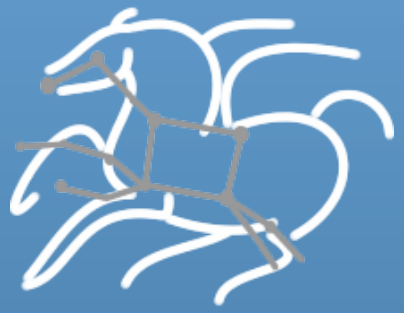


Introduction to Scientific Workflows and Pegasus

Karan Vahi

Science Automation Technologies Group

USC Information Sciences Institute

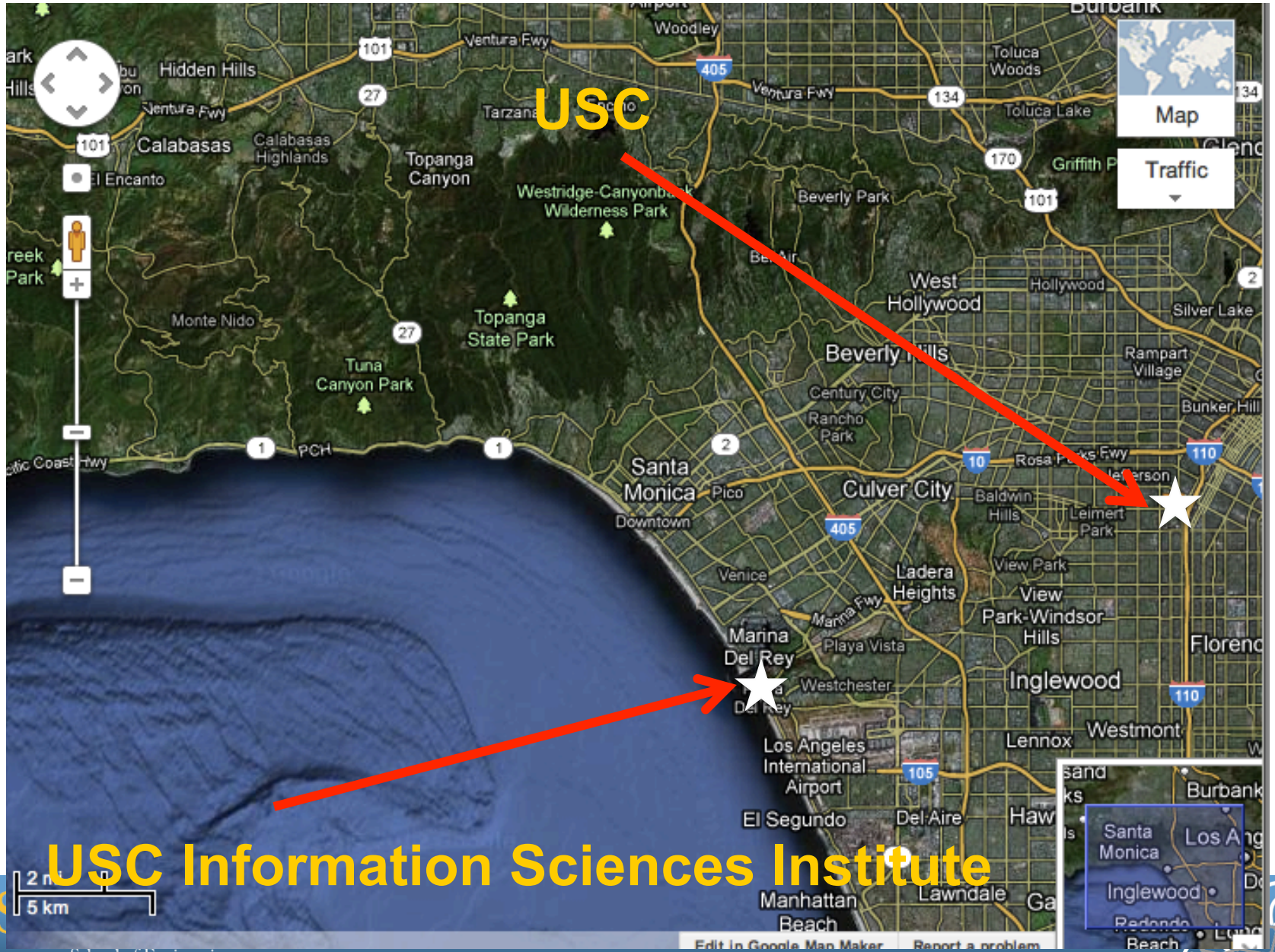
What is Information Sciences Institute?

