U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Clean. Reliable. Nuclear.

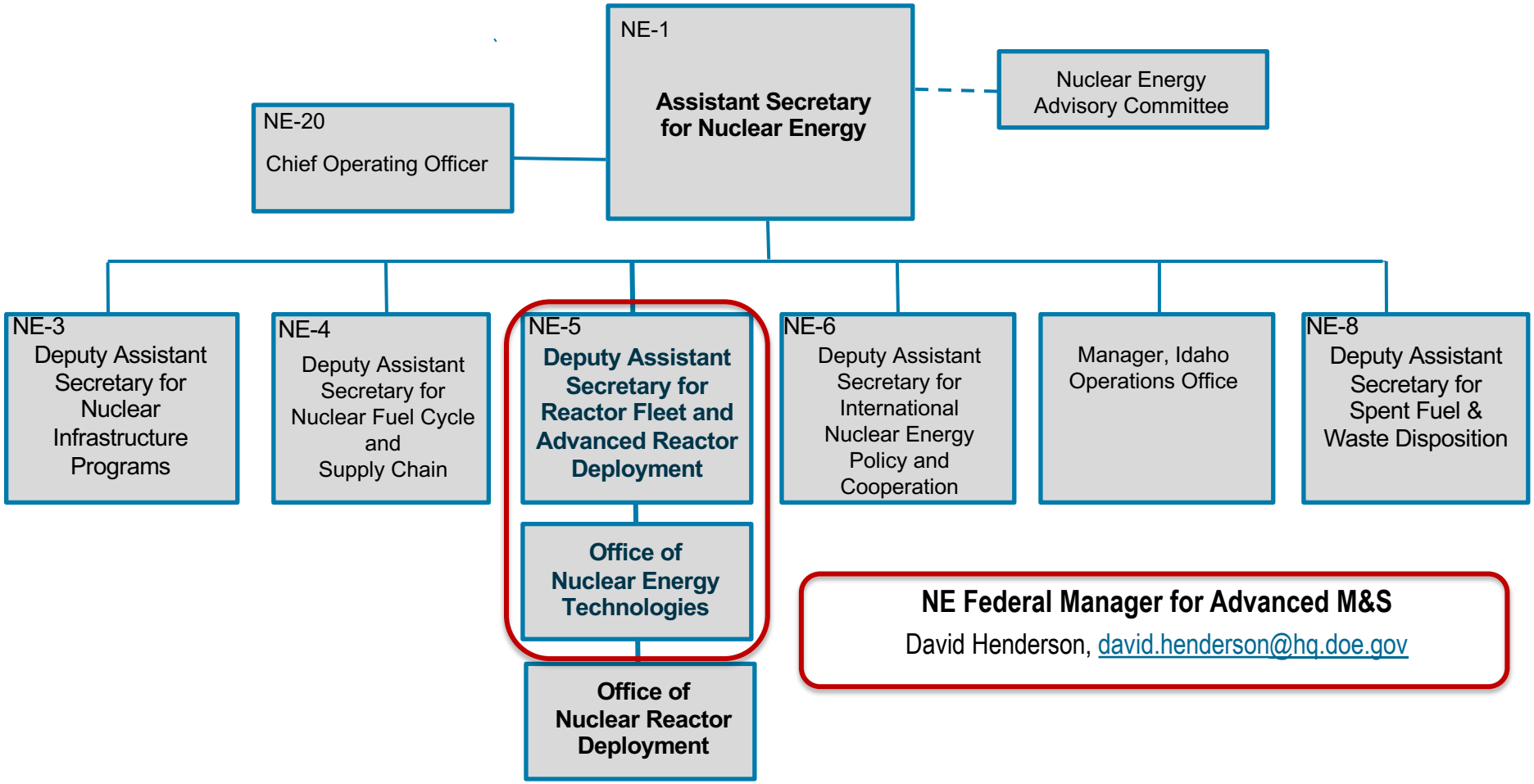
Nuclear Energy Advanced Modeling & Simulation

CINR Annual Planning Webinar - August 2019

Nuclear Energy University Programs (NEUP)
Consolidated Innovative Nuclear Research (CINR)
Office of Nuclear Energy
U.S. Department of Energy

Office of Nuclear Energy Organization

Where in NE are programs for developing and deploying advanced modeling and simulation tools managed? Who manages them?



