Scientific Workflows on the Grid

Goals

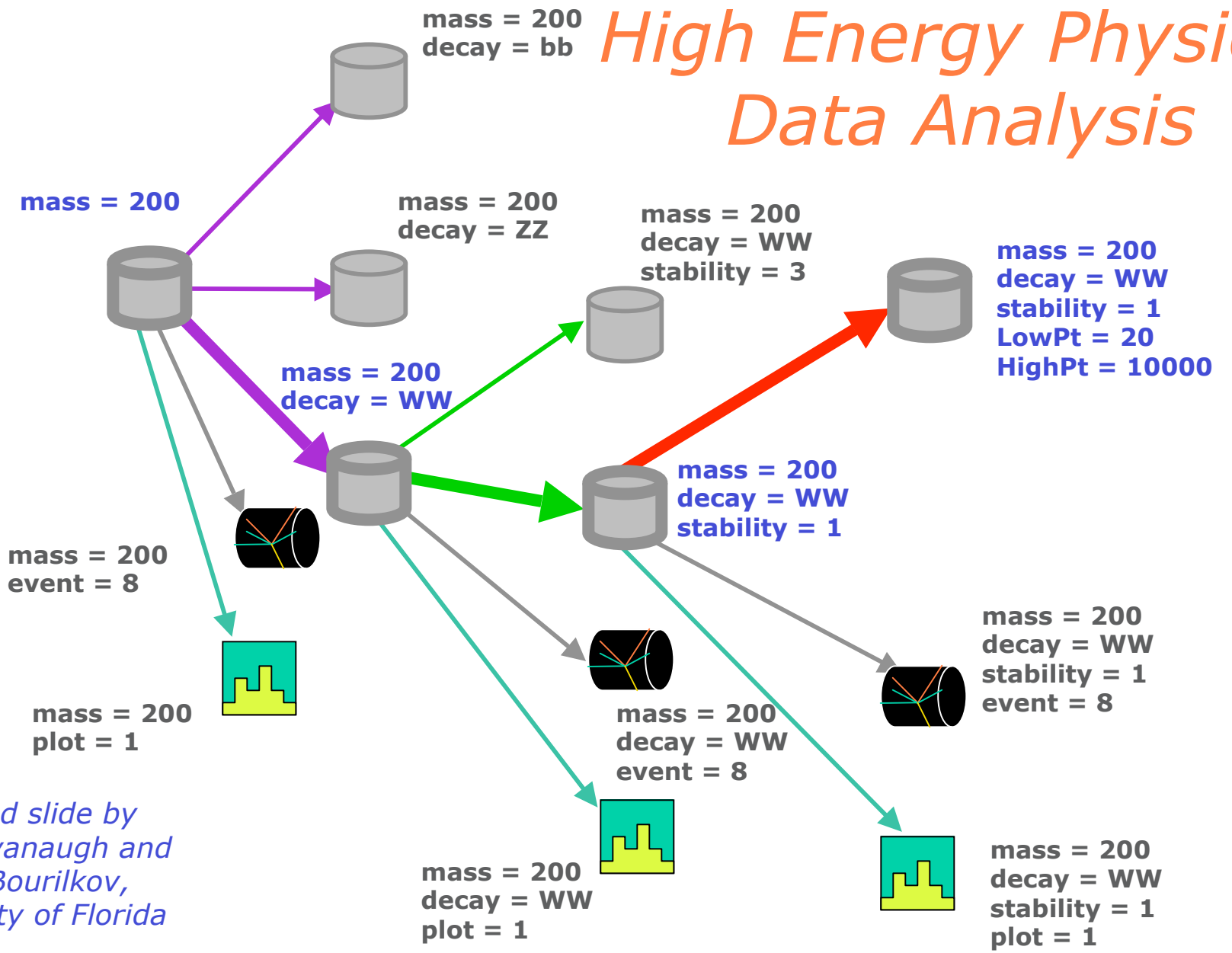
Enhance scientific productivity through:

- Discovery and application of datasets and programs at petabyte scale
- Enabling use of a worldwide data grid as a scientific workstation

Virtual Data and Workflows

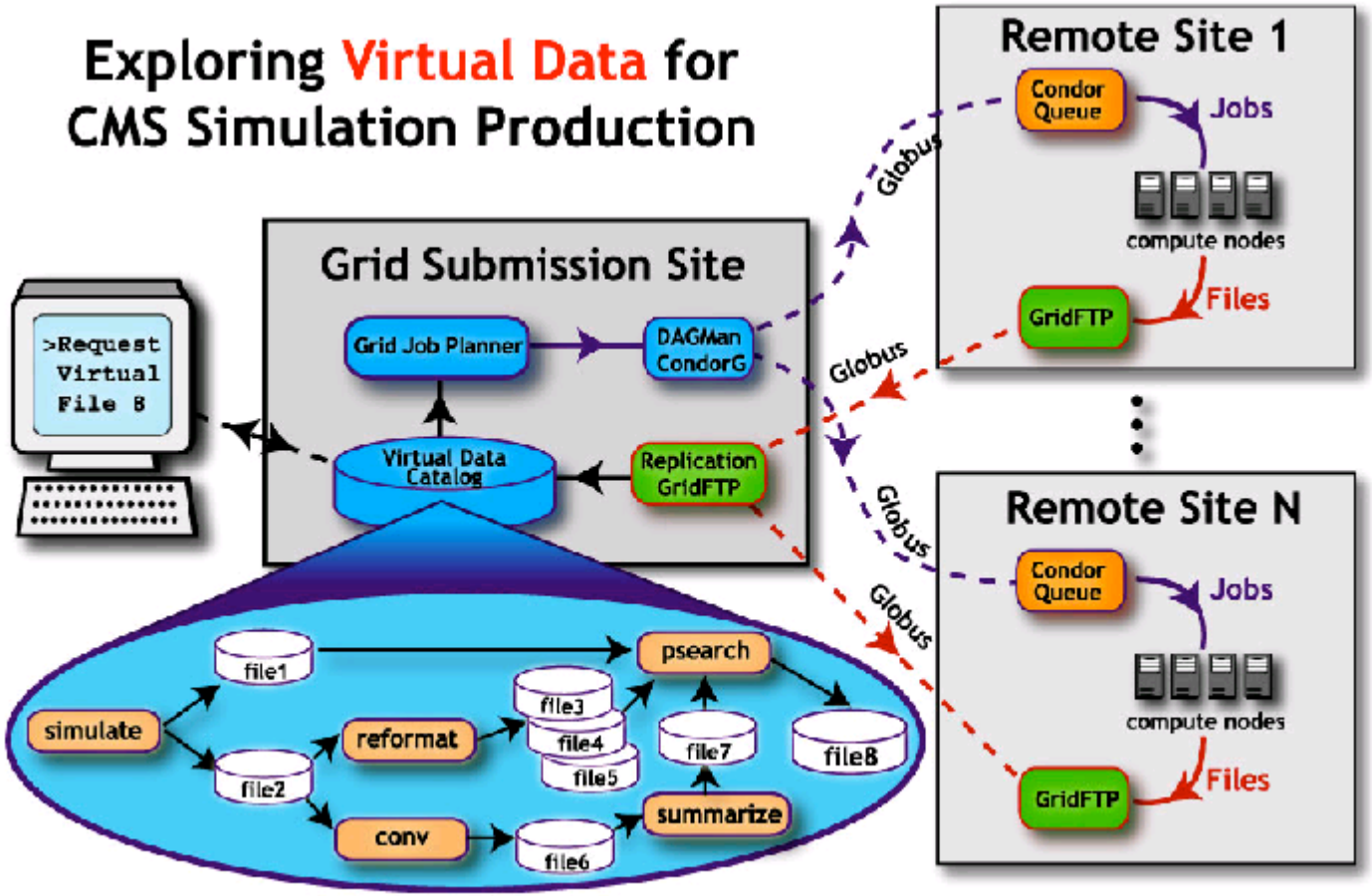
- Challenge is managing and organizing the vast computing and storage capabilities provided by Grids
- **Workflow** expresses computations in a form that can be readily mapped to Grids
- **Virtual data** keeps accurate track of data derivation methods and **provenance**
- Grid tools **virtualize** location and caching of data, and recovery from failures

Example Application: *High Energy Physics Data Analysis*



Work and slide by Rick Cavanaugh and Dimitri Bourilkov, University of Florida

Executing a scientific workflow



What must we "virtualize" to compute on the Grid?

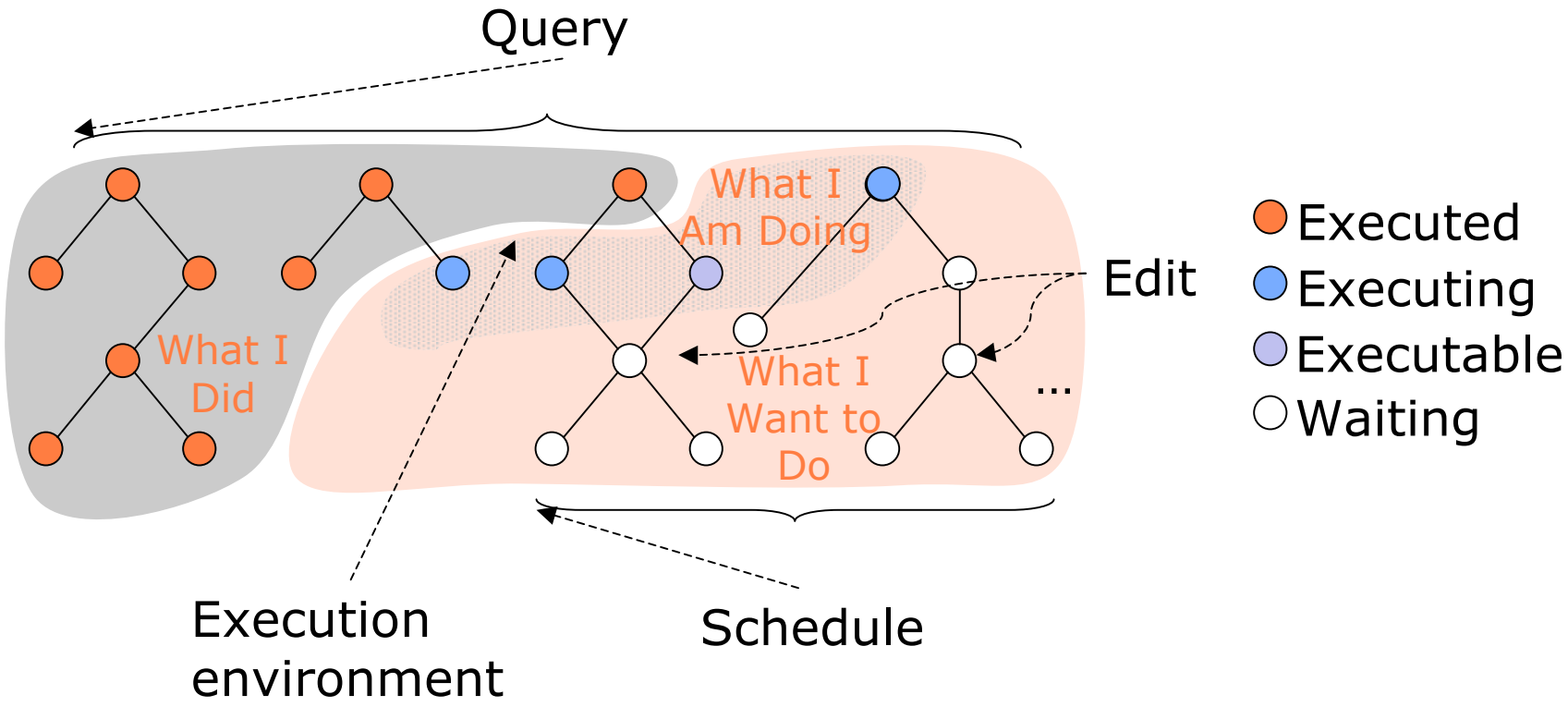
- Location-independent computing: represent all workflow in abstract terms
- Declarations not tied to specific entities:
  - sites
  - file systems
  - schedulers
- Failures – automated retry for data server and execution site un-availability

