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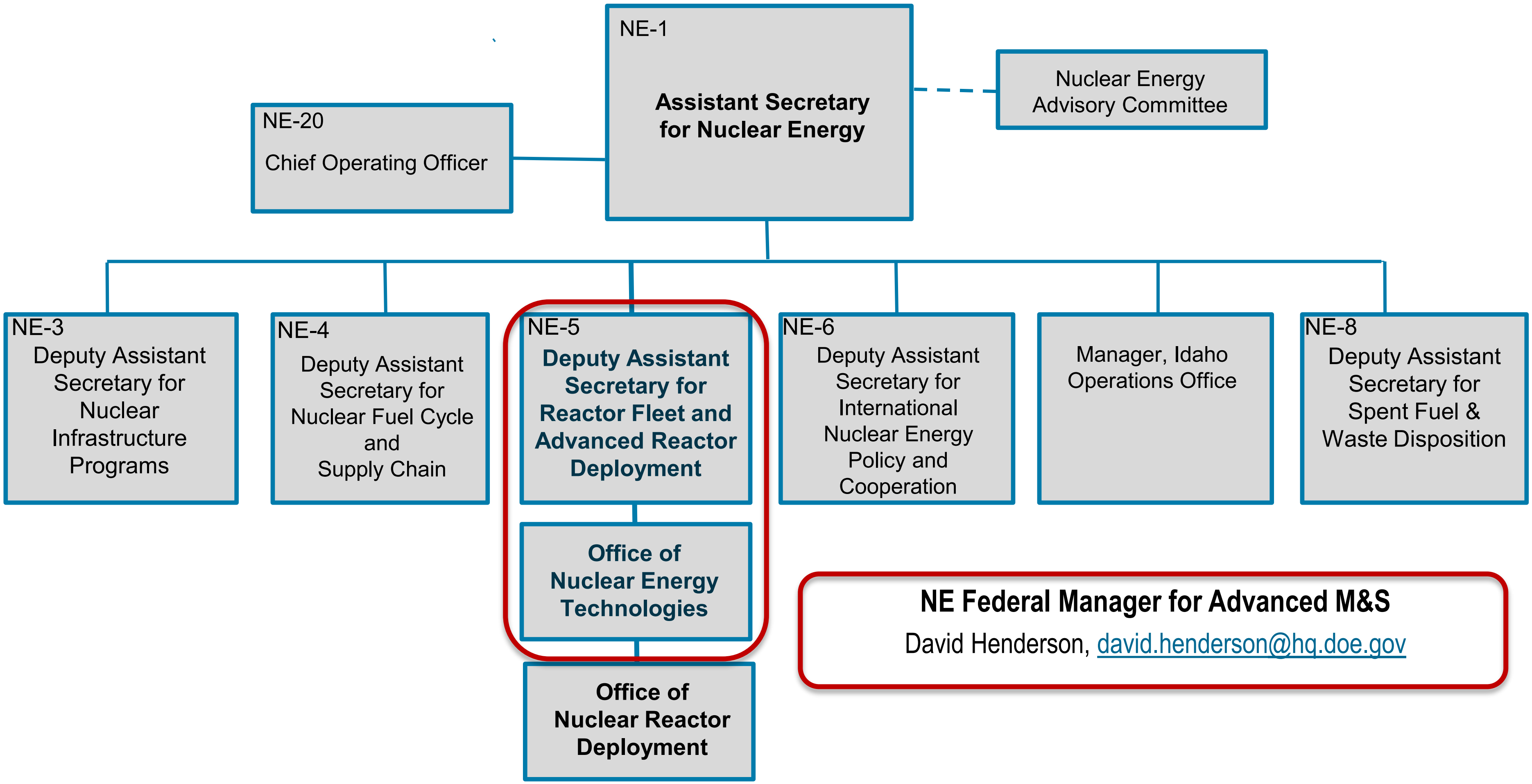
Nuclear Energy
Advanced Modeling & Simulation

CINR Annual Planning Webinar - August 2020

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?



