







# Science Impact of Sustained Cyberinfrastructure: The Pegasus Example

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University of Southern California,  
Information Sciences Institute

NSF Office of Advanced CyberInfrastructure Webinar  
May 17, 2018

Pegasus represents a long standing collaboration with Miron Livny, University of Wisconsin, Madison



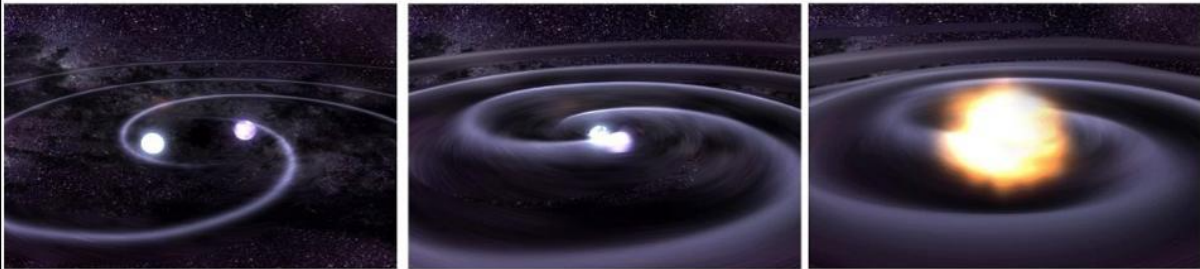
 <http://pegasus.isi.edu>

Slide 1: Title slide. Science Impact of Sustained Cyberinfrastructure: The Pegasus Example. Ewa Deelman, USC. Title slide also indicates that Pegasus represents a long standing collaboration with Miron Livny, University of Wisconsin, Madison

October 16<sup>th</sup> 2017: “ LIGO and Virgo make first detection of gravitational waves produced by colliding neutron stars”

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School of Engineering  
Information Systems Division

And kick off a new era of multi-messenger astronomy



*“The inspiral and merger of two neutron stars, as illustrated here, should produce a very specific gravitational wave signal, but the moment of the merger should also produce electromagnetic radiation that's unique and identifiable as such.”, credit LIGO*

NASA's Fermi space telescope had detected a burst of gamma rays at about the same time



<http://pegasus.isi.edu>


Images credit: LIGO Scientific Collaboration

Slide 2: Pictures depicting colliding neutron stars, before and during the merger

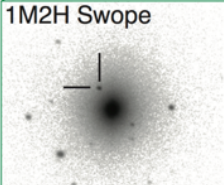
The caption for the picture is

*The inspiral and merger of two neutron stars, as illustrated here, should produce a very specific gravitational wave signal, but the moment of the merger should also produce electromagnetic radiation that's unique and identifiable as such.”, credit LIGO*

## Targeting Telescopes on the Neutron Star Merger

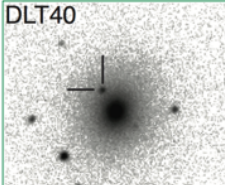


1M2H Swope



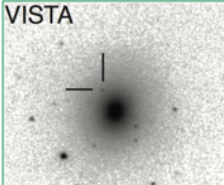
10.86h *i*

DLT40




11.08h *h*

VISTA



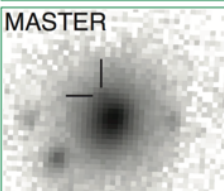
11.24h *YJK<sub>s</sub>*

Chandra



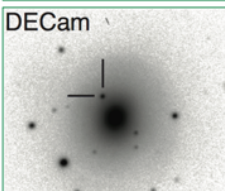
9d *X-ray*

MASTER



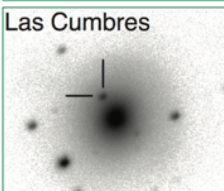
11.31h *w*

DECam



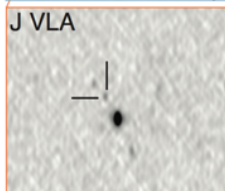
11.40h *iz*

Las Cumbres




11.57h *w*

J VLA



16.4d *Radio*

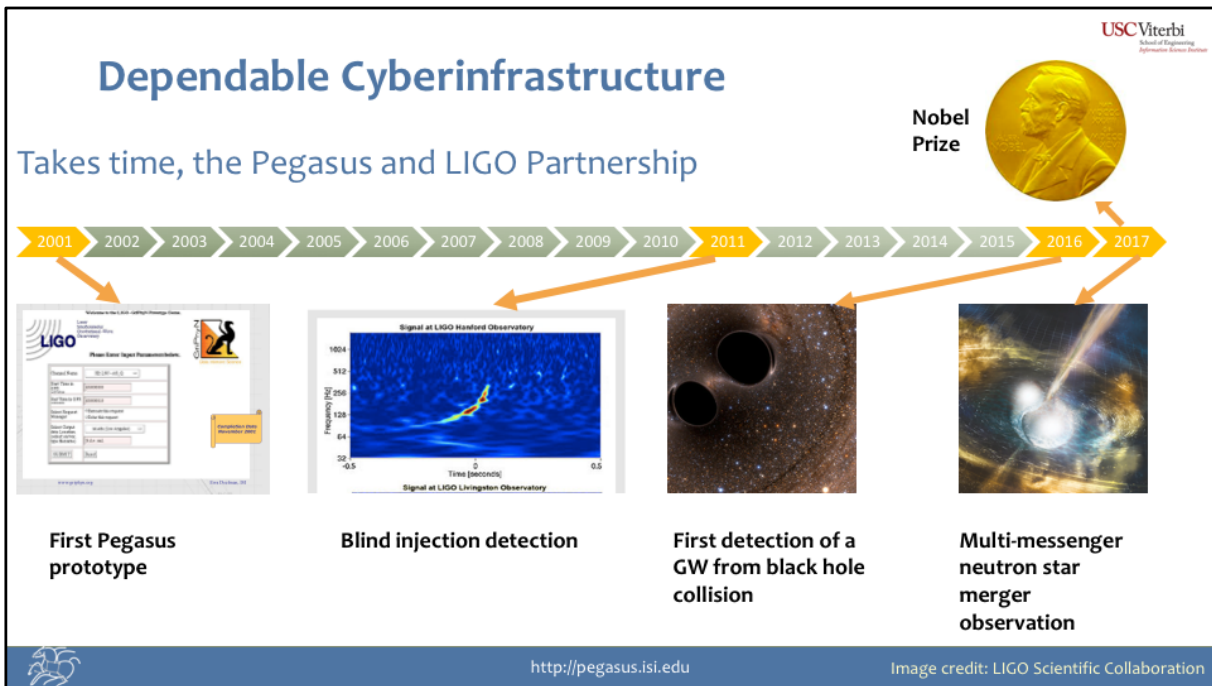
“aftermath of the BNS merger.. On the left are six optical images taken between 10 and 12 hours after the merger by different telescopes. On the right are images constructed from x-ray and radio observations. The x-ray image was taken 9 days after the merger by NASA's Chandra X-ray Observatory. 16 days after the merger NRAO's Jansky Very Large Array (VLA) captured the radio image” from LIGO.org



<http://pegasus.isi.edu>

Images credit: LIGO Scientific Collaboration

Slides 3: Pictures depict the colliding neutron stars as seen by various telescopes hours and days after the merger.



