Virginia Tech Nuclear Engineering Program
&
MRT Methodology and RAPID Code System for Neutronics Simulations

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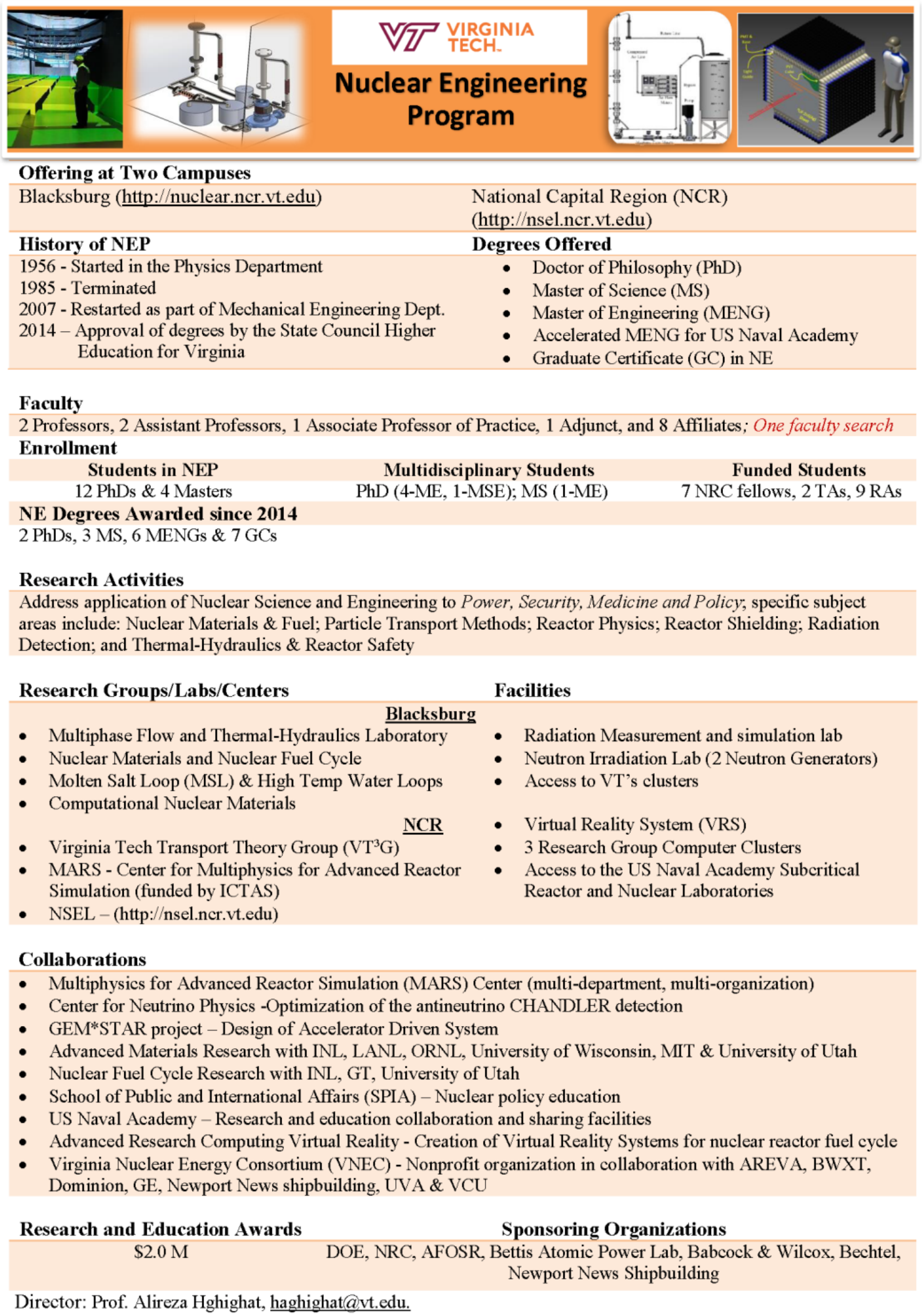
For presentation at the Idaho National Lab, Oct 24-25, 2017

NSEL
Nuclear Science and Engineering Laboratory
Virginia Tech Research Center. Arlington, VA

VIRGINIA TECH.

nuclear.ncr.vt.edu



VIRGINIA TECH.

Nuclear Engineering Program

Offering at Two Campuses

Blacksburg (http://nuclear.ncr.vt.edu)	National Capital Region (NCR) (http://nsel.ncr.vt.edu)

History of NEP	**Degrees Offered**
1956 - Started in the Physics Department 1985 - Terminated 2007 - Restarted as part of Mechanical Engineering Dept. 2014 – Approval of degrees by the State Council Higher Education for Virginia	• Doctor of Philosophy (PhD) • Master of Science (MS) • Master of Engineering (MENG) • Accelerated MENG for US Naval Academy • Graduate Certificate (GC) in NE

Faculty

2 Professors, 2 Assistant Professors, 1 Associate Professor of Practice, 1 Adjunct, and 8 Affiliates*; One faculty search*

Enrollment

Students in NEP	Multidisciplinary Students	Funded Students
12 PhDs & 4 Masters	PhD (4-ME, 1-MSE); MS (1-ME)	7 NRC fellows, 2 TAs, 9 RAs

NE Degrees Awarded since 2014

2 PhDs, 3 MS, 6 MENGs & 7 GCs

Research Activities

Address application of Nuclear Science and Engineering to *Power, Security, Medicine and Policy*; specific subject areas include: Nuclear Materials & Fuel; Particle Transport Methods; Reactor Physics; Reactor Shielding; Radiation Detection; and Thermal-Hydraulics & Reactor Safety

Research Groups/Labs/Centers	**Facilities**
Blacksburg	
• Multiphase Flow and Thermal-Hydraulics Laboratory • Nuclear Materials and Nuclear Fuel Cycle • Molten Salt Loop (MSL) & High Temp Water Loops • Computational Nuclear Materials	• Radiation Measurement and simulation lab • Neutron Irradiation Lab (2 Neutron Generators) • Access to VT's clusters
NCR	
• Virginia Tech Transport Theory Group (VT^{3}G) • MARS - Center for Multiphysics for Advanced Reactor Simulation (funded by ICTAS) • NSEL – (http://nsel.ncr.vt.edu)	• Virtual Reality System (VRS) • 3 Research Group Computer Clusters • Access to the US Naval Academy Subcritical Reactor and Nuclear Laboratories

Collaborations

- Multiphysics for Advanced Reactor Simulation (MARS) Center (multi-department, multi-organization)
- Center for Neutrino Physics -Optimization of the antineutrino CHANDLER detection
- GEM*STAR project – Design of Accelerator Driven System
- Advanced Materials Research with INL, LANL, ORNL, University of Wisconsin, MIT & University of Utah
- Nuclear Fuel Cycle Research with INL, GT, University of Utah
- School of Public and International Affairs (SPIA) – Nuclear policy education
- US Naval Academy – Research and education collaboration and sharing facilities
- Advanced Research Computing Virtual Reality - Creation of Virtual Reality Systems for nuclear reactor fuel cycle
- Virginia Nuclear Energy Consortium (VNEC) - Nonprofit organization in collaboration with AREVA, BWXT, Dominion, GE, Newport News shipbuilding, UVA & VCU

Research and Education Awards	**Sponsoring Organizations**
$2.0 M	DOE, NRC, AFOSR, Bettis Atomic Power Lab, Babcock & Wilcox, Bechtel, Newport News Shipbuilding

Director: Prof. Alireza Hghighat, haghighat@vt.edu.

Since 2014, offering *PhD, MS, MENG* degrees

Two Campuses:

- **Blacksburg**
- **National Capital Region (NCR)**

The only NE program in the Washington DC Metro area

2017, established an *accelerated MENG degree for the US Naval Academy (USNA)*

5 faculty, 1 faculty search, 8 affiliate faculty 1 adjunct

Faculty Research

Nuclear Materials Modeling

Dr. Celine Hin (Assistant Professor) (celhin@vt.edu)

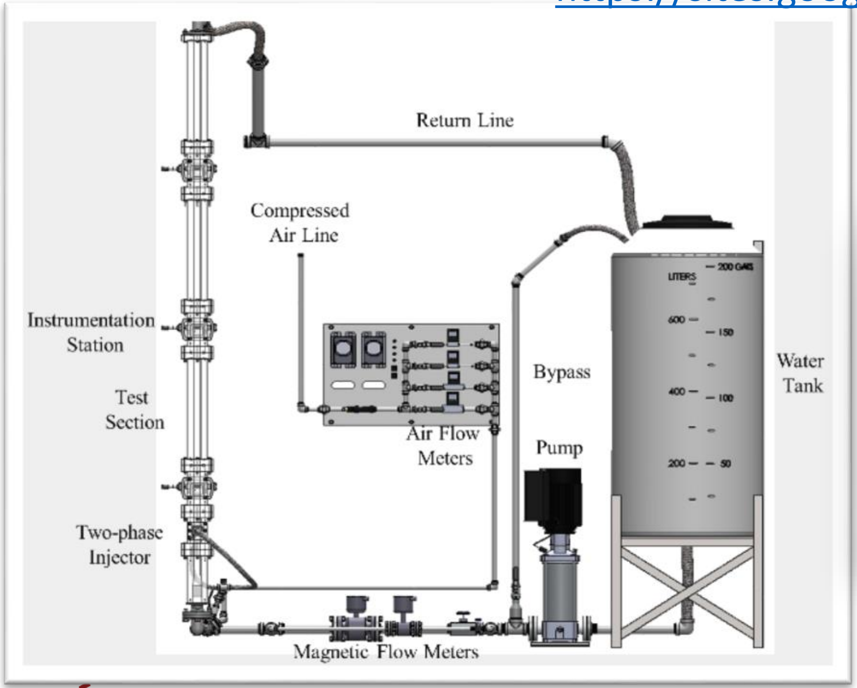
- Study of fuel and fuel cladding materials
- Development of *radiation resistant* materials
- Development of *kinetic Monte Carlo* code to study the microstructure evolution and corrosion under neutron radiation
- Study the effect of *point defects* on the integrity of nuclear materials using *density functional theory*

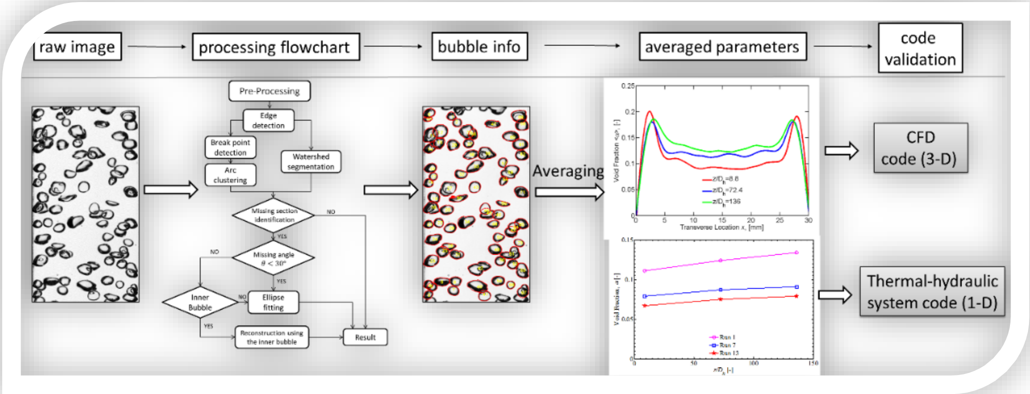
Multiphase Flow and Thermal-Hydraulics Lab (MFTL)

Dr. Yang Liu (Assistant Professor) (liu130@vt.edu)

- Thermal-hydraulic design and safety analysis
- Two-phase flow modeling, instrumentation and experiment
- Two-phase flow computational fluid dynamics (CFD)

https://sites.google.com/a/vt.edu/vtmftl/



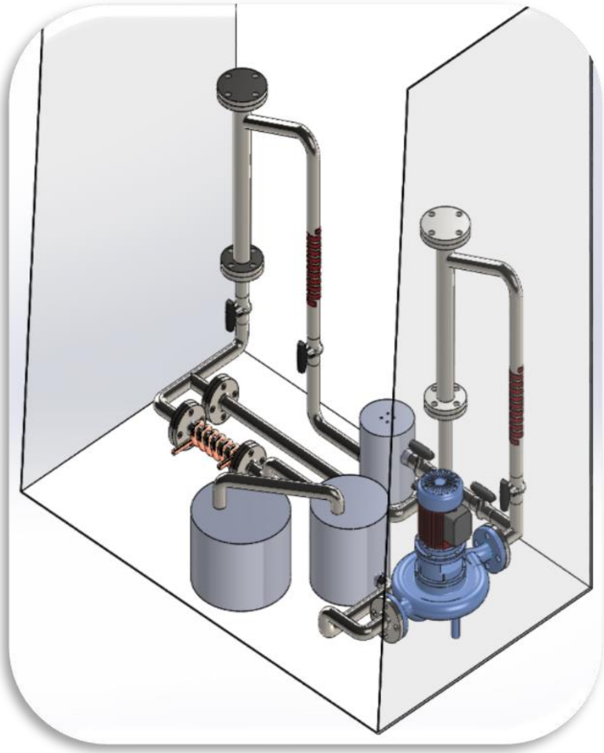


Nuclear Materials and Nuclear Fuel Cycle

Dr. Jinsuo Zhang (Professor) (zjinsuo@vt.edu)

- **Structural materials corrosion** and corrosion control in high temperature water, liquid metal, and molten salt
- **Chemistry** of fission products and actinides in molten chloride, fluoride salts and liquid sodium
- **Electrochemical separation** for used fuel treatment and molten salt purification
- **Fuel-cladding** chemical interactions (FCCI) of metallic fuels (mainly U-Zr)

Glovebox Systems, Molten Salt Loop & High Temp Water Loops



Faculty Search (2017-2018)

- **Nuclear Engineering and Sciences** (Open rank)**:** open to all areas of nuclear engineering including:
  - nuclear materials and fuels,
  - particle transport methods,
  - radiation detection,
  - reactor physics,
  - reactor safety,
  - reactor shielding,
  - reactor design,
  - medical and imaging applications,
  - nuclear security and safeguard,
  - nuclear non-proliferation and policy.

