

What is ModCon? Transformational AI Model Consortium (ModCon)

April 3, 2026



U.S. DEPARTMENT of ENERGY

ModCon

Transformational AI Models Consortium

Mission

- ⚡ Establish a consortium to accelerate the technical development and scientific discovery of the Model Teams
- ⚡ Develop and deliver domain cross-cutting services as an engine for transformational AI model development
- ⚡ Convene partners from industry, academia, and internationally to accelerate AI development and adoption

Deployed on Genesis Mission Infrastructure
The American Science Cloud

Four Core Teams

deliver support to Genesis Teams

IPPF
Partnerships and IP Management

DBS
Data Brokers & Standards

BPSW
Best Practices for Scientific Workflows

BASE
Cross-Cutting AI Capabilities

Partners
17 DOE Labs + Industry + Academia

What We Deliver

 **AI-Ready Data Pipelines**
Transform raw scientific data into training-ready datasets

 **Scientific Workflows**
Leaderboards, workflows, and upskilling for continuous discovery

 **Transformational Capabilities**

- Core Agentic Framework
- Self-Improving Models Harness
- Multimodal Reasoning Frontends
- Safety, Security, Assurance
- Evaluation

Genesis Mission Mapping
Data and Model Teams



Genesis Mission

Governance and DOE Engagement

Lab Council, ALDs, DOE Lab Reps
Partnership Council, External
Executive Voice

ModCon Office

Director

Rick Stevens, Argonne

Deputy Director

Court Corley, PNNL

Project Management

Emily Dietrich, Argonne

Model Team Coordinator

Tom Brettin, Argonne

AmSC Coordination

Neeraj Kumar, PNNL

Cross-Cutting Capabilities

IPPF: IP & Partnership Formation

Megan Clifford, Argonne
Daniel Ratner, SLAC
Jason Hales, INL

BPSW: Best Practices for Scientific Workflows

Franck Cappello, Argonne
Rafael Ferreira Da Silva, ORNL

DBS: Data Broker Standards

Lauren Biven, JLAB;
Jeren Browning, INL
Ray Grout, NLR

BASE: Baseline AI R&D Capabilities

Stefan Wild, LBNL
Nathan Hodas, PNNL

CAF: Core Agentic Framework

Ian Foster, Argonne

EVAL: Evaluation

Stefan Wild, LBNL

SAFE: AI Security & Safety

Nathan Hodas, PNNL

SIM: Self-Improving Models

Ana Gainaru, ORNL

DATA: AI-Ready Data

Shreyas Cholia, LBNL

MM: Multimodal Reasoning

Sandeep Madireddy, Argonne

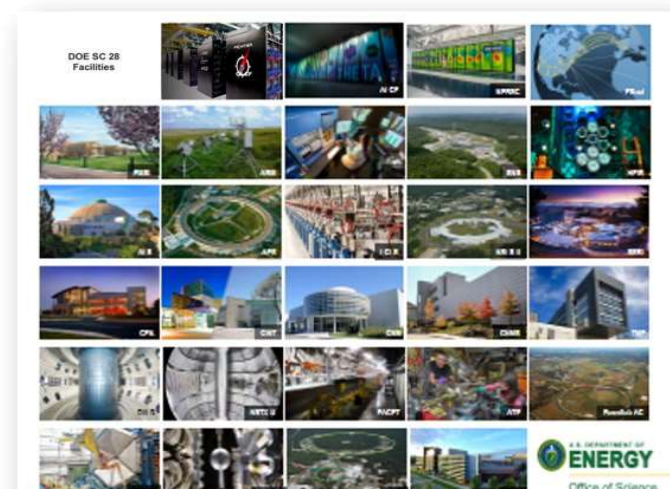


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American Science Cloud (AmSC)

A Unified Platform for Transformational AI and Science Across DOE

- AmSC is a secure, federated, and science-optimized cloud environment
 - *Not centralized servers but an environment supporting contributed tools, services, and ModCon core capabilities*
- Integrates DOE's world-leading computing, experimental facilities, data resources, and HPC networks
 - *A flexible structure to support integration of capabilities*
- Enables AI-ready end-to-end workflows across the complex
 - *Contributions from across the DOE lab complex, not predefined workflows*



Data Services

FAIR, AI-ready datasets across DOE



Model Services

State-of-the-art models for discovery



AI Services

Extreme-scale training & inference



Infrastructure

Secure compute, storage, networking

Genesis Mission defines ambition and urgency.
AmSC scaffolds a shared platform to execute.

DOE Labs and Infrastructure Partners

ANL · LBNL · BNL · FNAL · INL · JLab · NETL · NLR · ORNL · PNNL · PPPL · SLAC

<https://amsc.energy.gov/>



Genesis Mission



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ModCon Core Baseline AI Research & Development **BASE**



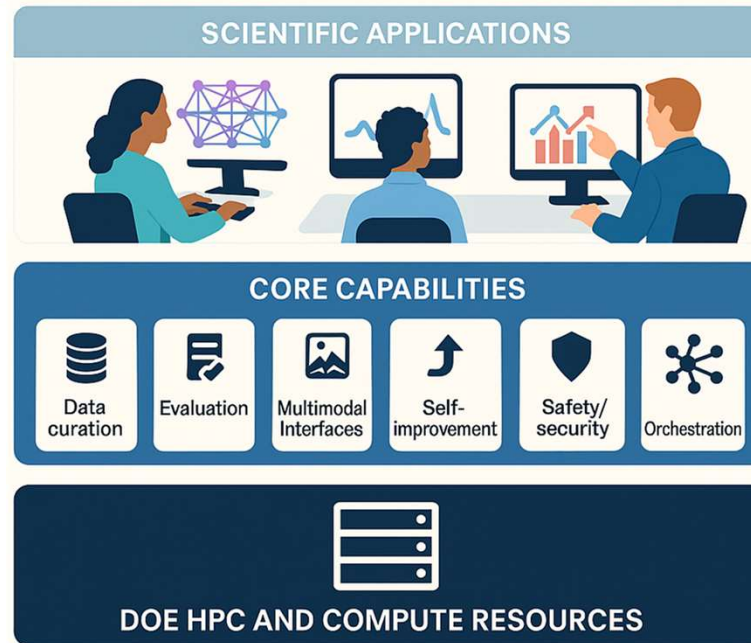
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Base R&D is Delivering Baseline AI Capabilities to the Genesis Mission

- Providing reusable methods, frameworks, and tools that underpin every Model Team
- Responsive to the requirements set by the BPSW, DBS, IPPF crosscuts
- Collaborating directly with Model Teams and AmSC

We are also:

- Genesis Mission's crosscutting AI dev team
- Filling in what is missing from the current AI ecosystem
- Helping inspire others to use the command line



**FASTER
SCIENCE**

SAFER AI

**SCALABLE
ORCHESTRATION**



Stefan Wild
(LBNL)



Nathan Hodas
(PNNL)

Base/CAF: Building a Common Agentic Framework



Ian Foster
(ANL)



Yadu Babuji
(ANL)



Matt Baughman
(PPPL)



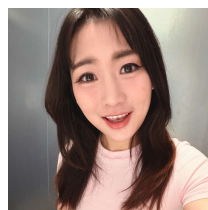
Kyle Chard
(ANL)



Tanwi Mallick
(ANL)



Fred Suter
(ORNL)

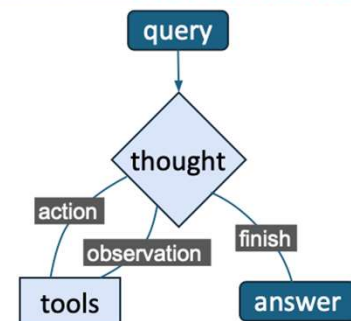


Bella Yang
(ANL)

Agents enable **closed-loop, autonomous scientific workflows** across complex, distributed systems

To enable agentic AI applications across AmSC at unprecedented scales, CAF is:

- **Developing scalable agentic orchestration** (1000s of concurrent LLMs, agents, tool calls; flexible inter-agent comms)
- **Promulgating best practices** for agent use in DOE environments



1. Local Agent Execution LangGraph, Academy Your on-ramp to CAF. Run persistent, stateful agents on a laptop or workstation—no federation required. Status: Mature	2. Federated Agent Execution LangGraph + Academy Cross-institutional agent execution under federated identity and policy. Status: Mature	3. Massively Parallel Agent Inference LangGraph, Aegis Fan out thousands of LLM requests in parallel on HPC. Status: Emerging
4. Governed Tool Use at Scale Academy governance Invoke expensive, stateful, or dangerous tools under proactive policy enforcement. Status: WIP	5. Multi-Agent Coordination Shared state + policy + budgets Many agents under shared governance—within one institution or across many. Status: Emerging	6. Long-Lived Autonomous Agents Lifecycle management Agents that persist for days to months, maintaining state, memory, and goals. Status: Emerging

<https://agents4science.github.io/Capabilities>

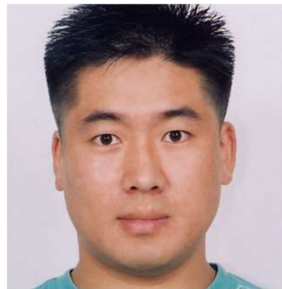
Base/Data: Automating the Data Preparation Pipeline



Lead: Shreyas Cholia
(LBNL)



Jean Luca Bez
(LBNL)



Jong Choi
(ORNL)



Rohith Varikoti
(PNNL)



Kyle Parfrey
(PPPL)



Andrew Tritt
(LBNL)



Aaron Tuor
(PNNL)

Developing an AI-agent driven data curation pipeline that autonomously transforms raw scientific data into AI-ready form

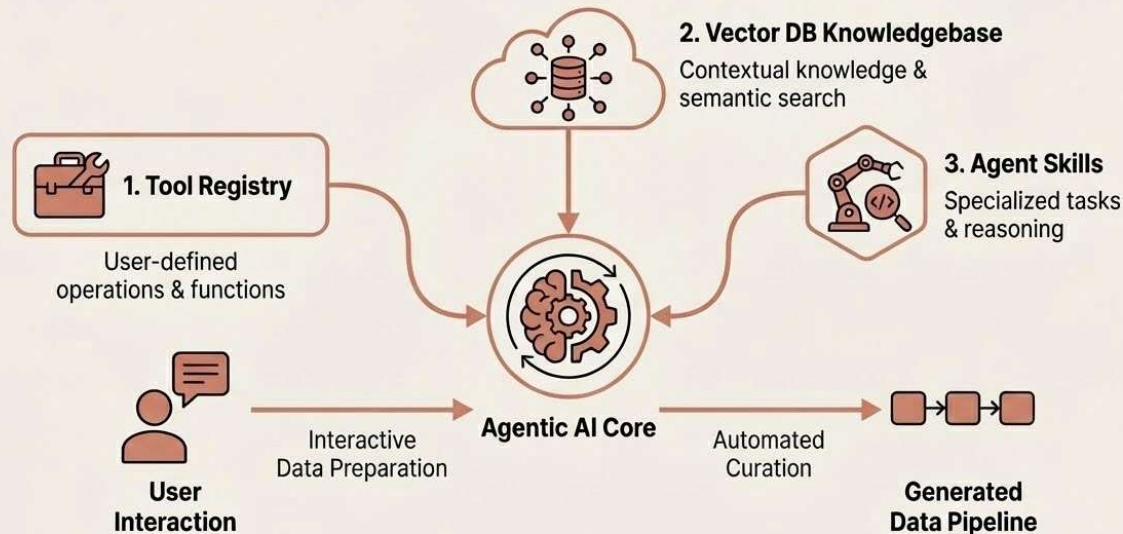
Contact:

SCholia@lbl.gov

Base/Data: Composable Data Pipeline Framework

Agentic Data Pipeline Builder

A flexible, interactive framework for generating AI-driven data preparation workflows.



