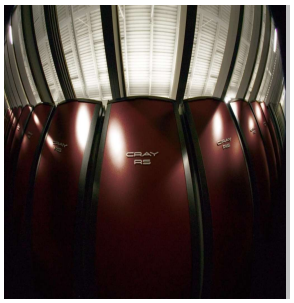

# Making Data Useful Through Metadata Techniques

Jay Lofstead

Sandia National Laboratories

*Exceptional service in the national interest*

HPC-IODC @ ISC

25 May 2023

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

# Problem Overview

Sandia National Laboratories

- Bits in a file are meaningless….unless you know:
  1. The file format/organization
  2. The application type/specific application that generated it

- For science, it can still be meaningless….unless you know:
  3. What configuration that application used
  4. What OS version, compiler, and TPLs were used
  5. Environment variables that affected the run
  6. And many others

# Problem Overview

Sandia National Laboratories

- Partial solutions:
  - Standard file formats and libraries
  - Provenance systems
  - Source repo
  - DevOps scripts and logs
  - Container construction manifests
- Biggest remaining problem:
  - Is there anything interesting in the data to look at?

# Solution Space

Sandia National Laboratories

## Specific problem definition:

*As an analyst evaluating simulation and observation data, what data properties exist within what file (object) within a dataset that may suit my explorations?*

# 3 Existing Tool Generations

Sandia National Laboratories

Generations refer to classes and development order rather than obsolescence!

- 1st generation: file level metadata, domain specific tools
- 2nd generation: raw data level indexing
- 3rd generation: data-level tagging

Provenance-related tools are a completely separate discussion (exercise left to the reader)

# First Generation Tools (Storage Sys)

Sandia National Laboratories

- POSIX extended attributes
  - Implementation and limitations varies by file system
  - File system may have to be mounted differently to enable them
  - Key-value pairs
  - Limited to block size for portability (1024 bytes for maximum compatibility)
  - Tools like `tar` may require special flags to save, if supported at all
- HPSS
  - Implements POSIX extended attributes
  - Stores all metadata in a RDBMS outside the tape archive for performant queries
  - Can export data for use in systems like Starfish (see next)

# First Generation Tools (Abstracted)

Sandia National Laboratories

- Starfish (https://starfishstorage.com/)
  - File level arbitrary metadata
  - Strong query capabilities
  - Integration with HPSS (possible, if not standard)
  - Works across storage systems
  - Depends on files being in a fixed location or location updated as files move in storage
- JAMO – Joint Genome Institute (JGI) Archive and Metadata Organizer
  - One example of a domain specific tool
  - Repository for data, metadata, and provenance with full query API
  - Standard + User defined Templates for metadata
  - Can tag at a more detailed level as well

# Second Generation Tools (indexing)

Sandia National Laboratories

Raw data indexing

- Exact value or binning

- FastBit
  - Make Bloom-filter style index on data.
  - Bins for value ranges with a 1/0 to indicate present/absent
  - Query capabilities: Does a value exist in this file/dataset?
    - Yes/no
    - No ability to know where

# Second Generation Tools (custom db)

Sandia National Laboratories

- SciDB
  - Built for astronomy images and other 2-D data sets originally
  - Multi-dimensional array data model
  - Indexing capabilities
  - SQL front-end
  - Query for data values or thresholds

# Second Generation Tools (IO libs)

Sandia National Laboratories

All offer an attribute capability, but it varies a bit

- NetCDF
  - Attach to a variable for things like units
  - Flat hierarchy makes it a linear search
- HDF5
  - Attach to any part of the hierarchy
  - Walk tree to search
- ADIOS
  - Attach to any part of the hierarchy
  - Separate attribute index for fast searching

# Third Generation Tools (features)

Sandia National Laboratories

- Associate tags data/parts of data
  - Region/var/run
  - Bounding box, simple tag
- Solutions use key-value and RDBMS approaches for different tradeoffs
- Key-value
  - Flat hierarchy with all encoding in key name
  - O(1) to get next item adjacent in sorted keys
  - O(n) to find something that is not exactly matching key

# Third Generation Tools (key-value)

Sandia National Laboratories

- SoMeta (LBL)
  - Developed as a way to see how to use a KV store to optimize data access for object stores
  - Encode tag information into key and use value for data location
  - Key searching speed based on key storage system

- TagIt (ORNL)
  - Integrated into storage system
  - Assuming distributed, shared nothing storage
  - Works like a distributed DB index placing index next to data for faster access

# Third Generation Tools (RDBMS)

Sandia National Laboratories

- Biomedical Image Metadata Manager (BIMM)
  - Image database with tags
  - Search for semantic features
  - Domain specific, but is really just image tagging capability
- EMPRESS
  - Embedded database(s) for tagging
  - Run, timestep, var, and hyperslab tagging
  - Flexible query API + ability to use SQL directly on database
  - Per process/node/job database granularity
  - In memory, hybrid, on persistent storage
  - Distributed shared nothing
  - Use logical locations to be file/object format independent

# State of the Art Summary

Sandia National Laboratories

- Long term data archiving
  - Which data set(s) contain what I want to study?
- Short/medium term data set identification
  - What does each set contain and which ones to save?
- Provenance largely focuses on environment
  - Critical, but insufficient/inefficient/impractical/fragile

*How do we look for complex data features we didn't think to annotate earlier?*

# Fourth Generation Tool

Sandia National Laboratories

Coeus project from US DOE ASCR funding

- Derived quantity information-based tagging
  - For a climate model, where is the pressure gradient greater than a particular value
- Problems!
  - Derived quantities take time to compute
  - Derived quantities can be as large as the original data

# Applying Metadata in the Large

Sandia National Laboratories

- National Science Data Fabric (NSDF) pilot project
  - Valerio Pascucci (Utah), Michela Taufer (UTK) PIs
- Materials Commons 2.0
- FAIR data principles focused (another separate discussion)

Sandia National Laboratories

NSDF

Vision

Mission

Catalyze the creation of a globally connected, democratized infrastructure in which scientific investigation and training are unhindered by the limitations of dealing with extreme amounts of data.

Democratize access to large-scale scientific data by developing production-grade, scalable solutions to data storage, movement, and processing that can be deployed on commodity hardware, cloud computing, and HPC resources.

(courtesy of Valerio Pascucci)

Sandia National Laboratories

# National Science Data Democratization Consortium


(courtesy of Valerio Pascucci)

# NSDF + Metadata Management

Sandia National Laboratories

- Generation 5?
  - Metadata management for multiple applications in distributed store
- Issues addressed:
  1. What part of the rich, but large metadata can we save to help for data selection?
  2. How do we distribute the metadata system as a local cache for large, distributed data storage system?
  3. How do we deal with different kinds of storage systems, file formats, data organizations, and other complexities?

# Thank you

Sandia National Laboratories

- gflofst@sandia.gov