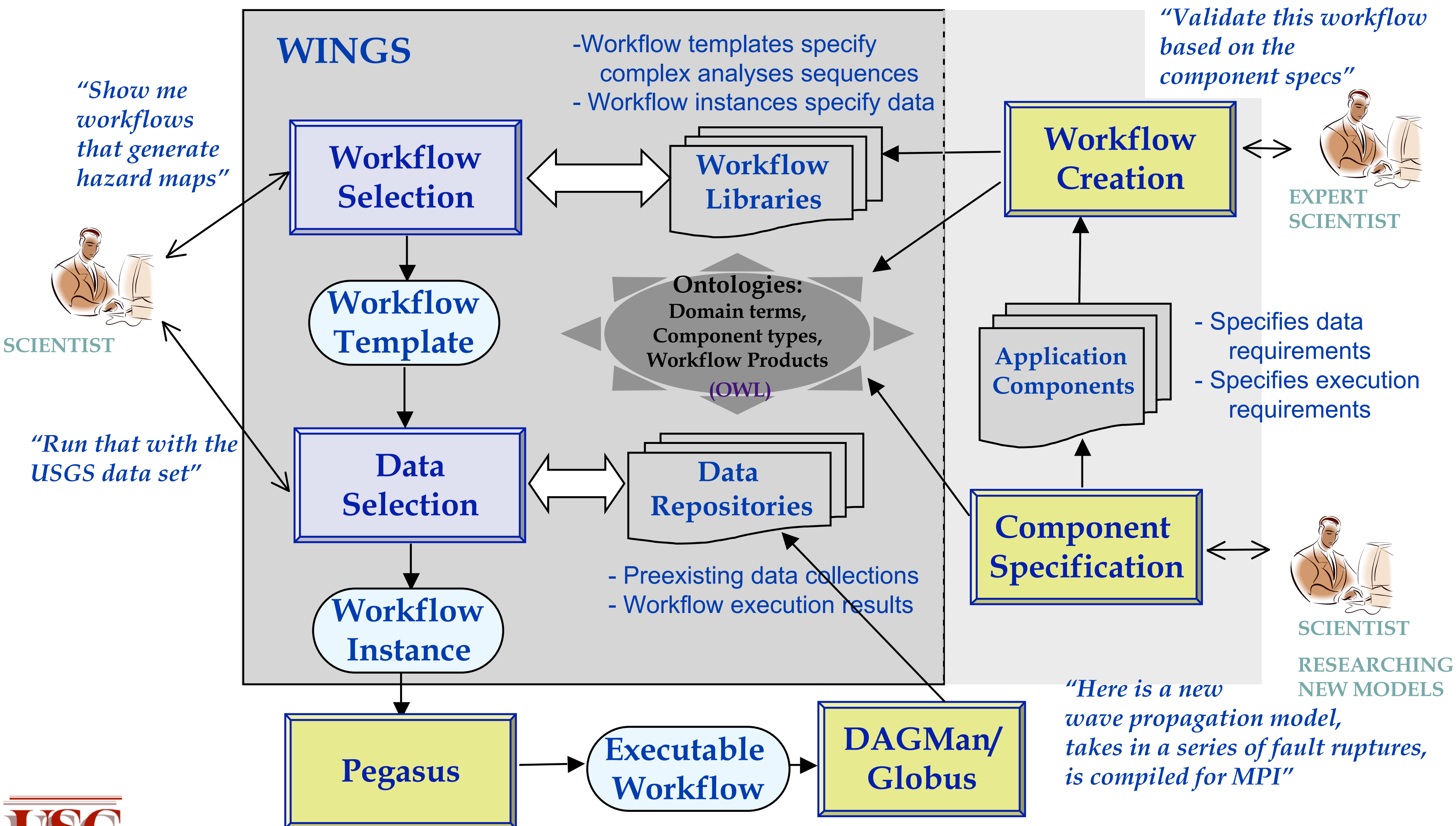


Workflow Instance



Executable Workflow

WINGS/Pegasus: Workflow Instance Generation and Selection, Using semantic technologies for workflow generation

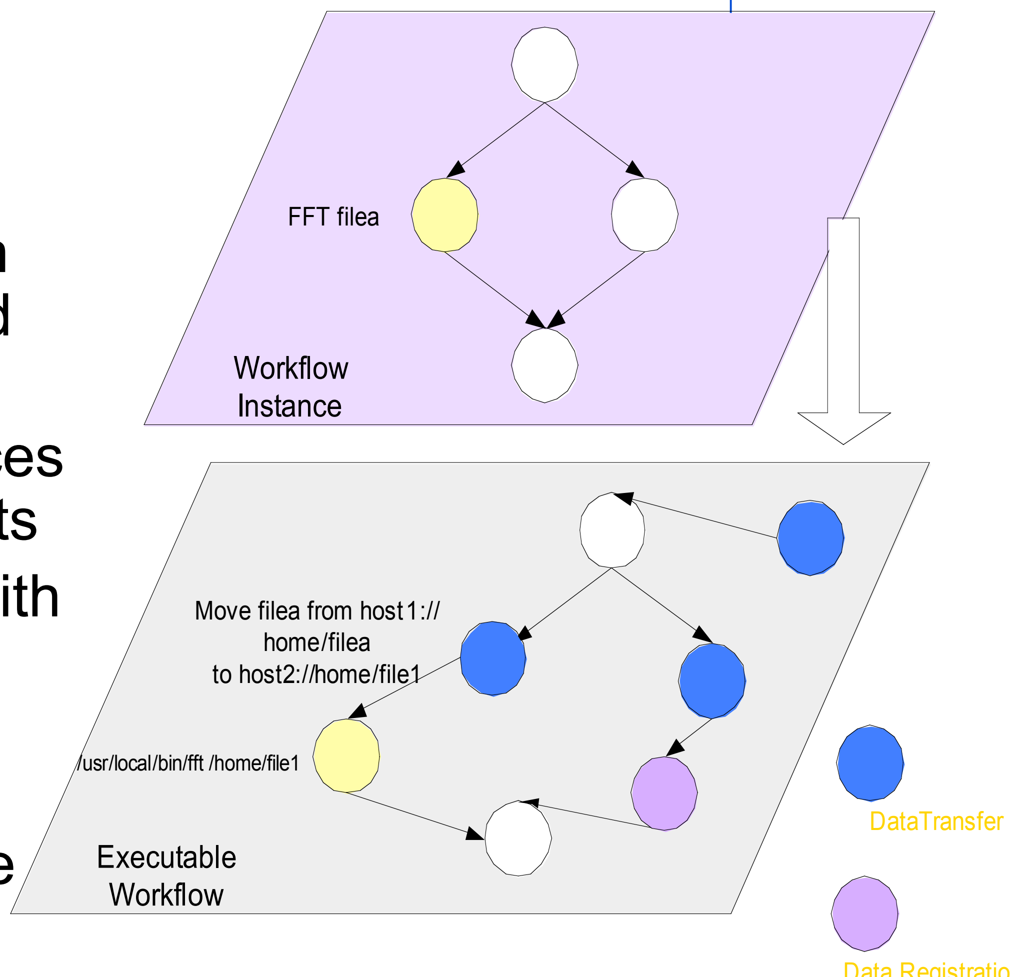


Wings for Pegasus: A Semantic Approach to Creating Very Large Scientific Workflows