NE Federal Manager for Advanced M&S

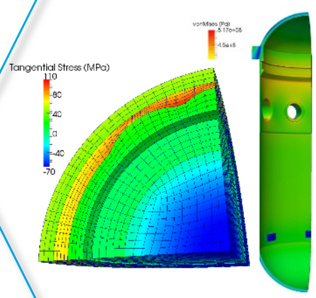
David Henderson, david.henderson@hq.doe.gov

Advanced Modeling & Simulation

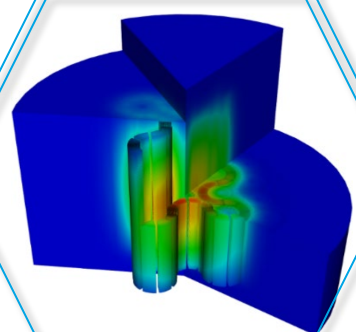
Mission: to develop, demonstrate, and deploy usable advanced modeling and simulation capabilities to enable the deployment of innovations that align with the NE Mission for the existing fleet, advanced reactors, and fuel cycles

Context: early stage R&D performed must be relevant to industry and coordinated with NRC

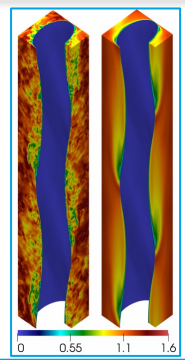
Focusing on core competencies to fill gaps:



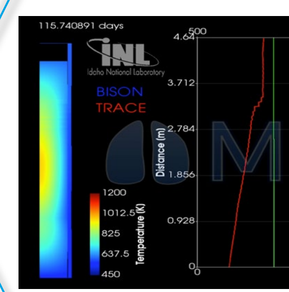
Multiscale fuel performance and structural materials degradation modeling: BISON, GRIZZLY, YellowJacket



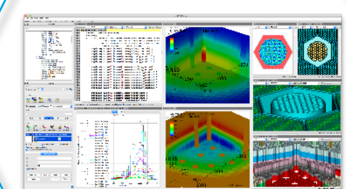
Reactor Physics: GRIFFIN, MPACT, Shift



Multiscale thermal fluids: SAM, PRONGHORN, Sockeye, Nek5000



Multiphysics: MOOSE, VERA



Workflow Management: Workbench

Advanced Modeling & Simulation
Underpins NE's Mission Focus Areas

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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

