OAK RIDGE National Laboratory

Activation Analysis with MAVRIC & ORIGEN for Advanced Reactors

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Steve Skutnik

SCALE Users' Group Workshop

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U.S. DEPARTMENT OF ENERGY

Outline

- Overview of MAVRIC
- Overview of ORIGEN
- Activation Analysis of Megapower microreactor concept
  - Brief description of model
  - Source generation with ORIGEN
  - Dose calculation with MAVRIC
- Summary

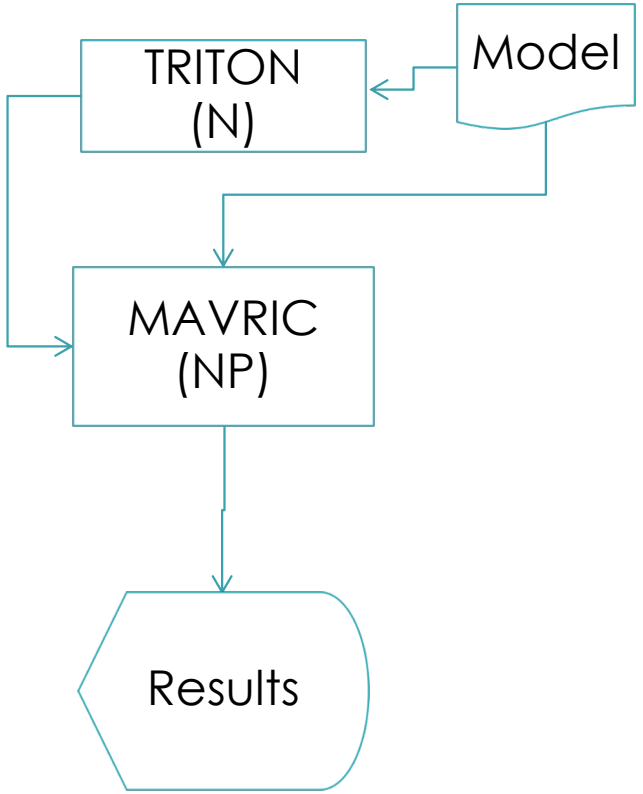
Goal

Demonstrate SCALE tools for calculation of dose rates due to activation fission products from an advanced reactor concept

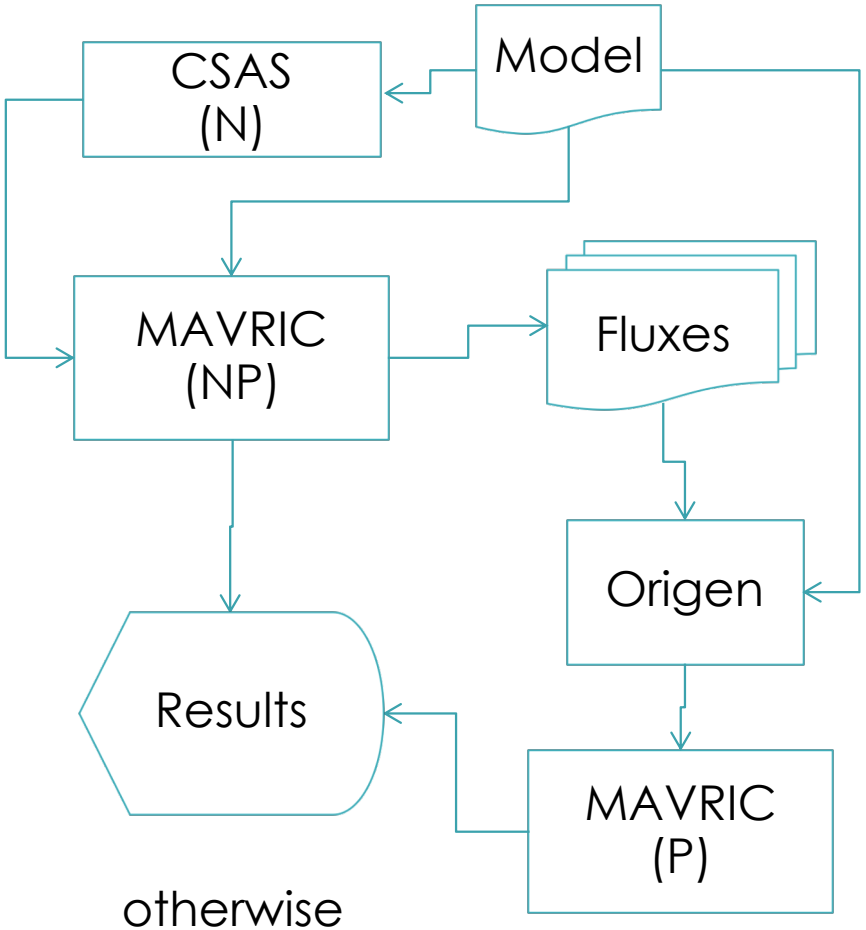
- **ORIGEN** is a general depletion/decay engine
- **CSAS** is a Monte Carlo criticality transport code (fission source)
- **MAVRIC** is a Monte Carlo radiation shielding code (fixed source)
  - powerful variance reduction methods
- **TRITON** is a depletion, activation, and source terms calculation code
  - uses CSAS & ORIGEN
  - no variance reduction

