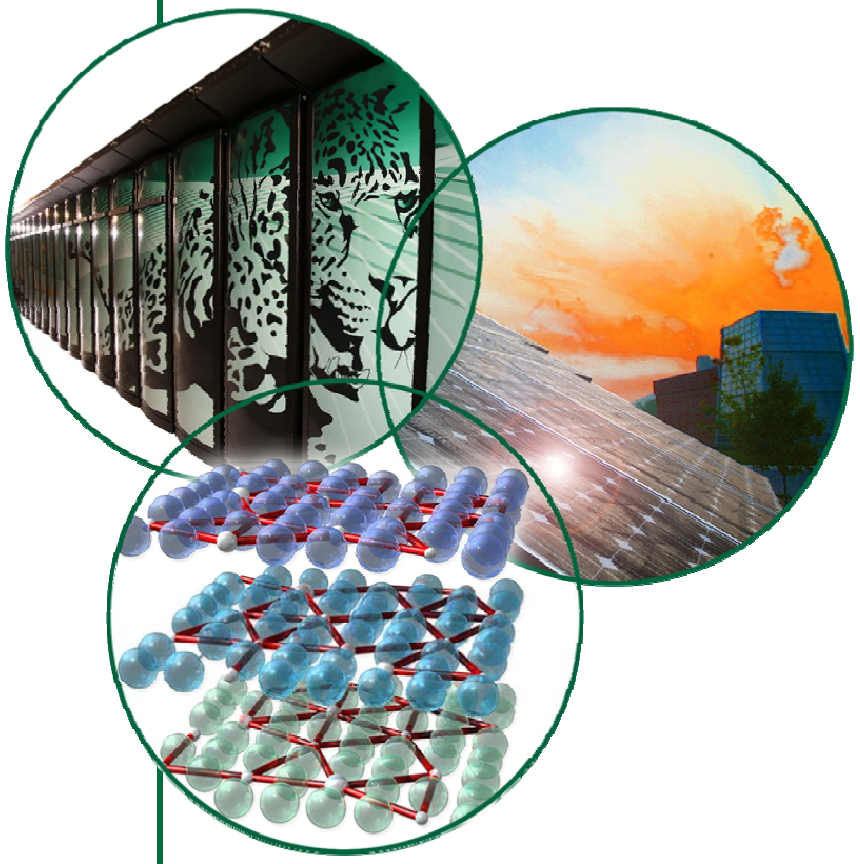
ORNL Modeling & Simulation Capabilities for Nuclear Analyses

Michael E. Dunn
Nuclear Data & Criticality Safety Group Leader

Nuclear Science & Technology Division



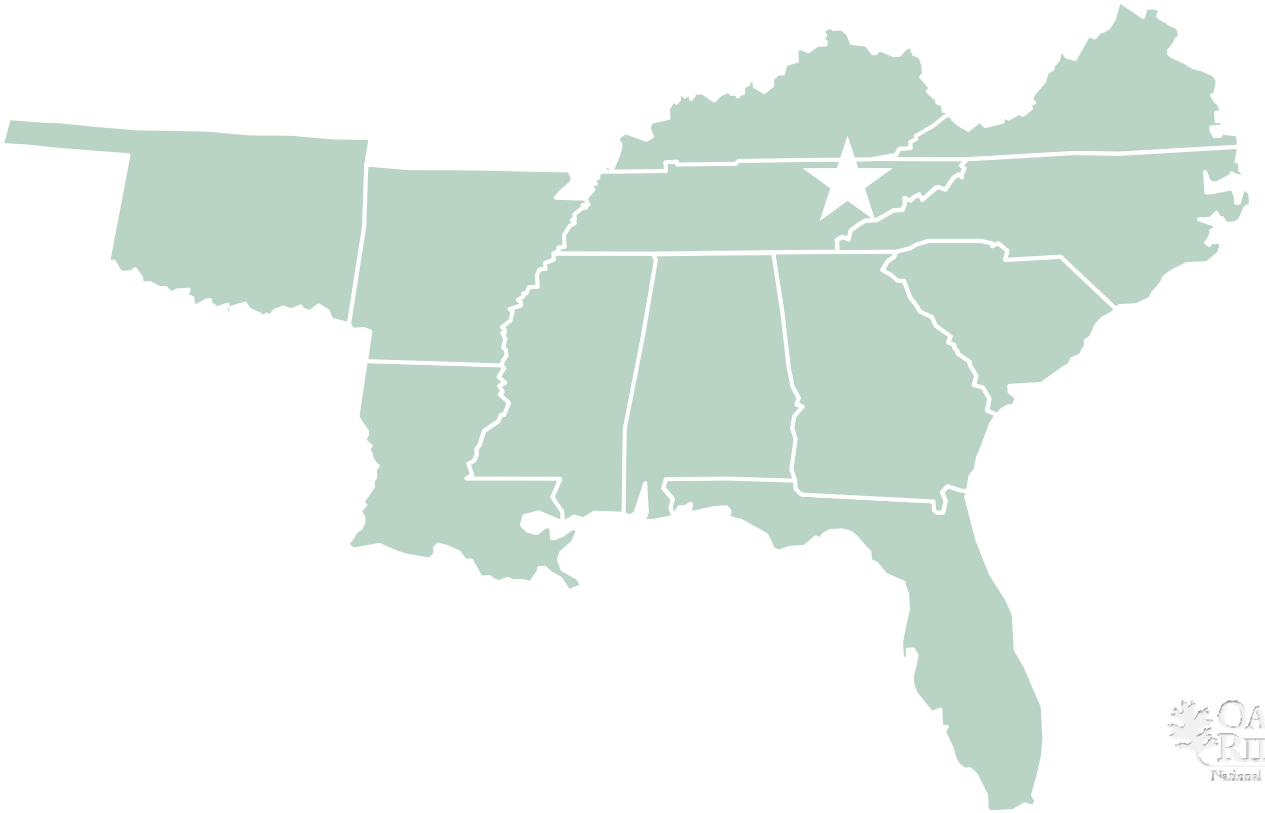
International Workshop on Accelerator-Driven Sub-Critical Systems & Th Utilization
Virginia Tech, VA
September 27-29, 2010

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Outline

- ORNL and NSTD at a Glance
- SCALE Radiation Transport Modeling & Simulation (M&S) Capabilities
- SCALE M&S Nuclear Applications Work
- Summary



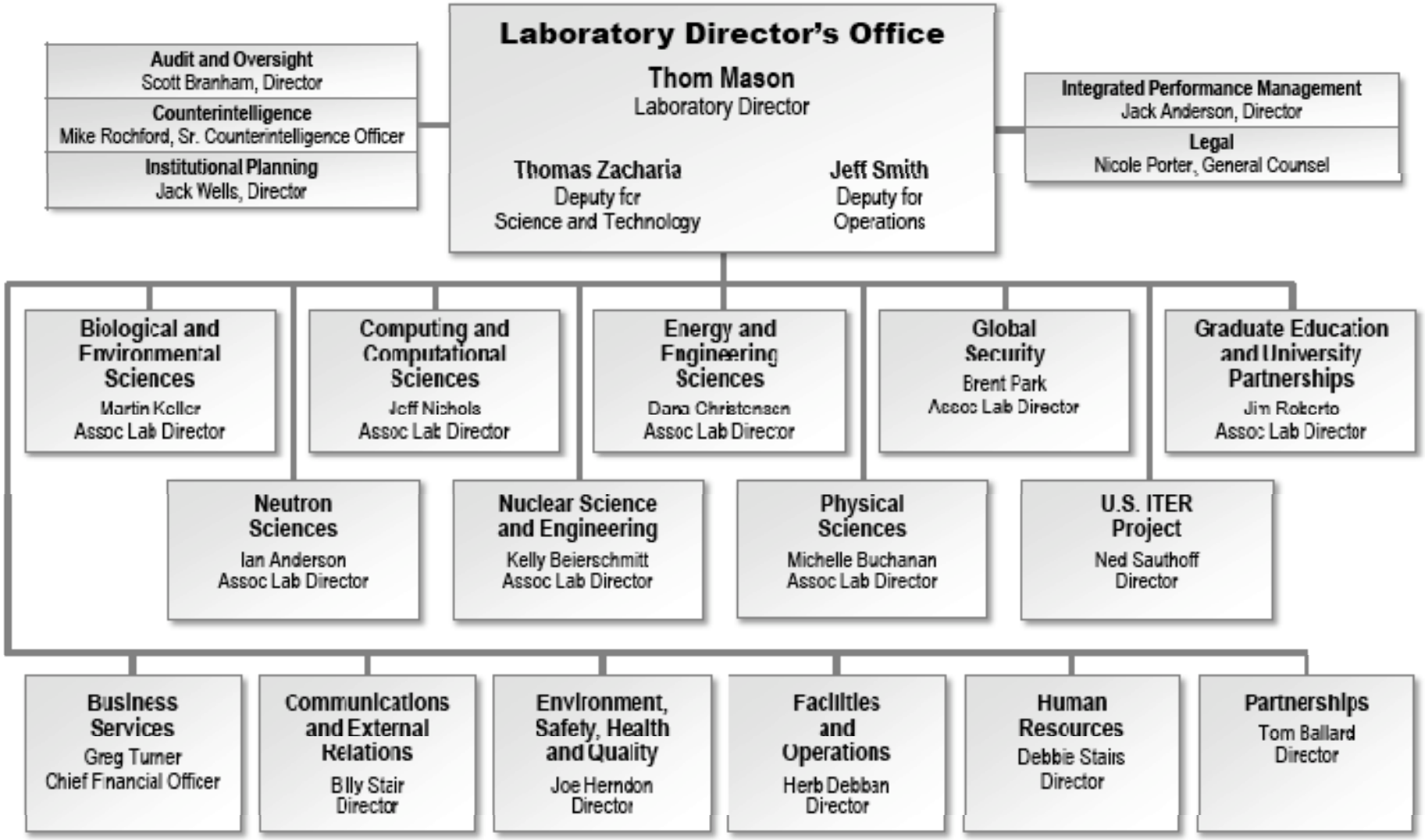
ORNL working to deliver science and technology for energy