Data Science Agent Toolkit (DSAGT):

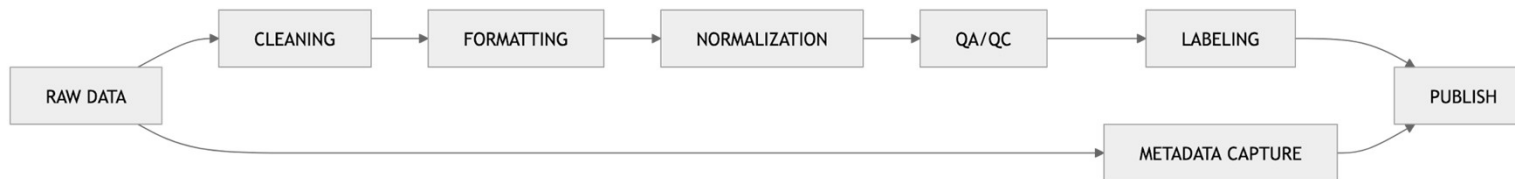
Agentic Harness to manage data preparation pipeline

- Use your favorite interactive LLM agent (Claude, Codex, OpenCode, Goose etc.)
- Support for data tool execution, RAG knowledge-bases, Agent Skills
- Use of "Skills" for agentic tasks: Data Card Generator, HDF5 data ...

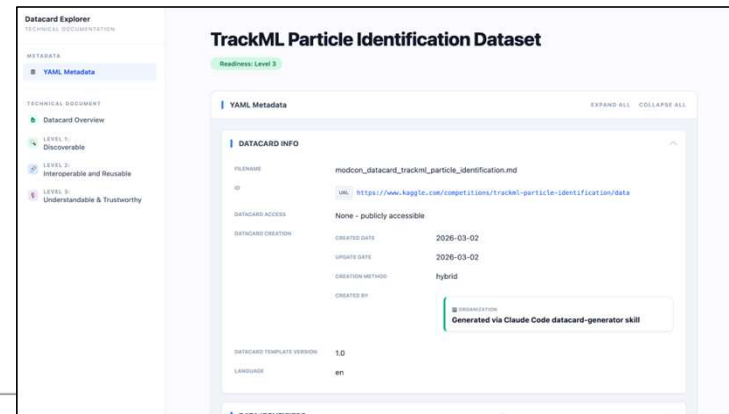
Base/Data: AI Readiness

AI Readiness

- Working with ModCon DBS on AI readiness tool list / metrics / evaluations.
- Practical definition of AI-readiness: Getting to **model.load(data)** + additional metadata
- Example pipelines / steps / definitions vary across model teams



- Data card generation and visualization tools
- Work with model teams on preparation pipeline to fit their needs



Base/Eval: Model Assessment and Evaluation



Stefan Wild
(LBNL)



Eric Chagnon
(LBNL)



Neil Getty
(ANL)



Fernando Llorente
(BNL)



Zarija Lukic
(LBNL)



Emily Saldanha
(PNNL)



Shashank
Subramanian (LBNL)



Fred Suter
(ORNL)



Angel Yanguas-Gil
(ANL)

Developing tools, benchmarks, & protocols that assess robustness, generalizability, reproducibility, & scientific validity under evolving data and uncertain ground truths

- Track multi-metric progress over time
- Serve as peer reviewer, ultimately with SME-HitL
- Integrating with AmSC UI/Infrastructure

Key principles

- Open-source framework, multiple techlanes
- Address non-language modes, domain-specific info
- Build to evolve and scale



Tools



Benchmarks

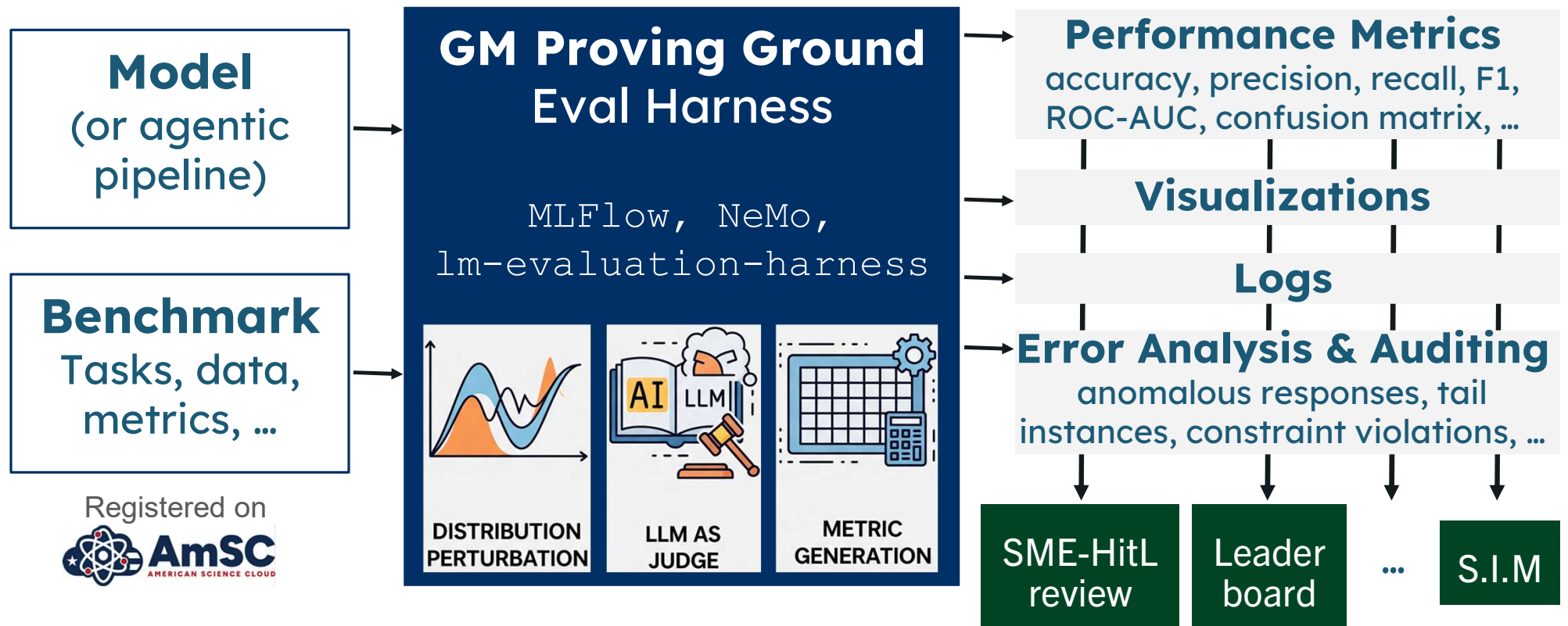


Protocols

+ AmSC & BPSW embedded liaisons

11 (Wahid Bhimji, Nhan Tran, Rafael Zamora-Resendiz)

Base/Eval: Delivering a Comprehensive Evaluation Suite



Base/MM: Multimodal Scientific Reasoning Models



Sandeep Madireddy
Argonne National Lab



Adarsha Balaji
Argonne National Lab



Guojing Cong
Oak Ridge National Lab



Patrick Emami
National Lab of the Rockies



Ben Erichson
Lawrence Berkeley
National Lab



Neil Getty
Argonne National Lab



Sam Wheeler
Argonne National Lab



Fangfang Xia
Argonne National Lab



Goal: *Develop multimodal scientific reasoning models and an intelligent conversational interface that accepts inputs across modalities, performs cross-modal reasoning, to answer complex scientific questions*



At-Scale Services / MLOps

Software: <https://github.com/AI-ModCon/BaseMM> PRISM/
Contact: Sandeep Madireddy (smadireddy@anl.gov)



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Base/MM: Multimodal Scientific Reasoning Models

PROJECT GOALS & CHALLENGES



Goal: Cross-modal reasoning across text, images and other structured data for scientific discovery



Capability: Utilize the best-in-class modality/domain encoders and enhance multimodal reasoning - tool-free capabilities and tool-based discovery and tasks.



Challenge: Bridging the gap between all diverse modalities, data quality, and enable flexible dialogue.

