U.S. DEPARTMENT OF ENERGY | Office of Nuclear Energy

An Overview of NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Prepared for NEAMS Workbench Collaborators

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Leader, NEAMS Integration Product Line

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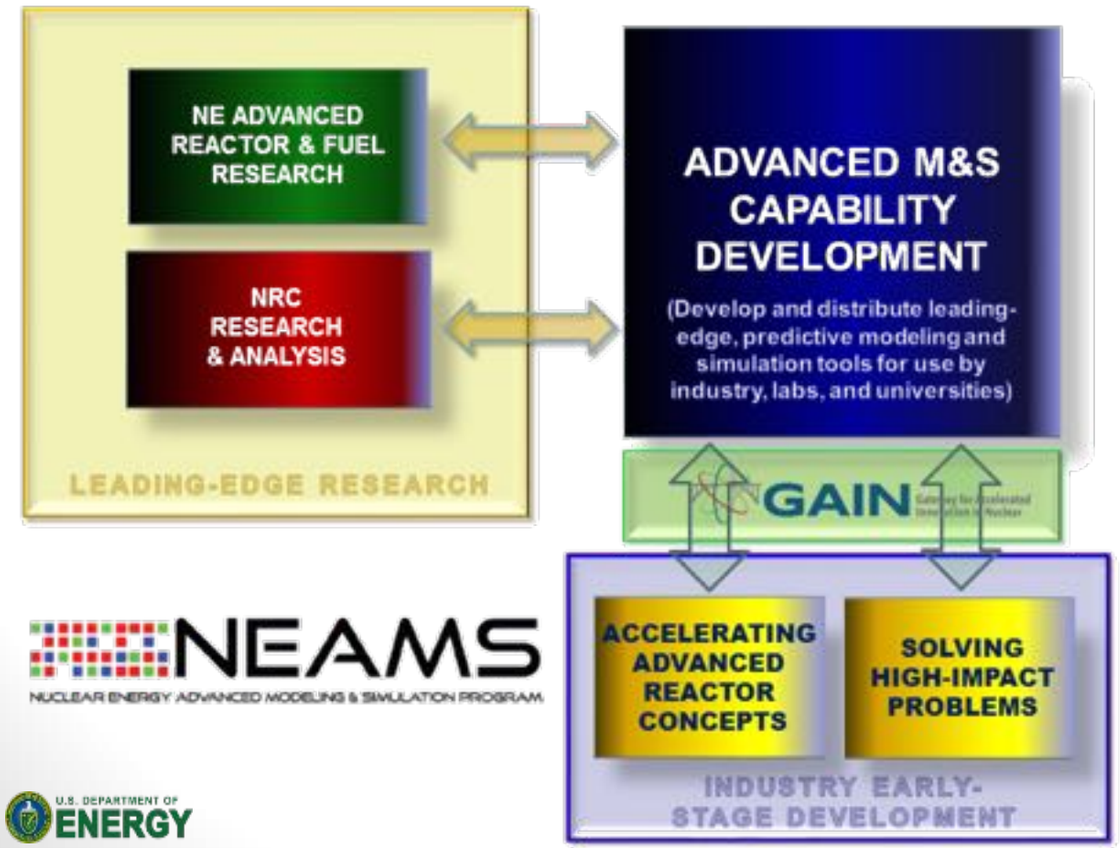
Nuclear Energy Advanced Modeling and Simulation (NEAMS)

The NEAMS Mission: provide leading-edge computational tools, currently not available to industry, for accelerating early-stage development of advanced reactor concepts and promoting innovative solutions to important nuclear industry problems; these advanced M&S capabilities will –



- Enable transformative scientific discovery and insights otherwise not attainable or affordable
- Solve problems identified as significant by industry, and consequently expand validation, application, and long-term utility of these advanced tools
- Enhance opportunity for industry to commercialize advanced concepts
- Allow industry to implement innovations that improve the economics of both existing and future nuclear power plants

NEAMS Organizational Structure

National Technical Director
Chris Stanek (LANL)

Leadership Council

ATF HIP
Jason Hales (INL)

Fuels Product Line
Steve Hayes (INL)

Integration Product Line
Brad Rearden (ORNL)

Reactors Product Line
Tanju Sofu (ANL)

SGFIV HIP
Elia Merzari (ANL)

Develop, apply, deploy, and support a predictive modeling and simulation toolkit for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities.