Extraordinary set of assets

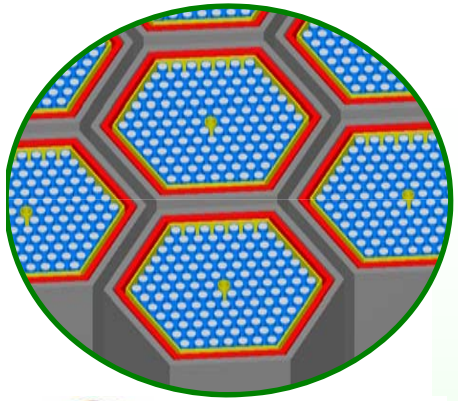
- **Outstanding tools for materials R&D**
- **World's most powerful system for open scientific computing**
- **Bioenergy Science Center**
- **The nation's broadest portfolio of energy programs**
- **Unique resources for nuclear technology**
- **Robust national security programs**

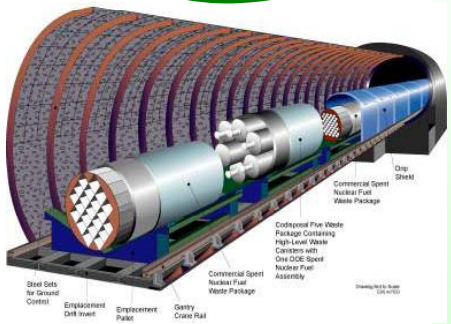
Challenge:
Use these assets to deliver results that are significant on both the national and the international scale

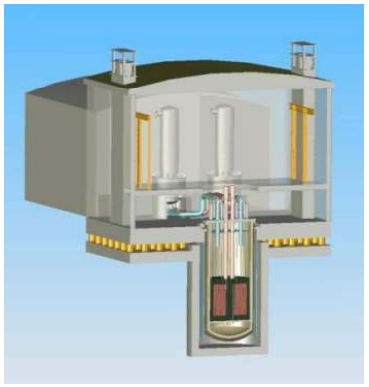
Oak Ridge National Laboratory



NSTD Nuclear Science and Technology Division







NUCLEAR MODELING, DESIGN, AND SAFETY

- Radiation shielding
- Radiation transport
- Reactor physics
- Criticality safety
- Nuclear data and codes
- Thermal hydraulics
- Material and fuel irradiation
- Advanced/Space reactors
- Information/Systems analysis
- Reactor/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

ORNL is the place for M&S

- *ORNL has assembled a unique, unmatched collection of M&S capabilities, expertise (people), and facilities that can be leveraged to address various nuclear applications needs*
  - Actively developed, advanced, unique radiation transport codes/methods running on the world's fastest computer
  - Actively developed, world-standard code (ORIGEN-S) for nuclear depletion/activation/decay simulations
  - Experience and active projects developing multi-physics simulation computational frameworks and capabilities for nuclear energy applications – strong tie between Nuclear S&T and Computational Sciences Divisions
  - National Leadership Computing Facility – computational resources, facilities, and expertise, including the world's fastest computer (ORNL's Cray XT5)
  - Depth and breadth of experience and expertise in nuclear security modeling for a variety of applications (e.g., urban modeling, SNM detection, forensics, weapons effects) and sponsors (e.g., NA-22, NA-24, DHS, DOD, FEMA, etc.)

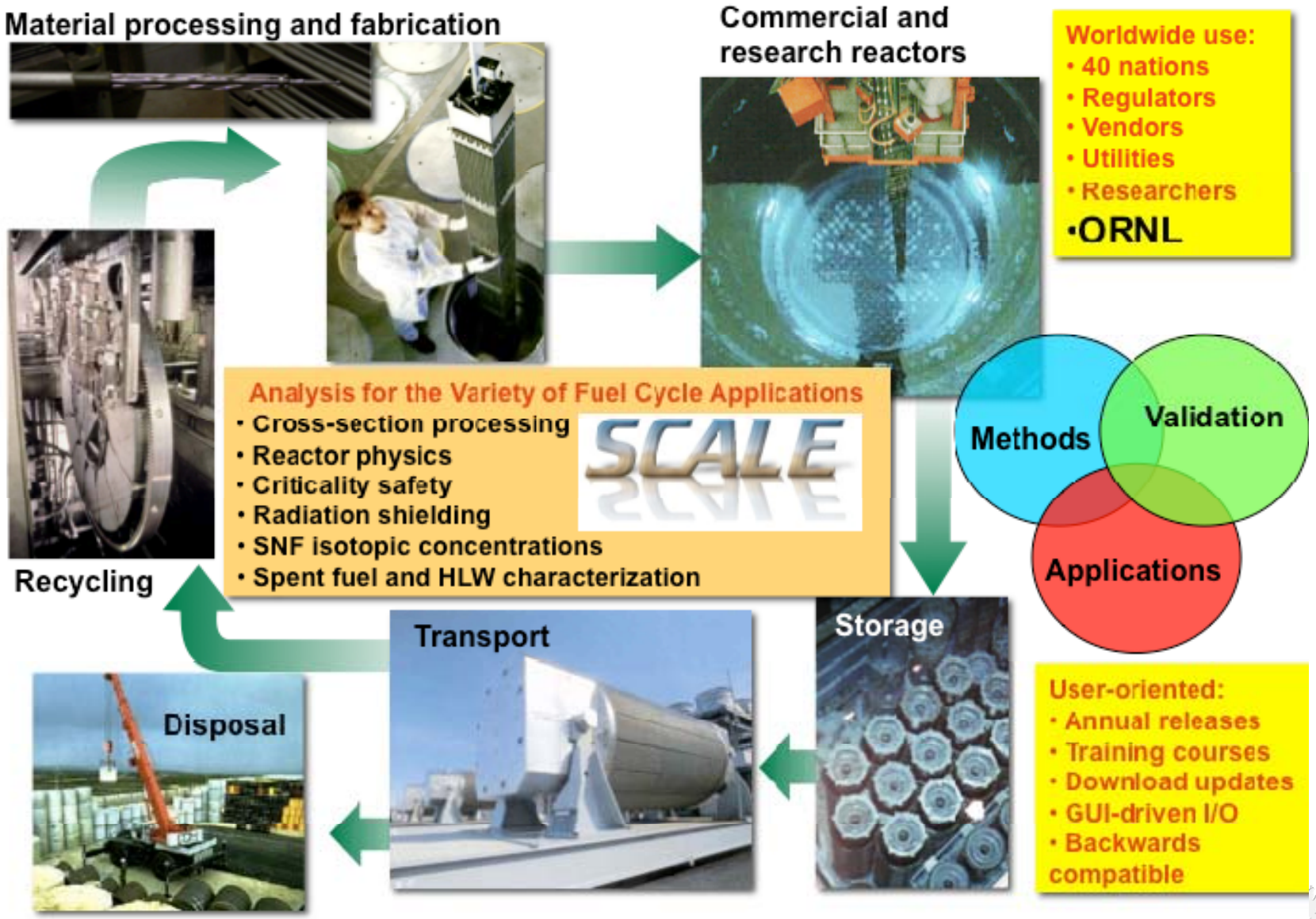
Standardized Computer Analyses for Licensing Evaluation (SCALE)

- Developed at ORNL for the NRC beginning in 1976
- Maintained/enhanced under co-sponsorship of NRC and DOE since 1987
- A collection of serial codes for performing analyses of nuclear facilities and packages. Capabilities include:
  - Cross-section processing
  - Criticality safety
  - Radiation protection & shielding
  - Reactor physics
  - SNF/HLW characterization (e.g., inventory, decay heat, radiation source and spectra)
- Latest version, SCALE 6
  - Next version, SCALE 6.1, to be released by Dec. 2010
- SCALE website: http://www.ornl.gov/sci/scale/

