Cross-Cutting Capabilities for Depletion, Nuclear Data, Uncertainty Quantification, and Benchmark Projects

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Messages we received

**HTGR @HTG** Reactor Neutronics and Depletion Codes @neams_doe

**HTGR @HTG** Shielding and Source Term Calculation Codes @neams_doe

**Fast Reactor @FR** Shielding and source term calculation codes: A code that takes the fuel isotopic inventory as input and can calculate releases under various accident scenarios for multiple types of reactors is crucial. @neams_doe

**HTGR @HTG** Nuclear Cross-section Generation Codes @neams_doe

**Molten Salt @MSR** Multi group Nuclear Data – Material composition and temperature characteristics of material – ultra fine nuclear data – self shielding. @neams_doe

**FHR @FHReactor** MSR (salt chemistry and corrosion, production transport of activation products including F-16 and tritium in primary salt loops). @neams_doe

**Molten Salt @MSR** Distribution of delayed neutrons @neams_doe

**Molten Salt @MSR** Tritium Transport/Corrosion Control. @neams_doe

**Fast Reactor @FR** Improved nuclear data and uncertainties @neams_doe

**HTGR @HTG** Verification and validation of commonly used codes @neams_doe

**Fast Reactor @FR** Need a comprehensive program for codes/tools V&V @neams_doe
There are known knowns; there are things we know that we know. There are known unknowns; that is to say, there are things that we now know we don't know. But there are also unknown unknowns – there are things we do not know we don't know.
—United States Secretary of Defense, Donald Rumsfeld, 2002

<table>
<thead>
<tr>
<th>KNOWN KNOWNS</th>
<th>KNOWN UNKNOWNS</th>
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<tbody>
<tr>
<td>Measurements/Observations</td>
<td>Uncertainty Quantification</td>
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<table>
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<tr>
<th>UNKNOWN KNOWNS*</th>
<th>UNKNOWN UNKNOWNS</th>
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<tr>
<td>Communication</td>
<td>Safety Margins</td>
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Topics to Discuss

- Depletion and source terms
- Nuclear data
- Uncertainty analysis
- Benchmark handbooks
Depletion and Source Terms

- Oak Ridge Isotope Generation code (ORIGEN)
- Irradiation and decay simulation code
- Fuel depletion and used fuel characterization
- Source terms for accident analyses (operating reactors, spent fuel handling, storage, etc.)
- Structural material activation (in-core, ex-core)
- Material feed and removal for fuel cycle and liquid fuel
- ORIGEN data enable comprehensive isotopic characterization of fuel over a large time scale, including repository analysis
ORIGEN Capabilities

Fuel depletion and used fuel characterization
- Nuclide concentrations (atoms and mass)
- Activities
- Decay heat
- Radiation emission rates and spectra (neutron and gamma)
- Radiotoxicity

Explicit simulation of nuclides in database
- 176 actinides
- 1151 fission products
- 910 structural activation nuclides

Explicit simulation of all pathways from neutron transmutation, fission, and decay
- ORIGEN tracks 2237 isotopes
- Includes all nuclides with half-lives > 1 ms
- Accurately represents the evaluated nuclear data
- Many physics codes track a small subset of isotopes

Multiple solvers

Modern API to interface with other tools

Available with SCALE 6.2

Integrated with many other tools
- PROTEUS
- BISON
- MPACT
- Shift
The ORIGEN Species

Notes
- DOE halted support for ORIGEN2 in 1989
- DOE and NRC continue to support development of ORIGEN in SCALE

- SHARP / PROTEUS
- BISON
- MPACT
- Shift
Destructive isotopic assay data
- 120 PWR samples, 60 nuclides

Decay heat measurements
- long decay time (years)
  - 121 PWR & BWR measurements
- short decay time (< 105 s)
  - thermal fission of $^{235}$U, $^{239}$Pu, and $^{241}$Pu
  - fast fission of $^{233}$U and $^{238}$U

Gamma spectra (burst fission)
- thermal fission of $^{235}$U, $^{239}$Pu, and $^{241}$Pu

Neutron spectra - SF and ($\alpha$,n) sources

Tritium production for MSRE

Need additional benchmark data for advanced reactors!
ORIGEN Runtimes

1946 nuclides, 35013 reactions

Depletion step without substeps
- Original solver: 44-152 ms (depending on step length)
- CRAM solver: 41-50 ms (depending on source order)