Advanced Modeling & Simulation

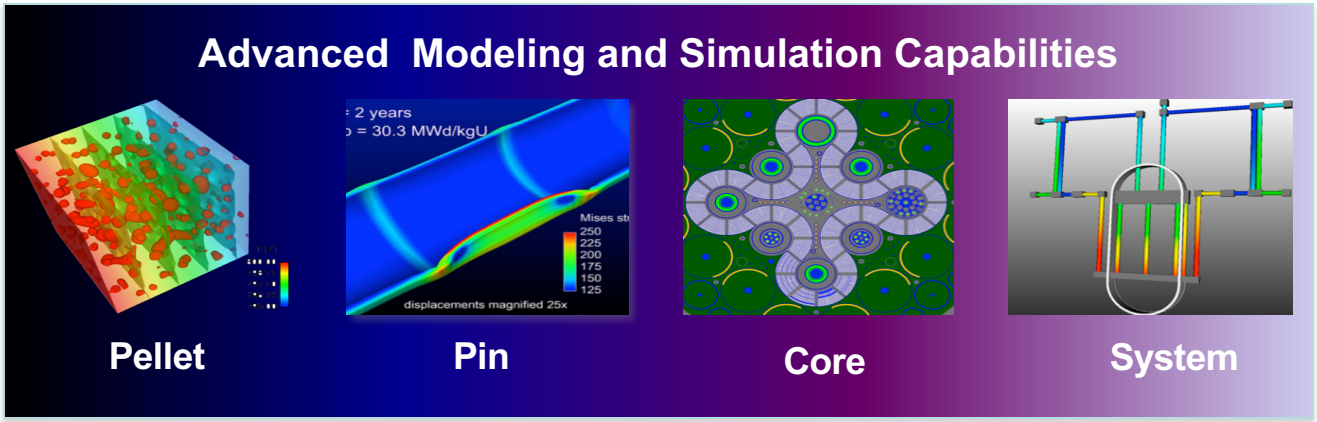
NE currently executes two complementary advanced M&S programs, each tailored to focus on a particular reactor technology area using computational tools uniquely suited to the particular reactor moderator(s) and fuel(s).

Energy Innovation Hub for Modeling and Simulation (Hub)

Objective: Develop and apply M&S tools focused on LWR technologies for an improved understanding of important operational and safety issues in existing reactors

Nuclear Energy Advanced Modeling & Simulation (NEAMS)

Objective: Develop and deploy predictive analytic computer methods for the analysis and design of advanced reactor and fuel cycle systems focused on non-LWR technologies



Advanced Modeling & Simulation
Underpins NE's Mission Focus Areas

Existing Fleet

- **Address core performance issues that increase operational costs**
- **Assure the long-term availability and market competitiveness of nuclear energy**

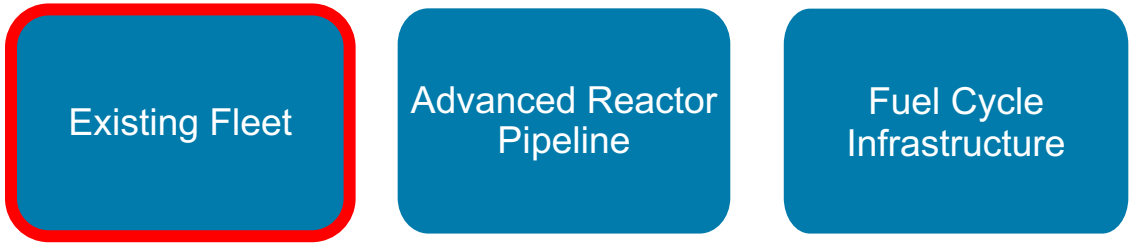
Advanced Reactor Pipeline

- **Accelerate concept development and commercialization**
- **Meet otherwise cost-prohibitive data needs**
- **Support NRC confirmatory analyses**

Fuel Cycle Infrastructure

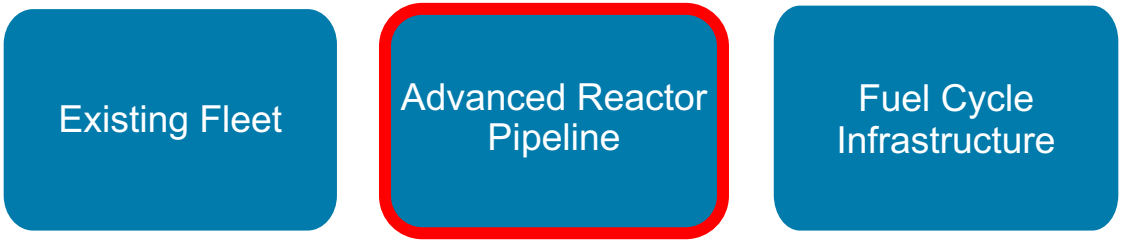
- **Confirm higher burn-up fuel strategies to slow production of used nuclear fuel (UNF) – VERA**
- **Support UNF R&D with high-fidelity analysis and prediction of fuel and cladding performance- NEAMS**