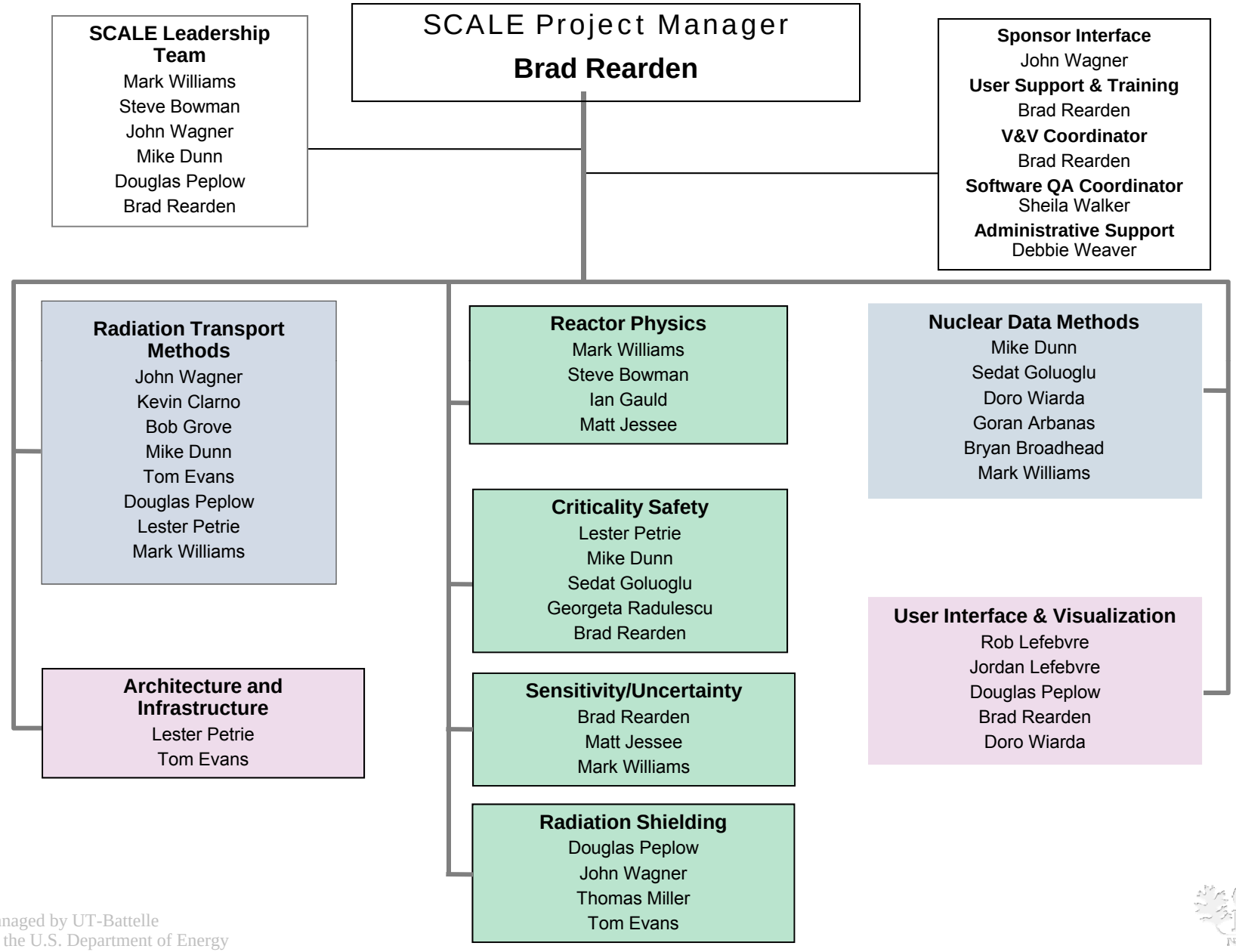
SCALE was originally developed for the NRC

~1800 SCALE users
From 40 nations

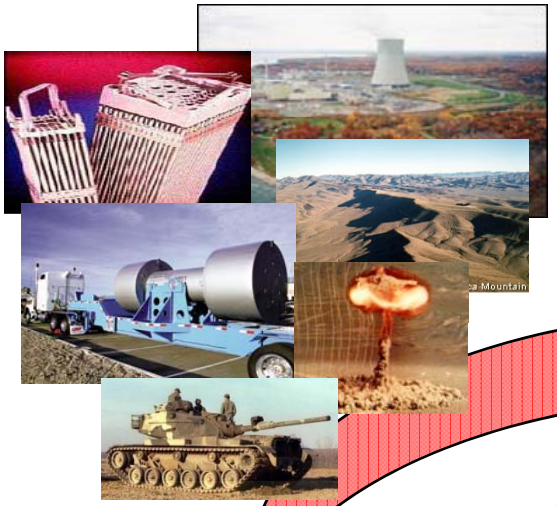
Standardized Computer Analyses for Licensing Evaluation (SCALE)



SCALE Project Team

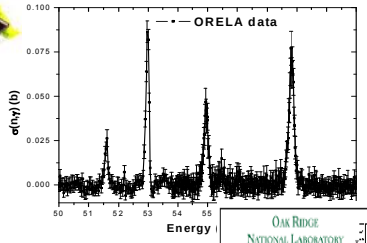


Applications

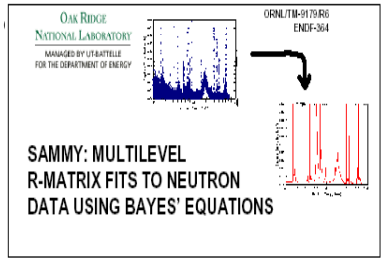


ORELA

Data Analyses



SAMMY

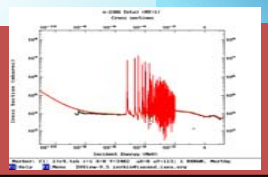


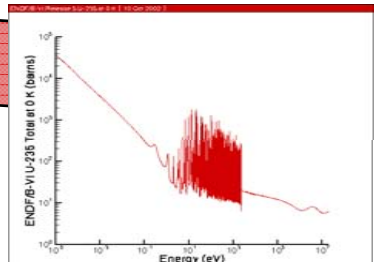
Measurements

ORNL capabilities span from nuclear data to M&S

Cross-Section Evaluations

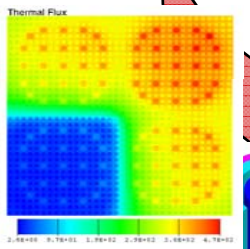
Evaluated Nuclear Data Files (ENDF/B)

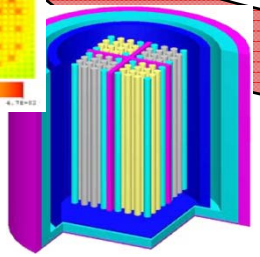




AMPX

Cross-Section Processing

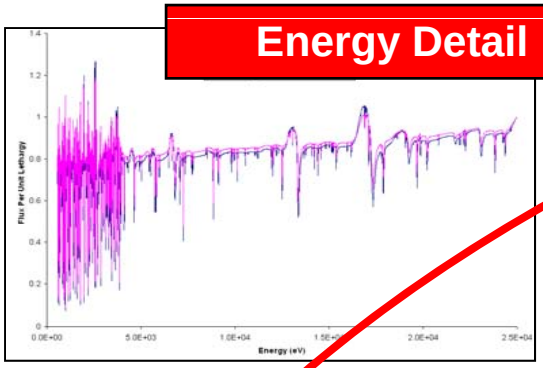


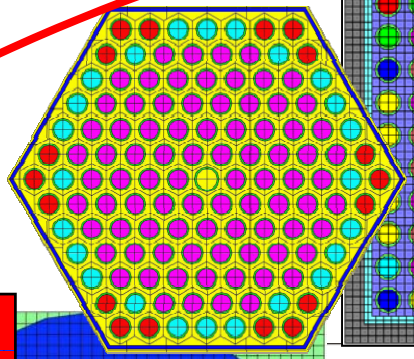


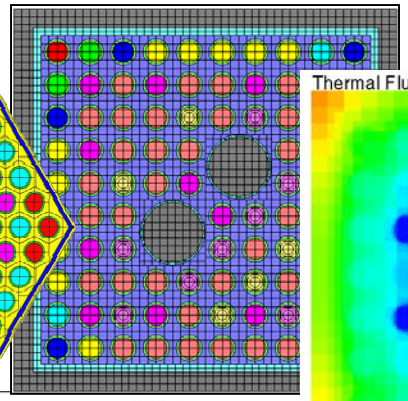
Computational Modeling

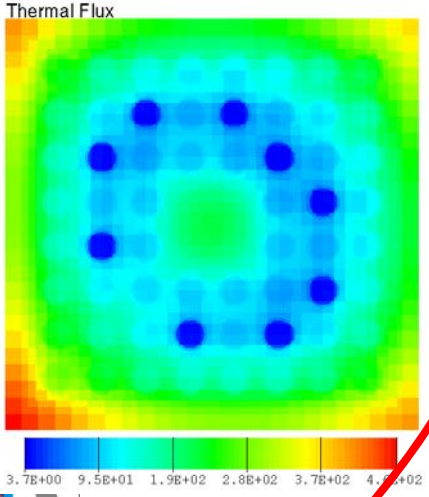
SCALE

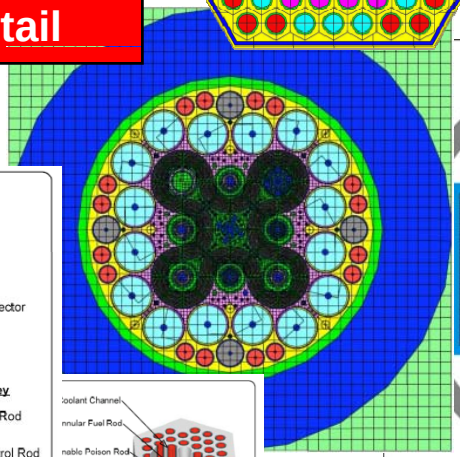
SCALE has rigorous lattice physics and depletion/decay capabilities that have been applied to all types of reactors