CURRENT STATUS



Scaling Training on Aurora, Perlmutter & Frontier

- 5x Throughput increase, efficient communication and memory optimization using FSDP, 85 samp/s → 420 samp/s via Native DDP



Projector Training & Modality Alignment (Stage 1 & 2)



Instruction Tuning: Joint Multimodal SFT (Stage 3)

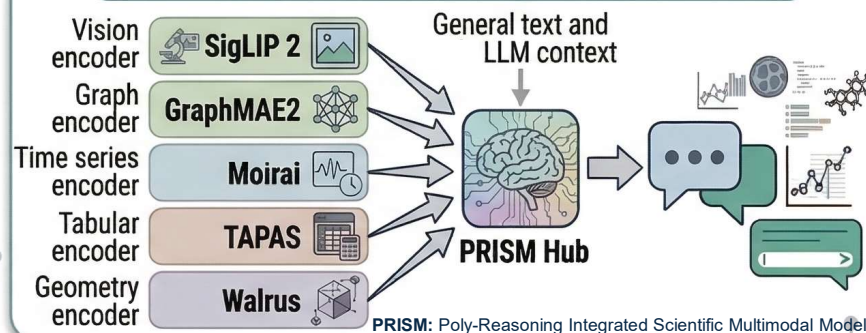


RL & Safety Pipelines with Reward/Policy Models (Stage 4)



Early results on reasoning: Image & Time Series modalities

PRISM HUB & SPOKE ARCHITECTURE



ONGOING RESEARCH & PLANS

- **Data Curation...**
 - ✓ Data Curation
 - ✓ Joint SFT
 - ✓ Ablating Core
 - ✓ Joint SFT
- **Evaluate multimodal/cross-modal reasoning**
- **Prototype** end-to-end 'GM Proving Ground' working on AmSC
- Standardize multimodal data ingestion, evaluation/safety, SIM interfaces
- Model-generated Synthetic Data for future training stages (feedback loop from SFT)

Base/Safe: Model Safety and Security



Nathan Hodas
(PNNL)



Robin Cosbey
(PNNL)



David Florey
(PNNL)



Natalie Isenberg
(PNNL)



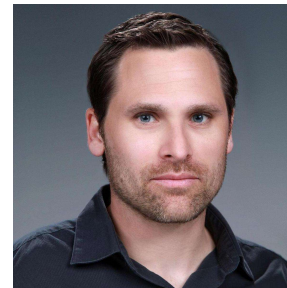
Steven Goldenberg
(JLAB)



Olivera Kotevska
(ORNL)



Reilly Raab
(PNNL)



Malachi Schram
(JLAB)

Developing
rigorous
frameworks,
scalable methods,
and institutional
safeguards that
guarantee safety
and security across
the scientific AI
lifecycle

Base/Safe: Agentic Framework with Flexible Execution Strategy for Model Teams



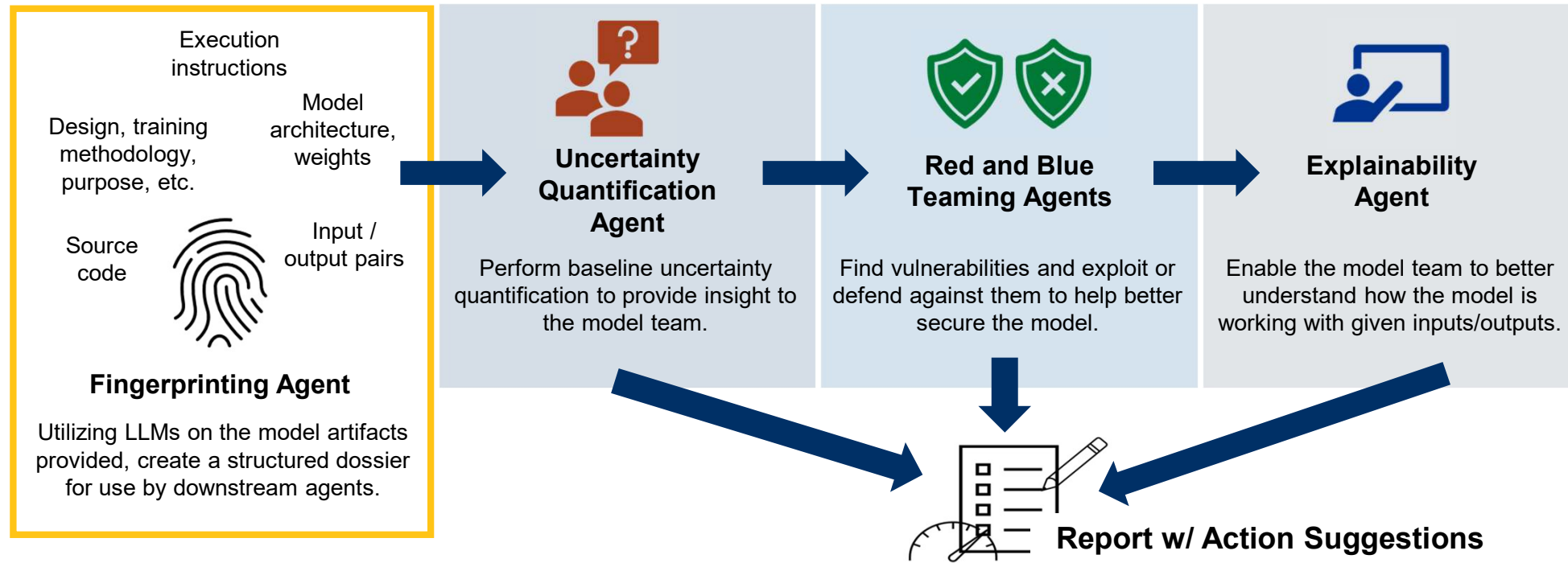
On Model Team (MT) laptop:
Either through command-line or embedded within VS Code IDE. Provides rich analysis tools directly in coding environment.



As a Continuous Integration (CI): Enables MT's to focus on functionality while the Base/Safe Agents focus on providing safety, uncertainty, and explainability insights.



Within testing environment:
This fully integrated approach enables more real-world analysis and insights.



Base/SIM: Enabling Self-Improving Models



Self-improving AI Models

Agentic framework for keeping domain science models up to date with data from new experimental and simulations



Software: <https://github.com/AI-ModCon/BaseSIM> APEIRON
Contact: gainarua@ornl.gov



Ana Gainaru
ORNL



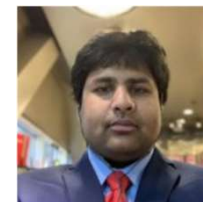
Steffen Schotthoefer
ORNL



Anna Quach
INL



Zilinghan Li
ANL



Krishnan Raghavan
ANL



Rafael Zamora-Resendiz
LBNL



Auralee Edelen
SLAC



Andrew Ayres
ORNL



Alvaro Sanchez-Villar
PPPL

Base/SIM: APEIRON's Continuous Self-Improvement



Goals

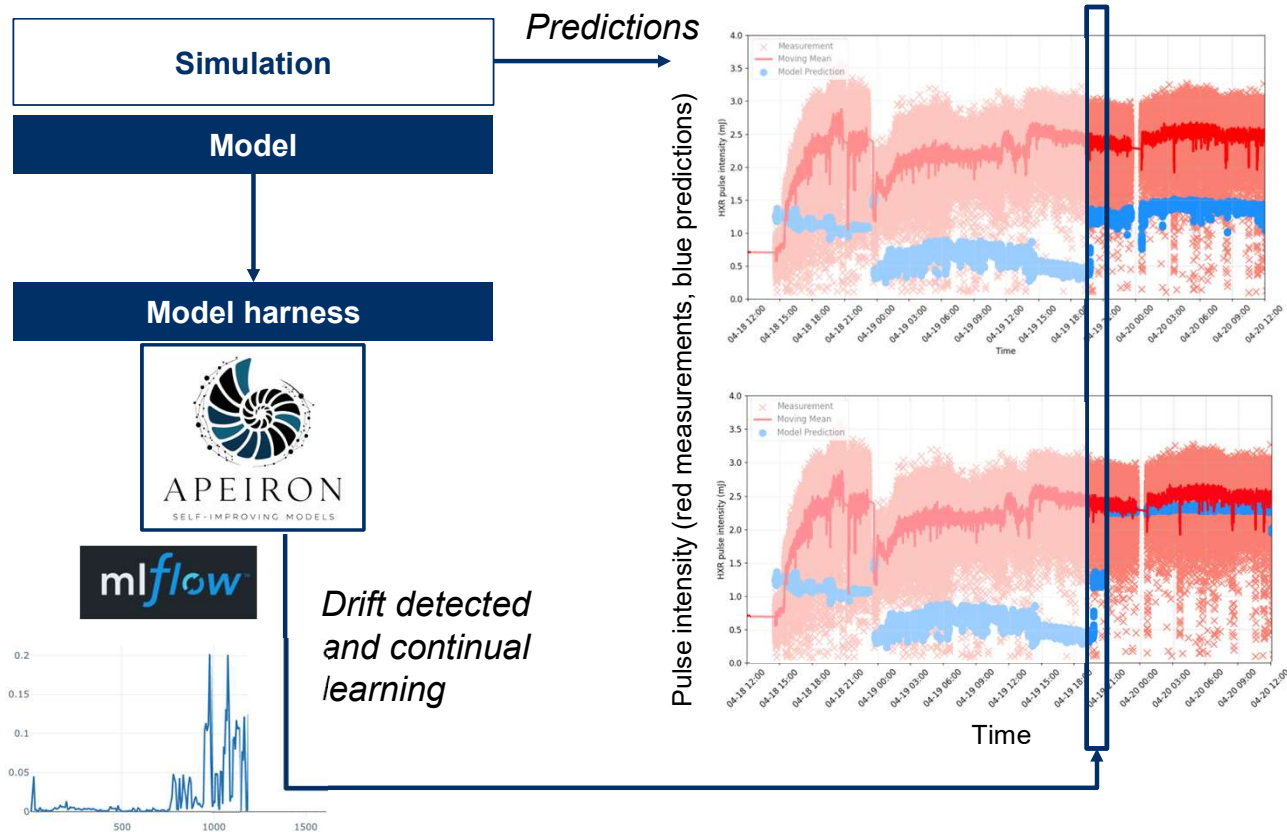
Keep domain-specific AI models synced to new experimental data and methods that emerge

