December 10, 2025

Casey Icenhour, PhD
Computational Scientist
Casey.Icenhour@inl.gov

Bringing together integrated simulation, surrogates, and data to support digital twins for fusion engineering

IAEA Workshop on Digital Engineering for Fusion Energy Research 2025

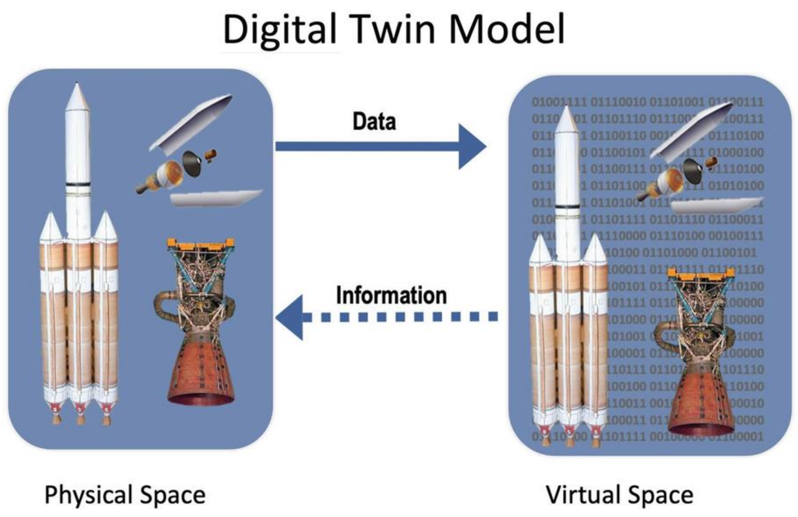
*Co-authors**: Pierre-Clément Simon, April Novak (UIUC), Corey DeChant, Cody Permann, Adriaan Riet, Matthew Anderson, Bradlee Jensen, Jeren Browning, Raffi Nazikian (General Atomics), Pattrick Calderoni*
***External affiliation noted where appropriate*

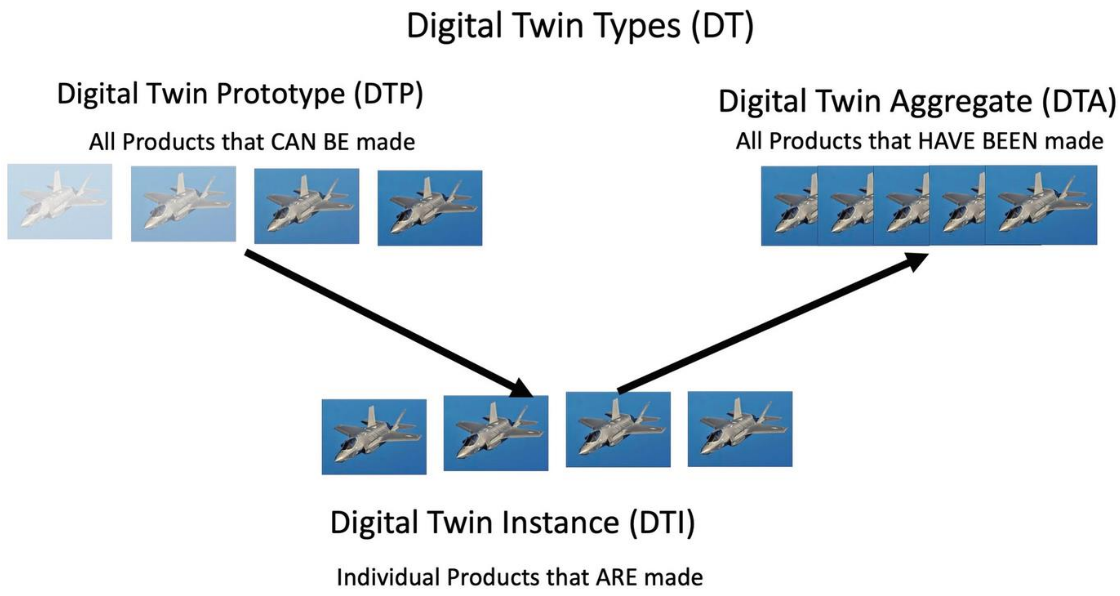
INL/CON-25-88100

Idaho National Laboratory

Digital Twin Development for Fusion

- Per Grieves, a DT should have three main elements:
    1. An actual or intended physical element (the ”Physical Twin” [PT]),
    2. A virtual or digital counterpart (the DT itself), and
    3. A communication channel of data and information between the two elements.
- As in aerospace (and many other fields!), executing on fusion requires immense amounts of data and interconnected systems.
    - Problem: Data from physical space is relatively sparse and hard to connect to form bases for DTPs.
    - Solution: Data aggregation (from exp. and sim.) and processing pipelines (for sim. and AI/ML) are essential to establishing both a DT and eventual PT on the timescales required.





Images: Grieves (2023) https://doi.org/10.1007/978-3-031-21343-4_4

Let's create data ecosystems for fusion to speed the development of DTs!

- Scale of the challenge and worldwide reach of the fusion community means we need a wide-ranging collaborative effort…
- …including validated, portable, simulations…
- …based on FAIR principles…
  - Findability
  - Accessibility
  - Interoperability
  - Reuse
- …and federating with established open databases and resources (e.g., NRDS, MatDB4Fusion).

Image Credit: General Atomics, nVidia

How are we working to push toward a digital twin?

- Modeling and Simulation
  - MOOSE
  - MOOSE Physics Modules
  - TMAP8, SALAMANDER, Cardinal, Zapdos
- Data Lake / Digital Engineering Toolbox (DeepLynx Nexus)
- Data Archives and Repositories (NRDS, FSP Archive)
- U.S. DOE FIRE Collaboratives
  - Blanket Nuclear Testing (BNT)
  - Blanket Component Test Facility (BCTF)
  - Solution-Oriented Workflow for Integrated Fusion Technology in Plasma-Facing Components (SWIFT-PFCs)
  - Fuel Cycle (FC) FIRE
  - **Fusion Energy Data Ecosystem and Repository (FEDER)**

MOOSE

Zapdos

SALAMANDER

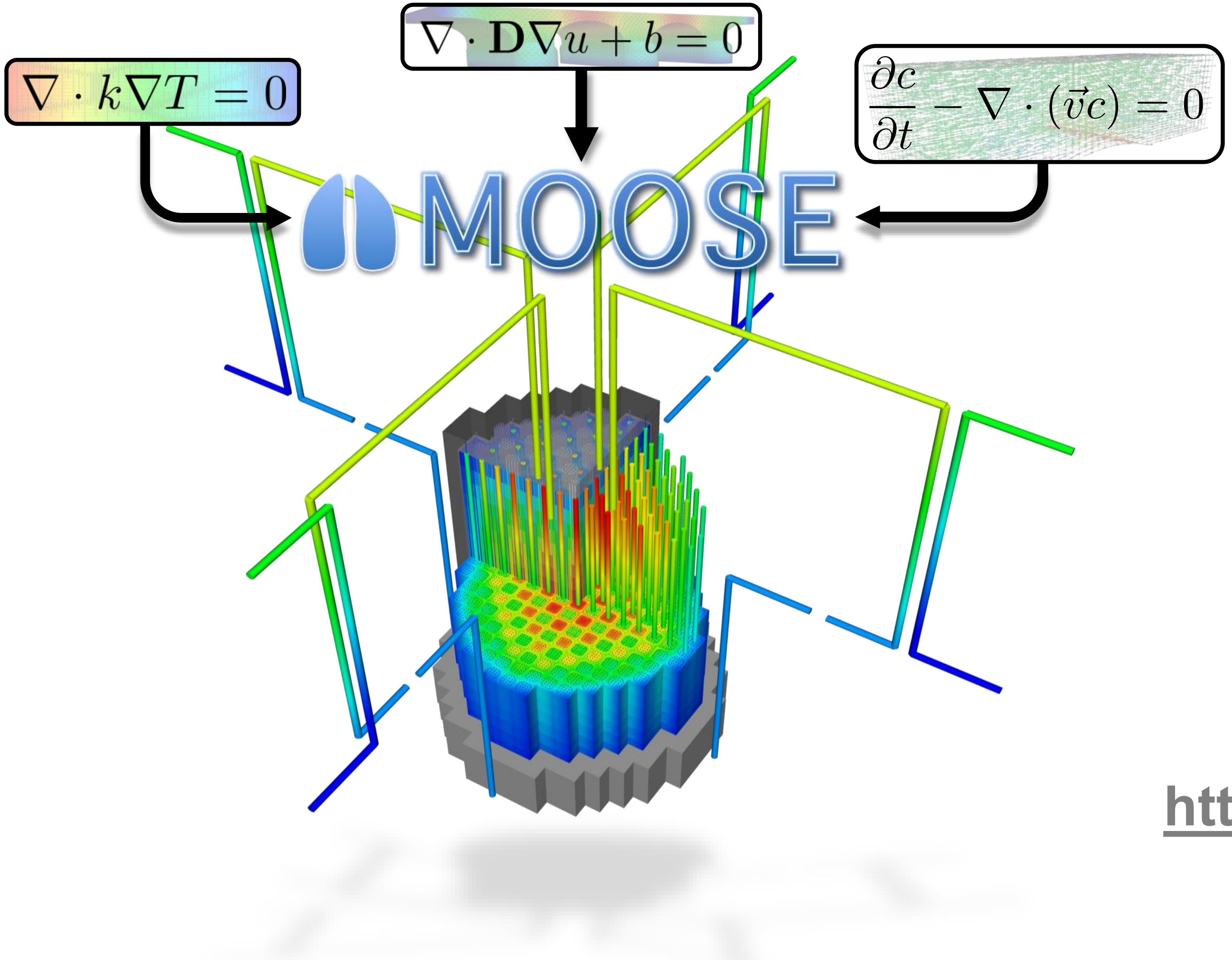
Cardinal

TMAP8

DeepLynx

FC FIRE

MOOSE Accelerates Development of High-Fidelity Modeling and Simulation Tools



What is MOOSE?