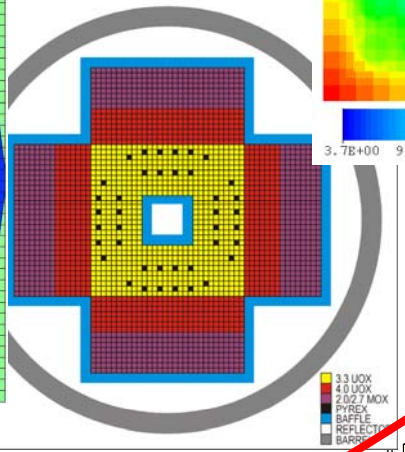


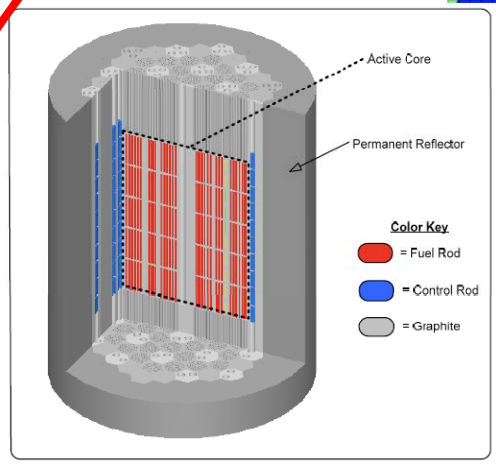


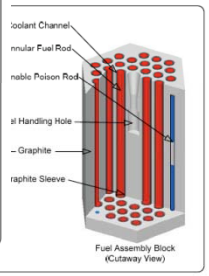


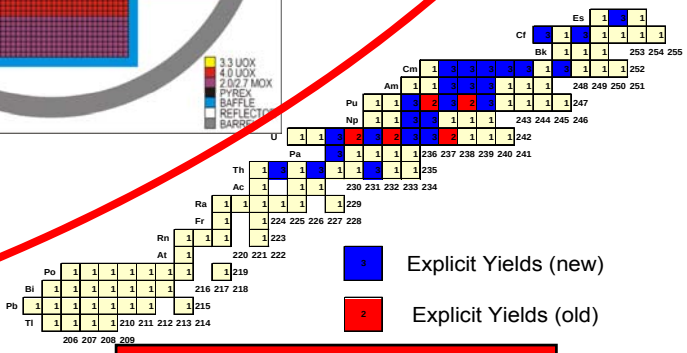








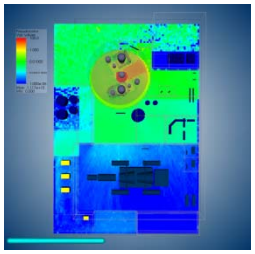
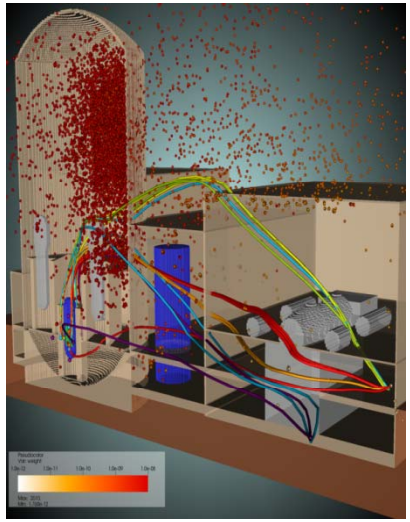
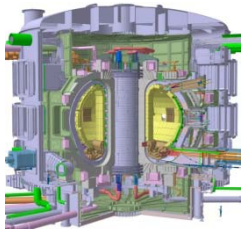
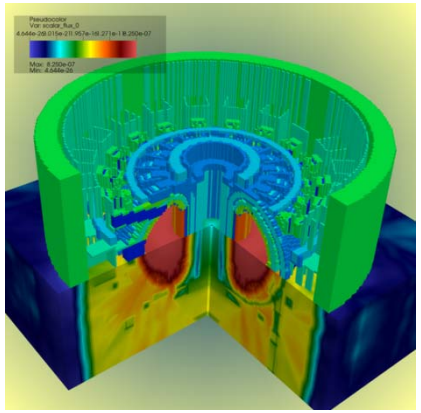


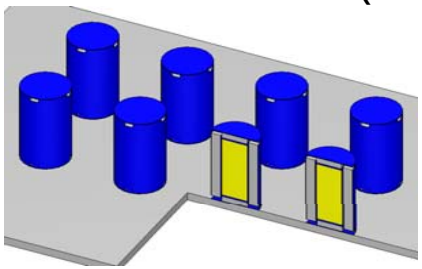


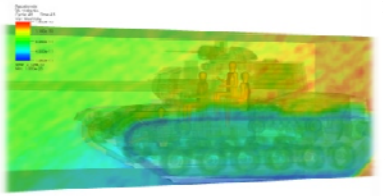
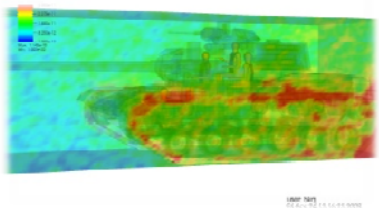
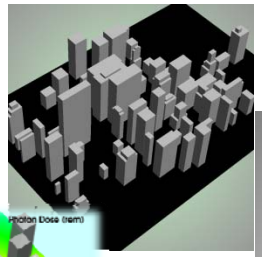
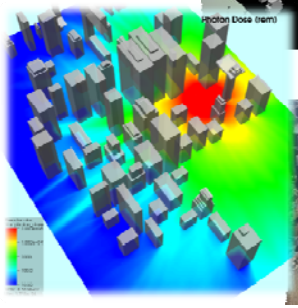
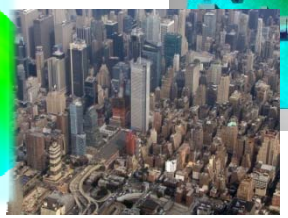
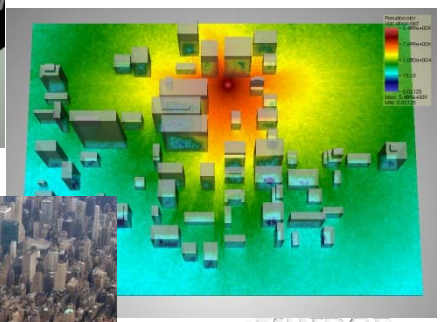
Isotopic Details (1946 nuclides)

Radiation transport capabilities have been enhanced for advanced applications

- Hybrid (deterministic and Monte Carlo) computational radiation transport tools expand potential for solving large, complex real-world problems
  - Radiation from a nuclear detonation
  - Monte Carlo reactor simulation
  - Cargo interrogation
  - Facility safety and safeguards
  - Fusion (ITER)



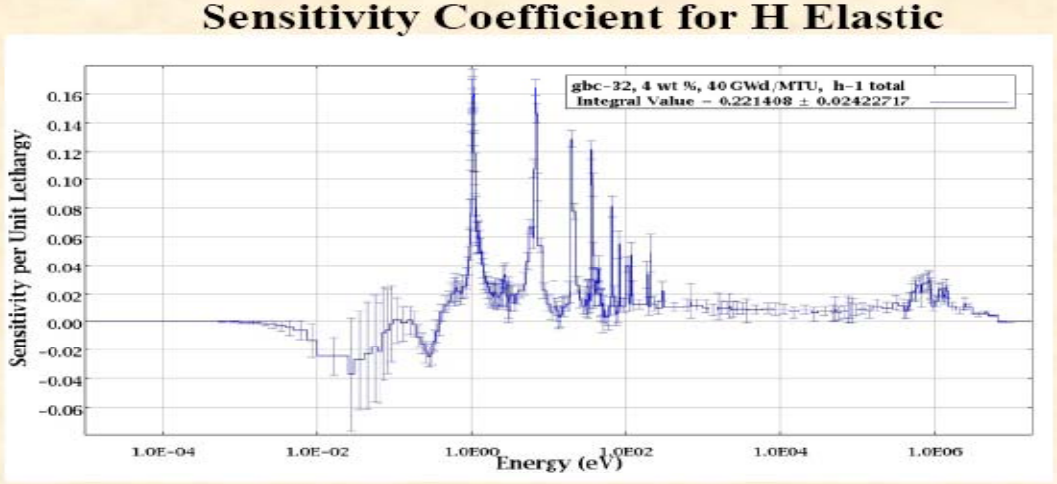







Problem: 25 mrem/y dose limit at controlled area boundary for ISFSI

SCALE Capabilities: Sensitivity/Uncertainty

- TSUNAMI calculates sensitivity coefficients for k-eff vs. cross section changes
  - Runs KENO V.a in forward and adjoint mode
  - Sensitivity data for each reaction of each nuclide on energy-dependent basis
  - Sensitivity profiles computed for experiments and applications can be compared to determine the degree of similarity

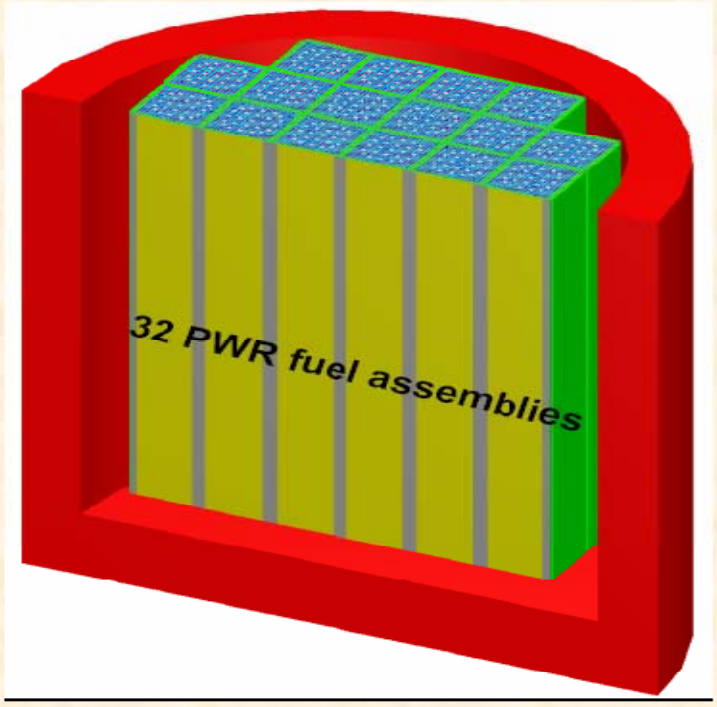
Monte Carlo Model for S/U Analysis of Spent-Fuel Cask