Yolanda Gil, Varun Ratnakar, Ewa Deelman, Marc Spraragen, and Jihie Kim, *OWL: Experiences and Directions 2006*

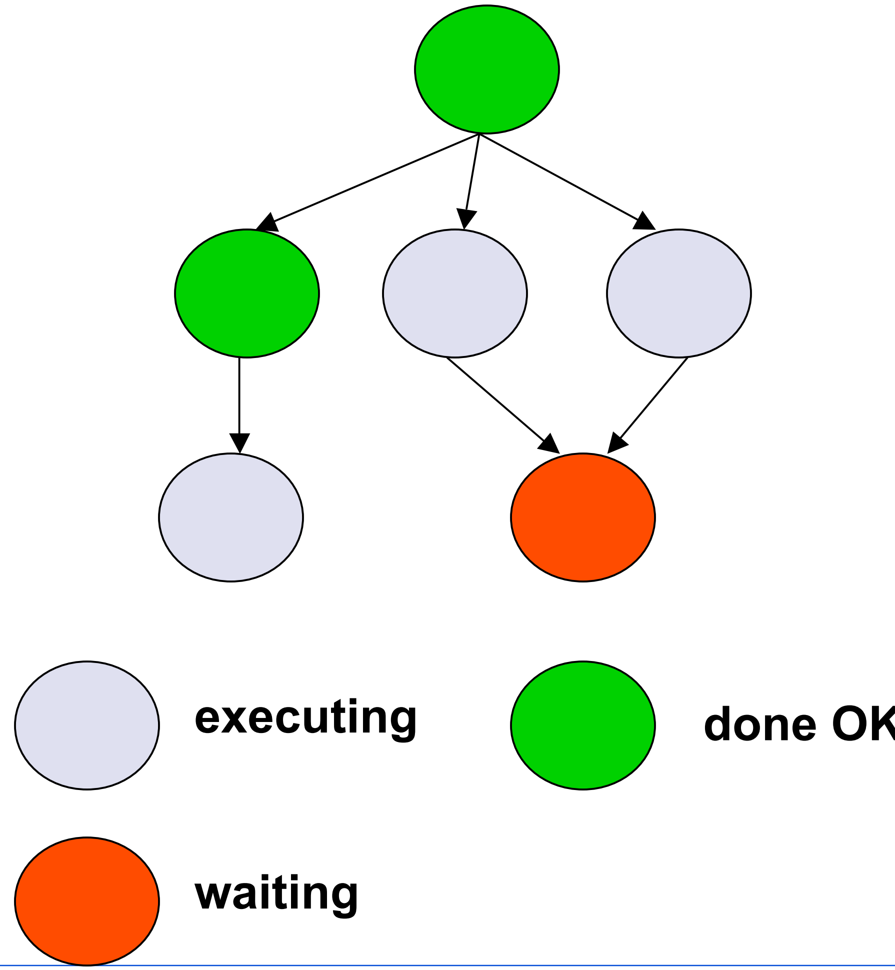
Pegasus: Planning for Execution in Grids

- Maps from workflow instance to executable workflow
- Automatically locates physical locations for both workflow components and data
- Finds appropriate resources to execute the components
- Augments the workflow with data staging and registration
- Reuses existing data products where applicable
- Publishes newly derived data products



Condor DAGMan (University of Wisconsin)

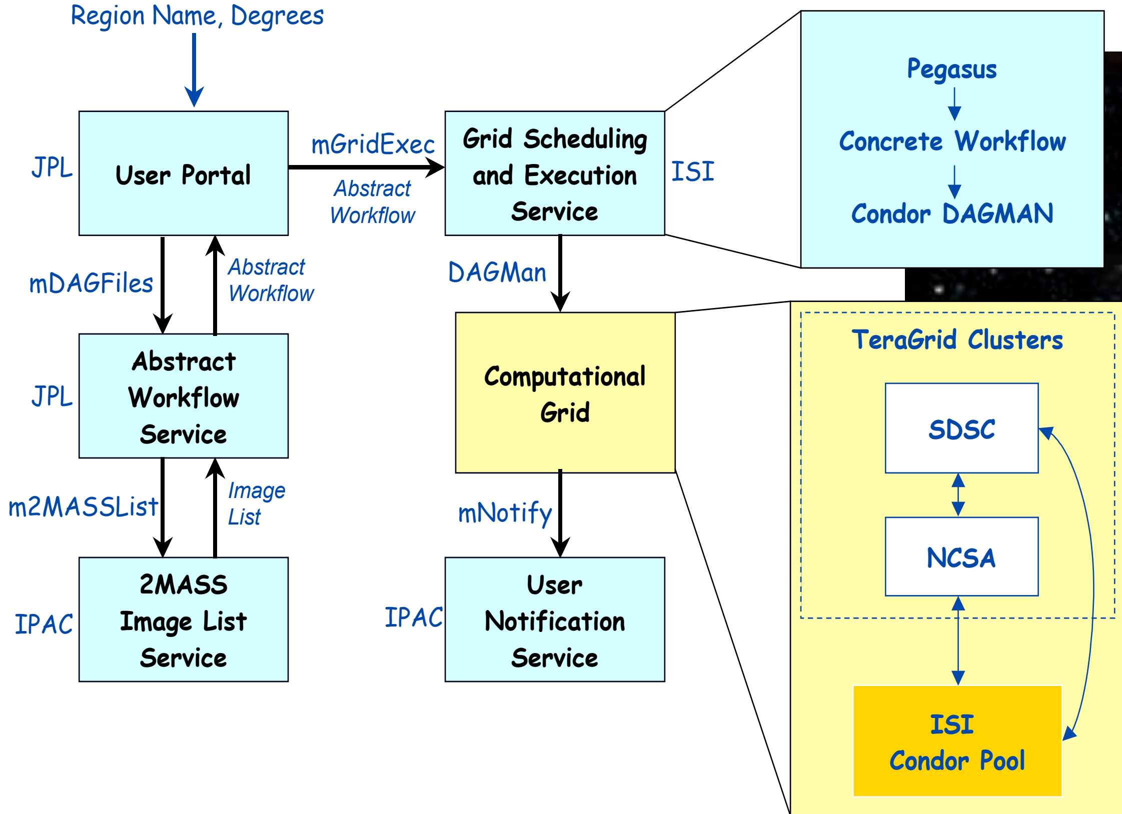
- Follows dependencies in workflow
- Releases nodes to execution (to Condor Q)
- Provides retry capabilities



