MODELING & SIMULATION NEEDS FOR ADVANCED REACTOR DESIGN AND LICENSING

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IMPORTANCE OF MODELING & SIMULATION

Bigger role for advanced reactors

- All early prototypes were largely an outcome of big experimental programs
  - Existing pressurized and boiling water reactor fleet also benefited from availability of substantial testing infrastructure

- M&S play a much bigger role in advanced reactor design and licensing
  - Wide range of advanced reactor concepts, each with multiple design variants
  - Diverging experimental needs with limited cross-cutting testing opportunities

- Legacy codes were developed using wealth of data from LWR operations and tests, but their applicability to different spectra, coolants and fuel forms is limited
  - Predictive analytical capabilities with reduced empiricism and closer-to-first-principles solutions are needed
  - Once validated, mechanistic models can be more confidently applied to new domains where the experimental data is sparse (but not absent)
  - M&S also helps with planning of more targeted testing programs
NEAMS PROGRAM

Nuclear Energy Advanced Modeling and Simulation

- A DOE-NE program to support development and deployment of advanced reactors and sustainability of operating LWRs
- Aims to expand the M&S basis for next generation reactors beyond the existing computer codes that were developed throughout 1970s
  - Fast reactors (SFR, LFR, GFR)
  - Thermal reactors (HTGR, FHR)
  - Molten salt fueled reactors (fluoride-thermal or chloride-fast spectrum MSRs)
  - Heat-pipe cooled fast or thermal micro-reactors
- Contributions from six national labs under six technical areas: Neutronics, thermal-fluids, fuels, structural/chemistry, multiphysics, and application drivers
- Program priorities are determined based on input from NRC, the industry council (coordinated by NEI), and other DOE programs like ART
NEAMS PROGRAM (Cont.)

- Multiscale (in space and time) simulation capabilities based on fundamental understanding of physical phenomena
  - Take advantage of advances in numerical methods and software engineering
  - Modern software quality assurance practices including V&V of physics models
  - Development of "best practices" to support their use in different applications

- Diverse interdependence of neutronic, fuel response, thermal-fluids, structural, and chemical phenomena also pose unique multiphysics M&S challenges
  - MSRs with moving fuel, chemistry and corrosion modeling
  - Pebble-bed concepts with double-heterogeneity in a gradually moving porous core
  - Fast reactors with a wider range of reactivity feedback phenomena
  - Micro-reactors with heat-pipe cooling
  - Applications that require moving-mesh multi-physics
  - Need for broad range of consequence analyses as part of risk-informed approach
MULTI-SCALE APPROACH

- Transient system analyses with which major physics of the entire plant and integral effects are captured but with large uncertainties
  - Geometry is coarsely modeled with empirical component models
  - Correlations (pressure drop and heat transfer) with limited validity
  - Point-kinetics to capture changes in core power with reactivity feedback
  - Supplementary models for transient fuel behavior (to identify cliff edges) and source term assessments

- Higher-order, high-fidelity solvers for more complex systems of equations that enable closer-to-first-principles solutions for core/component design/optimization
  - Computational Fluid Dynamics (CFD) for thermo-fluid calculations
  - Computational Structural Mechanics (CSM) for stress-strain evaluations
  - Space-time kinetics for variations in core power shape and level
  - Better accuracy allows reduced conservatism, increased safety assurance, and assessment of uncertainties in legacy tools and system simulations
FUNCTIONAL M&S AREAS

- Core design and assessment of reactor operations: GRIFFIN and SHIFT
  - Tools for entire neutronics analysis cycle from cross-section generation to neutron and radiation transport solutions, depletion calculations and sensitivity analyses
  - Deterministic analysis capabilities for complex, deformable geometries, transport-based perturbation theory for reactivity feedback evaluations

- Steady-state and transient fuel performance modeling: BISON and MARMOT
  - Multi-dimensional engineering scale assessment of new fuel forms
  - Mesoscale material development for prediction of microstructure evolution

- Thermal-fluids design support
  - System Analysis Module (SAM) for transient safety assessments
  - Multi-assembly subchannel analysis and distributed resistance models to calculate core-wide flow distributions and temperature profiles (Pronghorn)
  - CFD with DNS, LES, and URANS modeling options (Nek5000/NekRS)
  - Multi-phase heat transfer in a heat pipe for micro reactor concepts (Sockeye)
FUNCTIONAL M&S AREAS (Cont.)

- Structural mechanics and chemistry modeling (*Grizzly* and *YellowJacket*)
  - For modeling of degradation mechanisms and their progression for reactor structures, systems, and components subjected to aggressive thermal conditions
  - Multiphysics coupling with chemistry models for assessment of environmental degradation and corrosion concerns

- Source term assessments through models for radionuclide release, transport, retention, and dispersion through multiple barriers
  - MAR inventory assessments in the reactor, in/ex-vessel storage locations, coolant and cover-gas cleanup systems, and chemical processing/refueling systems
  - Identifying release pathways and phenomena associated with radionuclide transport and retention, and their modeling from source to environment
  - Application of these models to a spectrum of accidents (AOOs, DBAs, and BDBAs) for evaluation frequency/consequence evaluations and risk assessments
POTENTIAL ROLE OF ML&AI

- Machine learning can help building new models based on data when integrated with numerical and/or experimental techniques
  - Interface with DOE-ASCR program that provides ready-to-use machine learning techniques to explore their use in nuclear with high performance computing

- Some examples include:
  - Multiscale analysis of system transients for spatial/temporal integration of cascade of relevant scales
  - Development of a reduced order model (ROM) from more complex, high-fidelity models to capture system’s dominant response in engineering-scale simulations
  - Integration of fine-scale simulation techniques with distributed sensing technology for reconstructing high-resolution fields from sparse data
  - “Edge computing” through distributed sensors that can incorporate machine learning at the point of measurement

- This could be a potentially new focus area with greater ARPA-E collaboration
VALIDATION NEEDS

Test data is still gold

- NEAMS program does not directly support experiments but interfaces with other DOE programs like Advanced Reactor Technologies (ART) that offers sufficient test data for some advanced concepts (SFRs and HTGRs)
  - Integral tests from EBR-II, FFTF, and TREAT (leveraged in intl. collaborations for data from Monju, Phenix, CABRI, HTTR)
  - Separate effect tests at NSTF, HTTF and AGR (leveraged in intl. collaborations for data from SANA, PLANDTL, PLAJEST, TALL3D…)
  - New MSRE benchmark

- Still leaves a large “data deficit” for validation of M&S tools for some advanced reactor concepts and specialized tools/methods
  - Interfaces with DOE-NE University Program (NEUP) to close validation data gaps
  - DOE-NE’s ART Micro-Reactor Campaign is also planning an extensive testing program (SPHERE, MAGNET, MARVEL…)

Test data is still gold
SUMMARY

- Bigger role of M&S for next generation non-LWRs with multiple design variants due to differences in neutron spectra, coolant choices, and fuel types

- DOE-NE’s NEAMS program aims to expand the M&S basis for beyond the existing computer codes
  - Multi-scale neutronics, fuels, thermal-fluids, structural & chemistry core capabilities, and their multi-physics integration

- Program priorities based on NRC, industry council, and other DOE program input
  - Also looking forward to input from ARPA-E community

- Plans to continue addressing V&V needs through collaborations with DOE’s ART and NEUP programs (and potentially ARPA-E?)

- For more information about NEAMS codes and how to obtain them, pls contact:
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