Grid Workflows - Pegasus WMS

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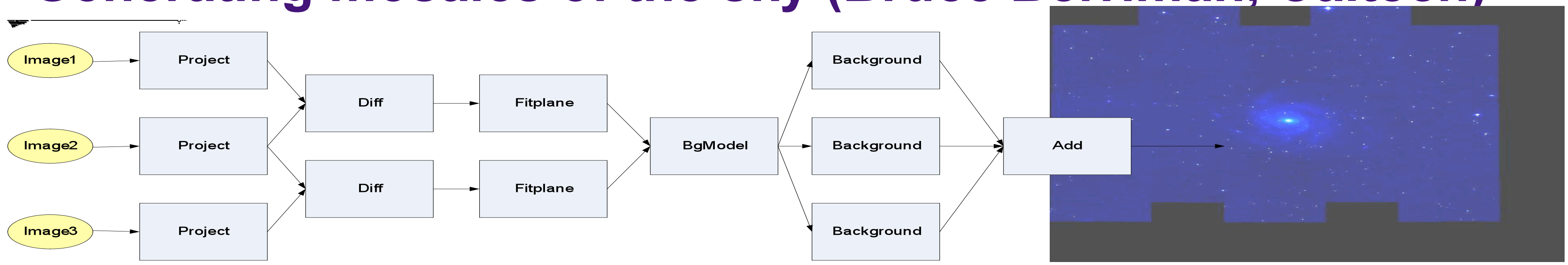
Outline

- What are scientific workflows
- Workflow lifecycle
- Workflow systems
- Pegasus-WMS
  - Pegasus mapper
  - DAGMan workflow engine

Generating mosaics of the sky (Bruce Berriman, Caltech)

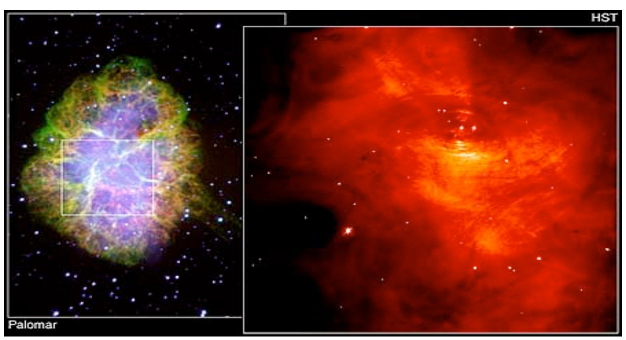


Size of the mosaic is degrees square*	Number of jobs	Number of input data files	Number of Intermediate files	Total data footprint	Approx. execution time (20 procs)
1	232	53	588	1.2GB	40 mins
2	1,444	212	3,906	5.5GB	49 mins
4	**4,856**	**747**	**13,061**	**20GB**	**1hr 46 mins**
6	8,586	1,444	22,850	38GB	2 hrs. 14 mins
10	20,652	3,722	54,434	97GB	6 hours

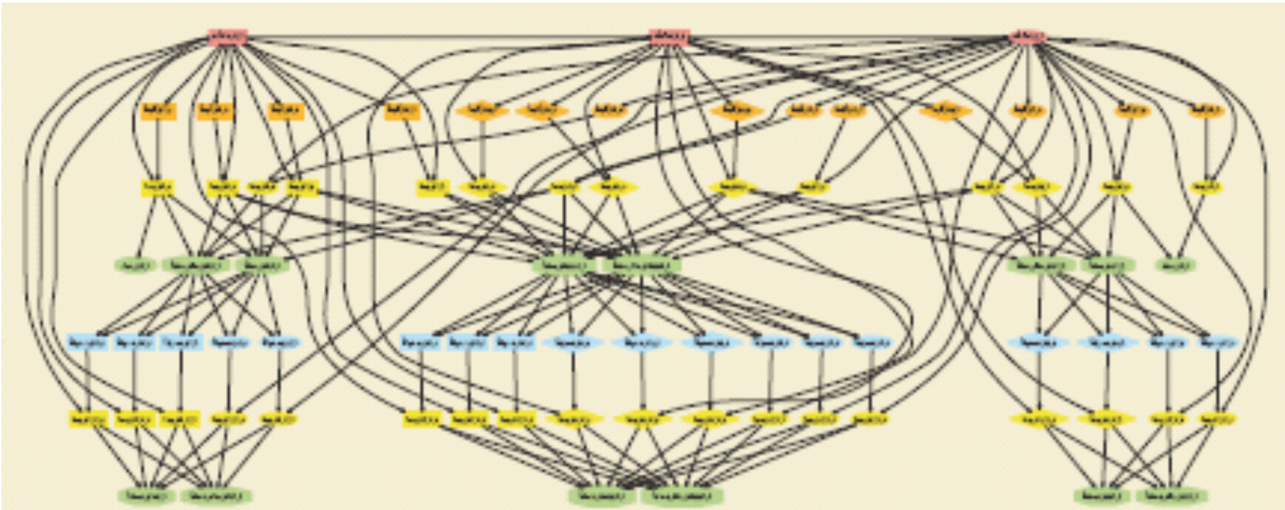
**The full moon is 0.5 deg. sq. when viewed form Earth, Full Sky is ~ 400,000 deg. sq.*

LIGO Scientific Collaboration

- Continuous gravitational waves are expected to be produced by a variety of celestial objects
- Only a small fraction of potential sources are known
- Need to perform blind searches, scanning the regions of the sky where we have no a priori information of the presence of a source
  - Wide area, wide frequency searches
- Search is performed for potential sources of continuous periodic waves near the Galactic Center and the galactic core
- Search for binary inspirals collapsing into black holes.
- The search is very compute and data intensive



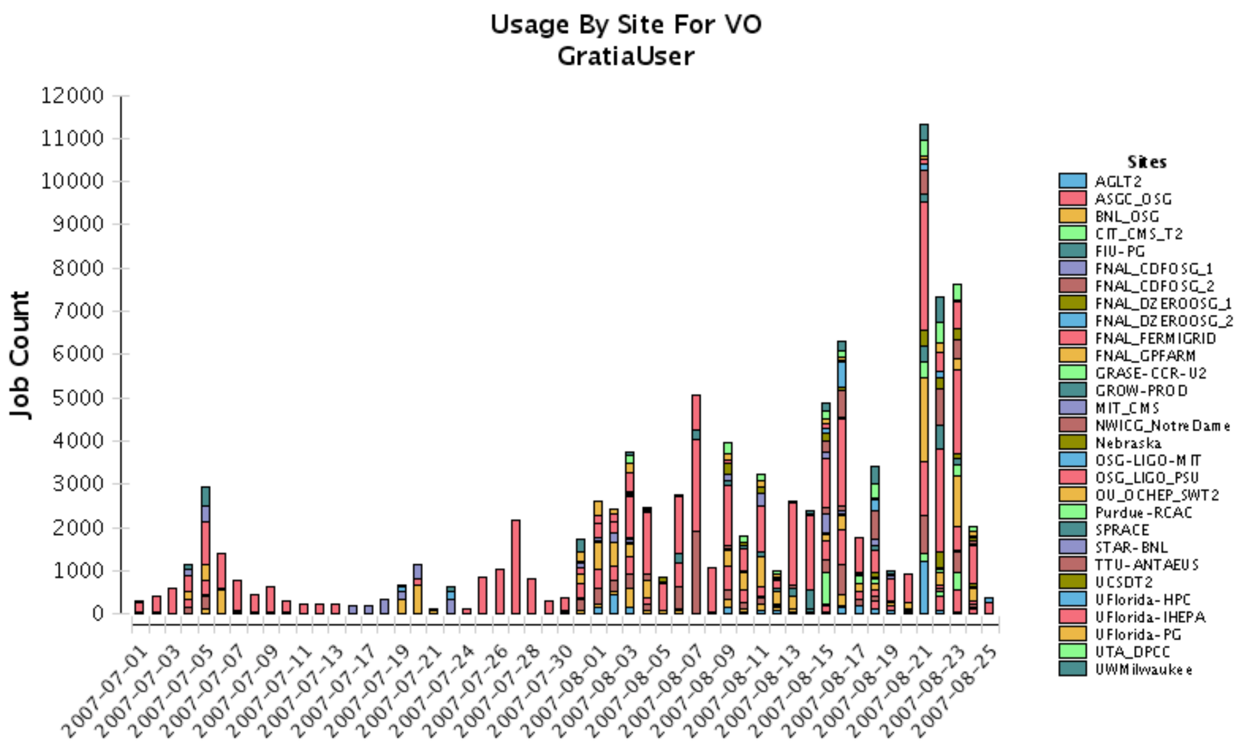
Pegasus Applications-LIGO



Support for LIGO on Open Science Grid

LIGO Workflows: 185,000 nodes, 466,000 edges 10 TB of input data, 1 TB of output data.