- Multiphysics
- 26 Physics, Solver, and Numerics Modules
- Open-source
- Laptop-to-HPC
- Flexible, modular
- NQA-1 Software Quality Assurance

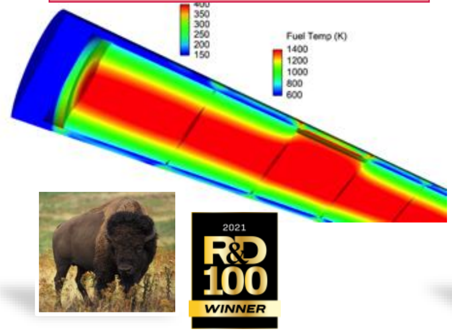
https://mooseframework.inl.gov

Accelerating Advanced Fission Reactor Deployment

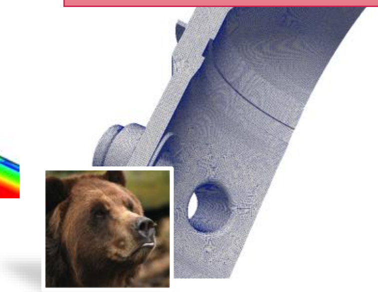
NEAMS

Accelerating Advanced Fission Reactor Deployment

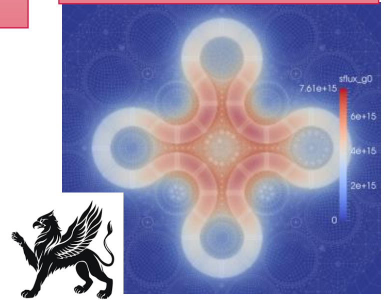
BISON
Nuclear Fuel Performance



Grizzly
Structural Mechanics for Component Aging

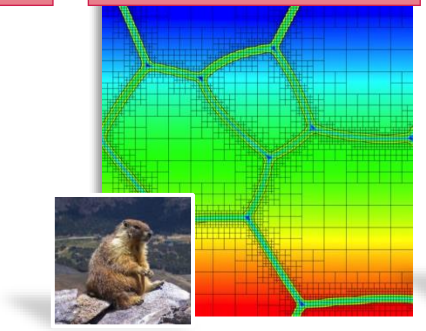


Griffin
Radiation Transport

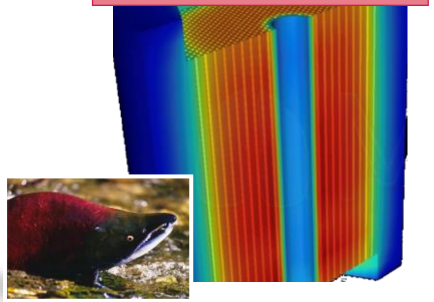


Pronghorn
Medium-fidelity CFD

Marmot
Mesoscale Materials



Sockeye
Heat pipe Simulation



U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

Kairos Power

RADIANT

Westinghouse

BWXT
Nuclear Energy Canada Inc.

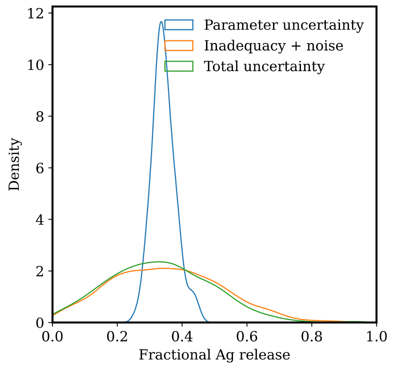
Structural Integrity Associates, Inc.®

EPRI

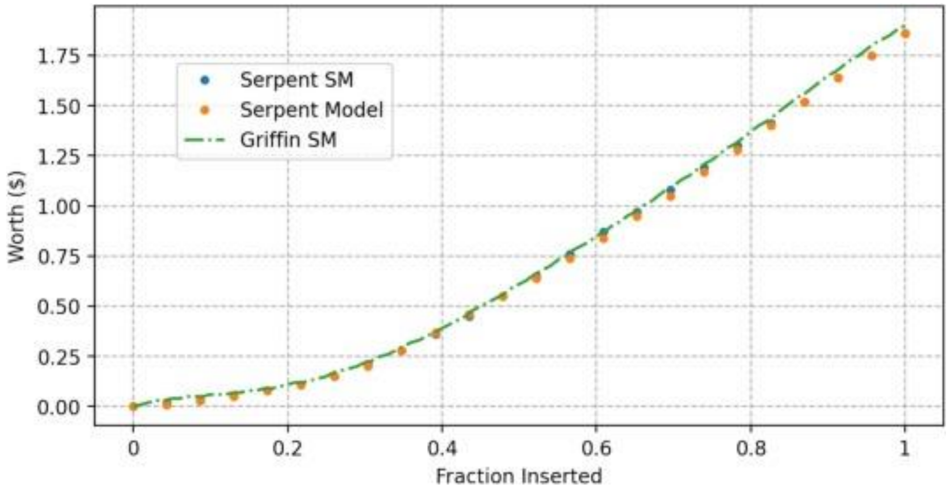
Example of impact:
Kairos Power release version 1.0.0 of KP-BISON, based on INL's BISON, used in support of NRC licensing of Hermes/Hermes 2 fission reactors

MOOSE Stochastic Tools Module (STM) enables surrogates and UQ for nuclear systems

- Provides a **MOOSE interface** for performing stochastic analysis on MOOSE-based models.
- Allows one to sample parameters, run applications, and gather data that is both **efficient** (memory and runtime) and **scalable**
- Performs uncertainty quantification (UQ) and sensitivity analysis with **distributed data** with **advanced variance reduction** methods
- Allows training of metamodels to develop fast-evaluating **surrogates** of a high-fidelity multiphysics model
  - Harnesses advanced machine learning capabilities through the C++ front end of Pytorch
  - Uses active learning models for building surrogates
- Provides a **pluggable** interface for these surrogates
- In the example on the right, an AGN-201 reactor design (more on this) and the Griffin neutron transport code were used as the basis for surrogate model development within the MOOSE STM



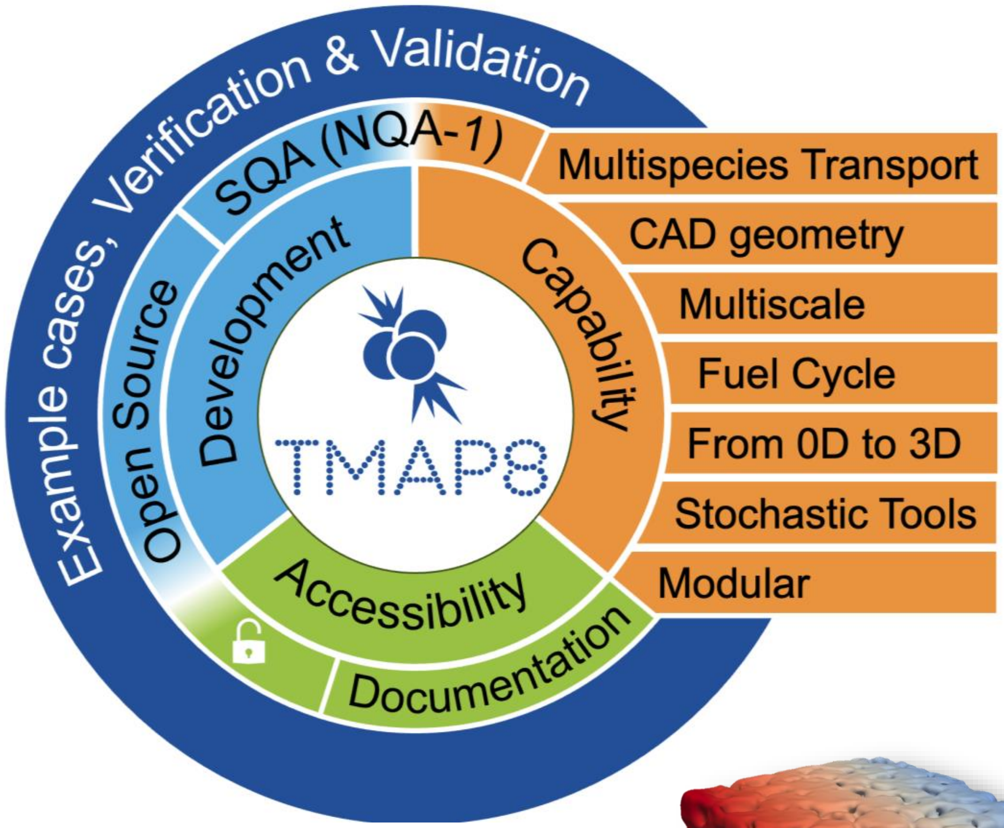
(Left) UQ on modeling Tristructural Isotropic (TRISO) particle Ag release.



