Science Impact of Sustained Cyberinfrastructure: The Pegasus Example

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

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
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
“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

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.
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
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

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.
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)

Slide 11: Describes workflow management challenges. The images show sample results from astronomy and earthquake science.
Slide 12: Describes the benefit of science workflow.

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 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.
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.
Our Approach: Submit locally, Compute globally

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 executonal 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)

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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
  - \textit{In situ workflows}

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
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.
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.
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.
Cross-pollination between domains is highly beneficial

Benefits the applications
Benefits the software

But, can make the software more complex

http://pegasus.isi.edu

Image credit: LIGO Scientific Collaboration
To sustain software, need many different funding sources and need to interleave research, software development, and user support

### Pegasus-related funding

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Application to bioinformatics: NIH
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

- 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?

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
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 heterogeneous
- 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

http://pegasus.isis.edu
Thank you to the team, collaborators and funders

Example Pegasus-enabled Applications

Cancer genetics
Clemson

Structural Protein-Ligand Interactome
Indiana U.

Molecular Dynamics
ORNL

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

For webinar Qs, email rramnath@nsf.gov
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