LIGO Collaborators: Kent Blackburn, Duncan Brown, Britta Daubert, Scott Koranda, Stephen Fairhurst, and others



Scientific Workflows

- Capture individual data transformation and analysis steps
- Large monolithic applications broken down to smaller jobs.
  - Smaller jobs can be independent or connected by some control flow/ data flow dependencies.
  - Usually expressed as a Directed Acyclic Graph of tasks

- Allows the scientists to modularize their application
- Scaled up execution over several computational resources

Types of Workflow Applications

- **Providing a service to a community (Montage project)**
  - Data and derived data products available to a broad range of users
  - A limited number of small computational requests can be handled locally
  - For large numbers of requests or large requests need to rely on shared cyberinfrastructure resources
  - On-the fly workflow generation, portable workflow definition
- **Supporting community-based analysis (SCEC project)**
  - Codes are collaboratively developed
  - Codes are "strung" together to model complex systems
  - Ability to correctly connect components, scalability
- **Processing large amounts of shared data on shared resources (LIGO project)**
  - Data captured by various instruments and cataloged in community data registries.
  - Amounts of data necessitate reaching out beyond local clusters
  - Automation, scalability and reliability

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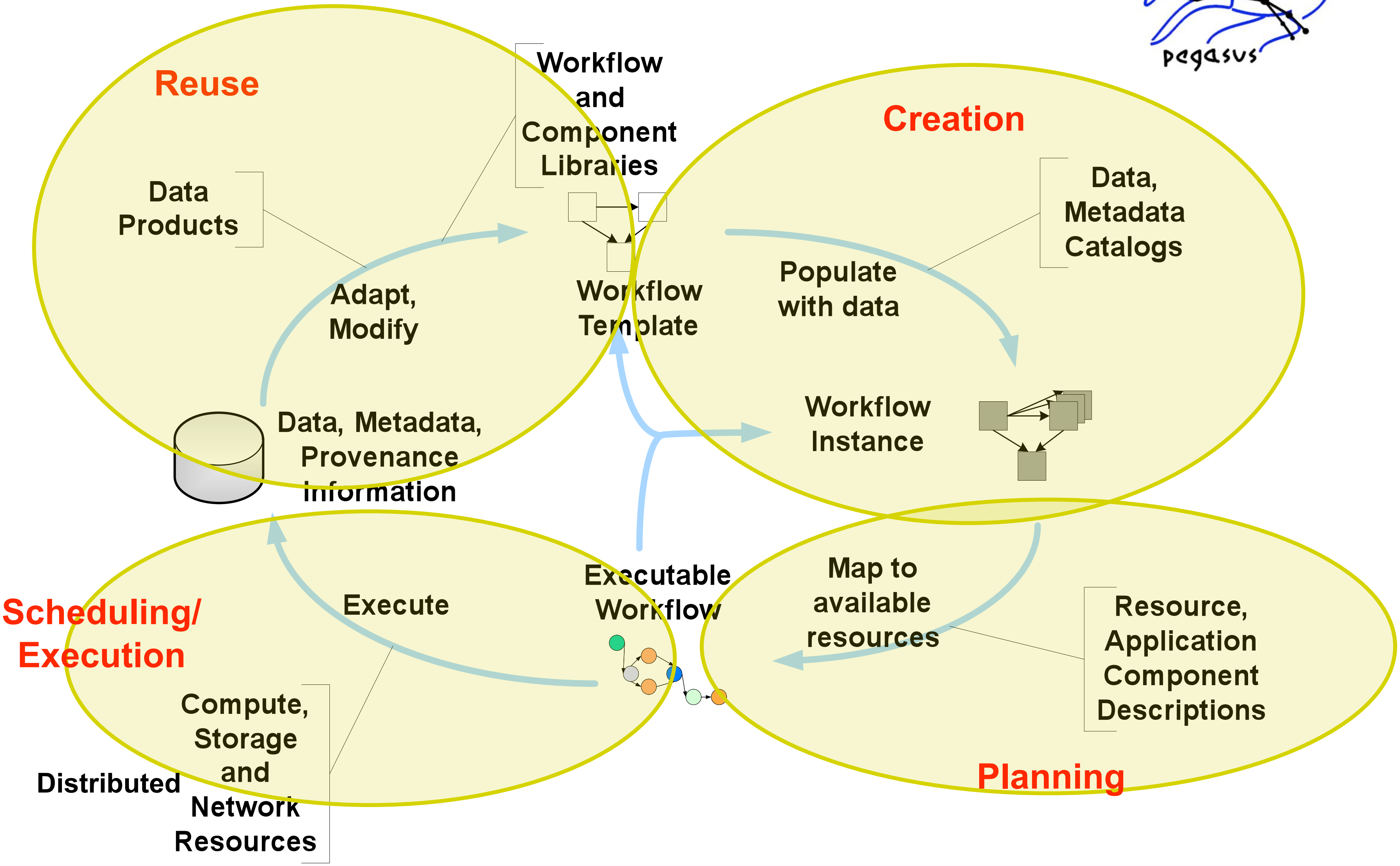
Workflow Lifecycle



Workflow Creation

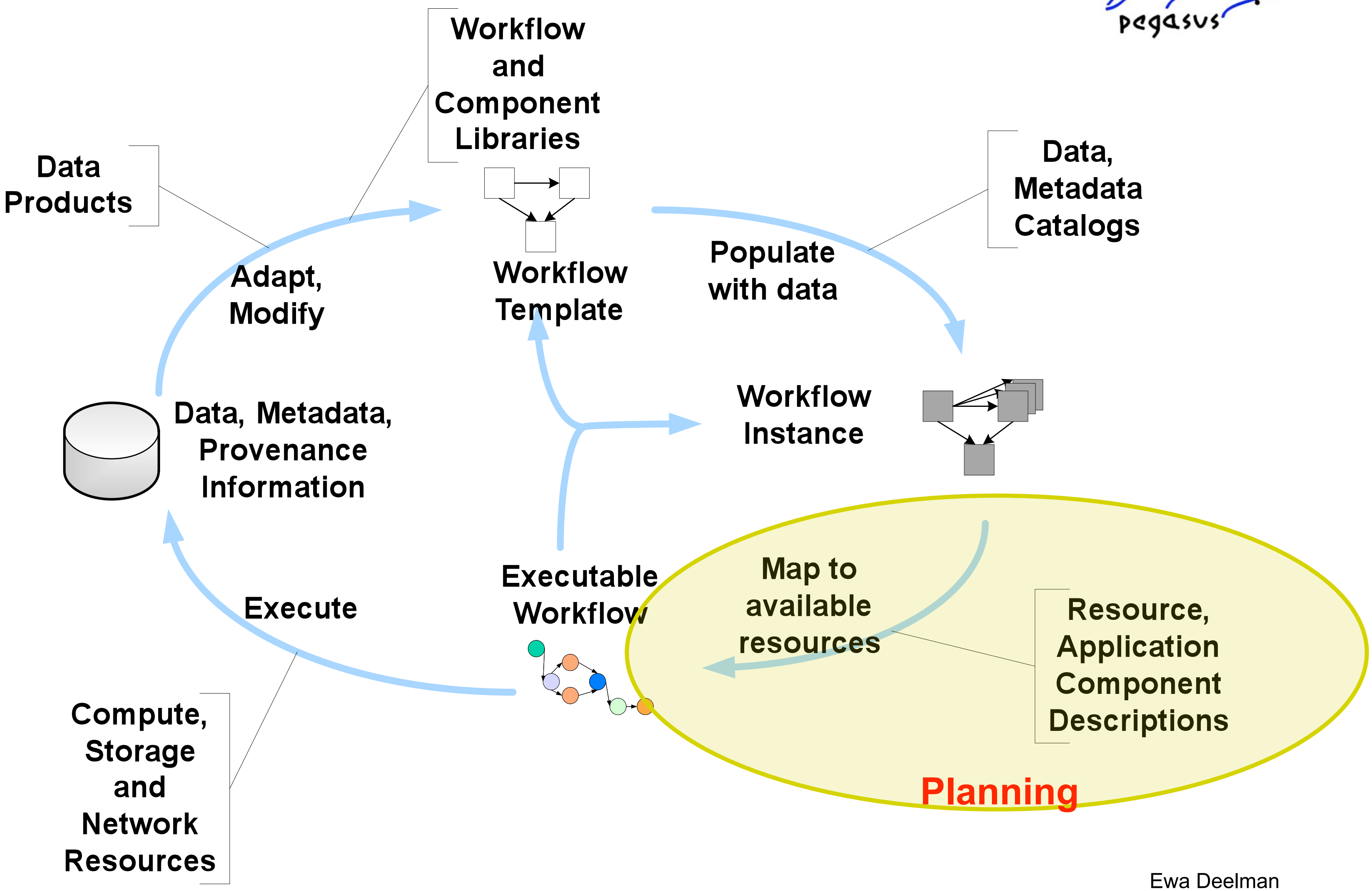
- Design a workflow (semantics info needed)
  - Find the right components
  - Set the right parameters
  - Find the right data
  - Connect appropriate pieces together
  - Find the right fillers