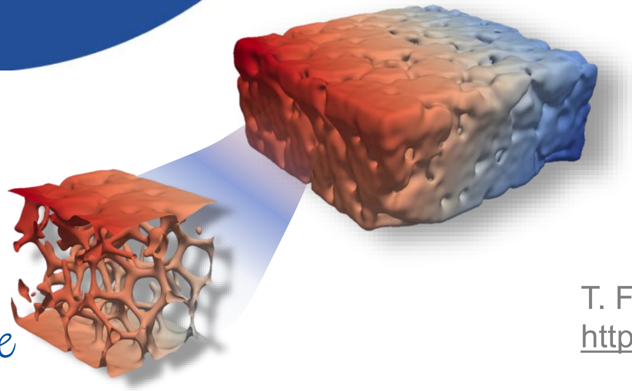
(Above) Coarse rod worth comparison between a Serpent model, Serpent surrogate model, and Griffin surrogate model. The Griffin surrogate is 7^{th}-order polynomial chaos surrogate trained on Latin-hypercube training sample containing 512 points.

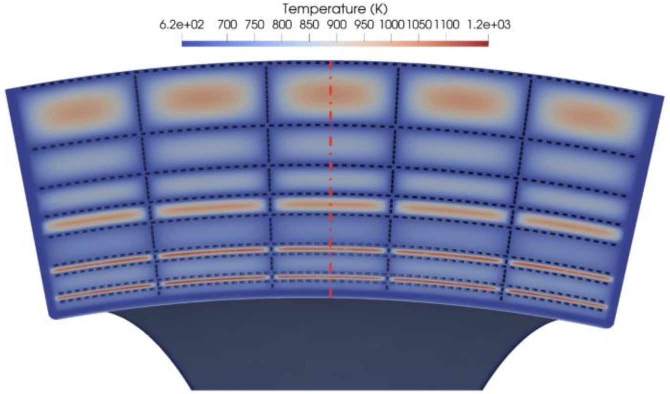
Stewart, et al. *Annals of Nuclear Energy,* **213**. 2025. https://doi.org/10.1016/j.anucene.2024.111041

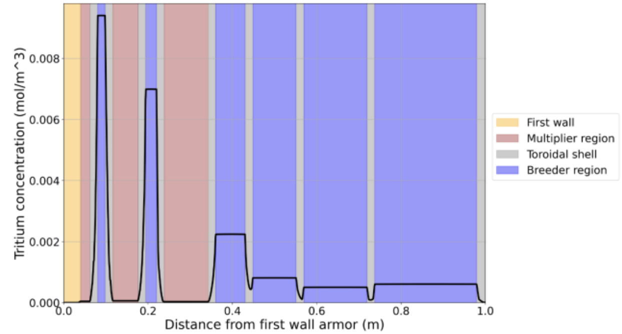
TMAP8, the MOOSE-based version of TMAP



- TMAP8, through its basis on MOOSE, enables multi-fidelity, multi-scale (pore-scale to system-scale), 3D, multispecies, multiphysics simulations of tritium transport, and offers massively parallel capabilities.
- Open-source, Nuclear Quality Assurance level 1 (NQA-1) compliant, and licensing (LGPL 2.1) enables public-private collaboration.
- 37 (and counting) V&V cases and examples available online





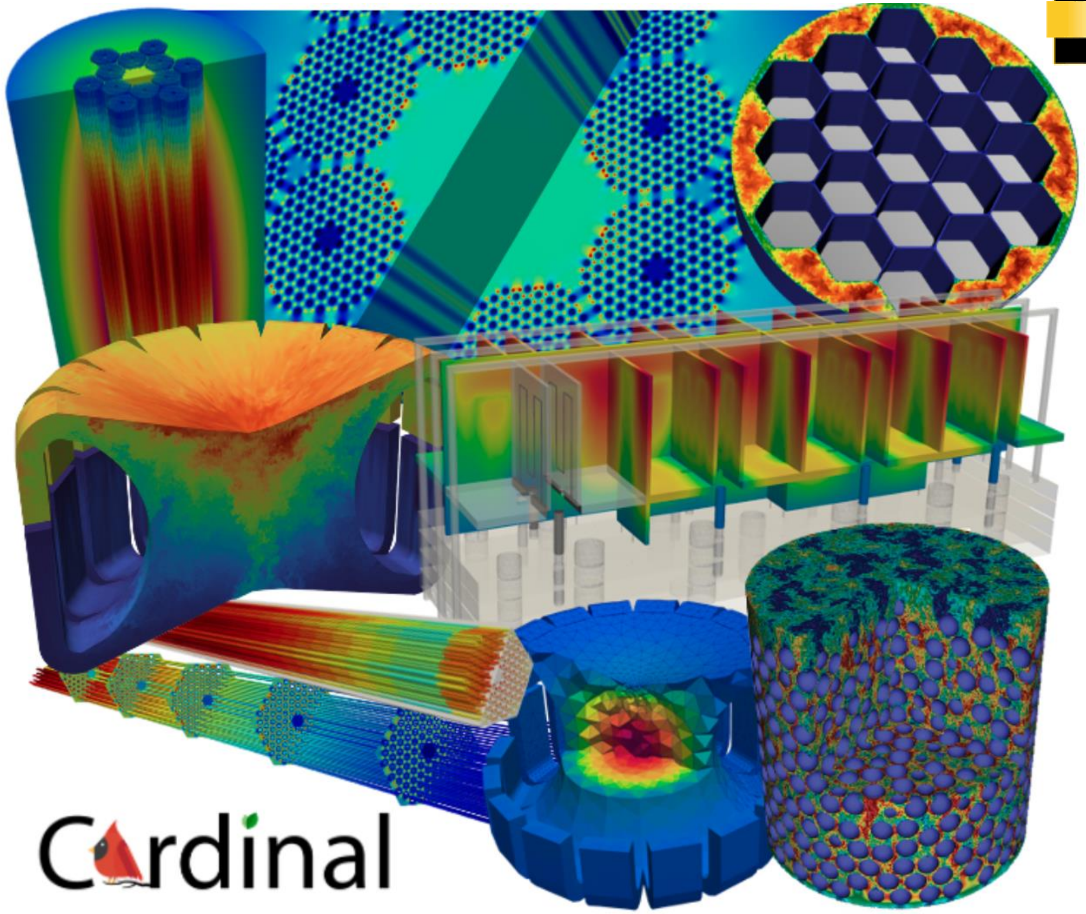


Website

T. Franklin et al., Fusion Engineering and Design, Volume 218, 2025, 115128. https://doi.org/10.1016/j.fusengdes.2025.115128.

Cardinal: Exascale Fission and Fusion Simulation

- Cardinal: MOOSE+OpenMC+NekRS
- Open-source showcase for coupling non-MOOSE-based applications
  - “MOOSE wrapping” feature used
- Many applications in fission, utilized in fusion most recently in breeder blanket module simulations with UKAEA (middle right in figure)
- Notably, used 27k GPUs on Summit HPC system (ORNL) to simulate a full pebble-bed reactor (350k pebbles)
- See April Novak’s Talk, **12/11, 9:55 AM**



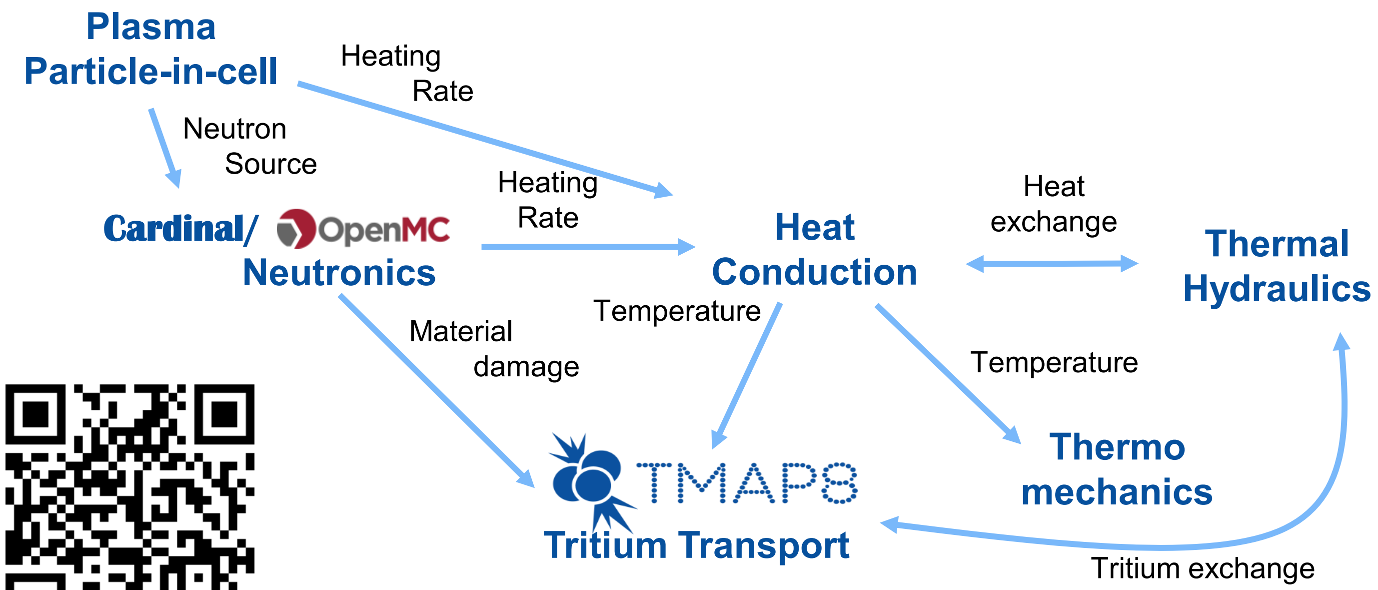
Cardinal Applications. Top row: neutron transport, fluid flow, and heat transfer in a gas-cooled microreactor; large eddy simulation in the core of a sodium fast reactor. Middle row: neutron transport and large eddy simulation in a molten salt fast reactor; coupled neutron-photon transport and heat conduction in a tritium breeder blanket module from the EU DEMO fusion plant. Bottom row: fluid flow and neutron transport in a high temperature gas reactor; fission heating simulated in a Computer Aided Design (CAD) geometry; large eddy simulation in a pebble bed reactor with 1568 pebbles.