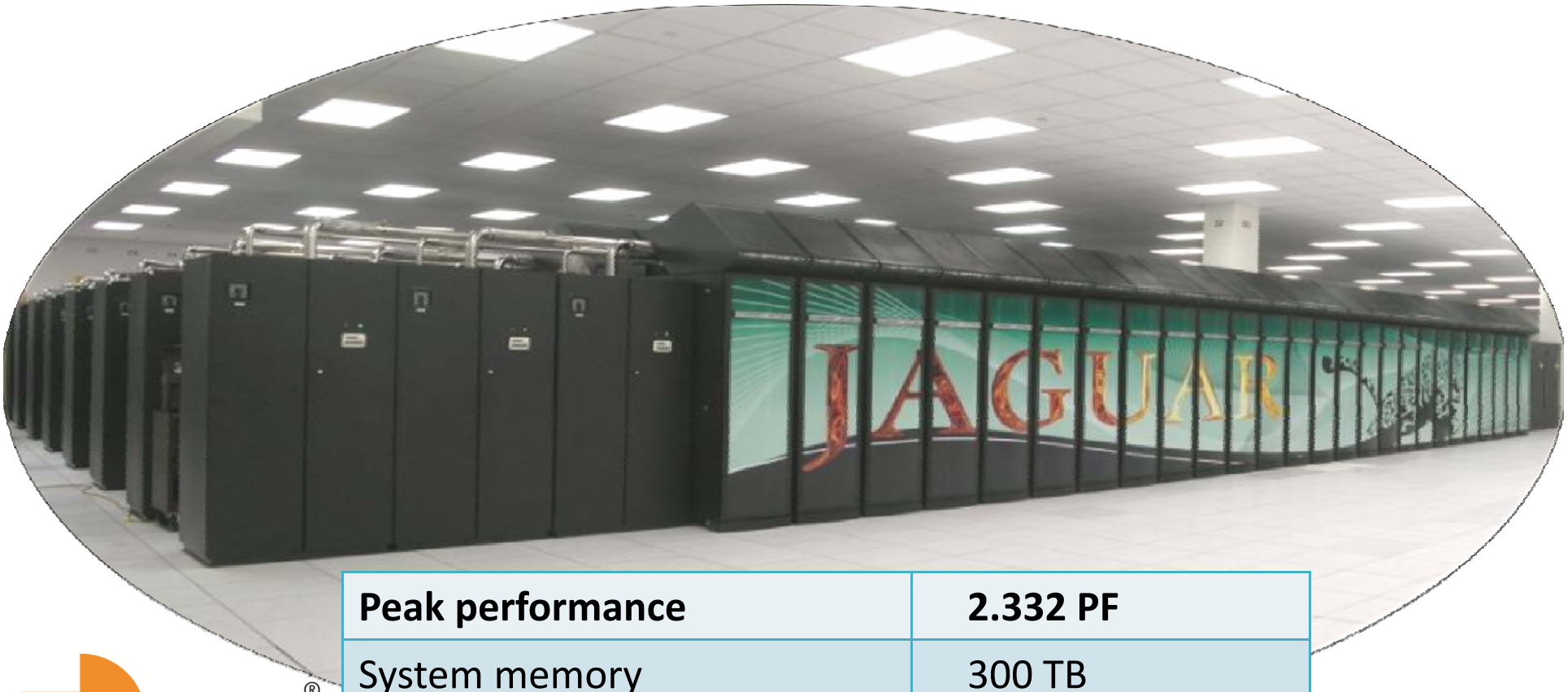
$$\mathrm{Var}(k) \equiv \mathbf{S}^{T}\mathbf{C}_{\alpha\alpha}\mathbf{S}$$

complete sensitivity

generic covariance



Jaguar: World's most powerful computer—Designed for science from the ground up



TOP500® SUPERCOMPUTER SITES

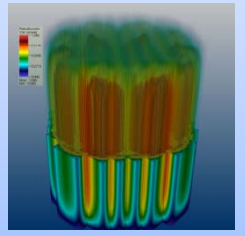
#1 Nov. 2009

Peak performance	**2.332 PF**
System memory	300 TB
Disk space	10 PB
Disk bandwidth	240+ GB/s
Interconnect bandwidth	374 TB/s

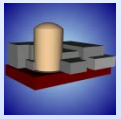
Denovo – massively parallel deterministic radiation transport code enabling solutions to enormous nuclear problems

- State of the Art Transport Methods
  - 3-D Discrete Ordinates (SN)
  - Multigroup energy, anisotropic PN scattering
  - 6 spatial discretization algorithms to choose from
- High Performance, Modern, Innovative Solvers
  - GMRES, BiCGStab. or Source Iteration options on within-group solves
  - DSA-preconditioning (SuperLU/ML-preconditioned CG)
  - Transport Two-Grid up-scatter acceleration of Gauss-Seidel MG iteration
  - Parallel first collision approximation
  - Eigenvalue (k_{eff}) and fixed-source problem modes
  - Krylov solvers provided by Trilinos Library

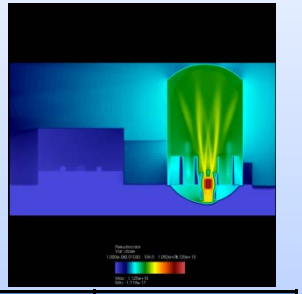
- Parallel Algorithms
  - Koch-Baker-Alcouffe (KBA) wavefront solve
  - Domain replicated & decomposed options for parallel first-collision source
  - Multi-level decompositions in energy and angle under development
  - Parallel I/O for massive problems
- Advanced Visualization and Run-Time Environment
  - Integrated Python front-end
  - Direct connection to SCALE geometry and data
  - HDF5 output directly interfaced with Visit



PWR Facility Modeling





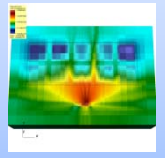


Zones	Angles	Groups	State Size (GB)	Output (GB)	Time (m)
103.7M	S_{24}/P_3	27	568.741	83.457	46.97
1,047.8M	S_{24}/P_3	27	5,746.180	843.189	79.43

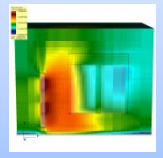
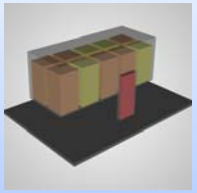
- **Highlights**
  - **2010 DOE Office of Science INCITE Award**
    Uncertainty Quantification for Three-Dimensional Reactor Assembly Simulations, 8M CPU-Hours
  - FY10 ASCR JOULE code
  - Key component of ORNL hybrid (Monte Carlo/deterministic) code/methods development
- **On-going and Future Directions**
  - 2 LDRDs (hybrid Monte Carlo and multilevel parallel decompositions)
  - Electron transport for home land security applications

Portal Monitoring

PNNL Generic Advanced Spectroscopy Panel (PGASP)

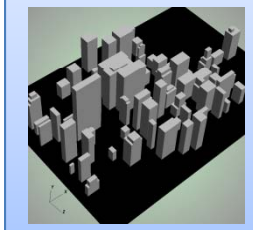
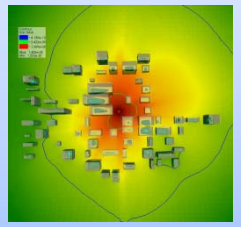
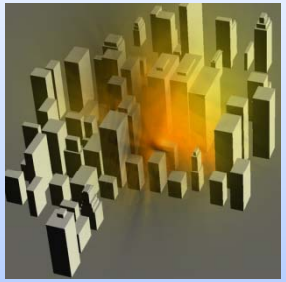


Denovo-generated importance functions for hybrid Monte Carlo

Urban Modeling

High-fidelity models of full cities

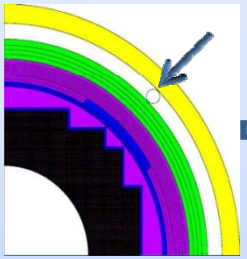




Neutron dose calculated on Jaguar XT5 in minutes

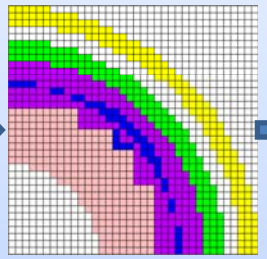
Hybrid radiation transport methods & codes developed at ORNL are making the impossible/impractical possible/practical

- Hybrid methods use the best attributes of Monte Carlo & deterministic methods in a complementary manner
- Methods & codes developed at ORNL are enabling high-fidelity Monte Carlo solutions for deep-penetration and answers-everywhere applications
  - CADIS – Consistent Adjoint Driven Importance Sampling, optimization of a single detector
  - FW-CADIS – Forward-Weighted CADIS, optimization of distributions (e.g., dose throughout a facility), as well as multiple detectors
- Hybrid codes
  - MAVRIC in publicly-released SCALE code system; uses Denovo (deterministic) and Monaco (Monte Carlo)
  - ADVANTG; uses deterministic and MCNP/X (Monte Carlo)

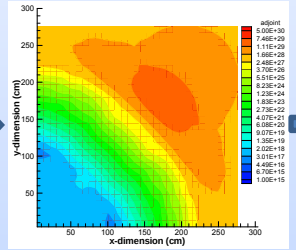
PWR Ex-Vessel Detector Modeling (CADIS)



