U.S. DEPARTMENT OF ENERGY | Nuclear Energy

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

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GAIN/EPRI Advanced Reactor Modeling and Simulation Workshop #2
EPRI Charlotte Campus
January 24-25, 2017

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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

Knowledge Management

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

KNOWN KNOWNS Measurements/Observations	**KNOWN UNKNOWNS** Uncertainty Quantification
UNKNOWN KNOWNS* Communication	**UNKNOWN UNKNOWNS** Safety Margins

All models are wrong, some are useful.
–George E. P. Box – Statistician, Professor, Univ. of Wisconsin

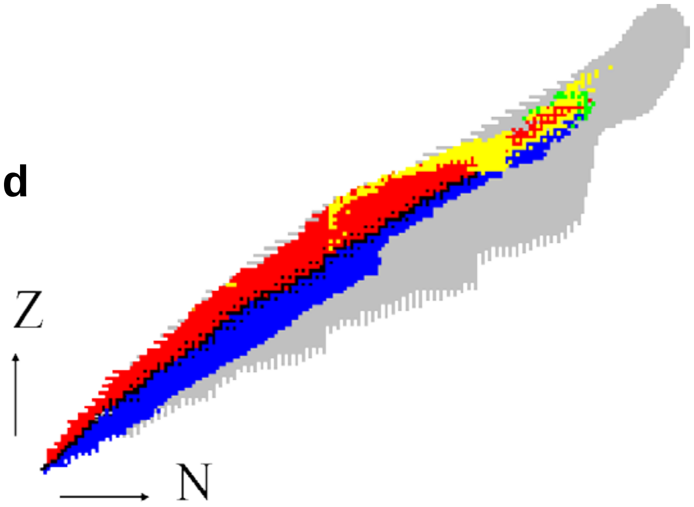
*Girard, John; Girard, JoAnn (2009-06-01). A Leader's Guide to Knowledge Management: Drawing on the Past to Enhance Future Performance. Business Expert Press.

Topics to Discuss

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

Depletion and Source Terms

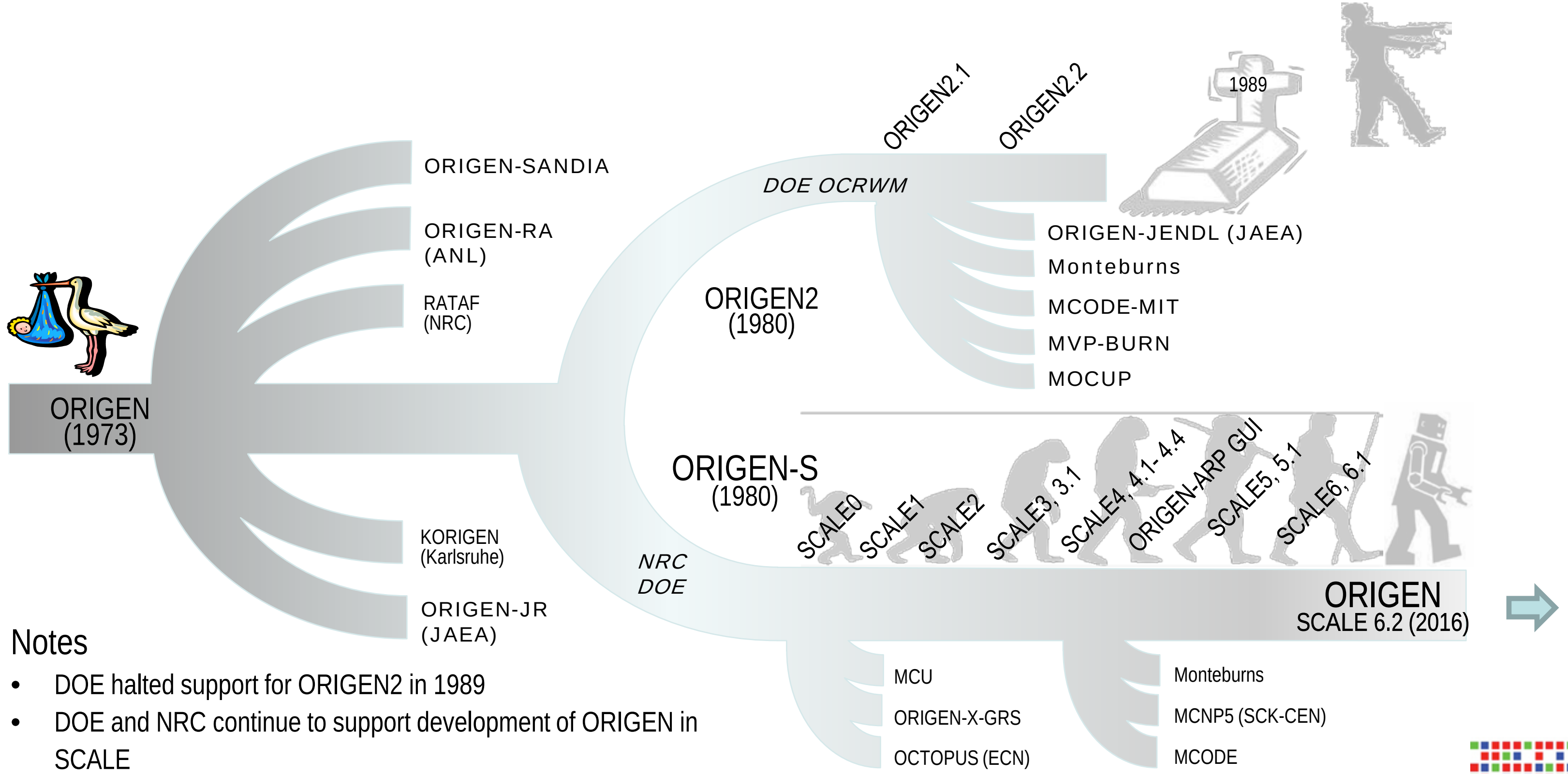
- Oak Ridge Isotope Generation code (ORIGEN)
- Irradiation and decay simulation code
- Fuel depletion and used fuel characterization
- Source terms for accident analyses (operating reactors, spent fuel handling, storage, etc.)
- Structural material activation (in-core, ex-core)
- Material feed and removal 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



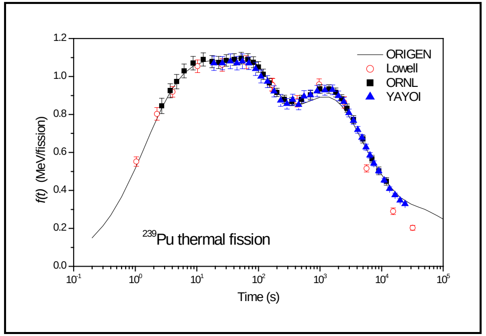
- SHARP / PROTEUS
- BISON
- MPACT
- Shift

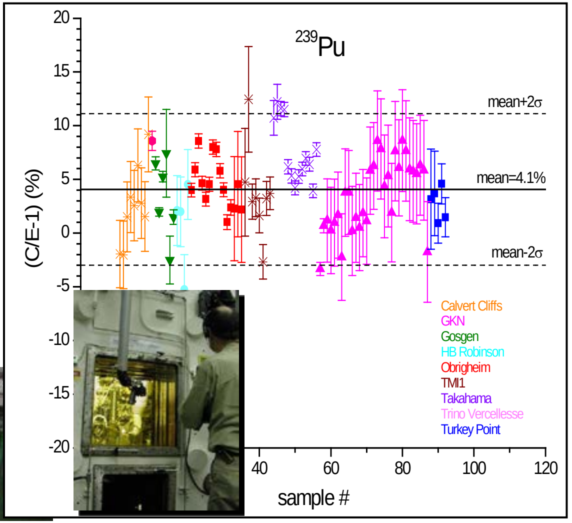
Notes

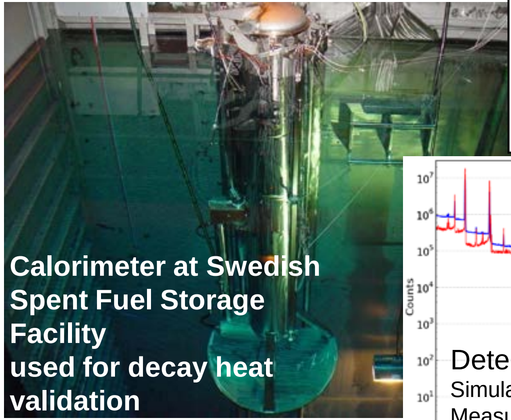
- DOE halted support for ORIGEN2 in 1989
- DOE and NRC continue to support development of ORIGEN in SCALE