Decay-only step without substeps
- Original solver: 4.2-6.7 ms
- CRAM solver: 12-13 ms

Substeps
- Original solver: 4-10 required for reliable results
- CRAM solver: usually none required, at most 2-4
Sources of Nuclear Data

Nuclear Energy

- **Decay data**
  - ENDF/B-VII.1
  - Natural isotopic abundances (NIST database)
  - ICRP 72 inhalation dose coefficients, EPA Report 12 external exposure

- **Neutron reaction cross section data**
  - JEFF 3.1/A special purpose activation file
  - ENDF/B-VII.0, -VII.1

- **Fission product yields**
  - ENDF/B-VII.0

- **Photon emission line-energy data**
  - Evaluated Nuclear Structure Data Files (ENSDF)
  - ENDF/B-VII.1

- **Neutron emission libraries**
  - SOURCES 4C code
  - Spontaneous fission decay and delayed neutron data
  - Alphas stopping powers, (α,n) cross sections, excitation levels
Cross-Section Generation for ORIGEN

ORIGEN requires a single space and energy-average (effective) cross section value per nuclide/reaction.

All reaction cross sections are collapsed using input neutron energy spectrum $\Phi(E)$ of the system from multigroup or continuous-energy eigenvalue calculation.
Accurate Simulations Require Accurate Nuclear Data Libraries

- Decay data are very well known and “constant” (relatively easy)
- Cross sections have much larger uncertainties
- Cross sections are problem dependent and must be determined for the system being analyzing – they depend on:
  - Fuel type
  - Enrichment
  - Burnup
  - Assembly design
  - Fuel temperatures
  - Moderator properties
  - Control rod/blade exposure etc.
ORIGEN Rapid Methodology for Burnup and Source Term Calculations

- Burnup calculation time is limited by flux solve time in assembly/core calculations.
- Can pre-compute finite set of burnup calculations covering some space of assembly design/operation to predict isotopics at arbitrary burnups/decay times.
- Could create isotopics "database" and interpolate.
- Better to create cross section "database" and re-solve depletion for the new system (depletion is fast).
Source Term Characterization

Input capabilities
- Axial moderator density/power distributions
- Radial composition/ORIGEN library assignment (enables approximate pin-by-pin 3D depletion)
- SCALE StdComp integration (e.g. zirc4)

Output capabilities
- Produces binary concentration file (f71)
- SCALE StdComp material file
- MCNP materials file
- Decay heat file

In production use
- NRC
- UNF-ST&DARDS
- NNSA, IAEA, Euratom, etc.

ORIGEN Reactor Libraries in SCALE 6.2
- Pressurized Water Reactors (PWRs)
- Boiling Water Reactors (BWRs)
- Mixed-oxide (MOX) libraries for typical BWRs and PWRs
- Russian VVER reactors
- Russian RBMK reactors
- Canadian CANDU reactors
- UK Advanced Gas Reactors (AGRs)
- MAGNOX Reactors
- IRT Reactors

Other reactor libraries can be generated by the user and/or developer, provided sufficient design information is available.
Source Term Generation with NEAMS Workbench / SCALE 6.2

Assembly-level calculation

Facility-level calculation
Cross-section measurements for resonance region (Data from facilities: IRMM, RPI, and ORELA)

Nuclear data analysis methods development (SAMMY)

Cross-section evaluation and preparation of ENDF/B nuclear data files

Cross-section processing methods development for generating nuclear data libraries (AMPX)

Identification of data needs through application to real-world problems
Continuous-energy data serve as reference solution to confirm multigroup approximations.

- Multigroup cross sections can be generated for any type of system
  - LWR, HTGR, MSR, FHR, SFR, etc. with appropriate energy group structure and weighting spectrum

- Uncertainties in cross sections (covariance data) quantify confidence in deployed data libraries

AMPX developed and deployed with SCALE

Uncertainty in $k_{\text{eff}}$ Due to Nuclear Data Uncertainties: 1,435 pcm!