- This position is directly related to VT's Intelligent Infrastructure Destination Area (a transdisciplinary initiative across many colleges.)

Nuclear Engineering R&D at National Capital Region (NCR)

http://nsel.ncr.vt.edu

NSEL (Nuclear Science and Enginnering Lab), Arlington, VA Operates under auspices of ICTAS* and Mechanical Engineering Department.

It engages with various entities/organizations at Virginia Tech and beyond, addressing different applications including:

- **power,**
- **security,**
- **medicine, and**
- **policy**

*Institute of Critical Technology and Applied Science

Virginia Tech Research Center
Arlington, VA

NSEL Collaborations
(nsel.ncr.vt.edu)

Key R&D	
Antineutrino detector – ***CHANDLER project*** for nuclear nonproliferation applications (funded by NSF & VT)	Neutron Physics Center, Physics Department Profs. Huber, Link & Mariani, Phys. Dept.
Multiphysics for Advanced nuclear Reactor Simulation (MARS) Center (funded by the ICTAS' Global Energy and Materials Initiative - **GEMI**);	**VT:** NE, Physics, ME & MSE **US:** Georgia Tech, NCSU, ORNL, Southern Nuclear **EU:** Paul Scherrer Institute & ecole polytechnique fédérale de lausanne, Switzerland; Politecnico di Torino, Italy
Creation of a Collaborative Virtual Reality System & Development of ***VRS-RAPID*** (funded by office of VP of NCR)	VT Advanced Computing Research - Visionarium Center Prof. Polys and Dr. Rajamohan, VT-ARC

NSEL Collaborations
(nsel.ncr.vt.edu)

Educational Programs	
US Naval Academy (USNA) **Vice Admiral Leidig & Prof. Millett**	**Accelerated Master of Engineering in Nuclear Engineering** (Jan 2017)
School of Public and International Affairs (SPIA) & Department of Science and Technology in Society **Profs. Roberts (SPIA) and Schmid (STS)**	Prepared an application for a ***graduate Certificate in Nuclear Science, Technology, and Policy (NSTP)*** (Fall 2018)
Mechanical Engineering Faculty @ NCR **Profs. Mahajan, Pitchumani & Rahman**	Establishing a CPE activity***: Energy Engineering & Innovation*** (Spring 2018)
In collaboration with local universities, government agencies & VT departments, centers and groups	Has organized various **forums, workshops and training courses** (technical & policy matters)

VirginiaNuclear
Energy Consortium

http://www.virginianuclear.org/

VNEC nonprofit organization

Organization	Activities	Location
Virginia Nuclear Energy Consortium (VNEC) nonprofit organization*	• Promotion of nuclear industry, education and research • Membership include: AREVA, B&W, Dominion, GE, Newport News Shipbuilding, UVA, VCU, and VT • Prof. Haghighat served as Chairman of the Board, Jan 2015 to July 2016; currently, he serves as the Vice Chairman of the Board	Virginia

*On June 6, 2016,with help from NEI, VNEC organized the first *Virginia Nuclear Energy Summit*, and Prof. Haghighat gave an opening talk and participated in two panel discussions.

NSEL – Organization of Workshops/Forums*

Year (date)	Title
2011 (Nov 7-11)	13th International Workshop on Particle Transport Simulation of Nuclear Systems (http://www.cpe.vt.edu/transport)
2012 (March 11-12)	Symposium on Low Power Critical Facilities (LPCF) in collaboration with SUNRISE (Southeast Universities Nuclear Reactors Institute for Science and Education) (http://www.cpe.vt.edu/lpcf)
2012 (Nov 5)	Forum on Nuclear Regimes: Future Outlooks; sponsors included AREVA, ICTAS, VT-NCR, and partners included Naval Postgraduate school, Federation of American Scientists, and George Washington's Elliot College of International Affairs (http://www.ictas.vt.edu/nuclear)
2013 (Aug 7)	Seminar on nuclear power & education for a group of international reporters (at the request of Department of State) (http://nsel.ncr.vt.edu)
2014 (July 20)	a half-day workshop on "Advanced particle transport methodologies/tools for nuclear safeguards and non-proliferation," INMM 55th Annual Meeting, Atlanta, Georgia. (In collaboration with Georgia Tech)
2014 (Sept 28)	A half-day workshop on "Hybrid particle transport methods for solving complex problems in real-time," PHYSOR 2014 International Conference, Kyoto, Japan. (In collaboration with Georgia Tech)
2014 (Dec 15-18)	MRT Methodologies for Real-Time Simulation of Nuclear Safeguards & Nonproliferation Problems,' Modeling and Simulation for Safeguards and Nonproliferation *Workshop ORNL.*

*visit http://nsel.ncr.vt.edu/events.html for further details on workshops and related presentations.

NSEL – Organization of Workshops/Forums (continued)*

Year (date)	Title
2015 (June 23-25)	1st Workshop on Methodologies for Spent Nuclear Fuel Pool Simulations (Safety and Safeguards) (http://www.cpe.vt.edu/nuclear)
2016 (May 6)	Prof. Haghighat was an invited panelist at the *2016 Energy Sustainability and Resiliency*, organized by VA Chamber of Commerce; VNEC set an information booth.
2016 (June 6)	*Virginia Nuclear Energy Summit*, organized by VNEC and NEI; Prof. Haghighat opened the Summit & served on two panels
2016 (Oct 5)	A half-day workshop on *MRT Methodologies for Real-Time Particle Transport Simulation of Nuclear Systems* at the *3th International Conference on Radiation Shielding (ICRS-13) & 19th Topical Meeting of the Radiation Protection & Shielding Division of the American Nuclear Society -2016 (RPSD-2016)* in Paris, France, Oct 3-6.

*visit http://nsel.ncr.vt.edu/events.html for further details on workshops and related presentations.

NSEL - Virginia Tech Transport Theory Group (VT^3G)

CHANDLER (Carbon Hydrogen An- tineutrino Detector with a Lithium Enhanced Raghavan) - A novel Detector Technology for Reactor antineutrino Detection (*Inverse beta decay (IBD) interaction:* $\bar{\nu}_e + p \rightarrow e^+ + n$)

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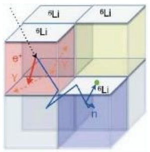
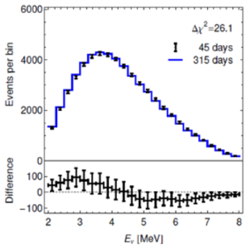
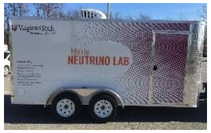
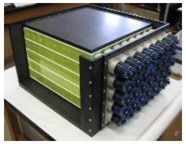


- **Why?**
  - Look for a new hypothetical particle called a sterile neutrino
  - Monitoring of nuclear reactors for non-proliferation and safeguards applications
  - Coupling with RAPID for reactor core physics monitoring

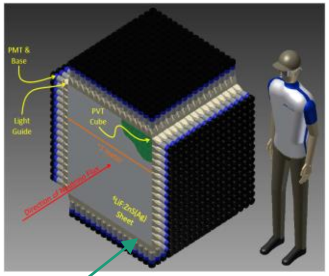


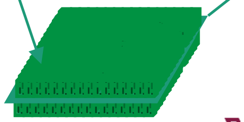
- **Status**
  - Has built a miniCHANDLER; for the last two months it has been placed outside the North Anna Power Station
  - Performed detailed neutronics studies
    - Removal of background cosmic-ray neutron events through spatial-temporal-energy correlations
    - Examined a simplified shield
  - Plan (seeking further funding)
    - Analyze the results of miniCHANDLER
    - Examine other coinciding events for reduction of background
    - Develop an effective shield design
    - Construct a full CHANDLER (1 m^3)
    - Perform experiments at the BR2 reactor facility, SCK.CEN, Belgium





16 layers of 16x16 wavelength-shifting scintillator cubes; 17 layers of LiF-ZnS(Ag)





Center for Multiphysics for Advanced nuclear Reactor Simulation (MARS)

Mission of Center:

Design and analysis of a **revolutionary nuclear reactor system** that is transformative and can significantly improve the availability of clean and affordable energy for all mankind. We are developing multi-physics algorithms for modeling and simulation of both **critical** and **subcritical** (driven with an accelerator) Molten Salt fueled reactors

Research team (PI, co-PI's, post-docs, students):

- Alireza Haghighat (Cluster Lead, PI), Nuclear Engineering Program, ME, haghighat@vt.edu
- Celine Hin (co-PI), Nuclear Engineering Program, ME&MSE, celhin@vt.edu
- Patrick Huber (co-PI), Physics, pahuber@vt.edu
- Yang Liu (co-PI), Nuclear Engineering Program, ME, liu130@vt.edu
- Bruce Vogelaar (co-PI), Physics, vogelaar@vt.edu
- Jinsuo Zhang* (co-PI), Nuclear Engineering Program, ME, zjinsuo@gmail.com (new faculty)
- Valerio Mascolino (Ph.D. student), Nuclear Engineering Program, ME, val@vt.edu
- Nathan J. Roskoff (Ph.D. student) , Nuclear Engineering Program, ME, roskofnj@vt.edu

Funding : Internally funded by ICTAS

Ongoing work: With limited funding is working on:

- *t*RAPID: time-dependent algorithms for RAPID for reactor kinetics (solid and liquid fuel);
- *b*RAPID: a 3-D, FM-based burnup calculation algorithm for RAPID; and,
- *A* response-function formulation is being developed for determination of detector response.

MARS Center led a multidisciplinary &multi-organization proposal

DoE-IRP Grand Challenge Proposal

(Feb 2017; not selected)

Title: Novel Multiphysics Software for Design and Safety Analysis of Molten Salt Reactors in Support of NEAMS

Virginia Tech is leading an Integrated Research Project (IRP) proposal for the multi-physics modeling and simulation of MSRs. US collaborators with outstanding technical accomplishments as well as EU partners with previous experience on MSR design are involved in the project:

US Academia

- Virginia Tech, Arlington/Blacksburg, VA, (Alireza Haghighat (PI), Jinsuo Zhang, Co-PI)
- Georgia Institute of Technology, Atlanta, GA (Bojan Petrovic, Farzad Rahnema, Dingkang Zhang, Co-PIs)
- North Carolina State University, Raleigh, NC (Maria Avramova, Kostadin Ivanov, Co-PIs)

US Industry

- Southern Company Services , Birmingham, AL (Nick Smith, Co-PI)

US National Laboratories

- Oak Ridge National Lab, Oak Ridge, TN (Kevin Robb, Ben Betzler, Co-PIs)

International Organizations

- Paul Scherrer Institute, Switzerland (Jiří Křepel, Andreas Pautz, Konstantin Mikityuk, Co-PIs)
- Politecnico di Torino, Italy (Piero Ravetto, Sandra Dulla, Co-PIs)

Creation of a Collaborative Virtual Reality System (VRS) & VRS-RAPID

Objective:

Development of a first-of-a-kind web application for the creation of a collaborative Virtual Reality System (VRS) for application to 3D interactive scientific computing.

Benefits:

- Offering theoretical and experimental courses, especially distance learning courses and those with laboratories or experiments involving hazardous materials
- Training of professionals
- Analysis of results of modeling and simulation of systems
- Development of tools for management of emergencies

Work done:

- Developed a collaborative VRS software for the RAPID (Real-time Analysis for Particle transport and In-situ Detection) code system. This software is referred to VRS-RAPID.*

Participants:

- Dr. Alireza Haghighat, Nuclear Engineering Program
- Dr. Nicholas Polys, Visionarium, Department of Computer Science
- Dr. Srijith Rajamohan, Visionarium, Department of Computer Science
- Valerio Mascolino, PhD Candidate, Nuclear Engineering Program
- Nathan Roskoff, PhD Candidate, Nuclear Engineering Program

Amount of funding and time frame:

- Internal funding

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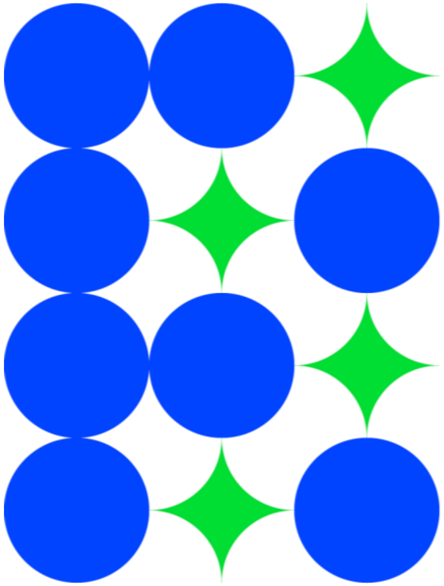
*Pending patent application



RAPID code system & VRS-RAPID

Neutronics Simulation Approaches

- **Deterministic Methods**
  - Solve the linear Boltzmann equation to obtain the expected flux in a phase space
- **Statistical Monte Carlo Methods**
  - Perform particle transport <u>experiments</u> using random numbers (RN's) on a computer to estimate average properties of a particle in phase space

Deterministic vs. Monte Carlo

Item	Deterministic	MC
Geometry	Discrete/ Exact	Exact
Energy treatment – cross section	Discrete	Exact
Direction	Discrete/ Truncated series	Exact
Input preparation	Difficult	simple
Computer memory	Large	Small
Computer time	Small	Large
Numerical issues	Convergence	Statistical uncertainty
Amount of information	Large	Limited
Parallel computing	Complex	Trivial

Why not MC only?

- Because of the difficulty in obtaining
  detail information
  with **reliable statistical** uncertainty
  in a **reasonable time; examples are:**
    - Real-time simulations
    - Obtaining energy-dependent flux distributions,
    - Time-dependent simulations,
    - Sensitivity analysis,
    - Determination of uncertainties

Why not use advanced hardware?

