

ORNL Nuclear Simulation and Analysis and Opportunities

for You...



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**Nuclear Science &
Technology Division**

**Oak Ridge National
Laboratory**

ANS Seminar
The University of Texas

Six Scientific Themes

*Born of necessity. Inspired by our quest to know.
We have always been called upon to address
America's greatest scientific challenges.*

BIOLOGICAL SYSTEMS

Developing New Options

Whether converting biomass to fuel or understanding the impacts of climate change, biological research at ORNL is helping develop new options for energy, environmental protection, and human health. mannre@ornl.gov

NEUTRON SCIENCE

Leading the World

The Spallation Neutron Source and the High Flux Isotope Reactor together make Oak Ridge the world's foremost center for neutron science.

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ADVANCED MATERIALS

Strengthening American Industry

With DOE's first Nanoscience Center, the world's most powerful electron microscope, and the High Temperature Materials Laboratory, Oak Ridge plays a critical role in American industrial competitiveness.

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"Men love to wonder, and that is the seed of science."

... Ralph Waldo Emerson

NATIONAL SECURITY

Guarding the Gates

From biochemical sensors to stopping the proliferation of nuclear weapons, technologies that make America safer are among the laboratory's top research priorities.

akersfhjr@ornl.gov



HIGH PERFORMANCE COMPUTING

Tackling the Big Problems

With unmatched computational capacity for open scientific research, Oak Ridge is on a path by 2009 to reach a petaFlop, or 1 quadrillion mathematical calculations per second, making it possible to model the most complex scientific problems.

zachariat@ornl.gov

ENERGY

Providing Energy Alternatives

Increased production, improved transmission, reduced consumption: Oak Ridge is addressing our energy challenges on all fronts, from safer nuclear power to more energy-efficient cars and homes.

christensend@ornl.gov



Nuclear @ ORNL

- **Nuclear Science & Technology Division**
 - ✦ All things nuclear
 - ◆ SCALE nuclear analysis code suite
- **Space Nuclear Power Program**
 - ✦ Electricity generation, propulsion, shielding, materials
- **Fusion Engineering Division**
 - ✦ Teamed with Princeton as the US lead for ITER
- **Spallation Neutron Source**
 - ✦ Neutron and atomic physics
- **Research Reactor Division (HFIR)**
 - ✦ Materials testing, irradiation research, and isotope production
- **Radiation biology, medical physics, astrophysics, etc.**



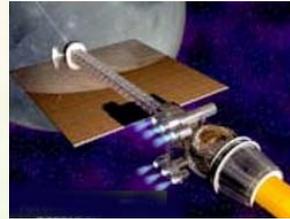
Nuclear Science and Technology Division

NUCLEAR SECURITY TECHNOLOGIES



- Material protection, control, and accounting
- Safeguards
- Arms control assessments
- Export control
- Nuclear threat reduction
- Radiation detection
- Radiation transport
- Transportation technologies
- Fissile material detection
- Fissile material disposition
- Instrumentation

NUCLEAR SYSTEMS ANALYSIS, DESIGN, AND SAFETY



- Nuclear data and codes
- Criticality safety
- Reactor physics
- Radiation shielding
- Advanced/Space reactors
- Thermal hydraulics
- Material and fuel irradiation
- Information/Systems analysis
- Facility safety
- Risk assessment
- Regulatory support
- System instrumentation and controls
- Enrichment technology