<table>
<thead>
<tr>
<th>nuclide-reaction</th>
<th>with</th>
<th>nuclide-reaction</th>
<th>% $\Delta k/k$ due to this matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>u-238 n,n'</td>
<td></td>
<td>u-238 n,n'</td>
<td>1.2053(9)</td>
</tr>
<tr>
<td>na-23 elastic</td>
<td></td>
<td>na-23 elastic</td>
<td>0.3242(2)</td>
</tr>
<tr>
<td>fe-56 elastic</td>
<td></td>
<td>fe-56 elastic</td>
<td>0.2590(3)</td>
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<tr>
<td>u-238 n,\gamma</td>
<td></td>
<td>u-238 n,\gamma</td>
<td>0.2435(1)</td>
</tr>
<tr>
<td>fe-56 n,n'</td>
<td></td>
<td>fe-56 n,n'</td>
<td>0.2388(1)</td>
</tr>
</tbody>
</table>

Incorrect group structure/weighting

Correct group structure/weighting
Uncertainties in nuclear data can be a limiting factor in the design of advanced reactors.

NEAMS is engaging in the development and use of nuclear data uncertainties to be responsive to Advanced Reactors Technology program and industry needs.

- Neutron cross section covariance library based on ENDF/B-VII.1
- Fission product yield covariances
- Decay data covariances
- Gamma yield covariances

From: N. Touran, "Sensitivities and Uncertainties due to Nuclear Data in a Traveling Wave Reactor", NEA/OECD SG 39 Meeting 2016-05-10
SCALE 6.2 Covariance Library

- ENDF/B-VII.1 for 187 isotopes
- Modified ENDF/B-VII.1 $^{239}$Pu nubar, $^{235}$U nubar, H capture, and several fission product uncertainties, with data contributed back to ENDF repository for ENDF/B-VIII
- "Low-fidelity" data for ~215 nuclides missing from ENDF/B-VII.1
- Fission spectrum (chi) uncertainties processed from ENDF/B-VII.1 and from JENDL 4.0 (minor actinides)
  - Previous SCALE chi uncertainties were generated from Watt spectrum data and data were missing for minor actinides
- 56- and 252-group energy structures
- 33-group fast reactor library in development
Sensitivity/Uncertainty (S/U) Analysis for M&S Validation

- Establish impact of data uncertainties on M&S Results (uncertainty quantification)
  - Bias margins for criticality safety
  - Design margins for advanced reactors
  - Safety margins for decay heat and criticality in UNF analysis

- Selection and design of benchmark experiments for M&S validation (similarity analysis)
  - Maximizes information contained in existing integral experiments
  - Enables design of more relevant experiments

- Consolidation of measured and computed results for improved reliability (assimilation/adjustment)
  - Provides adjusted data that reduces bias and uncertainty in calculations
  - Recommend data improvements to nuclear data evaluators
Two Approaches to Uncertainty Analysis

Stochastic Sampling (Dakota, SCALE/Sampler)

- Covariances of input data sampled; statistical analysis of output distribution gives uncertainties

- Pros
  - Typically minimally invasive to code
  - Can address complex simulations with coupled codes

- Cons
  - Quantification of separate effects (sensitivity coefficients) is challenging

Sensitivity Methods (SCALE/TSUNAMI, PERSENT)

- Sensitivities are computed and combined with covariances to obtain uncertainties

- Pros
  - Quantifies uncertainty contributors
  - Obtains all data sensitivities for a single response in single calculation

- Cons
  - Requires invasive implementation of adjoint solution in simulation codes
  - Limited to radiation transport applications
UQ analysis by Monte Carlo sampling can be applied to any type of SCALE calculation

- Sampler provides uncertainty in any computed result due to uncertainties in:
  - neutron cross sections ($\sigma$)
  - fission product yields ($Y_f$), decay data ($\lambda$), and branching fractions ($b$)
  - Model parameters such as dimensions ($x$) and compositions ($\rho$)
Uncertainties Evolve with Burnup/Decay

Pu isotopic Uncertainty

Decay Heat Uncertainty

Figure 5. Distribution in sampled multiplication factors at 60 GWD/T burnup.
Dakota: Suite of iterative mathematical and statistical methods that interface to computational models