- A research organization under the USC Viterbi Engineering. (http://www.isi.edu)
  - Birthplace of the internet.
  - 350 fulltime staff. Main Campus in Marina Del Rey.
  - Research Areas
    - Advanced electronics
    - Computational systems and technology
    - Informatics, grid computing , HPC
    - Intelligent Systems – AI , NLP.

- Science Automation Technologies Group (http://pegasus.isi.edu)
  - Develops tools and techniques that automate the computational processes.
  - Releases a scientific workflow management system Pegasus.
    - Allows users to run workflows on a variety of infrastructure (local clusters to clouds)
  - Works closely with users to solve their computational problems.
  - Close collaboration with groups at UPC and Keck
    - Southern California Earthquake Center (SCEC - http://scec.org)
    - Computational Biology and Bioinformatics (http://tingchenlab.cmb.usc.edu)
    - Jim Knowles group at Keck (http://keck.usc.edu/Research/Research_Institutes/Zilkha_Neurogenetic_Institute/Investigators.aspx)

Information Sciences Institute

- **Basic and applied research in:**
  - **Advanced electronics**
    - fabrication; novel electronics
  - **Computational systems and technology**
    - Software/hardware supercomputing, high-performance computing, cloud computing, scientific workflows
  - **Informatics**
    - Medical informatics, decision systems, computer networks, grid computing
  - **Intelligent systems / artificial intelligence**
    - Natural language, knowledge technologies, information
    - and geospatial integration, robotics


USC
USC Information Sciences Institute
Map
Traffic
Santa Monica
Marina Del Rey
Culver City
Beverly Hills
West Hollywood
Inglewood
Los Angeles International Airport
El Segundo
Manhattan Beach
Lawndale
Hidden Hills
Calabasas
Topanga Canyon
Topanga State Park
Tuna Canyon Park
Monte Nido
Westridge-Canyon Wilderness Park
Beverly Park
Rancho Park
Century City
Rampart Village
Silver Lake
Ladera Heights
View Park-Windsor Hills
Baldwin Hills
Leimert Park
Playa Vista
Westchester
Venice
Downtown
Pico
Lennox
Westmont
Del Aire
Toluca Woods
Toluca Lake
Griffith P
Woodley
Ventura Fwy
Rosa Parks Fwy
Marina Fwy
PCH
2 mi
5 km
Burbank
Santa Monica
Inglewood
Edit in Google Map Maker
Report a problem