Slide 4: Shows the timeline of the Pegasus and LIGO partnership since 2001 to 2017, includes the first prototype in 2001, the detection of the blind injection in 2011, the first ever direct detection of the gravitational wave from colliding black holes in 2016, and the Nobel Prize in 2017.

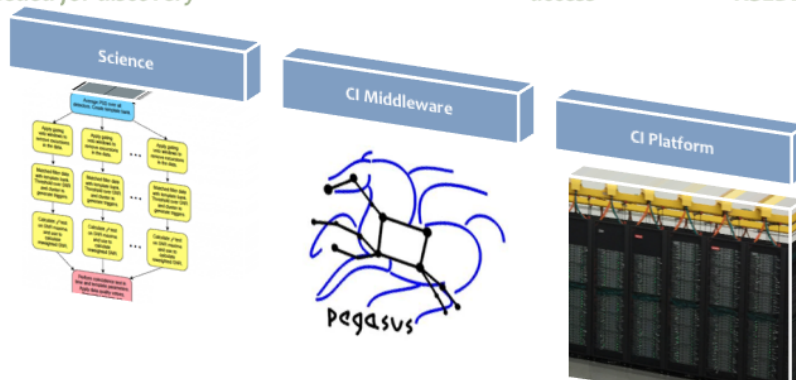
## First GW detection: Pegasus automated ~ 21K workflows with ~ 107M tasks

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*Science workflow:  
measure the statistical significance  
of data needed for discovery*

*Automated by Pegasus  
execution of tasks and data  
access*

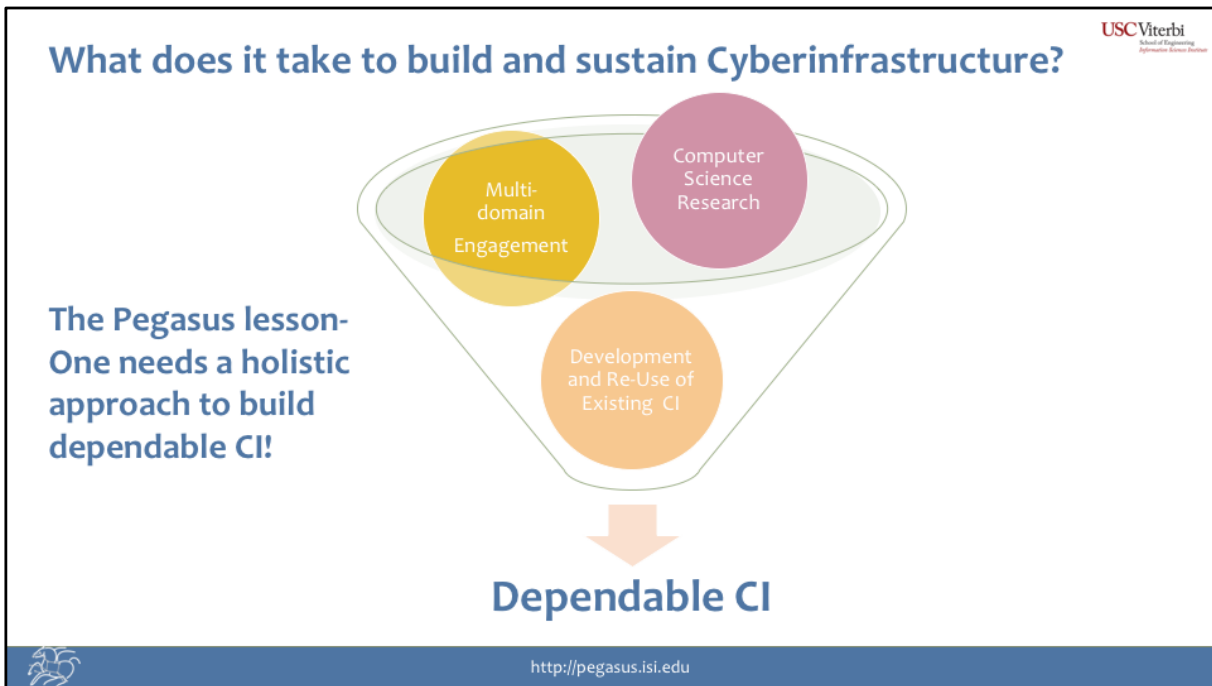
*Distributed Power  
LIGO, Open Science Grid,  
XSEDE, Blue Waters*



<http://pegasus.isi.edu>

Slide 5: Description of the Pegasus automated workflows.

Peter Couvares, data analysis computing manager for the Advanced LIGO project at Caltech: "When a workflow might consist of 600,000 jobs, we don't want to rerun them if we make a mistake. So we use DAGMan(Directed Acyclic Graph Manager, a meta-scheduler for HTCondor) and Pegasus workflow manager to optimize changes,"



Slide 6: Pictures depict three important aspects of CI. 1) Multi- domain engagement, 2) Computer science research, 3) development and re-use of existing CI



Slide 7: Timeline from 2000 to 2018 with Pegasus team members. Karan Vahi, the main Pegasus developer has been working on the project for 17 years.