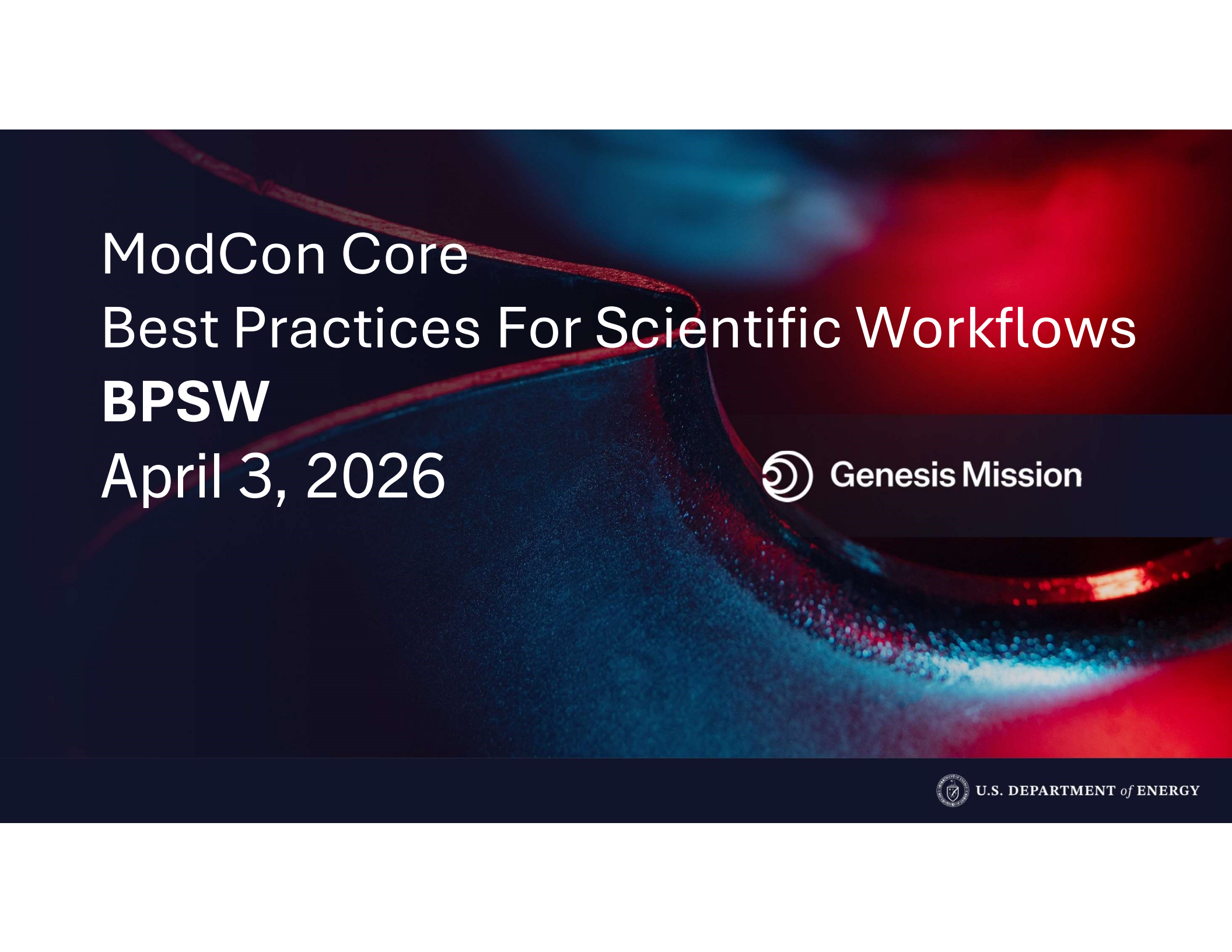
Monitor workflow runs
Detect data and model drift
Trigger continual learning
Monitor performance

Status

APEIRON framework has been developed and can connect to domain scientists through API calls

In progress: Deployment at scale
In progress: SKILLS / MCP tools





ModCon Core Best Practices For Scientific Workflows **BPSW** April 3, 2026

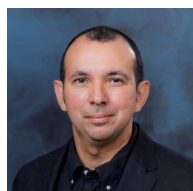


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BPSW 23 Members from 11 DOE Labs



Franck Cappello,
Co-lead, ANL



Rafael Ferreira da
Silva, Co-lead, ORNL



Robert Underwood,
Extended Team Lead,
ANL



Massimiliano Lupo
Pasini, Extended
Team Lead, ORNL



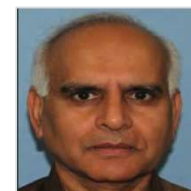
Rinku Gupta,
Extended Team
Lead, ANL



Neil Getty, ANL



Murat Keceli, ANL



Nagi Rao, ORNL



Jong Youl Choi,
ORNL



Helia Zandi, ORNL



Nathan Tallent,
PNNL



Natalie Isenberg,
PNNL



Anna Giannakou,
LBNL



Dan Gunter,
LBNL



Mohammad Abdo,
INL



Long Qi, AMES



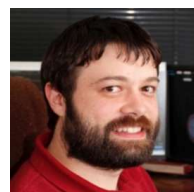
Mikhail Titov, BNL



Joseph Smith, NLR



Nhan Tran, FNAL



Thomas Britton, JLAB



Shantenu Jha, PPPL



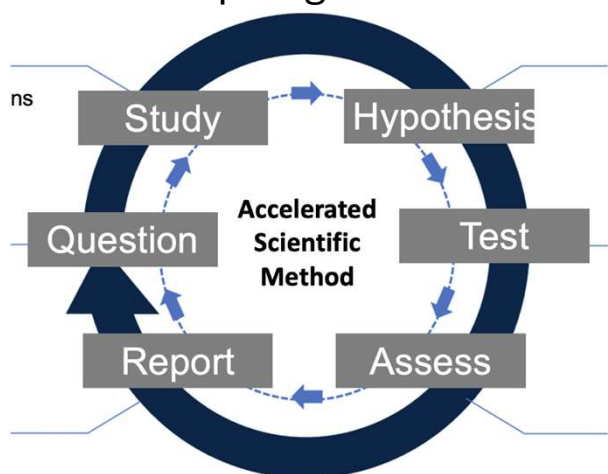
Thorsten Hellert,
LBNL



Amith Murthy,
SLAC

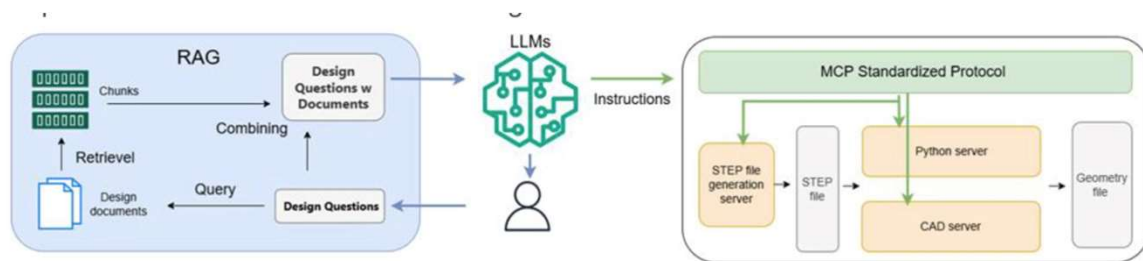
Scientific Workflows

BPSW considers every steps of the whole research workflow from the research questions to report generation.



Some teams implement the entire cycle.
Most teams focus on a subset of steps
(e.g. AI4HPC: LLM-based code translation workflow)

MOAT March Demo



End-to-End Loop: couples an LLMs to a RAG, MCP servers.

1. User's query is passed to the RAG to retrieve relevant documents ([Study](#)).
2. The LLM uses this context to generate a plan, which involves calling simulation tools via the MCP. ([Plan Generation](#))
3. The MCP executes the simulation and returns results (e.g., a STEP file for a CAD model). ([Test](#))
4. The process is iterated with human oversight. ([Assess](#))

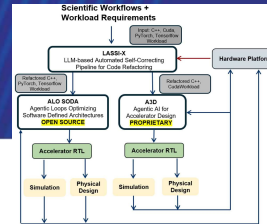
BPSW Specific Goals

- 1) Catalog the practices of AI integration in scientific workflows at DOE
- 2) From the catalog, Identify, catalog and develop training about best practices, the integration methods that provide the most acceleration
- 3) Identify the 20 most important tasks to accelerate with AI in scientific workflow
- 4) Identify where AI models break and define research directions to mitigate this (e.g. LLMs, Hypothesis Generation Multi-Agents)
- 5) Define AI integration templates that DOE workflows not using AI can use for acceleration

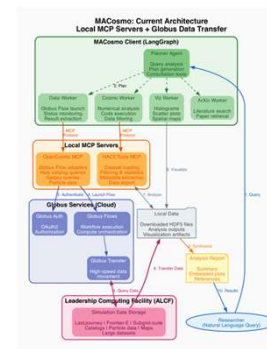
Examples of Workflows for March demos



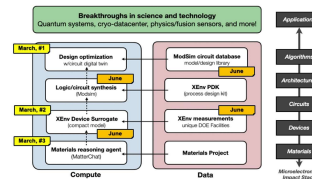
Microelectronics



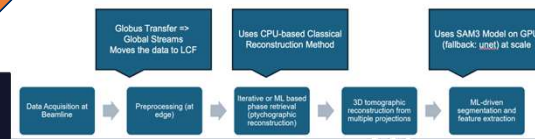
Q2C



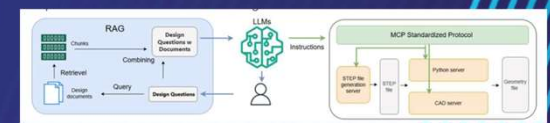
AXESS



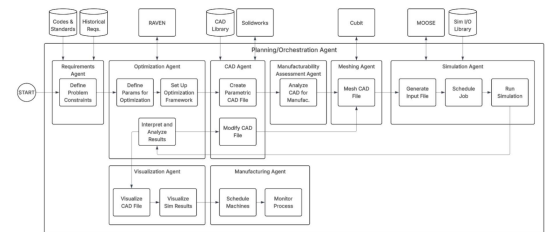
Synapse-I



MOAT



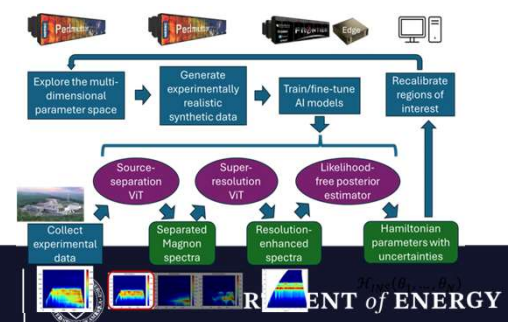
Prometheus



COMB-Flow



MAIQMAG



Catalog of Current Practices

Ran a survey collecting current practices within the DOE complex

144 workflow responses so far including AI

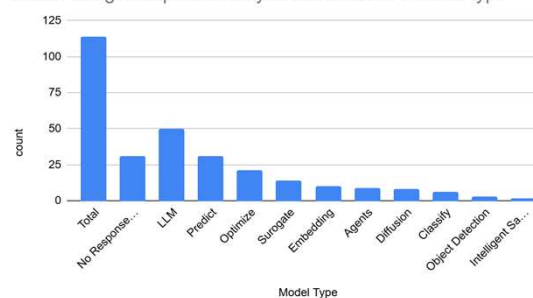
- We are targeting ~180-200 responses, but expect more
- Several labs are just now distributing the survey

This includes detailed Responses for **12 model teams** (not included: AI4Quantum, AI4HPC, and new model teams added Jan'25)

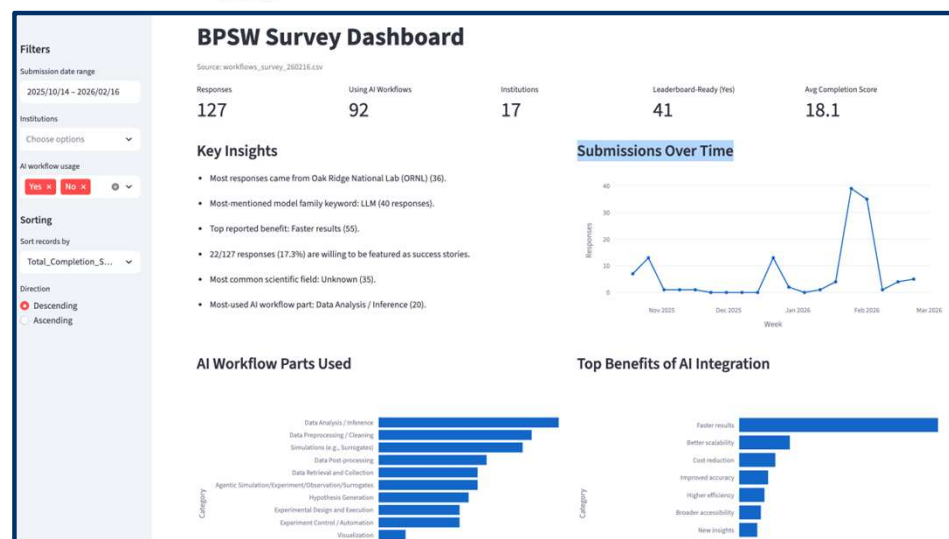
Developed a [dashboard](#) from the workflow survey responses, and working to deploy onto AmSc next week.

