# CST

Amber Boehnlein

# Outline

- IT News
- Sci Comp News
- Data Science News
- High Performance Data Facility

# IT News

- 2025: primary focus is on holding the fort
  - Penetration testing to check for vulnerabilities
  - Improving the enterprise risk assessment
- Glad to learn that access issues are improved!
  - Automation to assist Physical Security is planned
- Cyber Security
  - The intensity of the requirements flowing down to us match the intensity of the news reports.
  - Compliance focus
  - There will be changes that impact the users
    - User accounts might change to O365 with MFA—Still investigating
      - Evaluating not having email accounts for many Jlab users
      - Use home institution accounts
      - Account granted under false credentials—increased scrutiny on process
    - Zero Trust Architecture-impacts not yet known for scientific systems
    - We will do our best to keep the impacts to a reasonable level.

# New requirements from DOE on sharing research results

## 2023 DOE Public Access Plan

### Publications

- Move from 12-month embargo to immediate access upon publication
- Continue to submit accepted manuscripts via E-Link, but earlier in reporting process
- Provide access through DOE's designated repository, DOE PAGES®
- Emphasize author deposits of accepted manuscripts (green OA) – DOE

### Data

- Now Data Management and Sharing Plans (DMSPs)
- "Scientific Data" to validate and replicate research findings
- Data underlying publications should be made available at time of publication
- Timeline for sharing other scientific data
- Repository selection should align with NSTC Desirable Characteristics of Data Repositories guidance

### Persistent Identifiers

- Collect metadata associated with publications and data
- Metadata to include authors, affiliations and funding with associated PIDs, publication date, and PID for output
- Instruct researchers to obtain a PID for themselves and use when publishing and reporting R&D outputs
- Researcher PIDs must meet common/core standards
- PIDs for awards

*2023 DOE Public Access Plan: https://www.energy.gov/doe-public-access-plan*

U.S. Department of ENERGY | Office of Science 6 Energy.gov/science

Slide from Michael Cooke's presentation to ASCAC January 2025 https://science.osti.gov/ascr/ascac/Meetings/202501

# New requirements from DOE on sharing research results

**Jefferson Lab, Experimental Collaborations, and PIs have joint responsibilities in responding to the new requirements.**

Formal requirements will be added to the JLab contract (next slide)

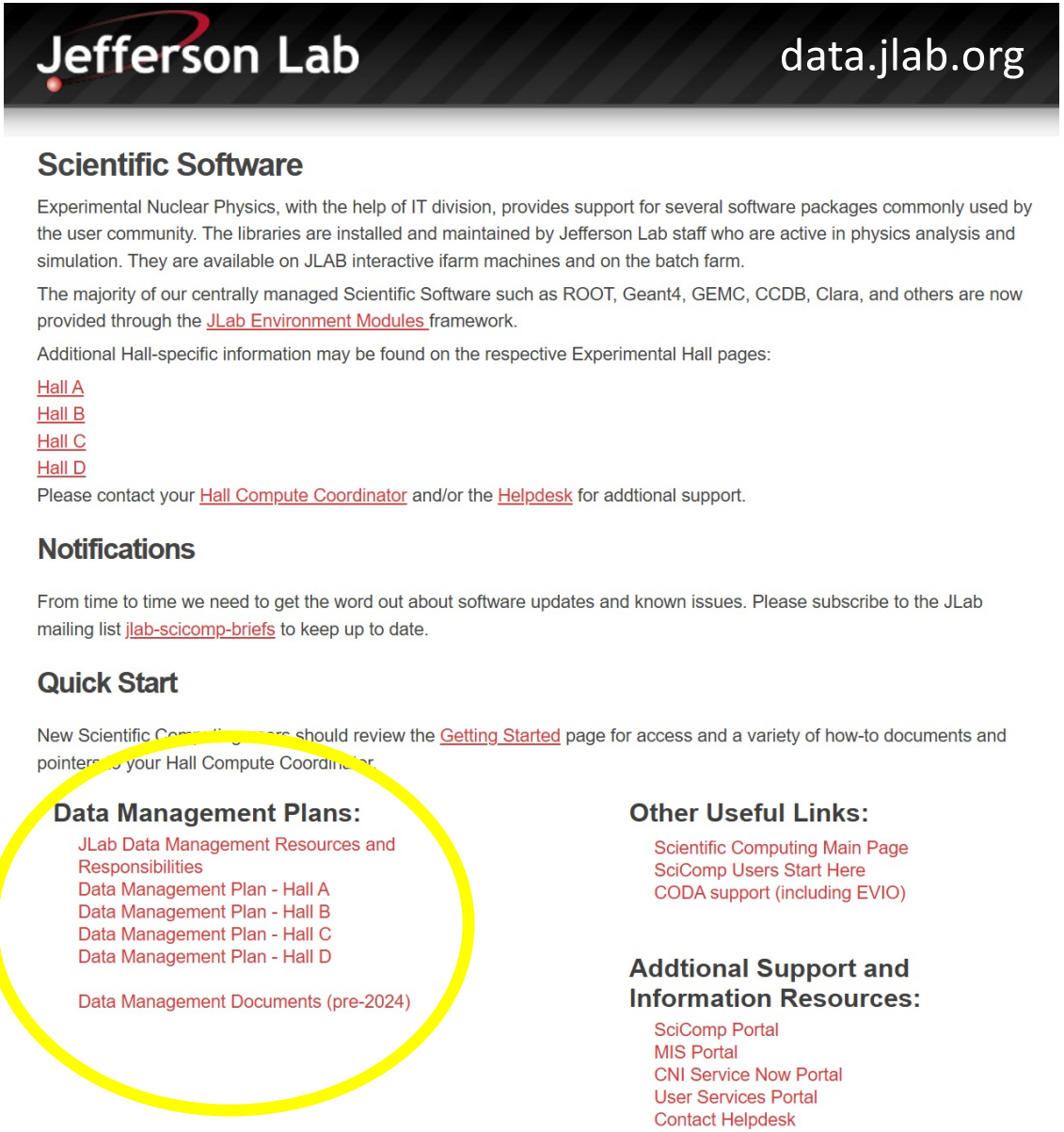
Updates for grantees are expected to appear in the Office of Science Statement on Digital Data Management