Novak, A. J., et al. "Coupled Monte Carlo and thermal-fluid modeling of high temperature gas reactors using Cardinal." *Annals of Nuclear Energy* 177 (2022): 109310.

Novak, A. J., et al. "Multiphysics Coupling of OpenMC CAD-Based Transport to MOOSE using Cardinal and Aurora." *M&C 2023*.

Software for Advanced Large-scale Analysis of MAgnetic confinement for Numerical Design, Engineering & Research

SALAMANDER

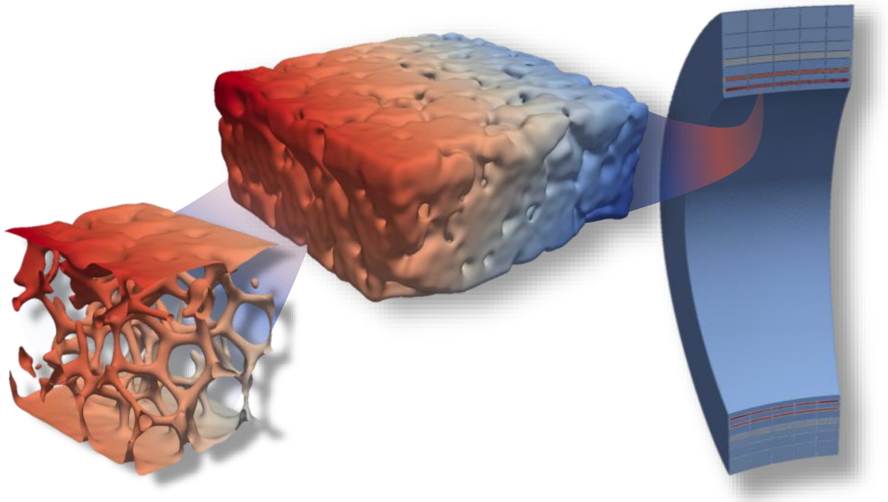


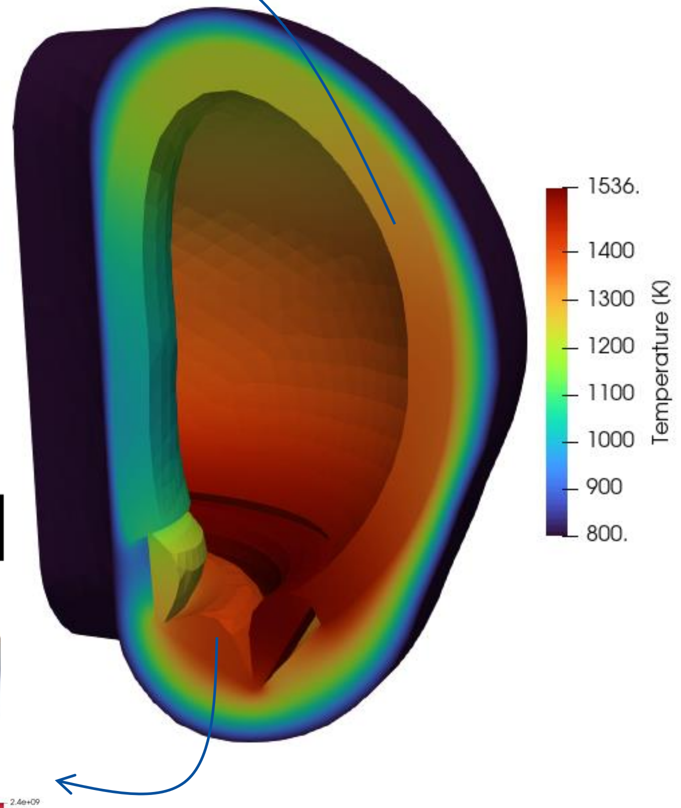
SALAMANDER is designed to perform multiphysics simulation and capture interactions between these physics.

Website

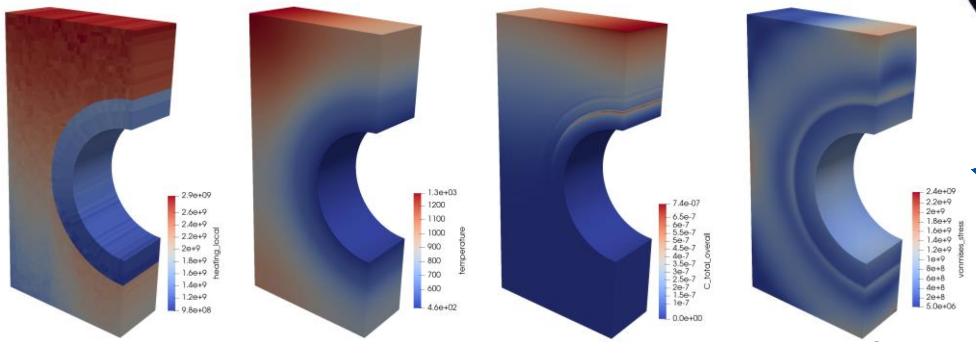
- SALAMANDER is an open-source MOOSE-based application that integrates multiphysics capabilities for multi-fidelity calculations of fusion materials, components, and systems.
- It inherits MOOSE features and contains fusion-specific capabilities.
- SALAMANDER is being developed to support design, engineering studies, and research efforts.

SALAMANDER-driven workflow for blanket design and evaluation





TMAP8 SALAMANDER Cardinal



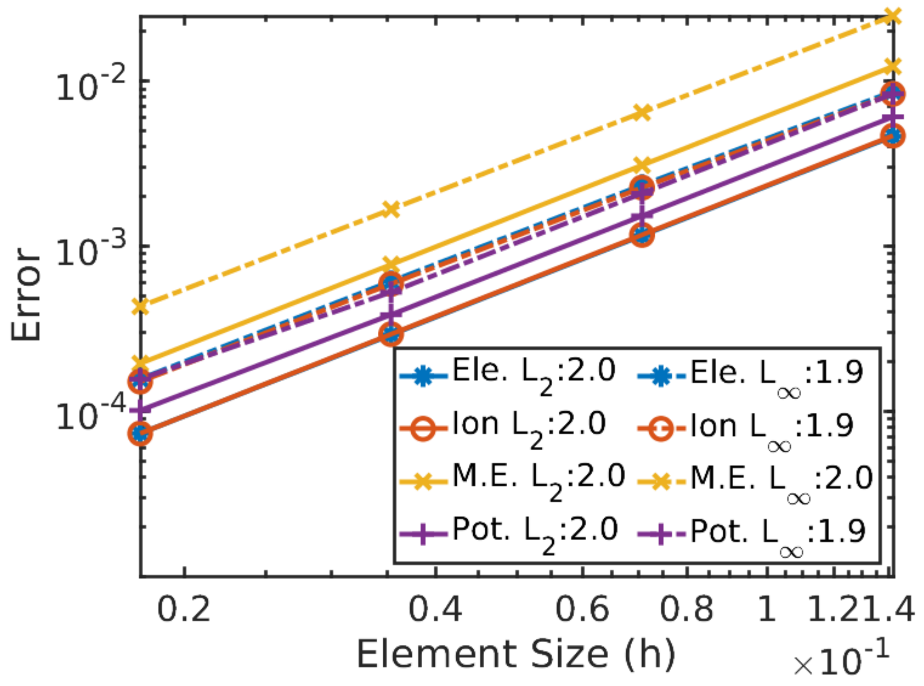
Volumetric heating rate from neutronics (J/m^{3}s) | Temperature (K) | Tritium concentration (atomic fraction) | Von Mises Stress (Pa)

- Integrated modeling and simulation studies are under development for connecting simulation insights across multiple scales and physics regimes.
- Tritium transport (TMAP8), neutronics (Cardinal/OpenMC), thermal hydraulics, heat conduction, and mechanics together bring a more holistic view of the performance and lifetime of a blanket module.
- See PC Simon’s Talk, **12/12 at 9:30 AM** for more detailed information about SALAMANDER!