Mapping the Science Process to workflows

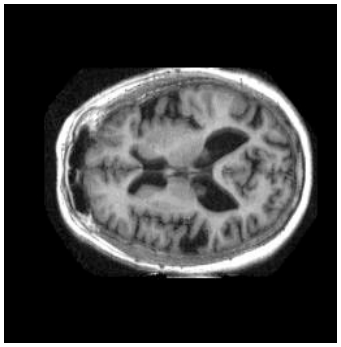
- Start with a single workflow
- Automate the generation of workflow for sets of files (datasets)
- Replicate workflow to explore many datasets
- Change Parameters
- Change code – add new transformations
- Build new workflows
- Use provenance info

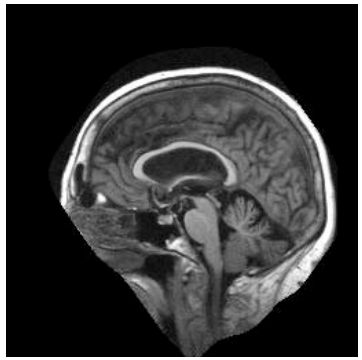
How does Workflow Relate to Provenance?

- Workflow – specifies what to do
- Provenance – tracks what was done



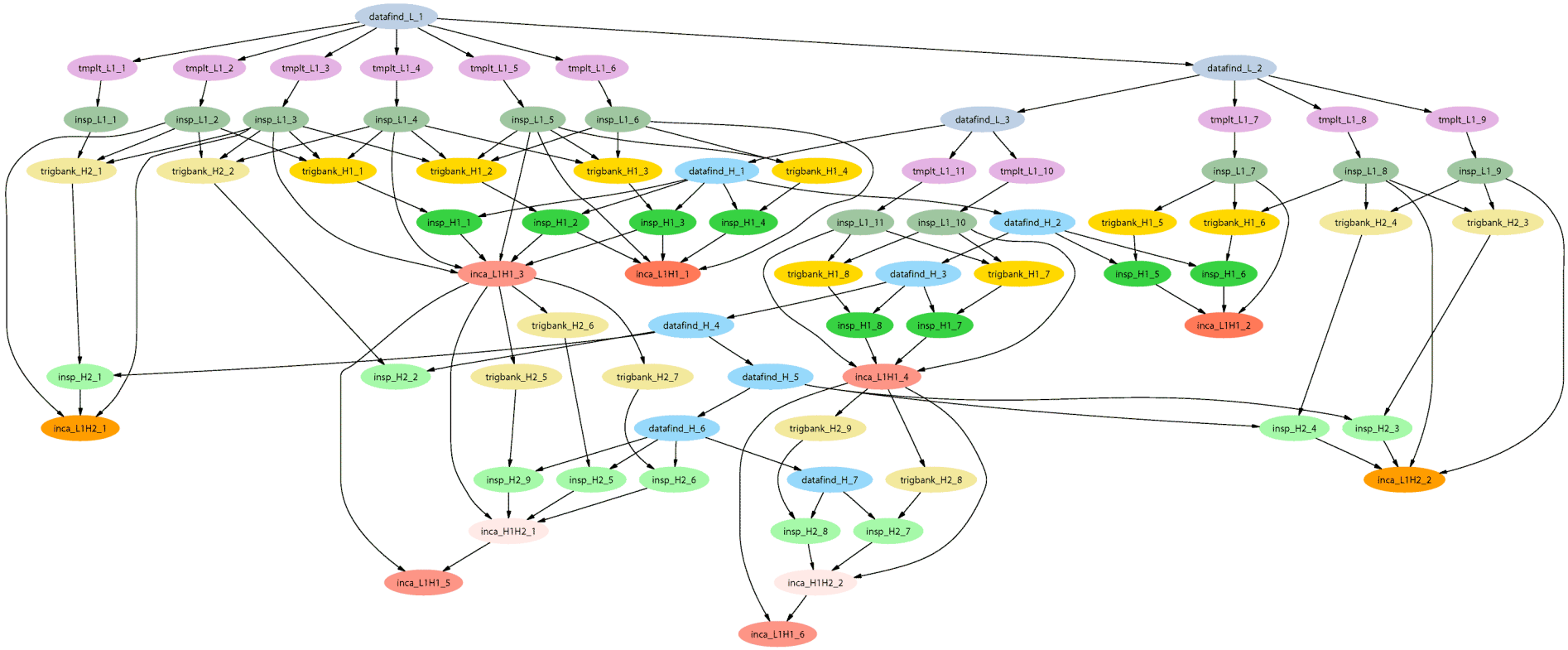
Functional MRI Analysis





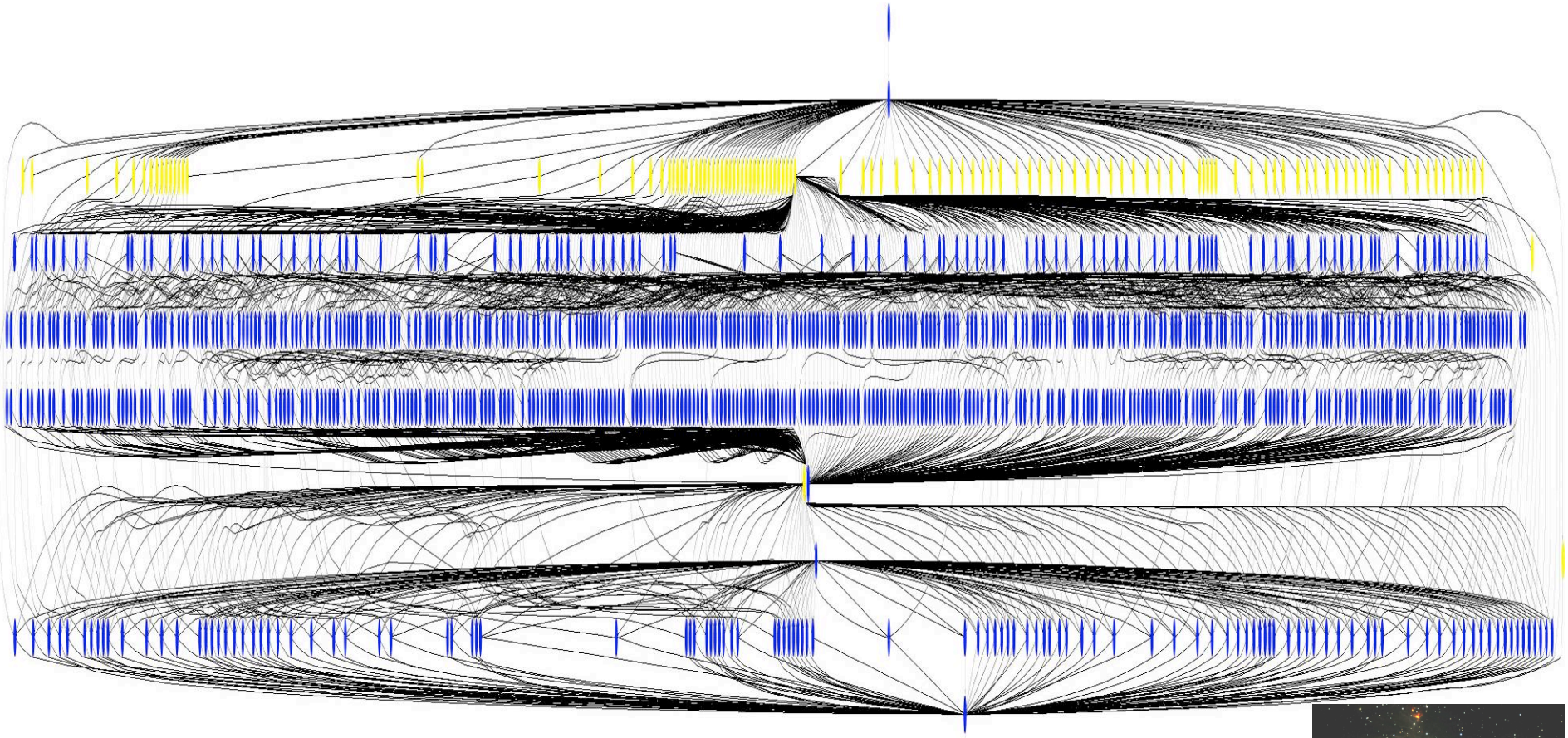
Workflow courtesy James Dobson, Dartmouth Brain Imaging Center

LIGO Inspiral Search Application



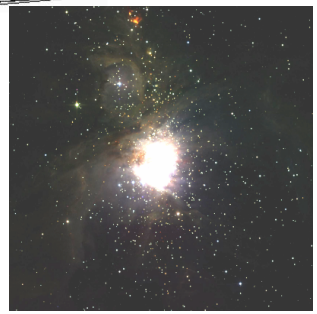
Inspiral workflow application is the work of Duncan Brown, Caltech, Scott Koranda, UW Milwaukee, and the LSC Inspiral group