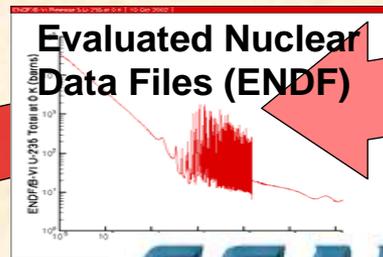
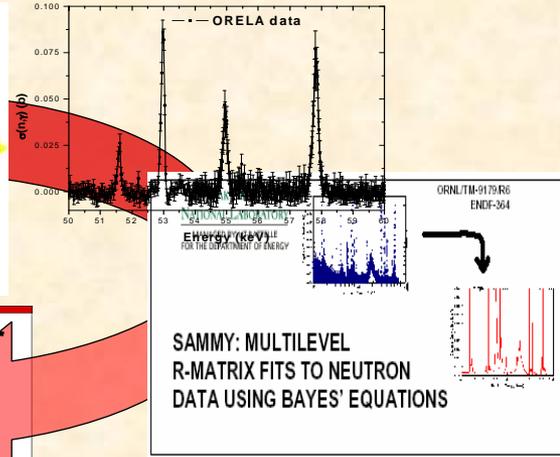
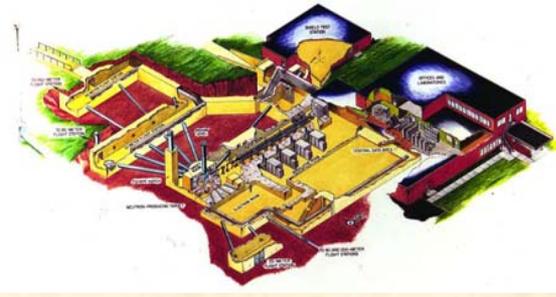
FUELS, ISOTOPES, AND NUCLEAR MATERIALS



- Nuclear fuels
- Heavy element production
- Stable/radioactive isotopes
- Medical isotope development
- Separations science and technology
- Nuclear process and equipment design
- Robotics
- Remote handling
- Chemical engineering

SCALE @ ORNL: Science to Applications

science

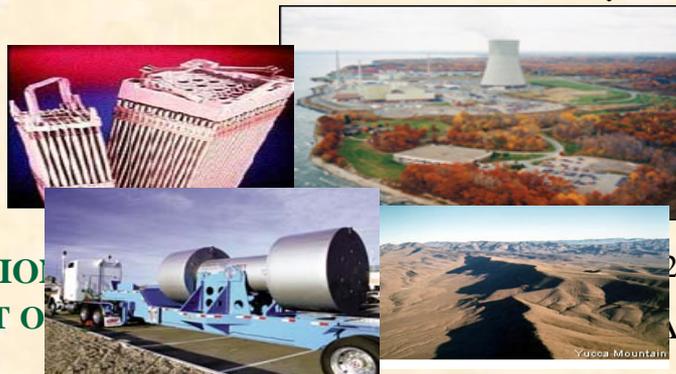


computational modeling

SCALE

AMPX

applications



Interface **science**
(the basic physics of
cross-section
measurements),
computational modeling
(SCALE),
and **applications**
expertise to support
evaluation and resolution
of nuclear engineering
and safety issues.

- Cross-section processing
- Criticality safety
- Radiation protection and shielding
- Reactor physics
- SNF/waste characterization (e.g., inventory, decay heat, radiation source and spectra)