- Support both experts and novices

Challenges in user experiences

- Users' expectations vary greatly
  - High-level descriptions
  - Detailed plans that include specific resources
- Users interactions can be exploratory
    - Or workflows can be iterative
  - Modifying portions of the workflow as the computation progresses
- Users need progress, failure information at the right level of detail
- There is no ONE user but many users with different knowledge and capabilities

Workflow Lifecycle



Specification: Place Y = F(x) at L
Execution Environment: Distributed

- Find where x is--- {S1,S2, …}
- Find where F can be computed--- {C1,C2, …}
- Choose *c* and *s* subject to constraints (performance, space availability,….)
- Move x from *s* to *c*

Error! ***x*** **was not at** ***s!***

  - *Move F to c*

Error! ***F(x)*** **failed!**

- Compute F(x) at *c*
- Move Y from *c* to L

Error! ***c*** **crashed!**

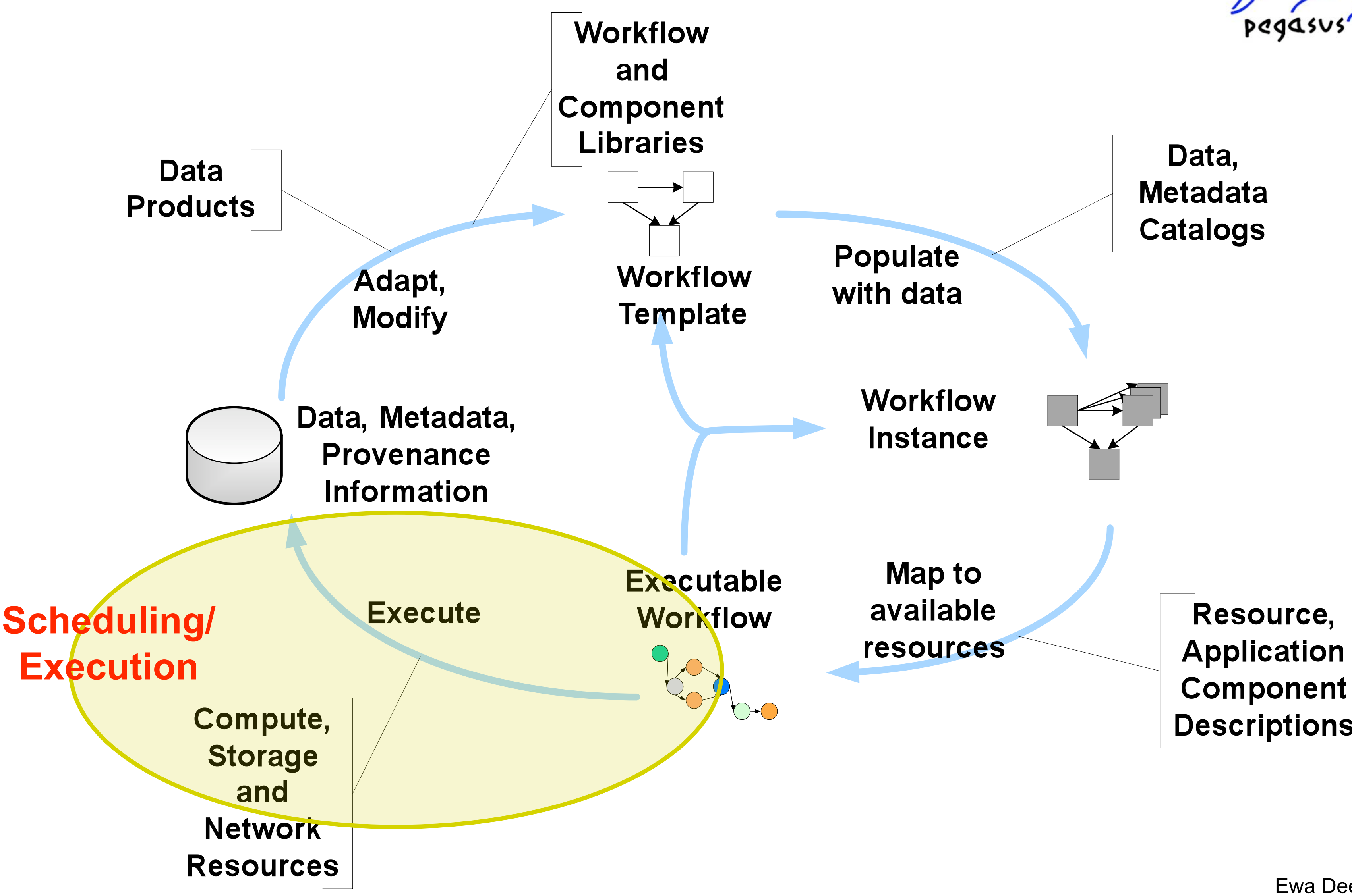
- Register Y in data registry
- Record provenance of Y, performance of F(x) at c

Error! ***there is not enough*** **space at L!**

Some challenges in workflow mapping

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

Workflow Lifecycle



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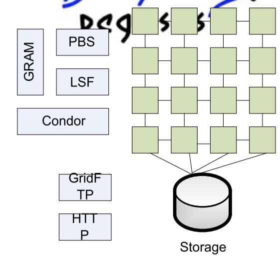
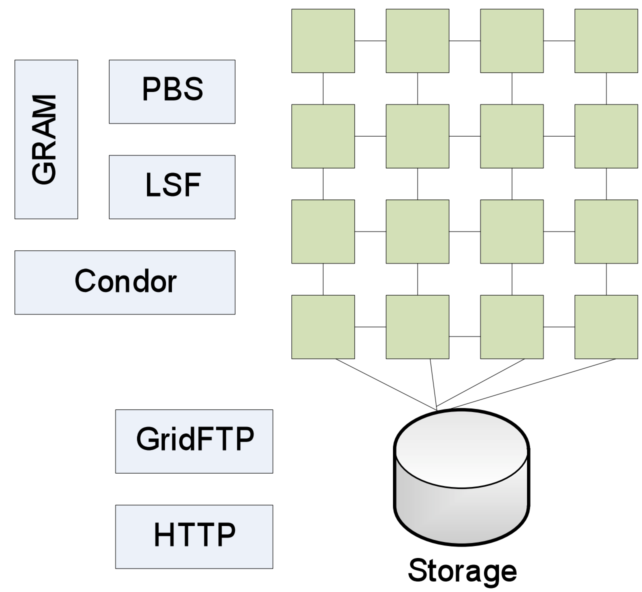
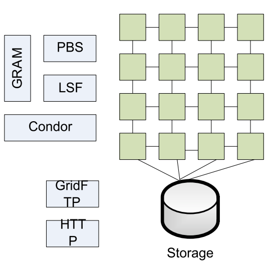
Execution Environment

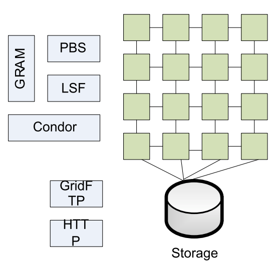


Globus and Condor Services for job scheduling
Globus Services for data transfer and Cataloging

Information Services:
--- information about data location
--- information about the execution sites