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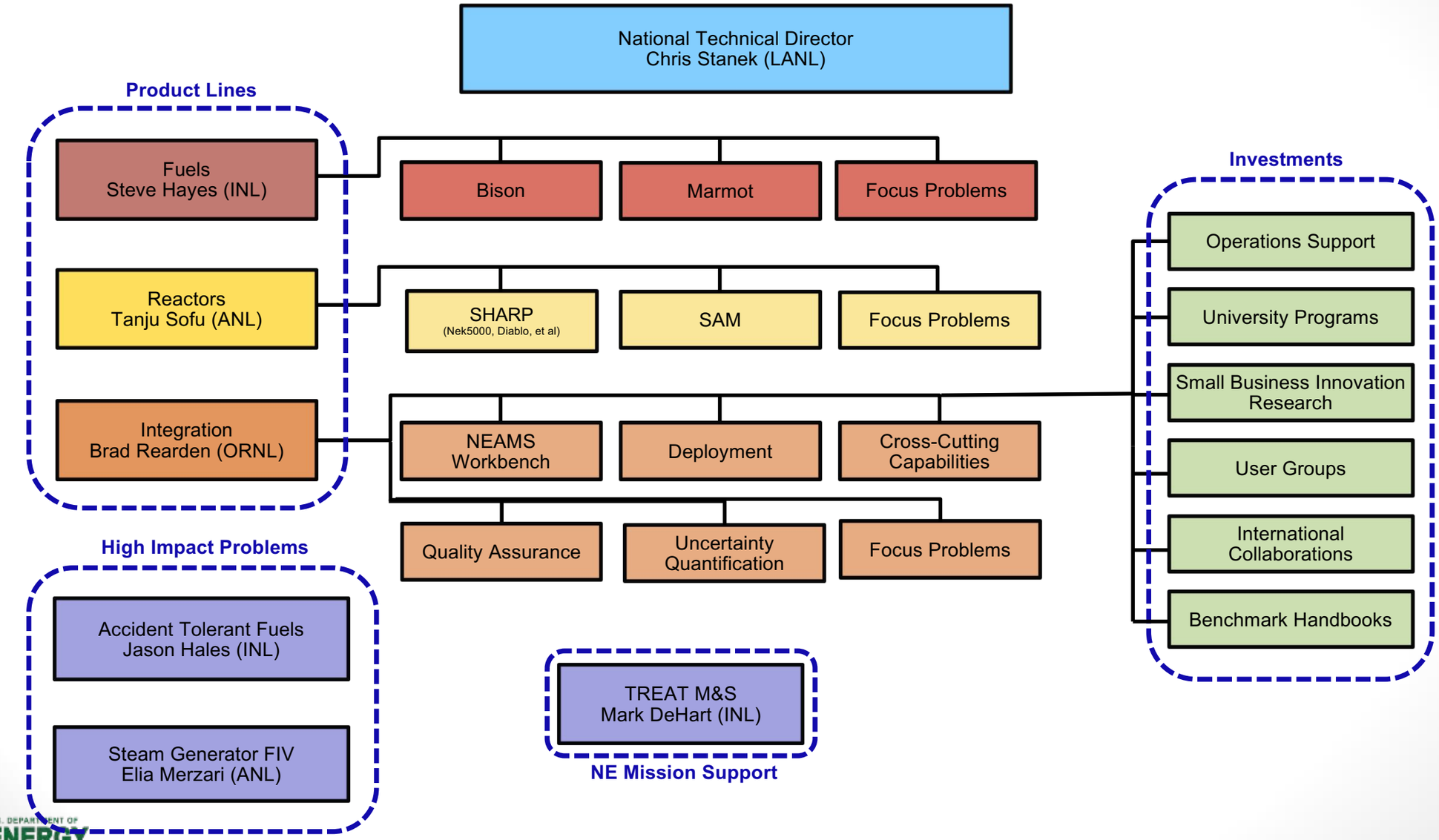
NEAMS Mission Areas