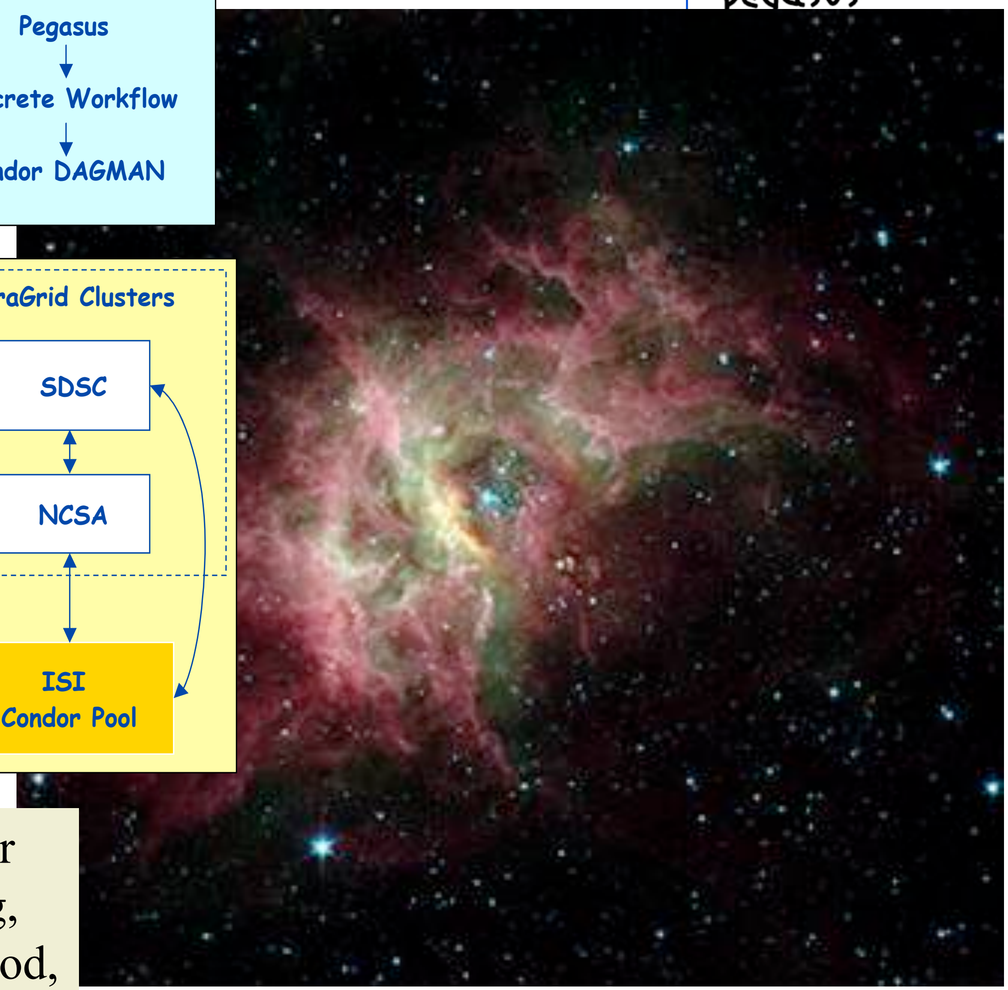
Challenges in user experiences

- Users' expectations vary greatly
  - High-level descriptions
  - Detailed plans that include specific resources
- Users interactions can be exploratory
  - Modifying portions of the workflow as the computation progresses
- *Users need progress, failure information at the right level of detail*

Portals, Providing high-level Interfaces

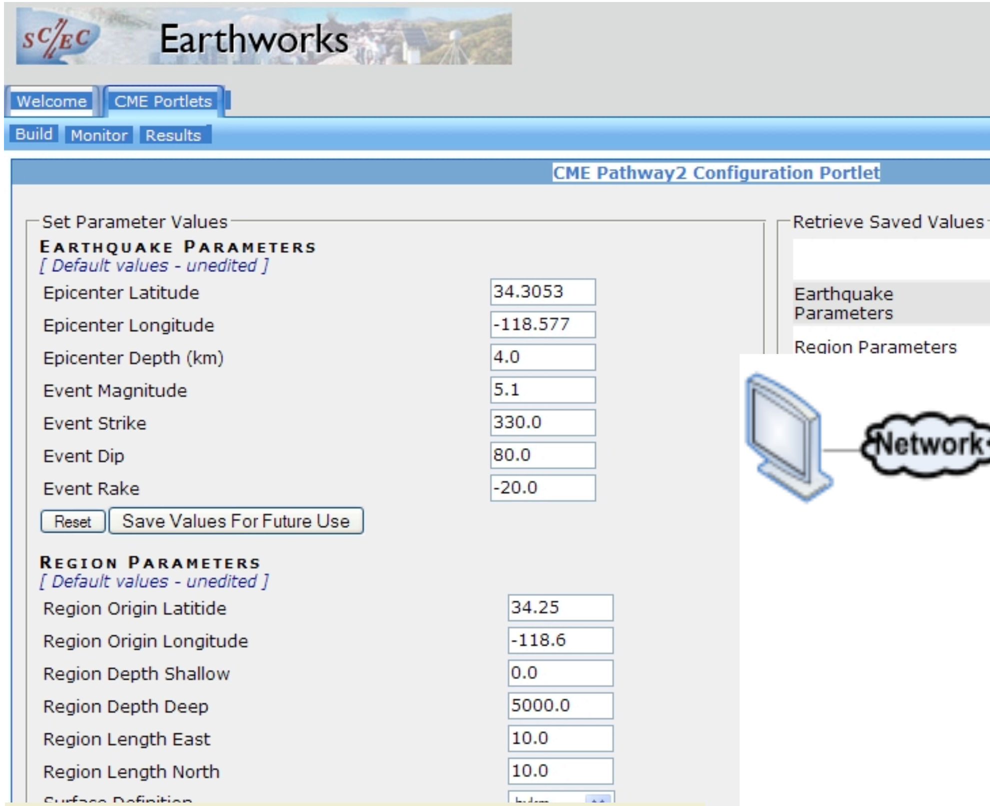


Montage: a grid portal and software toolkit for science-grade astronomical image mosaicking, J. C. Jacob, D. S. Katz, G. B. Berriman, J. Good, A. C. Laity, E. Deelman, C. Kesselman, G. Singh, M.-H. Su, T. A. Prince, R. Williams, , IJCSE*, to appear 2006*

