The Whole Tale: Merging Science and Cyberinfrastructure Pathways

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Motivation and Vision

• Many scientific experiments are difficult, if not impossible, to replicate, verify, and/or reproduce
• The scholarly publication has not kept pace with the changes in science:
  • **Data underpins most research** whether acquired, derived, or obtained from a repository
  • **Computation & software is an integral & inseparable component** via which most research takes place
  • WholeTale aims to **capture and preserve the journey towards discovery rather than just the endpoints**

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What is a "Tale"?

• A living publication that preserves all digital scholarly objects and can be shared and replayed
  • Input, intermediate, derived data
  • Software and environment
  • Workflow process
  • Publication narrative
• Captures computational steps and provide compute environment
• Provides unique identifiers to objects
• Publishable research object
Community Engagement

- Cyberinfrastructure and science working groups help drive development
  - Astrophysics, materials science, environmental science, bioinformatics, social sciences, reproducibility, information sciences, education and training
- Internship program
  - Reproducibility of published materials science machine learning models
  - Automated provenance capture when reconstructing environment conditions
  - Understanding infrastructure requirements to promote reproducible research
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User Interface
Upcoming Workshop

• Whole Tale Workshop: Tools and Approaches for Publishing Reproducible Research
• When: September 13-14, 2018
• Where: Big Ten Center, Chicago
• What:
  • Discuss initiatives to conduct, track, remix, and share research
  • How can Whole Tale make workflows easier and more reproducible?
• Who:
  • Domain scientists, computer scientists, infrastructure developers
COLDFRAME:
A Scalable Framework for Collaborative, Data-Intensive Research and Education

Nurturing collaborative data-intensive research in adverse conditions
Problem

- Data intensive science is increasingly collaborative
  - Diverse sets and levels of expertise
  - Geographically distributed teams

- Teams face challenge of enabling collaboration
  - Technical infrastructure
  - Rapidly evolving computational/research data management systems
  - Common patterns/architectures and tools

- NSF big idea: Harnessing the Data Revolution
  - Integrated data and computational infrastructure to accelerate data-intensive research and workforce development.
Coldframe

- Nascent initiative
- Framework to enable research teams to easily provide collaborative access to large research datasets and specialized computational resources
- Address needs identified through extensive work in the EarthCube, National Data Service (NDS), and Big Data Hub (BDHubs) communities
- Bridging the gap between interactive analysis and execution on cloud, High Performance Computing (HPC) and High Throughput Computing (HTC) resources
- Supports outreach and education on the system used for research
High-level architecture
Communities/Drivers

- EarthCube Coral Reef Science and Cyberinfrastructure Network (CRESCYNT)
  - Enabling collaborative, multi-disciplinary analysis of coral reef bleaching events
- High-throughput phenomics and genomics (TERRA-REF)
  - Supporting collaborative access to 2PB reference dataset and tools on a variety of resources
- Data science education for non-R1 institutions
  - Consortial/cooperative models for data science/CI education
- Access and sharing of fused satellite data (Terra Fusion)
  - How can they provide access to 3PB fused dataset for collaborators and future reuse?
- Computational astrophysics (Moesta)
  - How can they provide access to 300TB simulation for analysis/visualization?
Key features

- Multi-scale deployment
- Data ingest
- Access control and sharing
- Scale-out compute support
- Image preservation (research)
- External compute support
- External data management
- Community-created catalogs