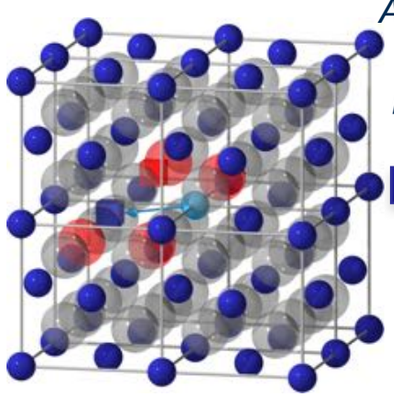


FPL

NEAMS - Fuels Product Line (FPL)

- **Empirical models can accurately interpolate between data, but cannot accurately extrapolate outside of test bounds**
- **Goal: Develop improved, mechanistic, and *predictive* models for fuel performance using hierarchical, multiscale modeling - applied to existing, advanced (including accident tolerant) and used fuel.**

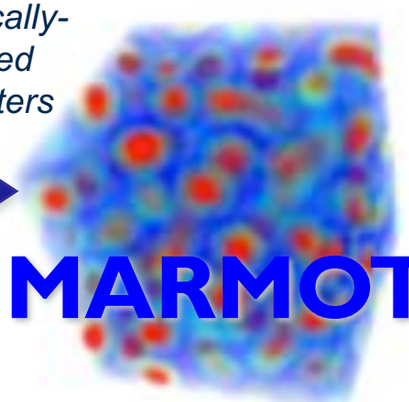
Atomistic simulations



Atomistically-informed parameters

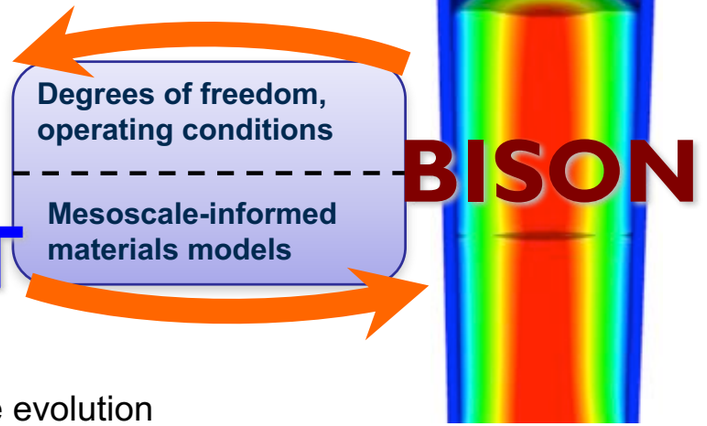
- Identify important mechanisms
- Determine material parameter values

Meso-scale models



- Predict microstructure evolution
- Determine effect of evolution on material properties

Engineering scale fuel performance



- Predict fuel performance and failure probability

MOOSE

Multiphysics Object-Oriented Simulation Environment

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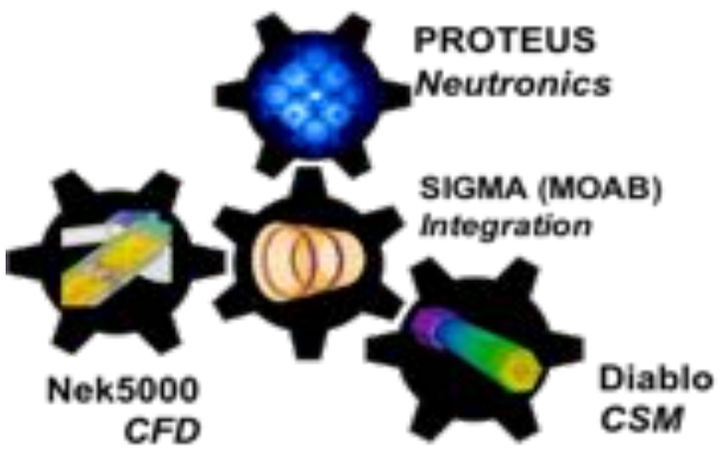
RPL

NEAMS - Reactors Product Line (RPL)

RPL Focus:

- **System Analysis Module (SAM)**
- **Simulation-based High-fidelity Advanced Reactor Prototyping (SHARP)**
  - Pin-by-pin neutronics, T/H, CFD and CSM modules
  - Capabilities to integrate these modules for multi-physics simulations
  - Primarily targets leadership class computing platforms
  - A range of reduced-order models/methods are also being pursued for more common computing platforms



SHARP is comprised of several physical modeling tools and capability to integrate these tools for multi-physics analyses