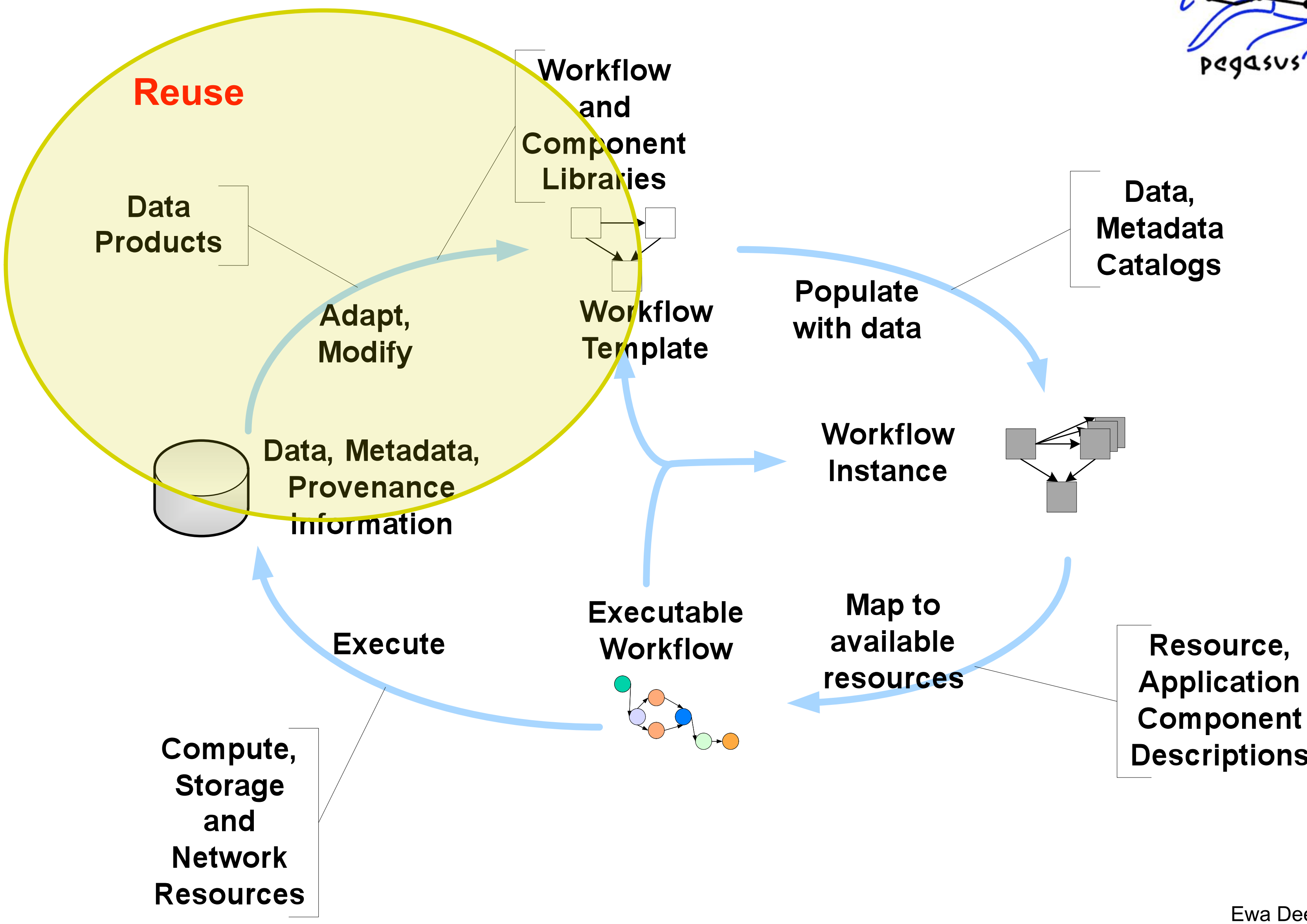




Challenges in Workflow Execution

- Resource provisioning
  - Which resources to provision if many possibilities?
  - How many resources to provision?
  - For how long?
- Fault Tolerance
  - How to recognize different types of failures
  - How to recover from failures?
- Efficient collaboration between the data and computation management systems
- Debugging
  - How to relate the workflow result (outcome) to workflow specification

Workflow Lifecycle



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Challenges in reuse and sharing

- How to find what is already there
- How to determine the quality of what's there
- How to invoke an existing workflow
- How to share a workflow with a colleague
- How to share a workflow with a competitor

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Swift programs

- A Swift script is a set of **functions**
  - Atomic functions wrap & invoke application programs
  - Composite functions invoke other functions
- Data is **typed** as composable arrays and structures of files and simple scalar types (int, float, string)
- Collections of **persistent file structures** (datasets) are **mapped** into this data model
- Members of datasets can be processed in **parallel**
- Statements in a procedure are executed in **data-flow** dependency order and concurrency
- Variables are **single assignment**
- **Provenance** is gathered as scripts execute

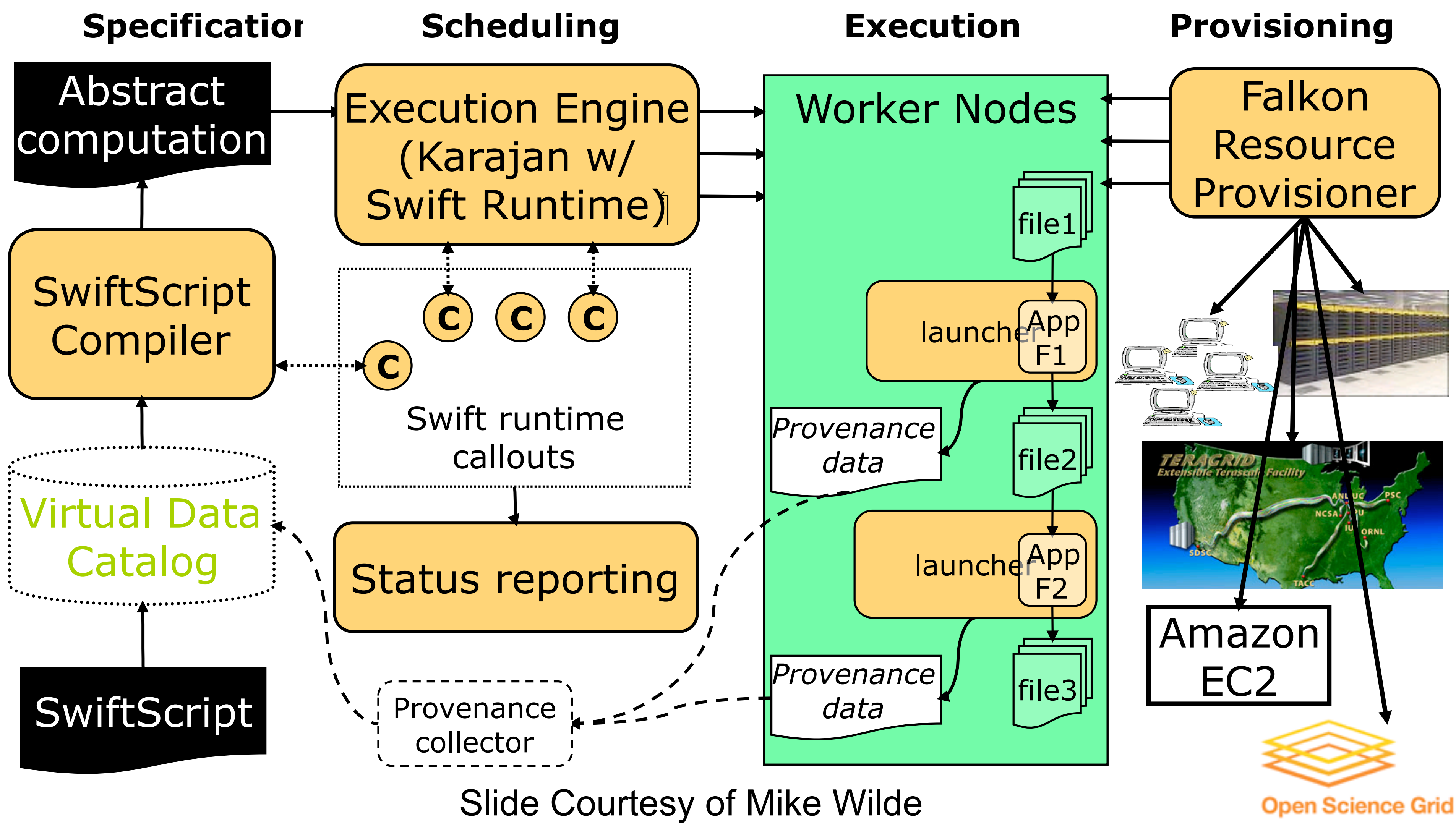
Slide Courtesy of Mike Wilde

Swift

- Clean separation of logical/physical concerns
  - XDTM specification of logical data structures
- Concise specification of parallel programs
  - SwiftScript, with iteration, etc.
- Efficient execution (on distributed resources)
  - **Karajan+Falkon**:
  - Grid Interface, light dispatch, pipelining, clustering, provisioning
- Rigorous provenance tracking and query
  - Records provenance data of each job executed

