CI/CS WORKSHOP

THE COMMUNITY TOGETHER

ResearchSOC | CI CoE PILOT
Mats Rynge: Workflows

USC Information Sciences Institute
www.isi.edu
Questions

- How pegasus takes care of protected data
- Have a few questions about feasibility of supporting workflow systems on a floating vessel
Trustworthy Data Working Group

Aims to provide guidance on data security for open science, to improve scientific productivity and trust in scientific results. Open science relies on data integrity, collaboration, high performance computing, and scalable tools to achieve results, but currently lacks effective cybersecurity programs that address the trustworthiness of scientific data.

Community Survey: Scientific Data Security Concerns and Practices
• 111 participants
• Report available: https://doi.org/10.5281/zenodo.3906865

PEARC’20 Workshop on Trustworthy Scientific Cyberinfrastructure

Next: creating a “Guidance for Science Projects and Cyberinfrastructure Developers” document
Protected Data?

Trustworthy Data?

**Integrity** - The data has not been altered.

**Reproducibility** - The data can be re-created, or the associated scientific results are replicable.

**Provenance** - The data's origin and lineage can be readily established.

**Methodology** - The processes and inputs used to create the data are well-established and accepted by the community.

**Responsible stewardship** - The ownership of the data is well managed and can be transferred.

**Accuracy** - The data is free from error.

**Reputation** - The data was generated by a credible or trusted source.

**Significance** - The data enables future research directions (with associated funding/support).

**Availability** - The data is there when I need it

**Authorization** - Way to vet and grant access

**Confidentiality** - Ensure repository hides/masks PII or other sensitive information from those not granted access

**Accountability** - Provision for metadata to describe the data, including provenance, versioning
Integrity Protection for Scientific Workflow Data: Motivation and Initial Experiences

Mats Rynge, Karan Vahi, Ewa Deelman  Information Sciences Institute - University of Southern California
Anirban Mandal, Ilya Baldin  RENCI - University of North Carolina, Chapel Hill
Omkar Bhide, Randy Heiland, Von Welch, Raquel Hill  Indiana University
William L. Poehlman, F. Alex Feltus  Clemson University
Pegasus Workflow Management System, Production Use

Last 12 months: Pegasus users ran 240K workflows, 145M jobs

Majority of these include data transfers, using LAN, the Internet, local and remote storage

https://pegasus.isi.edu/
**Goals:**

Provide additional assurances that a scientific workflow is not accidentally or maliciously tampered with during its execution.

Allow for detection of modification to its data or executables at later dates to facilitate reproducibility.

Integrate cryptographic support for data integrity into the Pegasus Workflow Management System.

PIs: Von Welch, Ilya Baldin, Ewa Deelman, Raquel Hill
Team: Omkar Bhide, Rafael Ferreira da Silva, Randy Heiland, Anirban Mandal, Rajiv Mayani, Mats Rynge, Karan Vahi
Our Talk

- Introduction and Motivations
- Our Approach
- Current Status
- Welcome to the Jungle
- Integrity Issues in the Wild
- Future Work
Data Integrity

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Challenges to Scientific Data Integrity

Modern IT systems are not perfect - errors creep in.

At modern “Big Data” sizes we are starting to see checksums breaking down.

Plus there is the threat of intentional changes: malicious attackers, insider threats, etc.

User Perception: “Am I not already protected? I have heard about TCP checksums, encrypted transfers, checksum validation, RAID and erasure coding – is that not enough?”
Motivation:
CERN/NEC Studies of Disk Errors

Examined Disk, Memory, RAID 5 errors.

“The error rates are at the $10^{-7}$ level, but with complicated patterns.” E.g. 80% of disk errors were 64k regions of corruption.

Explored many fixes and their often significant performance trade-offs.

A similar study by NEC found that 1 in 90 SATA drives will experience silent data corruption.

https://www.necam.com/docs/?id=54157f55-5de8-4966-a99d-341cf2cb27d3
Motivation: Network Corruption

Network router software inadvertently corrupts TCP data and/or checksum!

XSEDE and Internet2 example from 2013.

Second similar case in 2017: University of Chicago network upgrade caused data corruption for the FreeSurfer/Fsurf project.

https://www.xsede.org/news/-/news/item/6390
Motivation:
Software failures

Bug in StashCache data transfer software would occasionally cause silent failure (failed but returned zero).