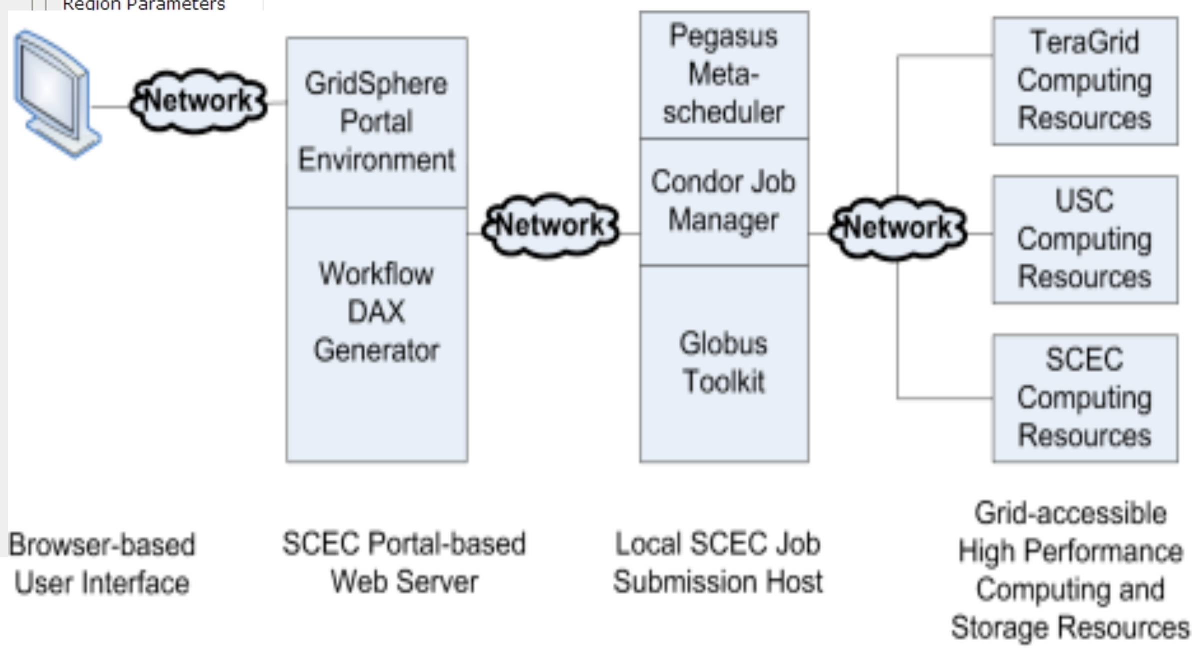


Galactic Star Formation Region RCW 49

Portals, Providing high-level Interfaces



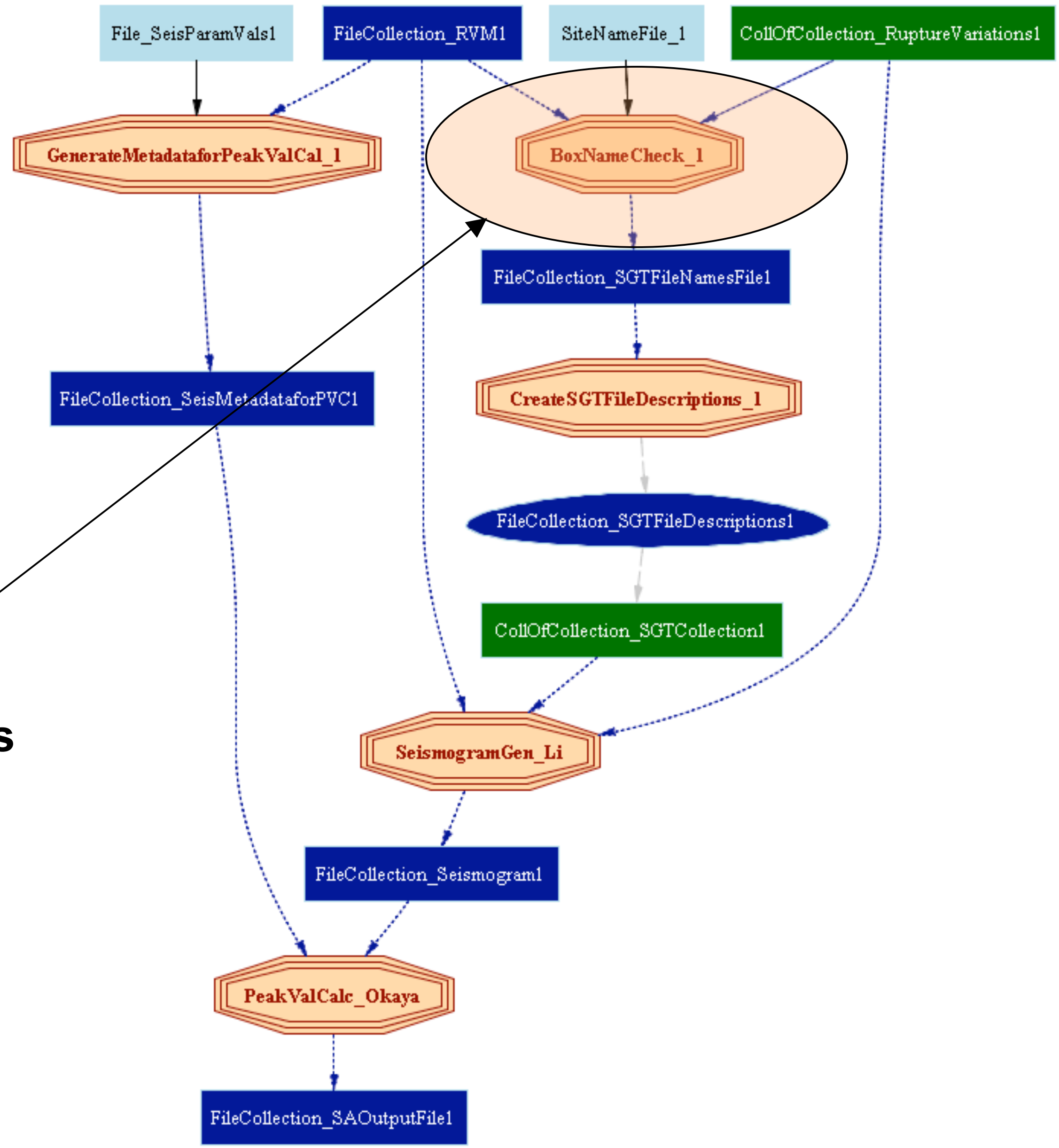
TG Science Gateway, Washington University



EarthWorks Project (SCEC), lead by with J. Muench P. Maechling, H. Francoeur, and others