**Back Row:** Tu Mai Anh Do, Mats Rynge, Karan Vahi, George Papadimitriou


**Front Row:** Rosa Filgueira, Ewa Deelman, Rajiv Mayani

**Missing:** Rafael Ferreira da Silva, Ashwin Venkatesha

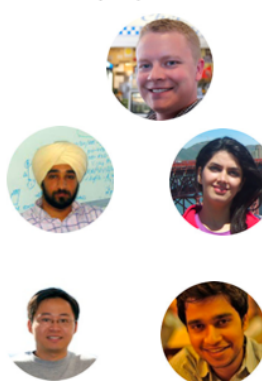
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Information Science Institute

## Takes Contributions from Many People


Developers



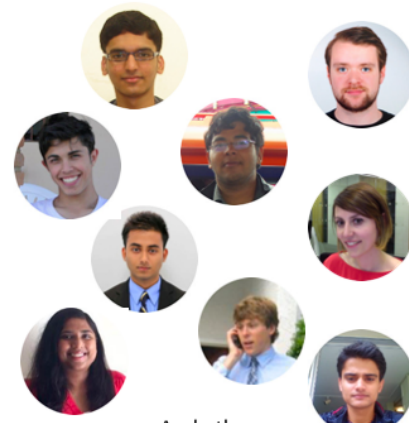
GRAs



PostDocs




Master Students and Visitors



Currently at Amazon, Google, NetApps, SpaceX, Samsung, startups

And others

## Takes Collaboration with Many CS and Domain Scientists



<http://pegasus.isi.edu>

Slide 8: Takes Collaboration with Many CS and Domain Scientists



## How did Pegasus Start?

Extend the concept of view materialization in DBs to distributed environments



### The Virtual Data Grid (VDG) Model

- Data suppliers publish data to the Grid
- Users request raw or derived data from Grid, without needing to know
  - Where data is located
  - Whether data is stored or computed

NSF ITR: GriPhyN Project: Ian Foster (PI), Paul Avery, Carl Kesselman, Miron Livny, (co-PIs)



### Virtual Data Scenario

- (LIGO) "Conduct a pulsar search on the data collected from Oct 16 2000 to Jan 1 2001"
- For each requested data value, need to
  - Understand the request
  - Determine if it is instantiated; if so, where; if not, how to compute it
  - Plan data movements and computations required to obtain all results
  - Execute this plan

How do you translate the Computer Science idea to the needs of science?

Circa. 2001



<http://pegasus.isi.edu>

Slide 9: Pictures describes the idea of Virtual Data Grid and Virtual Data Scenario.

## Challenge: How Translate a Science Request to an Actionable Plan?

Welcome to the LIGO-GrPhyN Prototype Demo.

**LIGO** Laser Interferometer Gravitational-Wave Observatory

**GrPhyN** Data Science

Please Enter Input Parameters below.

Channel Name:

Start Time in GPS:

End Time in GPS:

Select Request Manager:

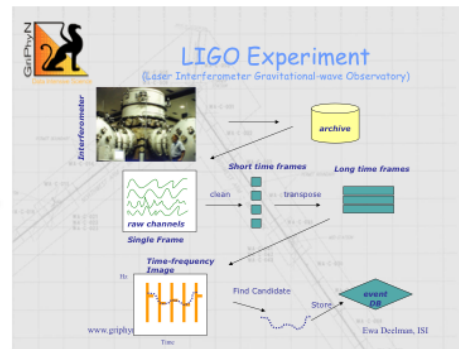
Select Output data Location (select server, type filename):

File:

Completion Date: November 2001

www.griphyn.org Ewa Declan, ISI

Explore AI  
planning  
techniques



Lost in translation: high-level abstraction for this science domain  
Found: new research direction: management of workflows in distributed environments

<http://pegasus.isi.edu>

Slide 10: On the left a picture of the user interface for the first LIGO prototype, on the right the resulting scientific workflow.

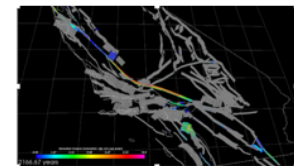


## Challenges of Workflow Management

- Working with LIGO and other applications (astronomy, earthquake science), found common challenges:
  - Need to describe complex workflows in a simple way
  - Need to access distributed, heterogeneous data and resources
  - Need to deal with resources/software that change over time
- Our focus:
  - Separation between workflow description and workflow execution
  - Workflow planning and scheduling (scalability, performance)
  - Task execution (monitoring, fault tolerance, debugging)



Sky mosaic, IPAC, Caltech



Earthquake simulation, SCEC, USC



Slide 11: Describes workflow management challenges. The images show sample results from astronomy and earthquake science.