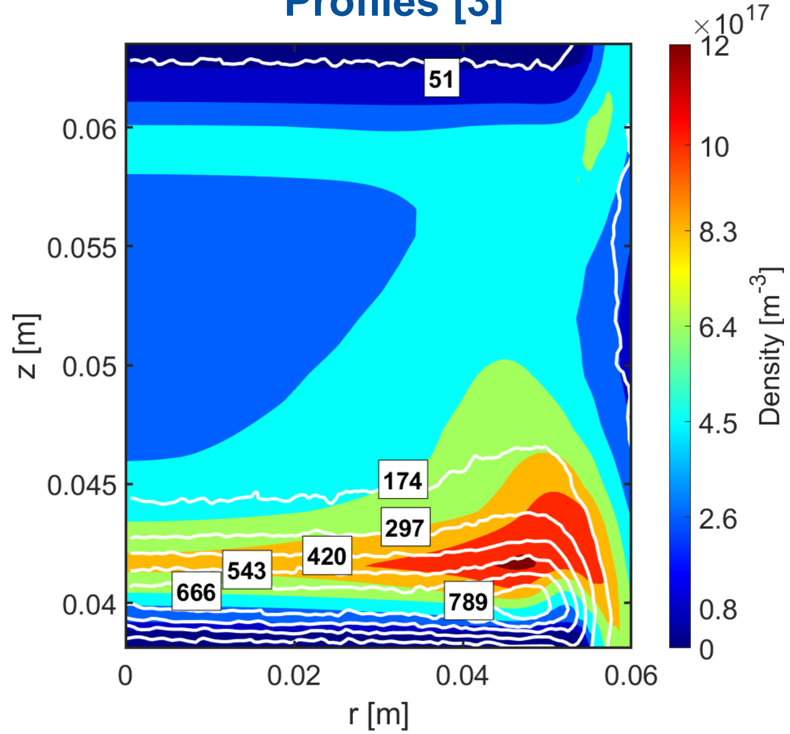
Multi-Fluid Plasma Code: Zapdos

- Zapdos is an open-source multi-fluid plasma code originally developed by Alex Lindsay to investigate plasma-water interfaces for DC discharges at atmospheric pressure [2].
- Zapdos is developed using thorough verification and validation practices for low-temperature plasma (both DC and microwave) [3].

Verification of Code Using Method of Manufactured Solutions (MMS) [3]



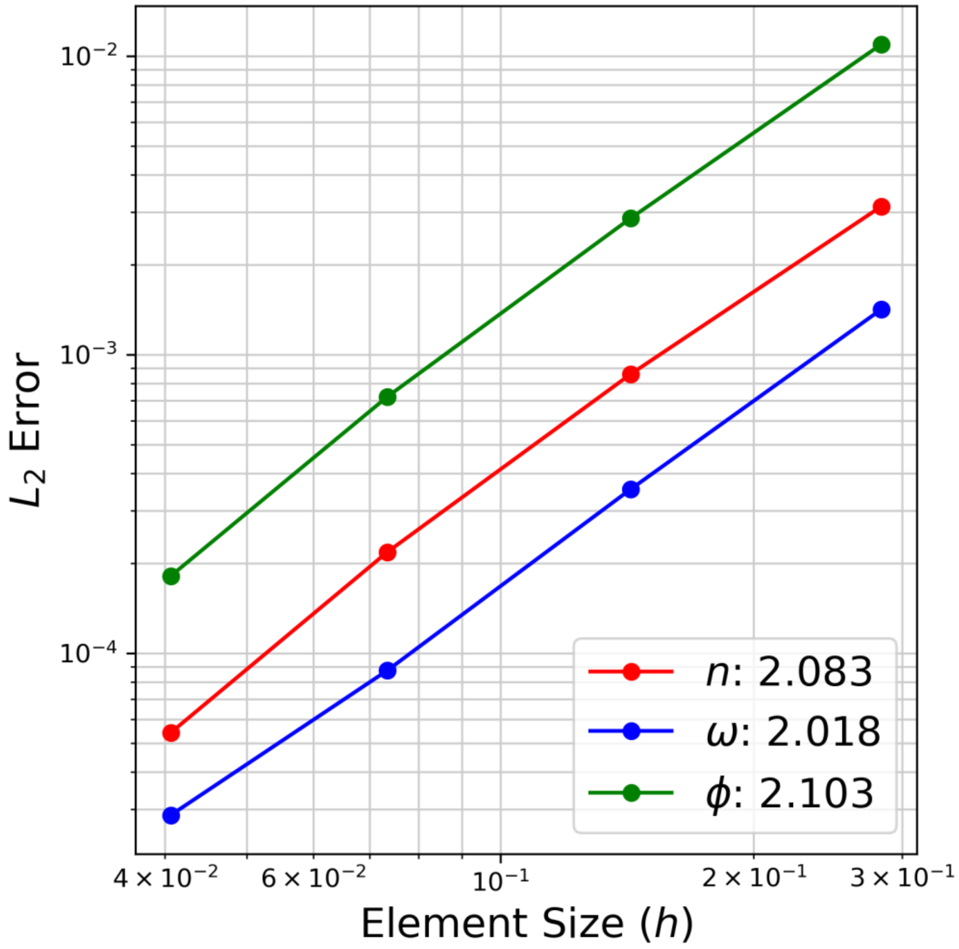
Experimental Validation of Metastable Profiles [3]



[2] Alexander D Lindsay et al. 2016 *J. Phys. D: Appl. Phys.* **49** 235204
[3] Corey DeChant et al. 2023 *Computer Physics Communications* **291** 108837

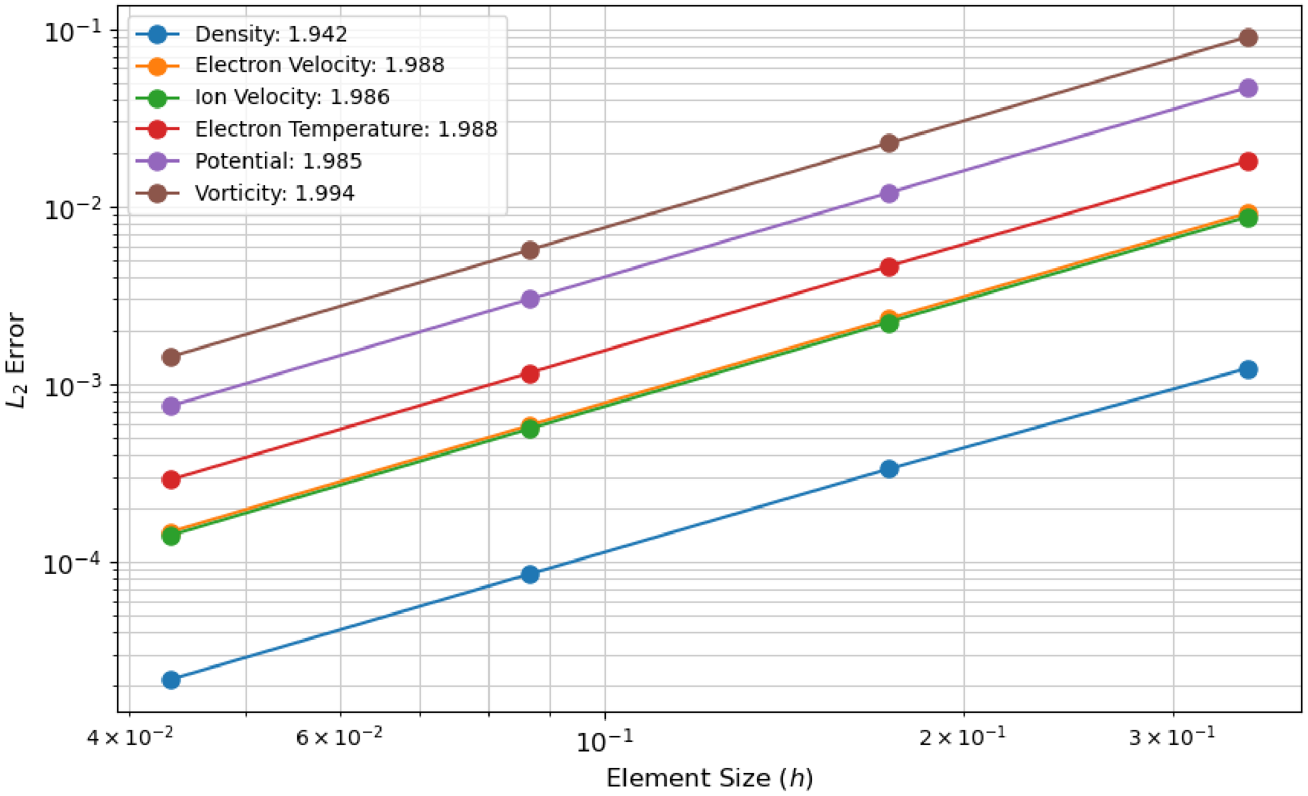
Verification of 2D Hasegawa-Wakatani Model

- New magnetic operators were introduced into Zapdos and tested individually.
- To test the integration of these operators, a simplified 2D model was chosen, the Hasegawa-Wakatani model, used to model electrostatic drift waves.
- The Hasegawa-Wakatani model includes the following:
  - $\frac{\partial n}{\partial t} = -\frac{1}{|B|}\vec{b} \times \nabla\phi \cdot \nabla n + \alpha(\phi - n) - k\frac{\partial \phi}{\partial y} + \nabla \cdot (D_{\perp n}\nabla_{\perp} n)$
  - $\frac{\partial \omega}{\partial t} = -\frac{1}{|B|}\vec{b} \times \nabla\phi \cdot \nabla \omega + \alpha(\phi - n) + \nabla \cdot (D_{\perp n}\nabla_{\perp} n)$
  - $\nabla \cdot (\nabla_{\perp}\phi) = \omega$
- Zapdos shows convergence close to the theoretical slope of 2, given the first-order Lagrange finite element discretization of the solution variables.