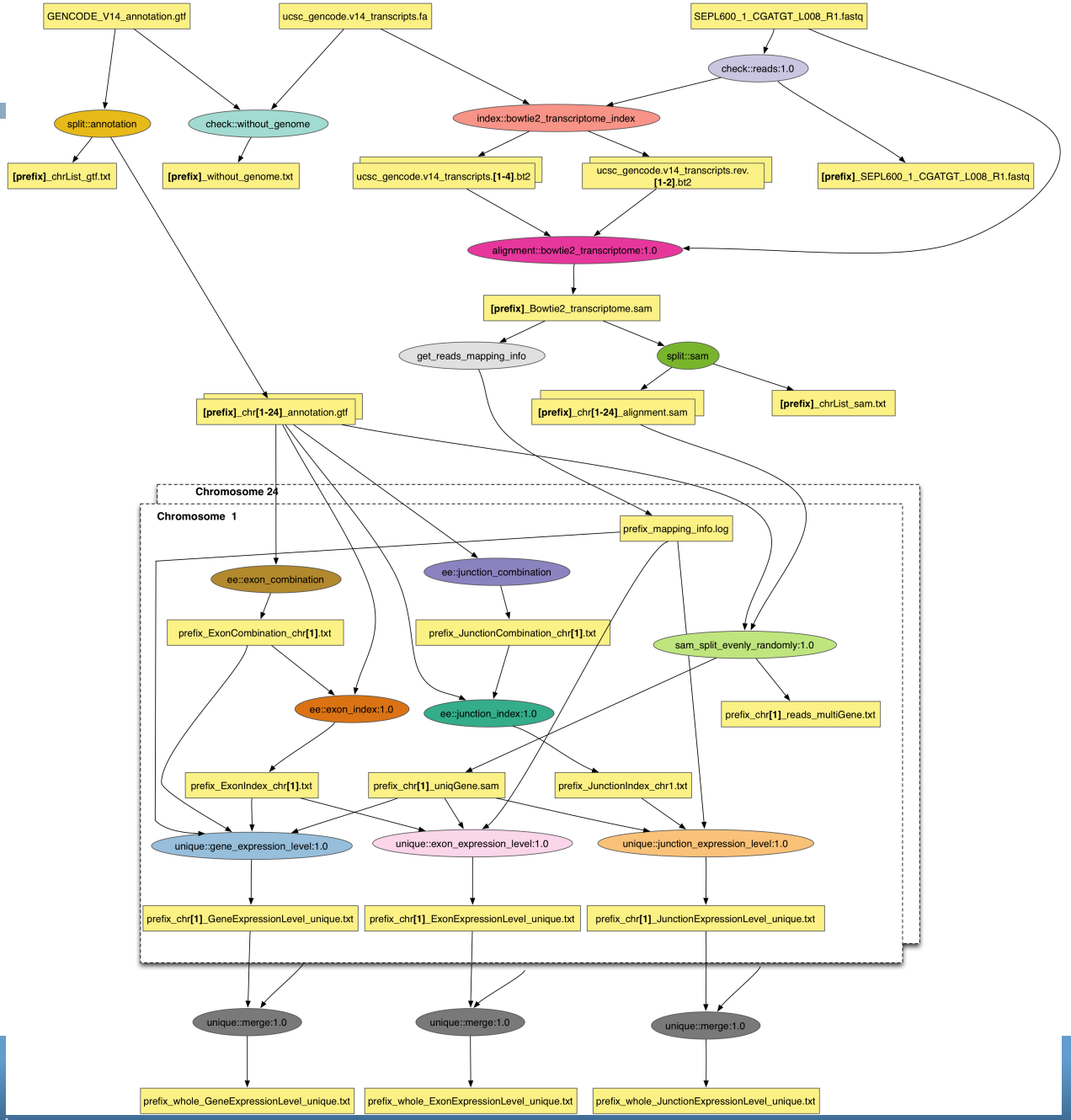
Scientific Workflows

- 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
- Provide automation
- Foster Collaborations

Workflows can be simple!

USC RNASEQ EXPRESSION ESTIMATION WORKFLOW

Workflow Developed By: Rajiv Mayani USC/ISI and Jennifer Herstein USC HSC



Computations: Users have same concerns!

- **Data Management**
  - How do you ship in the small/large amounts data required by your pipeline?
  - Different protocols for different sites: Can I use SRM? How about GridFTP? HTTP and Squid proxies?
  - Can I use Cloud based storage like S3 on EC2?