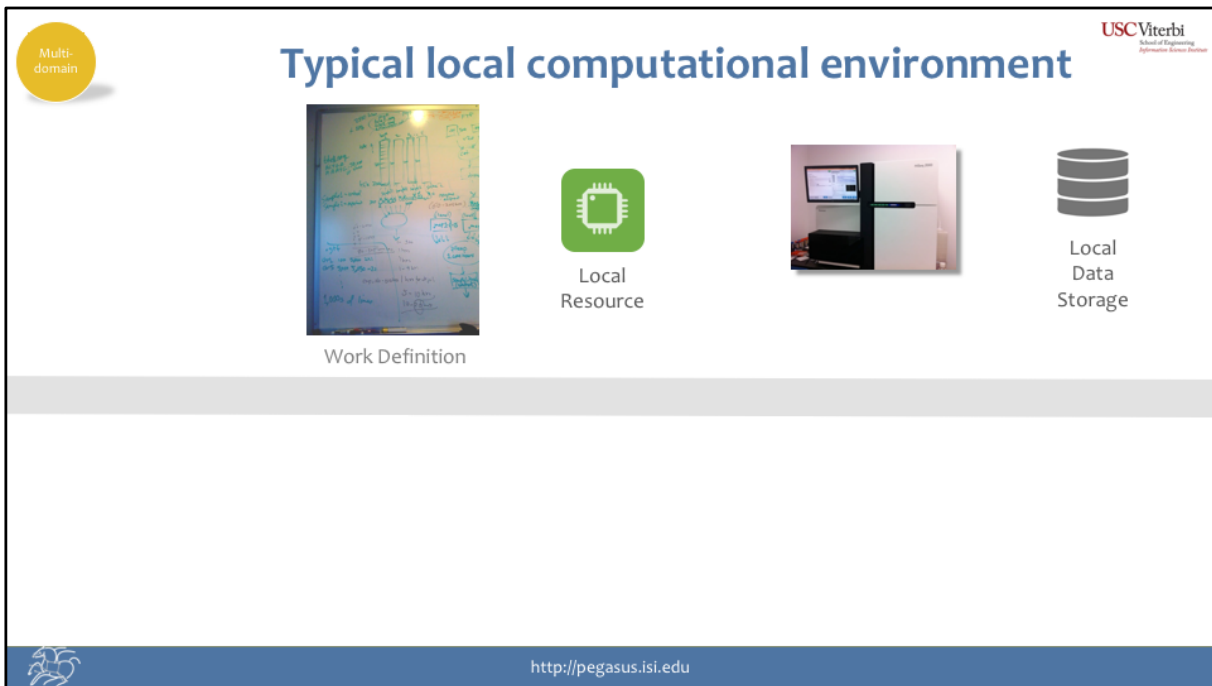


## Benefits of Scientific Workflows (from the point of view of an application scientist)

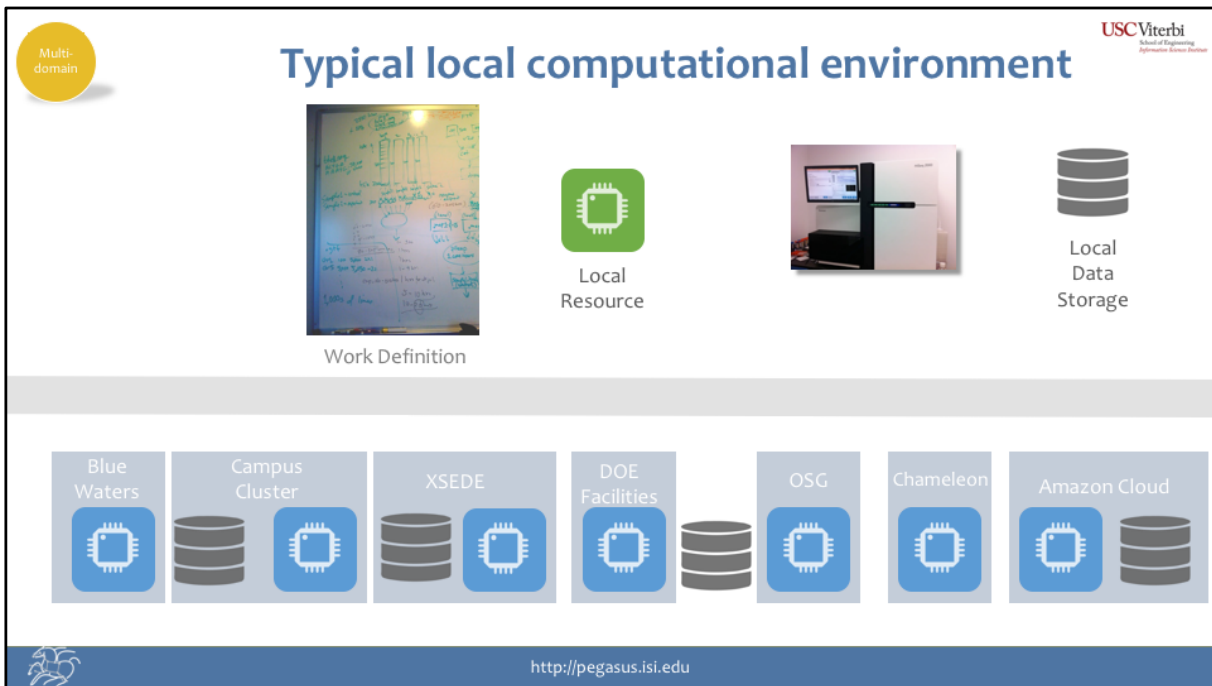
- Conducts a series of computational tasks
- Chaining (outputs become inputs) replaces manual hand-offs
- Ease of use: gives non-developers access to sophisticated codes
- Provides framework to host or assemble community set of applications, can be multi-disciplinary
- Framework to define common formats or standards when useful



Slide 12: Describes the benefit of science workflow.



Slide 13: Pictures describe typical computational workflow environment with local resources and storage.



Slide 14: Additional description of computational workflow environment that includes campus resources, national cyberinfrastructure, NSF and commercial clouds.

```

graph TD
    fa[f.a] --> hello((hello))
    hello --> fb[f.b]
    fb --> world((world))
    world --> fc[f.c]
  
```

## To run Hello World on TACC's Wrangler

- 1. Login to TACC**

```
localhost$ ssh -l deelman wrangler.tacc.utexas.edu
login1.wrangler$ emacs myjob.sub
```
- 2. Write submit script**

```
#!/bin/bash
#SBATCH -J myjob
#SBATCH -o myjob.o%j
#SBATCH -e myjob.e%j
#SBATCH -p normal
#SBATCH -N 1
#SBATCH -n 1
#SBATCH -t 01:30:00
#SBATCH --mail-
user: deelman@gmail.com
#SBATCH --mail-type=all
#SBATCH -A myproject

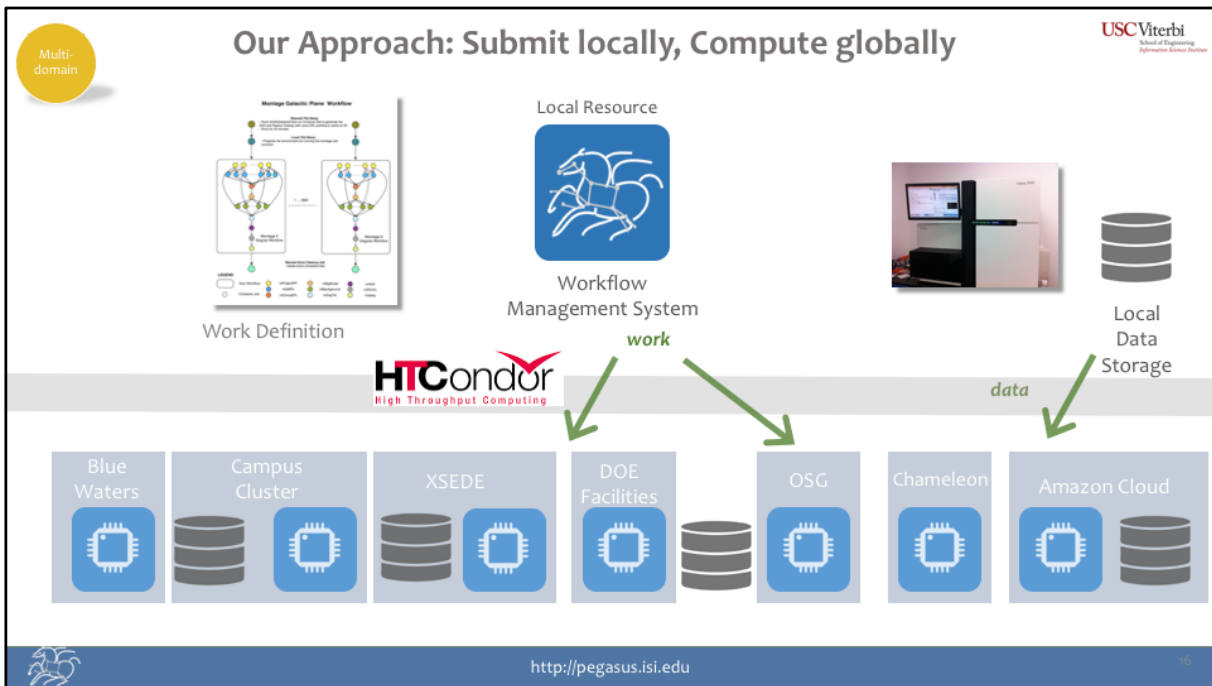
mkdir $WORK/helloworld
cd $WORK/helloworld
cp $WORK/data/inputs/* .
~/hello
~/world
cp * $WORK/data/outputs/
~/my_output_files/
```
- 3. Find and bring in your input data**
- 4. Submit script for execution**

```
login1.wrangler$ queue myjob.sub
```
- 5. Stage out data for further analysis**

What if Wrangler goes down/gets decommissioned? What if the job crashed? What about running on multiple platforms?