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

2008
ANS Seminar

UT-BATTELLE

There are many codes within SCALE

Input & Visualization

GeeWiz

KENO-3D

JAVAPENO

PLOTOPUS

Multi-Group Cross Sections

BONAMI

NITAWL

CENTRM

PMC

GEMINEWTRN

Radiation Transport

KENO-CE

KENO

MONACO

TORT

NEWT

XSDRN-PM

Feedback & Coupling

ORIGEN-S

STARBUCS

OPUS

KMART

Drivers to Simplify

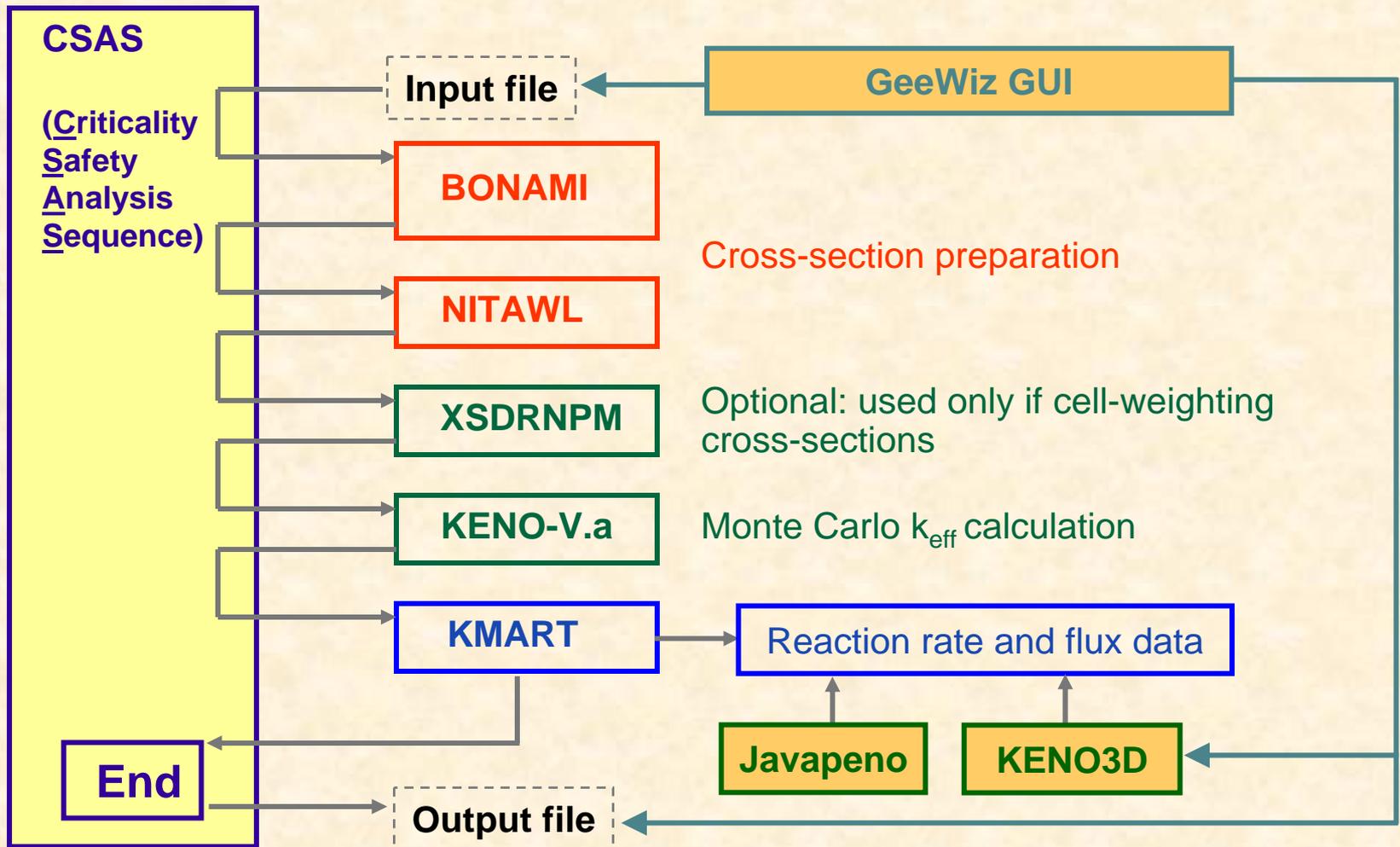
TRITON

CSAS

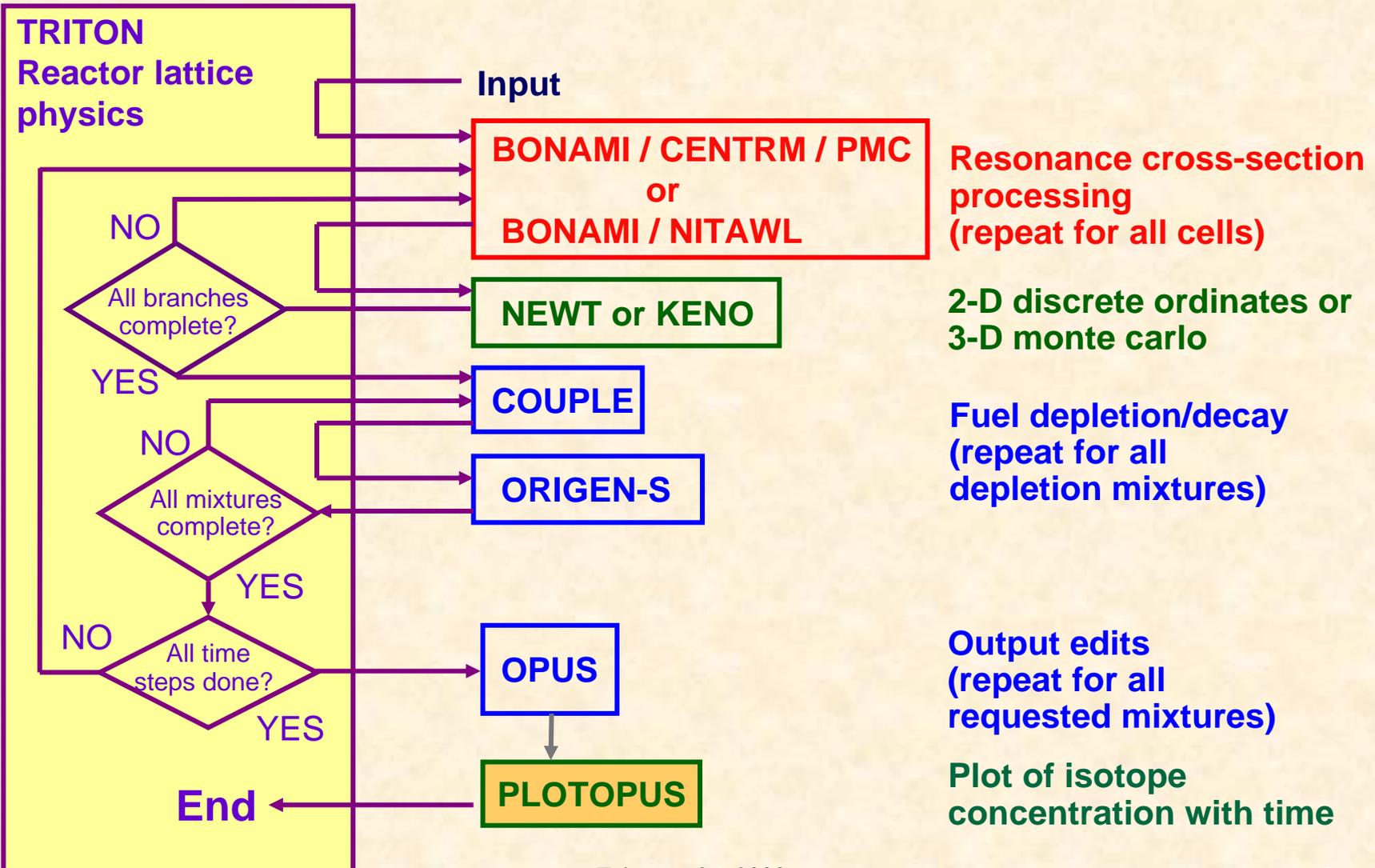
SAS

TSUNAMI

SCALE is built on a Modular Concept



Some drivers make many decisions



From Data to Cross Sections: Resonance Self-Shielding