**Stay tuned**: We are coordinating with DOE on the best way to work across the community.

# STIP program

- DOE O 241.1C contains the following new elements that we are working to implement:
  - Immediate public access to journal articles with no embargo
  - Persistent identifiers for STI:  OSTI will provide a DOI to all other STI (scientific data, technical reports and scientific software) if it is submitted to OSTI without one.
  - Scientific data that is made publicly available as a result of an approved DMP or DMSP is required to be submitted to E-Link
  - DMPs and DMSPs:  All R&D funded by DOE will require a data management plan (DMP) or data management and sharing plan (DMSP).
  - ORCIDs:  All users are highly encouraged to register for an ORCID.

# Data Management Plans




## 2024 Updates:

JLab DMP was renamed "***JLab Data Management Resources and Responsibilities***" to clarified its two-fold purpose:

1. Providing information about data management resources at the lab that can be used to inform DMPs submitted to funding organizations and
2. Articulating the responsibilities for data management and the responsibility to submit and experiment-specific DMP (EDMP) to the lab.

## Future Plans:

Over the next year, JLab will enhance the management of experimental data with the following activities.

1. Review Experimental Data Management Plans and data management practices to identify opportunities for streamlining and enhancing the value of data.
2. Explore the use of ORCIDs for scientific staff and CEBAF users.

# Email Changes

- Recognize that this a difficult topic
- Recognize that we have to ensure that we don't break mission
  - Our mission includes enabling users to work!
- Background
  - We have been running a separate in-house email service for users for many years and it is a significant risk due to the lack of MFA and compliance with other cyber requirements
- We have been exploring options for user email accounts for a while. All solutions have major downsides
  - ~~Can 'Do nothing'~~
  - ~~O365 is expensive~~
  - ~~Migrating to another in-house solution is extremely unlikely to get an 'Authority to Operate;~~
  - ✓ Using home institution emails
    - breaks some business processes

# What will change

- Timelines are TDB
- Proposed Solution:
  - Mix of O365 accounts for targeted users to preserve business processes with home institution email addresses for most users.
- End state for home institution:
  - The user's home institution email will be the primary email used for Jlab business
    - Internal process emails from Jlab to username@jlab.org will be forwarded
    - External emails will not be forwarded (this is true for staff who like to rely on a system besides O365 as well)
    - There are implications:
      - Burden on the user to keep JLIST up-to-date
      - Burden on the user to update any correspondence with external parties
      - if the jlab email address is used for a third-party product, the ability to reset a password is gone.
      - In many careers, Jlab is the long running institutional commitment.
  - Email messages that people still need will have to be migrated
  - The user email system will be decommissioned