Example Montage Workflow



~1200 node workflow, 7 levels

Mosaic of M42 created on the Teragrid using Pegasus



http://montage.ipac.caltech.edu/

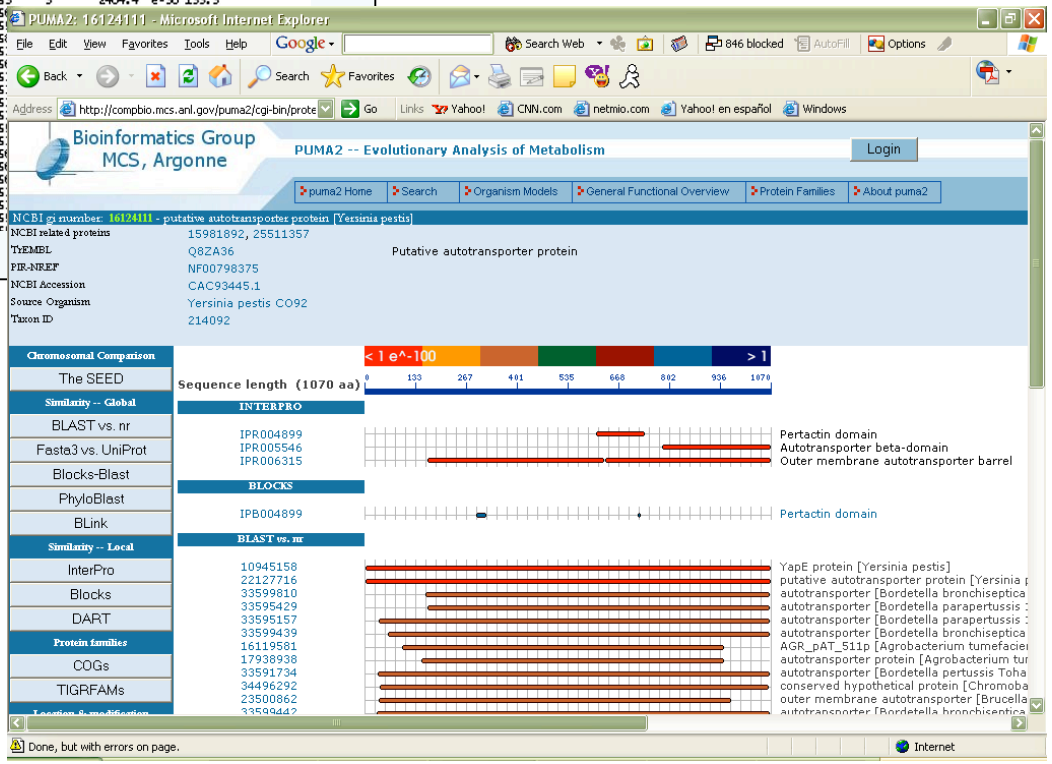
Blasting for Protein Knowledge

BLAST compare of complete nr database for sequence similarity and function characterization

REF_tigr|BRA0013	gi|39933731|ref|NP_946007.1|	34.90	255	131	1	15	257	8	2603.7	e-53	209.9
REF_tigr|BRA0013	gi|48782600|ref|ZP_00279106.1|	35.92	245	126	2	14	256	7	2591.1	e-49	198.4
REF_tigr|BRA0013	gi|41407534|ref|NP_960370.1|	36.09	266	125	2	15	258	3	2561.9	e-49	197.6
REF_tigr|BRA0013	gi|48851585|ref|ZP_00305793.1|	32.39	247	134	1	13	257	5	2476.1	e-48	192.6
REF_tigr|BRA0013	gi|15966306|ref|NP_386659.1|	36.50	263	138	3	18	257	5	2552.0	e-43	177.6
REF_tigr|BRA0013	gi|17548526|ref|NP_521866.1|	36.36	264	138	1	17	256	10	2602.7	e-43	177.2

Knowledge Base

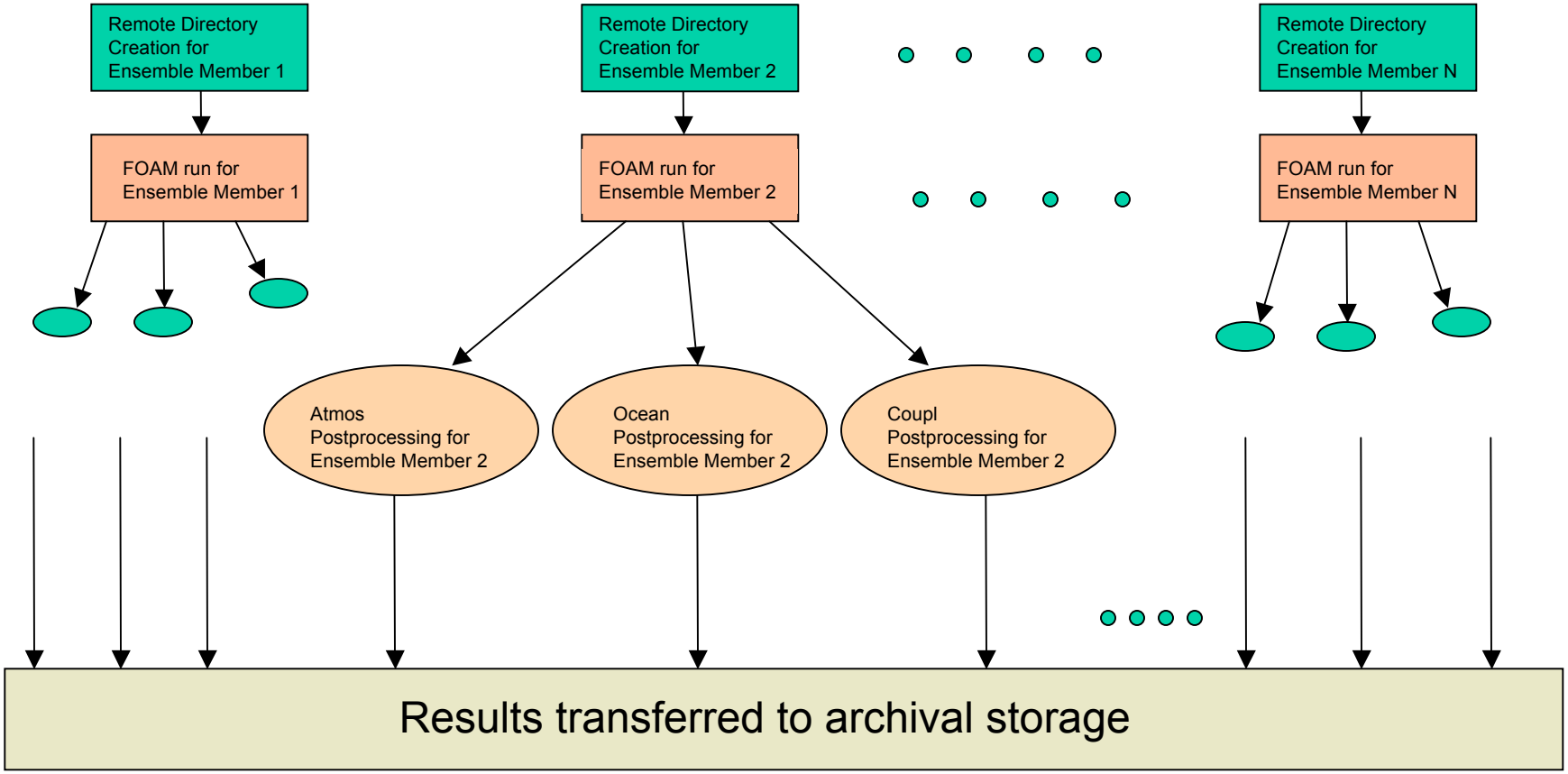
PUMA is an interface for the researchers to be able to find information about a specific protein after having been analyzed against the complete set of sequenced genomes (nr file ~ approximately 3 million sequences)



Analysis on the Grid

The analysis of the protein sequences occurs in the background in the grid environment. Millions of processes are started since several tools are run to analyze each sequence, such as finding out protein similarities (BLAST), protein family domain searches (BLOCKS), and structural characteristics of the protein.

FOAM:
Fast Ocean/Atmosphere Model
250-Member Ensemble
Run on TeraGrid under VDS

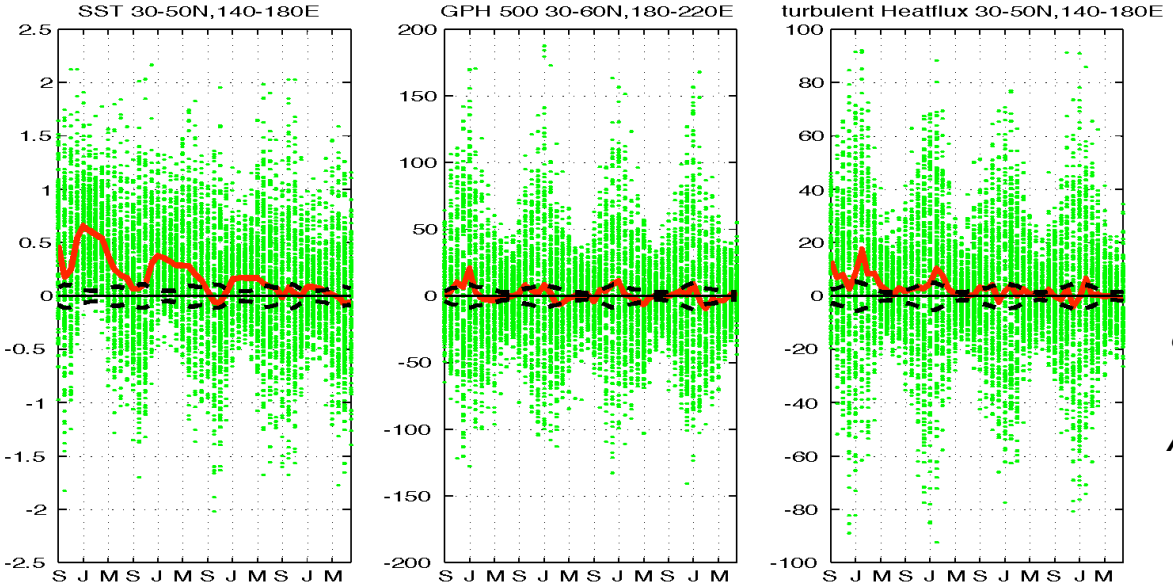


Work of: Rob Jacob (FOAM), Veronica Nefedova (Workflow design and execution)