➤ BONAMI: Bondarenko Method

- ✦ *Tabulated correction factor for temperature & concentration of an isotope*
- ✦ *Generally used in the unresolved energy range only*

➤ NITAWL: Nordheim Integral Treatment

- ✦ *Every resonance is treated independently*
- ✦ *Approximates problem-dependent geometry & material affects*
- ✦ *Fast, good accuracy with few high concentration isotopes (< ENDF/B-VI)*

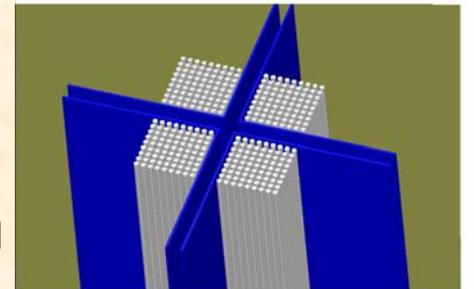
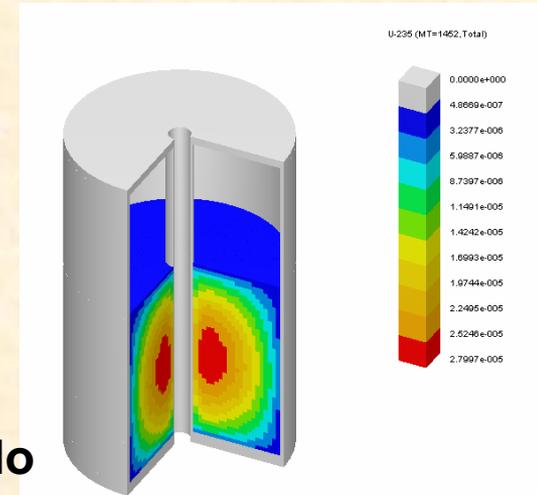
➤ CENTRM: Continuous Energy TRansport Module

for resolved resonance range (all libraries: ENDF/B-VI)

