Software Integrity with Pegasus: Securing Scientific Workflow Data

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SC17
Scientific Workflow Integrity with Pegasus
NSF CICI Awards 1642070, 1642053, and 1642090

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.

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Our Talk

● Problem Statement: Challenges to Data Integrity

● Our Approach: Adding integrity support to the popular Pegasus scientific workflow management system

● Challenges

● Next steps
Data Integrity: Seal ~ Signature ~ Authenticity ~ Trust

Q: How does one “sign” digital data?
Data Integrity

Important in Business, Arts, Politics, Science, ...

**FAKE NEWS!**  
Media Digitization and Preservation  
Reproducible Results

Former NOAA Scientist Confirms Colleagues Manipulated Climate Records  

vs.

No Data Manipulation in 2015 Climate Study, Researchers Say  
Our Focus: Science

“Scientific Workflow Integrity with Pegasus”

Modern day [computational] science uses workflows extensively. One popular workflow management system (WMS) used by several NSF projects is Pegasus. A WMS allows scientists to describe their process in a human-friendly way and then the software handles the details of the processing, dealing with tedious and repetitive steps and handling errors.

https://pegasus.isi.edu/
https://github.com/pegasus-isi/pegasus
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.
CERN Study 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.

Data integrity

Bernd Panzer-Steindel, CERN/IT
Draft 1.3  8. April 2007

Executive Summary

We have established that low level data corruptions exist and that they have several origins. The error rates are at the 10⁻⁷ level, but with complicated patterns. To cope with the problem one has to implement a variety of measures on the IT part and also on the experiment side. Checksum mechanisms have to be implemented and deployed everywhere. This will lead to additional operational work and the need for more hardware.

Introduction

During January and February 2007 we have done a systematic analysis of data corruption cases in the CERN computer center. The major work in the implementation of probes and automatic running schemes were done by Tim Bell, Olof barr and Peter Kelemen from the IT/FIO group. There have been similar problems reported in Fermilab and Desy and information exchange with them was done.

The following paper will provide results from this analysis, a judgment of the situation and a catalogue of measures needed to get the problem under control.

It is also to be seen as a starting point for further discussions with IT, the experiments and the T1 sites.

Network Corruption

Network router software inadvertently corrupts TCP data and checksum!

XSEDE and Internet2 example from 2013.

Second similar case in 2017 example with FreeSurfer/Fsurf project.

Brocade TSB 2013-162-A

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

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

Internal to the workflow this was detected when input to a stage of the workflow was detected as corrupted and retry invoked. (60k retries and an extra 2 years of cpu hours!)

However, failures in the final staging out of data were not detected because there was no workflow next stage to catch the errors.

The workflow management system, believing workflow was complete, cleaned up, so final data incomplete and all intermediary data lost. Ten CPU*years of computing came to naught.
Malicious attacks

- Script kiddies out for glory.
- Nation-states trying to disrupt/embarrass U.S. science.
- Disgruntled insiders.
- Grad students, post-docs, staff going for that publication with (bogus) phenomenal results.
Enter application-level checksums

Application-level checksums address these and other issues (e.g. malicious changes).

In use by many data transfer applications: scp, Globus/GridFTP, some parts of HTCondor, etc.

To include all aspects of the application workflow, requires either manual application by a researcher or integration into the application(s).
Some background

**Hash function** - a mathematical/algorithmic function that takes a set of bits (of **any length**) and maps them to another set of (hopefully **unique**) bits of **fixed length**.