Monte Carlo model



Deterministic model



Adjoint data

Results – O(10^4) Speedup

CASE	CPU TIME TO ACHIEVE RE=1% (H)	SPEEDUP
No VR	8.86E+4 (10.1 yrs)	1
Manual VR	13.6	6500
ADVANTG	**1.02**	**87000**

Calculate VR Parameters

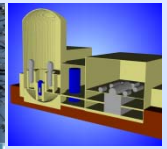
Source biasing

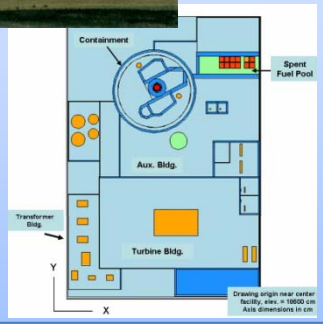
$$\hat{q}(\vec{r},E)=\frac{\phi^{+}(\vec{r},E)q(\vec{r},E)}{\int_V\int_E q(\vec{r},E)\phi^{+}(\vec{r},E)drdE'}$$

Transport biasing

$$w_i(\vec{r},E)=\frac{R}{\phi^{+}(\vec{r},E)\left(\frac{c_u+1}{2}\right)}$$

Full-Scale PWR Facility Modeling (FW-CADIS)

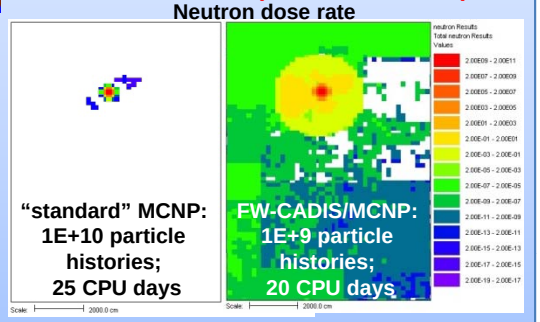




Simulation not possible with "standard" Monte Carlo

Simulation enabled with (ADVANTG-MCNP)

Neutron dose rate

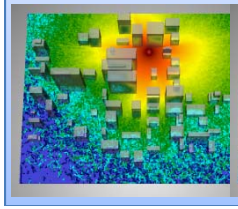


Note: scale is >30 orders of magnitude

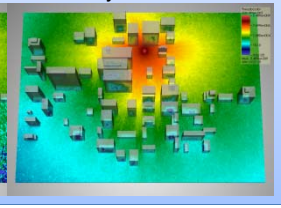
- **Highlights**
  - Enabled MC solutions for problems previously considered impossible
  - Routinely applied to nuclear energy, national security, & fusion applications
  - Unique capability at ORNL and key new capability in SCALE code system
- **On-going and Future Directions**
  - ORNL LDRD to extend hybrid methods for full-core MC reactor analysis
  - Extensions specific to national security applications
  - Implementation for accelerating Sensitivity/Uncertainty analyses

Urban Modeling (nuclear detonation)

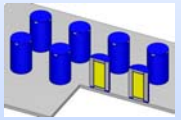
"standard' MC



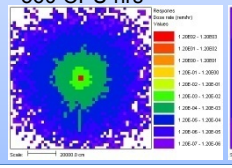
Hybrid MC



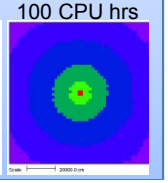
Reactor Site Boundary Dose (from spent fuel casks)



"standard' MC 560 CPU hrs



Hybrid MC 100 CPU hrs

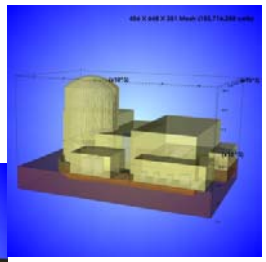


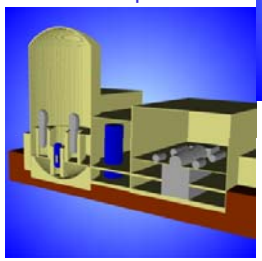
Nuclear Facility Modeling

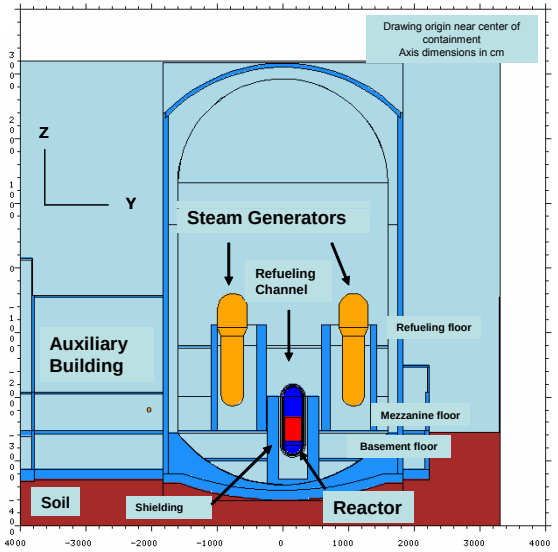
DTRA funded

- Full-scale PWR facility, including containment, auxiliary, turbine, and transformer buildings
  - Extent: 85 × 125 × 70 m
  - Sources modeled: reactor core, spent fuel pool, coolant activation

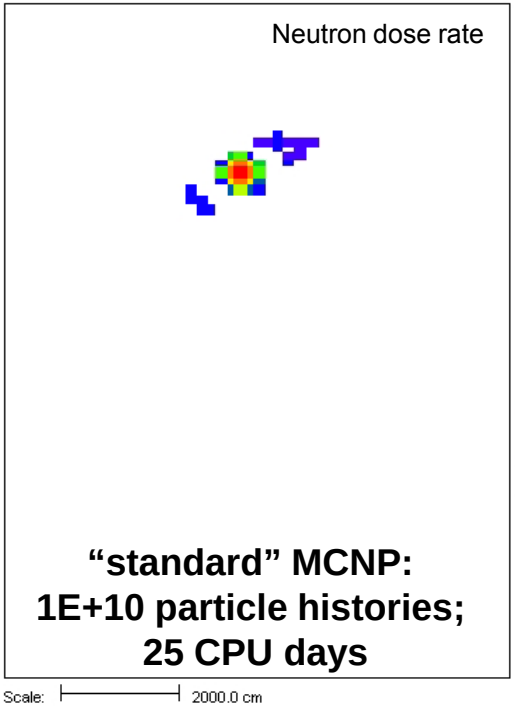
Denovo – deterministic transport model





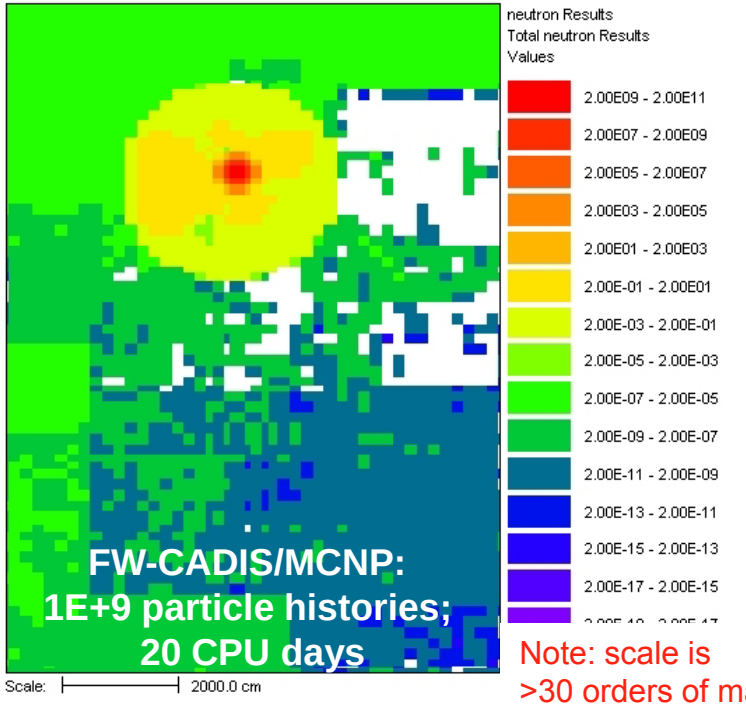


Simulation not possible with "standard" Monte Carlo

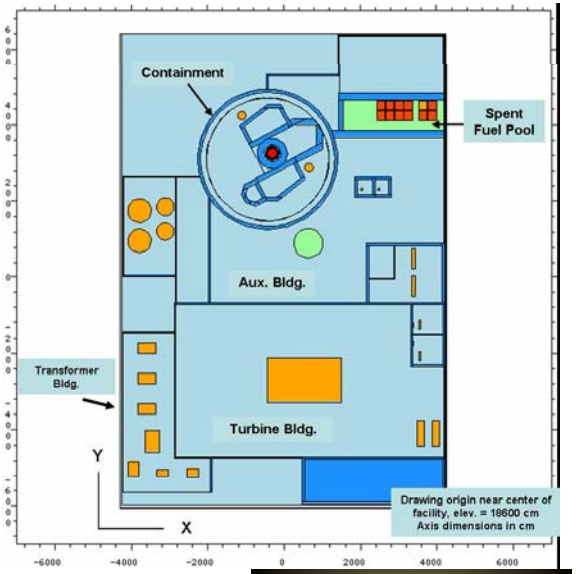


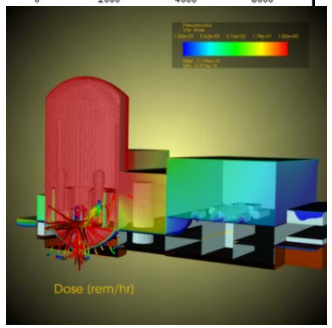
"standard" MCNP: 1E+10 particle histories; 25 CPU days