Chart shows AI model type usage across the surveyed scientific workflows

Model Usage: responses may use more than 1 model type



Responses only for the Model type question



Best Practices

Proven, evidence-based techniques or procedures that consistently deliver superior results and efficiency. Act as standards or benchmarks designed to minimize risk and optimize performance.

For AI-Based Workflows: “**Patterns**” of reusable AI integration techniques that have four elements:

- **Problem** (steps in the workflow) where AI-integration is it useful
- **Techniques** how to solve the problem (what AI, what training, what integration)
- **Consequences** of using the pattern (what benefits. e.g. speed, what risks)

Include policies (e.g. safety, security)

Goal in our case: **Provide guidance** on tasks such as AI design, model training, evaluation, integration, and deployment

Artifacts: user-guide, templates, trainings, and other resources

Adapted from Gamma et al, “Design Patterns for Object Oriented Software”

Some **Patterns** Identified in MT March Demo Workflows:

- LLM establishing a plan
- LLM calling multiple specialized agents
- Globus transfer to acquire, transfer data
- RAG requests to retrieve data
- Generation/Correction loops
- Calling surrogates for optimization.
- AI for data cleaning
- LLM as a judge for validation outputs

Prioritized AI Research Needs from the Model Teams

How was this list developed?

- Each team provided up to their top 5 needs
- Similar responses were grouped
- Ranked by the most top needs, most second needs etc.

Observations

- Currently based on a small subset of teams
- We expect that some tasks (e.g. #12) will become more important as teams gain experience
- We expect that more tasks will be identified as we expand to more teams

Next

- Collect more responses (send reminders, etc.)
- Participation in the International Forum on Detectors for Photon Science in Kyoto (April 2026)

Priority Research Tasks

1. Development of Surrogates (7 teams)
2. Code Development (5 teams)
3. Adversarial Evaluation (5 teams)
4. Optimization (4 teams)
5. AI+Modsim Orchestration (2 teams)
6. Data Sharing (2 teams)
7. Segmentation (1 team)
8. Data Integration (2 teams)
9. Hypothesis Generation (2 teams)
10. Real Time Visualization (2 teams)
11. Integrated Research Infrastructure (1 team)
- 12. Data Extraction and Cleaning (4 teams)**
13. Scientific/Technical Data Search (1 team)

Model/Agent Cards

Model/Agent Cards capture the capabilities, constraints, and intended use of DOE and community AI models & agents

Co-designed with stakeholders (AmSC, BASE-CAF, DBS, and leadership) to ensure consistency and adoption

- Scale is real: **330+ cards** already assembled and curated
- Broad coverage: spanning **30+ mission-relevant topics/domains**

Living inventory: continuously expanding as new models and agents emerge

<https://gitlab.osti.gov/genesis/modcon-bpsw>

The screenshot displays the 'Ornl_moat_sns_model Card' on the 'Genesis Mission | AI Resource Hub' website. The interface features a green header with the title and a navigation bar with tabs for 'project:genesis', 'team:MOAT', 'type:model', 'science:lightsource', 'science:accelerator', 'science:fusion', 'risk:general', and a license link. The main content area is divided into two columns. The left column contains sections for 'Pulsewatcher' (a description of the model), 'Developed by' (listing Kishan Rajput, Malachi Schram, Willem Blokland, Sasha Zhukov, and Anant Raj), 'Contributed by' (listing Timothy Robertson and Luis Caicedo Torres), 'Model Changelog' (listing a 2025-12-06 update), 'Model short description' (listing an autoencoder-based model for anomaly prediction), and 'Model description' (listing the base conditional auto-encoder model). The right column contains sections for 'Details' (listing development by Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Thomas Jefferson National Accelerator Facility), 'Languages' (listing Python), 'Datasets' (listing beam current, beam phase, and accelerator configuration), and 'Metrics' (listing training and validation reconstruction errors).

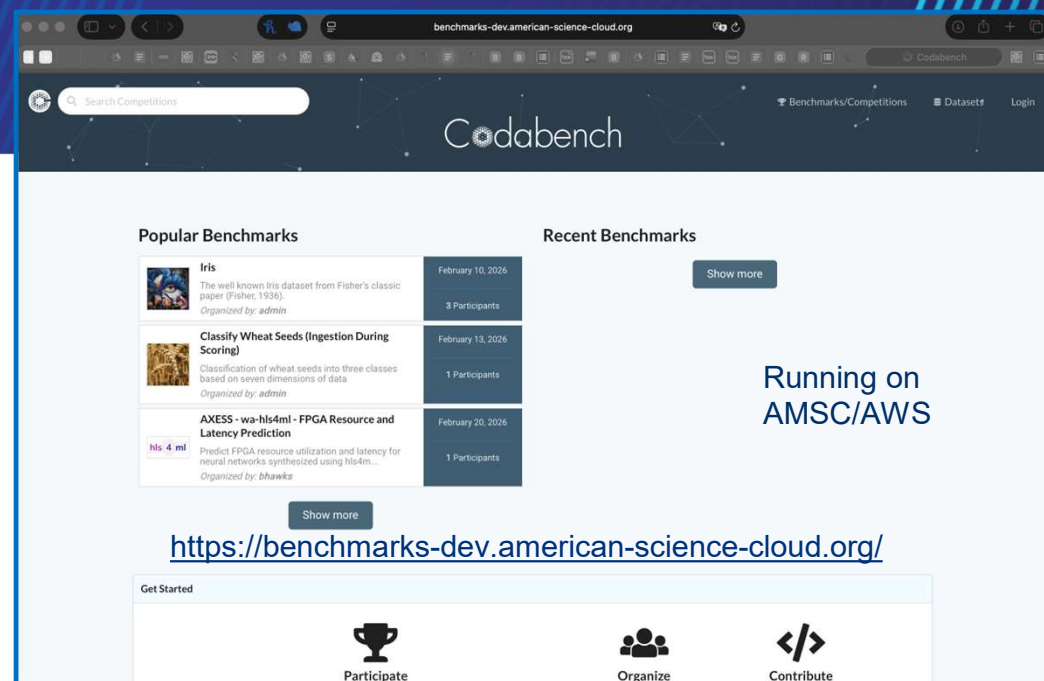
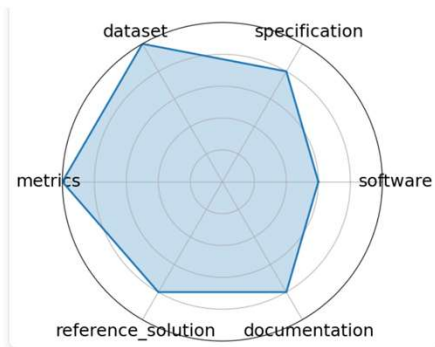
Leaderboard

The leaderboard will **expose the performance of different AI models on a selection of scientific workflow tasks** identified by the MTs and other DEO teams as critical for their scientific workflow accelerations.

The leaderboard will follow the general **format** of the benchmarks defined by **ML common**:
<https://mlcommons-science.github.io/benchmark>

Rigorous specifications of benchmark quality:

- Software environment
- Problem Specification and Constraints
- Dataset (FAIR)
- Performance Metrics
- Reference Solution
- Documentation



Hosted on the American Science Cloud (AWS)

Examples of benchmarks

- [LLMs] SciCode, CritPT
- [Agentic Evaluation] MOAT team
- [Surrogate Models] AXESS team
- [Segmentation] SYNAPS-I team