ORIGEN
Benchmarking and Validation

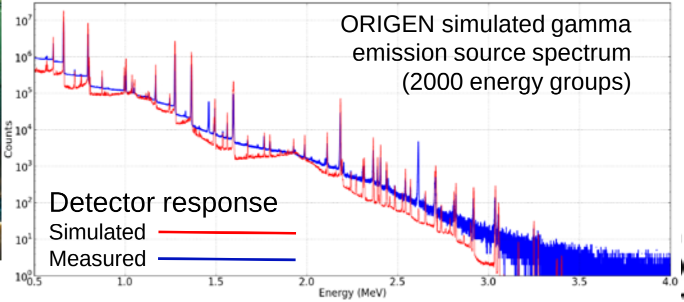
- **Destructive isotopic assay data**
  - 120 PWR samples, 60 nuclides
- **Decay heat measurements**
  - long decay time (years)
    - 121 PWR & BWR measurements
  - short decay time (< 105 s)
    - thermal fission of ^{235}U, ^{239}Pu, and ^{241}Pu
    - fast fission of 233U and 238U
- **Gamma spectra (burst fission)**
    - thermal fission of ^{235}U, ^{239}Pu, and ^{241}Pu
- **Neutron spectra - SF and (α,n) sources**
- **Tritium production for MSRE**
- **Need additional benchmark data for advanced reactors!**







Calorimeter at Swedish Spent Fuel Storage Facility used for decay heat validation

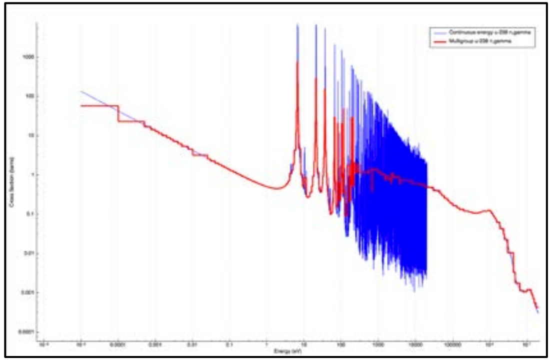


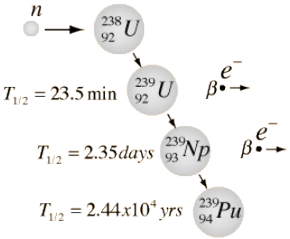
ORIGEN Runtimes

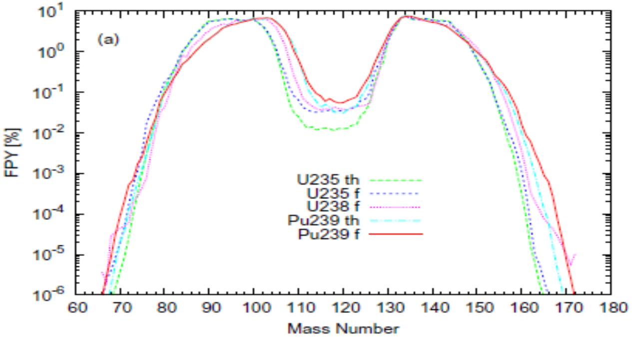
- **1946 nuclides, 35013 reactions**
- **Depletion step without substeps**
  - Original solver: 44-152 ms (depending on step length)
  - CRAM solver: 41-50 ms (depending on source order)
- **Decay-only step without substeps**
  - Original solver: 4.2-6.7 ms
  - CRAM solver: 12-13 ms
- **Substeps**
  - Original solver: 4-10 required for reliable results
  - CRAM solver: usually none required, at most 2-4

Sources of Nuclear Data

- **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







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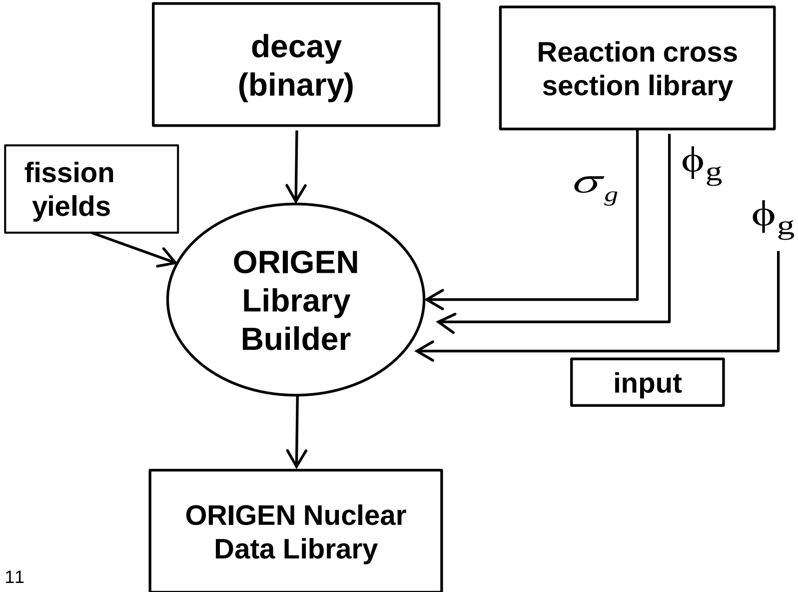
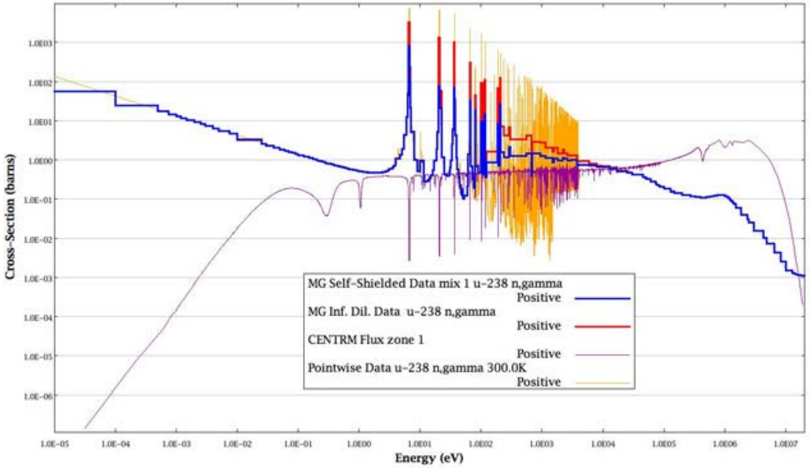
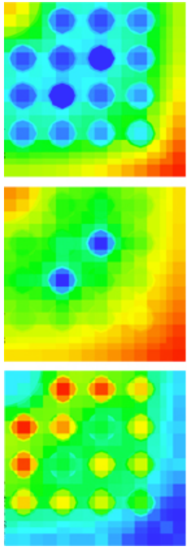
Cross-Section Generation for ORIGEN

- **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 Φ(E) of the system from multigroup or continuous-energy eigenvalue calculation**