Simulation enabled with hybrid methods/code



FW-CADIS/MCNP: 1E+9 particle histories; 20 CPU days

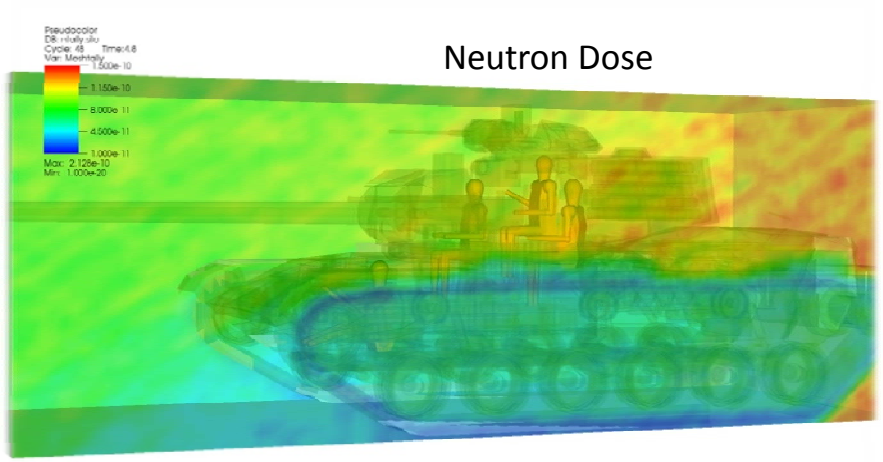


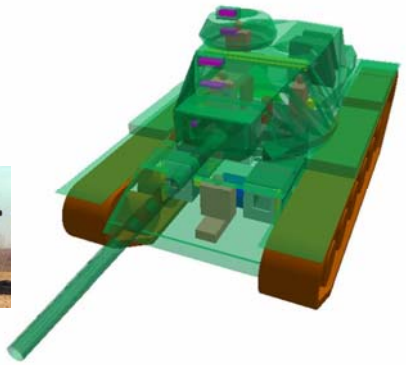


Note: scale is >30 orders of magnitude

Nuclear Vulnerability Analyses

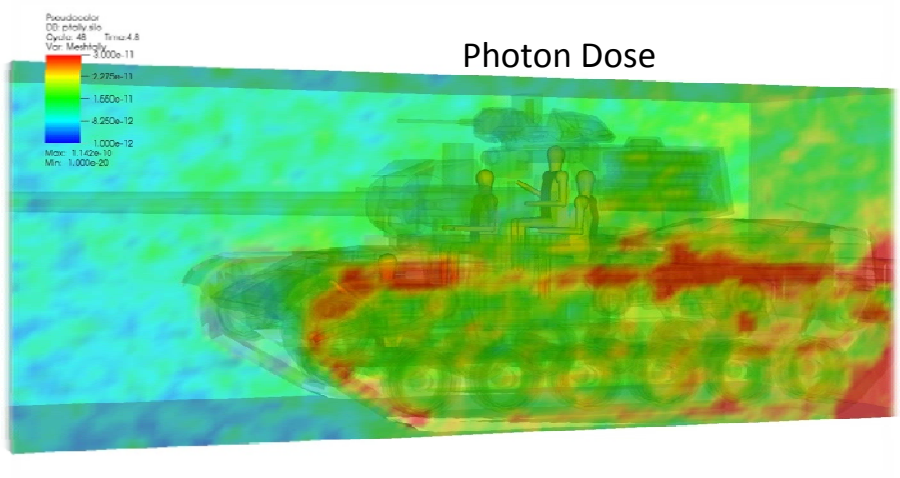
DTRA funded





BRL-CAD model of M60A1 tank

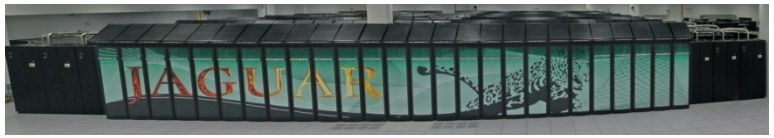
M60 Dosimetry Response to a Nuclear Event



- Objective – develop a modern nuclear analysis tool for performing radiation analyses for armored vehicles (replace MASH code system developed in '80s)
- Accomplishments
  - Developed relevant models to evaluate MCNP for this application
  - BRL-CAD interface developed & tested – MCNP-BRL provides linkage between MCNP5 and computer-aided design (CAD) packages
  - Hybrid methods applied/demonstrated

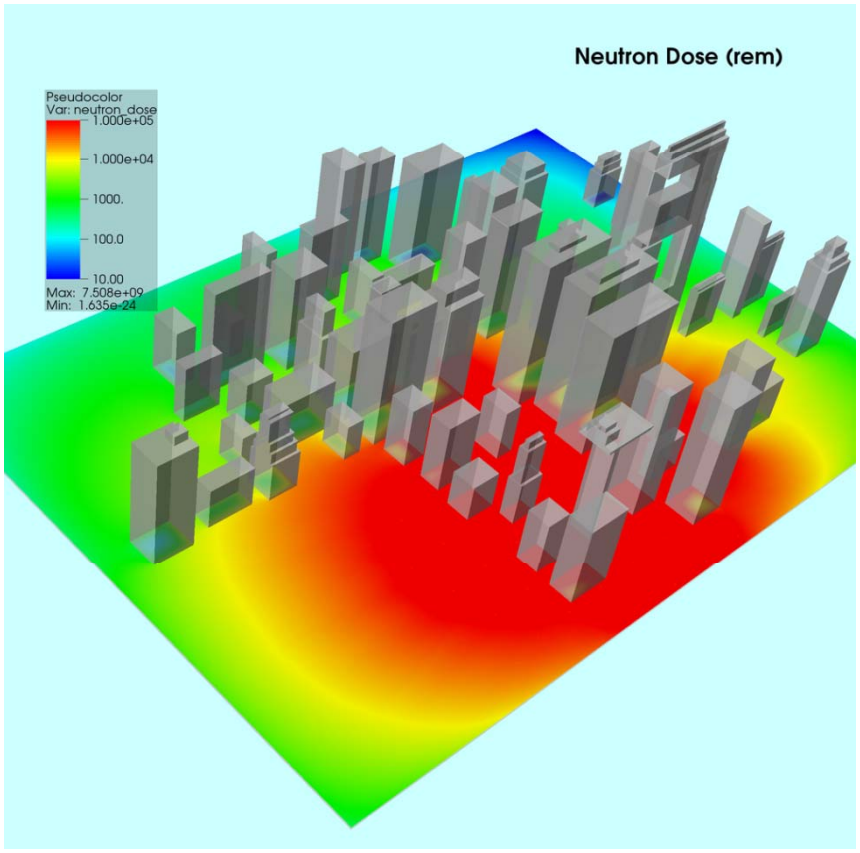
Urban IND Modeling

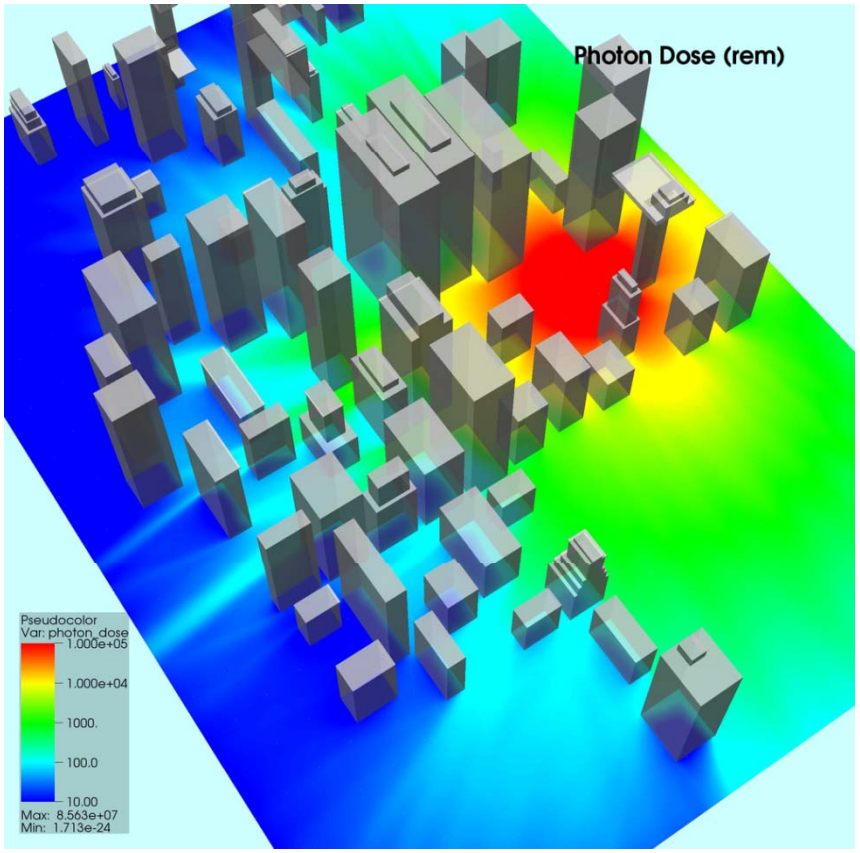
Denovo can run on PCs, workstation clusters, supercomputers



Jaguar – 1.64 PF Cray XT: 45,376 Quad-Core Processors, 362 TB memory

Enabling high-fidelity results in minutes





Neutron & Photon dose for a 1KT event (1×10^{23})