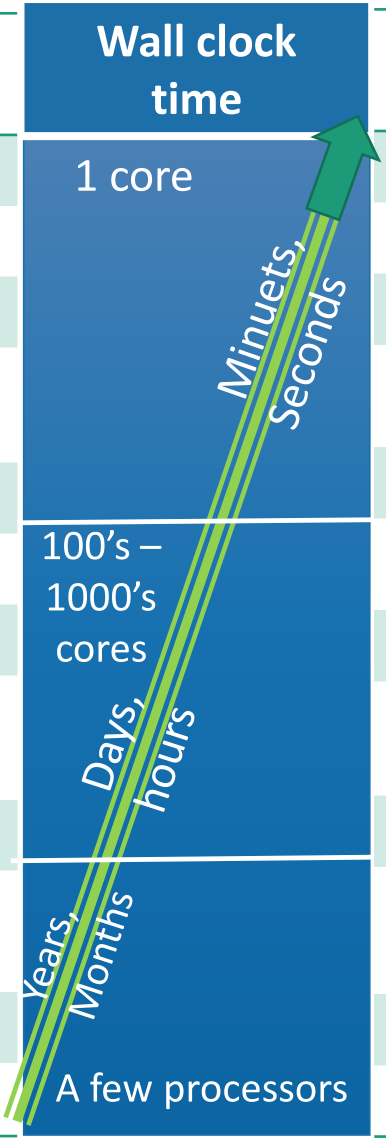
- VT^{3}G has developed vector and parallel algorithms:
  - Developed two large codes: PENTRAN (1996) and TITAN (2004)

Why not use hybrid methods?

- **Deterministic-deterministic** (differencing schemes, different numerical formulations, generation of multigroup cross sections, generation of angular quadratures, acceleration techniques)
  - VT^{3}G has developed various algorithms; a few have been implemented in PENTRAN and TITAN

- **Monte Carlo-deterministic** (variance reduction with the of use deterministic adjoint)
  - VT^{3}G has developed CADIS, A^{3}MCNP in 1997; *CADIS has become popular recently*!

My Journey
Particle Transport Algorithms Development



Year	Methodology	Computer code system	Former & Current Students
2017	VRS-MRT	VRS-RAPID	V. Mascolino
2016	MRT	RAPID	Dr. Walters & N. Roskoff
2015	MRT	TITAN-IR	Dr. Royston
2013	MRT	AIMS	Drs. Royston & W. Walters
2009	MRT	INSPCT-s	Dr. W. Walters
2007	Hybrid MC-det. (AVR)	ADIES (e^-)	Dr. B. Dionne
2005	Hybrid det. – det.	TITAN (n, ϒ)	Dr. C. Yi
1997	Hybrid MC-det. (automated VR - AVR)	A^{3}MCNP (n, ϒ)	Dr. J. Wagner
1996	Parallel (3-D)	PENTRAN (n, ϒ)	Dr. G. Sjoden
1992	Vector & parallel (2-D)		Drs. M. Hunter, R. Mattis & B. Petrovic
1989	Parallel processing (1-D)		
1986	Vector processing (1-D)		

Remarks

- Particle transport-based methodologies are needed for real-time simulation

- Even *‘Fast’ particle transport codes*, with parallel and hybrid algorithms, are slow because of large number of unknowns

Development of Particle Transport Formulations and Methodologies for Real-Time Calculations

- *Physics-Based transport methodologies* are needed:

  - ***Multi-stage, Response-function Transport (MRT) methodology*** *(Annals of Nuclear Energy, Vol. 87, 2016)*
    - Based on problem physics **partition** a problem into **stages** (sub-problems),
    - For each stage employ response method and/or adjoint function methodology
    - Pre-calculate response-function or adjoint-function using an accurate and fast transport code
    - Solve a linear system of equations to couple all the stages

Application of the *MRT Methodology*

- **Nondestructive testing:** Optimization of the Westinghouse's PGNNA active interrogation system for detection of RCRA (Resource Conversation and Recovery Act) (e.g., lead, mercury, cadmium) in waste drums (partial implementation of MRT; 1999)

- **Nuclear Safeguards:** Monitoring of spent fuel pools for detection of fuel diversion (funded by LLNL); Developed INSPCT-s code system (2007)

- **Nuclear nonproliferation:** Active interrogation of cargo containers for simulation of special nuclear materials (SNMs) (2013) (in collaboration with GaTech); developed the AIMS (Active Interrogation for Monitoring Special-nuclear-materials) code system (2013)

- **Image reconstruction for SPECT (Single Photon Emission Computed Tomography):** Real-time simulation of an SPECT device for generation of project images using an MRT methodology and Maximum Likelihood Estimation Maximization (MLEM); Developed the TITAN-IR code system (filed for a patent, June 2015)

- Simulation, Monitoring, and safeguards of nuclear systems: developed the RAPID (Real-time Analysis for Particle-transport and In-situ Detection) code system (2014) & more recently a Virtual Reality System for RAPID, VRS-RAPID (Sept 2017) (filed for patents for both concepts, Oct 2017)

Rapid

Real-time Analysis for Particle
Transport and In-situ Detection

Modeling of Nuclear Systems (cores, pools & casks)

- **Commonly used approach - Monte Carlo Simulation**
  - Source Convergence in eigenvalue MC is difficult due to undersampling (due to absorbers), HDR, inter-generation correlation
    - These effects are difficult to detect
  - Computation times are very long, especially to get detailed information
  - Changing system configuration (for design and analysis) requires complete recalculation

RAPID’s MRT Methodology

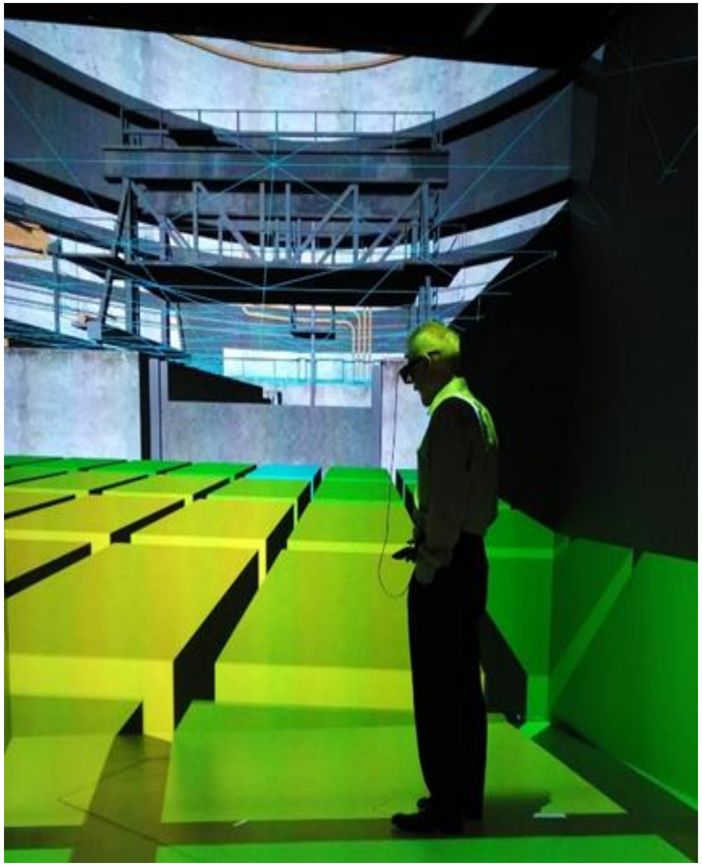
- **RAPID formulation is based on:**
  - Fission Matrix (FM) method
  - Adjoint function methodology, and

  it is expressed as a linear system of equations with pre-calculated coefficients and response functions.

- **Pre-calculations:**
  - FM coefficients and Adjoint-function distributions (or detector response coefficients) are pre-calculated via a *proprietary* MRT strategy for different assembly types, burnups, cooling times, and detector types and positions.

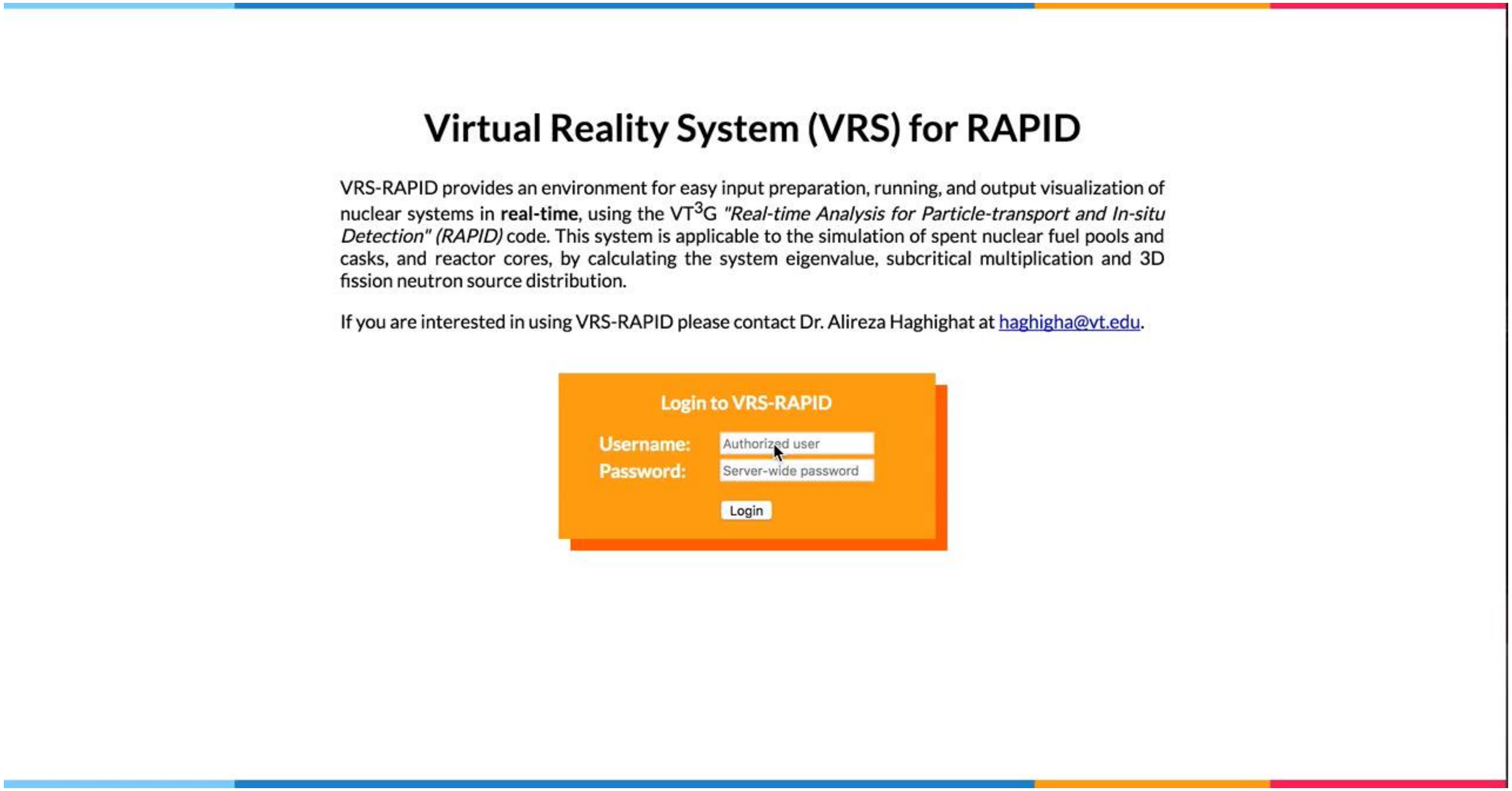
VRS-RAPID* Web Application

- RAPID is incorporated into a *Web application*, referred to as the Virtual Reality System (VRS) for RAPID.
- VRS-RAPID provides a collaborative Virtual Reality environment for a user to build models, perform simulation, and view 3-D diagrams in an interactive mode.
- 3-D diagrams can be projected onto a virtual system environment (e.g., a pool) for further analysis and training purposes.
- Additionally, VRS-RAPID outputs can be coupled with an immersive facility such as the VT's HyberCube System, as shown in this figure.



**Filed a patent application*

A Demo for the VRS-RAPID Web Application



Virtual Reality System (VRS) for RAPID

VRS-RAPID provides an environment for easy input preparation, running, and output visualization of nuclear systems in **real-time**, using the VT^{3}G *"Real-time Analysis for Particle-transport and In-situ Detection" (RAPID)* code. This system is applicable to the simulation of spent nuclear fuel pools and casks, and reactor cores, by calculating the system eigenvalue, subcritical multiplication and 3D fission neutron source distribution.

If you are interested in using VRS-RAPID please contact Dr. Alireza Haghighat at haghigha@vt.edu.

Login to VRS-RAPID

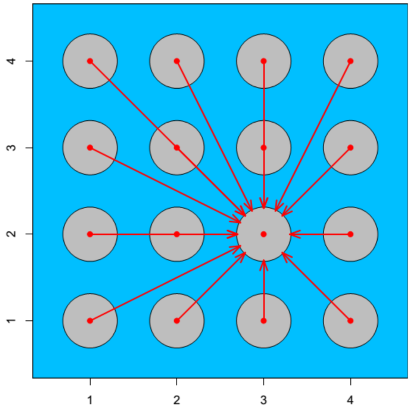
Username: Authorized user

Password: Server-wide password

Fission Matrix Method

- **Eigenvalue** formulation

$$F_i = \frac{1}{k}\sum_{j=1}^{N} a_{i,j}F_j$$



  - k is eigenvalue
  - F_j is fission source, S_j is fixed source in cell j
  - $a_{i,j}$ is the number of fission neutrons produced in cell i due to a fission neutron born in cell j.

- **Subcritical multiplication** formulation

$$F_i = \sum_{j=1}^{N}(a_{i,j}F_j + b_{i,j}S_j)\,,$$

  - $b_{i,j}$ is the number of fission neutrons produced in cell i due to a source neutron born in cell j.