Existing Fleet | Advanced Reactor Pipeline | Fuel Cycle Infrastructure

- **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

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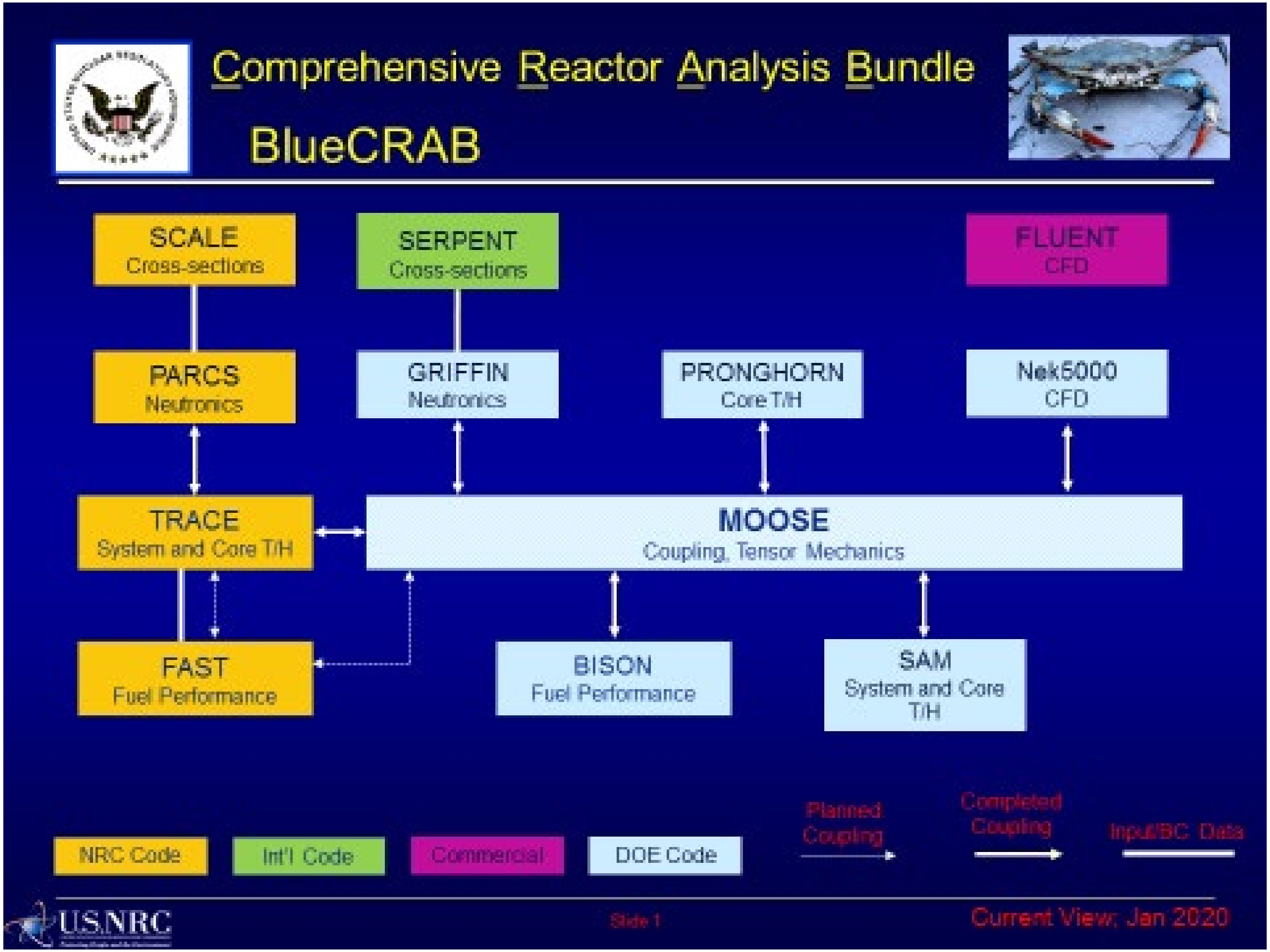
Advanced Modeling & Simulation
Supporting NE's Mission Focus Areas

Existing Fleet | **Advanced Reactor Pipeline** | Fuel Cycle Infrastructure

- **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*

		LWR	Non-LWR
Integration		MOOSE	MOOSE
System Analysis	Plant	VERA	SAM
Core Analysis	Neutronics-Pin Resolved	MPACT	Griffin (Rattlesnake, Proteus)
	Neutronics-Monte Carlo	Shift	Shift
	Neutronics-Kinetics/Depletion	MPACT	Griffin (MAMMOTH)
	Neutronics-Cross Sections	SCALE	Griffin (MAMMOTH)
	T-H Low Res	Cobra-TF (CTF)	SAM
	T-H Med Res		Pronghorn
	T-H Hi Res (CFD)	External codes/Nek5000	Nek5000
	Structural Mechanics	Grizzly Diablo	Grizzly Diablo
Fuel Analysis	Continuum	BISON	BISON
	Microstructure	Marmot	Marmot
	Component Aging	Grizzly Marmot	Grizzly Marmot
	Chemistry	MAMBA	MAMBA Yellowjacket (future)

NEAMS Chemistry Efforts

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Input from from MSR stakeholders has led to NEAMS instigating efforts in several areas of relevance to MSRs (which is being coordinated with ART-MSR Campaign and NE-4 efforts).