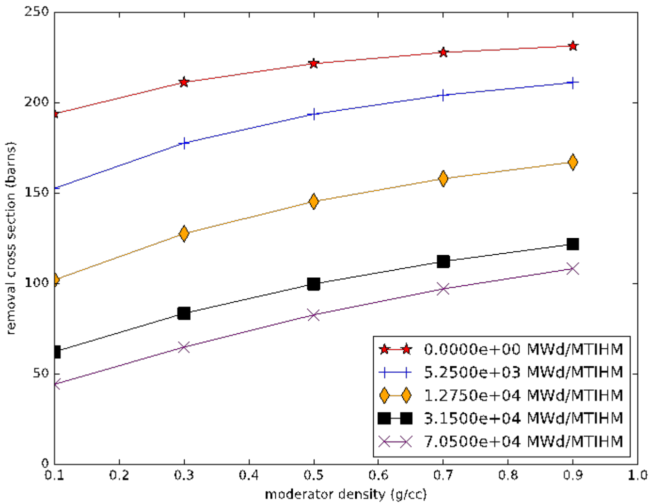






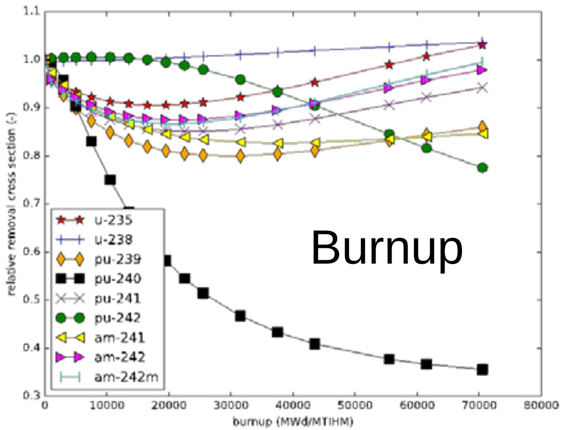
Accurate Simulations Require Accurate Nuclear Data Libraries

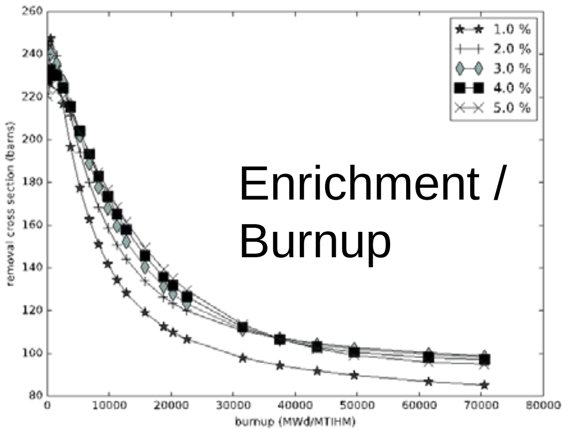
- Decay data are very well known and "constant" (relatively **easy**)
- Cross sections have much larger uncertainties
- Cross sections are problem dependent and must be determined for the system being analyzing – they depend on:
  - Fuel type
  - Enrichment
  - Burnup
  - Assembly design
  - Fuel temperatures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

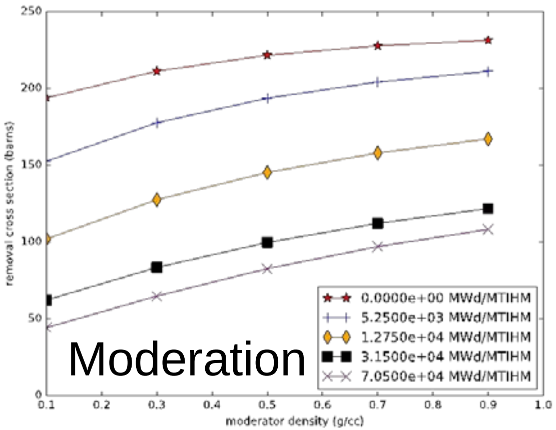


ORIGEN Rapid Methodology for Burnup and Source Term Calculations

- 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)



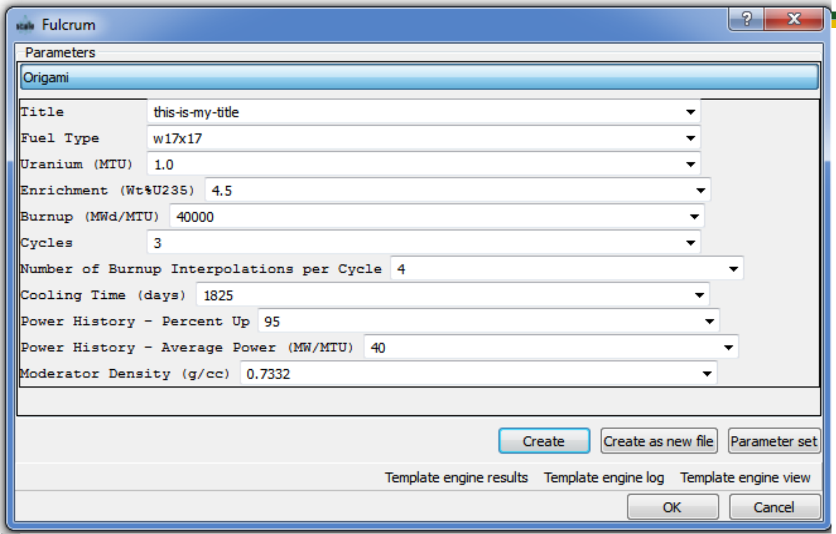




Source Term Characterization

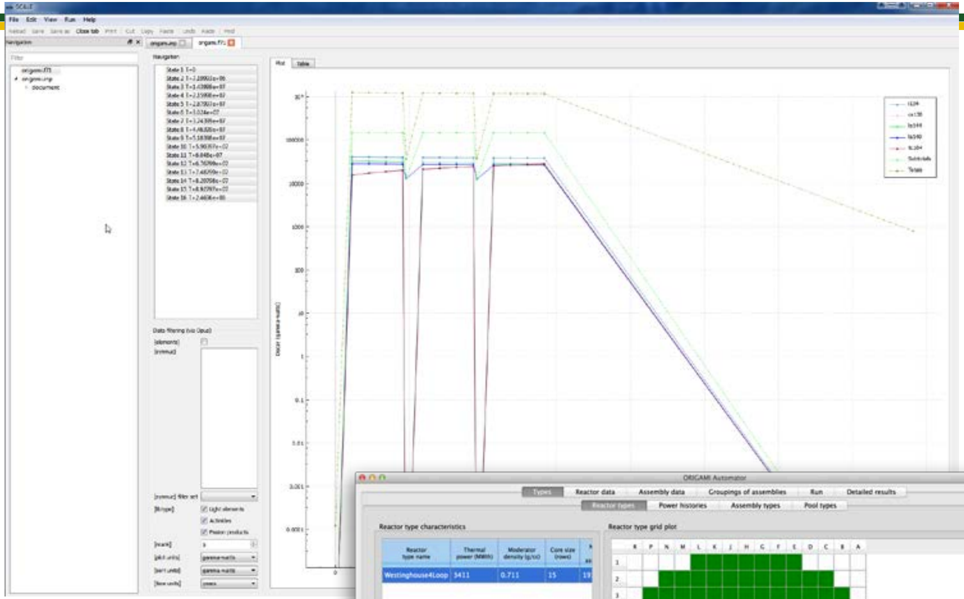
- **Input capabilities**
  - Axial moderator density/power distributions
  - Radial composition/ORIGEN library assignment (enables approximate pin-by-pin 3D depletion)
  - SCALE StdComp integration (e.g. zirc4)
- **Output capabilities**
  - Produces binary concentration file (f71)
  - SCALE StdComp material 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**

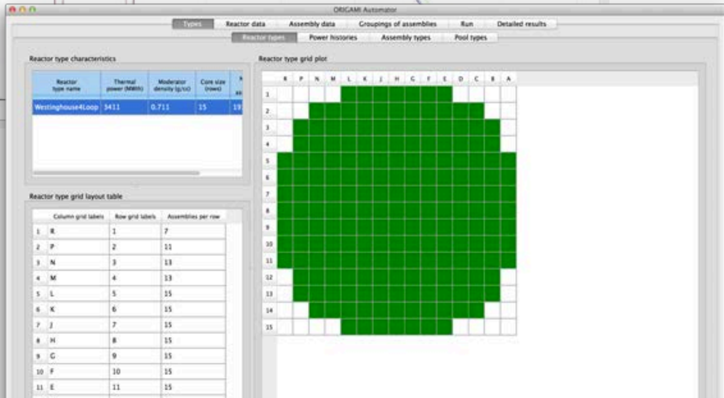
Source Term Generation with NEAMS Workbench / SCALE 6.2




```
options{ mtu=1.0 ft71=all}
libs=[ "w17x17" ]
fuelcomp{
  uox(fuel){ enrich=4.5 }
  mix(1){ comps=[ fuel=100 ] }
}
modz=[ 0.7332 ]
pz=[ 1.0 ]
hist[
  cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
  cycle{ power=40 burn=333.33 nlib=4 down=16.67 }
  cycle{ power=40 burn=333.33 nlib=4 down=0 }
  cycle{ down=1825 }
]
```