Determination of FM Coefficients (Pool - 81 Assemblies)

- **Brute force approach:**
  - For a typical spent nuclear fuel pool with a sub-region of 9x9 assemblies:

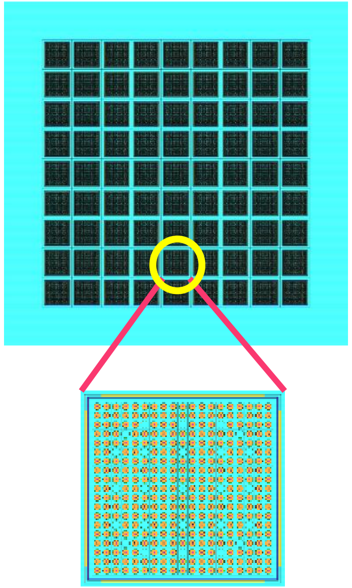
$$\boldsymbol{N = 9 \times 9 \times 264 = 21,384} \textbf{ total fuel pins}$$

    - Considering 24 axial segments per rod, then

$$\boldsymbol{N = 513{,}216}$$

  - Standard FM would require $N = 513{,}216$ separate fixed-source calculations to determine the coefficient matrix
    - A matrix of size *N x N* = 2.63391E+11 total coefficients (> 1 TB of memory is needed)

Pool - 9x9 array of assemblies



Assembly- 19x19 array

- The straightforward approach is clearly **NOT feasible**

- **Multi-layer, regional approach** (*filed for a patent*)
  - Determine coefficients as a function of different parameters
  - Process coefficients for problem of interest

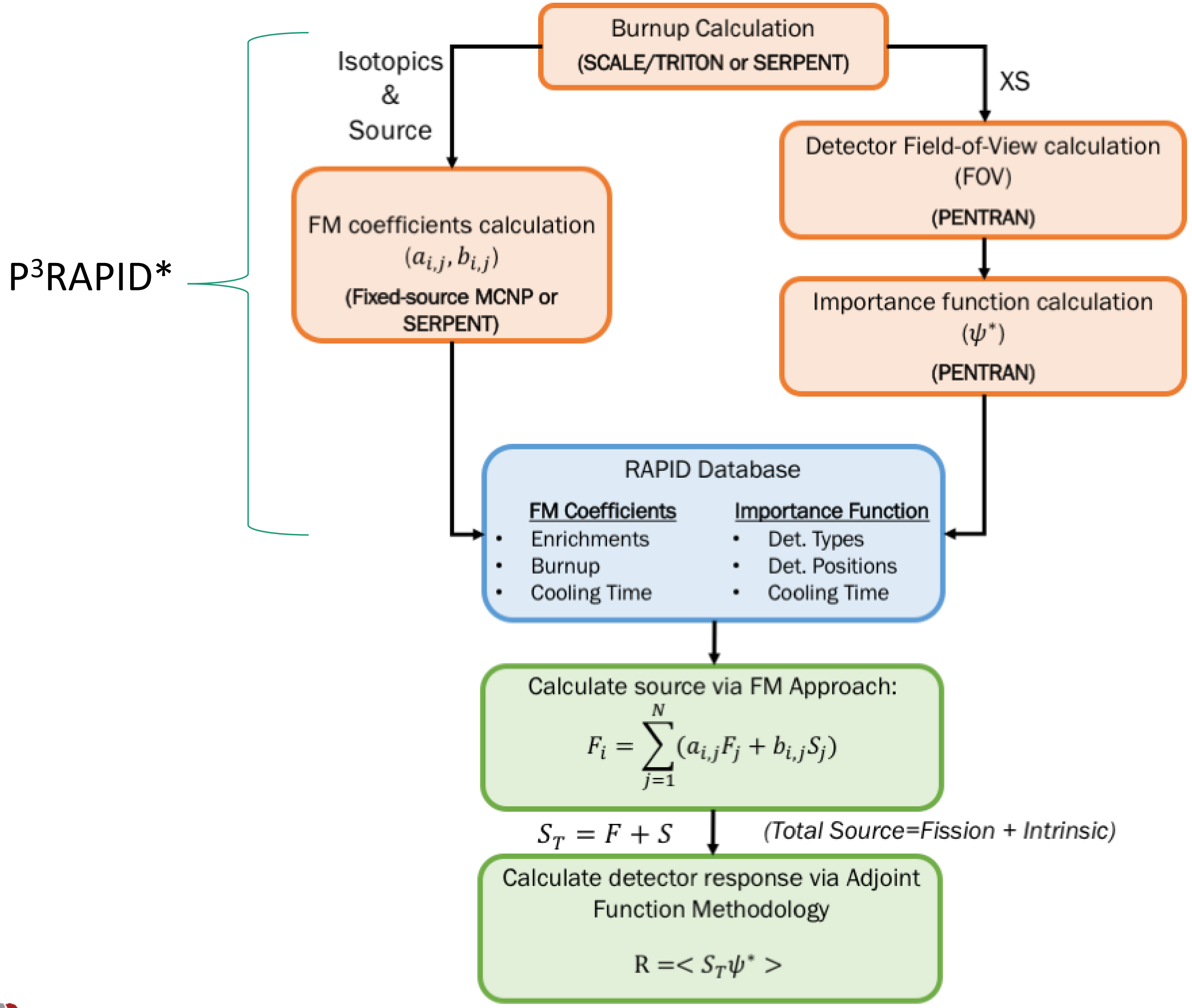
Status of RAPID

- Thus far, has been used for
  - simulation of spent fuel pools and storage casks, and reactor cores.

- Current capability
  - Calculates *system eigenvalue, subcritical multiplication, axially-dependent pin-wise fission* neutron, gamma, and/or antineutrino distributions, and detector responses or surface radiation dose.
  - When used in conjunction with measurements, e.g., for safeguards application, it can identity potential fuel diversion or misplacement.

- Ongoing work
  - *t*RAPID: time-dependent algorithms for RAPID for reactor kinetics (solid and liquid fuel);
  - *b*RAPID: a 3-D, FM-based burnup calculation algorithm for RAPID; and,
  - *A* response-function formulation is being developed for determination of detector response.

RAPID Code System Flowchart



Burnup Calculation

(SCALE/TRITON or SERPENT)

Isotopics & Source

XS

FM coefficients calculation

$(a_{i,j}, b_{i,j})$

(Fixed-source MCNP or SERPENT)

Detector Field-of-View calculation (FOV)

(PENTRAN)

Importance function calculation

(ψ^*)

(PENTRAN)

P^3RAPID*

RAPID Database

FM Coefficients
- Enrichments
- Burnup
- Cooling Time

Importance Function
- Det. Types
- Det. Positions
- Cooling Time

Calculate source via FM Approach:

$$F_i = \sum_{j=1}^{N} (a_{i,j}F_j + b_{i,j}S_j)$$

$S_T = F + S$ *(Total Source=Fission + Intrinsic)*

Calculate detector response via Adjoint Function Methodology

$$\mathrm{R} = < S_T \psi^* >$$

* P^3RAPID: Pre- and Post-Processing module for RAPID

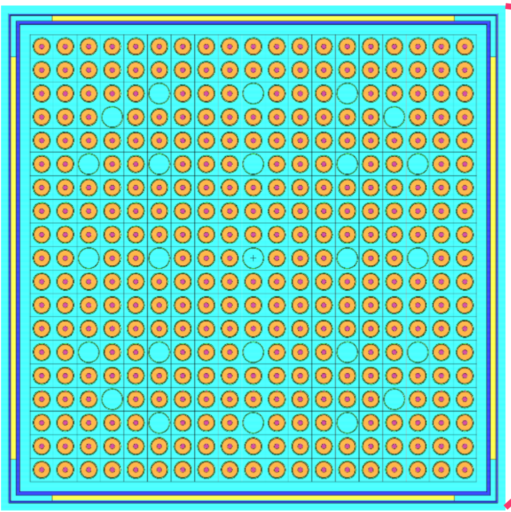
I^2S-LWR (Spent Fuel Pool)

I^2S-LWR FUEL ASSEMBLY

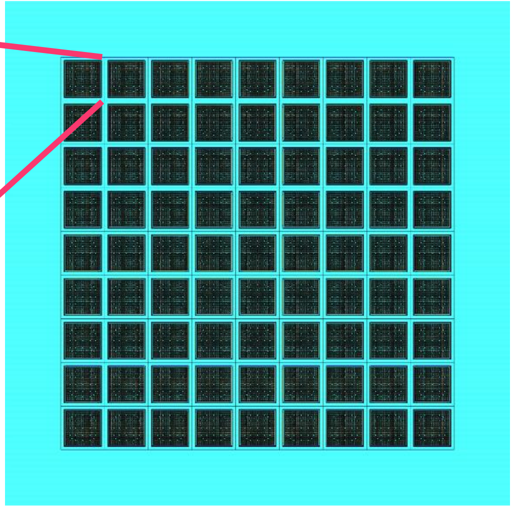
- 19x19 fuel lattice
  - 335 fuel rods, 24 control/guide tubes, 1 instrumentation tube
- U_3Si_2 fuel enriched to 4.95 wt-% ^{235}U

SPENT FUEL POOL

- Based on AP1000 SFP
- Consider a 9x9 segment of SFP (81 assemblies)
- Storage cell walls made of Metamic® (B4C-Al) between SS plates



Assembly in a Storage Cell

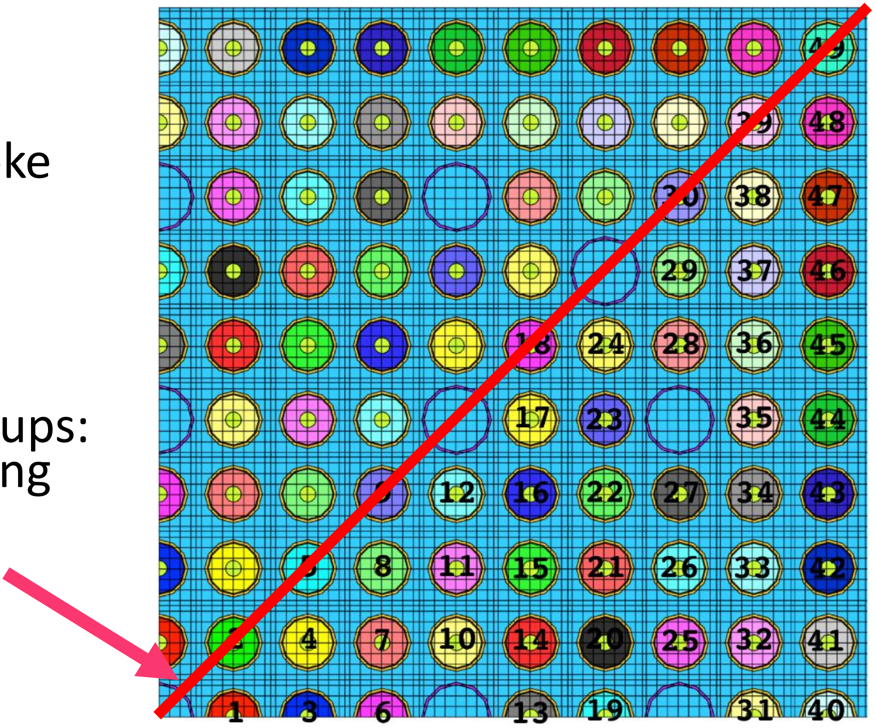


9x9 Segment of SFP

p^3RAPID – Burnup Calculation (SCALE-TRITON)

Stage 1

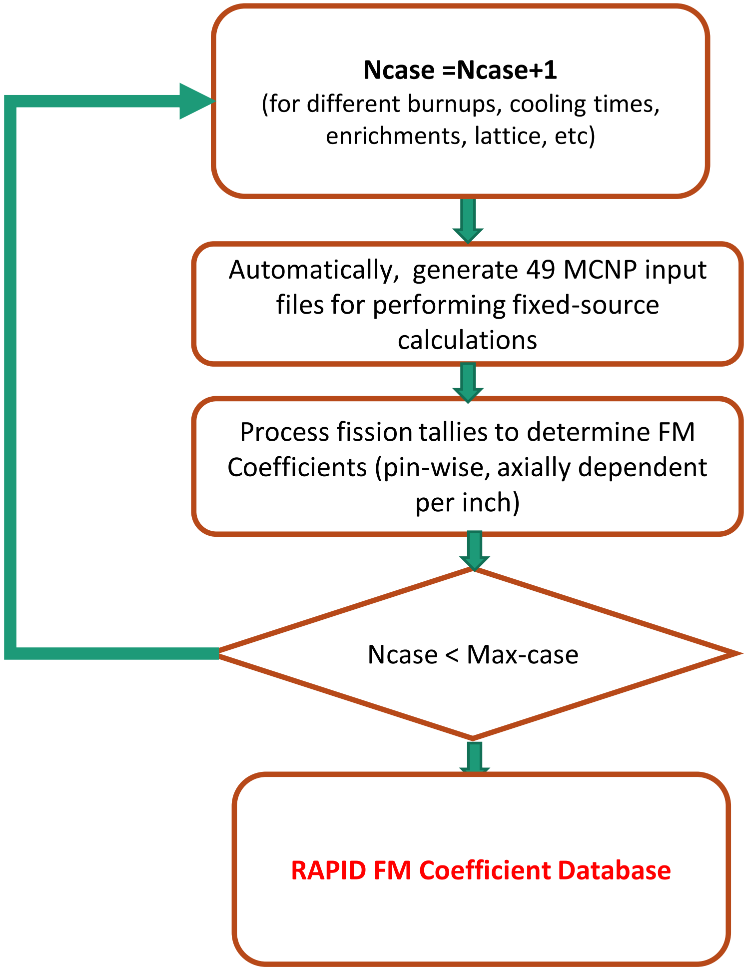
- **Need :** Material composition & Intrinsic source
- **Use:** SCALE 6.1 - TRITON
  - The TDEPL option used to invoke NEWT 2D & ORIGEN
- **For:**
  - enrichment of 4.95 wt-%; burnups: 37, 59 GWd/MTHM; and, Cooling Times: 14 days, 1 & 9 years
  - Quarter assembly model used.
  - 49 different fuel materials (considering octal symmetry)



p^3RAPID – FM Coefficient

Stage 2

- Using information from Stage 1,



Ncase =Ncase+1
(for different burnups, cooling times, enrichments, lattice, etc)