- Algorithms for design exploration and simulation credibility
- Makes sophisticated parametric exploration of simulations practical for a computational design-analyze-test cycle
- Provides scientists and engineers (analysts, designers, decision makers) greater perspective on model predictions:
  - Enhances understanding of risk by quantifying margins/uncertainties
  - Improves products through simulation-based design, calibration
  - Assesses simulation credibility through verification and validation

https://dakota.sandia.gov/
Spearman correlation coefficients for fuel thermal conductivity as a function of time for all outputs of interest for Halden irradiation experiment.
UQ analysis with sensitivities quantifies data contributors to uncertainty
SIMILARITY ANALYSIS: Identifying experiments representative of targeted application

\[ C_k^{(m,n)} = \frac{S^T_k C_{nm} S_k}{\sqrt{\text{Var}(k_m) \text{Var}(k_n)}} \]

- \( c_k = 0.91 \)
- \( c_k = 0.88 \)
S/U methods applied for investigation and design of experimental benchmarks and for safety margin assessment.

The 30B cylinder

These can contain 2270 kilograms of low-enriched uranium in the form of uranium hexafluoride. IAEA regulations include requirements for packages to meet the following test requirements: withstand a pressure test of at least 1.4 MPa; withstand a free drop test; withstand a thermal test at a temperature of 800 °C for 30 minutes. (World Nuclear News)
Availability of S/U Tools

**Dakota** (dakota.snl.gov)
- Stochastic sampling of input parameters, correlations, search, data calibration, etc.

- Eigenvalue S/U for $k_{\text{eff}}$ and reaction rates, integrated with Argonne ARC codes (e.g. DIF3D)

**SCALE 6.2** (scale.ornl.gov)
- TSUNAMI-3D: Monte Carlo with CE and MG eigenvalue S/U capability for $k_{\text{eff}}$ and reaction rates
- TSUNAMI-2D: lattice physics sensitivity analysis
- TSUNAMI-1D: prototyping sensitivity analysis
- TSAR: Reactivity coefficient sensitivity analysis
- Sampler: Stochastic sampling of input and data
- TSUNAMI-IP: Similarity assessment
- TSURFER: Data calibration

**Covariance Data**
- ENDF/B-VII.1; SCALE 6.2;
- COMMARA (fast reactor neutron data)
NEAMS IPL supports U.S. leadership of both the
• International Criticality Safety Benchmark Evaluation Project (ICSBEP) and the
• International Reactor Physics Benchmark Evaluation Project (IRPhEP).

Handbooks generated by these projects provide thousands of benchmark experiments from dozens of countries with an assessment of data integrity, quantification of experimental uncertainties, and thorough technical review with established deployment process.

Strong collaborations with Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA)
Benchmark Evaluation Process

Evaluation Process
- Identify
- Verify
- Evaluate
- Complete
- Calculate
- Document

Peer Review (National and International Exports)

Comprehensive Source of Externally Peer Reviewed Integral Benchmark Data

Future Use
- Advanced Modeling and Simulation
- Analytical Methods Development, Validation, and Verification
- Reactor Design and Licensing
- Training
- Criticality and Reactor Safety Analysis
- Fuel Cycle and Related Activities
- Range of Applicability and Experiment Design
- Nuclear Data Refinement

Short-Term Preservation
- Externally Available Technical Journals & Reports
- Informal Reports Letters & Memos
- Logbooks
- Drawings
- Experimenter’s Annotated Copy of Published Reports
- Experimenter (Retired or Working on Other Projects)
- Facilities Awaiting D&D

Benchmark Experiment Data
Benchmark Evaluation Process
International Handbook of Evaluated Criticality Safety Benchmark Experiments

- September 2016 Edition
- 22 Contributing Countries
- ~69,000 Pages
- 570 Evaluations
  - 4,913 Critical, Near-Critical, or Subcritical Configurations
  - 45 Criticality-Alarm-Placement/Shielding Configurations
  - 215 Configurations with Fundamental Physics Measurements
  - 829 Unacceptable Experiment Configurations

http://icsbep.inl.gov/
https://www.oecd-nea.org/science/wpnscs/icsbep/
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  - 147 Approved Benchmarks
  - 4 DRAFT Benchmarks

http://irpheap.inl.gov/
http://www.oecd-nea.org/science/wprs/irphe/
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