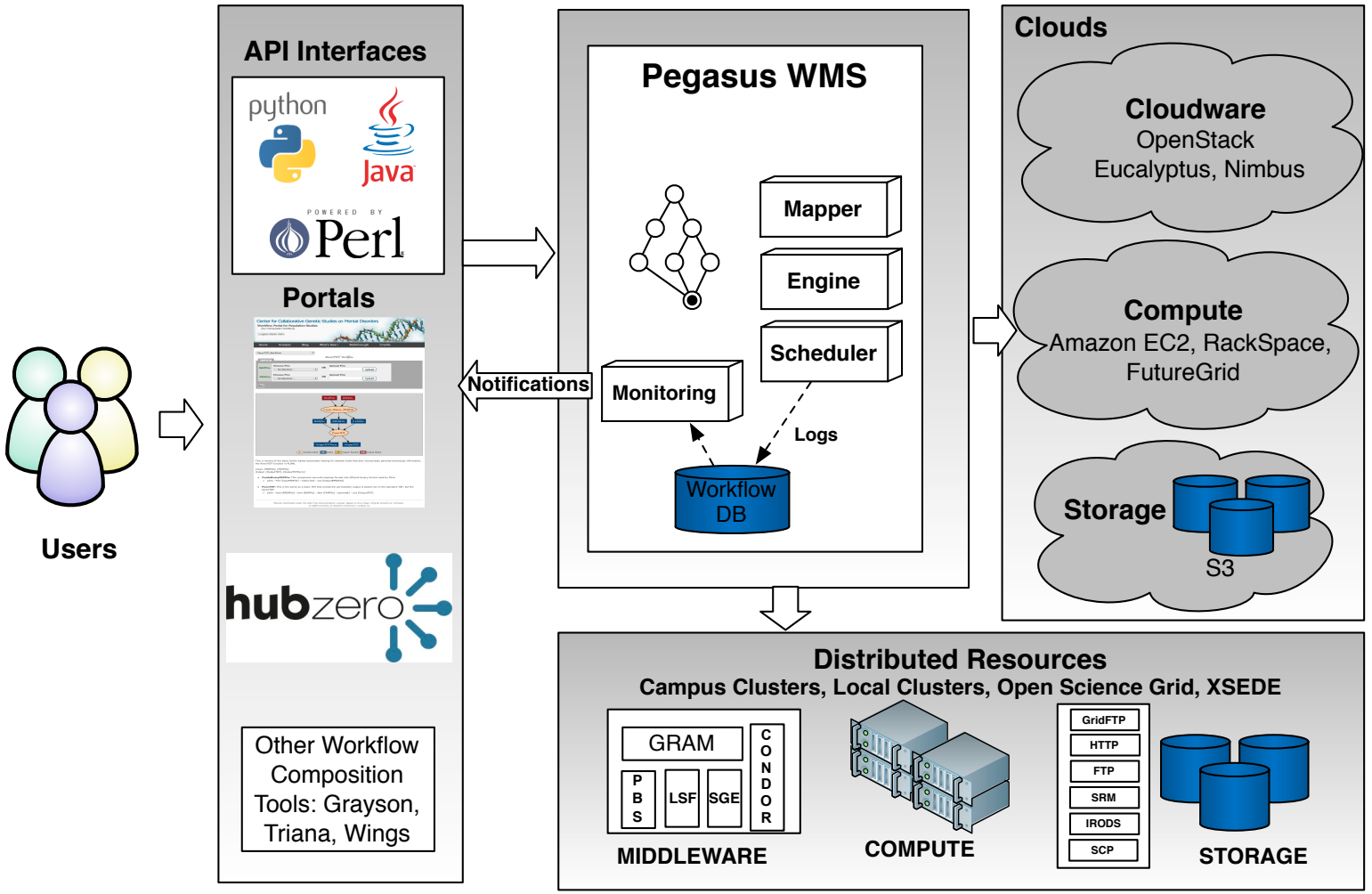
- **Debug and Monitor Computations.**
  - Users need automated tools to go through the log files
  - Need to correlate data across lots of log files
  - Need to know what host a job ran on and how it was invoked

- **Restructure Pipelines for Improved Performance**
  - Short running tasks?
  - Data placement?