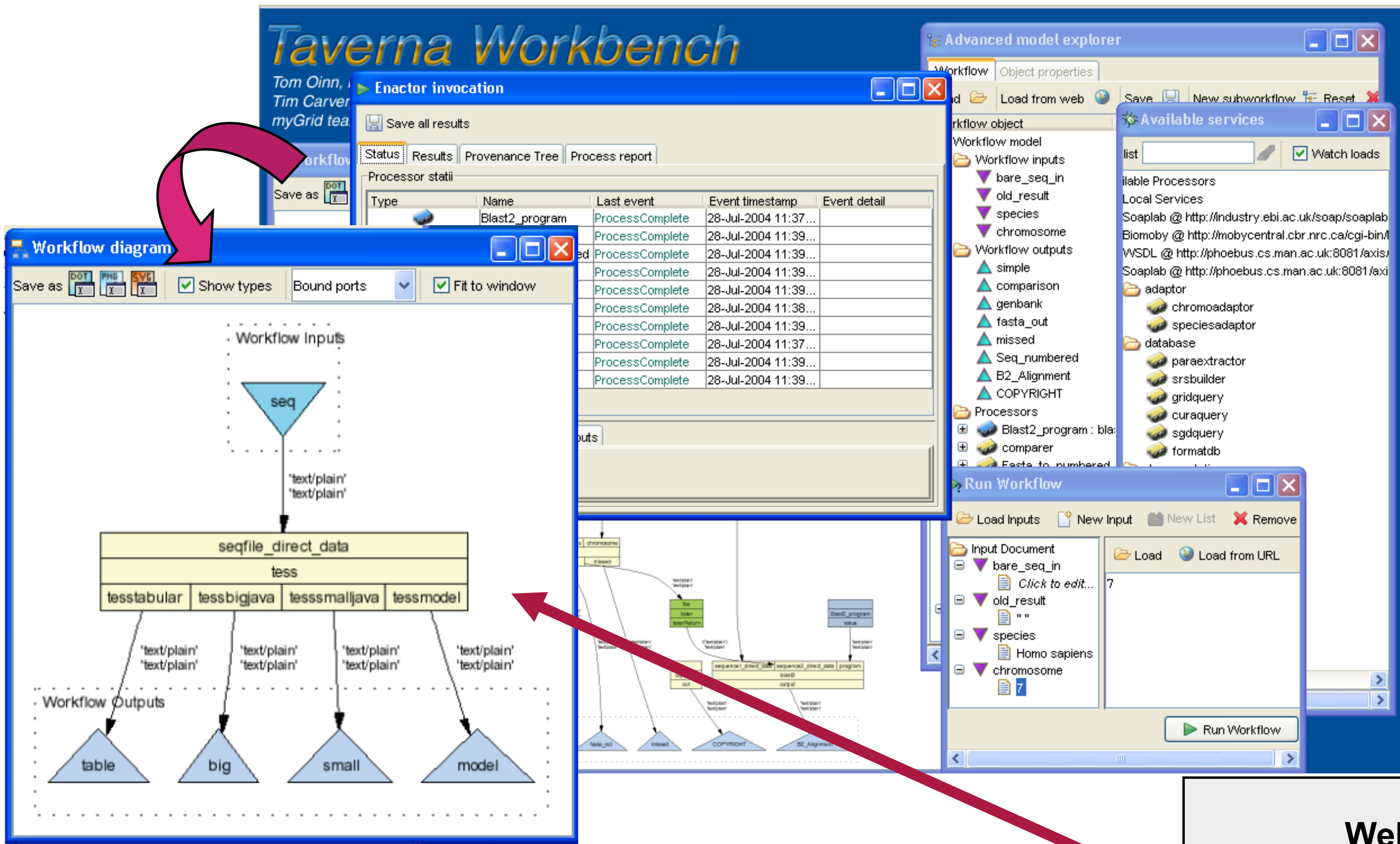
Slide Courtesy of Mike Wilde

Swift Architecture



Slide Courtesy of Mike Wilde

Taverna Workbench



Web S e.g. DDBJ BLAST

SOAP Web S Any Application

Scufl Simple Conceptual Unified Flow Language

Taverna Writing, running workflows & examining results

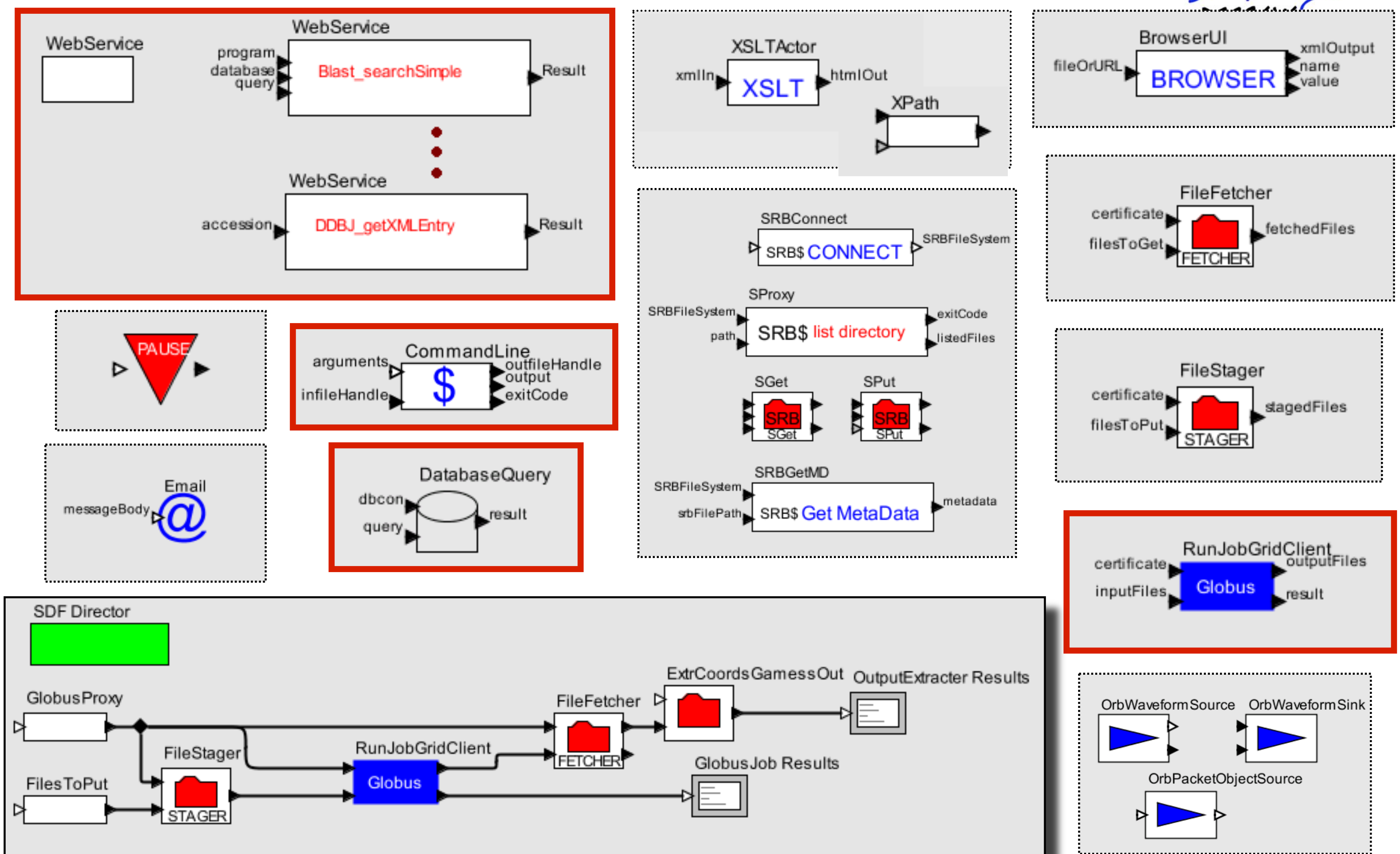
SOAPLAB Makes applications available

Slides courtesy of Katy Wolstencroft

Kepler (UCSD)

- Kepler is a software application for the analysis and modeling of scientific data
  - Builds on Ptolemy II framework and provides a GUI to construct workflows
- Actor Oriented Modeling
  - Each actor has input/output ports
  - Parameters are static ports
- Data Connections
  - Unidirectional communication channels connect output to input ports
- Composite Actors
  - Wrap sub workflows
  - Arbitrary Nesting
- Directors
  - Define the execution semantics of workflow graph
  - executes workflow graph (some schedule)
  - sub-workflows may have different directors promotes reusability

Everything is a service / actor…



Slides courtesy of Bertram Ludaesher

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Pegasus-Workflow Management System
a layered approach

A reliable, scalable workflow management system that an application or workflow composition service can depend on to get the job done

Workflow Mapping System	A decision system that develops strategies for reliable and efficient execution in a variety of environments
Workflow Execution System	Reliable and scalable execution of dependent tasks
Task Execution System	Reliable, scalable execution of independent tasks (locally, across the network), priorities, scheduling

Cyberinfrastructure: Local machine, cluster, Condor pool, Grid

Pegasus Workflow Management System

Abstract Workflow

A reliable, scalable workflow management system that an application or workflow composition service can depend on to get the job done

