DDDAS 2020 Government Panel

Sonia R. Sachs, Ph.D.
Program Manager
Advanced Scientific Computing Research
DOE Office of Science

Oct 4, 2020

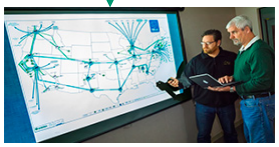
How DDDAS methods are relevant to DOE Office Science?

Basic Energy Sciences	•**Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels**
Biological and Environmental Research	•**Understanding and predicting complex biological, earth, and environmental systems**
Fusion Energy Sciences	•**Building the scientific foundations for a fusion energy source**
High Energy Physics	•**Understanding how the universe works at its most fundamental level**
Nuclear Physics	•**Discovering, exploring, and understanding all forms of nuclear matter**

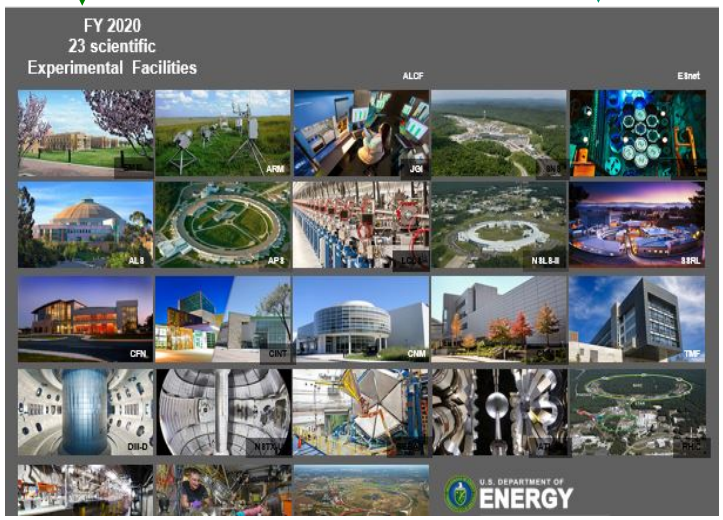
HPC Facilities

Simulation modeling and data analytics

manual, sequential, batch mode



ESnet



Experimental Facilities

Ongoing: Pilots that follow the DDDAS paradigm to create automated, real-time, or near-real time connection

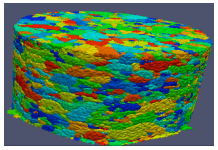
Boosting Light Source Productivity with *Swift* ALCF Data Analysis

H Sharma, J Almer (APS); J Wozniak, M Wilde, I Foster (MCS)

DD 2014
Mira 5M

Impact and Approach

- HEDM imaging and analysis shows granular material structure, non-destructively



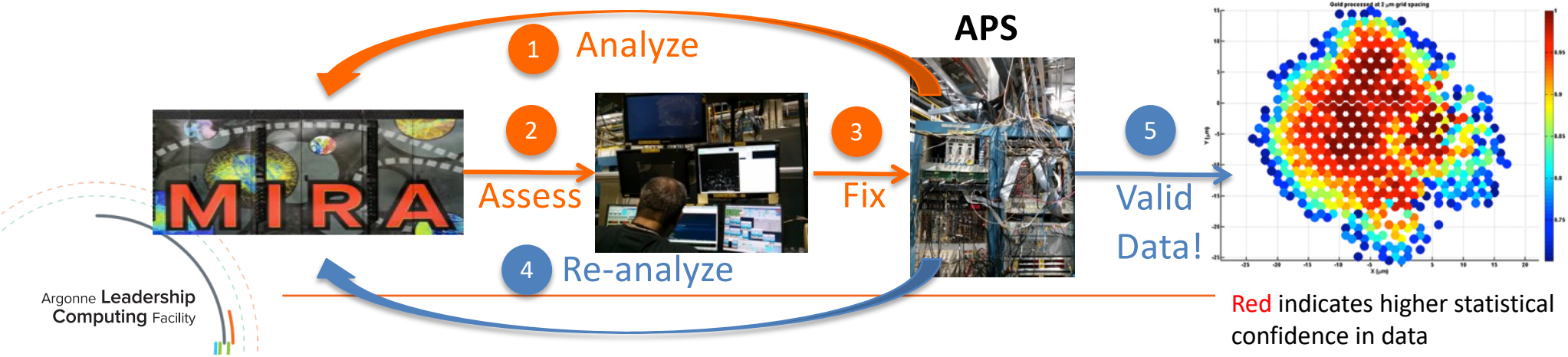
- APS Sector 1 scientists use Mira to process data from live HEDM experiments, providing real-time feedback to correct or improve in-progress experiments
- Scientists working with *Discovery Engines* LDRD developed new *Swift* analysis workflows to process APS data from Sectors 1, 6, and 11