Pegasus
Workflow Management System (est. 2001)

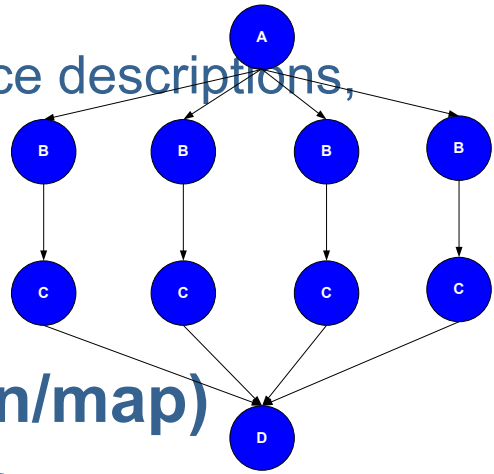
- A collaboration between USC and the Condor Team at UW Madison (includes DAGMan)
- Maps a resource-independent "abstract" workflow onto resources and executes the "executable" workflow
- Used by a number of applications in a variety of domains
- Provides reliability—can retry computations from the point of failure
- Provides scalability—can handle large data and many computations (kbytes-TB of data, 1-10^6 tasks)
- Infers data transfers, restructures workflows for performance
- Automatically captures provenance information
- Can run on resources distributed among institutions, laptop, campus cluster, Grid, Cloud

Pegasus WMS


API Interfaces
python
Java
POWERED BY
Perl
Portals
hubzero
Other Workflow Composition Tools: Grayson, Triana, Wings
Users
Notifications
Pegasus WMS
Mapper
Engine
Scheduler
Monitoring
Logs
Workflow DB
Clouds
Cloudware
OpenStack
Eucalyptus, Nimbus
Compute
Amazon EC2, RackSpace, FutureGrid
Storage
S3
Distributed Resources
Campus Clusters, Local Clusters, Open Science Grid, XSEDE
GRAM
PBS
LSF
SGE
CONDOR
MIDDLEWARE
COMPUTE
GridFTP
HTTP
FTP
SRM
IRODS
SCP
STORAGE

Pegasus Workflow Management System

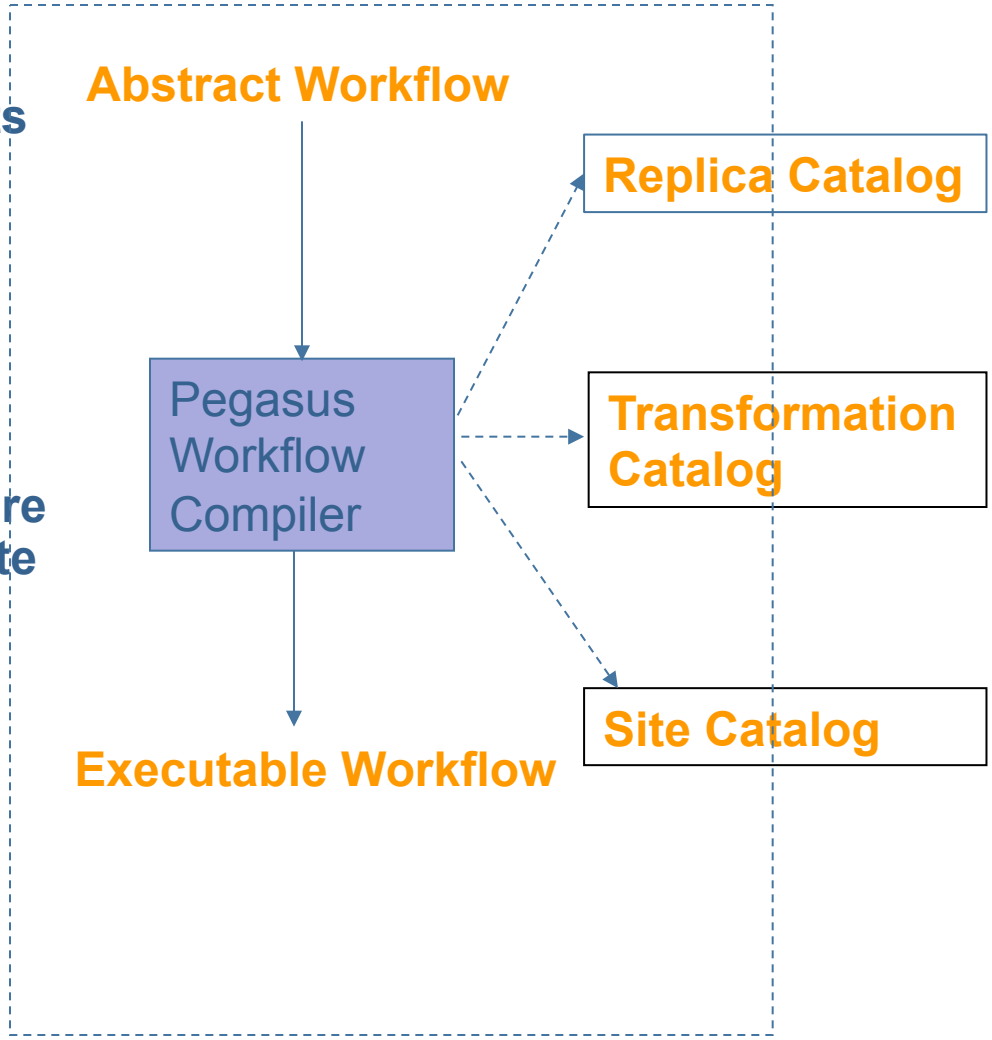
- **Abstract Workflows - Pegasus input workflow description**
  - Workflow “high-level language”
  - Only identifies the computation, devoid of resource descriptions, devoid of data locations
  - File Aware