→ primary purpose: detect changes in data

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()
'cbf296e175f02156cd60d6bf93aebd92893e72a0c4c48eaeedef092d0dc7e28fc1'
```

The fixed length result is the “hash value”, a.k.a. “checksum” or “digest”.
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SWIP Goals

● Provide assurances that a workflow is not accidentally or maliciously altered during 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 WMS.
Taking Advantage of Pegasus WMS

● Familiar interface to scientific projects (>700k Pegasus workflows from 2013 to 2015).

● Integrity-checking is tedious and error-prone. A WMS system, with its understanding of data ingest and creation is a good place to handle these tasks.

● Manages provenance and metadata, which we can protect.

● Maps abstract workflow to computing infrastructure and with understanding of security needs can choose appropriate infrastructure or even re-configure it.
Pegasus Workflow Management System

Discover what resources (computation, data, software) are available
Select the appropriate resources based on an architecture, availability of software, performance, reliability, availability of cycles, storage,..
Devise a plan:
  - What resources to use
  - How to best adapt the workflow to the resources
  - What protocols to use to access the data, to schedule jobs
  - What data to save
Execute the plan
  - In a reliable way
  - Keep track of what data was accessed, generated and how
Outside of the WMS functions
  - Resource provisioning
Key Pegasus benefits

Portability across heterogeneous infrastructure
  Separation of workflow description and execution
  Support for campus and leadership class clusters, OSG, XSEDE, academic and commercial clouds
  Can interact with a number of different storage systems (with different protocols)
Supports data reuse—useful in collaborations and ensemble workflow runs
Reliability
  Recover from failures, retry, workflow-level checkpointing
Scalability
  $O(\text{million})$ task, $O(\text{TB})$ data in a workflow
Restructures workflow for performance
Web-based monitoring and debugging tools
Can be included in various user-facing infrastructures
  (Graphical composition tools, Portals, HUBZero)
Open source, available on github
Workflow Execution Challenges and Capabilities

Failures in the execution environment or application
  Workflow-level checkpointing
  Retries
  Resubmit the workflow onto different resources (pick up where you left off)

Data storage limitations on execution sites
  Clean up data as you go along (automatically adds nodes to workflow)

Performance
  Small workflow tasks
  Task clustering, pilot jobs
  Data reuse

Heterogeneous execution architectures
  Specialized execution engines
  Support for a variety of storage layouts
  Support for most data transfer protocols
Pegasus, Production quality, In use since 2001

LIGO Laser Interferometer Gravitational Wave Observatory

Southern California Earthquake Center, USC

Syracuse U

Bioinformatics: SoyKB, University of Arizona

Pegasus LIGO PyCBC Workflow
Usage Since Sept 2015
Workflows: 20,942
Tasks: 107,576,294
Jobs: 55,915,928
Defined and Executed by Pegasus

Bioinformatics: Protein interactions, IU

Swamp, Montage, Caltech

cacr.iu.edu/projects/swip/
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.

Pegasus WMS is widely used (LIGO, SCEC, SoyKB, Montage, etc.) by the scientific community and is the target of our improvements.
Pegasus will perform integrity checksums on input files 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

Failure is triggered if checksums fail
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Challenges

Can we do more than know “something changed?”

Balance performance / integrity trade-off?

How do we handle storage without compute capabilities?

Are all errors in all types of data of equal concern?

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)?

→ Prof Steve Myers (Co-PI), IU SICE
Today’s Limits

We are not modifying operating systems, libraries, and software outside of Pegasus – this limits the strength of the assurances we can provide.

E.g. Modification of system libraries could fool our integrity checks.

As we encounter these limitations we will document how a next generation CI and Hardware stack could address them.

E.g. through the use of trusted computing (Intel Secure Guard Extension, etc.)
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?
Enter the Chaos Jungle!

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

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

Combining the two we get virtual infrastructure that intentionally corrupts data - randomly or predictably?

Now we can test how software runs under bad conditions.

https://commons.wikimedia.org/wiki/File:Tioman_Rainforest.JPG
Chaos Jungle Primer

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
Demonstration Overview

1. Launch workflow with Pegasus integrity checking enabled
2. Workflow data is fetched from http server hosted on Data node
3. Integrity check errors appear as events in the Kibana dashboard

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

HTCondor Master

HTCondor Worker - 0
HTCondor Worker - 1
HTCondor Worker - 2
HTCondor Worker - 3

Data Node

Workflow Data
Demonstration Overview
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Our three-year plan

**Year one:** Requirements analysis and prototyping

**Year two:** Iterate with partners to evaluate effectiveness and usability:
- LIGO, CyberShake, FreeSurfer, OSG, SPLINTER, Chameleon, NSFCloud
*We are just starting year two.*

**Year three:** Complete transition to production through release in Pegasus and ORCA.
Will release through existing open-source repositories and licenses.
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.
Practicing what we preach + research

http://download.pegasus.isi.edu/pegasus/4.7.4/sha256sums.txt (current Release version)

e58352f89e8325b92d13cac996c029fdc7950b019ea17b9a71a41f9ad9f9ec29a6 pegasus_4.7.4-1+deb7_amd64.deb
94750e8ef2cf381b6b0aaf68ab1412e3763098496b3e3f0b9a74719764ecbdb3 pegasus_4.7.4-1+deb8_amd64.deb
e0a15758815a21c7c1f296842daco79fbd14eeb2db624f49f1973b2cd08495baf pegasus-4.7.4-1.el6.x86_64.rpm
...
26257cfad6eb7e72507a5349c74f15535ed87475d5fc6ddb9b71b20d8a5af8 pegasus-worker-4.7.4-x86_rhel_6.tar.gz
Concerns over hash functions

- Collisions, i.e., non-unique hashes
- Computational expense
- "Big data"
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Limitation of TCP Checksum with Big Data

TCP has a 16-bit checksum.
This means 1/65,536 packets will randomly have the same checksum.
So packet corruption is 1/65,536 likely not to be detected by TCP checksum.

In 1999, Vern Paxson found corruption in 1/5000 packets.

Hence:
1/65,536 × 1/5000 ≈ 1/300 million packets will get corrupted and not detected by the TCP checksum.

If we assume 1 kbytes / packet, a 300GB transfer will have one undetected error.