Advanced Modeling & Simulation
Supporting NE's Mission Focus Areas



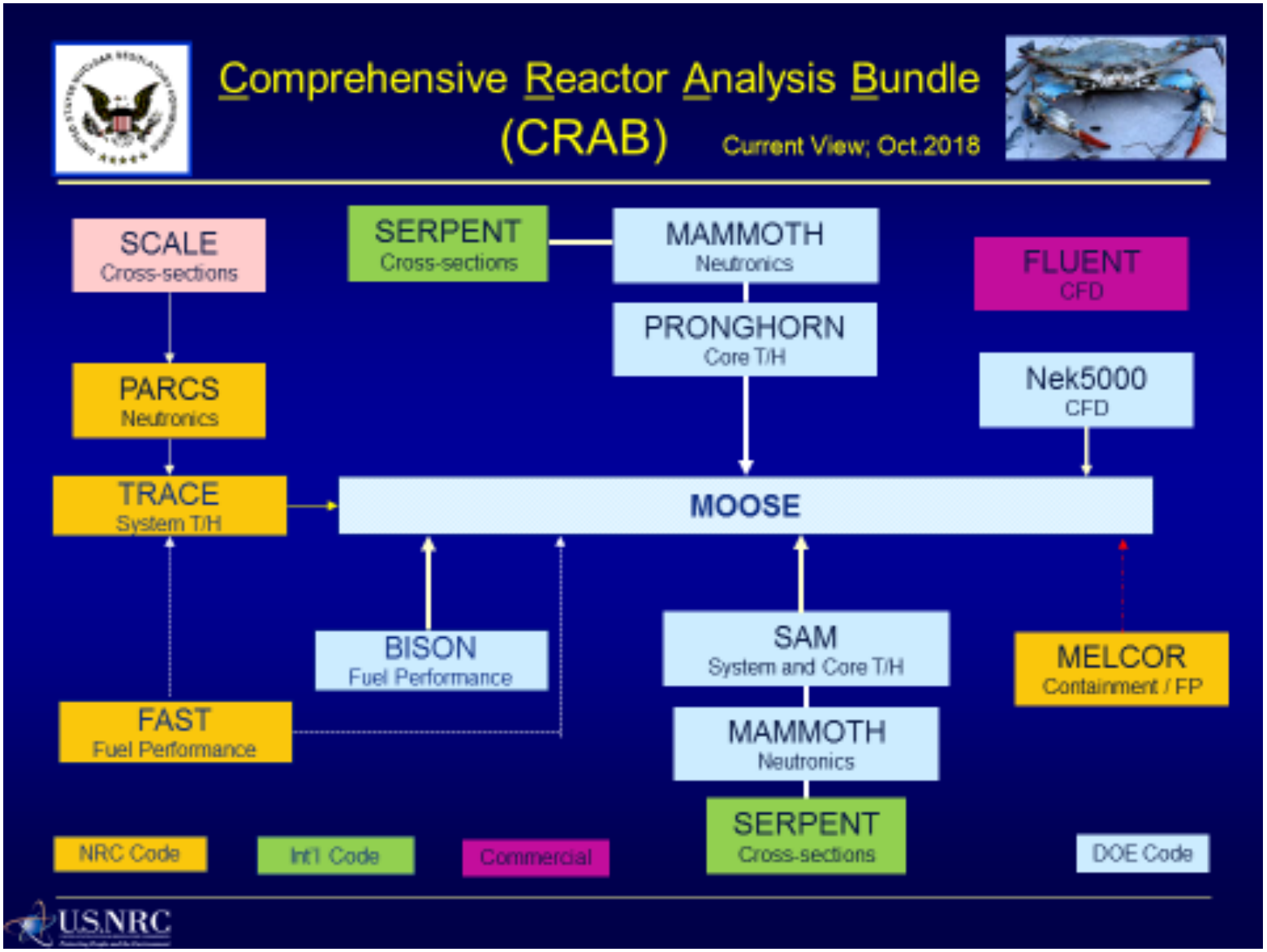
- **Allows the LWR vendors and utilities to develop innovative solutions to important fuel and core performance issues**
  - *Issues* – include power shifts, corrosion, fuel damage, and thermal performance, which add cost and limit affordability
  - *Solutions* – will help achieve significant reductions in reactor operational costs, which is an important component in the industry-wide initiative, "Delivering the Nuclear Promise"
- **Empowers the LWR community to take advantage of accident tolerant fuels (ATF), and implement load-following strategies for enhanced safety, improved economics, and greater versatility on the grid**
  - Accelerate development and approval of new ATF concepts (in fact, advanced M&S researchers have identified a promising new fuel, patent-pending)
  - Confirm viability of load-following with LWRs, to allow greater flexibility in meeting electrical demand, especially in combination with other renewable energy sources