FOAM: TeraGrid/VDSBenefits

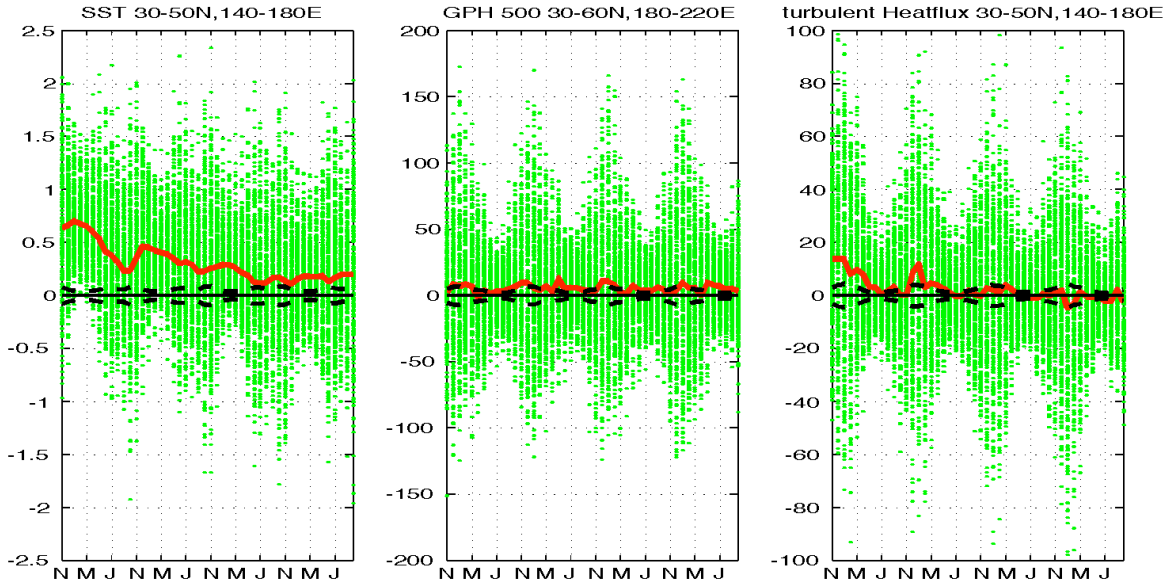
Climate Supercomputer

160 ensemble members = 2.5 months to run



TeraGrid with NMI and VDS

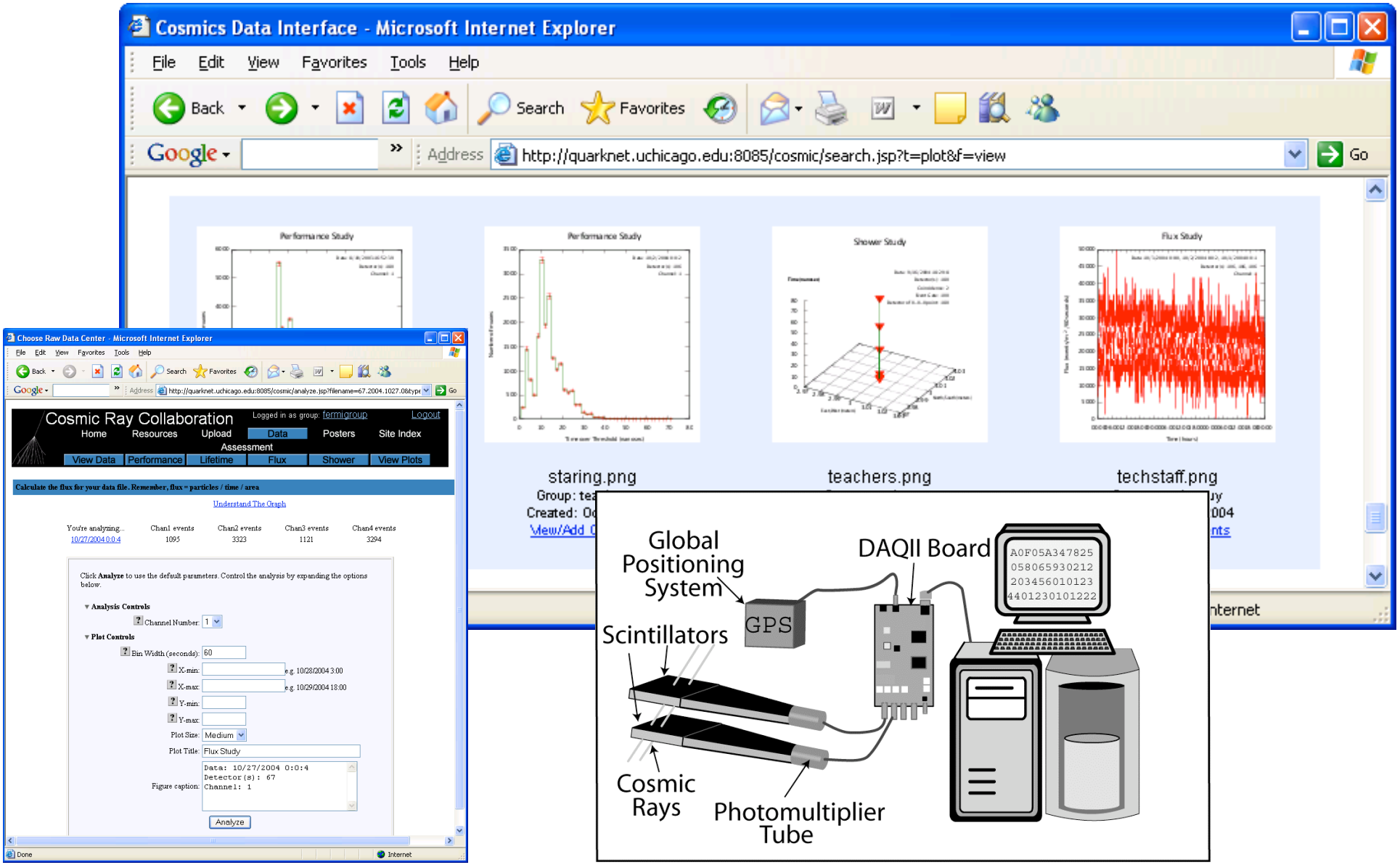
250 ensemble members = 4 days to run



Green: each ensemble Red: ensemble mean

FOAM application by Rob Jacob, Argonne; VDS workflow by Veronika Nefedova, Argonne Visualization courtesy Pat Behling and Yun Liu, UW Madison..

i2u2 - Leveraging Virtual Data for Science Education



VDS Applications

Application	Jobs / workflow	Levels	Status
ATLAS HEP Event Simulation	500K	1	In Use
LIGO Inspiral/Pulsar	~700	2-5	Inspiral In Use
NVO/NASA Montage/Morphology	1000s	7	In Use
GADU Genomics: BLAST,…	40K	1	In Use
fMRI AIR, freeSurfer prepro	100s	12	In Devel
QuarkNet CosmicRay science	<10	3-6	In Use
SDSS Coadd; Cluster Search	40K 500K	2 8	CS Research
FOAM Ocean/Atmos Model	2000 (core app runs 250 8-CPU jobs)	3	In use
GTOMO Image proc	1000s	1	In Devel
SCEC Earthquake sim	1000s		In use

Some workflow systems

- DAGman – part of Condor
- VDS – VDL+Pegasus
- Swift

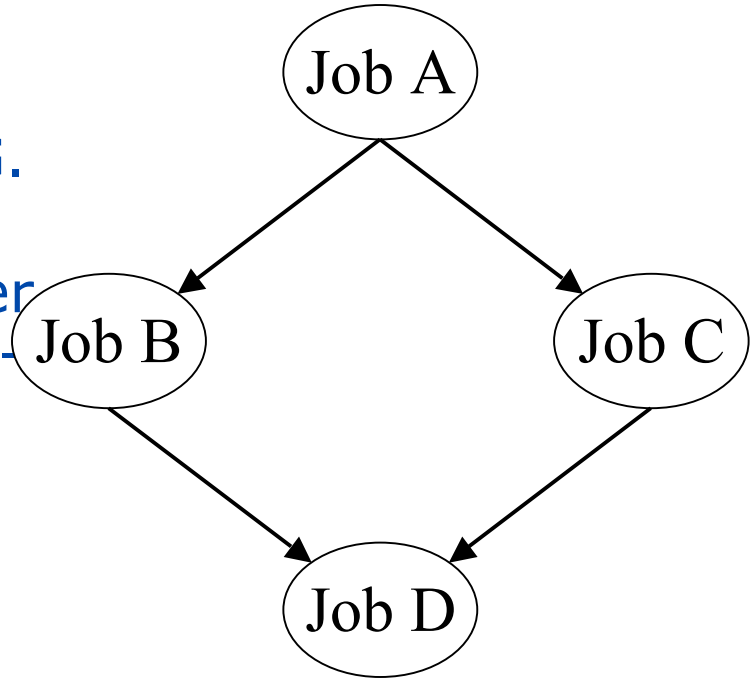
DAGMan

- **Directed Acyclic Graph Manager**

- DAGMan allows you to specify the *dependencies* between your Condor jobs, so it can *manage* them automatically for you.
  - By default, Condor may run your jobs in any order, or everything simultaneously, so we need DAGMan to enforce an ordering when necessary.
- Example: "Don't run job "B" until job "A" has completed successfully."

What is a DAG?

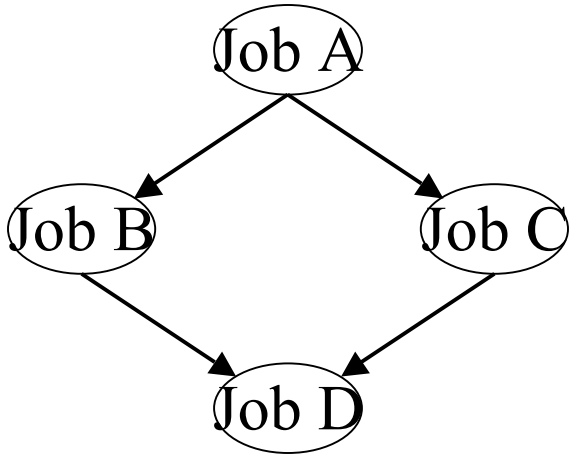
- A DAG is the data structure used by DAGMan to represent these dependencies.
- Each job is a "node" in the DAG.
- Each node can have any number of "parent" or "children" nodes – as long as there are no loops!