# Next Steps

- Continuing to struggle to get on the same page (even in IT)
- We all want to work together to minimize the disruption
  - Transition plan with dates and communication for the users (Matt, Brad, Amber)
  - Technical implementation plan (Andy and Kari)
  - Need to understand and document the criteria for O365 accounts (Brad)
  - Users who are below the criteria for O365 but depend the jlab.org account for their business processes
    - Need to understand the use cases to recommend mitigations
- Goal: User email updates begin Aug 1
- Goal is to reject incoming email by ‘late fall’
  - Read only mode for historical access and migration

- *My opinion:*
  - *There have been lots of changes for the users rolled out piecemeal*
  - *It would be wonderful if the Lab and User community came together to define what the user experience can look like for the next 40 years*

# Scientific Computing Updates for 2025

- Data from the Halls are at record levels as Accel stabilizes and high-data rate experiments ramp up
  - Peak flows of 5+ GB/sec sustained over many days
  - 3 PB raw data collected in May, June will likely exceed 6 PB

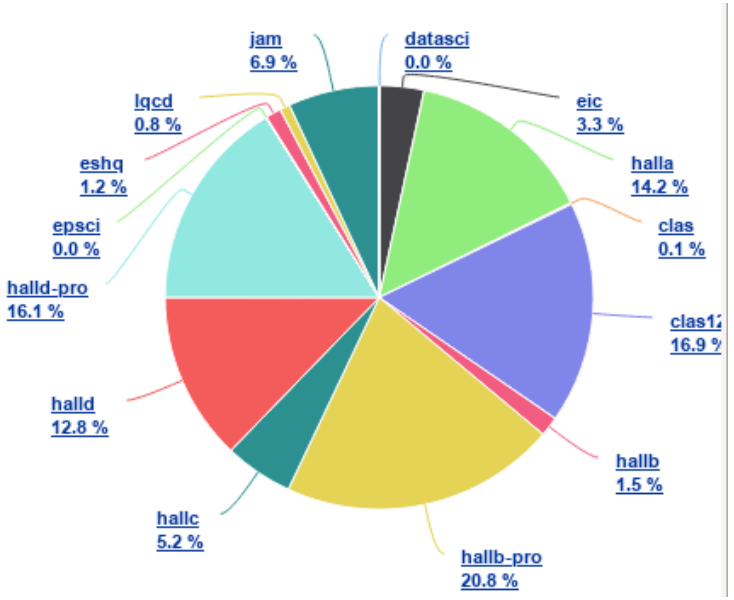
- New Hardware deployments
  - 20 new A800s GPUs deployed into the Farm pool (sciml* nodes) in May/June 2025
    - In addition to the A100s and older T4s and Titans
  - O(1PB) of new fast storage will be deployed to /work this Fall 2025
  - FY25 Farm CPU purchase should arrive late Summer, plan is to install in Sept 2025

- Farm uptime continues to be high
  - Monthly software maintenance is performed to keep pace with security and software updates.
- JLab Rucio deployment is reaching maturity
  - EIC simulation (early adopter) now in full production w/ Rucio + OSG
  - Next up are limited deployment for GlueX, CLAS sub-groups
- Open Science Grid
  - Support for MOLLER, SoLID, CLAS12, GlueX, and EIC projects
  - Support for increased I/O using XRootD and OSDF/Pelican with dedicated data transfer nodes (DTNs) and token-based authorization.
- User-facing GitLab instance (code.jlab.org) deployed last year is proving popular
  - federated logins support cross-institution collaboration
  - CI/CD pipelines and containerized workflows seeing rapid adoption
- Kubernetes / OpenShift cluster deployment maturing
  - First production use was to support on-premises CI/CD workflows from Gitlab
  - Add'l compute capacity will be to OpenShift cluster Fall 2025
  - Next up: Containers for services in Kubernetes
- Annual JLab Software and Computing Workshops for Users
  - Organizers: JLab Grad-Student/PostDoc Assoc. (GSPDA) + SciComp + JSA funding support
  - *Would like to do more of these!*