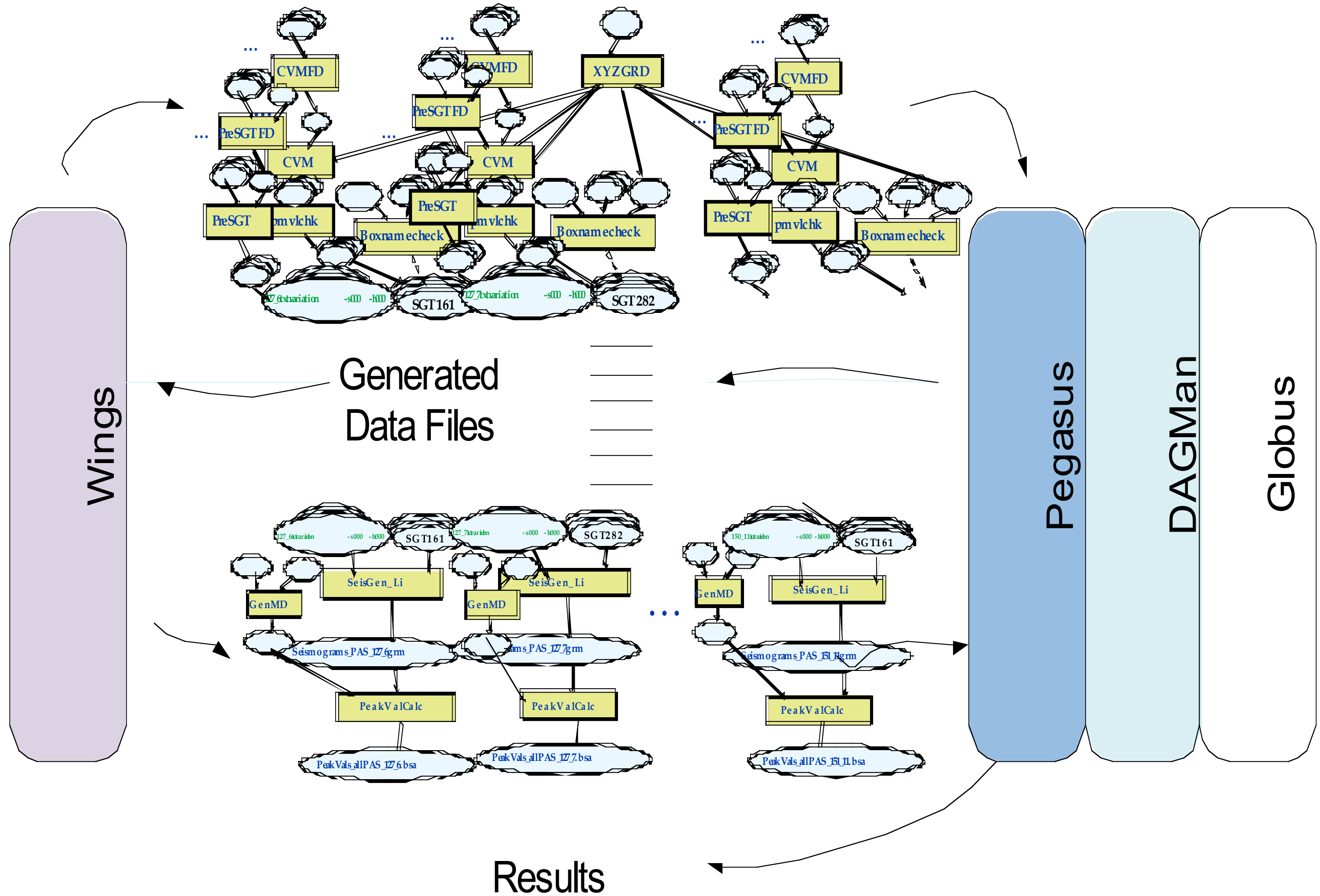
SCEC Earthworks: Community Access to Wave Propagation Simulations, J. Muench, H. Francoeur, D. Okaya, Y. Cui, P. Maechling, E. Deelman, G. Mehta, T. Jordan TG 2006

SCEC CyberShake Workflow, not a one shot workflow



Needs to run before rest of the workflow is instantiated

Iterative workflow instantiation, mapping and execution

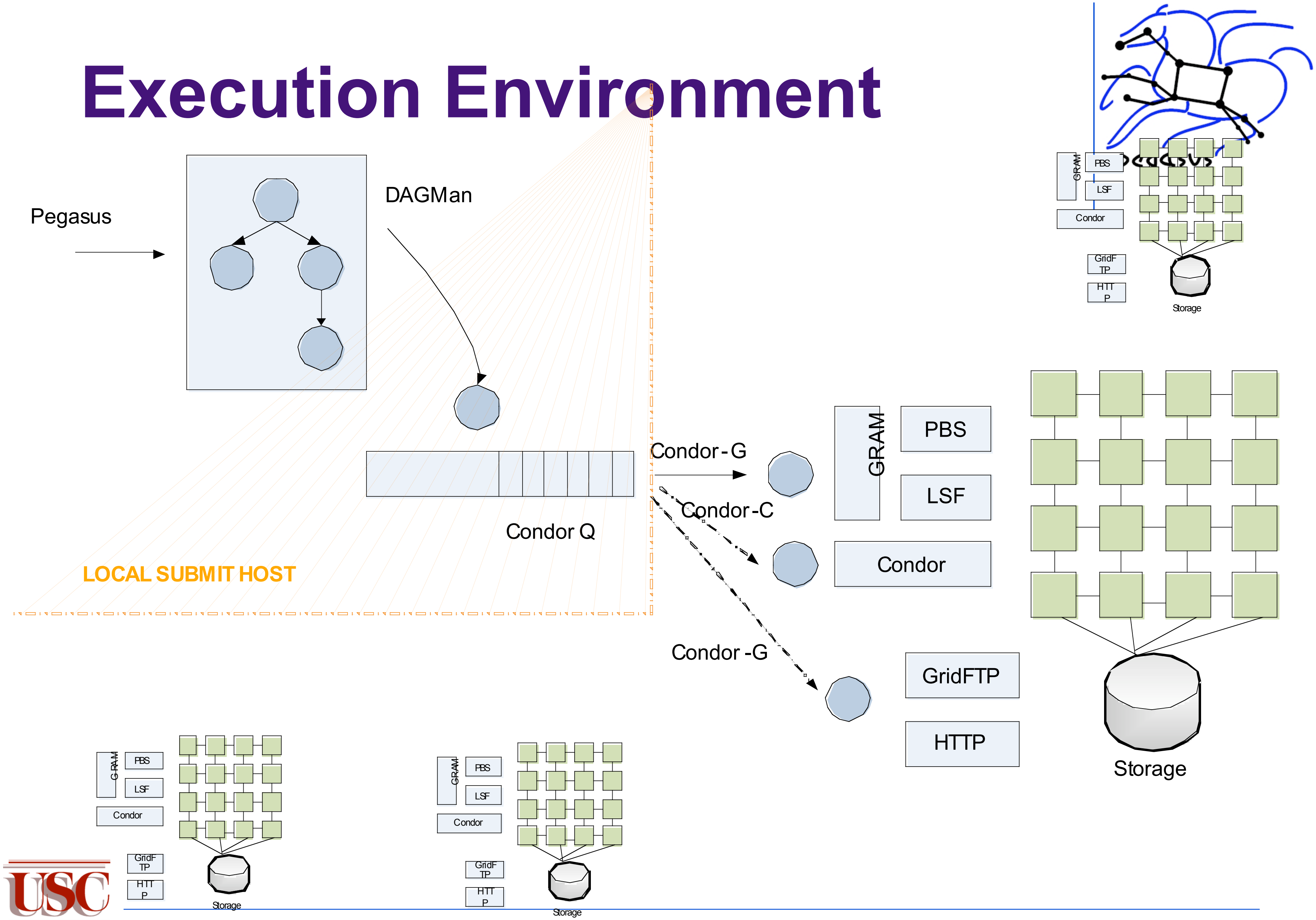


Wings for Pegasus: A Semantic Approach to Creating Very Large Scientific Workflows
Yolanda Gil, Varun Ratnakar, Ewa Deelman, Marc Spraragen, and Jihie Kim, *in submission*