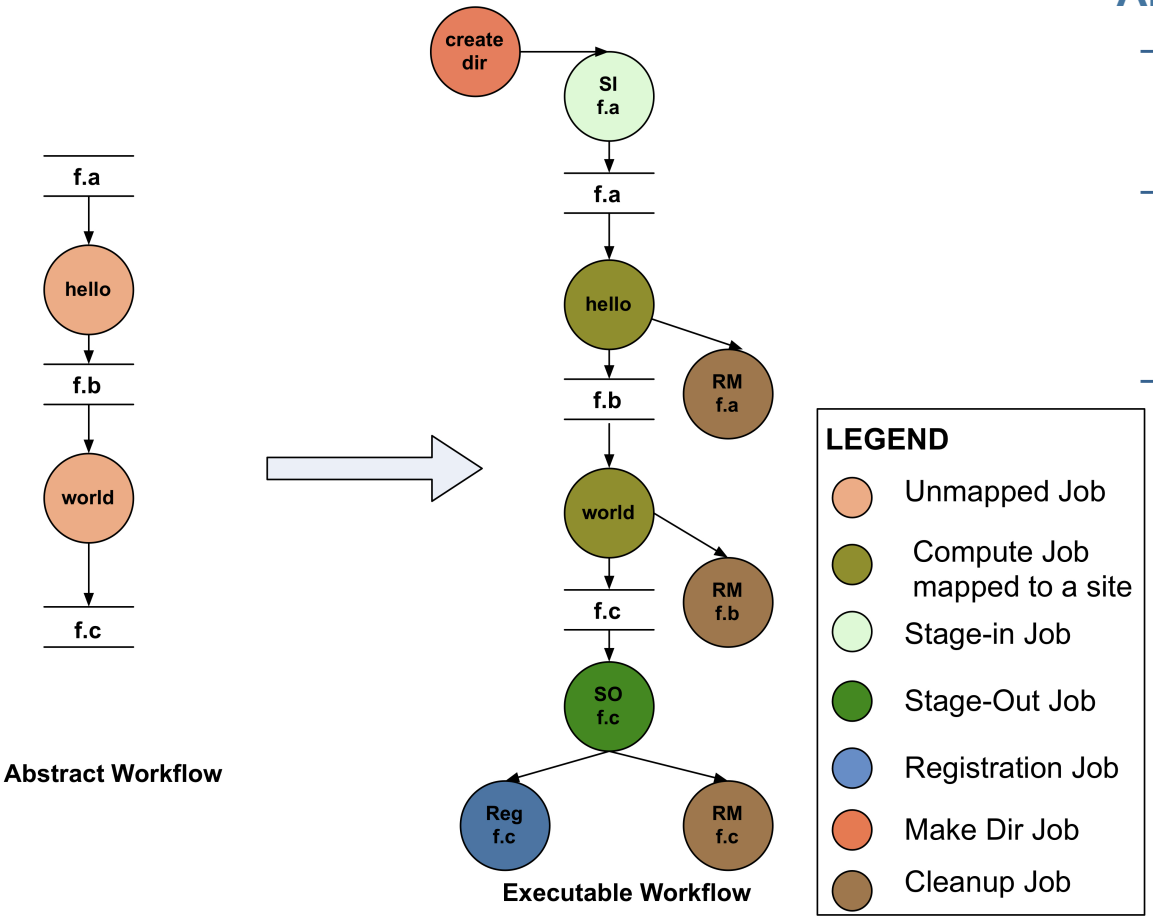
- **Pegasus is a workflow “compiler” (plan/map)**
  - Target is DAGMan DAGs and Condor submit files
  - Transforms the workflow for performance and reliability
  - Automatically locates physical locations for both workflow components and data
  - Collects runtime provenance