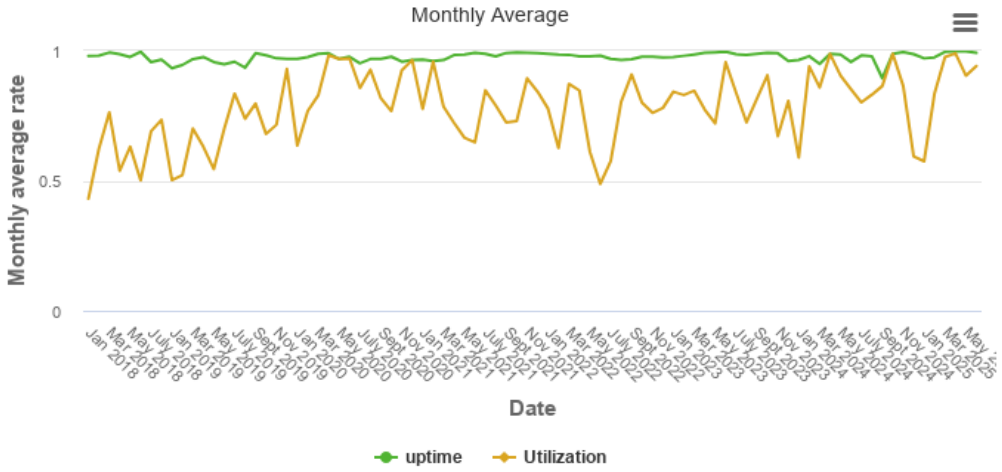
# CST: 2025 Performance Highlights (ENP Farm and OSG)

- The high uptime trend for the farm continues.
  - Most downtime is from scheduled upgrades, maintenance, and configuration changes.
  - Usage varies with demand; Not I/O constrained because of workflow management tools
- OSG usage >60M core hours/year as of 6/2025
- 2025 Largest share of farm use from CLAS12 and GlueX processing, but Hall A is now in the same category due to SBS data loads

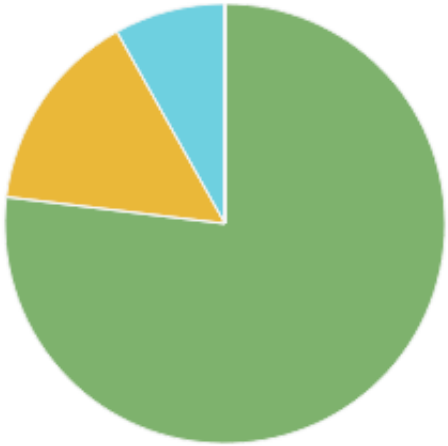
## 2025 Farm Usage by Project




## Farm Uptime and Usage




## 2025 OSG Usage by Project



| | total |
|---|---|
| CLAS12 | 45 Mil |
| ePIC | 9 Mil |
| gluex | 5 Mil |
| MOLLER | 39 K |
| EIC | 1 K |
| moller | 1.8 |
| GLUEX | 1.3 |
| solid | 0.2 |
| SOLID | 0.03 |