- ✦ **Performs 1-D S_n calculation for continuous-energy neutron spectra using with Point-Wise nuclear data**
- ✦ **Processes problem-dependent multigroup XS's using Point-Wise nuclear data and flux spectrum**

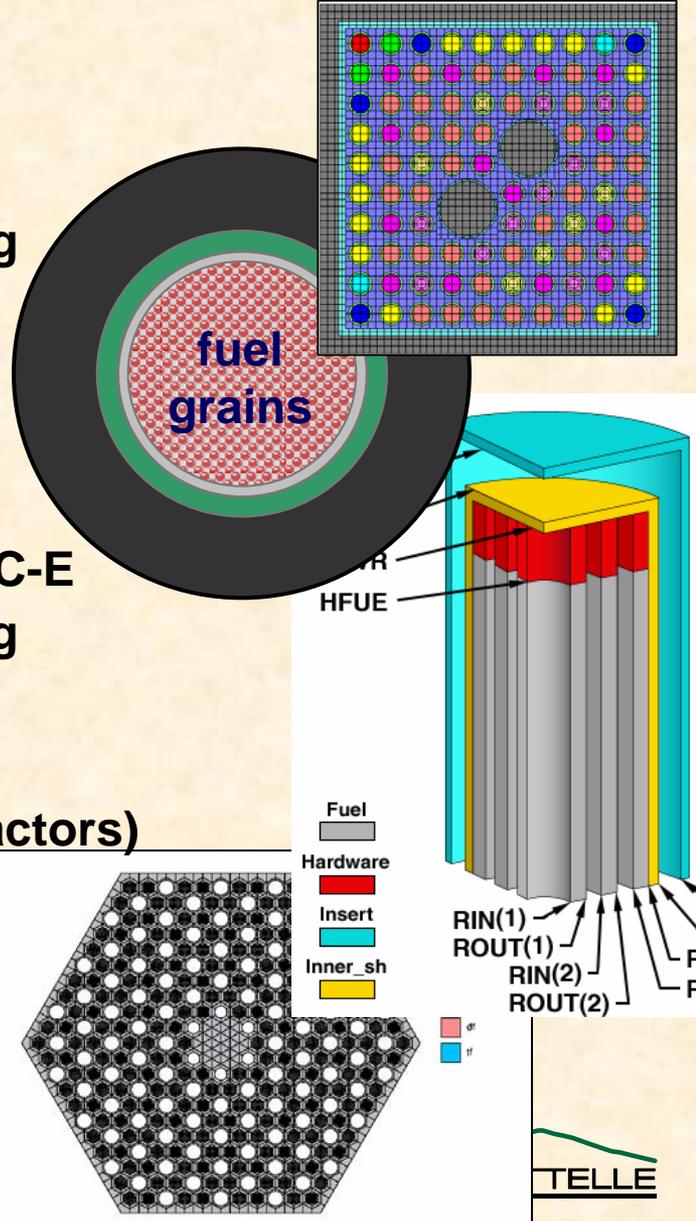
SCALE Stochastic Transport Methods

- **KENO-5 and KENO-VI multi-group Monte Carlo codes**
 - ✦ Developed for criticality safety applications
 - ✦ Much faster than continuous energy
 - ✦ Now integrated with TRITON for depletion
- **Continuous Energy KENO**
 - ✦ Currently under development
 - ✦ Provides the rigor of continuous energy Monte Carlo
- **MORSE/MONACO Monte Carlo Shielding**
 - ✦ Advanced variance reduction
- **A Single Consistent Geometry**
 - ✦ SCALE Generalized Geometry Package (SGGP) being adopted for all ORNL codes
 - ✦ Easily switch from NEWT to KENO-VI to CE-KENO