Pegasus mapper
DAGMan
Condor Schedd

A decision system that develops strategies for reliable and efficient execution in a variety of environments

Reliable and scalable execution of dependent tasks

Reliable, scalable execution of independent tasks (locally, across the network), priorities, scheduling

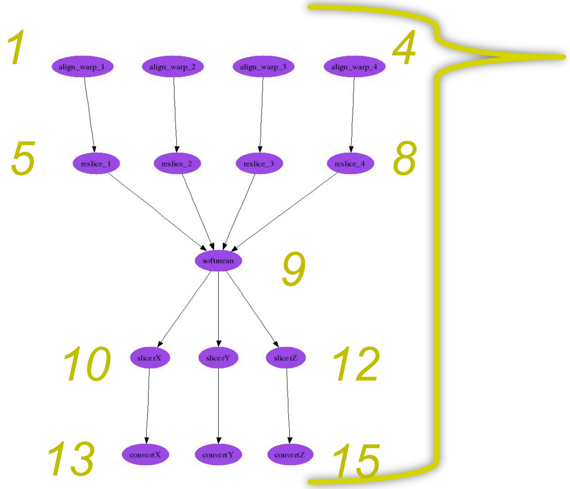
Cyberinfrastructure: Local machine, cluster, Condor pool, OSG, TeraGrid

Pegasus-Workflow Management System

- Leverages abstraction for workflow description to obtain ease of use, scalability, and portability
- Provides a compiler to map from high-level descriptions (workflow instances) to executable workflows
  - Correct mapping
  - Performance enhanced mapping
- Provides a runtime engine to carry out the instructions (Condor DAGMan)
  - Scalable manner
  - Reliable manner

In collaboration with Miron Livny, UW Madison, funded under NSF-OCI SDCI

Pegasus Workflow Mapping



Original workflow: 15 compute nodes devoid of resource assignment

Resulting workflow mapped onto 3 Grid sites:

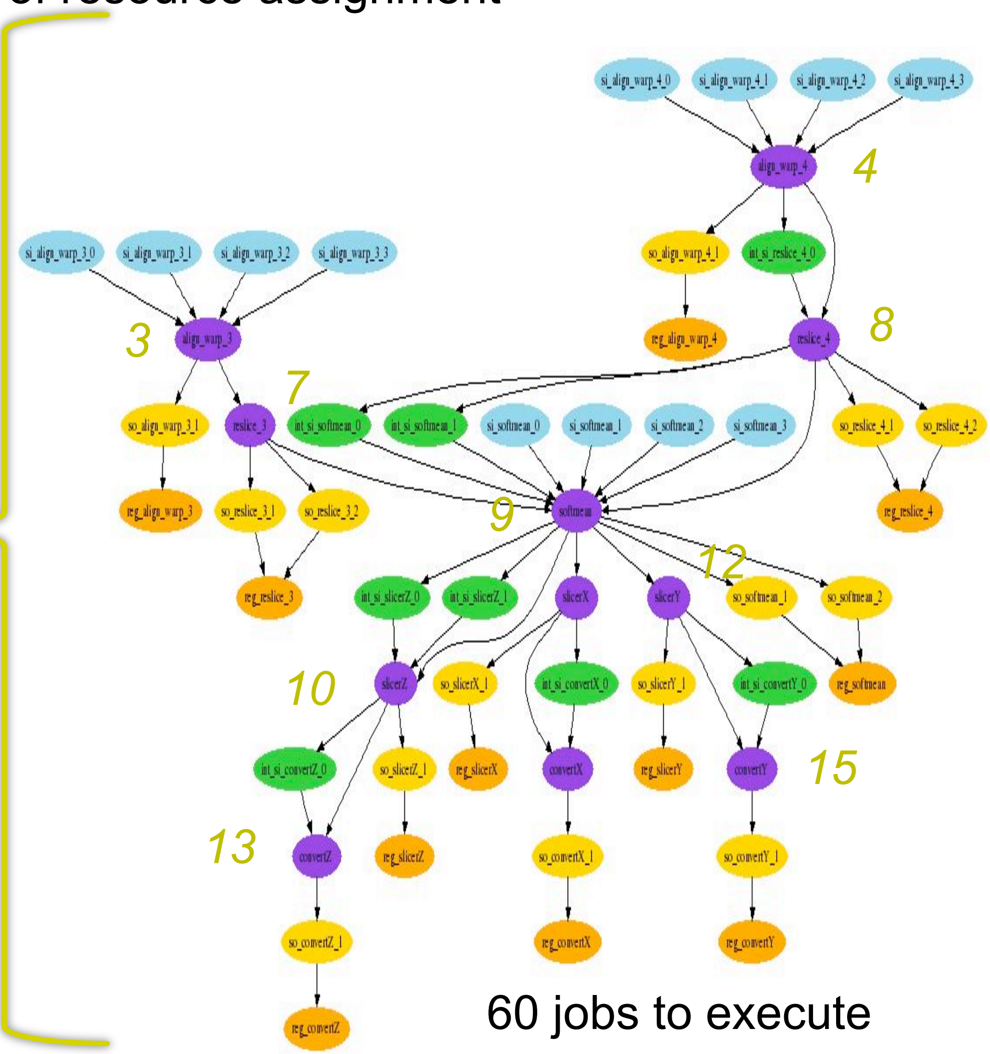
11 compute nodes (4 reduced based on available intermediate data)

12 data stage-in nodes

8 inter-site data transfers

14 data stage-out nodes to long-term storage

14 data registration nodes (data cataloging)



60 jobs to execute

Mapping Correctly

- Select where to run the computations
  - Apply a scheduling algorithm
    - HEFT, min-min, round-robin, random
    - Schedule in a data-aware fashion (data transfers, amount of storage)
    - The quality of the scheduling depends on the quality of information
  - Transform task nodes into nodes with executable descriptions
    - Execution location
    - Environment variables initializes
    - Appropriate command-line parameters set
- Select which data to access
  - Add stage-in nodes to move data to computations
  - Add stage-out nodes to transfer data out of remote sites to storage
  - Add data transfer nodes between computation nodes that execute on different resources
- Add nodes to create an execution directory on a remote site

Additional Mapping Elements

- Cluster compute nodes in small granularity applications
- Add data cleanup nodes to remove data from remote sites when no longer needed
  - reduces workflow data footprint
- Add nodes that register the newly-created data products
- Provide provenance capture steps
  - Information about source of data, executables invoked, environment variables, parameters, machines used, performance
- Scale matters--today we can handle:
  - 1 million tasks in the workflow instance (SCEC)
  - 10TB input data (LIGO)

Running in different environments

- Need to specify pegasus namespace profile keys with the sites in the site catalog.

- Submitting directly to condor pool
  - The submit host is a part of a local condor pool
  - Bypasses CondorG submissions avoiding Condor/GRAM delays.

- Using Condor GlideIn
  - User glides in nodes from a remote grid site to his local pool
  - Condor is deployed dynamically on glided in nodes for e.g. you glide in nodes from the teragrid site running PBS.
  - Only have to wait in the remote queue once when gliding in nodes.