Automatically, generate 49 MCNP input files for performing fixed-source calculations

Process fission tallies to determine FM Coefficients (pin-wise, axially dependent per inch)

Ncase < Max-case

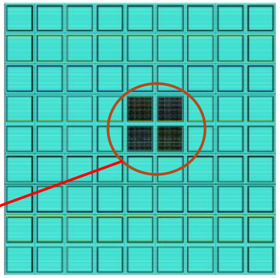
RAPID FM Coefficient Database

RAPID vs. MCNP

Spent fuel pool

Test Cases

- Performed eigenvalue calculations for a 2x2 segment of the reference SFP.
  - 4 test cases are defined, each containing different combinations of burnups/cooling times
  - Fuel region of the model partitioned into 32,256 fission regions (tallies) (for 1344 pins with 24 axial levels)
- Reference MCNP eigenvalue parameters are:
  - 10^6 particles per cycle, 400 skipped cycles 400 active cycles



Burnup [GWd/MTHM]

Cooling Time [years*]

CASE 1

0 GWd/MTHM 0 yr	37 GWd/MTHM 0 yr
37 GWd/MTHM 0 yr	0 GWd/MTHM 0 yr

CASE 2

0 GWd/MTHM 0 yr	59 GWd/MTHM 0 yr
59 GWd/MTHM 0 yr	0 GWd/MTHM 0 yr

CASE 3

59 GWd/MTHM 9 yr	37 GWd/MTHM 0 yr
37 GWd/MTHM 0 yr	59 GWd/MTHM 9 yr

CASE 4

59 GWd/MTHM 9 yr	37 GWd/MTHM 9 yr
37 GWd/MTHM 9 yr	59 GWd/MTHM 9 yr

*'0 year' cooling time refers to ~14 days

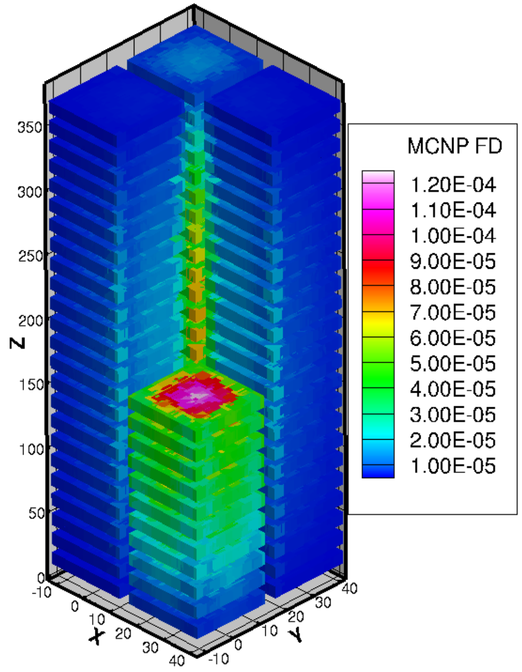
Comparison of Eigenvalues

Case	Keff		Rel. Diff. (RAPID vs. MCNP) (pcm)
	MCNP	RAPID	
1	0. 79998 (± 4 pcm)	0.80020	28
2	0.79511(± 4 pcm)	0.79532	26
3	0.60444(± 3 pcm)	0.60425	-31
4	0.58330(± 3 pcm)	0.58322	-14

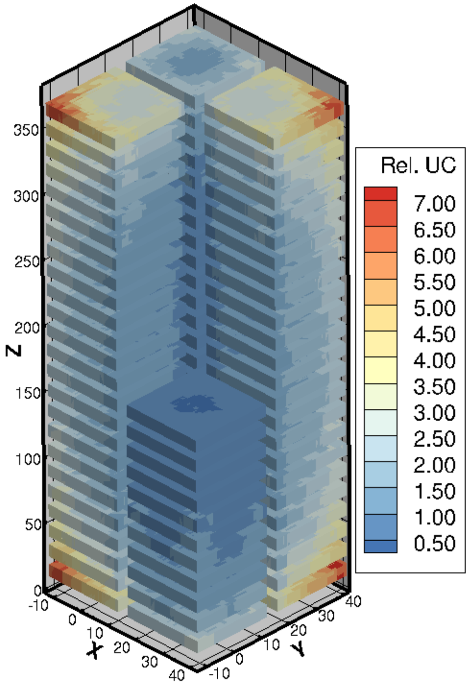
MCNP prediction – Fission Density (Case 1)

0 GWd/MTHM 0 yr	37 GWd/MTHM 0 yr
37 GWd/MTHM 0 yr	0 GWd/MTHM 0 yr

Fission Density



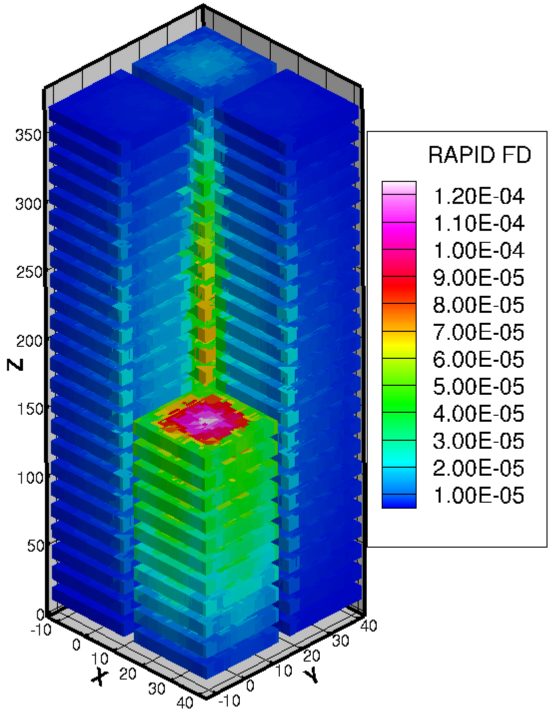
1-σ Relative Uncertainty



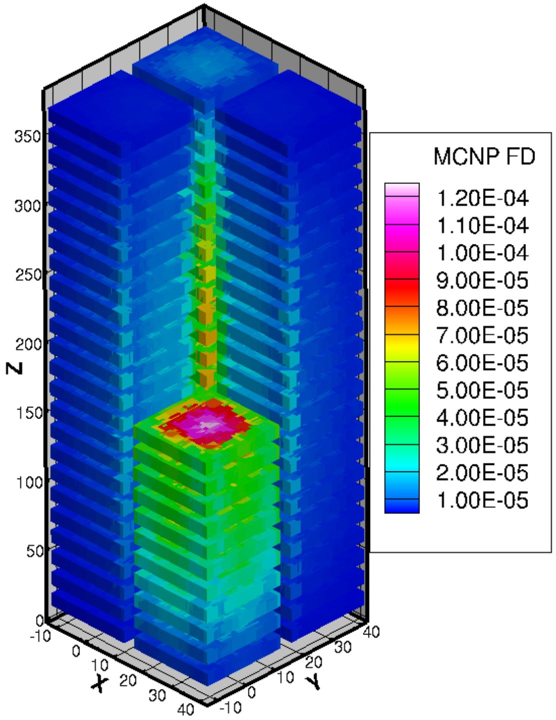
RAPID vs. MCNP – Fission Density (Case 1)

0 GWd/MTHM 0 yr	37 GWd/MTHM 0 yr
37 GWd/MTHM 0 yr	0 GWd/MTHM 0 yr

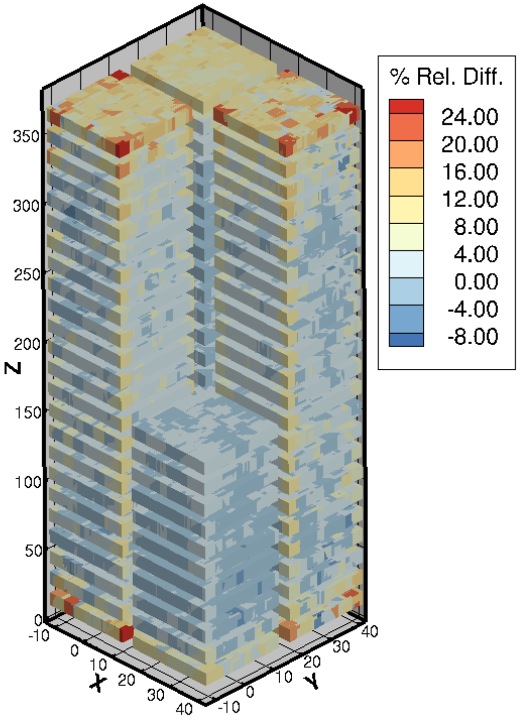
RAPID



MCNP



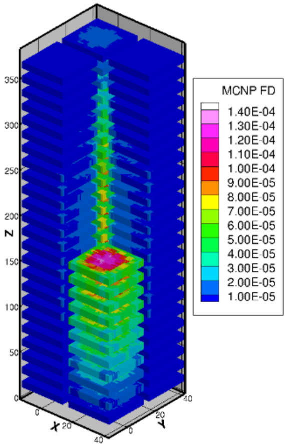
% Relative Difference



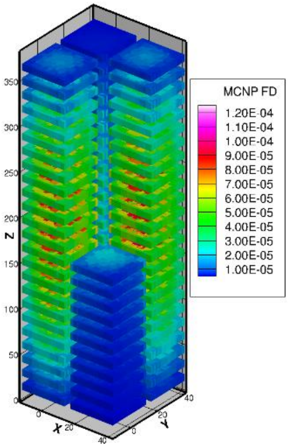
MCNP prediction – Fission Density (Cases 2-4)

Fission Density

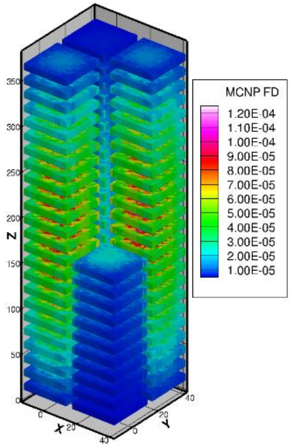
Case 2



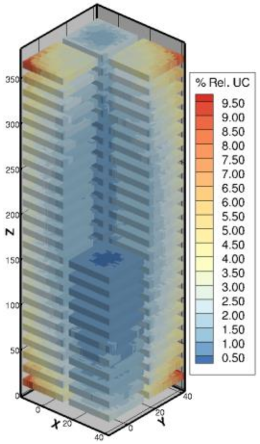
Case 3

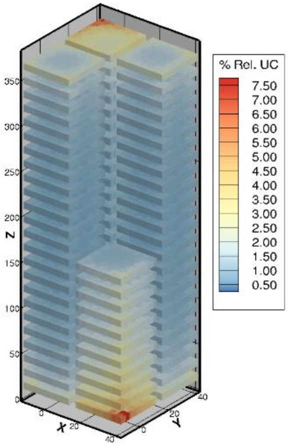


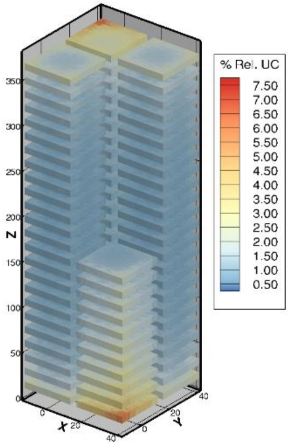
Case 4



1-σ Relative Uncertainty



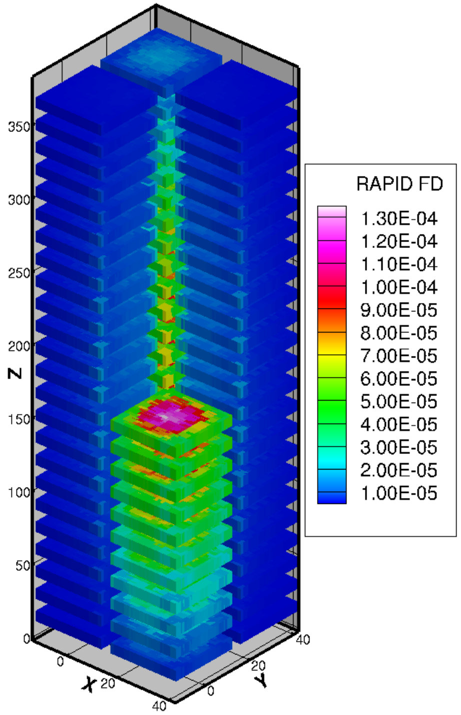




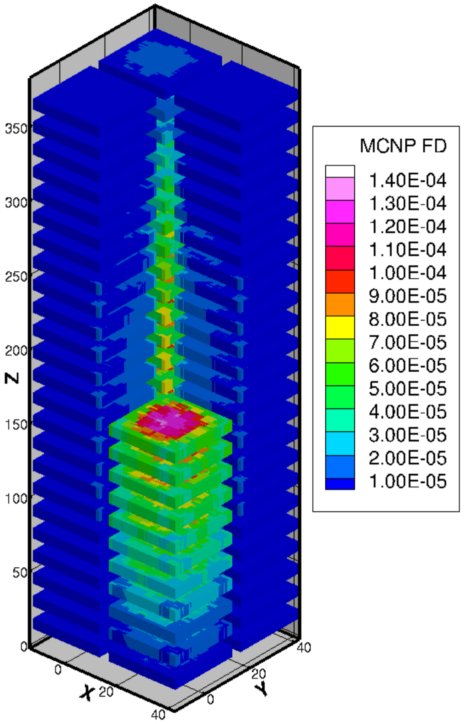
RAPID vs. MCNP – Fission Density (Case 2)