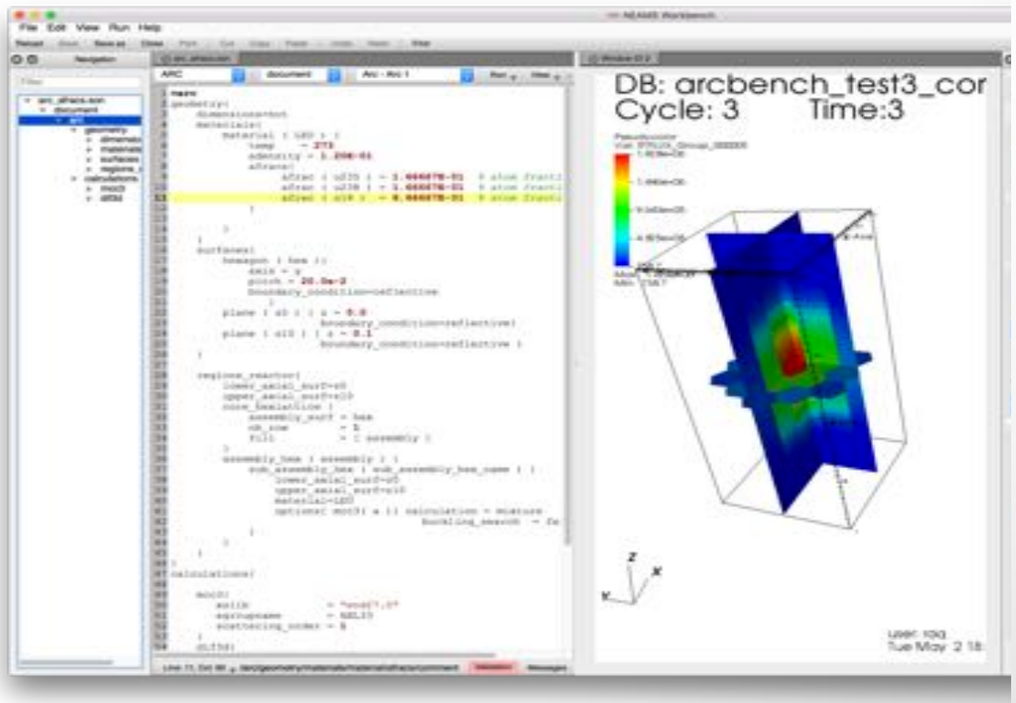
- PROTEUS/MC^2-3/PERSENT for neutronics
- Nek5000 for CFD and T/H
- Diablo for structural mechanics
- SIGMA interface for multi-physics coupling

NEAMS - Integration Product Line (IPL)

IPL

- **NEAMS FPL and RPL provide many advanced tools, but they often require large computational resources, can be difficult to install, and require expert knowledge to operate.**
- **Goal: Respond to needs of design and analysis communities by integrating robust multi-physics capabilities and current production tools in easy-to-use versioned deployments that enable end users to apply high-fidelity simulations to inform lower-order models for the design, analysis, and licensing of advanced nuclear systems.**

- **Desired attributes:**
  - Convenient access to high-fidelity simulations to inform lower-order models
  - Common user interface
  - Simplified common input to many codes
  - Visualization
  - Deployment
  - Quality assurance
  - Verification and validation
  - Uncertainty quantification
  - Application to design systems and recognized benchmarks