<http://pegasus.isi.edu>

Slide 15: Pictures walk the viewer through a programming workflow. 1) Login to computer, 2) Write script, 3) Find and download data, 4) Submit script to execute on system.




Slide 16: Pictures describe typical computational workflow environment with local resources and storage that accesses global resources to execute.

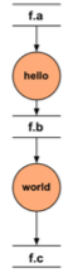


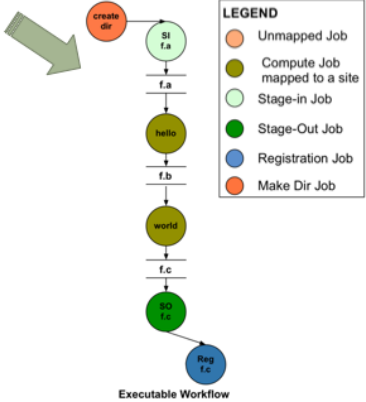


## Pegasus Today




- Scientists describe their computational processes (workflows) at a logical level, without including details of the underlying CI
  - Operates at the level of files and individual codes
- Pegasus maps the abstract workflow to the available resources and infers the needed data transfers
- Pegasus generates an executional workflow, writes out submit files, and executes the workflow
- Underpins other user facing portals: NanoHub (Purdue)
- Provides workflow management for workflow composition tools: Wings (USC)





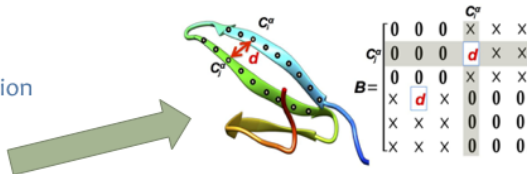
Executable Workflow


<http://pegasus.isi.edu>

Slide 17: add at the end: The picture on the left shows the abstract workflow that is devoid of resource description. The picture on the right shows the executable workflow generated by Pegasus and that include compute jobs mapped to an execution site, data stage-in and stage out jobs, data registration jobs, and make directory jobs.

## CS Principles Help in Cyberinfrastructure Development

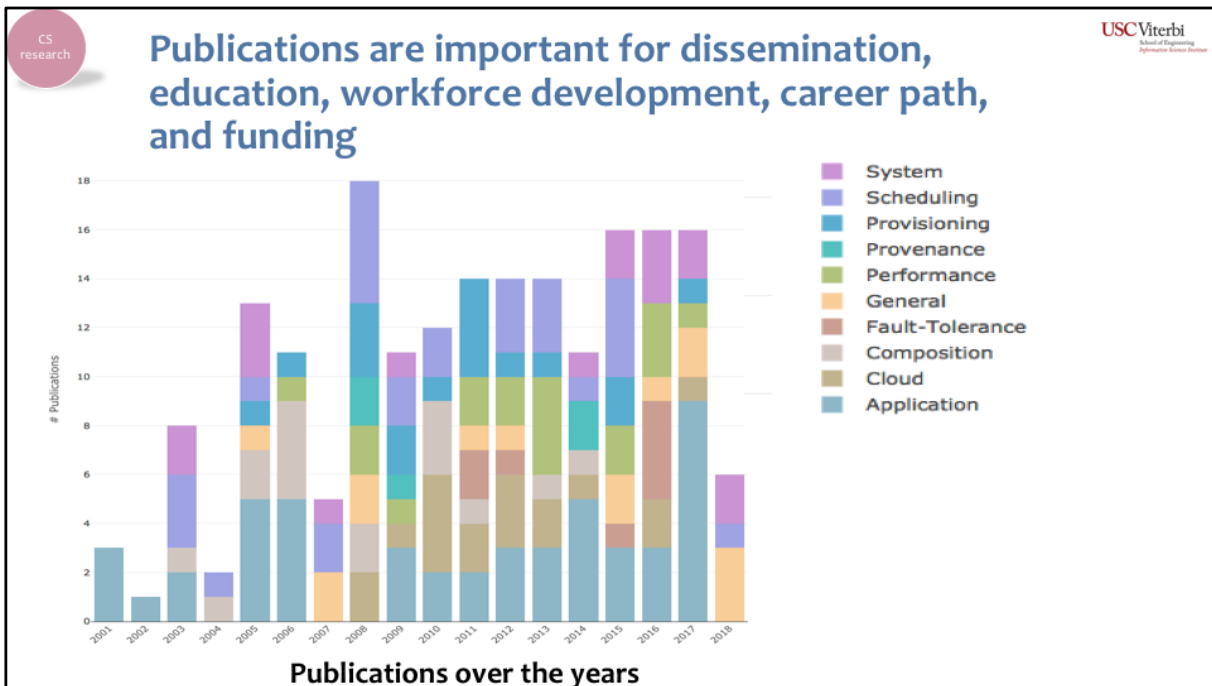
- Structure workflows as **directed acyclic graphs (DAGs)**
  - Re-use of graph traversal algorithms, node clustering, pruning, other complex graph transformation
- Use hierarchical structures in DAGs
  - To achieve scalability, recursion, dynamic behavior
- Develop new algorithms:
  - Task clustering
  - Data placement
  - Data re-use
  - Resource usage estimation
  - Resource provisioning
  - **In situ workflows**



**New Direction:**  
In-memory coupling  
of simulation and  
analytics  
Collaboration with U  
Delaware, Cornell,  
UTEP



Slide 18: Describes CS principles in helping to develop cyberinfrastructure.