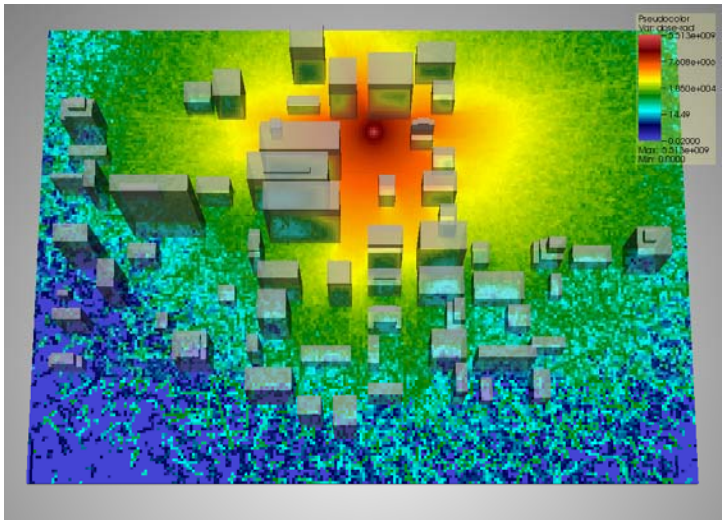
~70M cell problem (~1m^3 mesh), 27 neutron groups, P_3 Scattering, S-16 quadrature, 576 cores on JAGUAR - ~60 minutes

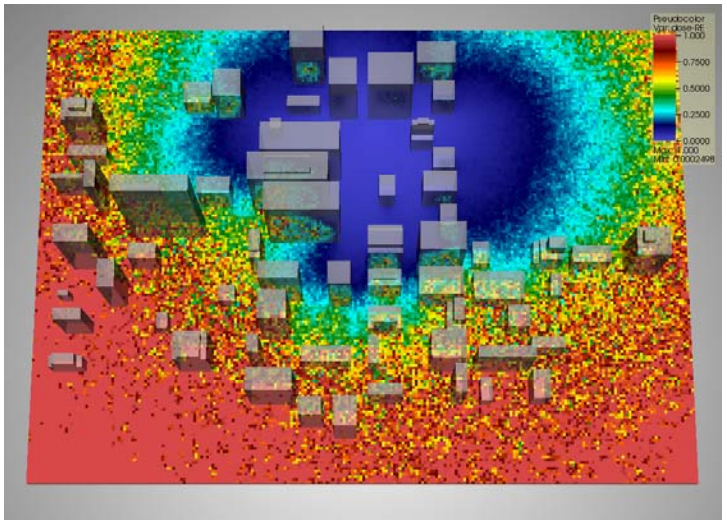
Urban IND Modeling

Hybrid methods enabling Monte Carlo-based results in reasonable computing times

24-hr Monte Carlo simulation of a 20kT Hiroshima-like weapon in a 1200×860×540m section of NYC

conventional

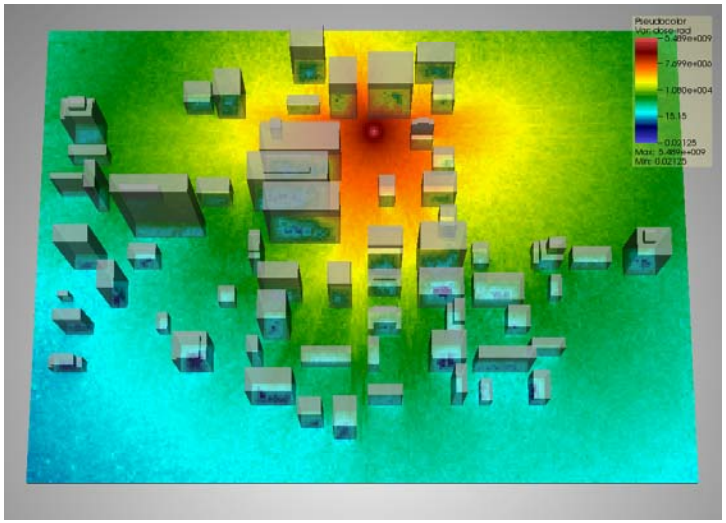


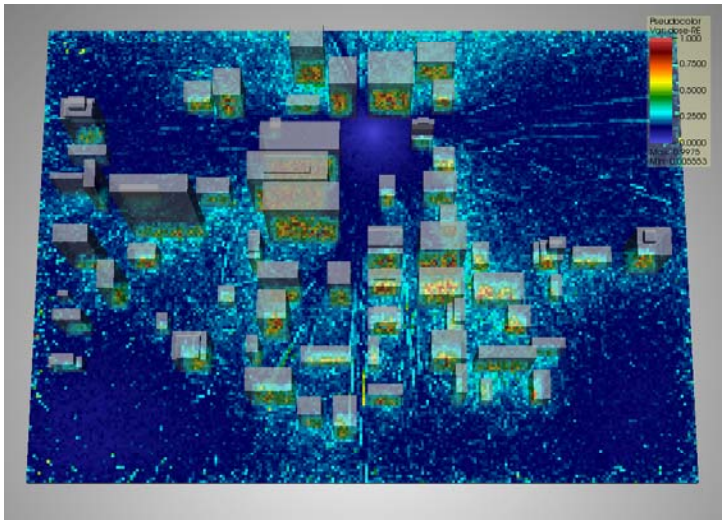


25% of cells have RE < 20%

48% of cells have RE < 50%

FW-CADIS





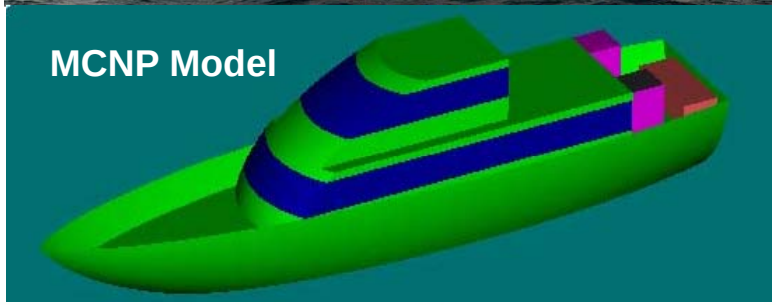
77% of cells have RE < 20%

97% of cells have RE < 50%

dose (rad)

relative uncertainty

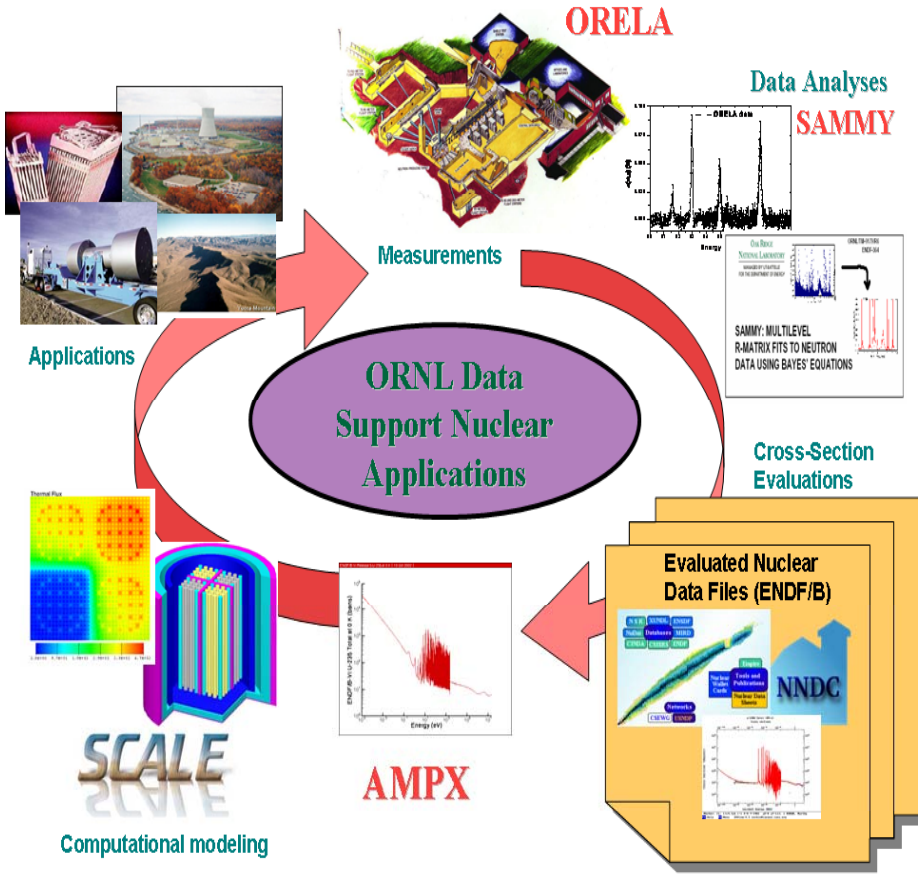
Active Interrogation Techniques to Detect SNM in Maritime Environments



- **Assessing the feasibility of current/projected active interrogation technologies on luxury yachts, fishing trawlers, break-bulk cargo ships and container ships**
- **Investigating boarded search and near proximity standoff detection scenarios**
- **Incorporating realistic background environments**
- **Analyzing the matrix of possible source/detector/shielding/cargo configurations**
- **Developing representative benchmark experiments of the two scenarios under investigation**

Summary

- ORNL has tightly coupled nuclear data and radiation transport capabilities:
  - Nuclear data measurements & evaluations
  - SCALE M&S tools for the entire nuclear fuel cycle
  - Sensitivity/uncertainty methods/tools for code validation, identification of nuclear data deficiencies, and focus experimental programs
  - Hybrid transport methods to enable full facility radiation protection and shielding design/analysis
    - Development of advanced tools for facility & packaging shield design optimization
  - Hybrid transport methods to enable Monte Carlo for neutronics portion of multi-physics core simulation
- Coupled data and transport capabilities provide valuable feedback loop to support nuclear data R&D for wide variety of nuclear applications



Opportunities for collaboration on nuclear data and radiation transport analyses

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+1 865 574-5260