0 GWd/MTHM 0 yr	59 GWd/MTHM 0 yr
59 GWd/MTHM 0 yr	0 GWd/MTHM 0 yr

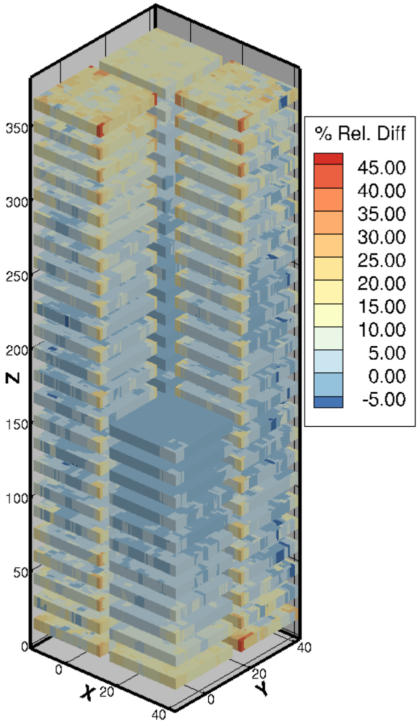
RAPID



MCNP



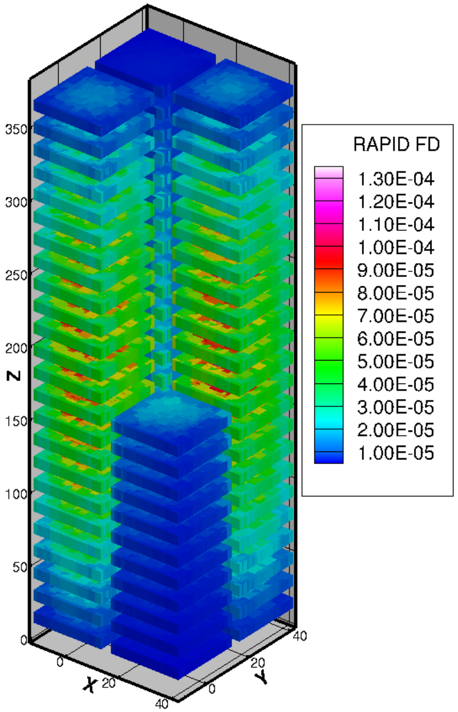
% Relative Difference



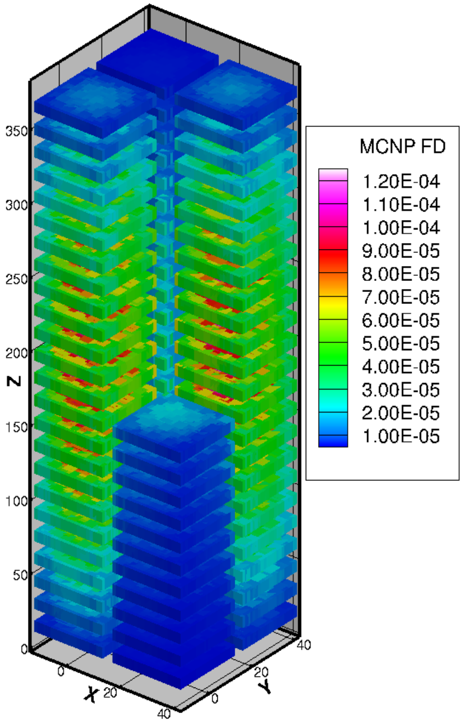
RAPID vs. MCNP – Fission Density (Case 3)

59 GWd/MTHM 9 yr	37 GWd/MTHM 0 yr
37 GWd/MTHM 0 yr	59 GWd/MTHM 9 yr

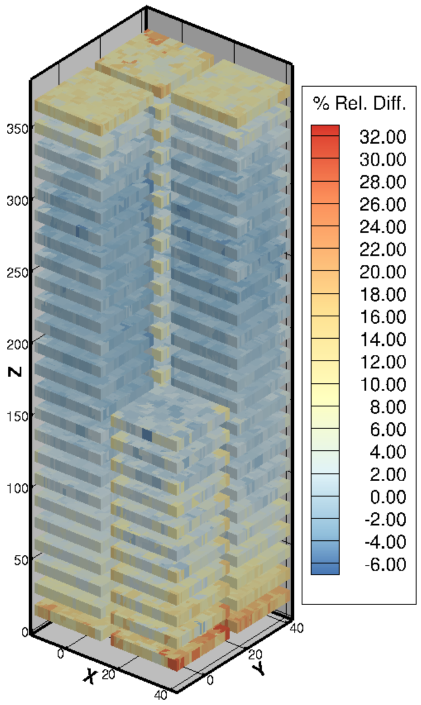
RAPID



MCNP



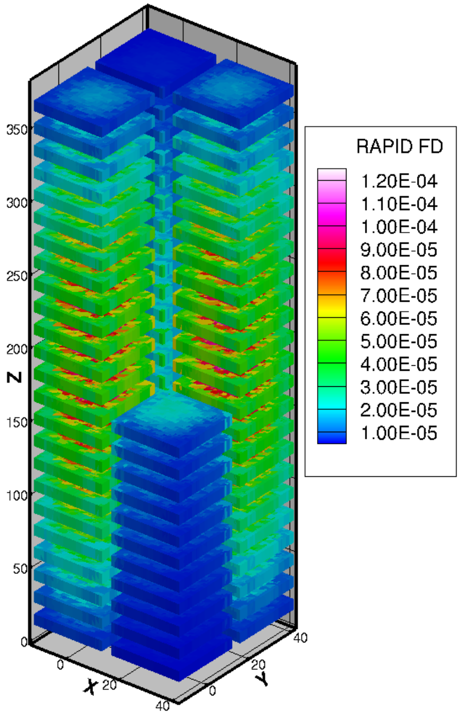
% Relative Difference



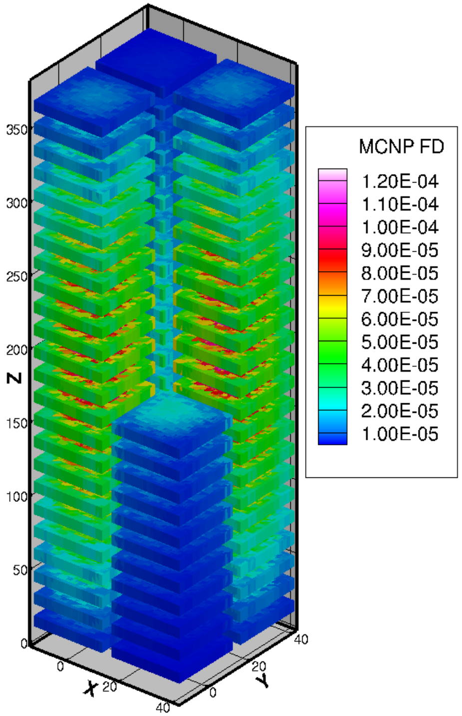
RAPID vs. MCNP – Fission Density (Case 4)

59 GWd/MTHM 9 yr	37 GWd/MTHM 9 yr
37 GWd/MTHM 9 yr	59 GWd/MTHM 9 yr

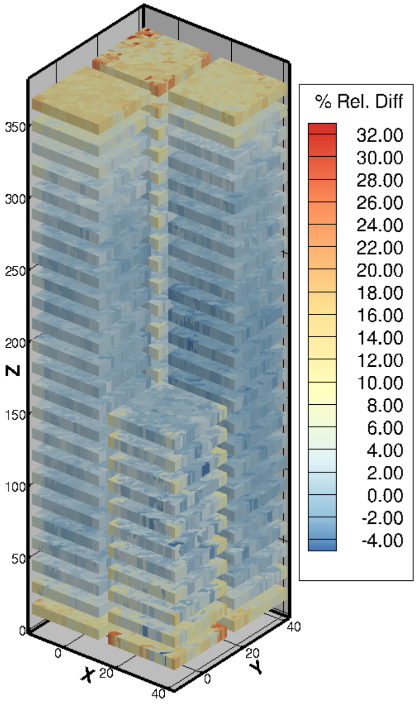
RAPID



MCNP



% Relative Difference



Computation Time

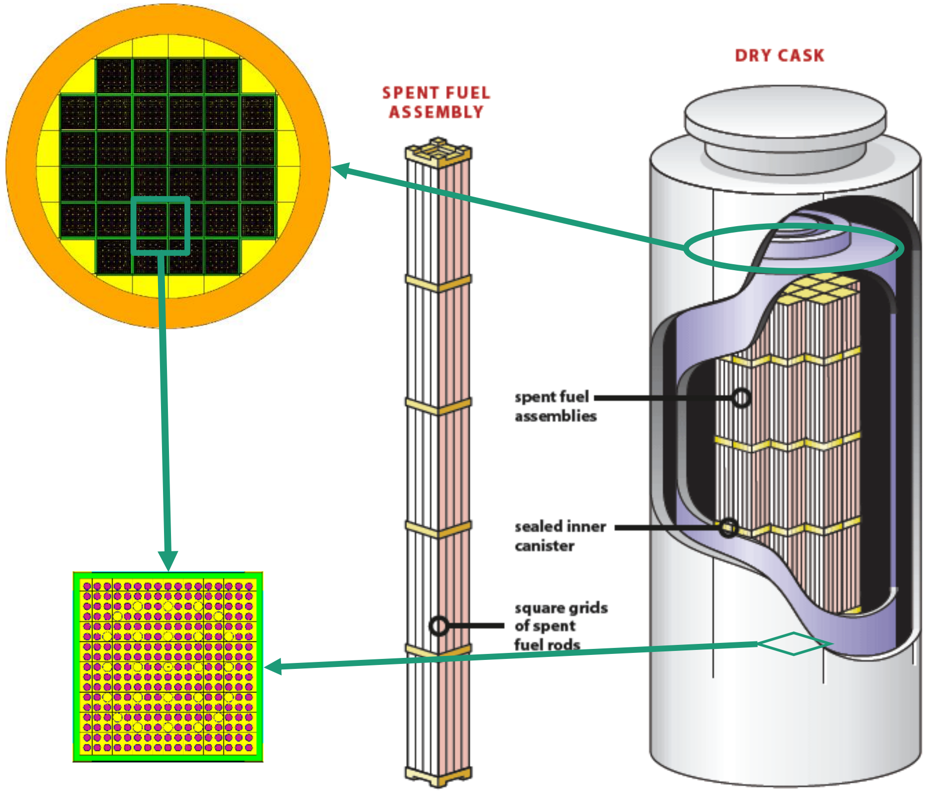
Case	MCNP		RAPID		
	Cores	Time (min)	Cores	Time (min)	Speedup
1	16	1020 (17 hrs)	1	0.50	2044
2	16	1013 (17 hrs)	1	0.51	1980
3	16	1082 (18 hrs)	1	0.50	2163
4	16	1149 (19 hrs)	1	0.50	2284

RAPID vs. MCNP

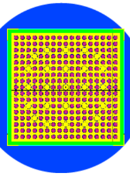
Spent Fuel Cask

GBC-32 Cask Computational Benchmark

- **Geometry**
  - 32 Fuel assemblies
  - Stainless steel (SS304) cylindrical canister
  - Inter-assembly Boral absorber panels
  - Height of the canister: 470.76 cm
- **Fuel assembly**
  - 17x17 Optimized Fuel Assembly (OFA)
  - 25 instrumentation guides
  - <u>Fresh</u> UO$_2$ 4% wt. enriched fuel pins
  - Active height: 365.76 cm



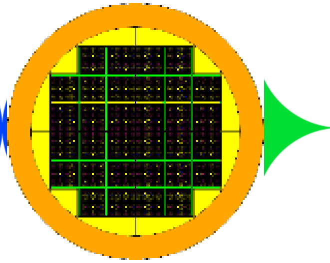
RAPID vs. MCNP – Single assembly model



pins = 264; #axial levels = 24; # tallies = 6336

Case	MCNP	RAPID
k_{eff}	1.18030 (± 2 pcm)	1.18092
k_{eff} relative difference	-	53 pcm
Fiss. density adjusted rel. uncertainty	0.48%	-
Fission density relative diff.	-	0.65%
Computer	16 cores	1 core
Time	666 min (11.1 hours)	0.1 min (6 seconds)
Speedup	-	6,666