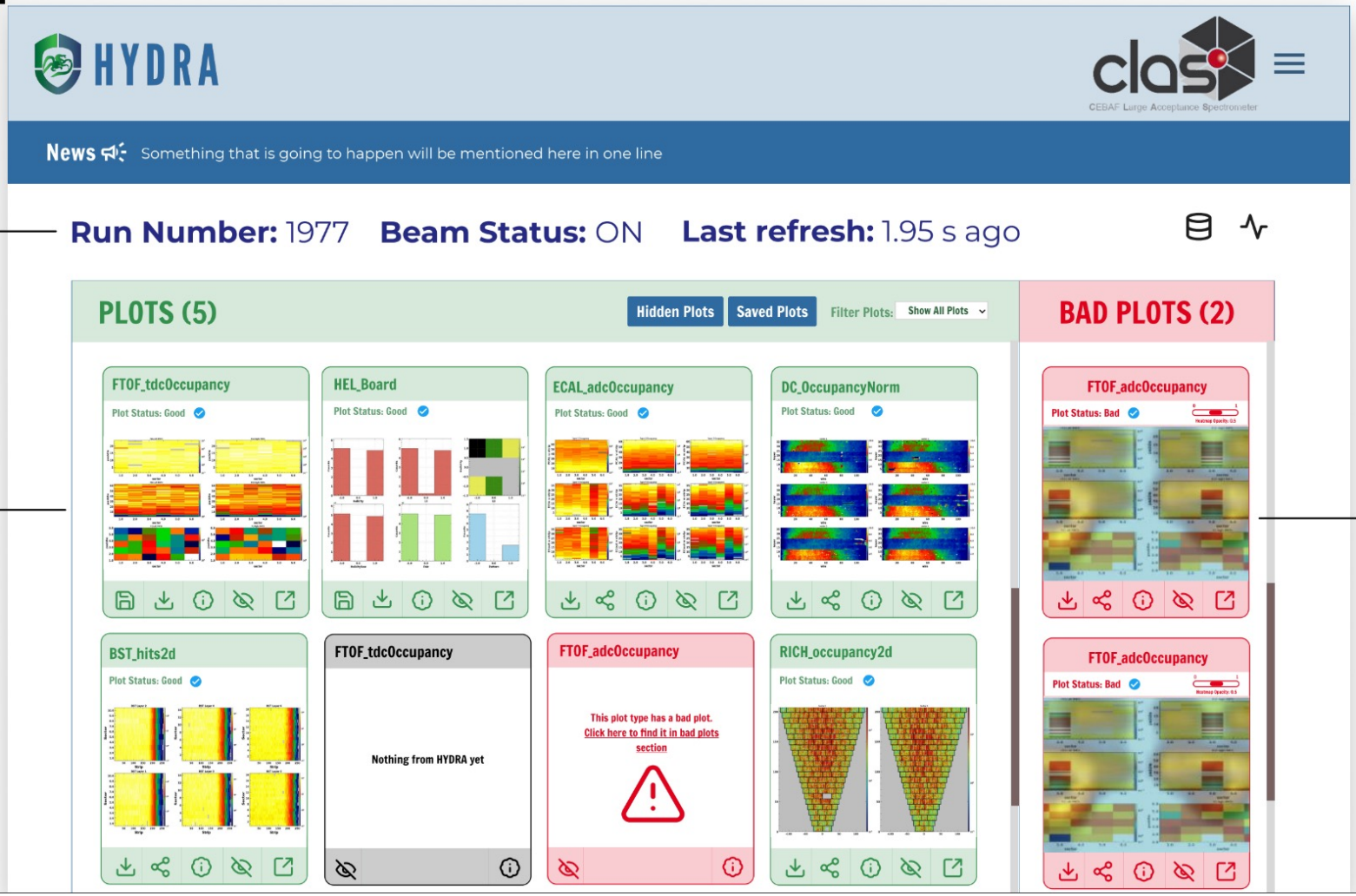


Jefferson Lab
Thomas Jefferson National Accelerator Facility

# AI Data Quality Monitoring

*New front-end user interface deployed for current(2025) Run*

**Run**




status indicators

Main image gallery

reserved for Bad plots

# AI Data Quality Monitoring


## By the numbers

**deployments**
7

**analyzed images**
3,001,442

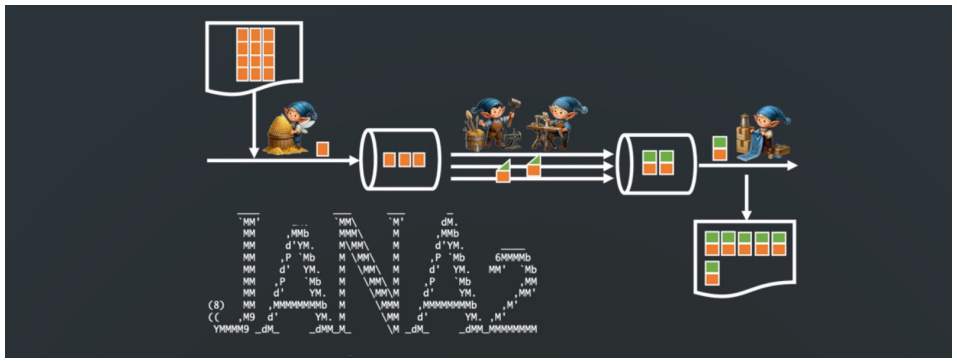
**human-labeled images**
982,422

**most labeled images by single human**
113,749

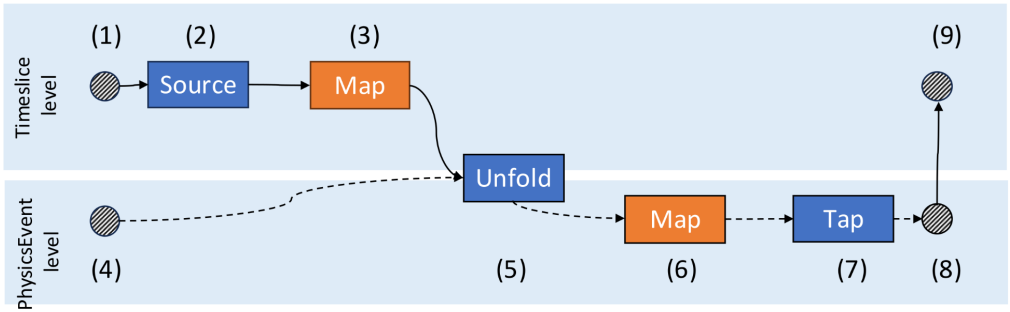
**trained models**
641
*not all in production

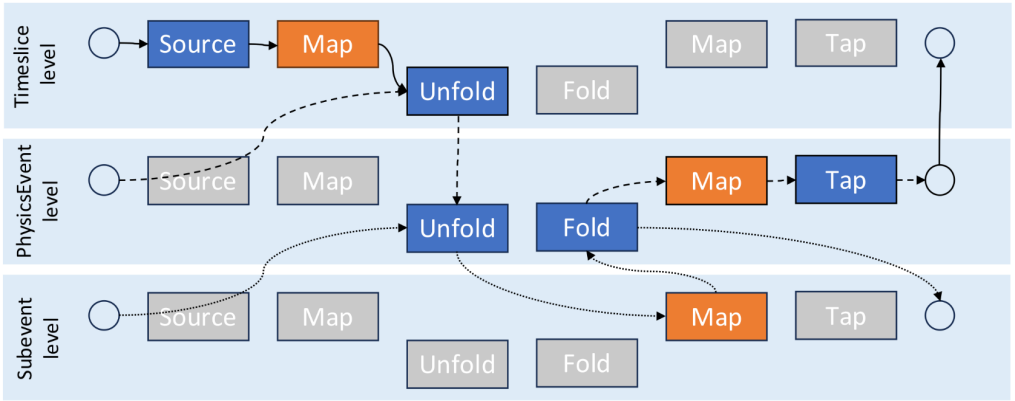
**individual runs with at least 1 bad image**
1,568
*Halls B and D

# JANA2 Event Reconstruction Framework




- C++ multithreaded reconstruction framework
- In production by GlueX and ePIC
- Is being adopted for SoLID and TDIS
- Support for streaming readout:
  - Software triggers and filtering
  - Timeframe splitting/event building
  - Subevents
- Users provide modular software components and JANA2 automatically infers the corresponding dataflow-parallel processing topology



# HPC in Scientific Data and Computing Department (CST div.)

## Performance Computing for Science Group

### Mission:

- Work closely with the Theory Center to advance Jefferson Lab's Lattice QCD (LQCD) efforts by leveraging state-of-the-art High Performance Computing (HPC) techniques, aiming to maximize the performance of LQCD software systems on DOE Leadership Computing Facilities and local computing clusters.
- Research and collaboration with universities and industrial partners to advance high performance computing.

### Notable achievements:

- Deeply involved in DOE LQCD Exascale Computing project (ECP), SciDAC5 and INCITE program.
- JIT (Just-In-Time) compilation technique via LLVM to convert LQCD parallel data C++ expression into LLVM IR (Intermediate Representation) code which can be converted into machine code for various GPUs and CPUs.
  - Enable Jefferson Lab LQCD software system Chroma to run on many GPUs efficiently using DOE supercomputers such as Frontier, Perlmutter and Aurora.
  - Collaborated with Intel to debug Intel OneAPI level zero runtime environment on Intel Ponte Vecchio GPUs.
- Research and development in portable parallel and distributed numerical algorithms targeting modern GPU and CPU architectures.
  - MgProton (MultiGrid), SuperbBlas (Distributed Blas for Tensor contraction), EigenSolver, Domain Decomposition.
- Graph contraction and scheduling algorithms to speed up calculations of correlation functions on GPUs and CPUs. Fast and portable GPU tensor contraction library with a GPU memory management system allowing oversubscription of the GPU memory.
  - Graph isomorphism, Graph partitions …