Defining a DAG

- A DAG is defined by a *.dag file*, listing each of its nodes and their dependencies:

```
# diamond.dag
Job A a.sub
Job B b.sub
Job C c.sub
Job D d.sub
Parent A Child B C
Parent B C Child D
```



- each node will run the Condor job specified by its accompanying Condor submit file

Submitting a DAG

- To start your DAG, just run ***condor_submit_dag*** with your .dag file, and Condor will start a personal DAGMan daemon which to begin running your jobs:

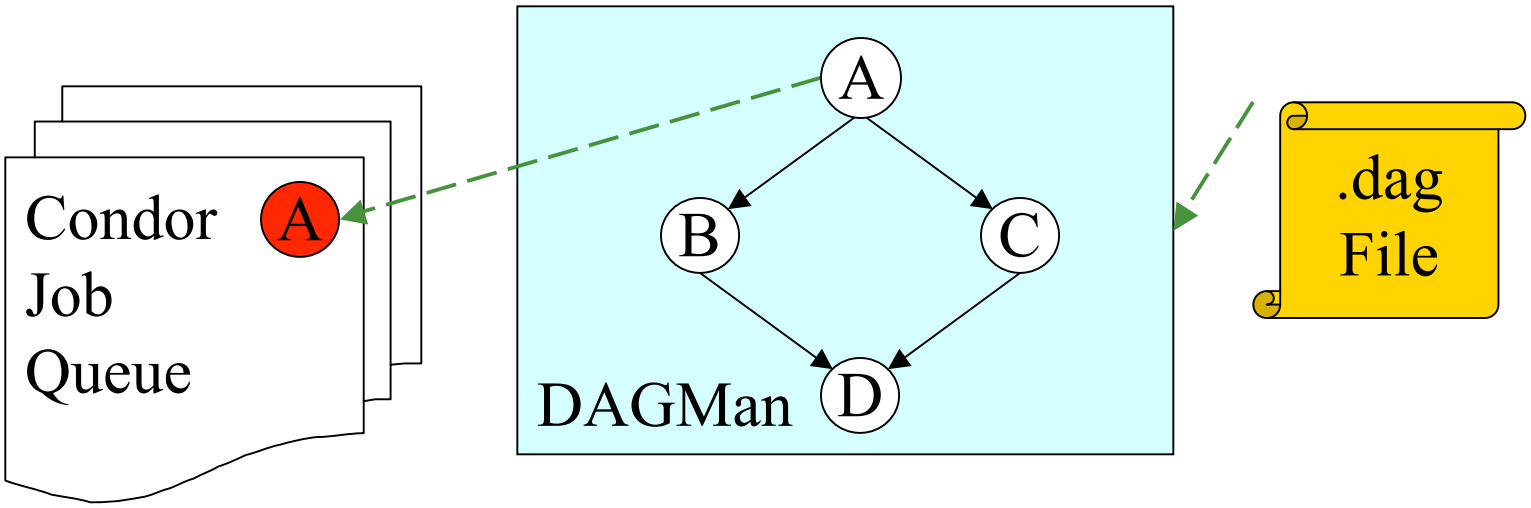
```
% condor_submit_dag diamond.dag
```

- condor_submit_dag submits a job with DAGMan as the executable.
  - This job happens to run on the submitting machine, not any other computer.

- Thus the DAGMan daemon itself runs as a Condor job, so you don't have to baby-sit it.

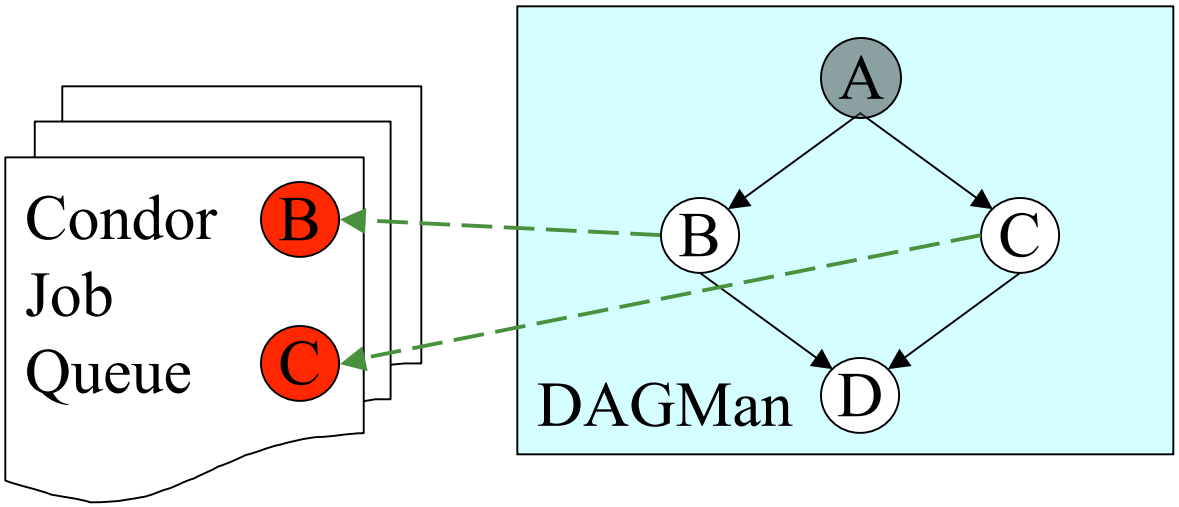
Running a DAG

- DAGMan acts as a “meta-scheduler”, managing the submission of your jobs to Condor based on the DAG dependencies.



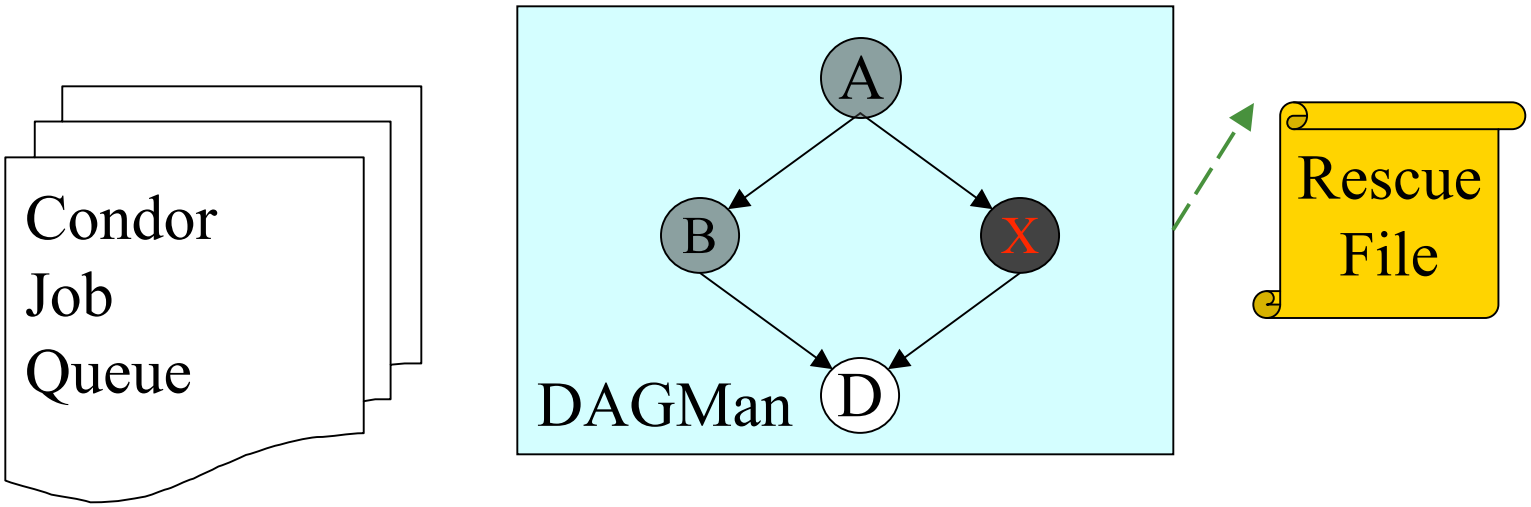
Running a DAG (cont'd)

- DAGMan holds & submits jobs to the Condor queue at the appropriate times.



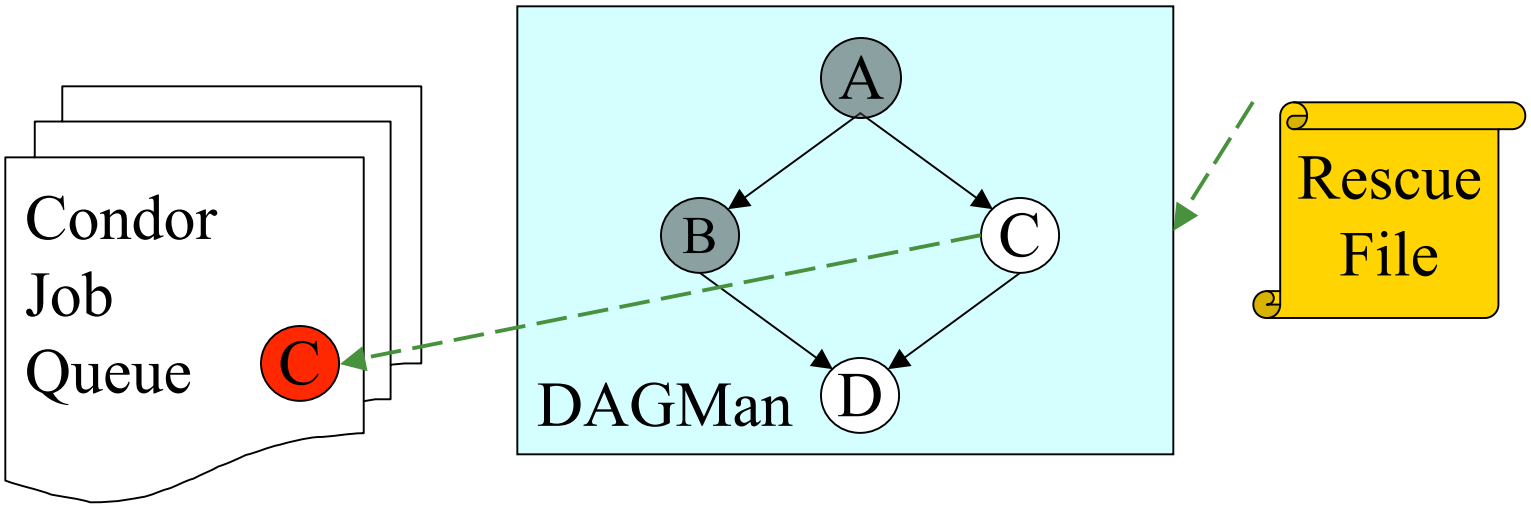
Running a DAG (cont'd)

- In case of a job failure, DAGMan continues until it can no longer make progress, and then creates a *"rescue" file* with the current state of the DAG.