Accomplishments

- Mira analyzes experiment in **10 mins vs. 5.2 hours** on APS cluster: **> 30X** improvement
- Scaling up to ~ 128K cores (driven by data features)
- **Cable flaw was found and fixed at start of experiment,** saving an entire multi-day experiment and valuable user time and APS beam time.
- **In press:** *High-Energy Synchrotron X-ray Techniques for Studying Irradiated Materials*, J-S Park et al, J. Mat. Res.
- *Big data staging with MPI-IO for interactive X-ray science*, J Wozniak et al, Big Data Conference, Dec 2014

ALCF Contributions

- Design, develop, support, and trial user engagement to make *Swift* workflow solution on ALCF systems a reliable, secure and supported production service
- Creation and support of the Petrel data server
- Reserved resources on Mira for APS HEDM experiment at Sector 1-ID beamline (8/10/2014 and future sessions in APS 2015 Run 1)

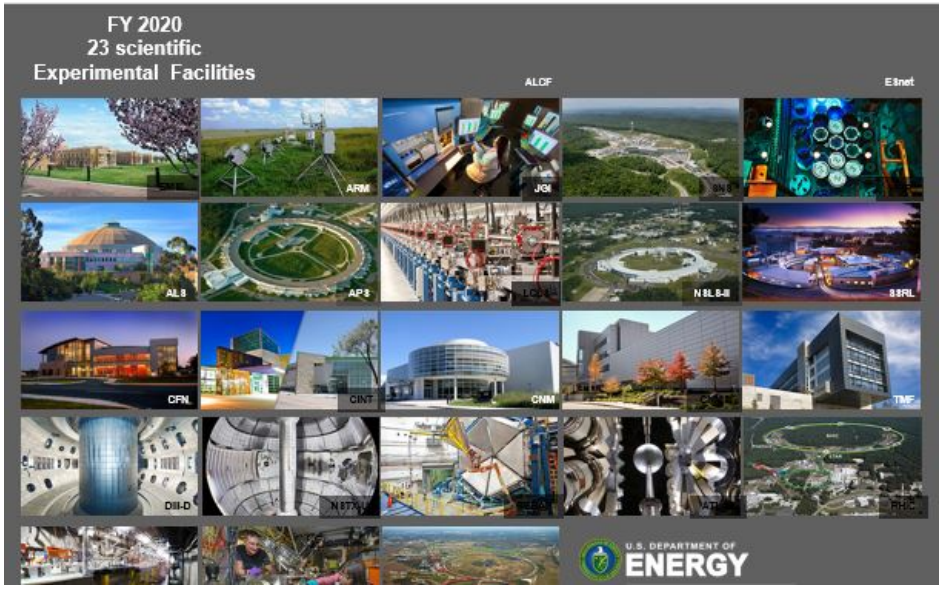


What are the growing needs for which DDDAS developments can enhance?