Advanced Modeling & Simulation
Supporting NE's Mission Focus Areas



- **Critical role in accelerating design and deployment of advanced reactors**
  - Design optimization is required to fully realize the economic and technological advantages of advanced concepts
  - Advanced M&S tools will help the NRC expand capabilities as needed to perform confirmatory analysis on advanced reactor concepts
- **Only way for vendors to economically address data needs, which otherwise could require cost-prohibitive experimentation**
  - Reduce the amount of experimental testing needed
  - Identify, design, execute, and analyze more effective high-value experiments
- **The advanced reactor industry is already using our Advanced M&S tools to:**
  - Reduce cost and time for license applications to the NRC
  - Enhance potential for successful commercialization - accelerated development crucial to economic viability

DOE Priority Codes



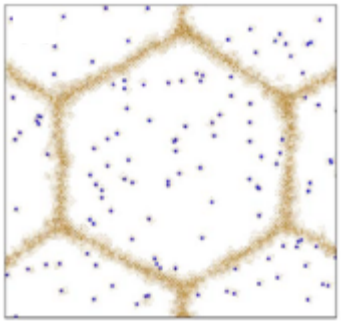
Advanced Modeling & Simulation:
Tools to Solve Advanced Reactor Priority Problems

		Advanced Reactors
Integration		MOOSE
System Analysis	Plant	SAM RELAP-7
Core Analysis	Neutronics-Pin Resolved	Rattlesnake Proteus
	Neutronics-Monte Carlo	External codes
	Neutronics-Kinetics/Depletion	MAMMOTH Rattlesnake
	Neutronics-Cross Sections	MAMMOTH MC2-3
	T-H Low Res	SAM RELAP-7
	T-H Med Res	Pronghorn
	T-H Hi Res (CFD)	Nek5000
	Structural Mechanics	Grizzly Diablo
Fuel Analysis	Continuum	BISON
	Microstructure	Marmot
	Component Aging	Grizzly Marmot
	Chemistry	MAMBA Yellowjacket (future)

BISON/MARMOT
Multiscale Mechanistic Modeling of Nuclear Fuels

- **Objective**: Use hierarchical, multiscale modeling for improved, mechanistic, and increasingly predictive models of fuel performance
- Mechanistic fuel behavior models: 1) minimize form errors, 2) provide insight were experimental data is sparse, and 3) may require less (or different) experimental data for validation

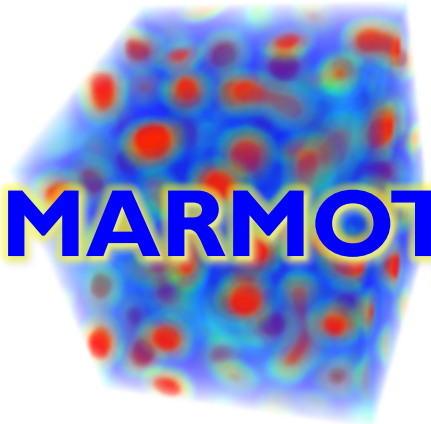
Atomistic simulations



- Identify important mechanisms
- Determine material parameter values

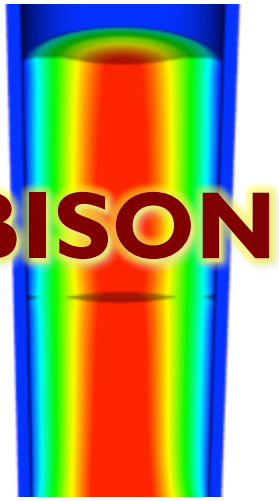
Atomistically-informed parameters

Meso-scale models



- Predict microstructure evolution
- Determine effect of evolution on material properties and fuel behaviors

Fuel performance models



- Predict fuel performance and failure probability

Advanced Modeling & Simulation
NEAMS-1: Generalized Multigroup Cross Sections

NEAMS-1 DEVELOPMENT OF GENERALIZED MULTIGROUP CROSS SECTIONS FOR ARBITRARY REACTOR GEOMETRIES (up to 3 years & $750,000)
TECHNICAL POC: David Kropaczek (ORNL)

- **Purpose:**
  - to have a consistent methodology for generating a multigroup cross section library applicable for use in reactor physics codes within the NEAMS program.
  - Running a continuous energy Monte Carlo calculation for a given problem allows for multigroup cross sections to be defined exactly for the 'snapshot' configuration. However, any significant changes in reactor system configuration invalidate the 'snapshot' result
- **Scope:**
  - Key considerations are 1) the geometry of the reactor system, 2) the energy spectrum of the neutron flux (including the presence of important resonances), 3) the consideration of feedback, such as that due to changes in fuel temperature
  - Methodology/approach should be demonstrated on a realistic test problem. (e.g. a thermal spectrum molten salt reactor with TRISO fuel over a number of fuel depletion steps at different fuel/salt temperatures representative of full power/zero power)
  - Comparison with Monte Carlo 'snapshot' cases at each of the conditions should be used to verify the methodology developed.