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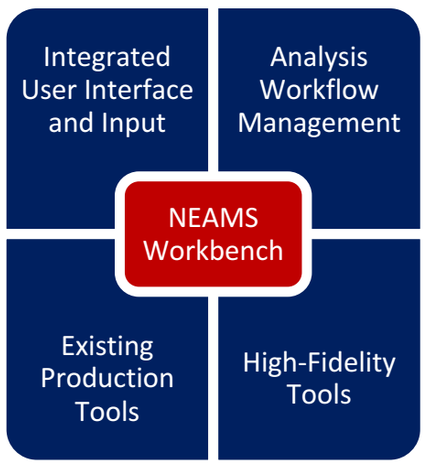
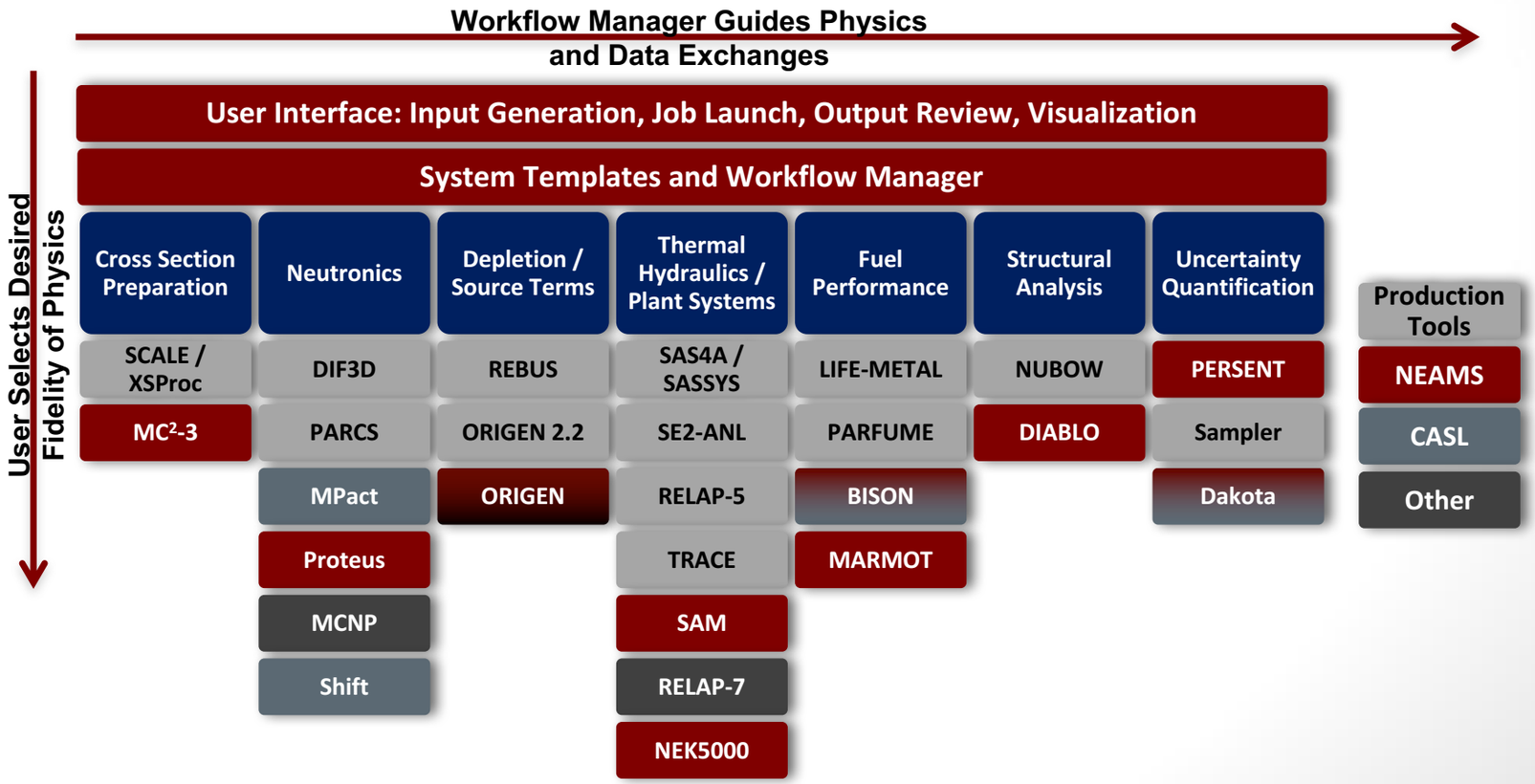
The NEAMS Workbench

IPL

- Integrate current production tools with advanced tools under an integrated user interface and workflow manager
- Leverage modern user interface from SCALE, which is co-sponsored by NRC
- Leverage templating/input expansion engine from UNF-ST&DARDS and SCALE so that engineering parameters can be expanded to specific input for analysis with varying levels of fidelity in several codes
- Desire to integrate many tools for many types of systems and demonstrate use of high-fidelity simulations to inform lower order models





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IPL

NEAMS – Workbench User Interface

Snapshot of Fulcrum (from SCALE)

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Templated Common Input – Use with Many Codes

IPL

Engineering-style problem specific input
(type of system, materials, dimensions, timesteps, etc)

Database of supported system configurations

- Known systems and customizable features
- Input requirements and options for each code
- Code and problem specific information (mesh geometry, etc.)