THERMODYNAMICS (MSTDB)

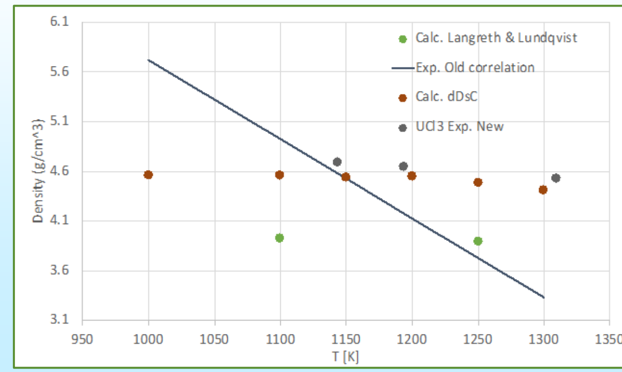
A particular emphasis of NEAMS program is our contribution to the development to the Molten Salt Thermodynamic Database (MSTDB)

54 pseudo-binary systems			26 pseudo-ternary systems	
NaF-LiF	UF_4-NaF	UF_4-ThF_4	LiF-BeF_2-UF_4	NaF-BeF_2-ThF_4
BeF_2-LiF	UF_3-NaF	CsF-ThF_4	LiF-BeF_2-ThF_4	NaF-BeF_2-UF_4
KF-LiF	CsF-NaF	CeF_3-ThF_4	LiF-BeF_2-NaF	NaF-BeF_2-PuF_3
RbF-LiF	LaF_3-NaF	UF_4-PuF_3	LiF-BeF_2-PuF_3	NaF-UF_4-ThF_4
CaF_2-LiF	ThF_4-BeF_2	CsF-PuF_3	LiF-NaF-UF_4	NaF-KF-CaF_2
ThF_4-LiF	PuF_3-BeF_2	LaF_3-PuF_3	LiF-ThF_4-PuF_3	LiF-KF-NaF
PuF_3-LiF	UF_4-BeF_2	RbF-UF_4	LiF-CaF_2-ThF_4	LiF-KF-CsF
UF_4-LiF	RbF-KF	CaF_2-UF_4	LiF-UF_4-PuF_3	LiF-KF-RbF
UF_3-LiF	CaF_2-KF	LaF_3-CsF	LiF-LaF_3-CsF	LiF-KF-CaF_2
CsF-LiF	PuF_3-KF	NaCl-$MgCl_2$	LiF-NaF-LaF_3	LiF-CaF_2-LaF_3
CeF_3-LiF	CsF-KF	NaCl-CsCl	LiF-NaF-RbF	LiF-CeF_3-ThF_4
LaF_3-LiF	LaF_3-KF	NaCl-$PuCl_3$	LiF-NaF-PuF_3	NaF-CaF_2-LaF_3
BeF_2-NaF	PuF_3-RbF	NaCl-UCl_3	LiF-CsF-PuF_3	BeF_2-UF_4-ThF_4
KF-NaF	CsF-RbF	$MgCl_2$-CsCl		
RbF-NaF	LaF_3-RbF	$MgCl_2$-$PuCl_3$		
CaF_2-NaF	ThF_4-CaF_2	$MgCl_2$-UCl_3		
ThF_4-NaF	LaF_3-CaF_2	$MgCl_2$-KCl		
PuF_3-NaF	PuF_3-ThF_4	$PuCl_3$-UCl_3		

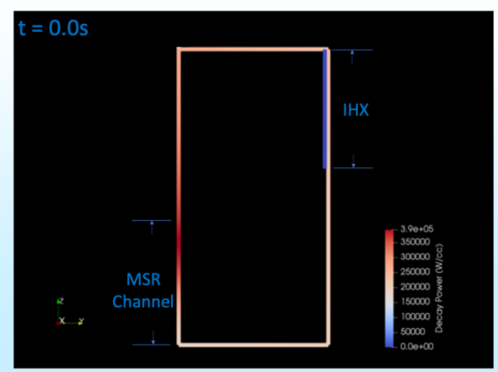
Recent NEUP award will expand investment in MSTDB by supporting research at Univ. of South Carolina ("Extension of MSTDB to Provide a High Quality, Validated Thermochemical Database for Predicting/Simulating Corrosion in Molten Salt Reactor Systems").