Assembly-level calculation





Facility-level calculation

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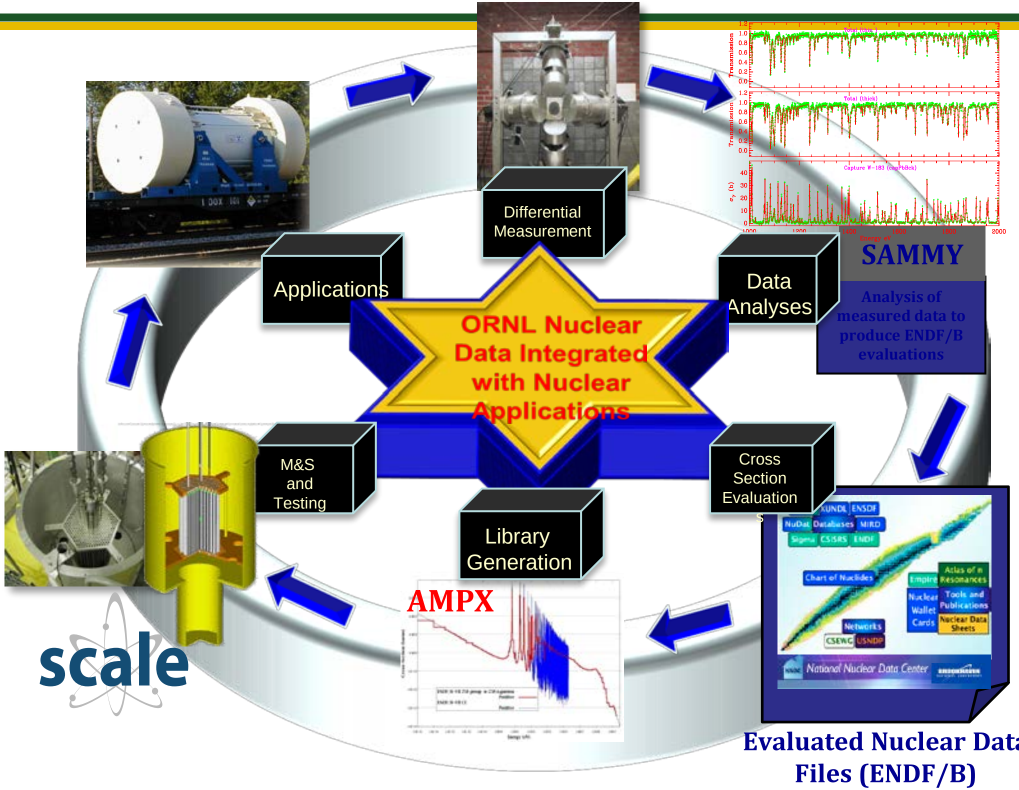
Nuclear Data Life Cycle

- **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



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Nuclear Data Libraries from AMPX (ex. SFR Benchmark)

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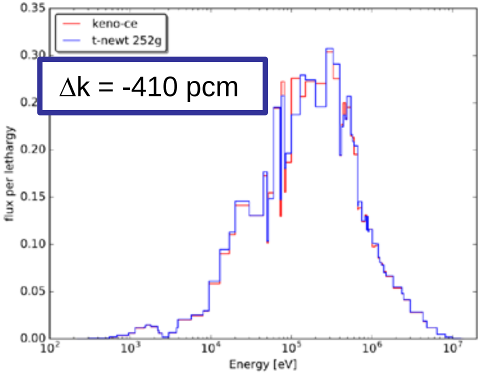
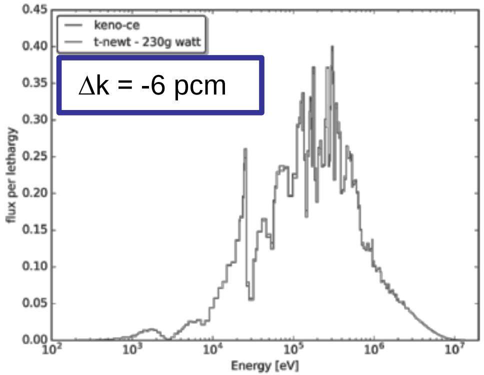
- **Continuous-energy data serve as reference solution to confirm multigroup approximations**
- **Multigroup cross sections can be generated for any type of system**
  - LWR, HTGR, MSR, FHR, SFR, etc. with appropriate energy group structure and weighting spectrum
- **Uncertainties in cross sections (covariance data) quantify confidence in deployed data libraries**
- **AMPX developed and deployed with SCALE**



Incorrect group structure/weighting



Correct group structure/weighting

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

covariance matrix nuclide-reaction	with	nuclide-reaction	% Δk/k due to this matrix
u-238 n,n'		u-238 n,n'	1.2053(9)
na-23 elastic		na-23 elastic	0.3242(2)
fe-56 elastic		fe-56 elastic	0.2590(3)
u-238 n,gamma		u-238 n,gamma	0.2435(1)
fe-56 n,n'		fe-56 n,n'	0.2388(1)

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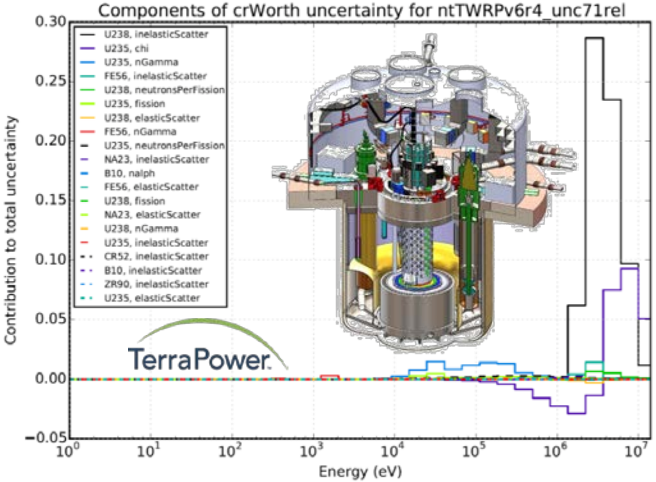
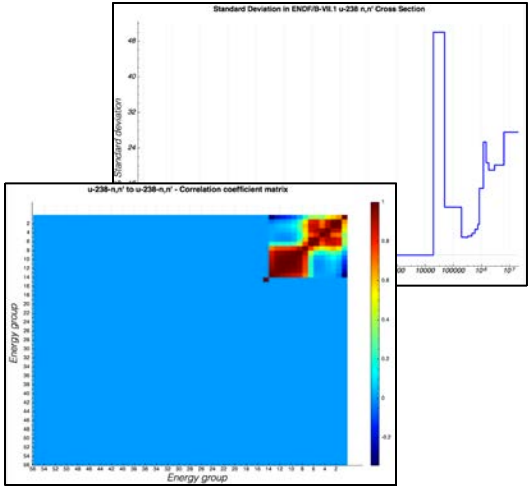
Nuclear Data Uncertainties