SCALE Deterministic Transport Methods

- **CENTRM**
 - ✦ 1-D, source-driven, continuous-energy
 - ✦ For problem-dependent resonance processing
- **XSDRN-PM**
 - ✦ 1-D, WDD, multi-group
 - ✦ Forward/adjoint with a host of uses
- **GEMINEWTRN**
 - ✦ 2-D arbitrary polygonal mesh, source-driven, C-E
 - ✦ For problem-dependent resonance processing
- **NEWT**
 - ✦ 2-D arbitrary polygonal mesh, multi-group
 - ✦ Forward/adjoint solutions for all analyses (reactors)
- **TORT**
 - ✦ 3-D orthogonal mesh, multi-group
 - ✦ For all analyses, widely-used in shielding



ORIGEN-S: Irradiation and decay simulation code

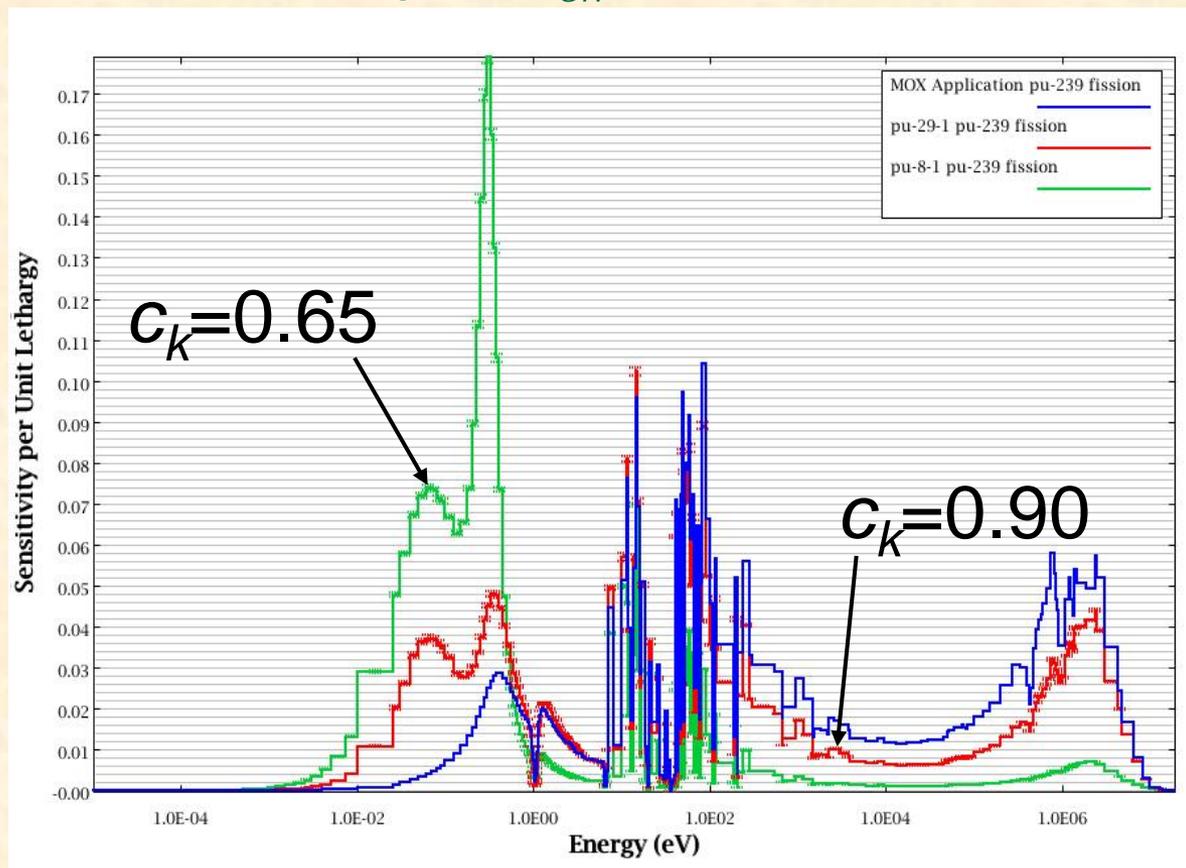
- Irradiation and decay simulation code
- Explicit simulation of 1484 unique nuclides (1946 nuclides in database)
 - ✦ 129 actinides
 - ✦ 1119 fission products
 - ✦ 698 structural activation materials
 - ✦ Other depletion codes typically track a minimum subset of isotopes that are important for reactivity
- Detailed radionuclide compositions
- Decay heat sources (neutron/photon), including energy spectra
- Radio-toxicity
- One of few codes available with comprehensive isotopic characterization of fuel over time scale of seconds to millennia
 - ✦ Accident analyses
 - ✦ Storage and handling
 - ✦ Transportation
 - ✦ Disposal or reprocessing
 - ✦ Repository analysis (storage, migration, dose assessment)