Abstract to Executable Workflow Mapping - Discovery

- **Data**
  - Where do the input datasets reside?
- **Executables**
  - Where are the executables installed ?
  - Do binaries exist somewhere that can be staged to remote grid sites?
- **Site Layout**
  - What does a execution site look like?



Abstract to Executable Workflow Mapping



- Abstraction provides
  - Ease of Use (do not need to worry about low-level execution details)
  - Portability (can use the same workflow description to run on a number of resources and/or across them)
  - Gives opportunities for optimization and fault tolerance
    - automatically restructure the workflow
    - automatically provide fault recovery (retry, choose different resource)

What Does Pegasus provide an Application - I

- **Portability / Reuse**
  - User created workflows can easily be mapped to and run in different environments without alteration.
- **Data Management**
  - Pegasus handles replica selection, data transfers and output registrations in data catalogs. These tasks are added to a workflow as auxiliary jobs by the Pegasus planner.
- **Performance**
  - The Pegasus mapper can reorder, group, and prioritize tasks in order to increase the overall workflow performance.

What Does Pegasus provide an Application - II

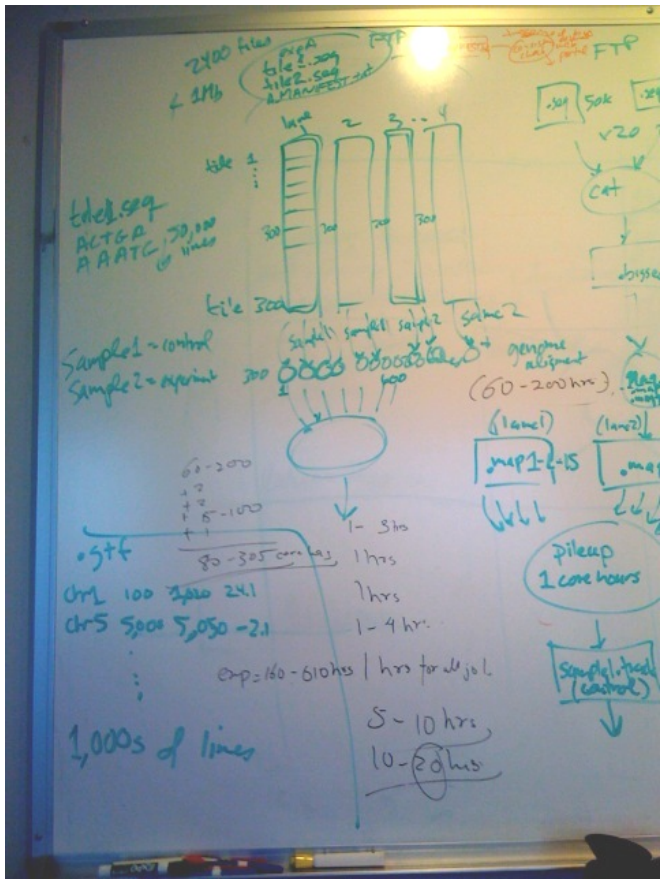
- **Provenance**
  - Provenance data is collected in a database, and the data can be summaries with tools such as pegasus-statistics, pegasus-plots, or directly with SQL queries.
- **Reliability and Debugging Tools**
  - Jobs and data transfers are automatically retried in case of failures. Debugging tools such as pegasus-analyzer helps the user to debug the workflow in case of non-recoverable failures.
- **Scalability**
  - Hierarchal workflows
  - Scale to hundreds of thousands of nodes in a workflow.