- 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



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



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

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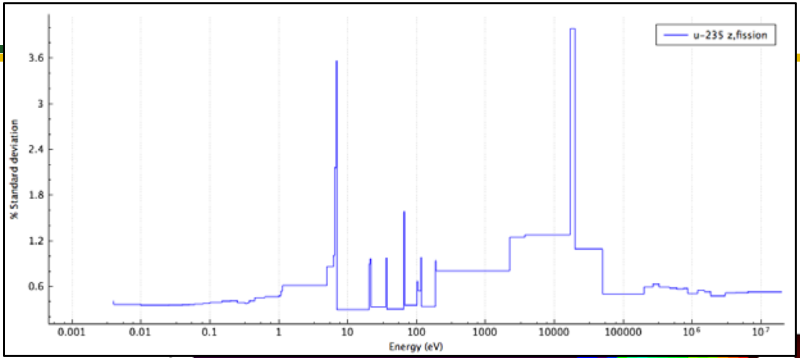
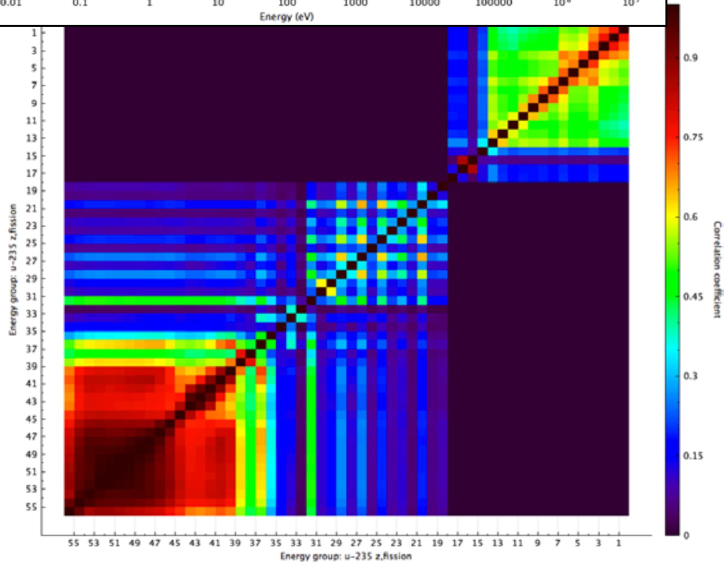
SCALE 6.2 Covariance Library

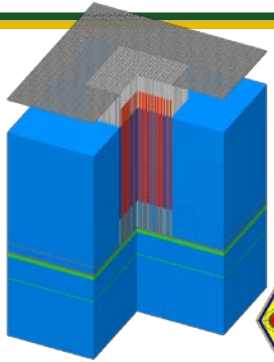
- **ENDF/B-VII.1 for 187 isotopes**
- **Modified ENDF/B-VII.1 ^{239}Pu nubar, ^{235}U nubar, H capture, and several fission product uncertainties, with data contributed back to ENDF repository for ENDF/B-VIII**
- **“Low-fidelity” data for ~215 nuclides missing from ENDF/B-VII.1**
- **Fission spectrum (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**

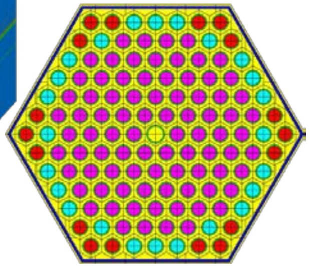


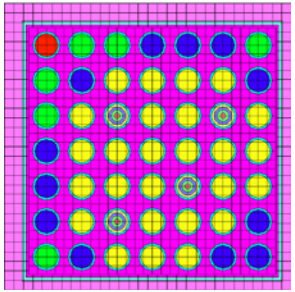


Sensitivity/Uncertainty (S/U) Analysis for M&S Validation

- **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)

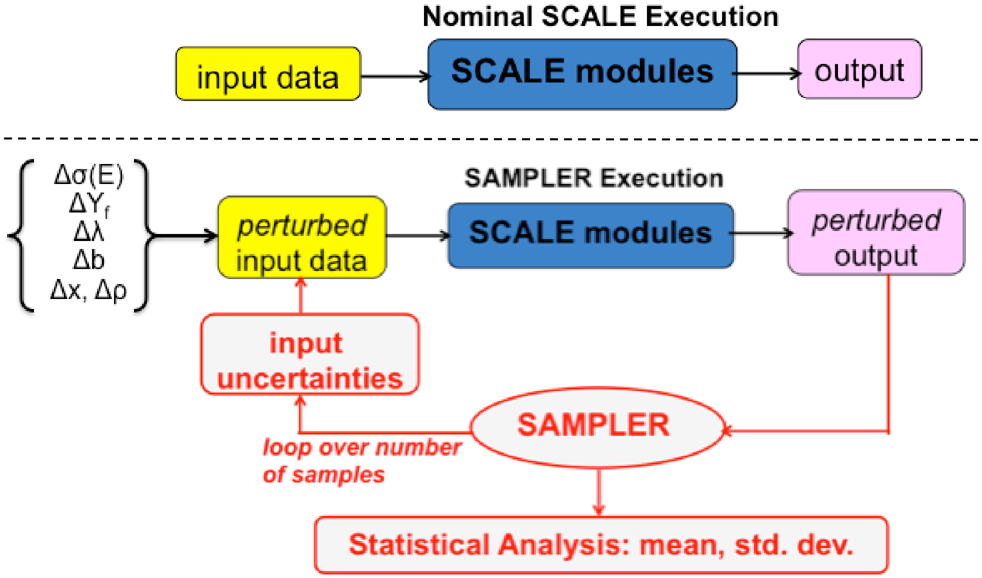
- **Covariances of input data sampled; statistical analysis of output distribution gives uncertainties**
- **Pros**
  - Typically minimally invasive to code
  - Can address complex simulations with coupled codes
- **Cons**
  - Quantification of separate effects (sensitivity coefficients) is challenging

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 (σ)
  - fission product yields (Y_f), decay data (λ), and branching fractions (b)
  - Model parameters such as dimensions(x) and compositions (ρ)



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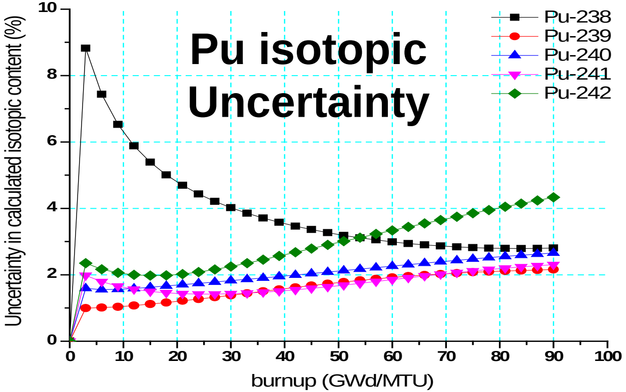
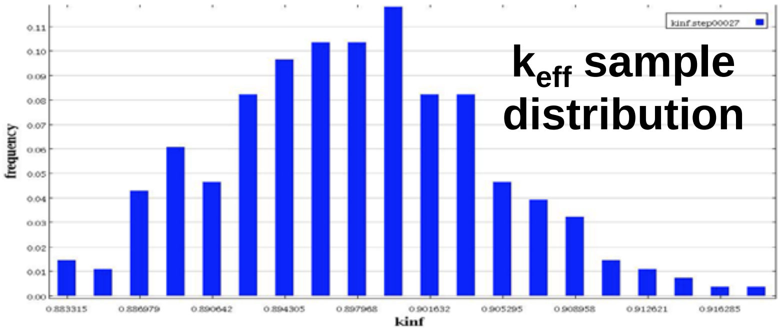
Uncertainties Evolve with Burnup/Decay





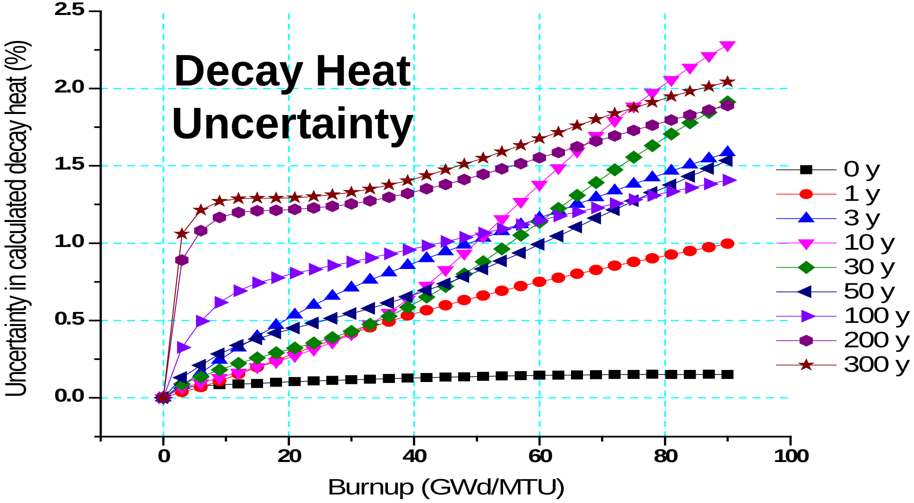


Figure 5. Distribution in sampled multiplication factors at 60 GWD/T burnup.