Verification of 3D Braginskii Model

- The 3D Braginskii model was chosen for the fluid description of the plasma edge.
- The Braginskii model within Zapdos currently:
  - Includes $\vec{v}_{\parallel e,i}$, $\vec{v}_{E\times B}$, $\vec{v}_{Dia}$ and $\nabla_{\perp}^{2}(f)$.
  - Is included only in the vorticity equation.
  - Includes effects from momentum transfer via collisions and for the electron heat flux as defined in [5].
- Currently, the cold ion assumption is used.
  - Next steps involve incorporating tracking ion temperature.
- Zapdos shows convergences close to the theoretical slope of 2.

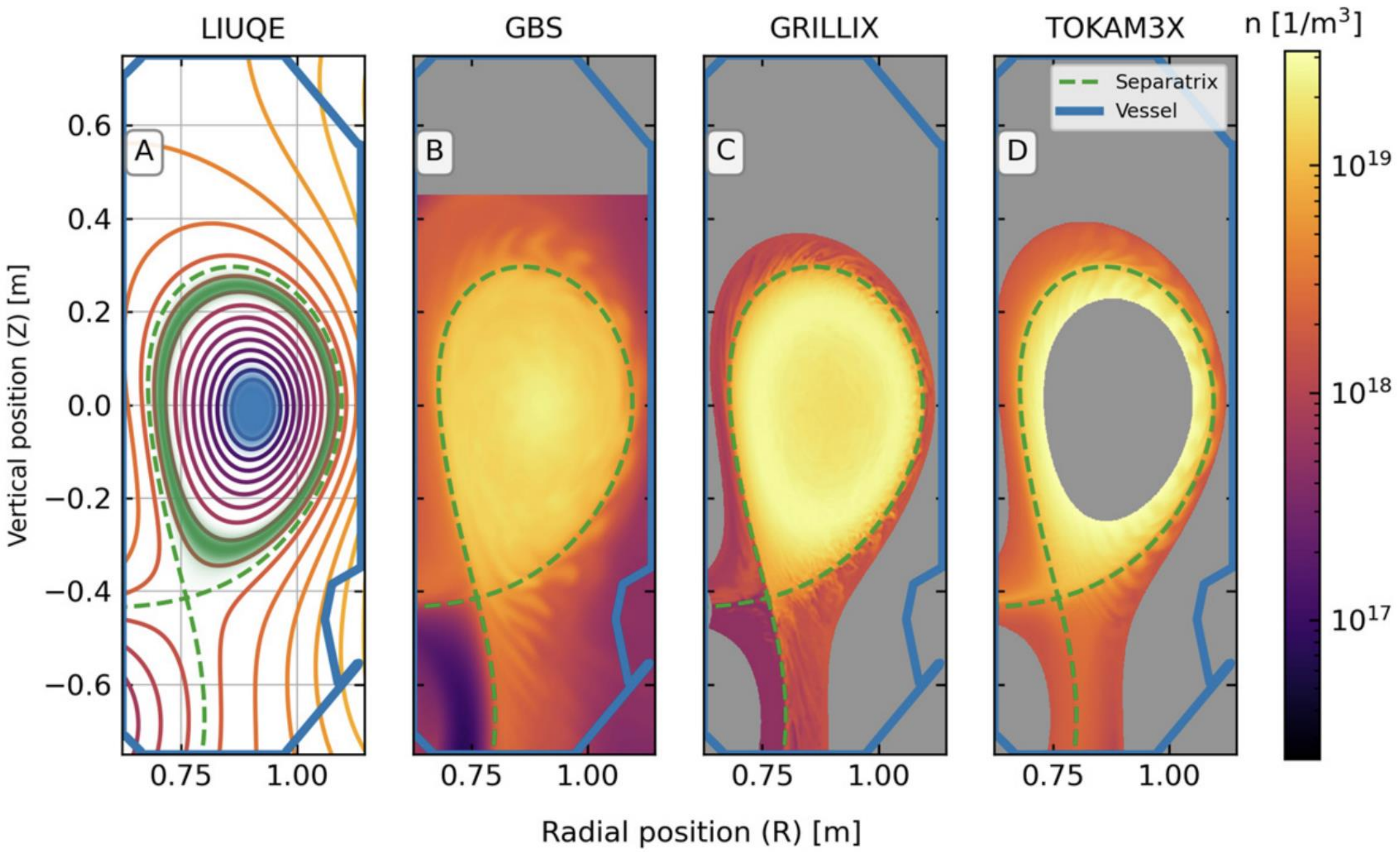


[5] Braginskii S. 1965 *Reviews of Plasma Physics* **1** (New York: Consultants Bureau)

Validation Case: TCV Fusion Device

- The TCV team has publicly shared shot data for a standard validation and benchmarking of fusion codes [6].
  - The data is on GitHub as TCV-X21 [7].
- The results in the first TCV-X21 paper serve as a great starting point in benchmarking, since:
  - Each code present includes different variations of the Braginskii model.
  - Modeling of neutrals was not included in these sets of simulations.

Previous Simulations of TCV-X21 [6]

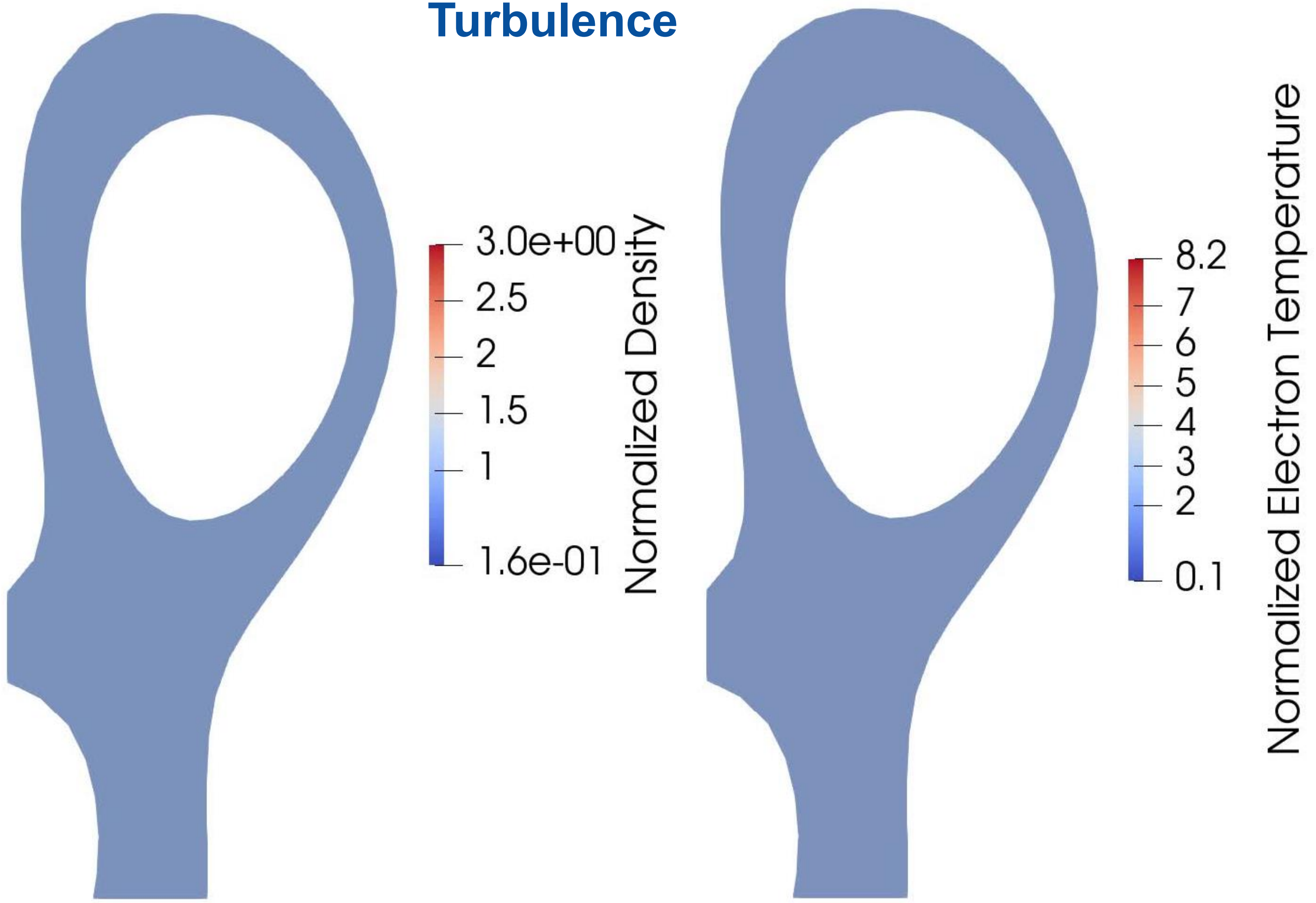


[6] D.S. Oliveira *et al* 2022 *Nucl. Fusion* **62** 096001
[7] https://github.com/SPCData/TCV-X21

Preliminary Results of TCV-X21

- The simulation included:
  - Uniform initial profile for all fields
  - The n and T_e values at the core is set higher than the initial profile
  - Bohm sheath criterion conditions for the outside boundary.
- Current simulation forms numerical instabilities as the n and T_e increase towards the inner wall.
- Similar instabilities were noted for GBS and GRILLIX for TCV-X21 [6]
  - For those codes, small additional sources were added to prevent numerical instabilities at very low temperatures or densities.