AI Discovery Engine

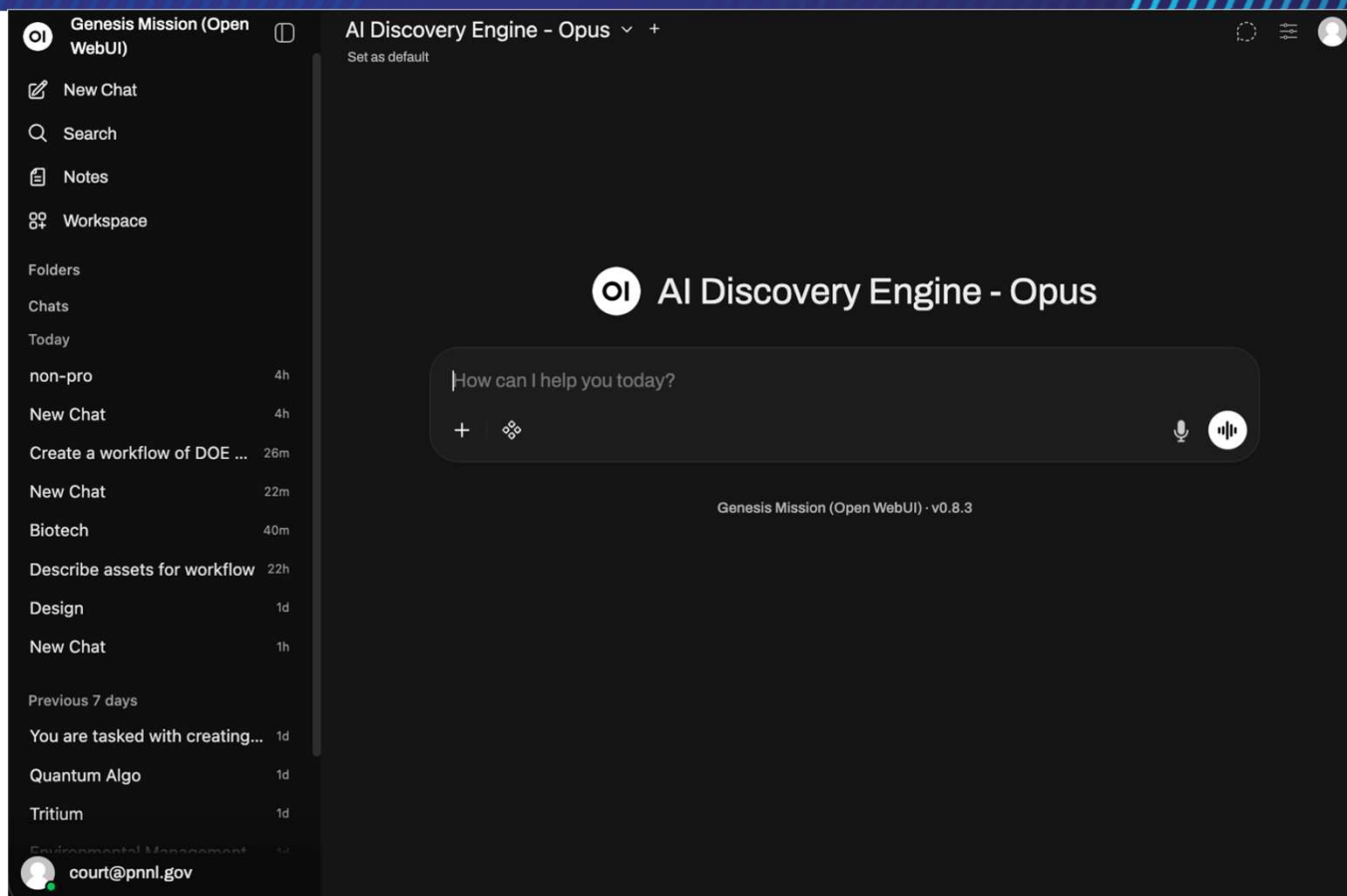
**Developed in partnership with PNNL

Natural language interface to compose and interrogate workflows of DOE and NNSA AI assets to solve national S&T challenges

~300 DOE and NNSA model and agent cards inform that possible workflows

Data and compute resources cards will be incorporated soon

AMSC deployment: to be hosted and operated within the AMSC environment



Establishing Scaling Laws Best Practices for MTs

- MTs are developing AI models where **efficient allocation of compute and data is critical**.
- **Scaling laws predict the performance relationship between model size, dataset size, and compute**.
- **BPSW Neil Getty and BASE Nathan Hodas** are establishing standardized best practices for Scaling Law analysis.
- **Conducted initial viability audit of MTs** using technical reports, model cards, and architecture documentation.
- **Will produce Scaling laws documentation and training materials**.

Tier	Name	Criteria
Tier 1	Scaling-Ready	Custom architecture trained from scratch; large dataset (>1B tokens); parametric code; well-defined loss; baselines available
Tier 2	Data-Scaling Only	Fine-tuning pre-trained models; cannot modify base model size; data scaling viable
Tier 3	Remediation Required / Not Applicable	Unclear metrics, no baselines, hard-coded architecture, workflow team, or not a trainable model

Metric	MTs
Tier 1 (Scaling-Ready)	7 (50%)
Tier 2 (Data-Scaling Only)	5 (36%)
Tier 3 (Remediation/N/A)	2 (14%)
High Confidence	8
Teams with >1B Tokens	6
Teams with De Novo Training	9
Teams Reporting FLOPs	1
Workflow/Agent Teams	2

What to consider in RFA proposals with respect to BPSW integration

Workflow patterns: Proposal can leverage, if relevant, one or more of the workflow patterns identified by BPSW.

Priority tasks: Proposal can focus, if relevant, on one (or more) of the priority tasks to accelerate with AI

Model/Agent Cards: Proposal can produce, if relevant and authorized, Models/Agent cards to include in the resource hub

Leaderboard: Proposal can produce benchmarks that will be included in the leaderboard

Scaling laws: Proposal can leverage the scaling law training material to include projections.

ModCon Core Data Brokers and Standards **DBS**

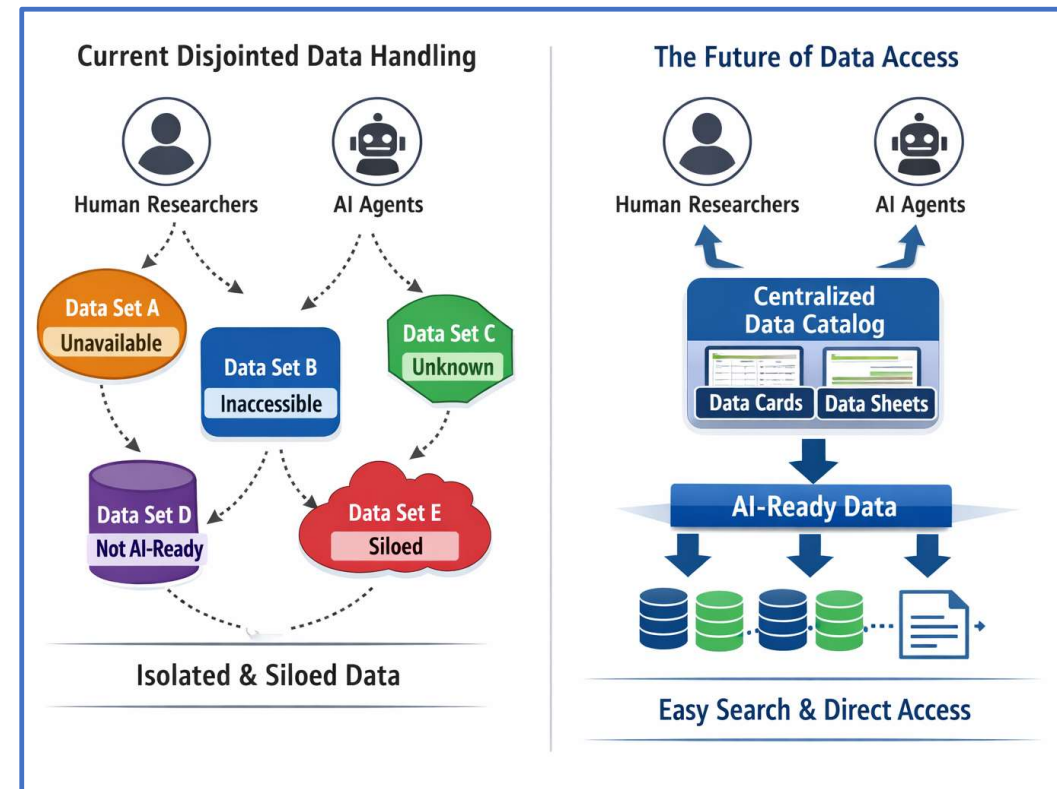


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DBS Enhances the Productivity of Science

DBS addresses current rate-limiters to scientific productivity and security by...

- improving the findability of data and related artifacts for people and agents
- developing secure, trustworthy frameworks for data sharing and publication
- automating data curation for AI-readiness



DBS Tasking

Current DBS work is organized into 5 Tasks:

- Task 1: Register Open, Curated Data in AmSC Catalog
- Task 2: Data Documentation
- Task 3: Curate, Publish, and Register New Data with AmSC
- Task 4: Automate Data Curation
- Task 5: Governance

Task 1: Register Open, Curated Data in AmSC Catalog

- 8 catalogs currently accessible through Genesis Central Catalog containing petabytes of data
- Catalogs and data repositories identified across all scientific domains



GENESIS MISSION
Genesis Central Catalog
8 catalogs indexed - 42.8 PB total known size

Energy Sciences & Technologies | Earth & Environmental Sciences | Life Sciences & Biosciences | Physical & Chemical Sciences | Fundamental & Basic Sciences

CATALOG / REPOSITORY	DOMAIN	ORIGIN URL	SIZE	STATUS
Energy Data eXchange (EDX)	Energy Sciences	https://edx.netl.doe.gov/	583 TB	Yes
Nuclear Research Data System (NRDS)	Energy Sciences	https://nrds.int.gov/	1 TB	Partial
ESS-DIVE	Earth	https://ess-dive.fsl.gov/	13.6 TB	Yes
National Microbiome Data Collaborative	Life Sciences	https://microbiomedata.org/	Unknown	Yes
Environmental Molecular Sciences Laboratory (EMSL)	Life Sciences	https://www.emsl.pnl.gov/	Unknown	Yes
MSDLive	Earth	https://msdlive.org/	190 TB	Yes
SLAC / Linac Coherent Light Source (LCLS)	Physical	https://www.slac.stanford.edu/facilities/lcls/experiments	42 PB	Yes
Fermi National Accelerator Laboratory (FNAL)	Fundamental	https://metacat.fnal.gov/9443/amsc_meta_prod/rep/gul/	39 TB	Yes

Task 2: Data Documentation

- V1 of metadata, data card, and data sheets available for use
- Tools and skills created for data card generation and viewing

Dataset Explorer

TECHNICAL DOCUMENTATION

METADATA

■ **YAML Metadata**

TECHNICAL DOCUMENT

1. Datascard Overview

2. LEVEL 1: Discoverable

3. LEVEL 2: Interoperable and Reusable

4. LEVEL 3: Understandable & Trustworthy

TrackML Particle Identification Dataset

Readiness: Level 3

YAML Metadata

EXPAND ALL

COLLAPSE ALL

■ DATACARD INFO

FILENAMEmodcon_datascard_trackml_particle_identification.md

ID

URL<https://www.kaggle.com/competitions/trackml-particle-identification/data>

DATACARD ACCESS

None - publicly accessible

DATACARD CREATION

CREATED DATE2026-03-02

UPDATE DATE2026-03-02

CREATION METHODhybrid

CREATED BY

ORGANIZATION

Generated via Claude Code datascard-generator skill

DATACARD TEMPLATE VERSION1.0

LANGUAGEen

■ DATA IDENTIFIERS

NAMETrackML_Particle Identification Dataset

Machine usability snapshot (top of datacard)

AI ready	License clarity	Machine access	Checksum / fixity	Semantic context
Yes / No / Conditional	Yes / No	Yes / No	Yes / No	Yes / No

Level 1 — Discoverable	Level 2 — Interoperable & reusable	Level 3 — Understandable & trustworthy
Identification & description - Title & dataset ID required - Persistent identifiers (DOI, handle, URL) required - Files & structure summary required - Dataset description — purpose, scope, context required - Keywords for discoverability - Citation (recommended format) - Dataset readiness level & confidence - Release status & review process - Data modalities, formats, splits	Access, provenance & context - Contact point (person + org) required - Access policy — sensitivity tier, authorization required - License (SPDX ID) required - Security markings — CUI, distribution statement - Science domain & ML task category - Funding & facilities (ROR IDs, grant numbers) - Dataset authors & contributors (ORCID) - Provenance — source data, processing steps, instrumentation - Related datasets, publications, software, AI models - Stewardship & update frequency	Quality, semantics & AI readiness - Data characteristics — variables, schema, missing data handling - Variable table — names, descriptions, units, value labels - Data quality — completeness, known issues, noise, uncertainty - Ontology & schema alignment (e.g., CF conventions, ENVO) - Controlled vocabularies - Integrity & fixity — checksum type, versioning strategy - AI/ML considerations — training/inference allowed, bias risks, safety - Dataset scale — record count, compressed & unpacked size - Data processing — preprocessing, calibration, labeling steps

Readiness levels describe usability & governance — not scientific quality or value.