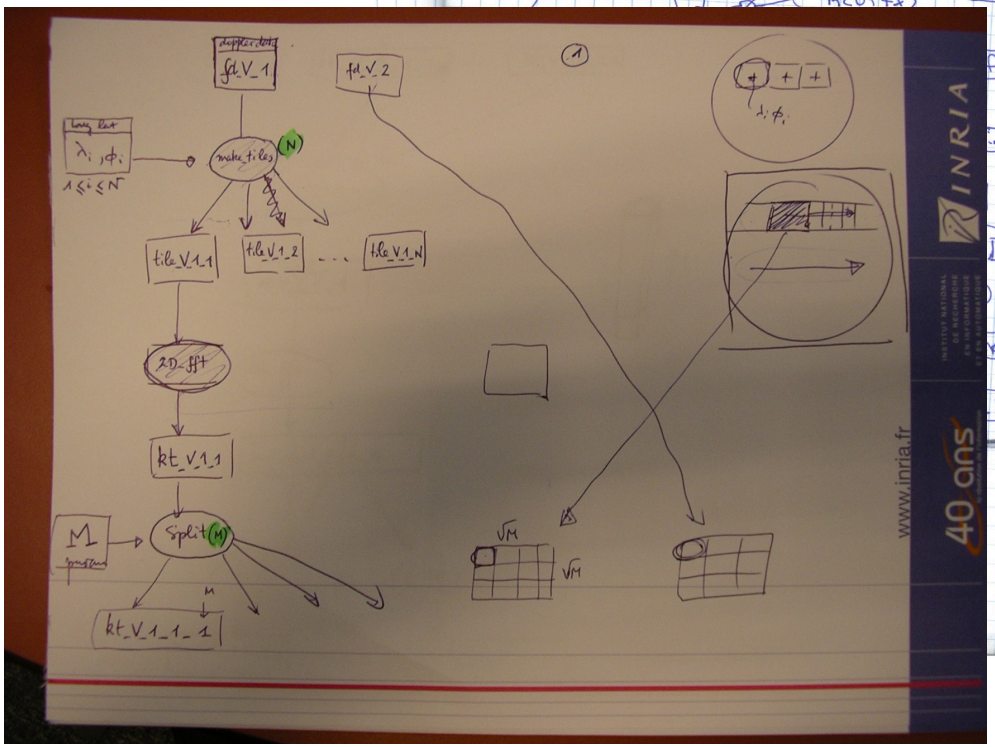
Simple Steps to Run Pegasus

1. **Specify your computation in terms of DAX**
   - Write a simple DAX generator
   - Python, Java , Perl based API provided with Pegasus
2. **Set up your catalogs**
   - Replica catalog, transformation catalog and site catalog.
3. **Plan and Submit your workflow**
   - Use *pegasus-plan* to generate your executable workflow that is mapped onto the target resources and submits it for execution
4. **Monitor and Analyze your workflow**
   - Use *pegasus-status* | *pegasus-analyzer* to monitor the execution of your workflow
5. **Workflow Statistics**
   - Run pegasus-statistics to generate statistics about your workflow run.

If you get stuck…

And you can draw….





We can help you!

Support: pegasus-support@isi.edu
pegasus-users@isi.edu

Relevant Links

- **Pegasus: http://pegasus.isi.edu**
- **Tutorial and documentation: http://pegasus.isi.edu/wms/docs/latest/**
- **Support: pegasus-users@isi.edu**
  pegasus-support@isi.edu

Acknowledgements

Pegasus Team, Condor Team, funding agencies, NSF, NIH, and everybody who uses Pegasus.