Slide 19: The graphs shows the publications by year starting in 2001 and ending in 2018. The publications span topics such as workflow system, job scheduling, resource provisioning, provenance, performance, general workflow management, fault

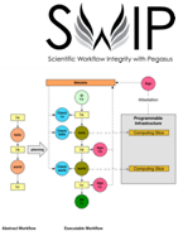

Re-use


## Leveraging Proven Solutions Key to Innovation

- Leveraged HTCondor's
  - Job submission to heterogeneous, distributed resources
  - Managing job dependencies expressed as DAGs
  - Job retries and error recovery
- Allowed us to focus on other aspects of automation:
  - Workflow planning, and re-planning in case of failures
  - Automated data management
  - Specialized workflow execution engines for HPC systems
  - APIs for workflow composition: Python, R, Java, Perl, Jupyter Notebook
  - User-friendly monitoring and debugging tools
  - Provenance tracking
  - Data integrity



Indiana University  
RENCI





<http://pegasus.isi.edu>


Slide 20: Mentions the SWIP data integrity project.

20

CS  
research

CI Dev.

## Using Real Applications Provides Realistic Testing and Evaluation




Montage: Important application for CS and CI

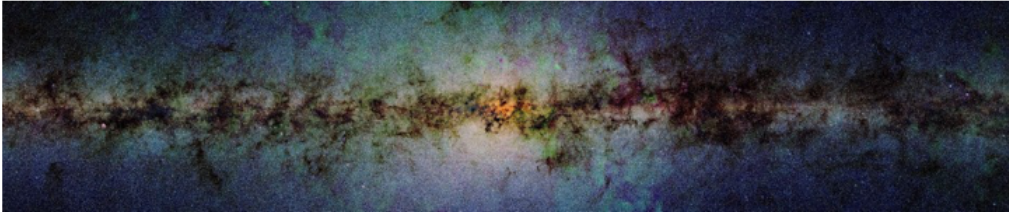
Open source, open data, scalable, robust

Helps advance CS and test CI: workflow scheduling, resource provisioning, provenance tracking


One of the workflows used in Pegasus' nightly build and test



Montage, an important astronomy application, collaboration with Caltech since 2002



Montage, an important astronomy application, collaboration with Caltech since 2002



<http://pegasus.isi.edu>

Slide credit: B.Berriman, J.Good, Caltech

Slide 21: Describes the Montage astronomy application. The application is also important for computer science research and for the testing of the cyberinfrastructure. Pegasus uses it as one of the applications for nightly builds and tests.

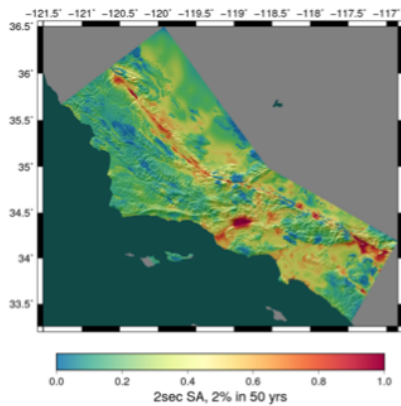
The picture shows the galactic plane generated by Montage.



## Need applications that push the boundaries of what you can do

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**SCEC's CyberShake: What will peak earthquake shaking be over the next 50 years?**



Useful information for:  
Building engineers  
Disaster planners  
Insurance agencies

**2017: 21.6 million core  
hours, 777TB of data**

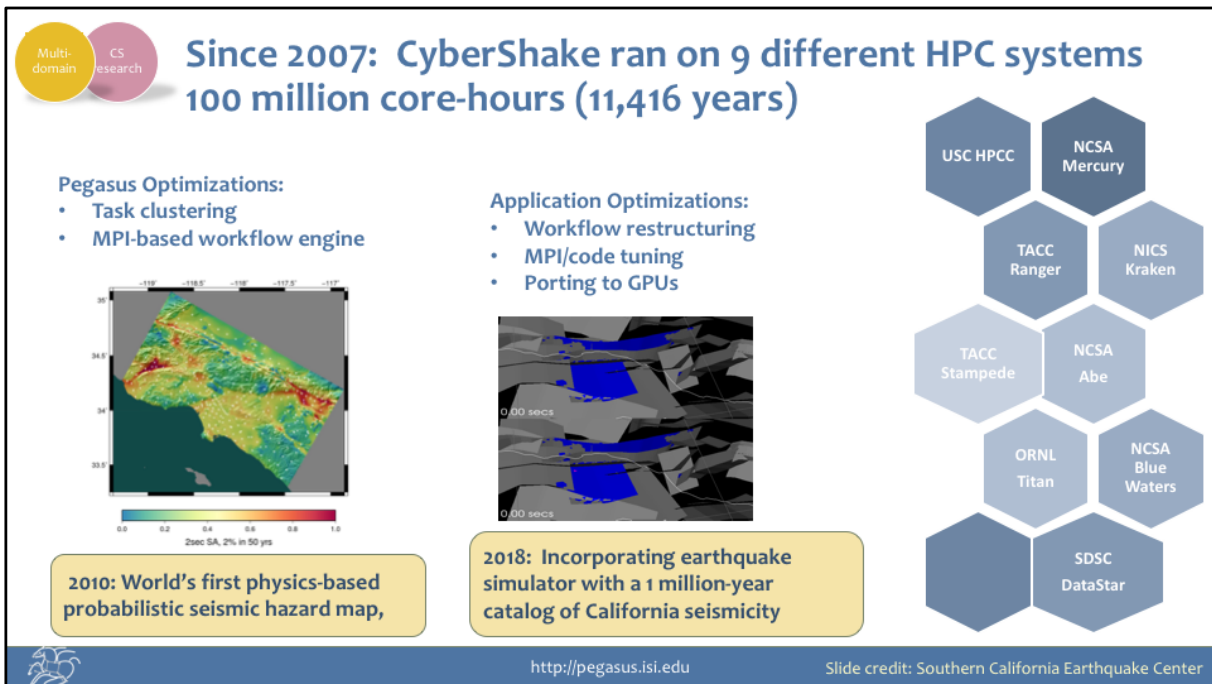
**On ORNL's Titan and  
NCSA's Blue Waters**