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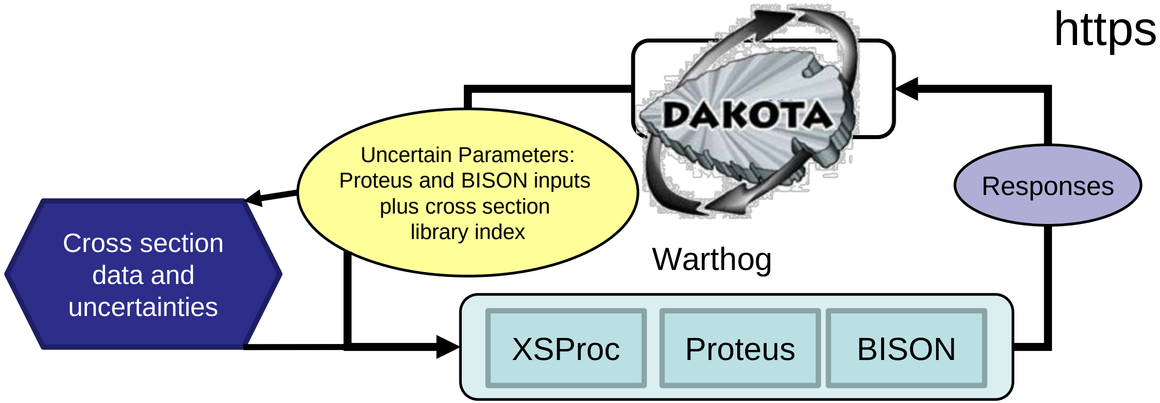
Dakota: Suite of iterative mathematical and statistical methods that interface to computational models

- **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/



Dakota/BISON Correlation Analysis for OECD/NEA WPRS UAM Benchmark Problem 4a

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- Spearman correlation coefficients for fuel thermal conductivity as a function of time for all outputs of interest for Halden irradiation experiment.

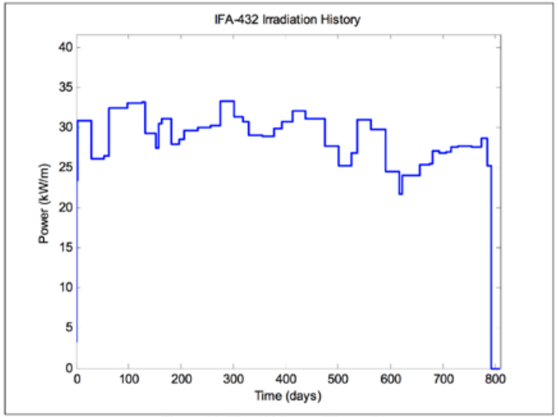
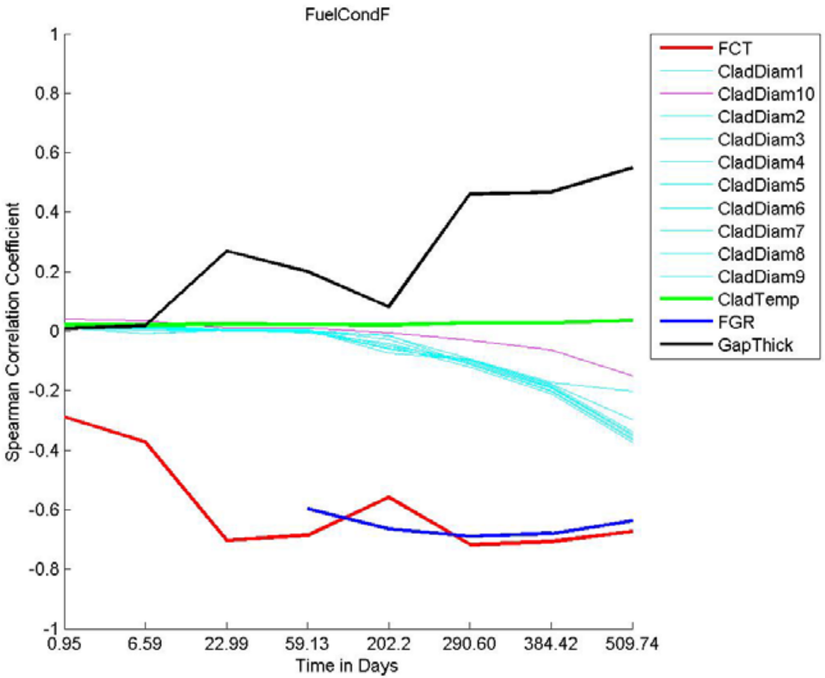


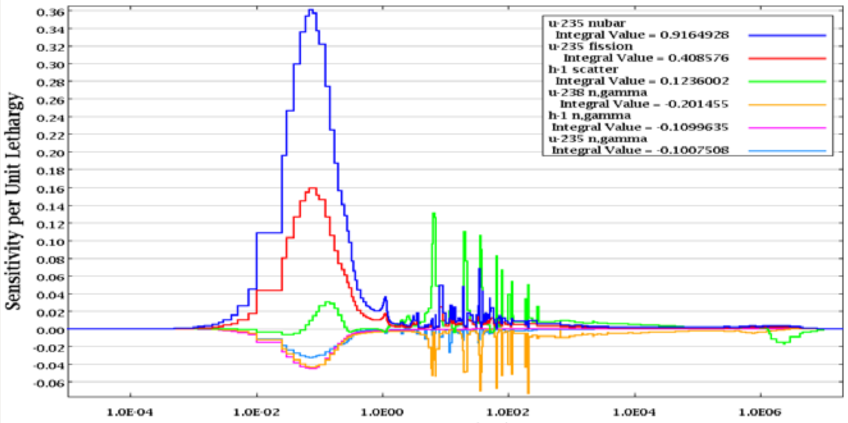
Figure 14: IFA-432 Power History Plot

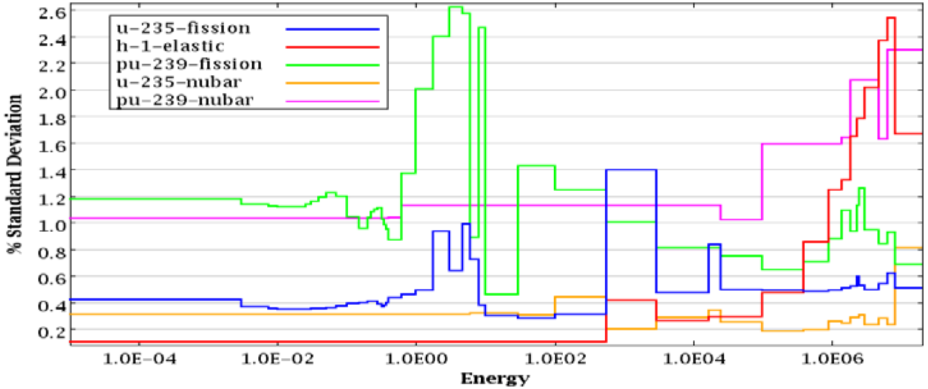


UQ analysis with sensitivities quantifies data contributors to uncertainty

$$\mathrm{Var}(k) \equiv \underbrace{S^{T}}_{\text{sensitivity}} \underbrace{C_{\alpha\alpha}}_{\text{covariance}} S$$

Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{238}U n,gamma	^{238}U n,gamma	2.7427E-01
^{235}U nubar	^{235}U nubar	2.7122E-01
^{235}U n,gamma	^{235}U n,gamma	1.4000E-01
^{235}U fission	^{235}U fission	1.3666E-01
^{238}U n,n'	^{238}U n,n'	1.2864E-01





SIMILARITY ANALYSIS: Identifying experiments representative of targeted application