Advanced Modeling & Simulation
NEAMS-2: Near-wall Gas-Flow Correlations in Pebble Bed

NEAMS-2: NEAR-WALL GAS-FLOW CORRELATIONS IN PEBBLE BED REACTORS (UP TO 3 YEARS AND $750,000)

TECHNICAL POC: Richard Martineau (INL)

- **Background:**
  - The INL/ANL approach to multiscale, multiphysics simulation for pebble-bed reactors (as well as others) is unique cutting edge modeling and simulation technology.
  - The NEAMS MOOSE Framework is capable of on-the-fly multiscale coupling of Nek5000 to any NEAMS TH code or to compute a distribution of closure relations for table lookup or functional evaluations.
- **Desired Scope:**
  - Experimenters must be able to reduce data into second-order or higher closure correlations.
  - Must include efforts to obtain closure data for turbulent heat flux and viscous and form drag
  - Must obtain data for non-isothermal Helium temperature distribution with a maximum solid phase temperature of 1000C
  - Pebble and near wall surrogates must be manufactured to match characteristics of graphite
  - Must include a large enough pebble field to account for radial variation in volume fraction (porosity)

Advanced Modeling & Simulation
NEAMS-3: Molten Salt Chemistry Modeling

NEAMS-3: Molten Salt Chemistry Modeling (up to 3 yrs & $750,000)

TECHNICAL POC: David Andersson (LANL)

- **Desired Scope:**
  - Development of a high-quality validated database based on thermodynamic, thermophysical and corrosion data that can be used for predictions of complex multi-component salt properties
  - The database format and methodology should follow standards agreed upon by the international research community, such as the international Molten Salt Thermochemical Database (MSTD) project for salt thermodynamics.
  - Proposals should identify and address specific gaps in existing models and databases, which may include some data generation by new experiments and atomic scale simulations.
- **Differentiation:**
  - Existing NEUP projects focus on data generation through experiments and simulations and some method development
  - The present request for proposals aims to put this and other information together into a validated database for use in established approaches to thermodynamic and corrosion analysis.
  - We do not seek proposals that only emphasize data generation by either experiments or modeling using, for example, ab initio molecular dynamics, empirical potential development or similar techniques.

Advanced Modeling & Simulation
MS-NEAMS-1: SAM BASELINE DEVELOPMENT

MS-NEAMS-1: SAM BASELINE DEVELOPMENT (up to 18 months & $300,000)

Technical POC – Tanju Sofu (ANL)

- **Multi-scale thermal fluid simulation**
  - **Robust and accurate** schemes for coupling between 1D system code and 3D CFD codes at the fluid-to-fluid interface; (more tightly coupled schemes are being sought other than the loose coupling approach in the literature)
  - And/or the coupling schemes of conjugate heat transfer between 2D structure & 3D fluid flow
  - Perform direct comparison of existing or new datasets with simulations using NEAMS codes (SAM-Nek5000);
  - Not seeking for pure CFD validation experiments.

- **Integrate material models into SAM**
  - Develop computationally-efficient material models for advanced reactors safety assessment; (new)
  - Phenomena important to advanced reactor licensing, such as tritium transport, source term evaluations, precipitation and corrosion, etc.
  - Implement those models into system-level analysis code SAM for transient safety evaluations
  - Not seeking for new experimental data on material transport and modeling.

Advanced Modeling & Simulation
Integrated Research Project (IRP)Scopes

General

- **Urgency to accelerate development and deployment of DOE-NE mod-sim capabilities to meet industry and NRC needs**
- **A specific goal of this call is to recruit a team of university researchers to participate within the program, working closely with national laboratory colleagues in support the overall programmatic effort**
- **In addition to technical contributions, university partners will assist with the definition of programmatic priorities and deliverables as well as potentially serving in program leadership positions**
- **When appropriate, university partners are also expected to serve as representatives of the program representatives, much like their national laboratory counterparts, presenting technical progress at meetings, conferences, etc.**

Two separate scopes – each $3M over 3 years

Advanced Modeling & Simulation
Integrated Research Project (IRP)Scope

IRP-NEAMS-1.1 Thermal Fluids Applications in Nuclear Energy

- **Focus is to include a university team as a key component of the NEAMS Center for Thermal Fluids Applications**
- **Main goal of Center:**
  - To create a clear "front-door" to stakeholders (primarily industry and NRC) for access to DOE-NE thermal hydraulics modeling and simulation capabilities in order to perform research on novel solution strategies for various fluid flow and fluid related issues
- **What is different about Center approach:**
  - It is “pragmatically multiscale”
  - The approach developed that combines three natural, though overlapping, length and time scales in a hierarchal multi-scale approach to avoid the temptation and pitfalls of attempting to develop a single "solve all" algorithm for physical fluid flow problems that will span 9 orders of magnitude in spatial and temporal scales.
- **Scope should include:**
  - Clear articulation of a university team that becomes a component of the lab-led Center
  - Technically, contributions to CFD framework for the simulation of single-phase flow with the primary goal of facilitating the design and assessment of advanced reactors.
  - Finally, proposals should identify plans to integrate results with the advanced models in the overall multiscale approach of the Center, supporting the creation of reduced order models or novel closures for use in systems codes (e.g., SAM).