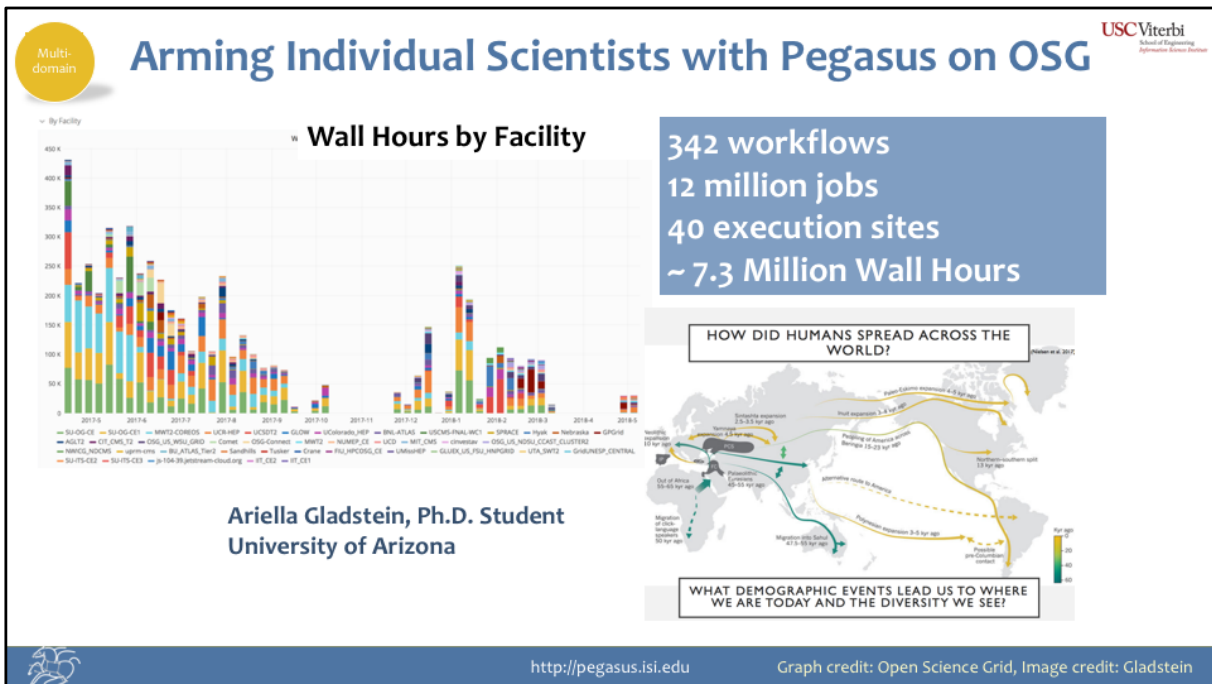
<http://pegasus.isi.edu>

Slide credit: Southern California Earthquake Center

Slide 22: The picture shows a seismic hazard map for Southern California.

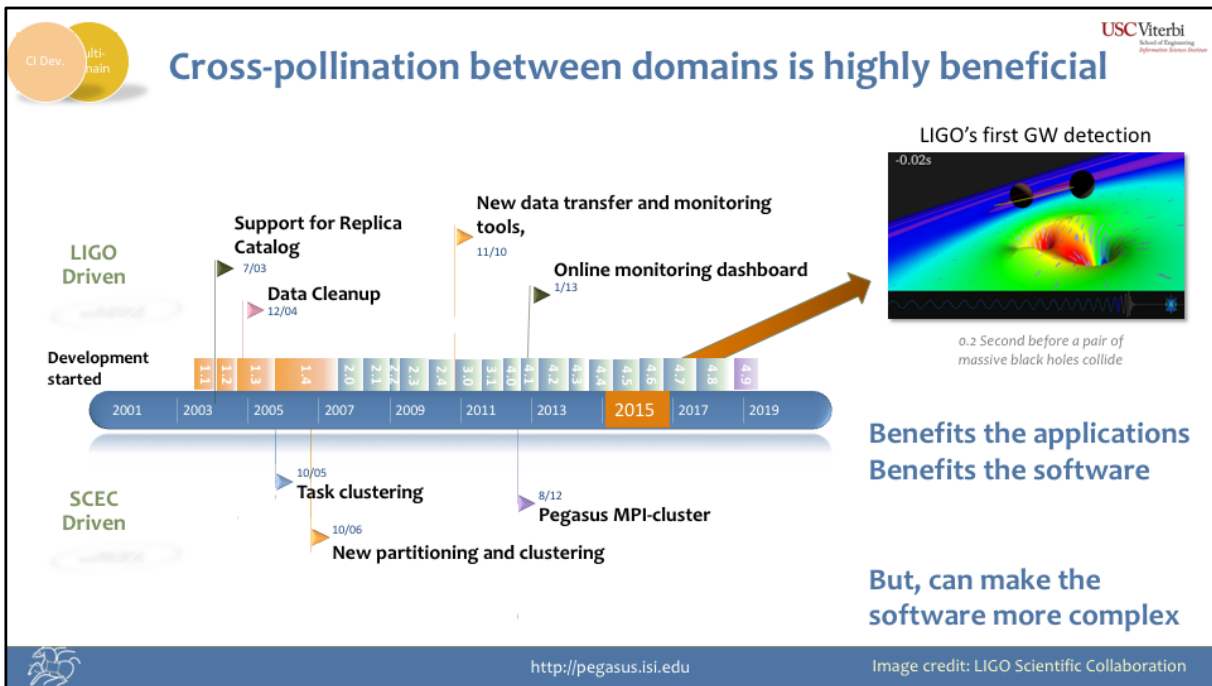


Slide 23: Shows the Cybershake map from 2010 and the results from the 2018 simulation of a million year of California seismicity. Also names the various HPC systems that CyberShake used over the last 16 years: USC, NCSA Mercury, TACC Ranger, NICS Kraken, TACC Stampede, NCSA Abe, ORNL Titan, NCSA Blue Waters, SDSC DataStar



Slide 24: Shows the amount of computing used by bioinformatics application supported by Pegasus on the Open Science Grid.