Poloidal Cross Section: Onset of Turbulence



[6] D.S. Oliveira *et al* 2022 *Nucl. Fusion* **62** 096001

The DeepLynx Ecosystem

https://github.com/idaholab/DeepLynx

Unified Data Catalog

- Centralized data repository with hierarchical organization and granular role-based access controls

Ecosystem Extensions

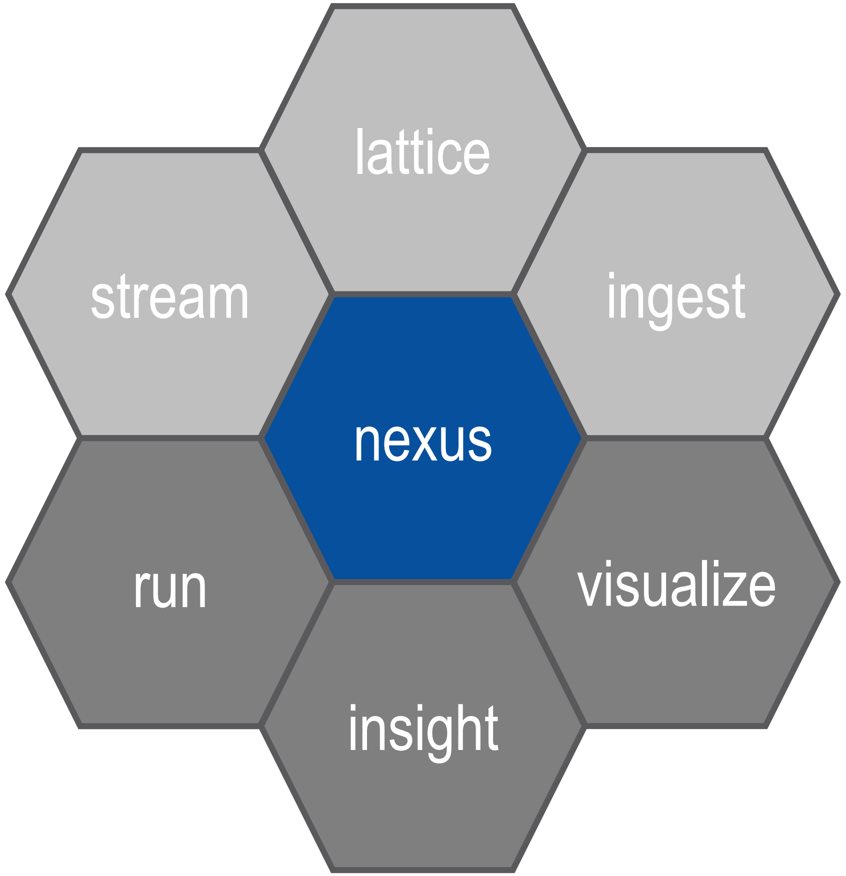
- Distributed architecture of specialized services providing comprehensive data management capabilities

Streamlined Microservice Design

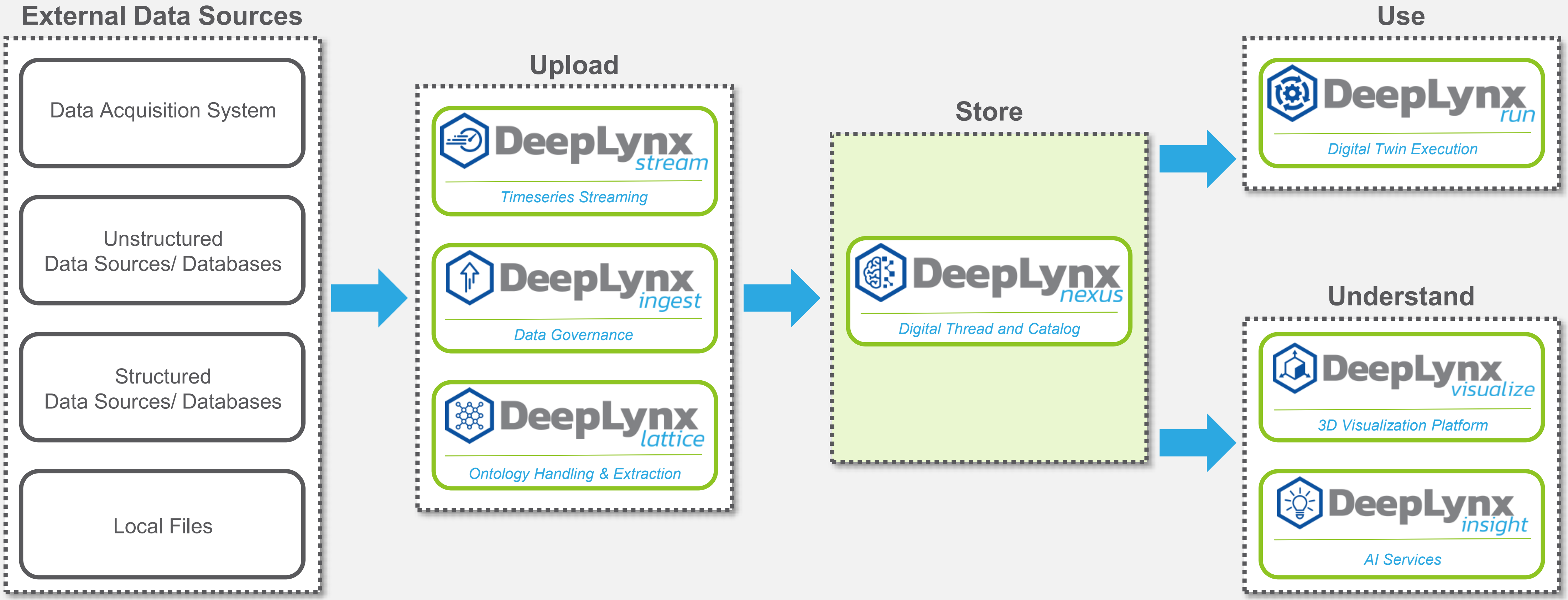
- Simplified, modular architecture enabling scalability and maintainable growth

Flexible Deployment Options

- Configured for on-premise, cloud, or hybrid infrastructure to meet organizational requirements



How Does the DeepLynx Ecosystem Work?



Digital Twin of the AGN-201 Research Reactor

- 5 W Reactor operated at Idaho State University
  - 9 polyethylene fuel disks of UO_2 (Core), thermal safety fuse, graphite/lead/water shield
- Reactor data collected and sent to DeepLynx (Azure cloud), continuously (<5 second intervals) during reactor operation
- ML and surrogate model codes access data and runs predictions.
- Prediction data uploaded to DeepLynx for use in visualization or further AI/ML workloads.

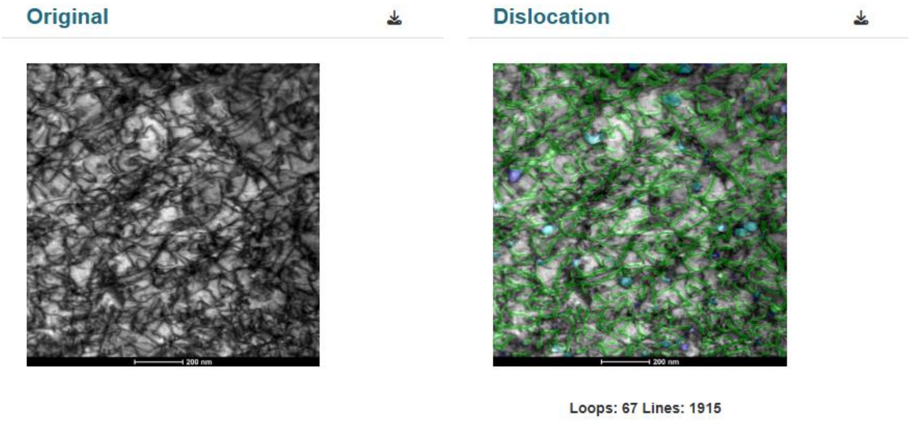
Stewart, et al. *Annals of Nuclear Energy*, **213**. 2025.
https://doi.org/10.1016/j.anucene.2024.111041

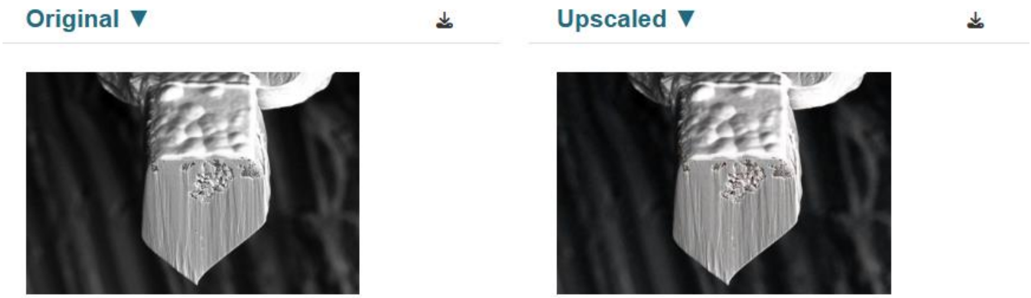
Nuclear Research Data System (NRDS)

https://nrds.inl.gov

- Seeks to make curation and distribution of data “FpAIRe”
  - Findability – metadata collection (DOIs, exp. info, license, tags)
  - **Peekable** – Drag-and-drop and preview for files within a project
  - Accessible, Interoperable – Collaborative project spaces, citable data
  - Reusable, **Extensible** – Downloadable data, access to HPC GPUs and AI execution
- Data close to compute – enables high speed analysis and AI/ML workflows

(Right) Dislocation loops and lines detected in high-noise micrographs using PANDA model.