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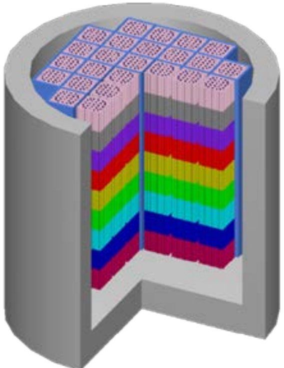
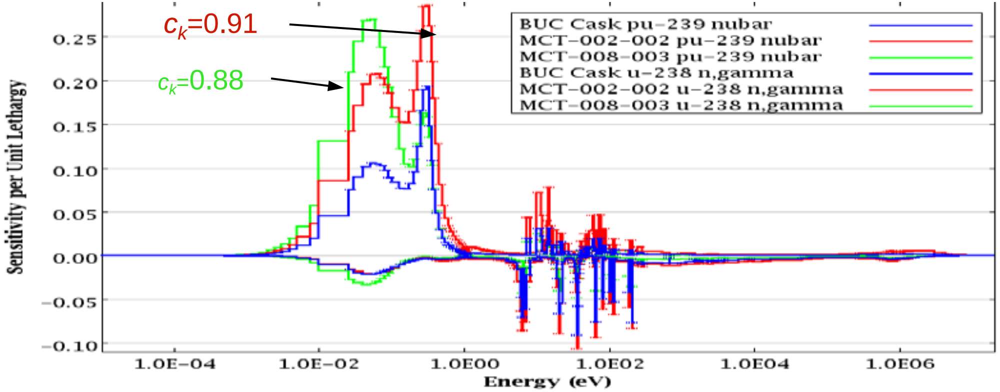
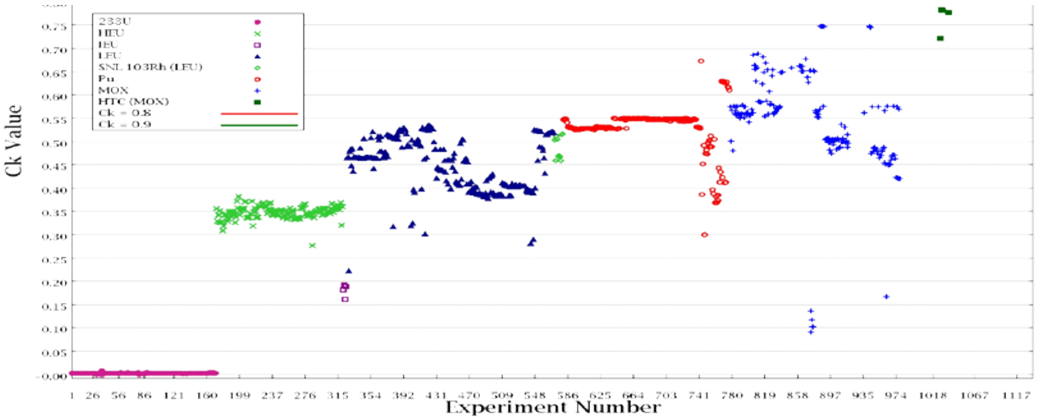
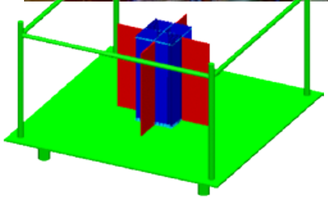
$$c_k^{(m,n)} = \frac{\mathbf{S}_{k_m}^{T}\mathbf{C}_{\alpha\alpha}\mathbf{S}_{k_n}}{\sqrt{Var(k_m)\,Var(k_n)}}$$

APPLICATION

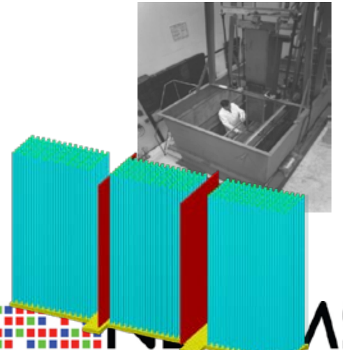








NUCLEAR CRITICALITY EXPERIMENTS

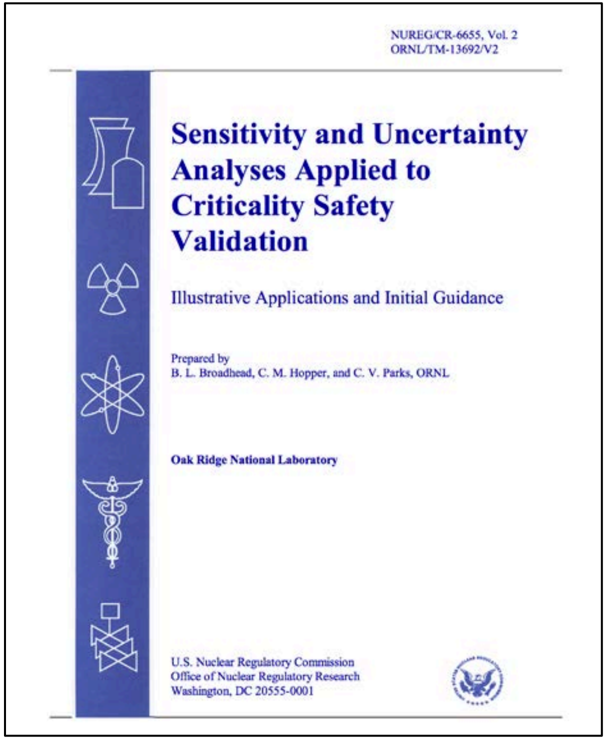


Fuel Cycle Licensing for >5%-wt Fuels

- **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)



NUREG/CR-6655, Vol. 2
ORNL/TM-13692/V2

Sensitivity and Uncertainty Analyses Applied to Criticality Safety Validation

Illustrative Applications and Initial Guidance

Prepared by
B. L. Broadhead, C. M. Hopper, and C. V. Parks, ORNL

Oak Ridge National Laboratory

U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Washington, DC 20555-0001

FISSION REACTORS

KEYWORDS: *sensitivity and uncertainty analysis, experiment design, highly enriched fuel*

USE OF SENSITIVITY AND UNCERTAINTY ANALYSIS IN THE DESIGN OF REACTOR PHYSICS AND CRITICALITY BENCHMARK EXPERIMENTS FOR ADVANCED NUCLEAR FUEL

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Received June 4, 2004
Accepted for Publication September 14, 2004

Framatome ANP, Sandia National Laboratories (SNL), Oak Ridge National Laboratory (ORNL), and the University of Florida are cooperating on the U.S. Department of Energy Nuclear Energy Research Initiative (NERI) project 2001-0124 to design, assemble, execute, analyze, and document a series of critical experiments to validate reactor physics and criticality safety codes for the analysis of commercial power reactor fuels consisting of UO_2 with ^{235}U enrichments ≥5 wt%. The experiments will be conducted at the SNL Pulsed Reactor Facility.

Framatome ANP and SNL produced two series of conceptual experiment designs based on typical parameters, such as fuel-to-moderator ratios, that meet the programmatic requirements of this project within the given restraints on available materials and facilities. ORNL used the Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) to assess, from a detailed physics-based perspective, the similarity of the experiment designs to the commercial systems they are intended to validate. Based on the results of the TSUNAMI analysis, one series of experiments was found to be preferable to the other and will provide significant new data for the validation of reactor physics and criticality safety codes.

I. INTRODUCTION

Framatome ANP, Sandia National Laboratories (SNL), Oak Ridge National Laboratory (ORNL), and the University of Florida (UF) are collaborating on the U.S. Department of Energy Nuclear Energy Research Initiative (NERI) project 2001-0124 to design, assemble, analyze, and document a series of critical experiments to validate reactor physics and criticality safety codes for the analysis of commercial pressurized water reactor (PWR) and boiling water reactor (BWR) UO_2 fuels with ^{235}U enrichments ≥5 wt%.