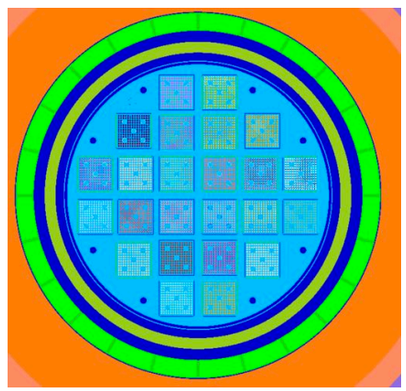
Template Engine Expansion

Input for Code A

Input for Code B

Input for Code C

Similar to CASL VERA-IN concept; Leverages Template Engine used for UNF-ST&DARDS and SCALE

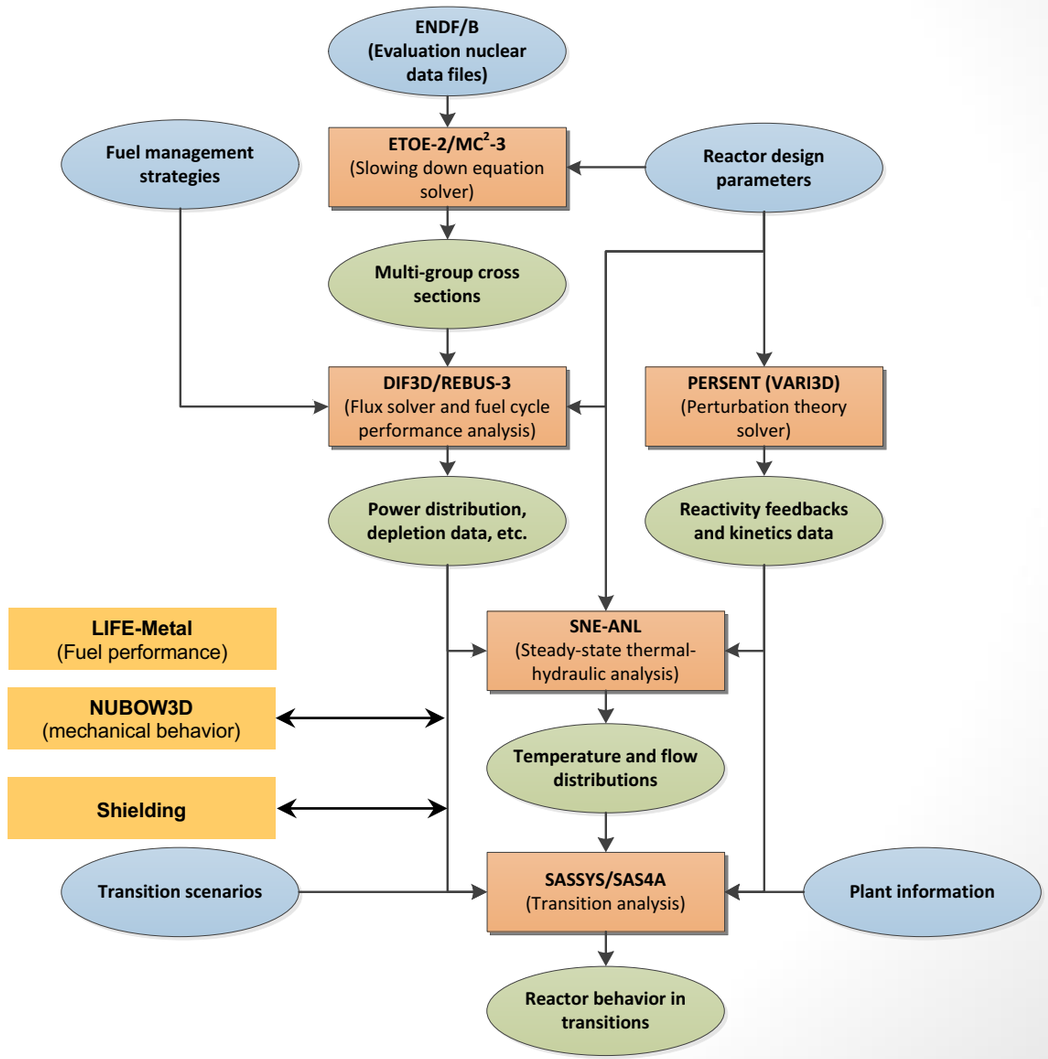


Workbench Integration of Legacy Codes: Advanced Reactor Codes (ARC)