Failures in the final staging out of data were not detected.

The workflow management system, believing workflow was complete, cleaned up. With the final data being incomplete and all intermediary data lost, ten CPU-years of computing came to naught.

How is this an data integrity issue? The workflow system should have verified that the data at the storage system after the transfer, is the expected data.
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Our High Level Plan...

• Workflow Management Systems (WMS) are great places to tackle data integrity.

• They understand what data is created and ingested and do not mind tedious tasks such as generating and checking checksums.

• Placement is important within the workflow of generate/validate checksums.

• Pegasus WMS is widely used (LIGO, SCEC, SoyKB, Montage, etc.) by the scientific community and is the target of our improvements.
Application-level Checksums – SHA256

- Application-level checksums (hashes) allow for detection of changes.
- Explored some more advanced solutions, but at the end simplicity won.
- Checksums already in use by many data transfer applications: scp, Globus/GridFTP, some parts of HTCondor, etc, but SWIP is focusing on end-to-end as well as over longer time periods.

e.g. using a SHA in Python:
```python
>>> hashlib.sha256(b"The Answer to the Ultimate Question of Life, the Universe, and Everything is 42").hexdigest()
'8a72856cf94464dd641f0a2620ab604dd7a3f50293784a3a399acf6dc5b651cb'
```
```python
>>> hashlib.sha256(b"The Answer To the Ultimate Question of Life, the Universe, and Everything is 42").hexdigest()
'a39be9fd272f2569aa95a07134a55f032ecb5c51cef6d66fe4032ec30bf4f1b6'
```
```python
>>> hashlib.sha256(b"The Answer is 42").hexdigest()
'cbf296e175f02156cd60d6bf93aebd92893e72a0c4c48eadeb092d0dc7e28fc1'
```
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Integrity validation is on by default since the Pegasus 4.9.0 release (Oct 31\textsuperscript{st}, 2018). Users who upgrade will automatically get the protection, but can opt out.

Sharing of detailed monitoring data with the Pegasus team is off by default. Users can opt-in. (We will come back to this at the end of the talk)
Automatic Integrity Checking in Pegasus

Pegasus performs integrity checksums on input files right before a job starts on the remote node.

- For raw inputs, checksums specified in the input replica catalog along with file locations
- All intermediate and output files checksums are generated and tracked within the system.
- Support for sha256 checksums

Job failure is triggered if checksums fail
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How do you know your integrity protection is working?

• Imagine the following: You finish adding integrity protection to your software. You run a workflow and all goes smoothly.

• Was there no integrity problem or did you just fail to detect it?

• How do you reliably and repeatedly test integrity protection?
Confidence in the implementation: Bamboo

• At commit, for each target platform:
  1. Build binary, workers, RPMs, DEBs, ....
  2. Run unit tests for Java, Python, and C components
  3. ~ 100 unit tests

• Nightly:
  1. Run functional tests. These are full workflows, configured to provide good code coverage
  2. ~ 85 workflows
Enter the Chaos Jungle!

https://github.com/RENCI-NRIG/chaos-jungle

Inspired by Netflix’s Chaos Monkey.
https://github.com/Netflix/chaosmonkey

Goal of Chaos Jungle (CJ) is to introduce different kinds of impairments into the virtual infrastructure - network, compute, storage.

The RENCI ORCA software creates virtual infrastructure on ExoGENI testbed. CJ software introduces impairments into data transfers.

We get virtual infrastructure that intentionally corrupts data

Randomly or predictably?

Now we can test how software runs under bad conditions.
Chaos Jungle

Uses Linux eBPF (extended Berkeley Packet Filters) functionality

Introduces a small eBPF program into the kernel attaching to either TC filter or XDP hooks

Inspects received packets and modifies some of those that match flow descriptors without affecting the appropriate checksums.

The packets thus look valid on the receiving end, however contain invalid data.