PHYSICAL PROPERTIES (DFT)

UCl_3 Density



SYSTEMS ANALYSIS (SAM)



NEAMS-1 ADVANCING MATERIAL MODELING IN SYSTEM ANALYSIS MODULE (SAM) CODE (up to 2 years & $400,000) TECHNICAL POC: Rui Hu (ANL)

- **Purpose:**
  - To support the development of materials transport modeling capabilities for non-LWR reactor safety assessment and source term evaluation
  - Material performance under high temperature irradiative and corrosive environments remains a key challenge for non-LWR reactor applications
- **Scope:**
  - Additional capabilities in the SAM code, such as:
    - Materials transport of contamination species in the primary loop
    - Capabilities for coolant-material interactions and the transport of fission products at the system level
    - Computationally efficient yet accurate lumped parameter material models into system-level analysis code SAM for both normal operation and transient safety evaluations
    - Advanced reduced-order material models (such as production, transport, precipitation and corrosion) and integrating those into SAM

Advanced Modeling & Simulation

NEAMS-2: Corrosion in Molten-Salt Components

NEAMS-2: CORROSION MODELING FOR MOLTEN-SALT-FACING STRUCTURAL COMPONENTS (UP TO 3 YEARS AND $700,000)

TECHNICAL POC: Ben Spencer (INL)

- **Background:**
  - Multiple non-LWR reactor designs are currently being developed that employ either fuel-bearing molten salts or non-fueled salts for a coolant.
  - The corrosive nature of these salts imposes significant challenges to the structural integrity of the components interfacing with the salt.
  - Robust mod-sim capabilities that can predict the evolution of corrosion in such components at scales of engineering relevance are essential for understanding the implications of design decisions on the service lives of such reactors.
- **Desired Scope:**
  - Develop capabilities for simulating the processes involved in corrosion in alloys relevant for these reactors.
  - Physically realistic models of these processes at the mesoscale are essential, and there must be a clear path to allow the results of mesoscale simulations to be used to inform predictive engineering-scale models
  - **Work done in response to this call must be captured and made deployable as part of the NEAMS-supported tools (finite-element-based codes using the MOOSE platform – Grizzly and Yellowjacket – and spectral-solver-based NEAMS codes (contact TPOC)**

Advanced Modeling & Simulation
NEAMS-3: High-Fidelity Pebble Bed Simulation

NEAMS-3: NEXT GENERATION, HIGH-FIDELITY PEBBLE-BED SIMULATION (up to 3 yrs & $600,000)

TECHNICAL POC: TBD

- **Background:**
  - One major challenge to current PBR analysis is the creation of accurate multigroup cross sections during the depletion cycle
  - The spectrum a pebble of a certain burnup sees in the core does not only depend on where in the core it is, but also on the composition of the pebbles around it; these conditions constantly change making a traditional precomputing and tabulation approach infeasible
  - Another challenge is the reliance on homogenized pebble depletion models
  - Flow of pebbles is currently modeled as incompressible flow and single pebbles are not resolved
  - NEAMS reactor physics code Griffin is developing pebble tracking transport (PTT) method, but PTT has not yet been extended to pebble depletion
- **Desired Scope:**
  - Proposals that address above issues and transcend the accuracy and fidelity of current models for pebble-bed reactor depletion – both the equilibrium core (asymptotic state after long enough runtime) and the running-in phases (transient phase before reaching the equilibrium core)
  - New methods should address challenges with current models and allow for “reference calculations” which can benchmark lower-fidelity solutions
  - Integration of capabilities into the NEAMS tool Griffin is desired

NEAMS-4: FUNDAMENTALS OF MULTIPHASE BOILING FLOW FOR HIGH-PRESSURE, HIGH-VOID CONDITIONS (up to 3 years & $800,000)

Technical POC – Rui Hu (ANL)