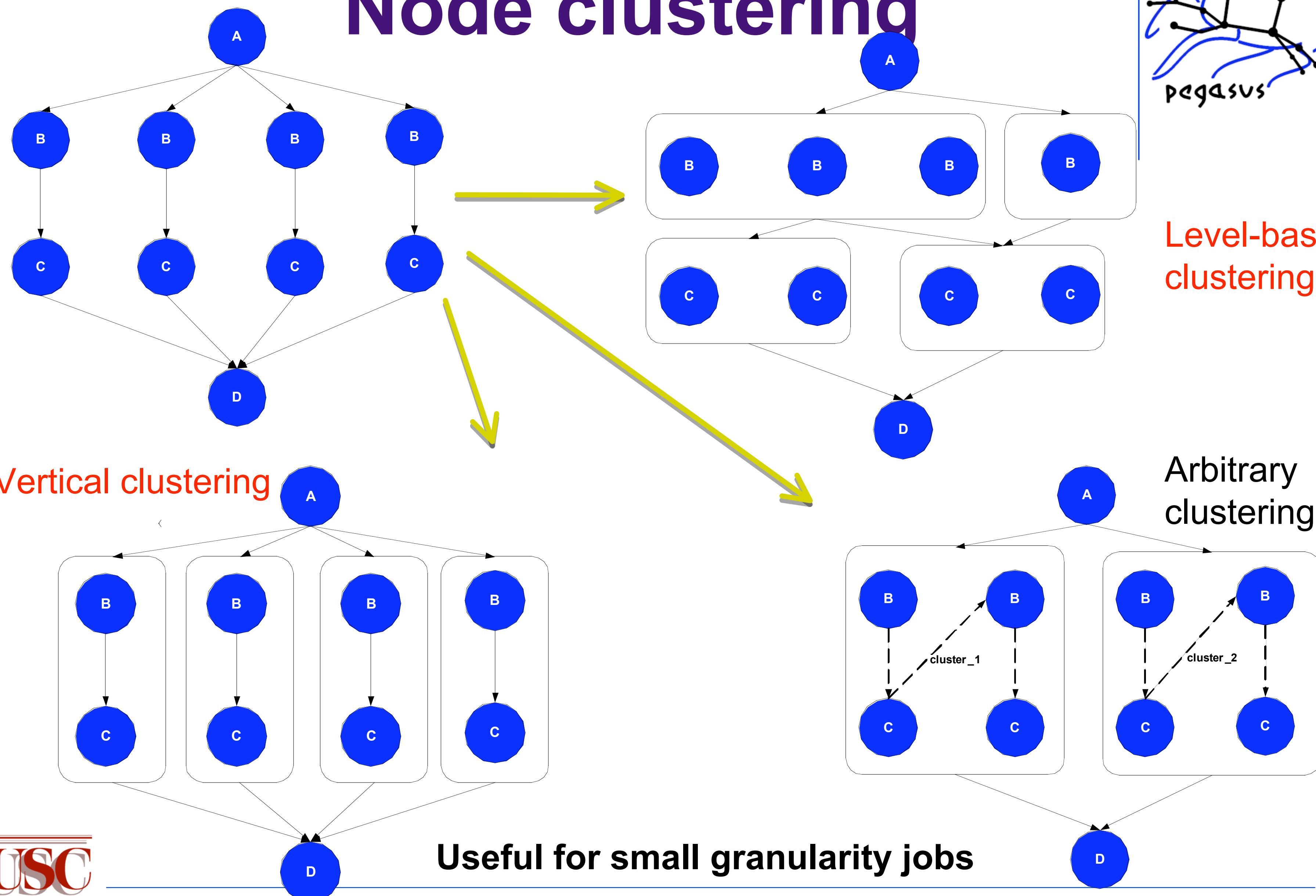
Some challenges in workflow mapping

- Automated management of data
  - Through workflow modification
- Efficient mapping the workflow instances to resources
  - Performance
  - Data space optimizations
  - Fault tolerance (involves interfacing with the workflow execution system)
    - Recovery by replanning
    - plan "B"
- Providing feedback to the user
  - Feasibility, time estimates