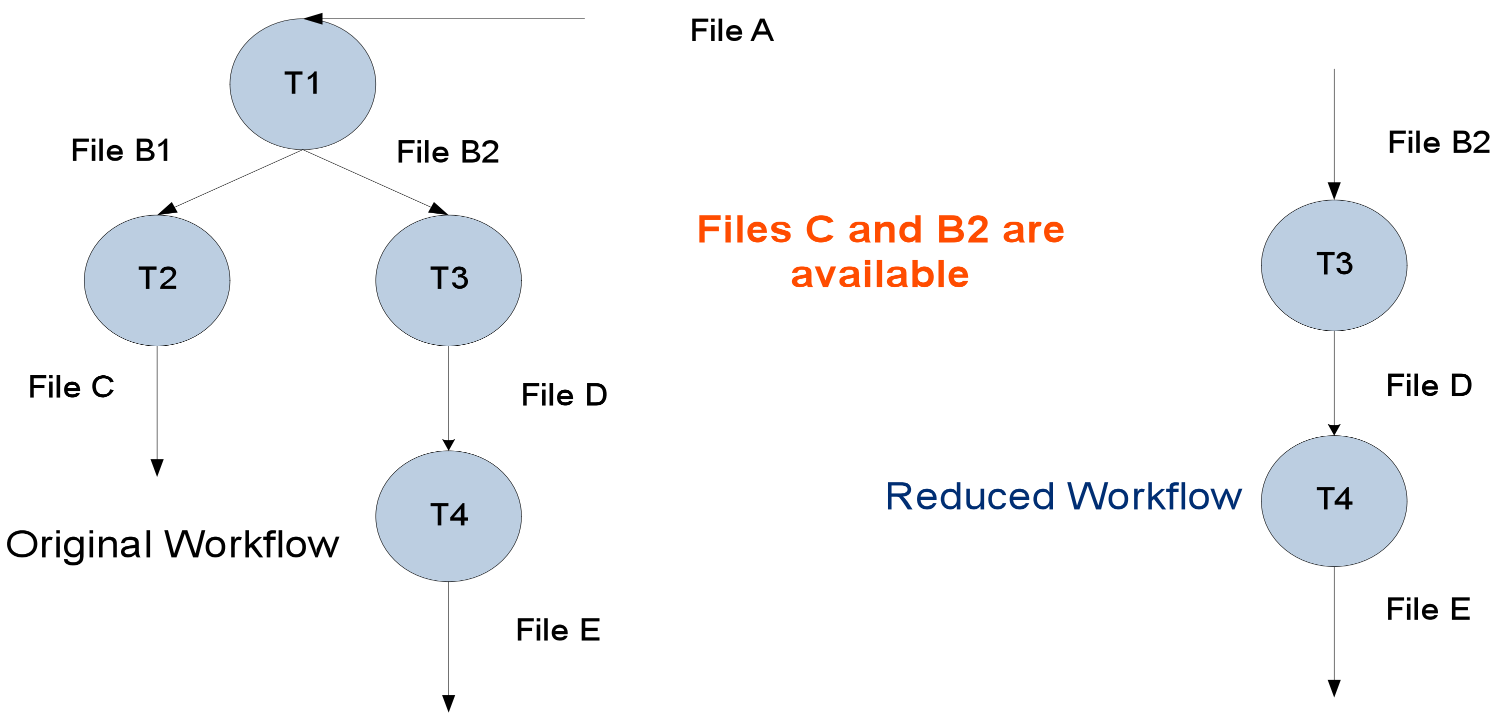
Optimizations during Mapping

- Node clustering for fine-grained computations
  - Can obtain significant performance benefits for some applications (in Montage ~80%, SCEC ~50%)
- Data reuse in case intermediate data products are available
  - Performance and reliability advantages—workflow-level checkpointing
- Data cleanup nodes can reduce workflow data footprint
  - by ~50% for Montage, applications such as LIGO need restructuring
- Workflow partitioning to adapt to changes in the environment
  - Map and execute small portions of the workflow at a time

Data Reuse

Sometimes it is cheaper to access the data than to regenerate it

Keeping track of data as it is generated supports workflow-level checkpointing

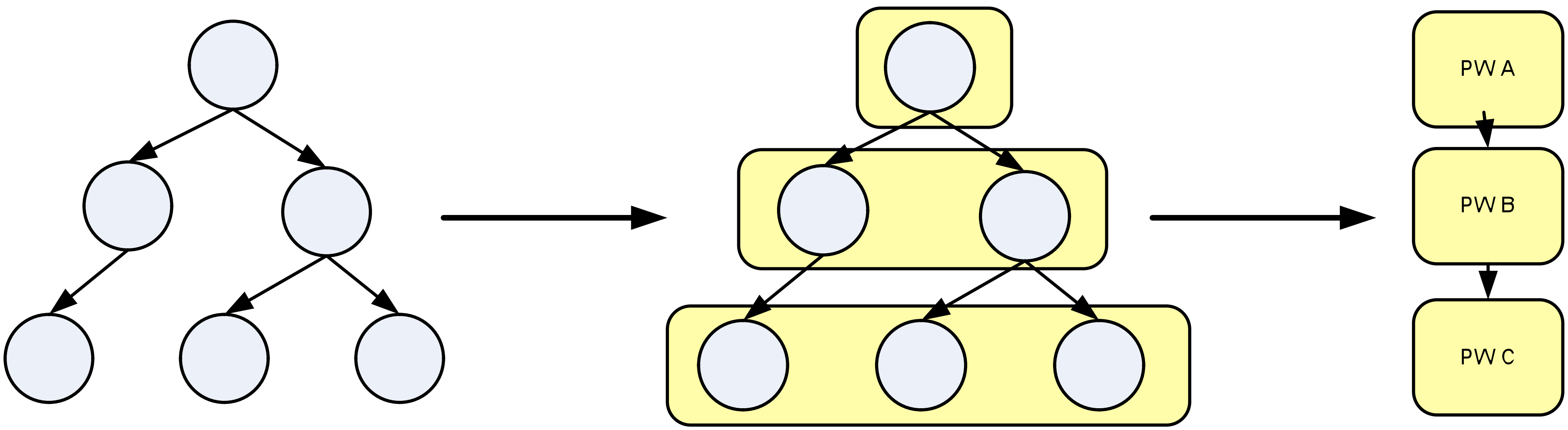


Mapping Complex Workflows Onto Grid Environments, E. Deelman, J. Blythe, Y. Gil, C. Kesselman, G. Mehta, K. Vahi, K. Backburn, A. Lazzarini, A. Arbee, R. Cavanaugh, S. Koranda, *Journal of Grid Computing, Vol.1, No. 1, 2003., pp25-39.*

File cleanup

- Problem: Running out of space on shared scratch
  - In OSG scratch space is limited to 30Gb for all users
- Why does it occur
  - Workflows bring in huge amounts of data
  - Data is generated during workflow execution
  - Users don’t worry about cleaning up after they are done
- Solution
  - Do cleanup after workflows finish
    - Does not work as the scratch may get filled much before during execution.
  - Interleave cleanup automatically during workflow execution.
    - Requires an analysis of the workflow to determine, when a file is no longer required.