● Level 1 ● Level 2 ● Level 3 **required** Required field at that level

Metadata v1 Summary

Data Card Viewer

Task 3: Curate, Publish, and Register New Data with AmSC

- AI-Readiness workshop series launched
 - Identify datasets, assist in curation, certify for Genesis Mission use

UNTAPPED DATA IDENTIFIED FOR AI READINESS

BNL image data
Brookhaven Natl. Lab
~500 PB

Dynamic protein structures
ALS — cryogenic imaging
~100 TB

RNA modification data
Modification detection protocols
~10 TB

Plant phenotyping + cryoEM
LiDAR, images, unanalyzed cryoEM
>1 PB

More datasets
To be identified via workshops
TBD

AI READINESS WORKSHOP PIPELINE

Datasets identified

Inventory of untapped GM data built

Ongoing

Workshop series launched

Engaging data owners to define needs

In progress

AI readiness specs drafted

Requirements defined per dataset

Up next

AI readiness certified

Data cards, metadata, lineage applied

Planned

National challenge use

Searchable, API-accessible, AI-ready

Planned

■ Complete / active ■ Current focus ■ Planned *None of these datasets are currently in use by model teams — this pipeline unlocks them.*

Task 4: Automate Data Curation

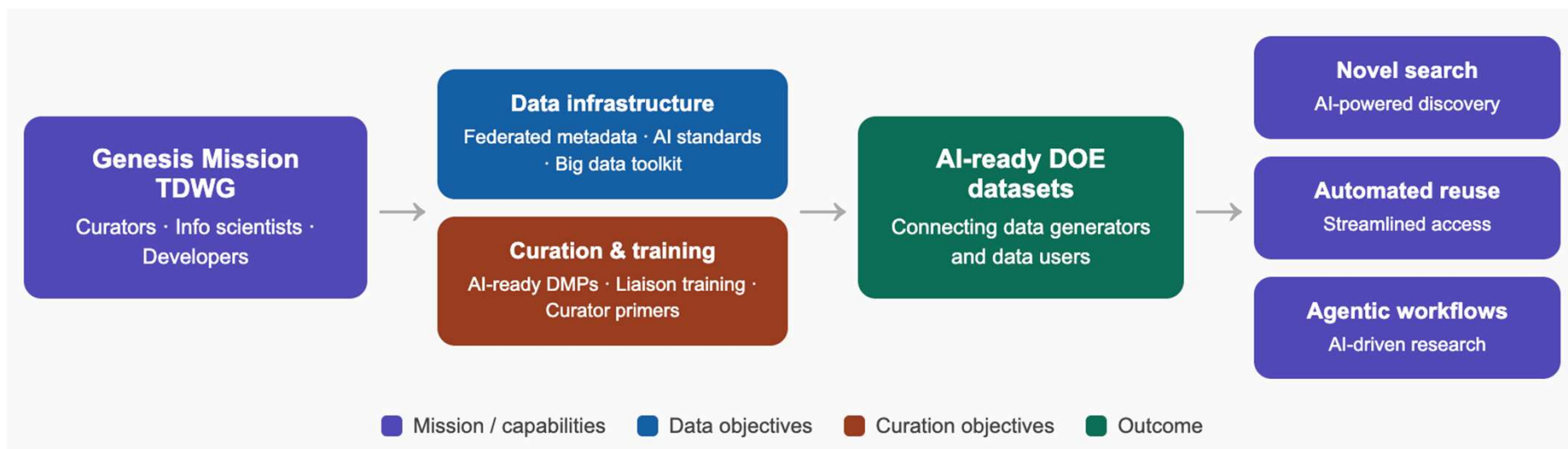
- Testing AI-readiness assessment tools on registered data to inform tool choice and usage

Tool	Python API	CLI Interface	Tabular Data	Scientific / Domain Formats	Distributed Processing	Data Quality Metrics	FAIR Compliance Assessment	Fairness / Bias Metrics	Privacy Metrics	Custom Metrics / Extensions	Automated Data Transformation	LLM / AI-Assisted Features	Metadata / Schema Management	Multi-dataset / Batch Support	GPU Acceleration	Domain Agnostic
YData Profiling	Yes	Yes	Yes	No	Partial	Yes	No	Partial	Yes	Partial	No	No	No	No	No	Yes
Evidently	Yes	No	Yes	No	No	Yes	No	No	No	Yes	Partial	Yes	No	Yes	No	Yes
Anemol-datasets	Yes	Yes	No	Yes	Yes	No	No	No	No	Partial	Yes	No	Yes	Yes	No	No
PhysicsNeMo Curator	Yes	Yes	No	Yes	Partial	Partial	No	No	No	Yes	Yes	No	No	Yes	Yes	No
NVIDIA NeMo Curator	Yes	Partial	No	No	Yes	Partial	No	No	Yes	Yes	Yes	Yes	No	Yes	Yes	Partial
draviz	No	Yes	N/A	No	N/A	No	No	No	No	Partial	No	No	No	Partial	No	Partial
DREAMER	Yes	No	Yes	No	Partial	Yes	No	No	No	No	Yes	No	No	No	No	Partial
Great Expectations	Yes	Yes	Yes	No	Partial	Yes	No	No	No	Yes	No	No	Yes	Yes	No	Yes
Soda Core	Yes	Yes	Yes	No	Yes	Yes	No	No	No	Yes	No	No	Yes	Yes	No	Yes
F-UJI	Yes	No	No	No	No	No	Yes	No	No	Yes	No	No	Yes	No	No	Yes
AIDRIN	Yes	Yes	Yes	Yes	Partial	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Partial	No	No	Yes
DSAGT	No	Yes	Yes	Yes	No	No	No	No	No	Yes	Yes	Yes	Partial	Yes	No	Yes
Bridge2AI	No	No	No	No	No	No	Yes	Yes	Partial	Partial	No	No	Yes	N/A	No	No
REDI	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	Partial	Yes	Yes	Yes	Yes	Yes	No	Partial

* Table generated by Sonnet based on collected report from the evaluation by the team. Missing or undocumented information might introduce mismatching results. Some tools are under heavy development (e.g., DSAGT, AIDRIN, REDI) or have not been published yet (e.g. REDI).

Task 5: Data Governance

- Established a Technical Data Working Group, in conjunction with partnerships teams
- TDWG is establishing federated metadata harvesting, AI-centric ontologies, FAIR-aligned infrastructure, best practices for data management plans, and specialized training and documentation to support AI-driven research



Putting it all together: Document-based search, access, reuse

Transforms DOE datasets into AI-ready resources by **centralizing access to metadata, datacards, and datasheets** and establishing clear standards and policies for data usage.

Bridges data generators and data users and enables:

- Novel search capabilities
- Automated access and reuse
- Integration into agentic workflows

metadata

- Highly structured (JSON, XML, RDF)
- Often standardized fields
- Possible to automated
- Enables data to be found, indexed, managed, and understood by software systems/AI

agent cards

model cards

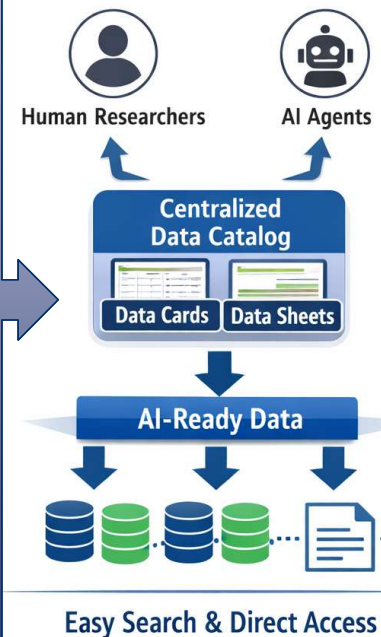
datacard / README

- Introduces and explains dataset background, context, organization & file structure, data details, methodological info, access & reuse
- Possible to automated
- Human & AI-readable
- Adjacent to files in the data repo
- Published & unpublished datasets

datasheet

- Comprehensive documentation of creation, scope, intended use, limitations, & ethical/technical considerations
- Intentionally human-written (possibilities to automate an initial draft)
- Capture tacit information & community knowledge
- Enables frontier models to leverage rich, unstructured dataset information
- For published, **elite** datasets

The Future of Data Access



DBS Members

DBS Leads

Laura Biven JLab
Jeren Browning INL
Ray Grout NLR

Genesis Data Pillar Leads

Ana Kupresanin LBNL
Dana Grisham SNL

Le	Chen	ANL
Nicholas	Schwarz	ANL
Rajeev	Thakur	ANL
Yi	Huang	BNL
Yihui (Ray)	Ren	BNL
Adam	Lyon	FNAL
Oliver	Gutsche	FNAL
Victor	Walker	INL
Brad	Sawatzky	JLAB
Diana	McSpadden	JLAB
Jai	Sachdev	PPPL
Jean Luca	Bez	LBNL

Kjiersten	Fagnan	LBNL
Sam	Blau	LBNL
Kelly	Rose	NETL
Nick	Wunder	NLR
Ray	Grout	NLR
Steven	Spurgeon	NLR
Struan	Clark	NLR
Ana	Gainarua	ORNL
Christian	Engelmann	ORNL
Mayanka	Chandra Shekar	ORNL
Olga	Kuchar	ORNL
Chitra	Sivaraman	PNNL
Terao	Kazuhiro	SLAC
Lindsay	Roy	SRNL

DBS Liaisons for each Model Team

Accelerating Scientific Discovery through AI-Driven Code Development	Diana McSpadden
AI Driven Co-Design for Microelectronics	YQ Chen
AI for Efficient Quantum Algorithms	Le Chen
AI for Planning and Operation of the US Power Grid	Chitra Sivaraman
AI Foundational Model Transforming Combustion Science and Technology for Energy and National Security	Lindsay Roy
America's AI Revolution Transforms Scientific Discovery at the Speed of Light	Nicholas Schwartz
CM ² US: Critical Minerals and Materials to Unlock Supply	Steven Spurgeon
FAMOUS: Foundational AI Models for Optimizing and Understanding Biological Systems	Kjiersten Fagnan
From Quarks to Cosmos through the Lens of AI	Brad Sawatzky and Terao Kazuhiro
Fusion-FM: A Foundational Model for Magnetic Confinement Fusion	Jai Sachdev
MAIQMag: Multimodal AI for 2D Quantum Magnets	Yihui Ren
MOAT: Multi-Office Particle Accelerator Team	Yi Huang
PROMETHEUS: A Revolution in Design and Operation of Nuclear Power Plants	Victor Walker
Specs-to-Silicon Microelectronics in Extreme Environments for Transformative Science	Adam Lyon