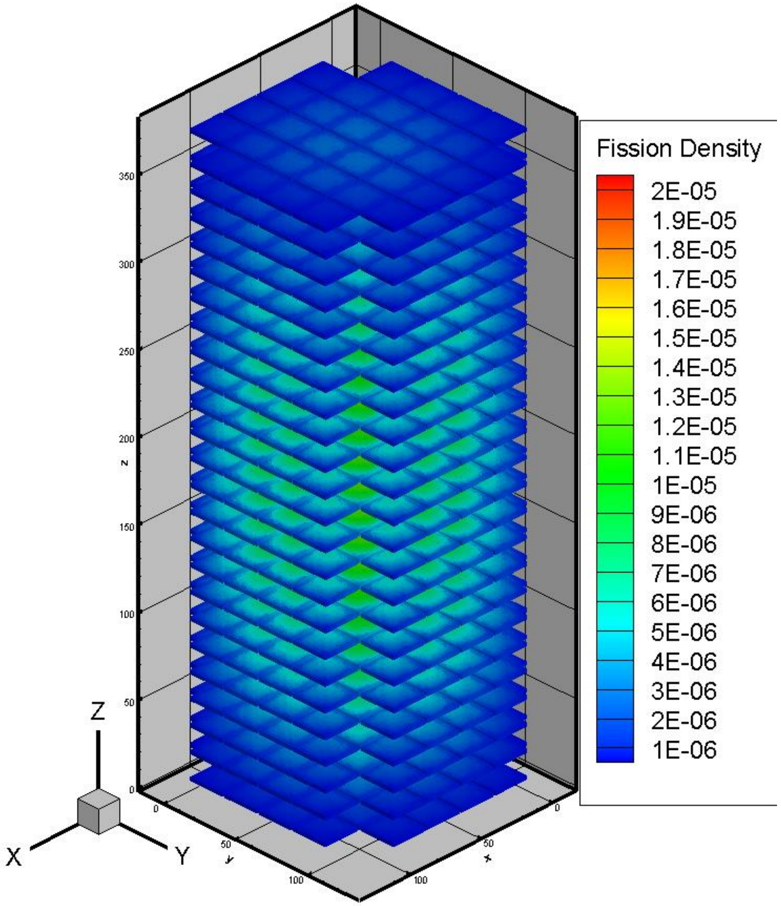
RAPID vs. MCNP – FULL Cask model



#assemblies = 32; # pins = 264; #axial levels = 24; # tallies = 202,752

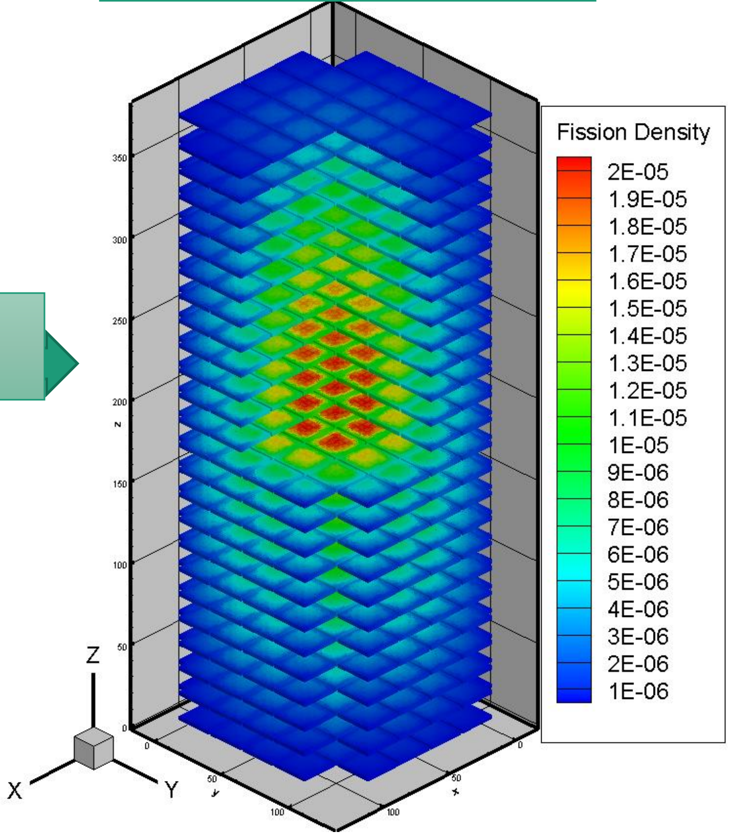
Case	MCNP	RAPID
k_{eff}	1.14545 (± 1 pcm)	1.14590
Relative Difference	-	39 pcm
Fission density rel. uncertainty	1.15%	-
Fission density relative diff.	-	1.56%
Computer	16 cores	1 core
Time	13,767 min (9.5 days)	0.585 min (35 seconds)
Speedup	-	23,533

Calculated Axially-Dependent, Pin-wise Fission Density in the GBC-32 Benchmark Using RAPID



Inside view

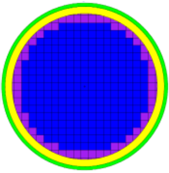
With a quarter Blanked



RAPID vs. SERPENT

Reactor Core

RAPID vs. SERPENT – PWR Core model*

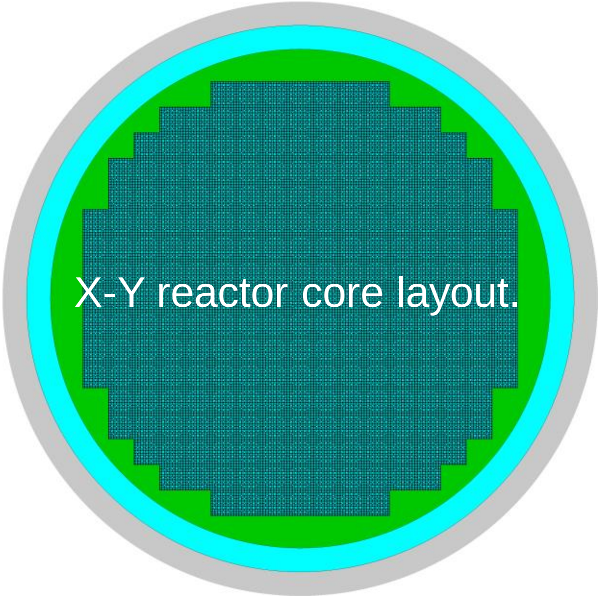


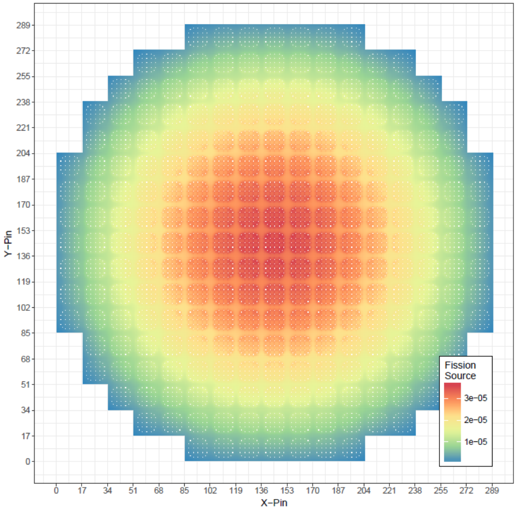
- RAPID has been applied to several large PWR problems, based on the NEA/OECD Monte Carlo Performance Benchmark Problem.
  - 241 assemblies, 264 pins per assembly
  - 100 axial levels
  - 6.4 million cells

- FM coefficients are pre-calculated using the SERPENT Monte Carlo code for different core configurations.

*A paper has been submitted for publication

Sample Result
RAPID vs. SERPENT – K_{eff} & Fission Density




Pin-wise Fission Source

k-eigenvalue

SERPENT: 1.000855 $\pm 1.0\ pcm$

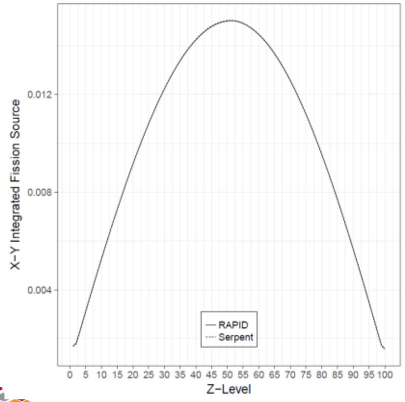
RAPID : 1.000912 $\pm 1.4\ pcm$

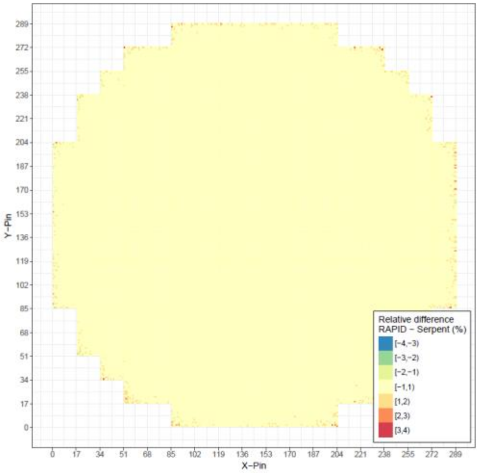
Diff. : 5.3 pcm

Pin-wise fission source

RMS error : 0.30%

SERPENT 1σ : 0.20%


Axial source comparison


RAPID-Serpent Difference

Computation time

SERPENT requires **1000 hrs**

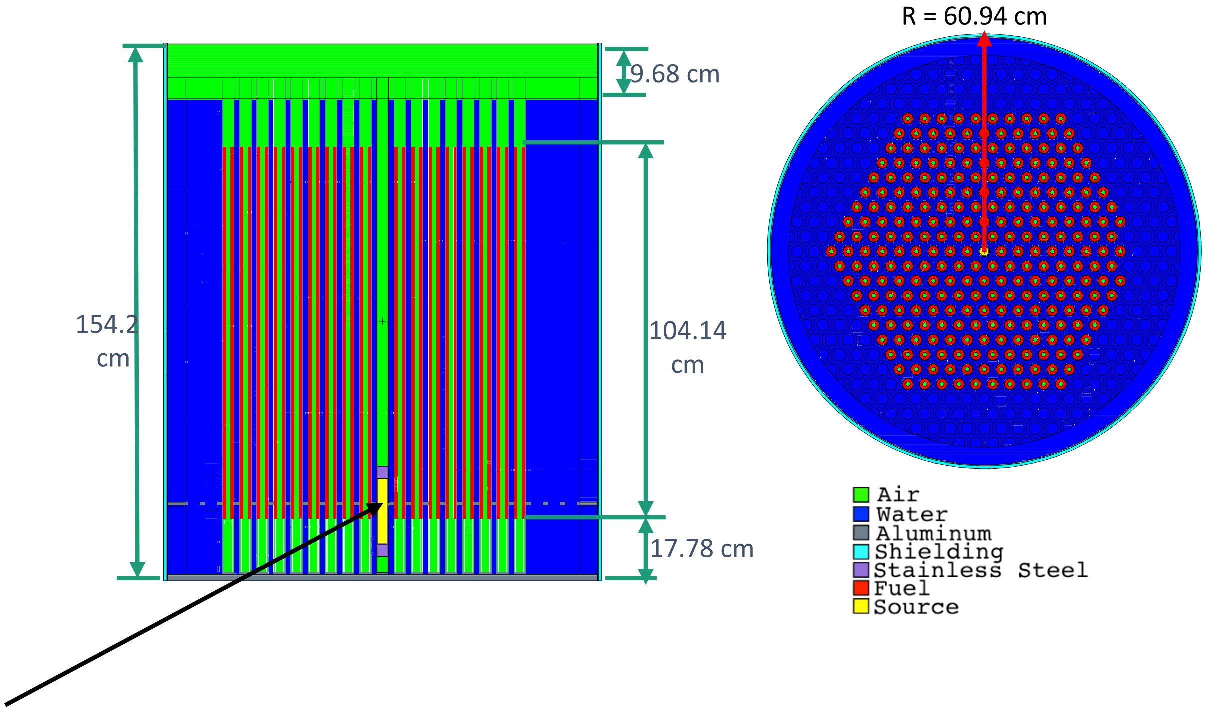
RAPID requires **0.23 Hrs**

Experimental Benchmarking of RAPID

US Naval Academy Subcritical Facility

Model Description - USNA-SC

- A cylindrical pool with natural uranium (fuel) and light water (moderator)
- There are a total of 268 fuel rods, arranged in a hexagonal lattice
- Fuel: hollow aluminum tubes containing 5 annular fuel slugs



- Neutron source: PuBe

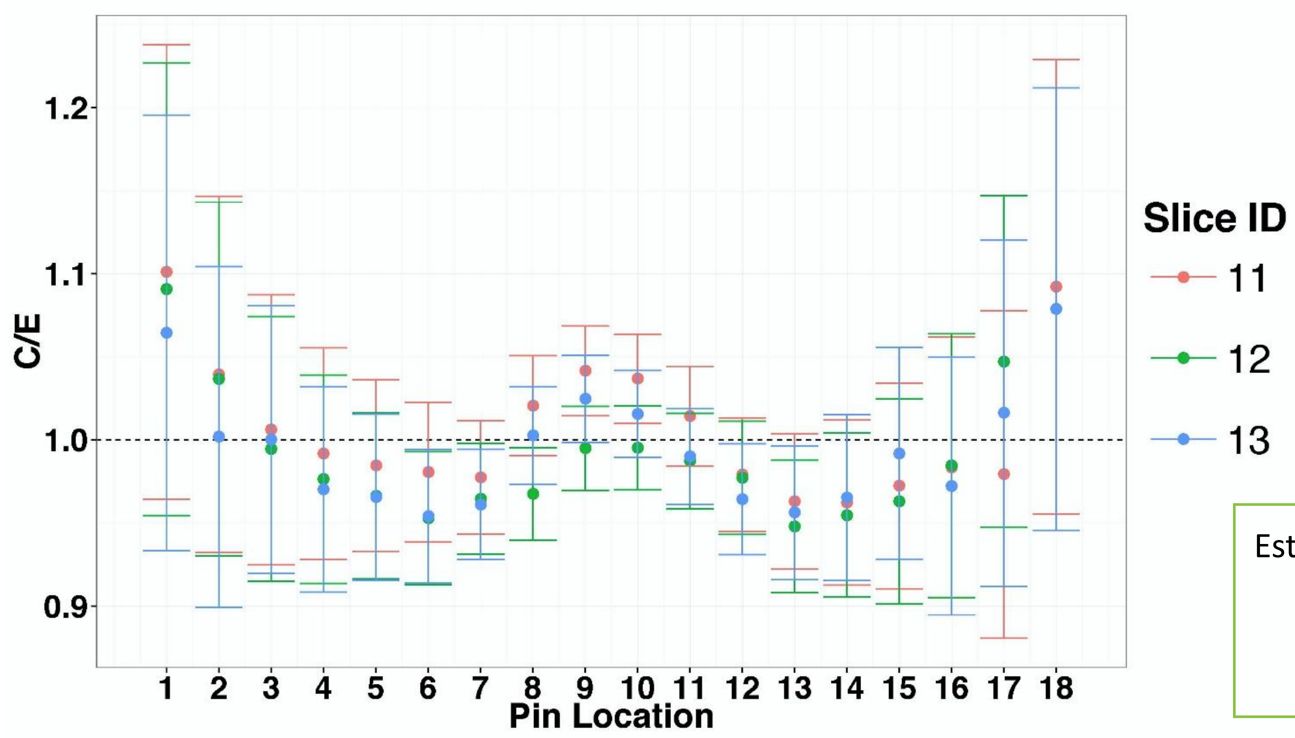
Comparison of Calculation vs. Experiment