IPL

- ARC suite of codes developed at ANL with >30 years of experience:
  - Highly efficient
  - Good accuracy (validated)
- Different codes use:
  - Similar design information
  - Different input logic
- Scripts were developed by users to assist with input generation

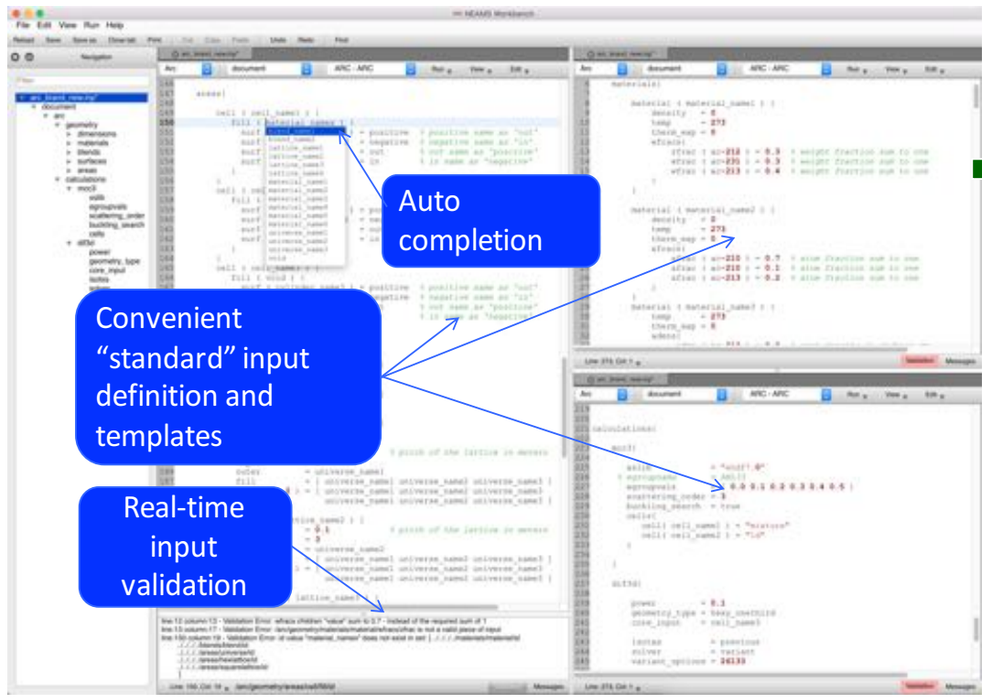
- Difficult for new users to get started
- Limited user community



Workbench Integration of Legacy Codes: Advanced Reactor Codes (ARC)

IPL

- Convenient input structure based on MCNP logic:
  - Well known logic
  - Very flexible and compatible with a wide range of other codes (PROTEUS, MCNP, *etc.*)
- Developed in close collaboration with:
  - ARC code system users
  - Code developers
- Challenges:
  - Keep input simple/attractive while compatible with deterministic codes' specific options
  - Interpret complex models and translate for lower fidelity code inputs



Workflow Manager

- Pre-processing:
  - Atom density calculation
  - Thermal expansion
  - …
- Translation into codes' input language
- Runtime environment