- **Background**
  - Prediction of two-phase flow behavior is essential to the operational performance and safety of LWRs as well as the power generation systems in many non-LWRs
  - Key parameters of interest are: void and pressure distribution over the range of boiling flow regimes that includes bubbly, slug, churn, and annular flow. Especially important is the film boiling behavior at which dry-out conditions occur that can lead to fuel failure
  - Fundamental understanding of two-phase flow, including the measurement of high-resolution, high pedigree data, is essential to advancing the predictive simulation capabilities
- **Scope:**

  Characterizing flow boiling characteristics in high-pressure, high-void-fraction flow regimes relevant to the operation and safety of reactor systems. Key aspects include:
  - High-res, multi-phase TH testing for nuclear energy applications, including evaluation of surface effects, void fraction distributions and phasic velocities.
  - Development of relevant closure models for prediction of slug, droplet and film phenomena in multi-phase computational fluid dynamics and subchannel analysis tools (Nek2P and CTF).
  - Establishment of a high-fidelity database for validation of high-void-fraction flow regime models and simulations

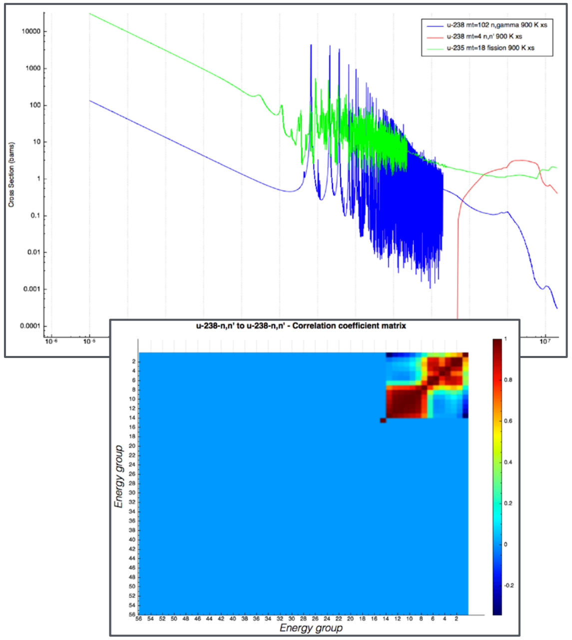
NEAMS-5: TIME-DEPENDENT MONTE CARLO SIMULATION CAPABILITY DEVELOPMENT (up to 3 years & $600,000)

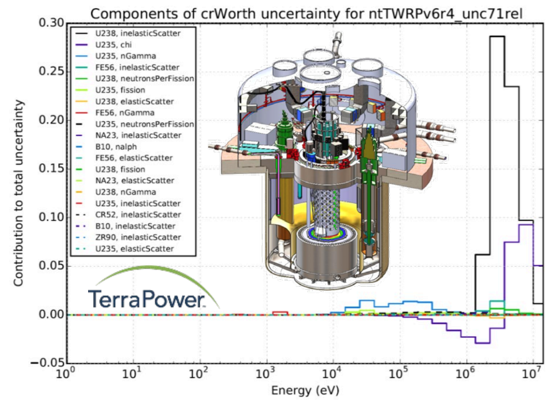
Technical POC – Matt Jessee (ORNL)

- **Background**
  - Continuous-energy Monte Carlo (MC) is generally limited to steady-state calculations of critical core configurations and fixed-source fluence analysis
  - Challenges with time-dependent MC analysis are well-known and include, for example, the need to achieve sufficient particle histories required for converged reaction rates for a given set of tally regions
- **Scope:**
  - Development of computationally efficient, robust MC time-dependent capabilities for reference solutions for NEAMS codes (Griffin and VERA) for transient and depletion ModSim
  - Proposals should focus on methods and algorithms that address the statistical nature of the MC method via novel approaches for error control, hybrid approaches for efficient importance sampling, and/or acceleration approaches for performing multiphysics iterations
  - Comparisons against a brute force approach of large particle history reactor simulation with user-defined time-dependent reactor state conditions should be part of the proposal
  - Proposed capabilities must be able to be implemented in the Shift Monte Carlo code, and demonstration of the approach in/with Shift is preferred

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 2016-05-18

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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