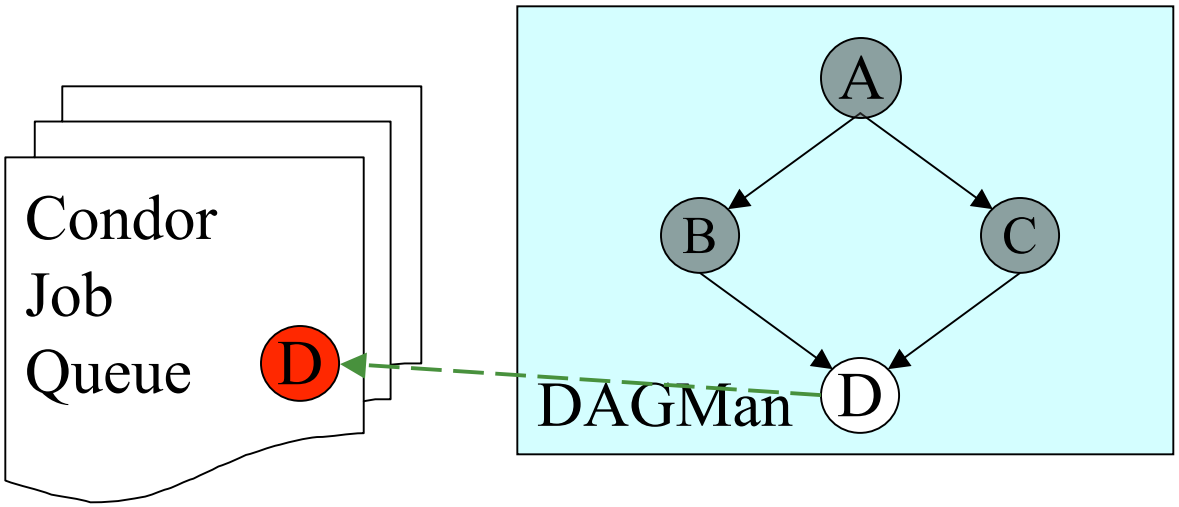
Recovering a DAG

- Once the failed job is ready to be re-run, the rescue file can be used to restore the prior state of the DAG.



Recovering a DAG (cont'd)

- Once that job completes, DAGMan will continue the DAG as if the failure never happened.



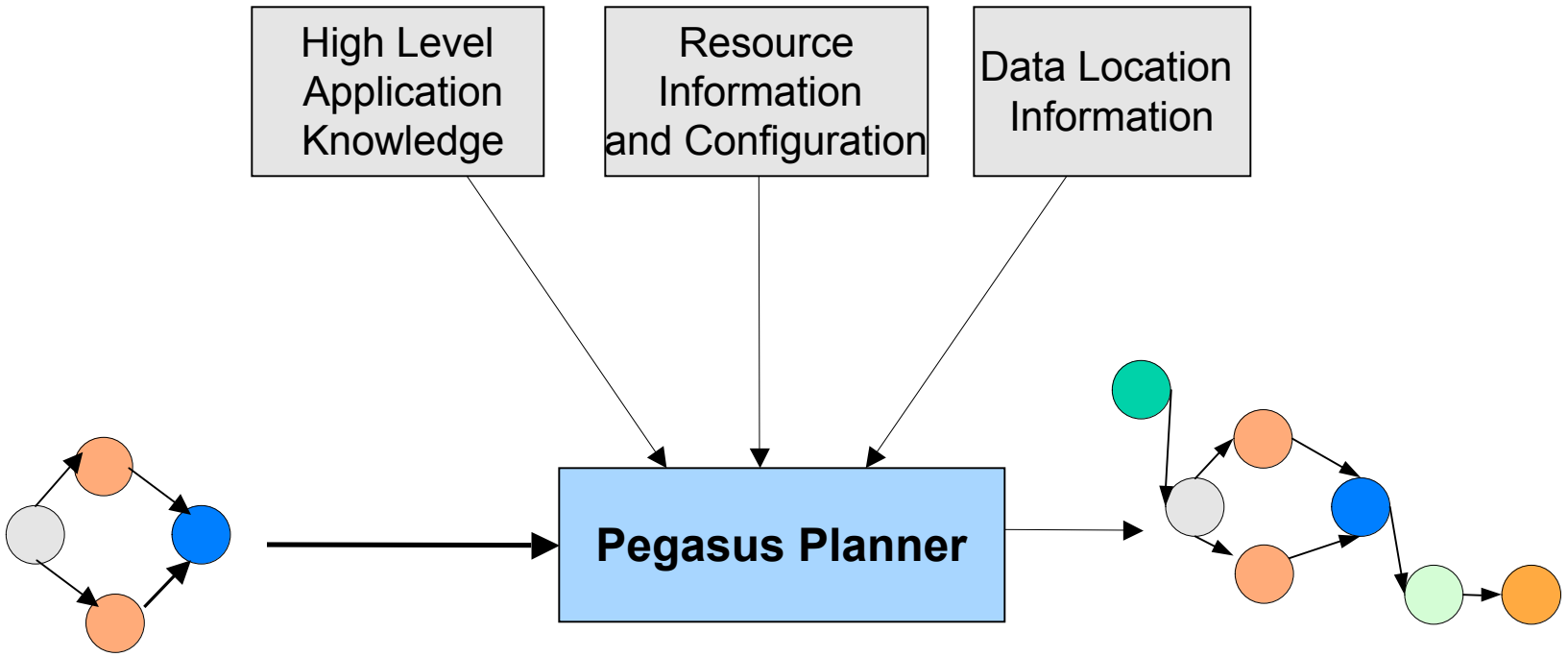
VDS

- Virtual Data System
  - Virtual Data Language (VDL)
    - A language to express workflows
  - Pegasus planner
    - Decides how the workflow will run
  - Virtual Data Catalog (VDC)
    - Stores information about workflows
    - Stores provenance of data

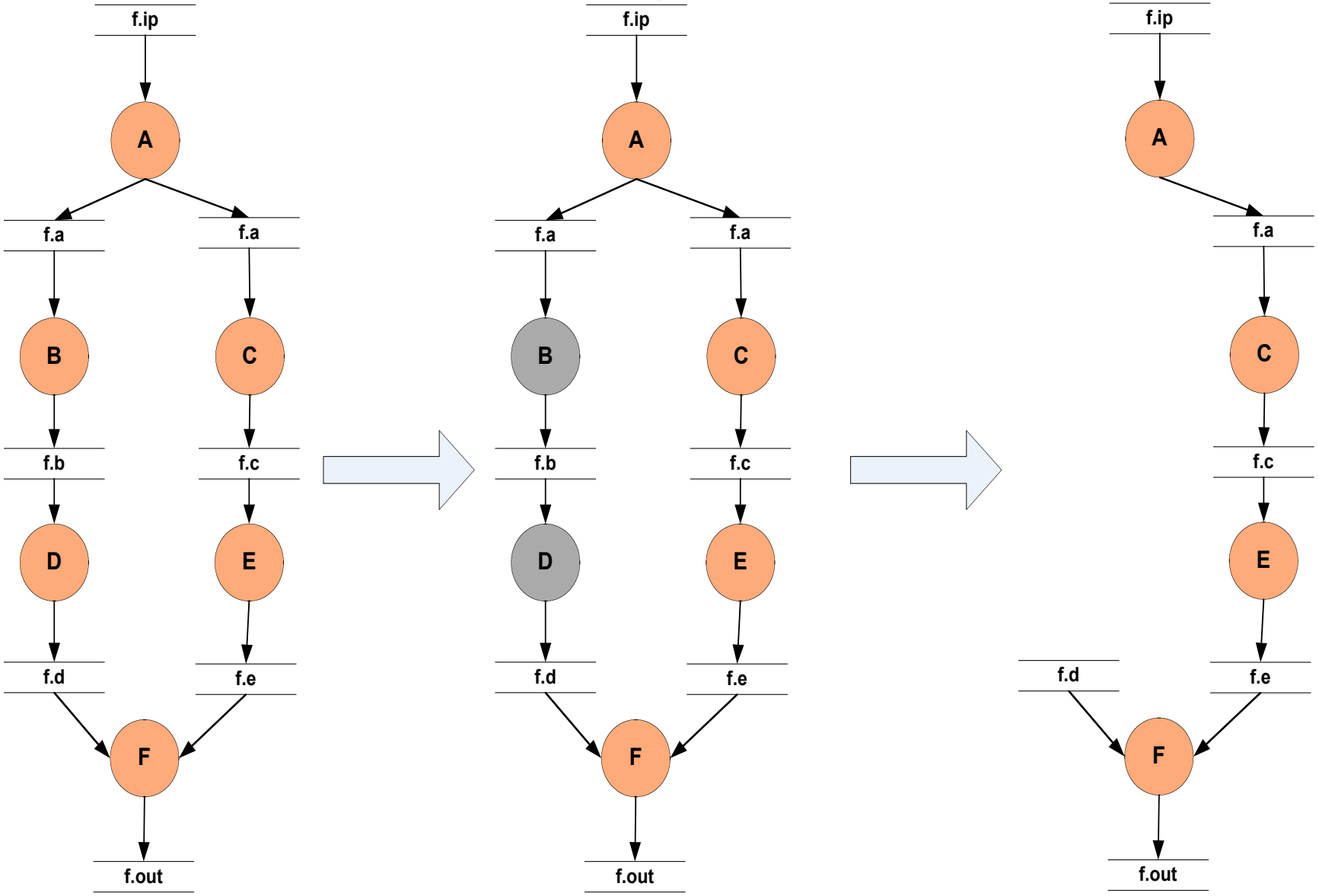
Virtual Data Process

- Describe data derivation or analysis steps in a high-level workflow language (VDL)
- VDL is cataloged in a database for sharing by the community
- Grid workflows are generated from VDL
- Provenance of derived results stored in database for assessment or verification