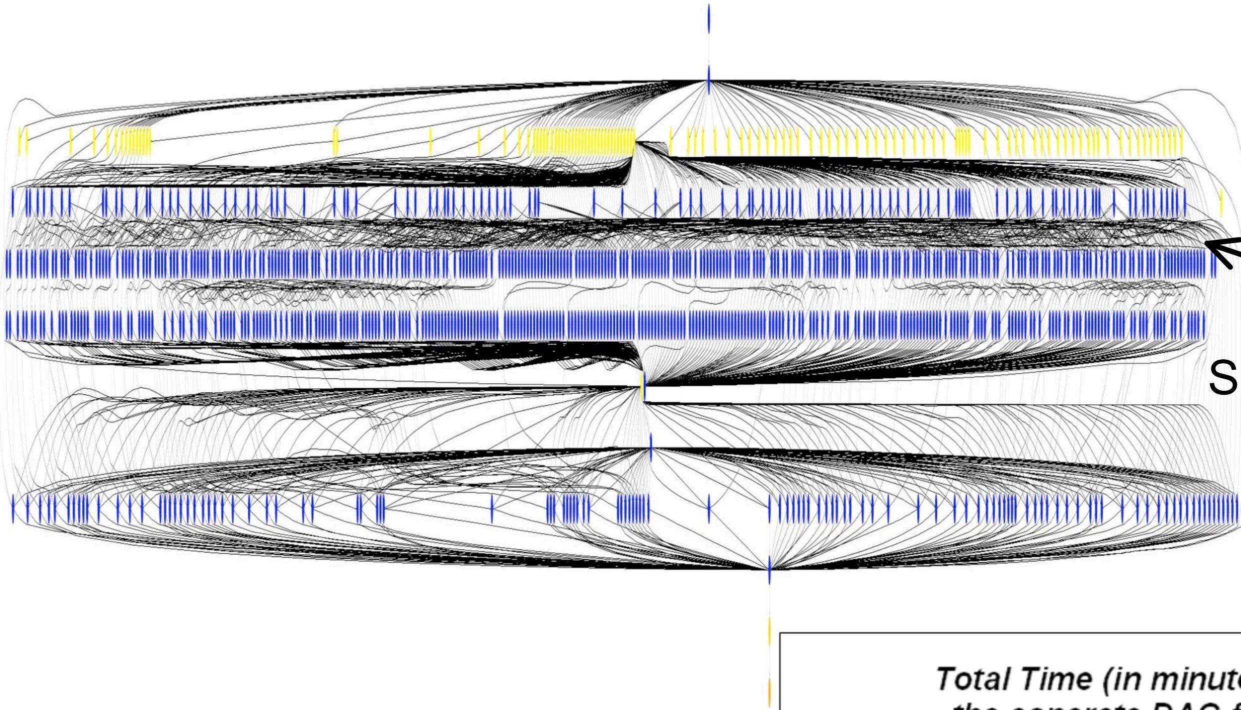
Execution Environment



Node clustering

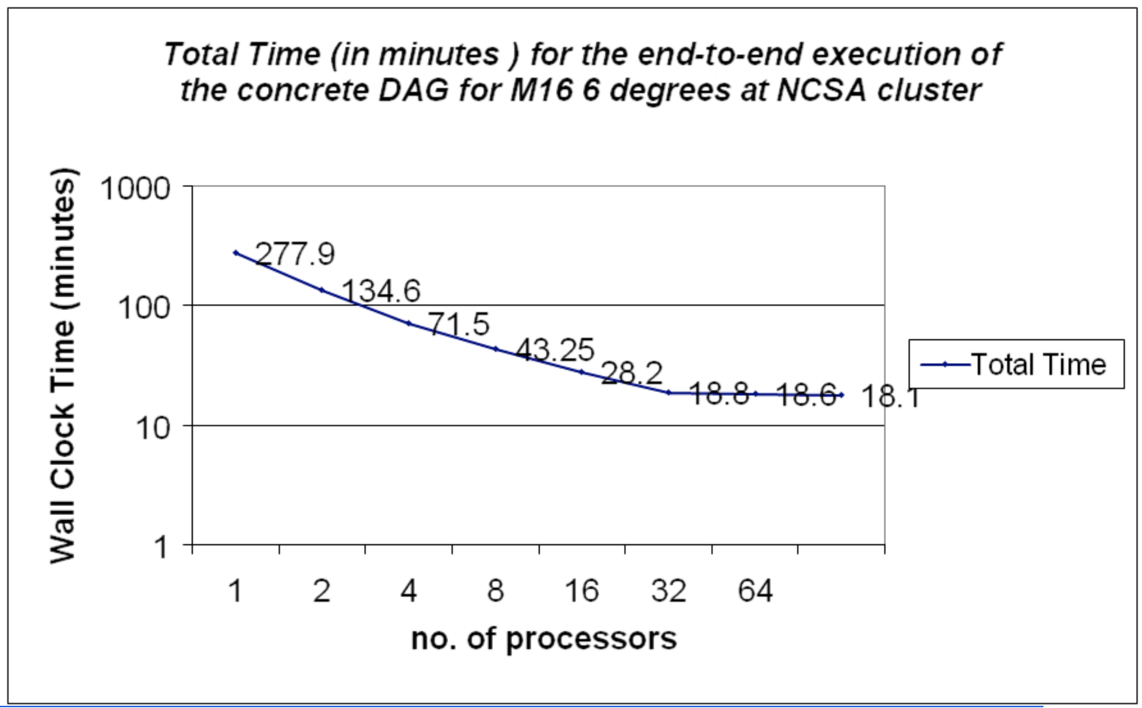


Useful for small granularity jobs



Small 1,200 Montage Workflow

Montage application
~7,000 compute jobs in instance
~10,000 nodes in the executable workflow
same number of clusters as processors
speedup of ~15 on 32 processors



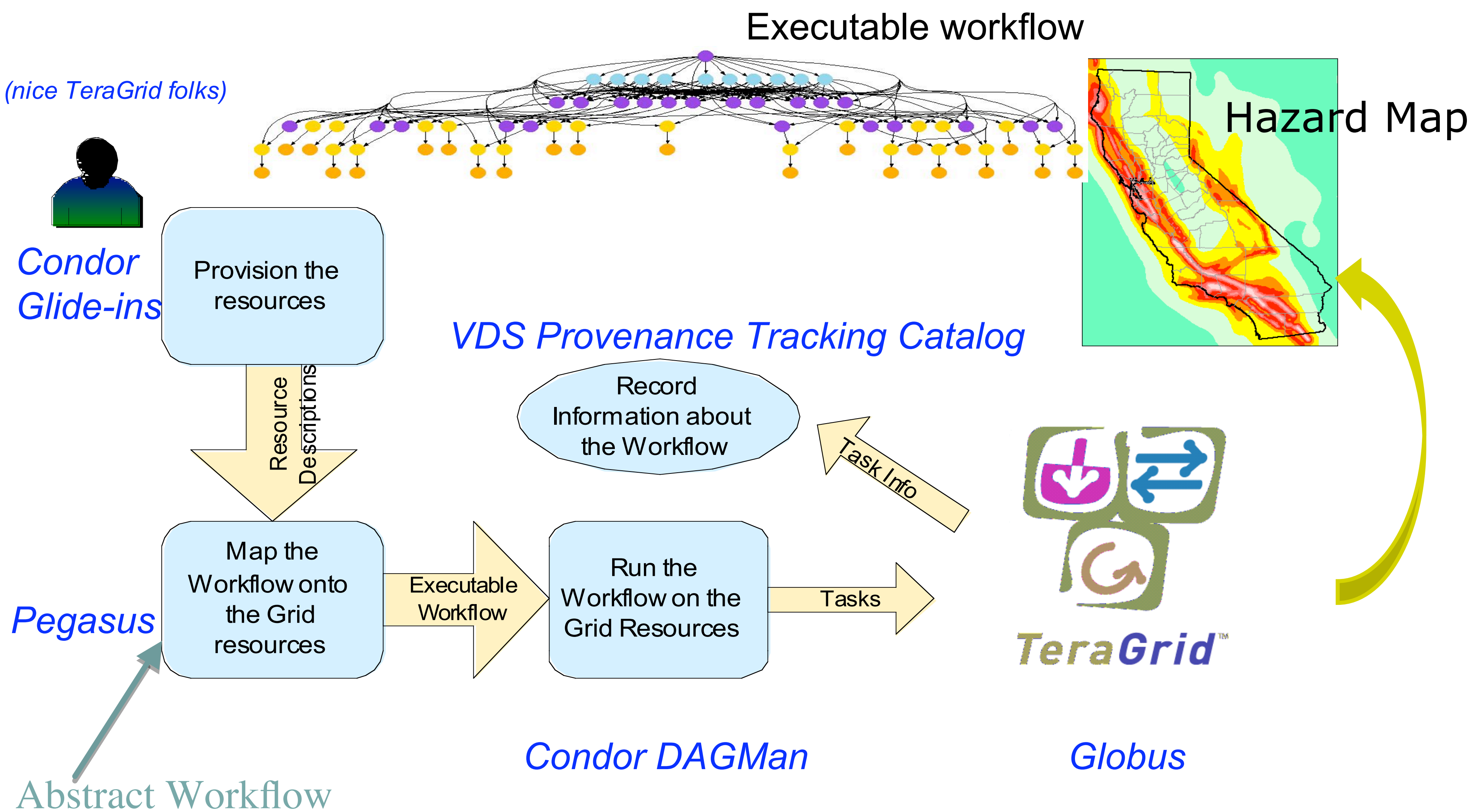
Efficient data handling

- Input data is staged dynamically, new data products are generated during execution
- For large workflows 10,000+ files
  - Similar order of intermediate and output files
  - Total space occupied is far greater than available space—failures occur
- Solution:
  - Determine which data is no longer needed and when
  - Add nodes to the workflow do cleanup data along the way
- Issues:
  - minimize the number of nodes and dependencies added so as not to slow down workflow execution
  - deal with portions of workflows scheduled to multiple sites
  - deal with files on partition boundaries

Challenges in Workflow Execution

- Provide fault tolerance
  - Mask errors, Interact with the workflow planner
- Support resource provisioning
- Provide monitoring information
- Providing execution-level provenance
- Support debugging
  - Provide workflow traces for easy replay