Advanced Modeling & Simulation
Integrated Research Project (IRP)Scope

IRP-NEAMS-1.2 Multiscale Nuclear Fuel Performance

- **Focus is to include a university team as a key component of the NEAMS Fuels Technical Area**
- **Purpose – to enlist university team to:**
  - help accelerate the development of the BISON fuel performance code for advanced reactor fuels, to enable the qualification of non-LWR fuel
  - participate within the program, working closely with national laboratory colleagues in support the overall programmatic effort
- **Priority:**
  - Accelerated development of BISON for particle fuel (gas reactors, FHRs and micro reactors)
  - Focus on developing capabilities to simulate thermomechanical response of particle fuel during AOO and accident scenarios, as well as tracking fission gas and other radioisotopes
  - University team will work with NEAMS to engage the NRC and vendors to ensure NEAMS work is relevant to fuel qualification efforts and complementary to previous experiments
  - Proposals that couple BISON to other NEAMS codes contained in the CRAB framework
  - Proposals should focus on finite element model development and multiphysics, rather than multiscale methods

- MS-NE-1 – Integral Benchmark Evaluations
- MS-NE-2 – Nuclear Data

ICSBEP (*International Criticality Safety Benchmark Evaluation Project*) & IRPhEP (*International Reactor Physics Evaluation Project*)

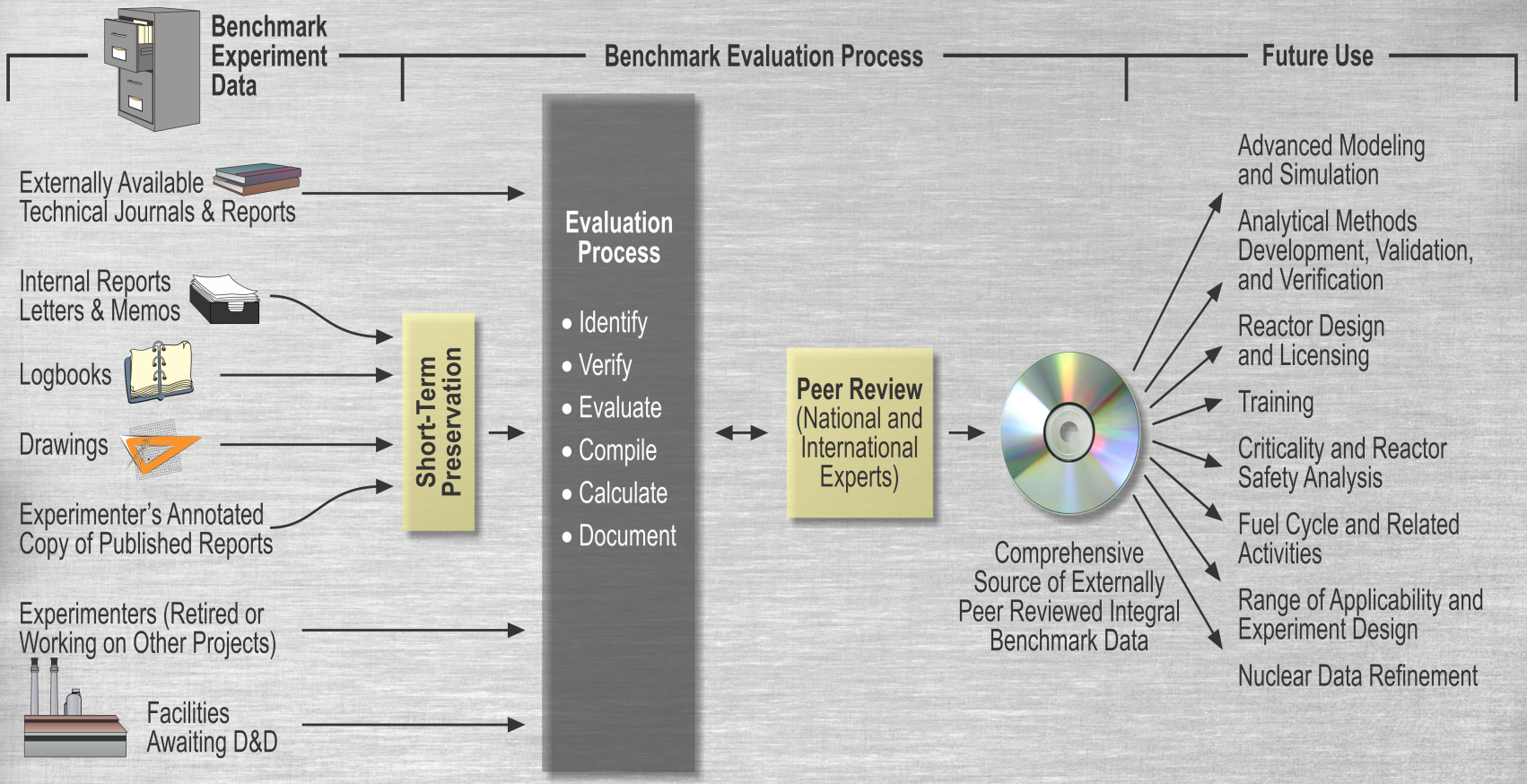
- **These are OECD NEA international activities involving expert groups focused on updating and publishing Handbooks that support:**
  - characterization of reactor core and methods
  - neutronics components of multiphysics measurements
  - validation of nuclear data; including cross sections; and
  - reactor and criticality safety, including modeling, simulation, and training
- **These benchmark development efforts:**
  - Compile benchmark-experiment data into standardized format
    - *Can be readily used to validate computational techniques and cross section data*
  - Evaluate the data
    - *Quantify overall uncertainties through various types of sensitivity analyses*
  - Eliminate the a large part of the tedious and redundant research and processing of experiment data that other researchers/analysts/designers would have to perform
  - Streamline necessary step of validating computer codes and nuclear data with experimental data
  - Preserve valuable experimental data
    - *Experiments represent significant investment of time, infrastructure, expertise, and cost that might not have received adequate documentation*
    - *The opportunity to repeat most of these measurements has long since passed*