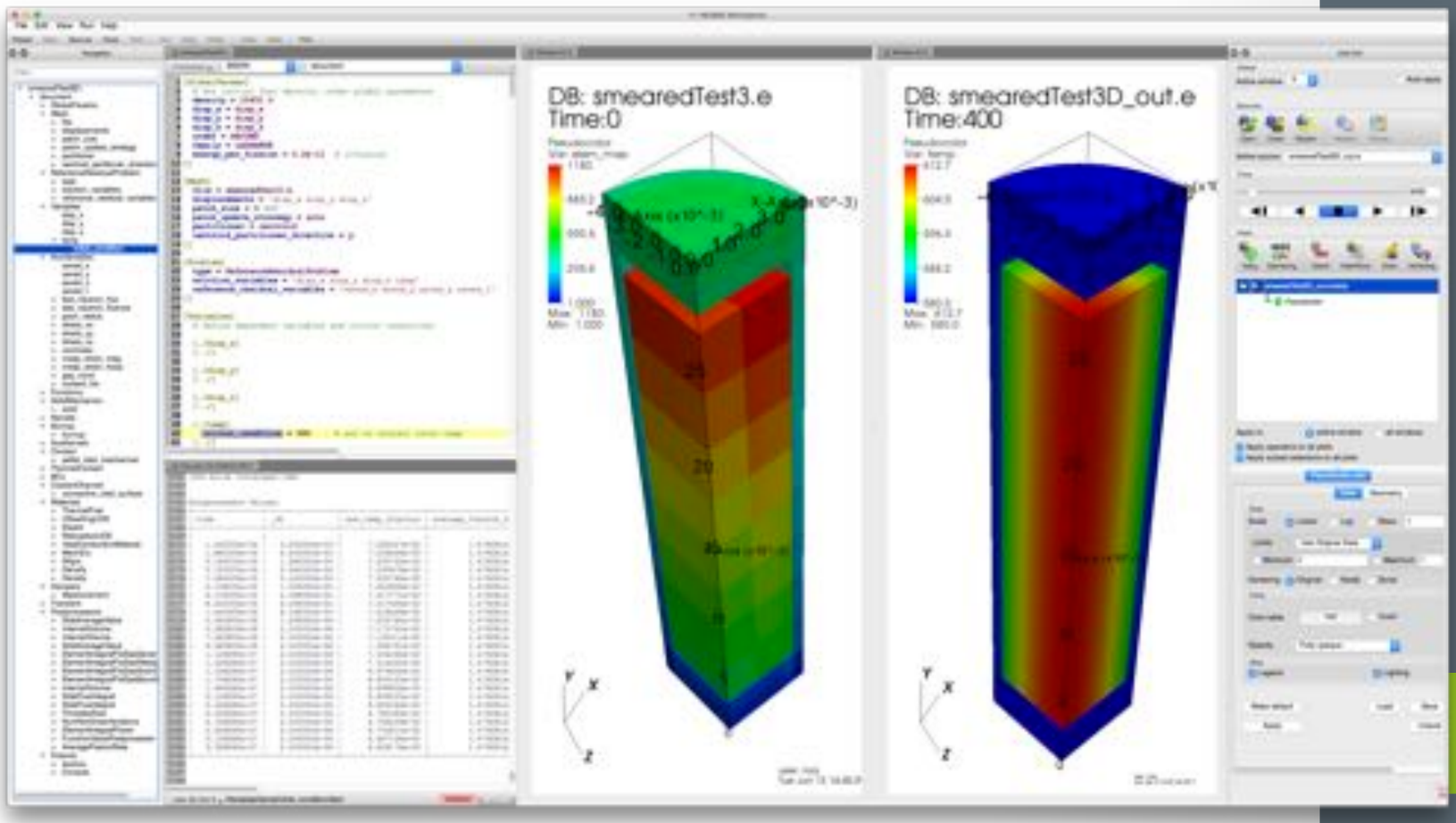
ARC Code Inputs

DIF3D | REBUS | PERSENT | MCC3

Workbench Integration of Modern Codes: MOOSE/BISON

IPL

- MOOSE applications easily enabled under Workbench with uniform input standards available through MOOSE
- Runtime updated to execute BISON
- MOOSE's input module updated to generate files needed by Workbench, even for new applications even when generated by external teams



Ongoing and Near-Term Code Integration Plans for the NEAMS Workbench

IPL

Tool	Application	Production Tool	NEAMS Tool	Integration Lead
BISON	Fuel performance		x	ORNL
MOOSE	General purpose multiphysics framework		x	ORNL/INL
Warthog	Multiphysics neutronics and fuel performance		x	ORNL
ARC	Fast reactor analysis	x	x	ANL
SCALE	Widely-used multipurpose neutronics and shielding analysis	x	x	ORNL
Dakota	Uncertainty quantification and model optimization	x	x	SNL/ORNL
VisIt	Mesh Visualization	x	x	LBNL
PROTEUS	Three-dimensional unstructured grid finite element neutron transport solver		x	RPI
MCNP	Widely-used Monte Carlo radiation transport code	x		RPI