ModCon Core Intellectual Property & Partnership Formation

IPPF

April 3, 2026



U.S. DEPARTMENT of ENERGY

Background

Intellectual Property and Partnerships

Team (IPPF or P3)

Partnerships (INL-led)

IP and Agreements (ANL-led)

Partnerships Team Focus

Partner alignment with labs

Cross-lab coordination

Intellectual Property (IP) and Agreements

Team Focus

Responsive to EO section 5(c)(i) and (ii)

Model Agreements for industry collaborators

Inter-lab alignments (“Virtual Lab”)

Requirements for non-open data protections

Master Scope of Work

LAUNCHING THE GENESIS MISSION

Executive Orders | November 24, 2025

(c) The Secretary, in coordination with the APST and the Special Advisor for AI and Crypto, shall establish mechanisms for agency collaboration with external partners possessing advanced AI, data, or computing capabilities or scientific domain expertise, including through cooperative research and development agreements, user facility partnerships, or other appropriate arrangements with external entities to support and enhance the activities of the Mission, and shall ensure that such partnerships are structured to preserve the security of Federal research assets and maximize public benefit. To facilitate these collaborations, the Secretary shall:

(i) develop standardized partnership frameworks, including cooperative research and development or other appropriate agreements, and data-use and model-sharing agreements;

(ii) establish clear policies for ownership, licensing, trade-secret protections, and commercialization of intellectual property developed under the Mission, including innovations arising from AI-directed experiments;

(iii) implement uniform and stringent data access and management processes and cybersecurity standards for non-Federal collaborators accessing datasets, models, and computing environments, including measures requiring compliance with classification, privacy, and export-control requirements, as well as other applicable laws; and

DOE/Genesis-level Partnerships

- Genesis Mission teams are strongly encouraged to work with industry, academia, and public-sector partners
- Partnerships can take many forms: data/model sharing, collaborative R&D, in-kind contributions on shared tasks, etc., and range from Genesis-wide to individual PIs.
- PIs are encouraged to work with their local lab tech-transfer office to understand partnering process and scope of agreements

DOE/Genesis-level Consortium

- The Genesis mission consortium established to manage public-private partnerships
- DOE has signed MOUs with 26 partners to be initial consortium members.
- Non-members can also participate in consortium, including partner-matching

Anthropic	Dell Technologies
OpenAI	Accenture Federal
Google	Services
Microsoft	Cerebras Systems
Amazon Web	Groq
Services	CoreWeave
Oracle	DrivenData
NVIDIA	Armada Systems,
Intel	Inc.
Advanced Micro	Periodic Labs, Inc.
Devices	Radical AI, Inc.
IBM	XPRIZE Foundation,
Hewlett Packard	Inc.
Enterprise	Project Prometheus

IP and Agreements – Accomplishments

External - DOE approved agreements

- SOW template (short 1.5 pager) – first step toward an agreement between MT and industry (contact your MT P3 POC)
- AI Agreement for Open Science Projects
- Agreement for AI Projects (non-open data / science)
 - Project Data Use Addendum (to handle proprietary / sensitive project data)
- 1-page NDA for initial project discussions between labs and companies
- Bridge Agreement (for anticipated PIA funded projects)
- Lab's existing agreements may be used

Inter-lab Collaboration Mechanisms

- Virtual Lab Teaming Framework – all 17 labs aligned
- Intellectual Property (IP) Advisory Committee to identify, coordinate, and support tech transfer and IP matters
- Data Use Plan (DUP) for MT projects (in coordination with Data team)
 - Ensure project work's deployment per mission objective
 - Lower risks of unauthorized data use / release
- Genesis Master Scope of Work (MSW) - eliminates local site office approvals for domestic Genesis agreements
- Blanket approval on Project Data protection (requested, with DOE IPL)
- Inter-lab project 1-pager (links Project Lead Lab to other Project Labs)

IP and Agreements – What's next

Current developments

- Internal and partner discussions started
- Records of partnerships and potential partnerships being developed
- MTs developing statements of work to establish agreements
- Data tracking and protections discussions started; joining DBS and Data Team discussions

Next steps

- Labs to sign Genesis consortium agreement
- Convert aligned SOWs to agreements
- Proliferate MSW across labs
- Continue identifying ways to reduce duplicative efforts (e.g., DOE reviews, foreign vetting)

P3 POCS IN MODEL TEAMS

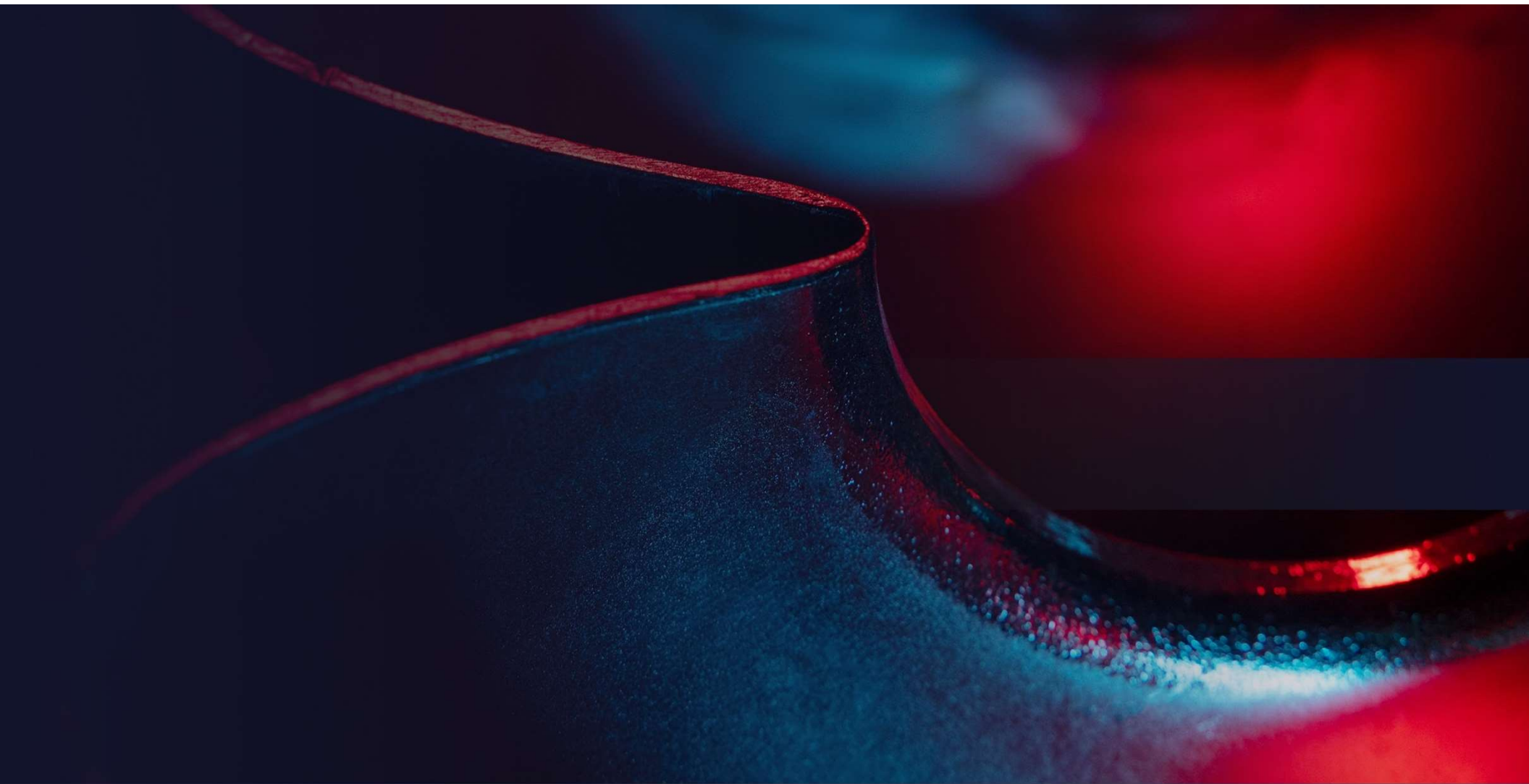
Seed Model Teams (MTs)	P3 POC	P3 POC Email Address
AI-Driven Code Development	Charlie Catlett, Demetra Adrahtas, Christina Lomasney	catlett@anl.gov, dadrahtas@anl.gov, christina.lomasney@pnnl.gov
AI Driven Co-Design for Microelectronics	Charlie Catlett, Phil Smith	catlett@anl.gov, pesmith@anl.gov
AI for Efficient Quantum Algorithms	Charlie Catlett, Phil Smith	catlett@anl.gov, pesmith@anl.gov
AI for the US Power Grid	Ray Grout, Eric Payne	ray.grout@nrel.gov, eric.payne@nrel.gov
Combustion Science and Technology	Charlie Catlett, Hemant Bhimnathwala	catlett@anl.gov, hbbhimnathwala@anl.gov
Scientific Discovery at the Speed of Light	David Martin, Peter Nugent, Gail Chen, Sebastian Ainslie	demartin@lbl.gov, penugent@lbl.gov, gailchen@lbl.gov, sainslie@lbl.gov
CM ² US	Charlie Catlett, Maricely Ramirez, Julianne Krennrich	catlett@anl.gov, mrhernandez@anl.gov, jmkrenn@ameslab.gov
FAMOUS	Christina Lomasney-Mattis, Paul Rigor	christina.lomasney@pnnl.gov, paul.rigor@pnnl.gov
From Quarks to Cosmos	Charlie Catlett, Peter Nugent, Ilya Kats	catlett@anl.gov, penugent@lbl.gov, ikats@anl.gov
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MAIQMag:	Shaun Gleason	gleasonss@ornl.gov
MOAT:	David Martin, Peter Nugent, Gail Chen, Sebastian Ainslie	demartin@lbl.gov, penugent@lbl.gov, gailchen@lbl.gov, sainslie@lbl.gov
Prometheus:	Jason Hales, Jason Stolworthy	jason.hales@inl.gov, jason.stolworthy@inl.gov
Specs-to-Silicon Microelectronics	Whitney Hastings, James Amundson	whasting@fnal.gov, amundson@fnal.gov



Genesis Mission



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