# Data Science:

- Started regular AI G17 monthly meeting:
  - Discuss AI activities (e.g. private, cross agencies, DOE, and the Administration)

- DOE AI JAMs:
  - 3 DOE AI JAM:
    - 1000 scientists: OpenAI, Anthropic
    - Director's exploration: OpenAI, Anthropic, Google, Microsoft, Amazon
    - Data Centers and Geo-Informatics w/ Google DeepMind

- AI+ Expo (DC):
  - Prepared for the DOE booth and gave JLAB AI talk

# Data Science at Jefferson Lab

**Mission Statement:**

Our mission is to deliver cutting-edge data science solutions that drive innovation and progress across the Department of Energy (DOE) complex by collaborating with subject matter experts at Jefferson Lab, partner laboratories, and universities. We aim to provide tailored data science support for scientific applications relevant to our regional community.

**Vision:**

We envision a future where:

1. **Capacity Building**: Our team expands the capabilities and capacity of data science within Jefferson Lab, fostering a culture of innovation and excellence.
2. **Collaborative Research Hub**: We establish a collaborative research hub that brings together experts from academia, industry, and government to tackle complex scientific challenges.
3. **Education & Outreach**: We foster education and research opportunities with regional universities and industries, promoting knowledge sharing and skill development.
4. **Sustainability**: By optimizing our data science workflow and algorithms, we strive to reduce the carbon footprint from our algorithms and deployment solutions.

# Data Science at Jefferson Lab

**Scope:**

The scope of the department involves the development and application of advanced Artificial Intelligence (AI) and Machine Learning (ML) techniques to address complex challenges in various research areas.

**1. Application Research Area**:

- Particle Physics, Accelerator, and Detectors
- Environmental Science, Health & Medical Applications
- Computer Science & Advanced and Resource Efficient Algorithms

**2. Data Science Methods:**

- **Anomaly Detection & Prediction**: Develop AI/ML models for identifying unusual patterns, predicting anomalies, and detecting potential issues in complex systems.
- **Uncertainty Quantification**: Create methods to quantify uncertainty in predictions, allowing for more informed decision-making under uncertainty.
- **Optimization & Control**: Apply optimization techniques (e.g., reinforcement learning) to optimize system performance, resource allocation, and process control.
- **Continual Learning**: Develop algorithms and infrastructure that enable machines to learn continuously from new data, adapting to changing conditions and improving over time.
- **HPC Scalable ML**: Design AI/ML systems that can execute on super-computers at DOE LCFs
- **Generative AI:** Leverage and develop new solutions based on existing LLM and generative techniques for scientific discoveries
- **Edge ML**: Implement Machine Learning solutions for low power edge devices

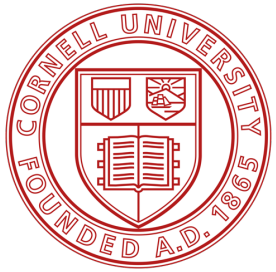
# Building Collaborations


















# DOE Projects (Accelerators – BES, HEP, NP)

Title: **Machine Learning for Improving Accelerator and Target Performance**
Partners: Oak Ridge National Laboratory
AI/ML Techniques: Anomaly Prediction, Uncertainty Quantification, Reinforcement Learning

Title: **Next Generation Compact SRF Accelerators for Industrial Applications**
Partners: Fermi National Accelerator Laboratory, Florida International University
AI/ML Techniques: Anomaly Prediction, Uncertainty Quantification, Reinforcement Learning, Meta-Learning

Title: **Beam polarization increase in the BNL hadron injectors through physics-informed Bayesian Learning**
Partners: Brookhaven National Laboratory, Cornell University, SLAC National Accelerator Laboratory
AI/ML Techniques: Uncertainty Quantification, Reinforcement Learning

Title: **AI for CEBAF**
Partners: Old Dominion University
AI/ML Techniques: Anomaly Prediction, Optimization, Uncertainty Quantification

Title: **Tuning LCLS FEL**
Partners: SLAC National Accelerator Laboratory, DESY
AI/ML Techniques: Reinforcement Learning

# DOE Projects (NP)

Title: **Femtoscale Imaging of Nuclei using Exascale Platforms**
Partners: Argonne National Laboratory, Virginia Tech, Old Dominion University, National Renewable Energy Laboratory, Ohio State University
AI/ML Techniques: Scalable ML, Generative AI, Optimization