Transfer learning super resolution analysis of non-scanning electron microscopy images using a generative adversarial network model.

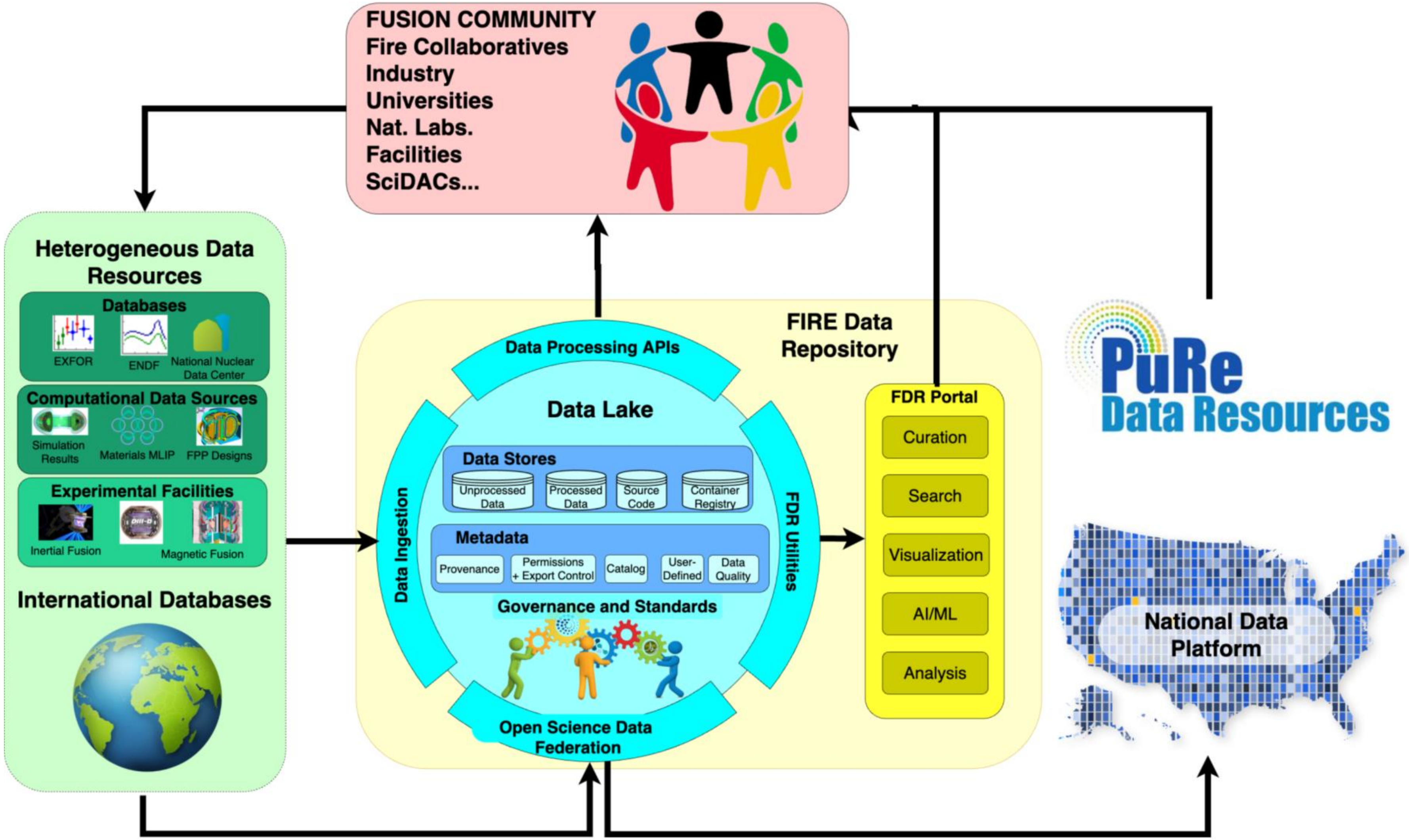
INL Fusion Safety Archive

The INL Fusion Safety Program (FSP) established by the U.S. DOE in 1979, focused on "*lithium fire safety, activation product analysis, superconducting magnet safety, safety design criteria, safety analysis methodology, safety data base development, and tritium and lithium fire modeling*." [*DOE Inventory, FY 1979*]

- Much of the FSP program archive prior to the 2000s was paper-based or stored on non-archival disks.
- A DOE-funded initiative was begun late 2024 to digitize and make these records and datasets available to the fusion community, supported by an LLM-driven search and accessibility front-end.
- Initial cataloging & digitization was completed in Summer 2025
  - Total documents: 2782
  - Books: 128
  - Existing URL: 1248
  - Digitized (internal): 307
  - Digitized (public): 52
- We would like to work toward inclusion of other legacy archives (e.g., UW design memos) – reach out if interested!

Word cloud generated from digitized records

What is this feeding into (amongst many others)? The Fusion Energy Data Ecosystem and Repository (FEDER) FIRE Collaborative



How do the projects discussed here tie into FEDER?

MOOSE

Cardinal

Zapdos

TMAP8

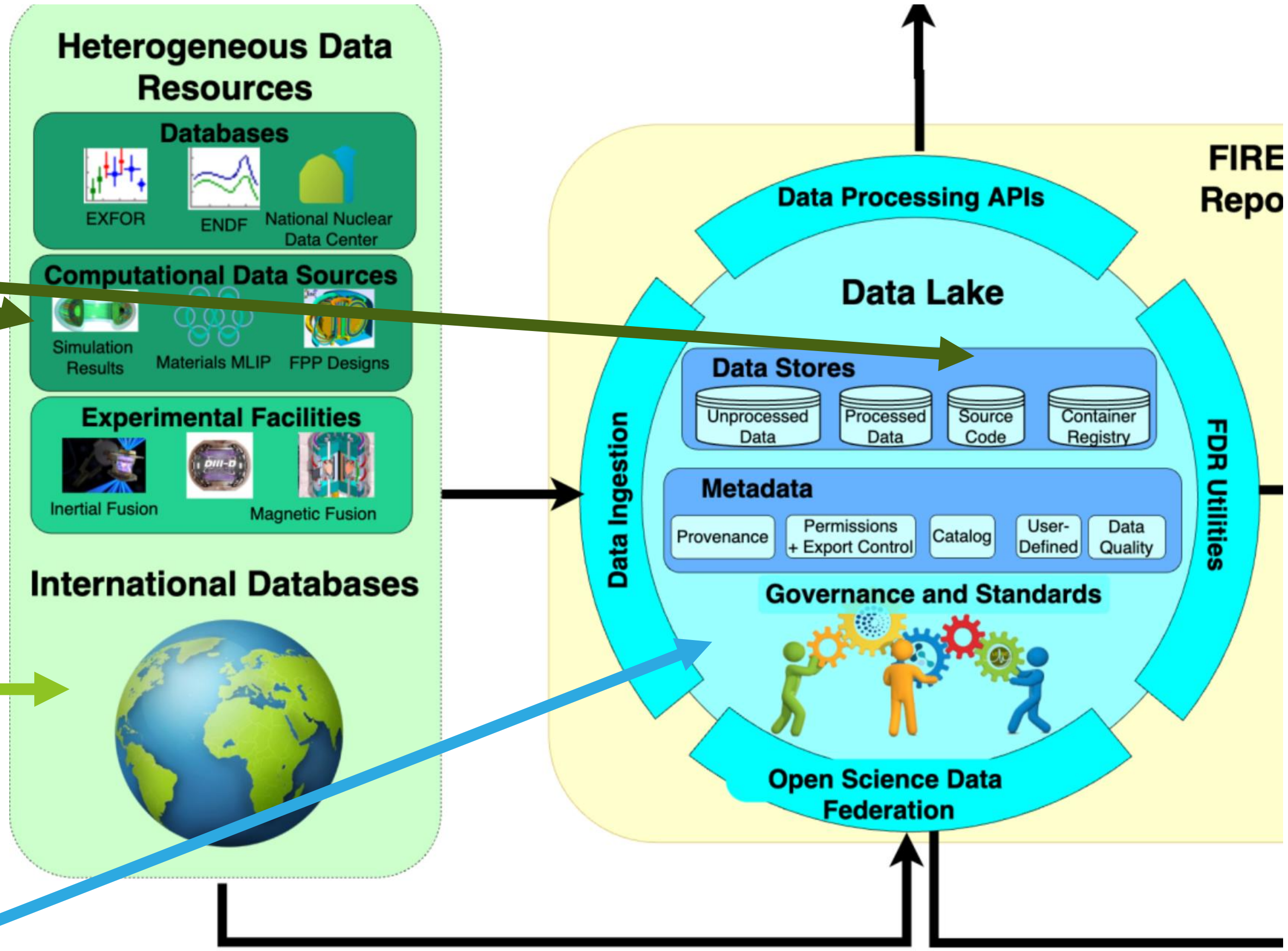
SALAMANDER

NRDS Nuclear Research Data System

FSP Archive

NRDS Nuclear Research Data System

DeepLynx



Slide Courtesy: Raffi Nazikian

Idaho National Laboratory

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy. INL is the nation's center for nuclear energy research and development, and also performs research in each of DOE's strategic goal areas: energy, national security, science and the environment.