INTERNATIONAL BENCHMARK PROGRAMS

NEA NUCLEAR ENERGY AGENCY

OECD BETTER POLICIES FOR BETTER LIVES

INL Idaho National Laboratory

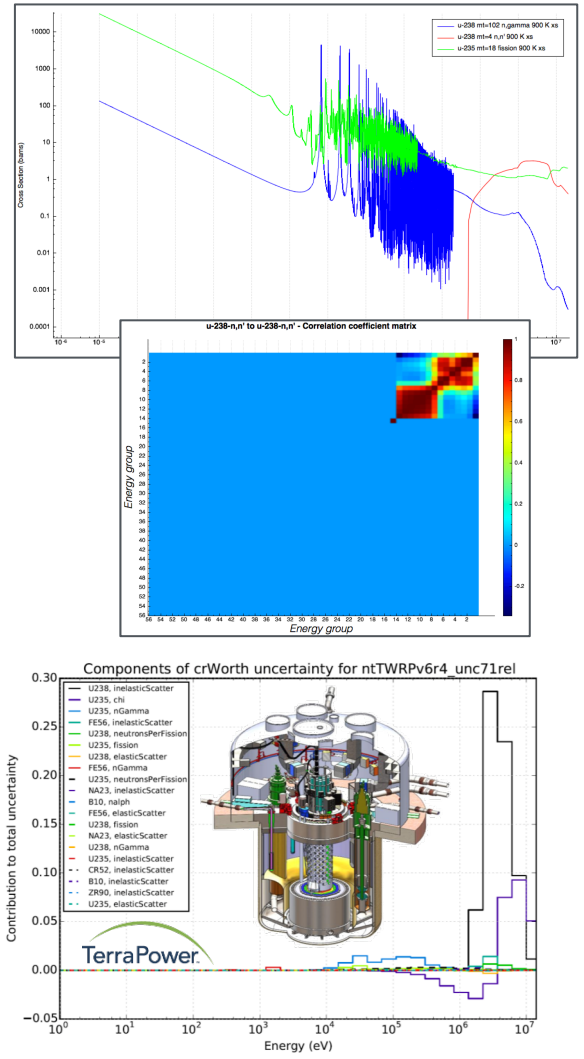


MS-NE-1 – Integral Benchmark Evaluations
Work-scope Description

- MS-NE-1 – Integral Benchmark Evaluations for inclusion in the International Reactor Physics Experiment Evaluation Project (IRPhEP) and International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbooks (TPOC – John Bess, john.bess@inl.gov)
  - Benchmark evaluation proposals are sought which would use existing experimental data, and would support NE programs (e.g., TREAT, LWRS, FCT, ART, and NE's Advanced Modeling and Simulation Program)
  - Measurements of interest include critical, subcritical, buckling, spectral characteristics, reactivity effects, reactivity coefficients, kinetics, reaction-rate and power distributions, and other miscellaneous types of neutron and gamma transport measurements
  - A growing area of interest includes evaluation of transient benchmark experiment data for light water reactor systems, such as PWRs and BWRs
  - To avoid duplication, please take into account ongoing work in these recent projects:
  - All evaluations must be completed according to the IRPhEP and ICSBEP requirements, including peer review
  - Multiphysics benchmarks are allowed