Title: **AI/ML Optimized Polarization**
Partners: Carnegie Mellon, College of William and Mary
AI/ML Techniques: Uncertainty Quantification, Reinforcement Learning

Title: **Graph Neural Networks for Particle Tracking**
Partners: University of Virginia
AI/ML Techniques: Graph Neural Networks, ML at the Edge

Title: **Generative AI Framework for Nuclear Physics**
Partners: Old Dominion University, University of Glasgow, National Institute for Nuclear Physics - INFN
AI/ML Techniques: Generative AI, Composable ML workflows

# Other DOE Related Projects

Title: **ML4BOPS**
Partners: Jefferson Lab Operations
AI/ML Techniques: Generative AI, LLMs

Title: **ML4NPTheory**
Partners: College of William and Mary
AI/ML Techniques: Generative AI, Transformers

Title: **CL4Fusion**
Partners: General Atomics
AI/ML Techniques: Uncertainty Quantification

# Advanced Computing for Environmental Studies

Joint Institute lead by Jefferson Lab and Old Dominion University
"an open opportunity to collaborate"

Title: **Flood Modeling**
Partners: Old Dominion University, University of Virginia
AI/ML Techniques: Regression, Uncertainty Quantification, Fourier Neural Operators

Title: **Air Quality Modeling**
Partners: Old Dominion University, Children's Hospital of The King's Daughters
AI/ML Techniques: Regression, Uncertainty Quantification

Title: **Health/Medical Studies**
Partners: Old Dominion University, Eastern Virginia Medical School
AI/ML Techniques: Anomaly Detection, Uncertainty Quantification, Generative AI

# Data Science:

- Accelerator related activities:
  - Streaming Monitoring/Diagnostic and Control Agent Framework
    - Containerized framework that can access remote data streams with continually learning to provide monitoring
    - Testing using FNAL and UITF remote sensors
  - SNS/ORNL:
    - Algorithm for imitation learning RL work for advanced accelerator control
    - Continuous Learning for Particle Accelerators paper accepted
  - BNL:
    - Using SOCT for BNL accelerator bunch merge Beam Transfer Line
  - CEBAF:
    - Differentiable conditional multi-objective optimization for CEBAF accepted
    - CEBAF radiation paper accepted
  - 5th ICFA Beam Dynamics Workshop on Machine Learning Applications for Particle Accelerators (2025)
    - 2 staff are part of the Scientific Organizing Committee
    - 6 abstracts accepted;3 talks given; 1 tutorial given
- SciDAC QuantOm project:
  - Scalable Asynchronous Generative AI paper accepted
- Advanced Computing for Environmental Studies:
  - Significant progress in the ultrasound anomaly project with EVMS/ODU
  - Published results on flood modeling with VB/ODU
  - Working on streaming real-time agent-based forecasting for VB flood application
- Mentored two ODU capstone projects

# HPDF

# Working towards CD-1

## Community outreach

- ✓ 6-way Light Sources meeting (Jan, in-person)
- ✓ IRI Management Council (April, virtual)
- ✓ FES PI meeting (June, in-person)
- ✓ HPDF/IRI workshop (July, in-person)
- ✓ Small-group interviews with groups identified through initial HPDF workshop (summer/fall, virtual)
- ✓ Supercomputing '24 (November, in-person) - presented to other ASCR facilities and a DOE booth talk
- Set up more meetings to give feedback

## Working toward CD-1

- ✓ Preliminary feedback from outreach analyzed to extract required capabilities
- ✓ Defining Project vs Facility scope; HPDF as a facility has larger aspirations than the project can deliver
- ✓ Using examples from similar projects to develop documents for design review
- Meeting with vendors and software communities to identify scope implementation options

## Next Steps

- Complete vendor interviews and incorporate product roadmaps into design specifications
- Document project scope, facility scope, and technical conceptual design
- Update analysis of alternatives and work breakdown, complete CD-1 documents – prepare for review

Please reach out if you have a DOE program or community meeting that we can participate in for outreach!

# Stay Informed

https://hpdf.science

https://linkedin.com/company/doe-hpdf

https://www.youtube.com/@doe-HPDF

**Share your thoughts!**
Answers will be provided via a website FAQ within a few weeks.