TSUNAMI: Tool for S/U Analysis with XSDRN (1-D) and KENO-VI (3-D)

- **Determination of critical experiment benchmark applicability to nuclear criticality safety analyses**
- **The design of critical general physics experiments (GPE)**
- **The estimation of computational biases and uncertainties for the determination of safety subcritical margins**

^{239}Pu Fission Sensitivity Profiles:
Sensitivity of k_{eff} to cross-section



That is what we have...

but what are we doing?

➤ Analysis

✦ Reactors

- ◆ Gen-IV / GNEP (DOE)
 - AHTR
- ◆ Gen-III, III+ (NRC)
- ◆ Space Reactors (NASA)

✦ Shielding / criticality safety

- ◆ Transportation
- ◆ Space
- ◆ Facilities

✦ Optimization and S/U

- ◆ GA system optimization
- ◆ S/U of design on nuclear data

✦ Others

- ◆ Medical physics
- ◆ Yucca mountain
- ◆ Nuclear materials

➤ Code Development

✦ Incorporation and integration

- ◆ Generalized geometry input
- ◆ TORT within SCALE
- ◆ TSUNAMI with NEWT/TRITON

✦ Incremental improvements

- ◆ MONACO variance reduction
- ◆ Uncertainty propagation
- ◆ ORIGEN-S improvements
- ◆ Many others...

✦ High-performance computing

- ◆ Multi-physics Reactor Simulation
- ◆ Multi-physics Fuel Simulation
- ◆ Genetic Algorithm Design Optimization

Your opportunities at ORNL

- **NESLS – Physics & Engineering Students**
 - ✦ Nuclear Science & Technology Division
 - ✦ Highly competitive stipends
 - ✦ www.ornl.gov/sci/nuclear_science_technology/nstip/internship.htm

- **SULI – Nuclear Engineering Students**
 - ✦ Less competitive, but only \$475/week
 - ✦ <http://www.scied.science.doe.gov/SciEd/erulf/about.html>

- **Full-time Staff and Post-Doc Positions**
 - ✦ <http://jobs.ornl.gov/>
 - ✦ Radiation Transport and Criticality Group
 - ◆ 2694, 2695, 2696
 - ✦ Advanced Reactor Systems and Safety Group
 - ◆ 2538
 - ✦ Reactor Analysis Group
 - ◆ Two are soon to be posted

- **SCALE is cheap**
 - ✦ Source code is free to NE students and faculty
 - ✦ Training is only ~\$500 (cheap for a professor)

| NESLS | Weekly Stipend |
|-------------------------|----------------|
| First Year (Freshman) | \$634 |
| Second Year (Sophomore) | \$698 |
| Third Year (Junior) | \$758 |
| Fourth Year (Senior) | \$831 |
| Fifth Year (Graduate) | \$968 |
| Masters Completed | \$1040 |

Conclusions

- **ORNL has a complete set of nuclear analysis tools**
 - ✦ Nuclear data and data analysis
 - ✦ Advanced cross section generation techniques
 - ✦ Deterministic & stochastic transport with CE and MG
 - ✦ Sensitivity and uncertainty propagation and assessment
- **We are utilizing these tools for many applications**
 - ✦ Reactors: air, land, and sea
 - ✦ Shield design & criticality safety
 - ✦ Fuel performance, waste and transportation
- **You can join us to learn in a 3-month job interview, explore Knoxville and the Smokies, and get paid very well**