Automatic, real-time, near real-time simulation modeling steering

ESnet

HPC Facilities

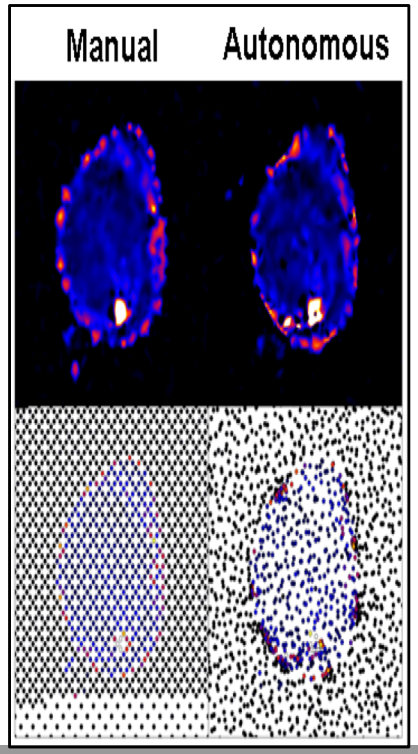


Experimental Facilities + **Edge** Instruments

Automatic, real-time, near real-time experiment steering

Has AI/ML impacted the scope or directions of programs in DOE? How do they align with DDDAS?

- DOE AI for Science Report https://www.osti.gov/biblio/1604756/
- New AI methods enable autonomous experimentation
- Example: X-ray scattering beamline autonomous experiment https://www.nature.com/articles/s41598-019-48114-3
  - X-rays from each experiment probe a portion of the material specimen
  - AI launches best sequence of experiments for revealing the internal structure
  - Collaboration between BNL, LBNL, Light source (NSLS-II), Nanoscale science (CFN), and Center for Advanced Mathematics in Energy Applications



Key Objective: Create an AI ecosystem, a seamlessly integrated suite of resources for scientific

✓ Discovery – 6x faster

✓ Competitiveness – more accurate

✓ Innovation – smart, self-driving experiments.

Slide material from Steve Lee, DOE ASCR

What opportunities are there for community coordination (e.g., academics-industry-gov)?

- **DOE open science HPC facilities** (ALCF, OLCF, NERSC) enable large collaborative projects (academics-industry-government)
- **DOE Initiatives** include coordination/collaboration with USG agencies, universities, industry and non-profit organizations.
  - **Artificial Intelligence and Machine Learning**
    - Cuts across all SC research programs and many DOE programs
    - Cuts across multiple USG Agencies, including VA, NIH, DoD, NASA, NOOA
    - DOE Artificial Intelligence and Technology Office (AITO) and Microsoft announced five consortiums in Aug 2020: using deep learning algorithms to provide near real-time data to improve the decision making for first responders, wildfire prediction and fire line containment; damage assessment, search and rescue and natural disasters including hurricanes and tornadoes.
    - The “First Five” consortium participants includes government, industry, universities, and non-profits..
  - **Microelectronics Innovation,** focusing on Materials, chemistry, and device physics; Component integration, architecture, and algorithms; Next-generation tools for synthesis, fabrication, and characterization of devices and systems
  - **National Isotope Strategy:** Impacts other Agencies (DoD, NIH, HHS, NASA). Cuts across SC, NE, and NNSA. Provides science, technology, production capacity, and radiochemical processing for strategic stable & radioactive isotopes
  - **Quantum Information Science:** Cuts across all SC research programs. Cuts across several other DOE programs (OE, NNSA)

What opportunities are there for community coordination (e.g., academics-industry-gov)?

DOE New Initiatives

- **Multi-program within DOE:**
  - Integrated Computational and Data Infrastructure for Scientific Discovery: Next Generation Biology Initiative
  - Rare Earth / Separation Science Initiative
  - Revolutionizing Polymer Upcycling
  - Strategic Accelerator Technology Initiative
  - U.S. Fusion Program Acceleration
- **Data and Computational Collaboration with NIH**
  - DOE provides advanced scientific computing and data resources for significant national issues/problems; leverage existing partnership with NCI to integrate artificial intelligence techniques to data analysis of Cancer data; leverage coordination on Brain Connectome and other ongoing collaborations with NIH