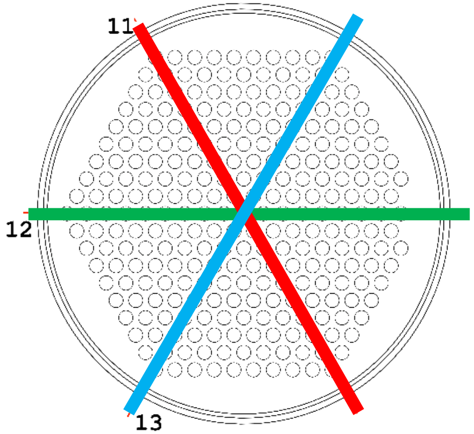
- ^{3}He detector is used to measure neutron count rates throughout the core
- To compare the measured and calculated counts, we obtain a detector efficiency factor (*Eff*)
- *Eff* is obtained based on least-squares minimization of calculate (*c*) and measure (*m*) counts as follows

$$Eff = \frac{\sum_i c_i m_i}{\sum_i c_i^2}$$

Where, *i refers to position within the core*

Calculated C/E and Estimated Uncertainty





Estimation of uncertainty in $f = \frac{c}{m}$

$$= \sqrt{\frac{\sigma_c^2}{m^2} + \frac{c^2\sigma_m^2}{m^4}}$$

RAPID

Detector Response or Surface Dose Calculation

Determination of Detector Response (R) or Surface Dose (D)

- "Forward" transport

$$\boldsymbol{R \text{ or } D = <\psi d_n>}$$

Where,

- ○ $R,\ [d_n = \Sigma_d \left(\frac{1}{cm}\right)]$, *or*
- ○ $D,\ [d_n = f_n(\frac{\frac{mrem}{hr}}{\frac{\#}{cm^2-s}})]$

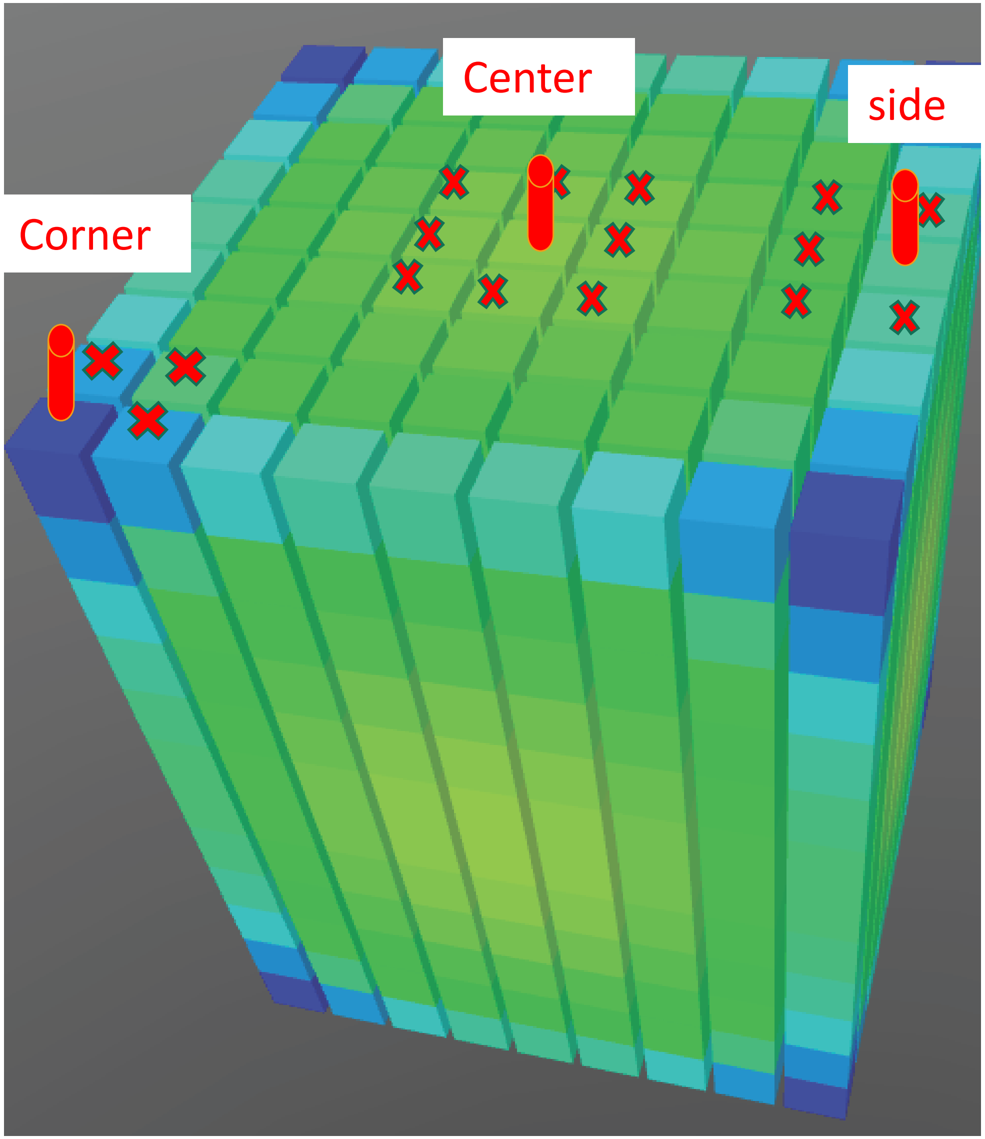
- "Adjoint-function" methodology by

$$\boldsymbol{R \text{ or } D = <\psi^* S>}$$

Where,

$$\boldsymbol{H^* \psi^* = d_n}$$

Determination of Detector Response in a Spent Fuel Pool

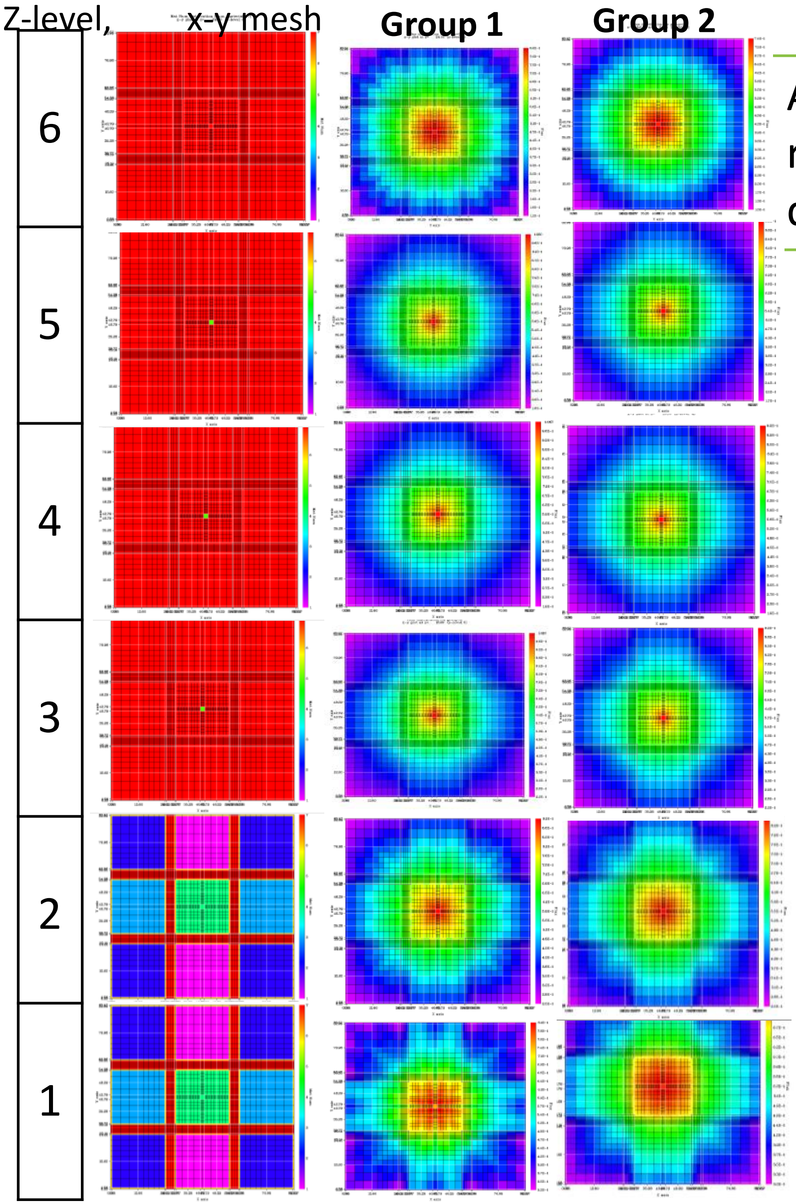


- Detector is placed on top of a fuel assembly
- Model contains surrounding assemblies: three types of assemblies (shown in figure) are identified:
  - Center
  - Side
  - Corner
- A 3-D PENTRAN Adjoint model is developed for each assembly type
- Axially, models include 15 cm of fuel plus a detector of height 5 cm and 10 cm of water on top of the detector

PENTRAN Adjoint Calculation – For a Center Assembly

Information on PENTRAN Calculation

- Model size 83.57x83.57x29 cm^3
- 2 groups
- S10 Quadrature set
- 94,578 meshes
- Wall-clock time = 279 sec, on one core



Adjoint-function, radial distribution at different z-levels

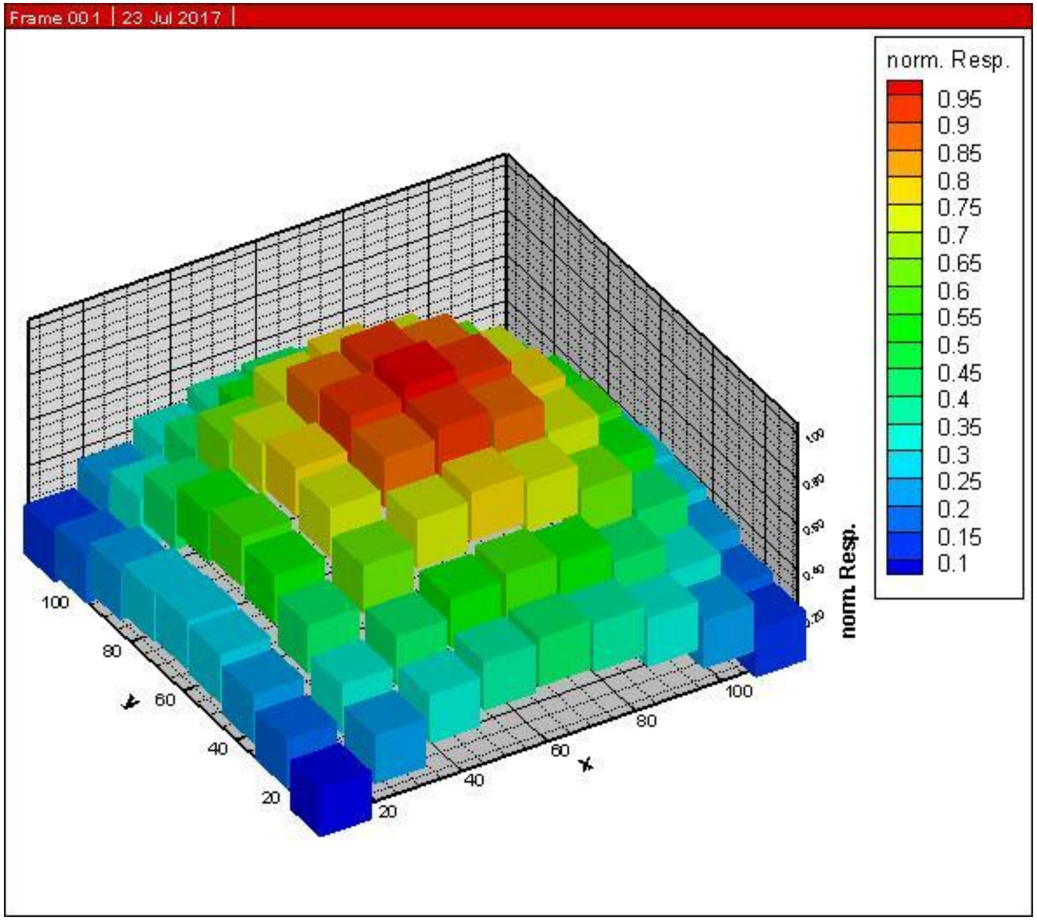
Determination of a detector response, as placed on top each fuel assembly

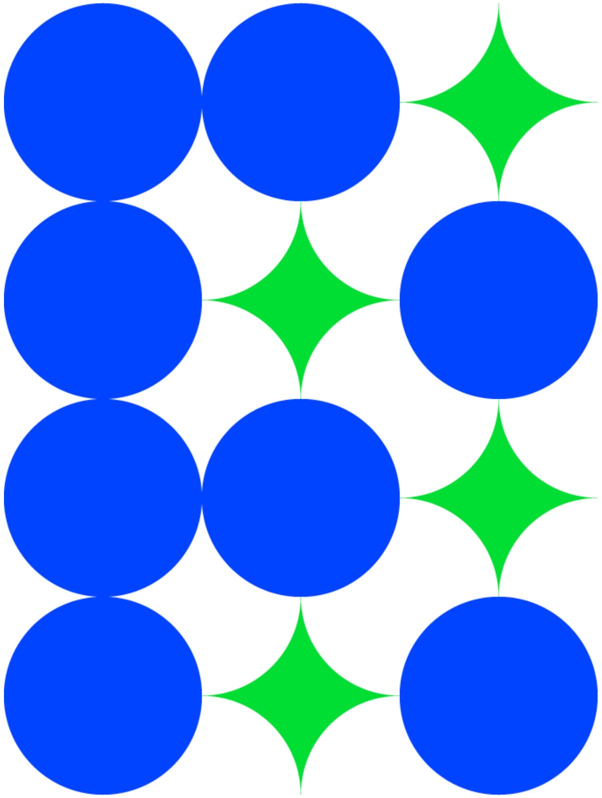
- By moving the detector on top of each fuel assembly in the pool of 9x9 assemblies

- RAPID calculates detector response by using

$$R= \sum_{g=1}^{2}\sum_{i=1}^{N_{cell}} \psi_{i,g}^{*}\,(\chi_g S_i)$$

Normalized detector response





Thanks!
Questions?