Planning with Pegasus



Abstract to Concrete, Step 1: Workflow Reduction

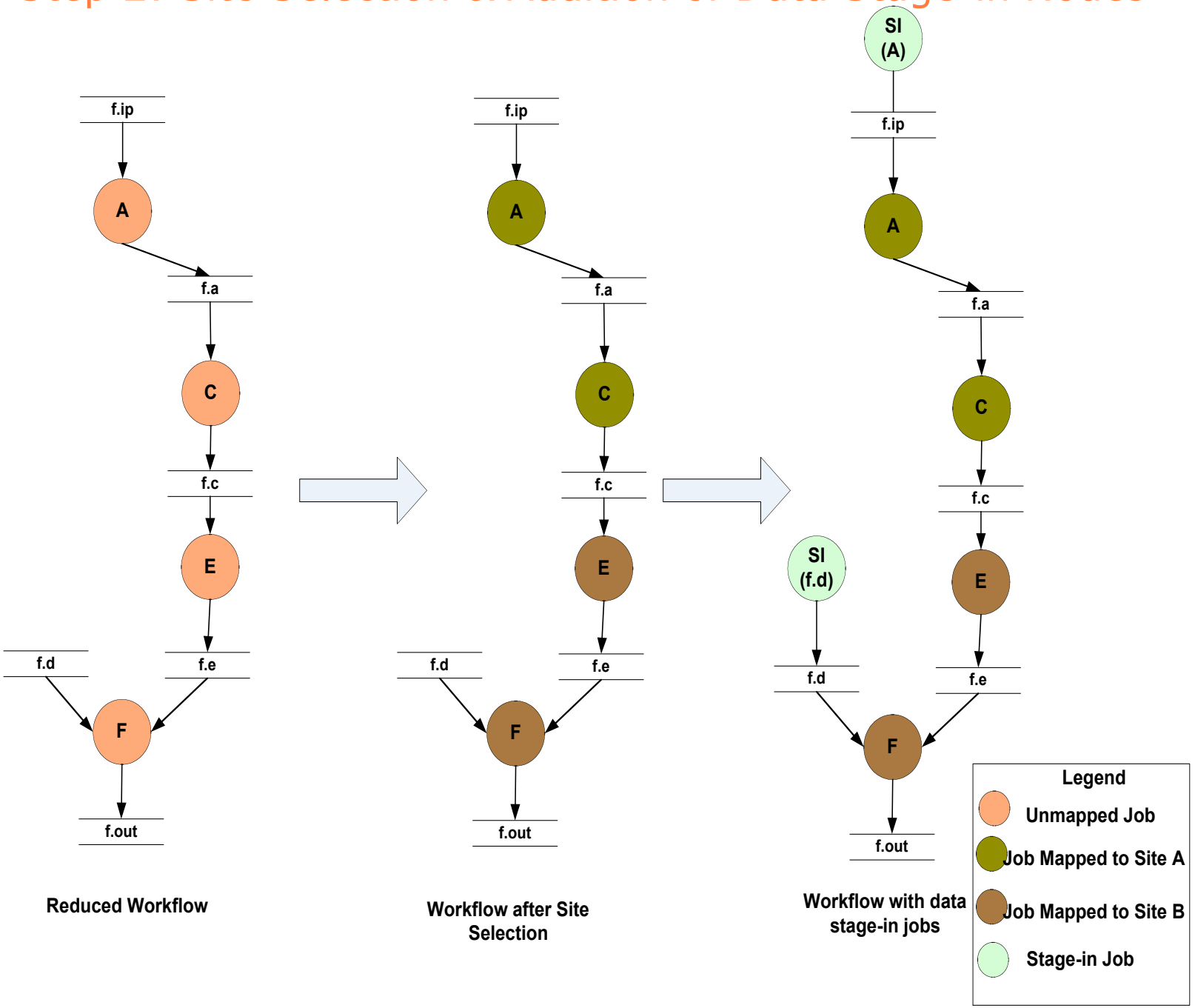


Abstract Workflow

File f.d exists somewhere.
Reuse it.
Mark Jobs D and B to delete

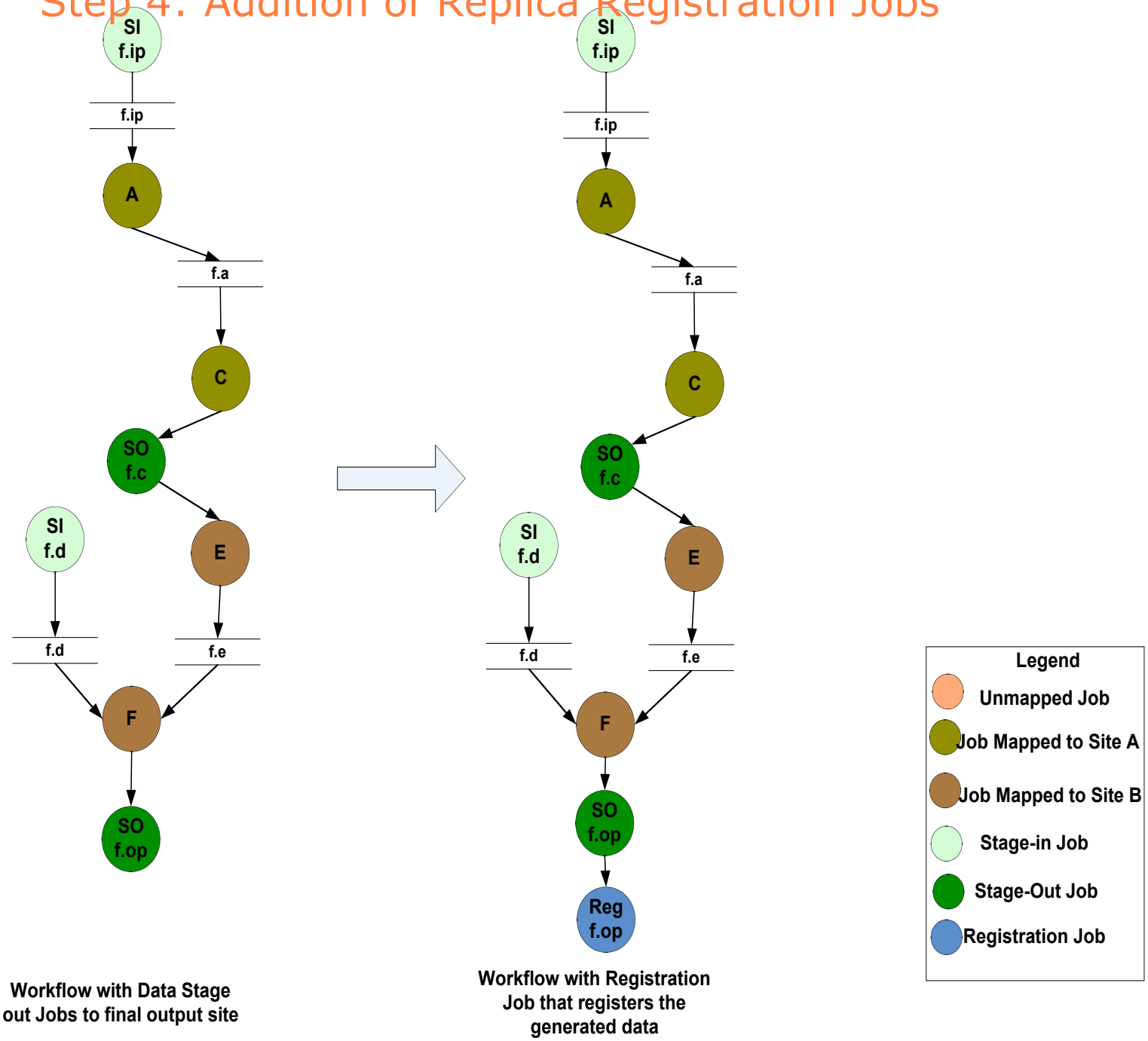
Delete Job D and Job B

Step 2: Site Selection & Addition of Data Stage-in Nodes



Step 3: Addition of Data Stage-out Nodes

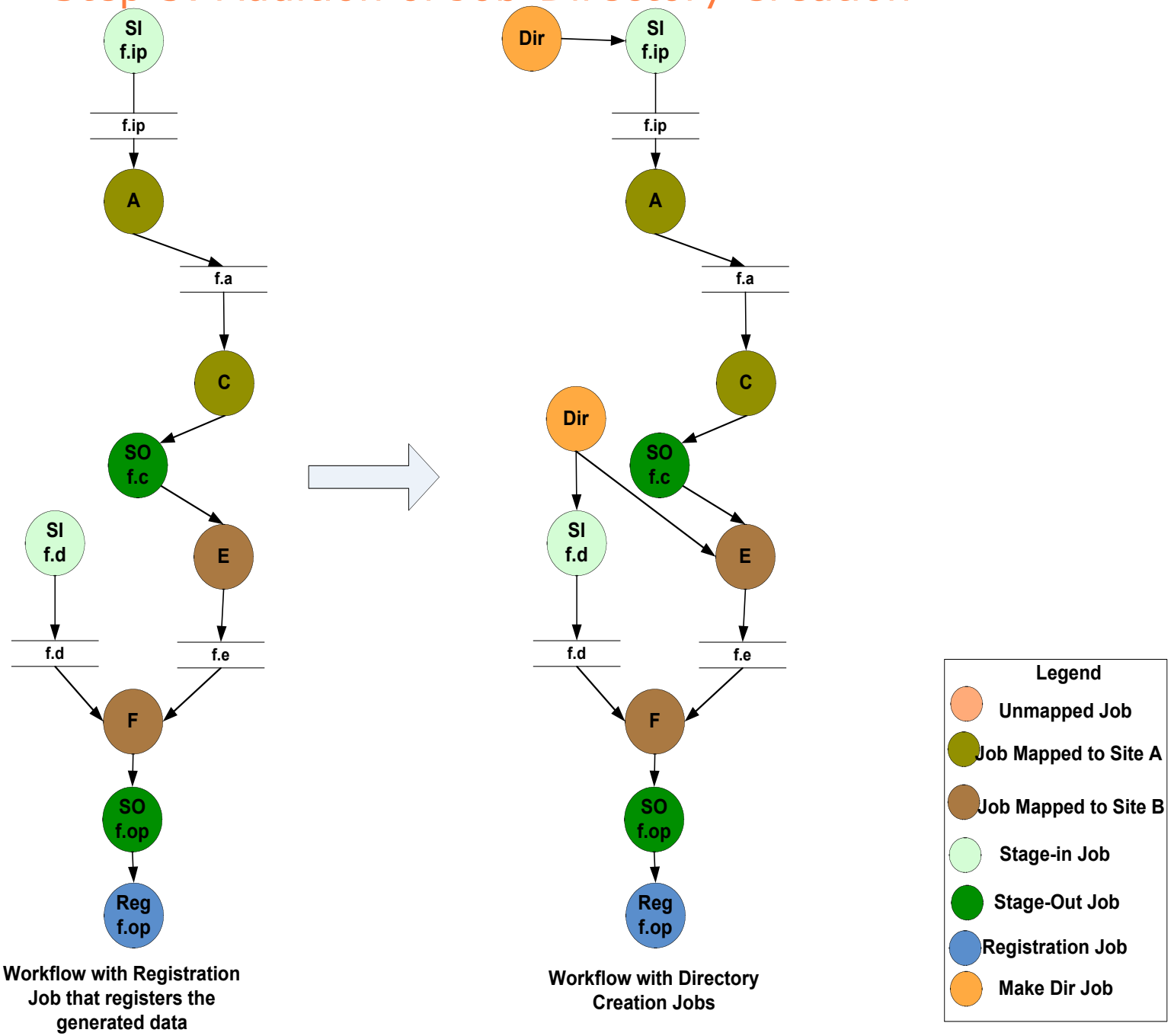
Step 4: Addition of Replica Registration Jobs