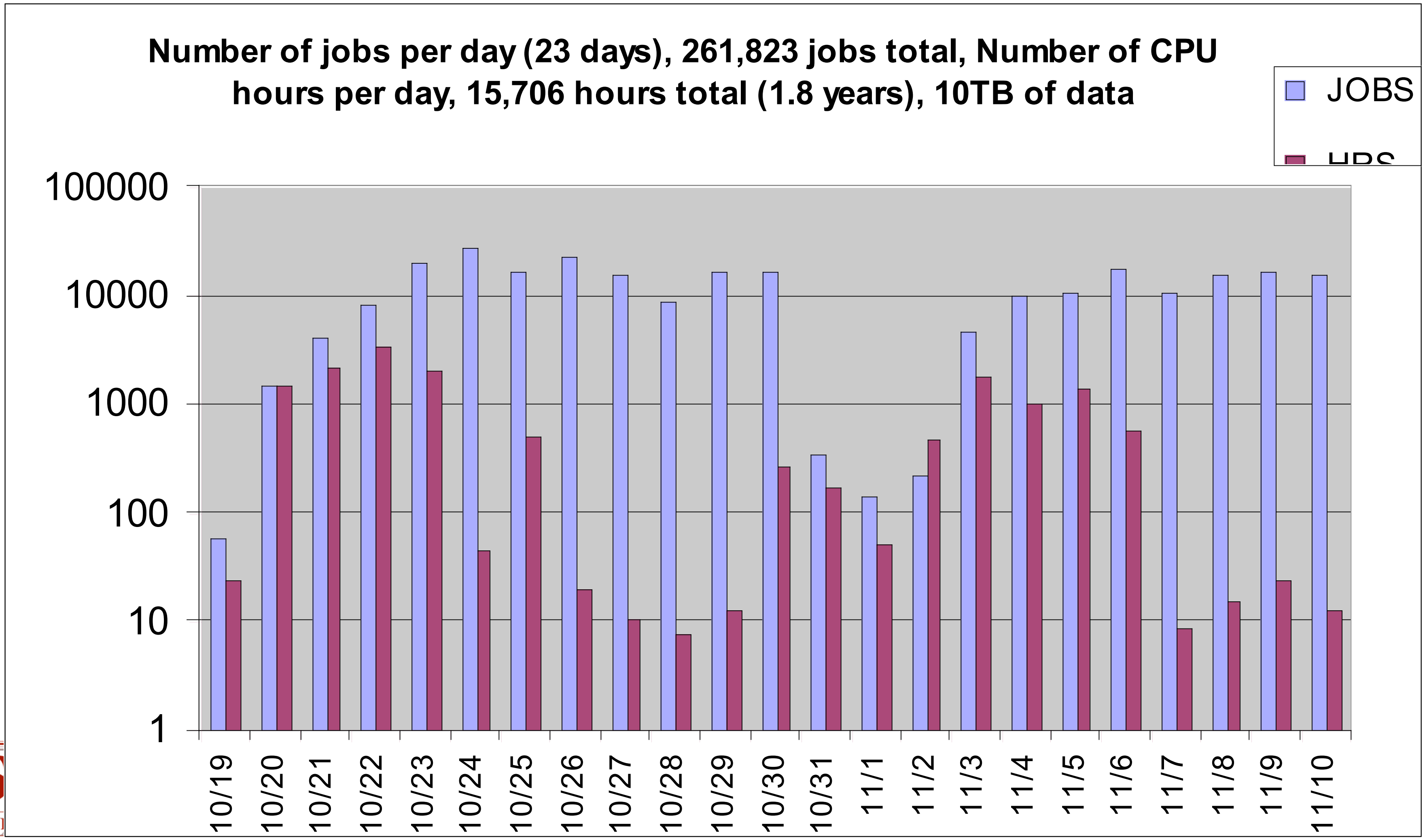
Southern California Earthquake Center (SCEC) workflows on the TeraGrid



Joint work with: R. Graves, T. Jordan, C. Kesselman, P. Maechling, D. Okaya & others

Gurmeet Singh et al. “Application-level Resource Provisioning”, Wednesday, M15, 14:30-16:00 session

SCEC on the TeraGrid Fall 2006



Benefits of Scientific Workflows

(from the point of view of an application scientist)

- Conducts a series of computational tasks.
  - Resources distributed across Internet.
- Chaining (outputs become inputs) replaces manual hand-offs.
  - Accelerated creation of products.
- Ease of use - gives non-developers access to sophisticated codes.
  - Avoids need to download-install-learn how to use someone else's code.
- Provides framework to host or assemble community set of applications.
  - Honors original codes. Allows for heterogeneous coding styles.
- Framework to define common formats or standards when useful.
  - Promotes exchange of data, products, codes. Community metadata.
- Multi-disciplinary workflows can promote even broader collaborations.
  - E.g., ground motions fed into simulation of building shaking.
- Certain rules or guidelines make it easier to add a code into a workflow.

Slide courtesy of David Okaya, SCEC, USC

Workflows for education and sharing

- Application specialists design individual application components
- Domain experts compose workflows using application components
  - Set correct parameters for components
  - Pick appropriate data sets
- Students run sophisticated workflows on training data sets
- Young researchers run sophisticated workflows on data sets of interest to them
- Scientist share workflows across collaborations to validate a hypothesis
- Need to develop tools, workflow libraries, component libraries

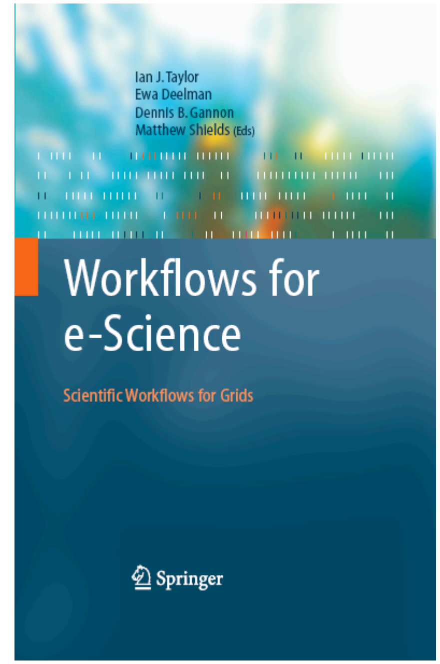
Current and Future Research

- Resource selection
- Resource provisioning
- Workflow restructuring
- Adaptive computing
  - Workflow refinement adapts to changing execution environment
- Workflow provenance (including provenance of the mapping process) – new collaboration with Luc Moreau
- Management and optimization across multiple workflows
- Workflow debugging
- Streaming data workflows
- Automated guidance for workflow restructuring
- Support for long-lived and recurrent workflows

General Conclusions

- Workflows are recipes for CyberInfrastructure
- Need to support the dynamic nature of science
- Support for long-lived and recurrent workflows
- Many challenges and many workflow tools out there
  - Interoperability is desired
- Need common representations that can be used by various workflow management systems
  - Maybe semantic technologies?
- Need common provenance tracking capabilities
  - See IPAW 06, and the Provenance Challenge
- To make forward progress
  - collaboration with application scientists is essential
  - collaboration between workflow system designers is essential

Scientific Workflows—a very active area



- Many workshops
- Special issues of SIGMOD 2005, JOGC 2005, SciProg 2006 (*to appear*)
- Book on e-Science Workflows (Taylor, Deelman, Gannon, Shields eds.) *to appear 2006*
- Bill Gate's SC 2005 Keynote
- NSF Workshop on the Challenges of Scientific Workflows (co-chaired with Yolanda Gil), May 2006, http://vtcpc.isi.edu/wiki

Acknowledgments

- Pegasus is being developed at ISI by Gaurang Mehta, Mei-Hui Su, and Karan Vahi
  - http://pegasus.isi.edu
- Wings is lead by Yolanda Gil, Jihie Kim, Varun Ratnakar
  - www.isi.edu/ikcap/wings/
- DAGMan is lead by Miron Livny
  - www.cs.wisc.edu/condor/
- Many application scientists made the workflows happen (GriPhyN, NVO, LIGO, Telescience, SCEC)