Fast and performant.

https://github.com/RENCI-NRIG/chaos-jungle
Chaos Jungle Experiment Setup

1. Launch workflow with Pegasus integrity checking enabled

HTCondor Master

2. Workflow data is fetched from http server hosted on Data node

Data Node

3. Integrity check errors appear as events in the Grafana dashboard

Workflow Data

0. Chaos jungle scripts executed on the HTCondor workers; Script mangles packets while preserving checksum
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Production Workflows

• Large workflows with lots of data transfers
• “Unprotected” protocols - no SSL or other protocol level protections
• Open Science Grid - WAN transfers
• Collecting the data is on an opt-in basis
Initial Results with Integrity Checking on

• OSG-KINC workflow (50,606 jobs) encountered 60 integrity errors in the wild (production OSG). The problematic jobs were automatically retried and the workflow finished successfully.

• The 60 errors took place on 3 different hosts. The first one at UColorado, and group 2 and 3 at UNL hosts.

• Error Analysis (by hand)
  • 1 input file error at University of Colorado.
  • 3 input file (kinc executable) errors on one node at University of Nebraska. The timespan across the failures was 16 seconds. We suspect that the node level cache got corrupted.
  • 56 input file errors on a different compute nodes at University of Nebraska. The timespan across the failures was 1,752 seconds. We suspect that the site level cache got corrupted.
Initial Results – VERITAS / Nepomuk Otte, GATech

Seeing very small, but steady stream of corrected integrity errors from reporting back to Pegasus dashboard.

For VERITAS, \(~.04\%\) of transfers fail with integrity errors. (~1 / 2500 transfers)

Cause uncertain (diagnosis is harder than detection).

Possibly errors in http based transfers (s3 protocol against CEPH)
Checksum Overheads

• We have instrumented overheads and are available to end users via pegasus-statistics.

<table>
<thead>
<tr>
<th>Type</th>
<th>Succeeded</th>
<th>Failed</th>
<th>Incomplete</th>
<th>Total</th>
<th>Retries</th>
<th>Total+Retries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jobs</td>
<td>1606</td>
<td>0</td>
<td>0</td>
<td>1606</td>
<td>31</td>
<td>1637</td>
</tr>
</tbody>
</table>

Workflow wall time: 7 hrs, 59 mins
Cumulative job wall time: 17 days, 23 hrs

# Integrity Metrics
3944 files checksums compared with total duration of 9 mins, 18 secs
1947 files checksums generated with total duration of 4 mins, 37 secs

# Integrity Errors
Failures: 0 jobs encountered integrity errors

• Other sample overheads on real world workflows
  
  • Ariella Gladstein’s population modeling workflow
    
    • A 5,000 job workflow used up 167 days and 16 hours of core hours, while spending 2 hours and 42 minutes doing checksum verification, with an overhead of 0.068%.

  • A smaller example is the Dark Energy Survey Weak Lensing Pipeline with 131 jobs.

    • It used up 2 hours and 19 minutes of cumulative core hours, and 8 minutes and 43 seconds of checksum verification. The overhead was 0.062%.

1000 Node OSG Kinc Workflow Overhead of 0.054 % incurred
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Challenges

• Can we do more than know “something changed?”

• Detecting error easier than diagnosing error.

• Balance performance / integrity trade-off?

• How do we handle storage without compute capabilities?

• Long data life: today’s cryptographic algorithms will probably not last as long as we need the science data. E.g. what threats will Quantum computing bring?

• When do we hit limits of cryptographic algorithms (collisions)?

• Are all errors in all types of data of equal concern?
Going Forward: Integrity Introspection for Scientific Workflows (IRIS)

• National Science Foundation CICI IRIS Grant #1839900

• SWIP addresses integrity checking making sure that workflow computations are protected from integrity errors, but
  — Doesn’t address analysis of integrity errors discovered, i.e. tracing the source of error or doing root cause analysis to remedy the problem.

• IRIS goal: Detect, diagnose, and pinpoint the source of unintentional integrity anomalies in scientific workflow executions on distributed cyberinfrastructure. (integrity analysis)
IRIS Overall Approach

Train ML algorithms on controlled testbeds and validate on national CI by integrating framework with Pegasus.

Engage with science application partners to deploy the analysis framework.

IRIS proposed framework
We thank the National Science Foundation for funding this work (Grants 1642070, 1642053, 1642090). Views expressed may not necessarily be the views of the NSF. Thanks to Eli Dart for Brocade TSB details.
Pegasus - a dHTC friendly workflow manager

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https://pegasus.isi.edu
Pegasus Concepts

Users describe their pipelines in a portable format called Abstract Workflow, without worrying about low level execution details.