Workflow with Data Stage out Jobs to final output site

Workflow with Registration Job that registers the generated data

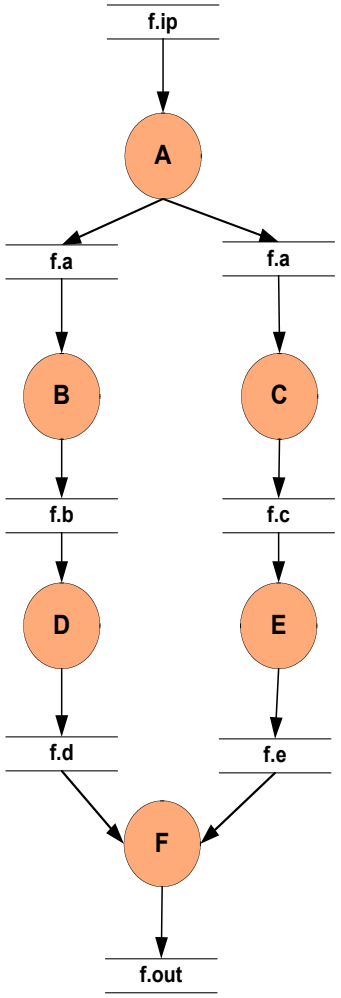
Step 5: Addition of Job-Directory Creation



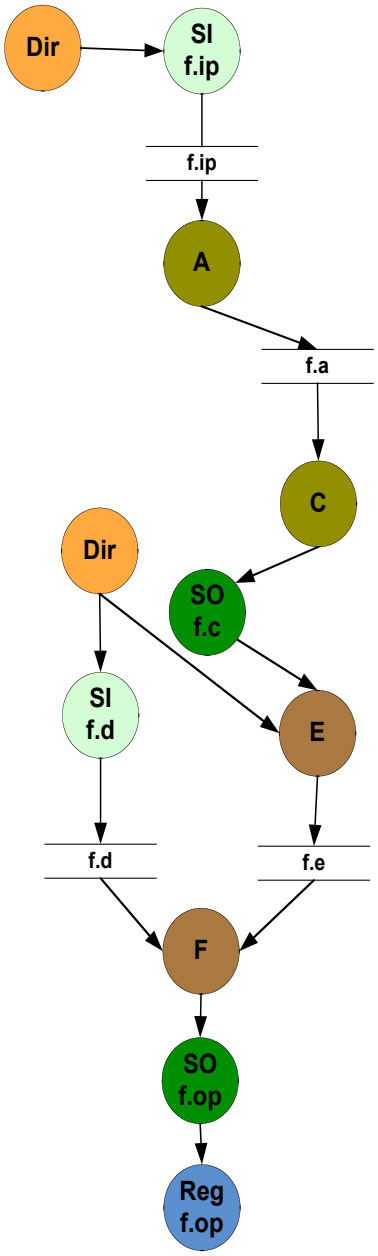
Workflow with Registration Job that registers the generated data

Workflow with Directory Creation Jobs

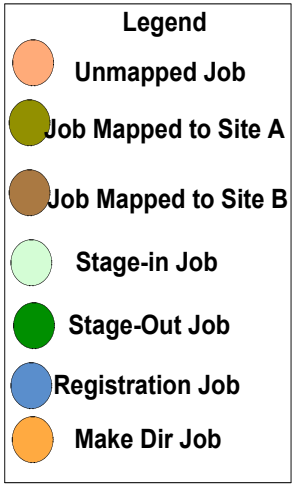
Final Result of Abstract-to-Concrete Process



Abstract Workflow



Final Concrete Workflow



Swift System

- 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
  - Lightweight threading, dynamic provisioning, Grid interfaces, pipelining, load balancing

+ Rigorous provenance tracking and query
  - Virtual data schema & automated recording

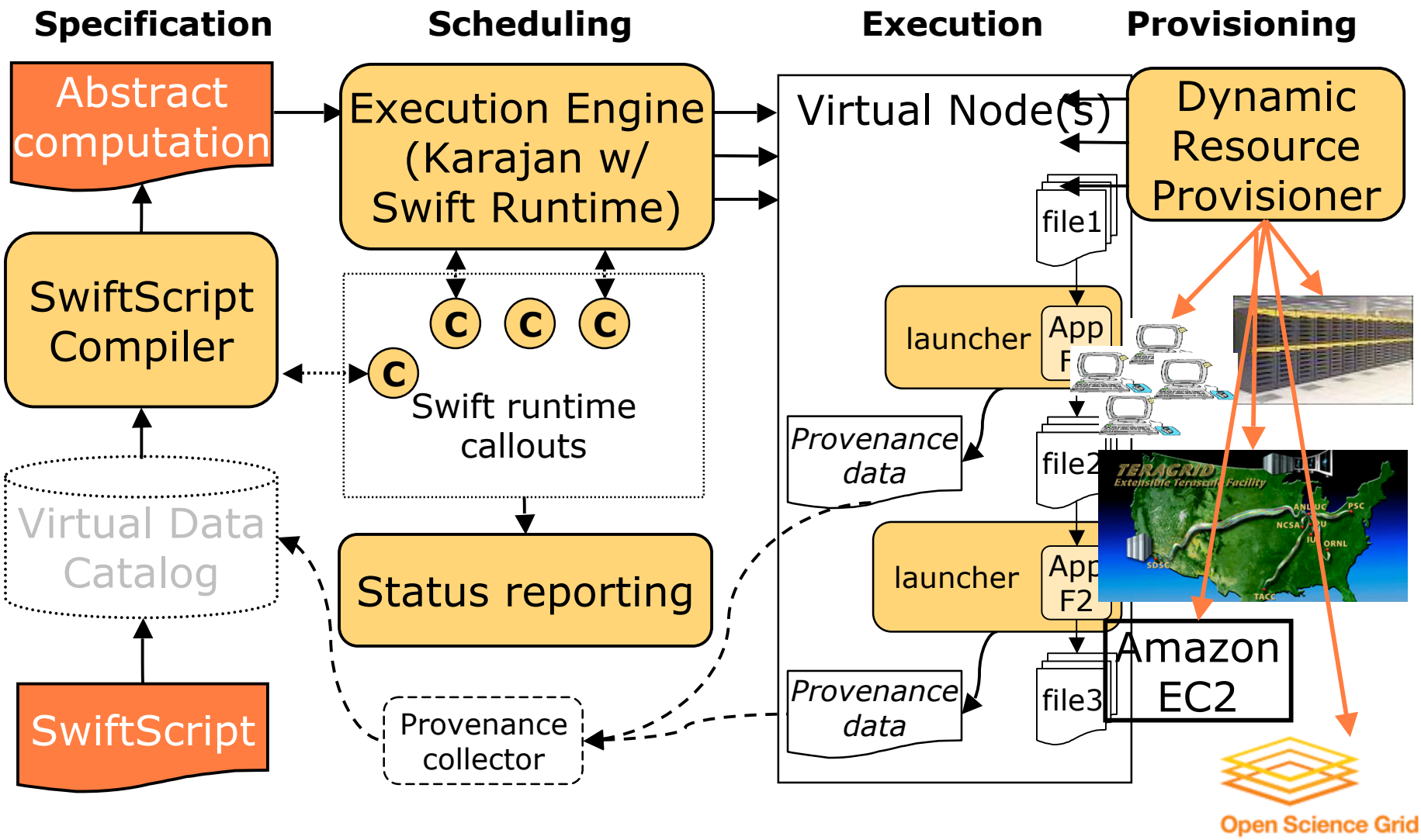
→ **Improved usability and productivity**
  - Demonstrated in numerous applications

AIRSN Program Definition

```
(Run snr) functional ( Run r, NormAnat a,
                       Air shrink ) {
    Run yroRun = reorientRun( r , "y" );
    Run roRun = reorientRun( yroRun , "x" );
    Volume std = roRun[0];
    Run rndr = random_select( roRun, 0.1 );
    AirVector rndAirVec = align_linearRun( rndr, std, 12, 1000, 1000, "81 3 3" );
    Run reslicedRndr = resliceRun( rndr, rndAirVec, "o", "k" );
    Volume meanRand = softmean( reslicedRndr, "y", "null" );
    Air mnQAAir = alignlinear( a.nHires, meanRand, 6, 1000, 4, "81 3 3" );
    Warp boldNormWarp = combinewarp( shrink, a.aWarp, mnQAAir );
    Run nr = reslice_warp_run( boldNormWarp, roRun );
    Volume meanAll = strictmean( nr, "y", "null" )
    Volume boldMask = binarize( meanAll, "y" );
    snr = gsmoothRun( nr, boldMask, "6 6 6" );
}
```

```
(Run or) reorientRun (Run ir,
                      string direction) {
    foreach Volume iv, i in ir.v {
        or.v[i] = reorient(iv, direction);
    }
}
```

Swift Architecture



Based on: The Virtual Data System – *a workflow toolkit for science applications*

OSG Summer Grid Workshop
Lecture 8
June 29, 2006

Based on: Fast, Reliable, Loosely Coupled Parallel Computation

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Computation Institute

University of Chicago & Argonne National Laboratory

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Based on: Lecture 5 Grid Resources and Job Management

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Condor Project,

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Grid Summer Workshop

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