At the inception of this project, a supply of nuclear fuel, originally manufactured for the PATHFINDER system intended for assembly at The Pennsylvania State University (Penn State) in the 1960s, was identified for use in the experiments. The PATHFINDER program was eventually canceled; the fuel was never irradiated and has been in storage at Penn State for many years. For this current project, the PATHFINDER fuel has been shipped to SNL for disassembly. Disassembly is necessary because the PATHFINDER fuel is ~2 m long and bundled

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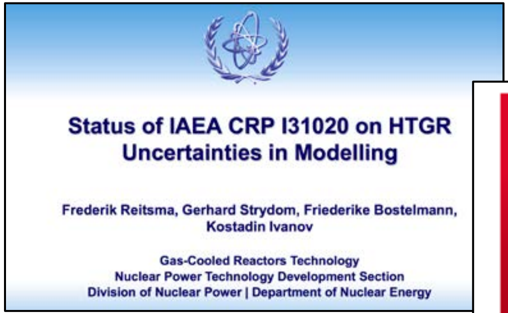
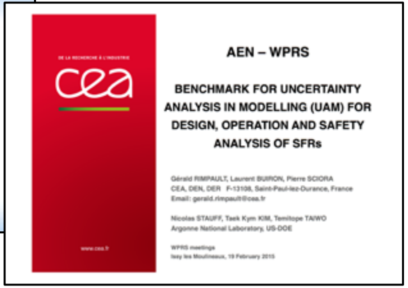
Availability of S/U Tools

- **Dakota** (dakota.snl.gov)
  - Stochastic sampling of input parameters, correlations, search, data calibration, etc.
- **ARC/PERSENT (**https://rsicc.ornl.gov/codes/ccc/ccc8/ccc-823.html)
  - Eigenvalue S/U for k_{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_{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)


Status of IAEA CRP I31020 on HTGR Uncertainties in Modelling

Frederik Reitsma, Gerhard Strydom, Friederike Bostelmann, Kostadin Ivanov

Gas-Cooled Reactors Technology
Nuclear Power Technology Development Section
Division of Nuclear Power | Department of Nuclear Energy



AEN – WPRS

BENCHMARK FOR UNCERTAINTY ANALYSIS IN MODELLING (UAM) FOR DESIGN, OPERATION AND SAFETY ANALYSIS OF SFRs

Gérald RIMPAULT, Laurent BUIRON, Pierre SCIORA
CEA, DEN, DER F-13108, Saint-Paul-lez-Durance, France
Email: gerald.rimpault@cea.fr

Nicolas STAUFF, Taek Kym KIM, Temitope TAIWO
Argonne National Laboratory, US-DOE

WPRS meetings
Issy les Moulineaux, 19 February 2015

International Benchmark Evaluation Projects

- **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)**

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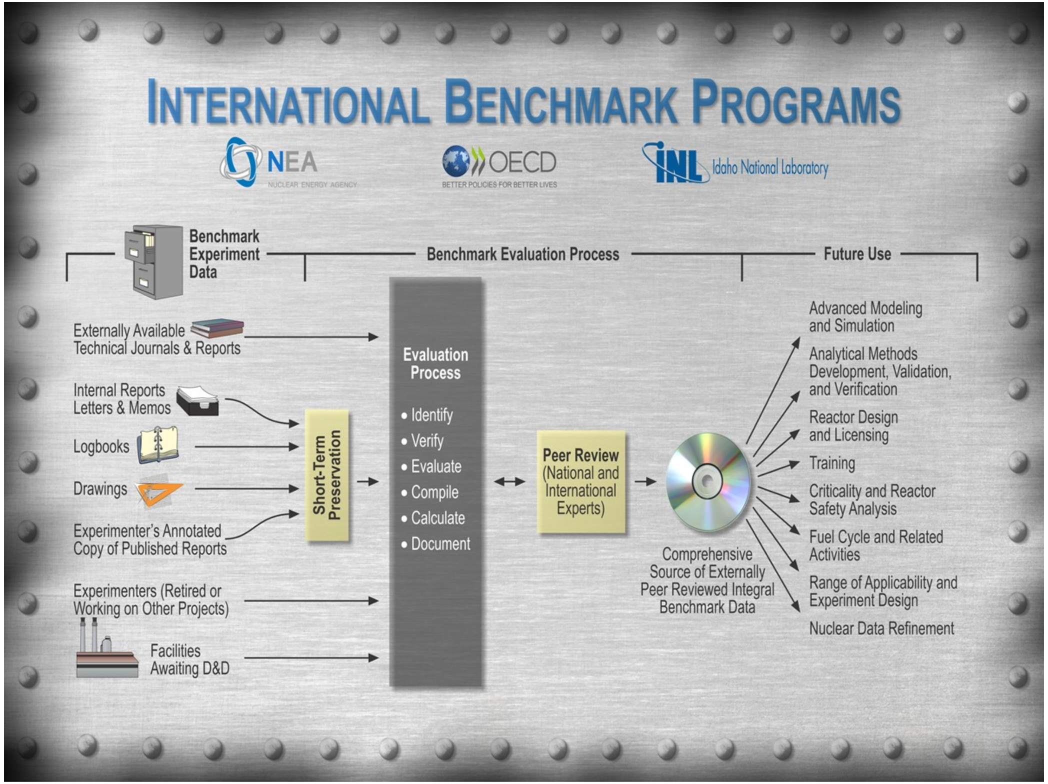
Benchmark Evaluation Process



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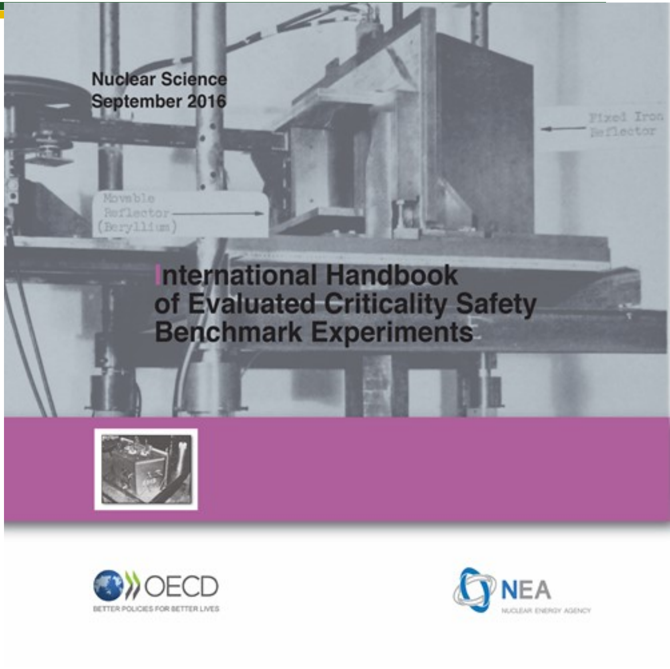
International Handbook of Evaluated Criticality Safety Benchmark Experiments

- **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/wpncs/icsbep/

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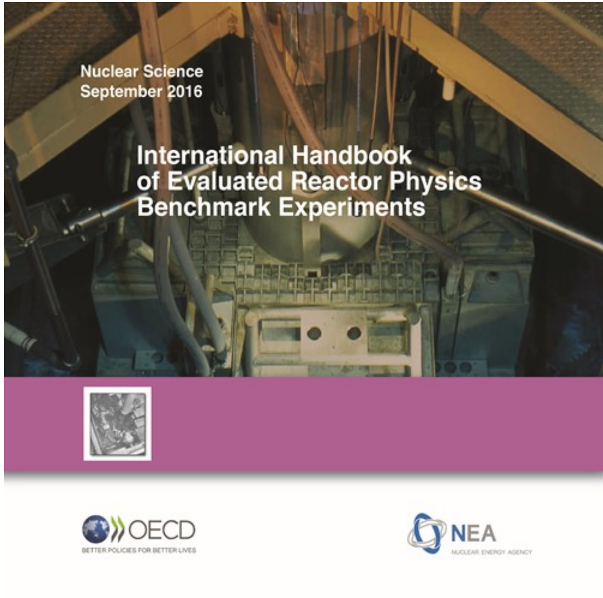
  - 147 Approved Benchmarks
  - 4 DRAFT Benchmarks



http://irphep.inl.gov/

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

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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

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