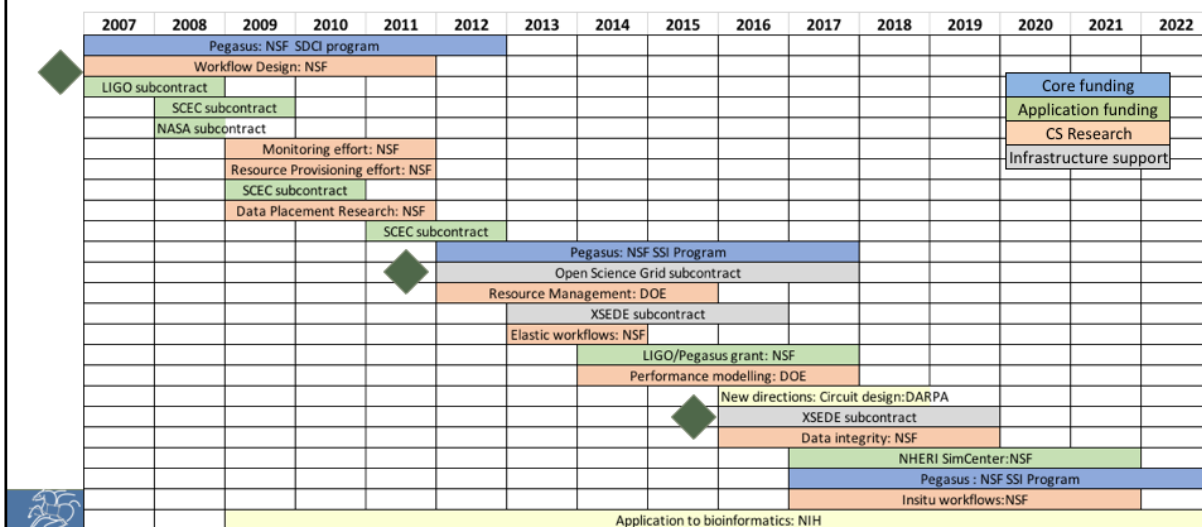


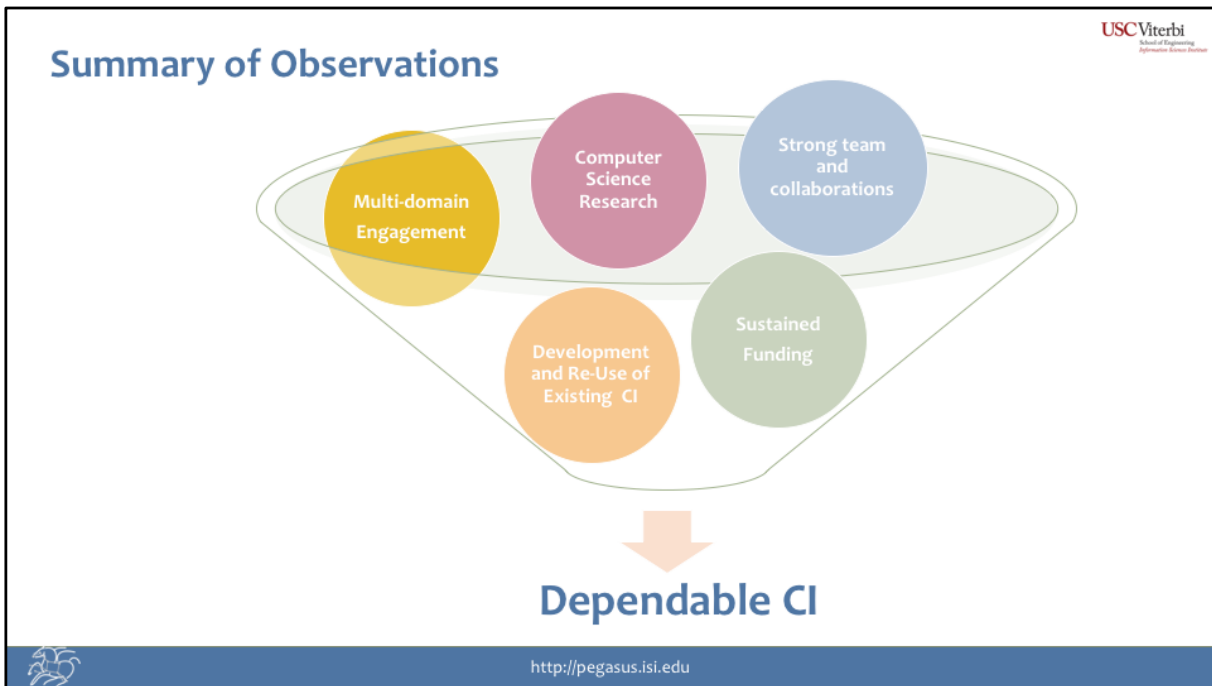




# To sustain software, need many different funding sources and need to interleave research, software development, and user support

## Pegasus-related funding

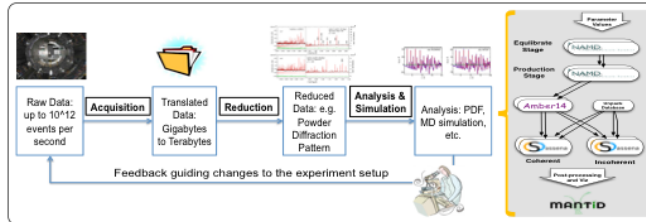




Slide 27: Slides shows the ingredients of dependable cyberinfrastructure: computer science research, multi-domain engagement, strong team and collaboration, development and re-use of existing cyberinfrastructure, sustained funding.

## Looking ahead: Application Trends

Spallation Neutron Source



### Planned CyberShake for Northern California:

- 869 geographic sites
- 16,000 workflow jobs
- 70 million core-hours on Blue Waters and Titan
- 800 TB of data

- More complex
- Faster time to solution: instrument steering
- More individual researchers in need of significant CI
  - Need intuitive workflow composition, better monitoring, error handling, assisted debugging

### Outreach: How do you reach scientists that don't know you are out-there?

Many scientists are going through the same pain

Leverage/enhance existing engagement: NSF's Campus efforts? OSG/XSEDE outreach?

Education and outreach at instruments and experimental facilities?



## Looking ahead: Growing Demand for Automation

### HPC Systems

- Complex
- Heterogeneous
- Specialized data storage
- Increasingly faulty

### Distributed Systems

- Software Defined capabilities
- Specialized data storage

### Clouds

- New platform for science
- Very heterogenous
- Can be costly

## Resource Management is Key

Constraints: time to solution, budget


Faulty environment: failure detection and attribution

Heterogenous storage: memory, burst buffers, file systems, data xfer nodes

Need to keep track of big data technologies and machine learning solutions that are being developed at a rapid pace by industry

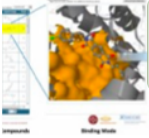


**Cancer genetics**



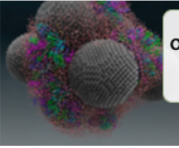
Clemson

**Structural Protein-Ligand Interactome**



Indiana U.

**Molecular Dynamics**

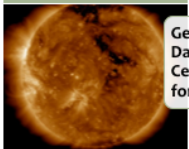


ORNL

**Thank you to the team, collaborators and funders**


**Example Pegasus-enabled Applications**

**Helioseismology**



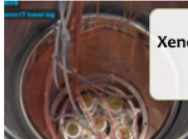
German Data Center for SDO

**Next Generation Sequencing**



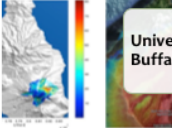
Children's Hospital of Philadelphia

**Dark Matter Detection**




Xenon1T

**Volcano Mass Flow**




University of Buffalo

**Soybean Studies**



University of Missouri

**Weak Gravitational Lensing**



Fermi National Lab

**We look forward to future collaborations**

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[pegasus-support@isi.edu](mailto:pegasus-support@isi.edu)