Workflows are DAGs
- Nodes: jobs, edges: dependencies
- No while loops, no conditional branches
- Jobs are standalone executables
- All data is tracked

Pegasus takes this and generates an executable workflow
- Data management tasks added
- Transforms the workflow for performance and reliability
- HTCondor DAGMan DAG

Planning occurs before execution
New and fresh Python3 API to compose, submit and monitor workflows, and configure catalogs

New Catalog Formats

Python 3
  - All Pegasus tools are Python 3 compliant
  - Python PIP packages for workflow composition and monitoring

Zero configuration required to submit to local HTCondor pool.

Data Management Improvements
  - New output replica catalog that registers outputs including file metadata such as size and checksums
  - Improved support for hierarchical workflows
  - Major documentation improvements
    - https://pegasus.isi.edu/docs/5.0.0dev/index.html
Optimizations

Task clustering

Hierarchical workflows
Enacts the execution of millions of tasks
Also enables loops and conditionals in DAGs

Task-resource co-allocation

Data Reuse
Jobs which output data is already available are pruned from the DAG
Pegasus Workflow Management System, Production Use

Last 12 months: Pegasus users ran **240K workflows, 145M jobs**

Majority of these include data transfers, using LAN, the Internet, local and remote storage

https://pegasus.isi.edu/
Data Staging Configurations

**HTCondor I/O** (HTCondor pools, OSG, …)
- Worker nodes do not share a file system
- Data is pulled from / pushed to the submit host via HTCondor file transfers
- Staging site is the submit host

**Non-shared File System** (Clouds, OSG, …)
- Worker nodes do not share a file system
- Data is pulled / pushed from a staging site, possibly not co-located with the computation

**Shared File System** (HPC sites, XSEDE, Campus clusters, …)
- I/O is directly against the shared file system
Directory creation, file removal

- If protocol can support it, also used for cleanup

Two stage transfers between incompatible protocols

- e.g., GridFTP to S3 is executed as: GridFTP to local file, local file to S3

Parallel transfers

Automatic retries

Credential management

- Uses the appropriate credential for each site and each protocol (even 3rd party transfers)
Containers are data too!

Users can specify to use images from Docker Hub, Singularity Library, or a file using URLs

The image is pulled down as a tar file as part of data stage-in jobs in the workflow

- The exported tar file / image file is then transferred to the job as any other piece of data
- Motivation: Avoid overwhelming Docker Hub/Singularity Library/… with by repeatedly requesting the same image
- Motivation: Optimize workflow data placement and movement

Symlink against a container image if available on shared file systems. For example, CVMFS hosted images on Open Science Grid
Advanced LIGO – Laser Interferometer Gravitational Wave Observatory

40,000 compute tasks
Inputs files: 1,100
Output files: 63
Processed Data: 725 GB

Executing on LIGO Data Grid, EGI, Open Science Grid and XSEDE
Pegasus performs integrity checksums on input files right before a job starts, ensuring the computation is on the expected piece of data.

- For inputs from external sources, checksums specified in the input replica catalog along with file locations, or generated first time we encounter the file.

- All intermediate and output files checksums are generated and tracked within the system.

Checksums validation failures is a job failure.
Seeing very small, but steady stream of corrected integrity errors from reporting back to Pegasus dashboard.

For VERITAS, \(~0.04%\) of transfers fail with integrity errors. (\(~1 / 2,500\) transfers)

Cause uncertain (diagnosis is harder than detection).
Possibly errors in http based transfers (s3 protocol against CEPH)
Pegasu est. 2001
Automate, recover, and debug scientific computations.

Get Started

Pegasus Website
https://pegasus.isi.edu

Users Mailing List
pegasus-users@isi.edu

Support
pegasus-support@isi.edu

Pegasus Online Office Hours
https://pegasus.isi.edu/blog/online-pegasus-office-hours/

Bi-monthly basis on second Friday of the month, where we address user questions and also apprise the community of new developments
See you at 1PM EST for CI/CS Workshop’s Panel: Ups and Downs of Cloud Computing in Open Science