Managing execution environment changes through partitioning



Original Abstract Workflow

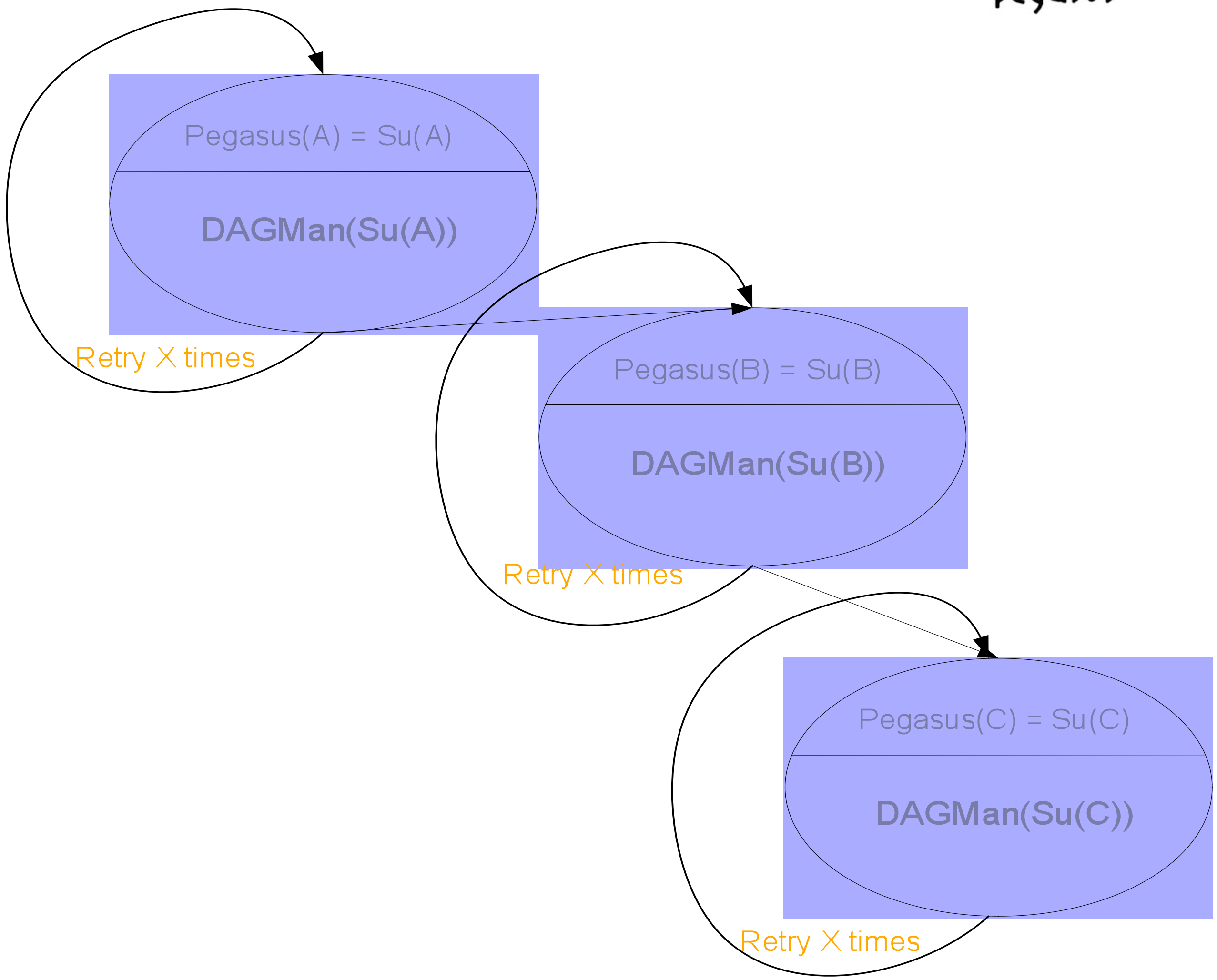
A Particular Partitioning

New Abstract Worfklow

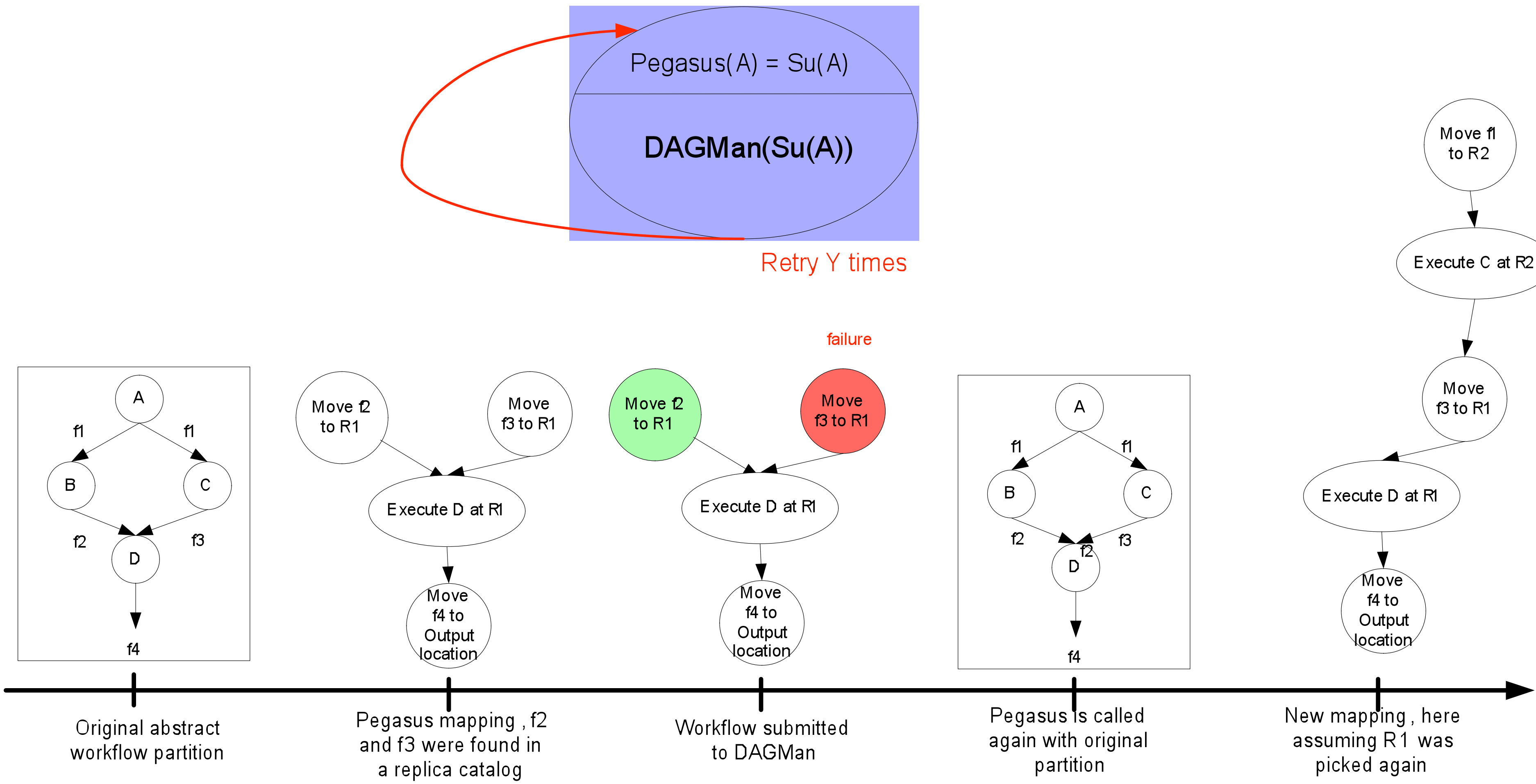
Resulting Meta-Workflow

Pegasus(X): Pegasus generates the concrete workflow and the submit files for Partition X -- Su(X)

DAGMan(Su(X): DAGMan executes the concrete workflow for X



Workflow-level checkpointing



DAGMan ("under the hood" of Pegasus)

- Pegasus uses DAGMan to run the executable workflow
- Users may not have to interact with DAGMan directly…
- …but they may (for debugging, optimization)
- Pegasus doesn't expose all DAGMan features

DAGMan (Directed Acyclic Graph MANager)

- Runs workflows that can be specified as Directed Acyclic Graphs
- Enforces DAG dependencies
- Progresses as far as possible in the face of failures
- Provides retries, throttling, etc.
- Runs on top of Condor (and is itself a Condor job)
- Doesn’t “care” whether node jobs are local or Grid jobs

Reliability Features of Pegasus-WMS

- Provides workflow-level checkpointing through data re-use
- Allows for automatic re-tries of
  - task execution
  - overall workflow execution
  - workflow mapping
- Tries alternative data sources for staging data
- Provides a rescue-DAG when all else fails

- Clustering techniques can reduce some of failures
  - Reduces load on CI services

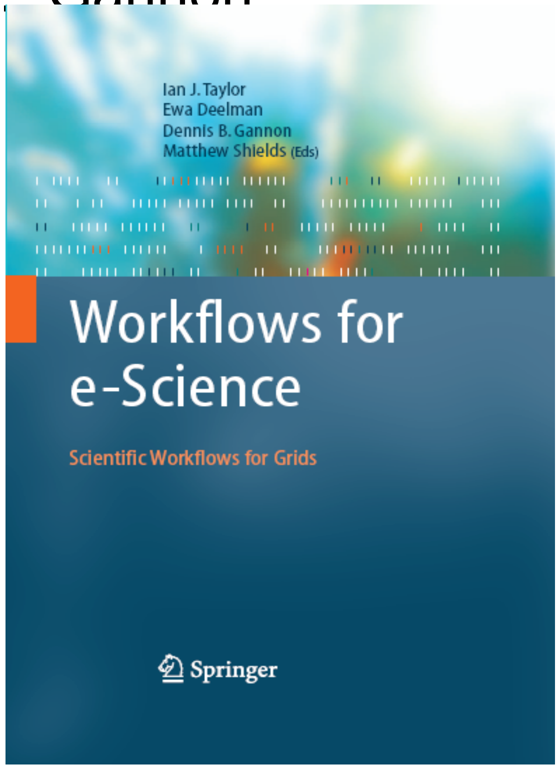
Acknowledgments

- Pegasus: Ewa Deelman, Mei-Hui Su, Karan Vahi, Arun Ramakrishnan (USC)
- DAGMan (in Pegasus-WMS): Miron Livny, and the Condor team (Wisconsin Madison)
- Wings: Yolanda Gil, Jihie Kim, Varun Ratnakar, Paul Groth (USC)
- LIGO: Kent Blackburn, Duncan Brown, Stephen Fairhurst, Scott Koranda (Caltech)
- Montage: Bruce Berriman, John Good, Dan Katz, and Joe Jacobs (Caltech, JPL)
- SCEC: Tom Jordan, Robert Graves, Phil Maechling, David Okaya, Li Zhao (USC, UCSD, others)

Relevant Links

- Pegasus: pegasus.isi.edu
- DAGMan: www.cs.wisc.edu/condor/dagman
- For more questions: pegasus@isi.edu

- NSF Workshop on Challenges of Scientific Workflows : www.isi.edu/nsf-workflows06, E. Deelman and Y. Gil (chairs)
- Workflows for e-Science, Taylor, I.J.; Deelman, E.; Gannon D.B.; Shields, M. (Eds.), Dec. 2006



- Open Science Grid: www.opensciencegrid.org
- LIGO: www.ligo.caltech.edu/
- SCEC: www.scec.org
- Montage: montage.ipac.caltech.edu/
- Condor: www.cs.wisc.edu/condor/
- Globus: www.globus.org
- TeraGrid: www.teragrid.org