MS-NE-2 – Nuclear Data
for Nuclear Energy Applications

- Many nuclear data measurements and evaluations are decades old and updates are needed, especially for new high-fidelity analysis approaches and emerging nuclear energy systems
- Nuclear data measurements are very complex, yet only a few neutron scattering facilities remain, and new capabilities are needed
- Changes in cross section data from one ENDF evaluation to the next can have a significant impact on design, licensing, and operational decisions including:
  - ENDF/B-VII.1 updates to uncertainties in ^{235}U and ^{239}Pu ν change the uncertainty in used fuel systems and affect applicability of benchmark experiments for validation
  - ENDF/B-VII.1 update to $^{35}Cl(n,p)$ reaction leads to1000s of pcm reactivity change for fast-spectrum molten chloride salt reactors
  - Missing nuclear data or older evaluations with large uncertainties for materials of interest can be a limiting factor in the design of advanced reactors
  - Pending thermal scattering data for graphite leads to a 900 pcm improvement in reactivity of TREAT with similar effects for HTGR and FHR systems
  - Many other nuclear data needs can be demonstrated through the use of sensitivity/uncertainty methods for relevant applications

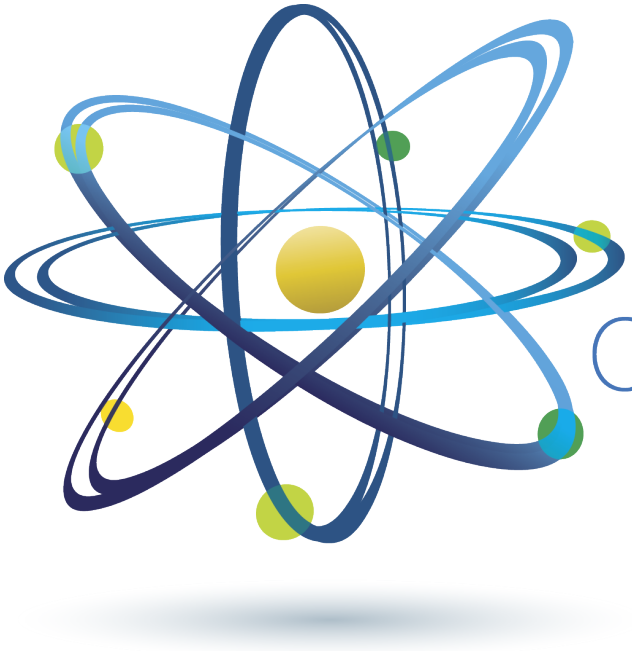


From: N. Touran, "Sensitivities and Uncertainties due to Nuclear Data in a Traveling Wave Reactor", NEA/OECD SG 39 Meeting 2016-05-10

MS-NE-2 – Nuclear Data
Work-scope Description

- MS-NE-2: Improvements to address nuclear data needs that are clearly demonstrated to be a limiting factor in nuclear fuel and reactor design, analysis, safety, and licensing calculations in NE missions areas. (TPOC – TBD)
  - Proposals are sought for achieving relevant nuclear data improvements that address one or more stated needs by developing and demonstrating the enhancements through the entire nuclear data pipeline, from:
    - *1) new nuclear data measurements*
    - *2) evaluation in the appropriate format (e.g. ENDF)*
    - *3) inclusion of nuclear data covariances*
    - *4) processing into usable forms for application codes*
    - *5) confirmation of improved predictions and uncertainties through application studies and validation; &*
    - *6) deployment through the National Nuclear Data Center at BNL for inclusion by external users in quality-assured design, analysis, safety, and licensing calculations*
  - Use of sensitivity and uncertainty analysis methods in proposed efforts is encouraged to demonstrate these needs and how they are being met
  - Many nuclear data needs for NE may be found in the NEA Nuclear Data High Priority Request List (HPRL) (https://www.oecd-nea.org/dbdata/hprl/); also of interest:
    - *continued investigations of thermal scattering data in high-temperature graphite, thermal scattering data for fluorine-based molten salt reactors, and chlorine reactions for fast spectrum molten salt reactors*
    - *documented needs for industry and DOE-NE missions especially as aligned with GAIN (e.g., NEAMS, CASL, ART, TREAT, FCR&D, LWRS)*
  - Proposals must demonstrate the importance of the proposed work to deployment or operation of a reactor (e.g. letter of support/impact from industry)

Questions?



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