How to calculate dose from activation?

- Separate prompt and delayed particle transport
  - CSAS for fission source generation
  - MAVRIC for prompt neutron and gamma transport
  - ORIGEN for activation & fission product gamma sources
  - MAVRIC for delayed gamma transport with ORIGEN-generated sources



easy way out!



otherwise

MAVRIC

Monaco with **A**utomated **V**ariance **R**eduction using **I**mportance **C**alculations

- Fixed source Monte Carlo code for radiation shielding applications
- Supports MG and CE libraries
  - neutron, photon, and coupled modes
- Built-in variance reduction methods
  - CADIS, FW-CADIS
- Comes with utilities
- Supports source importing
  - fission mesh source (CAAS)
  - ORIGEN decay and activation sources
- Built-in flux-to-dose conversion factors
  - ICRU, ANSI, Henderson, Caliborne-Trubey
- Flexible and user-friendly definitions and parameters

MAVRIC Model

- Material, geometry, and global parameters
  - comes in a variety of flavors
  - needed for any kind of simulations
- Definitions
  - locations, distributions, responses, meshes, and energy bounds
- Tallies
  - point detector, region and mesh tallies
- Sources
  - spatial, energy, and angular distributions
- Importance map
  - parameters for CADIS and FW-CADIS
- Utilities for mesh tallies
  - Boolean operations, masking/filtering, modifying, importing/exporting, etc.

CADIS in MAVRIC

Consistent Adjoint Driven Importance Sampling

- Improves the FOM for one detector, at the expense of:
  - tracking particles in unimportant areas
  - convergence of the other detectors

- Perform an adjoint discrete ordinates calculation with $q^{+}(\vec{r},E) = \sigma_d(\vec{r},E)$
- Develop importance map for weight windows
  - $\overline{w}(\vec{r},E) = \frac{c}{\phi^{+}(\vec{r},E)}$
- Develop biased source
  - $\hat{q}(\vec{r},E) = \frac{1}{c} q(\vec{r},E)\ \phi^{+}(\vec{r},E)$
- Estimate the responses $R(\vec{r},E)$everywhere
- Construct the CADIS adjoint source but weight the source strength with $1/R(\vec{r},E)$

Forward Weighted CADIS in MAVRIC

- Improves the FOM for multiple detectors
  - not as much as CADIS
- Good for finding global solutions

- Perform a forward discrete ordinates calculation
- Estimate the responses $R(\vec{r}, E)$everywhere
- Construct the CADIS adjoint source but weight the source strength with $\frac{1}{R(\vec{r},E)}$

- CADIS

ORIGEN

Oak **R**idge **I**sotope **Gen**eration

- Irradiation and decay simulation code for general purpose isotopics tracking, *not tracking an application-specific subset of isotopes*
  - 2237 isotopes
    - 176 actinides
    - 1151 fission products
    - 910 structural activation nuclides
  - 54000 transitions between isotopes
    - all pathways in modern nuclear data for neutron transmutation, fission, and decay
    - all nuclides with half-lives > 1 ms

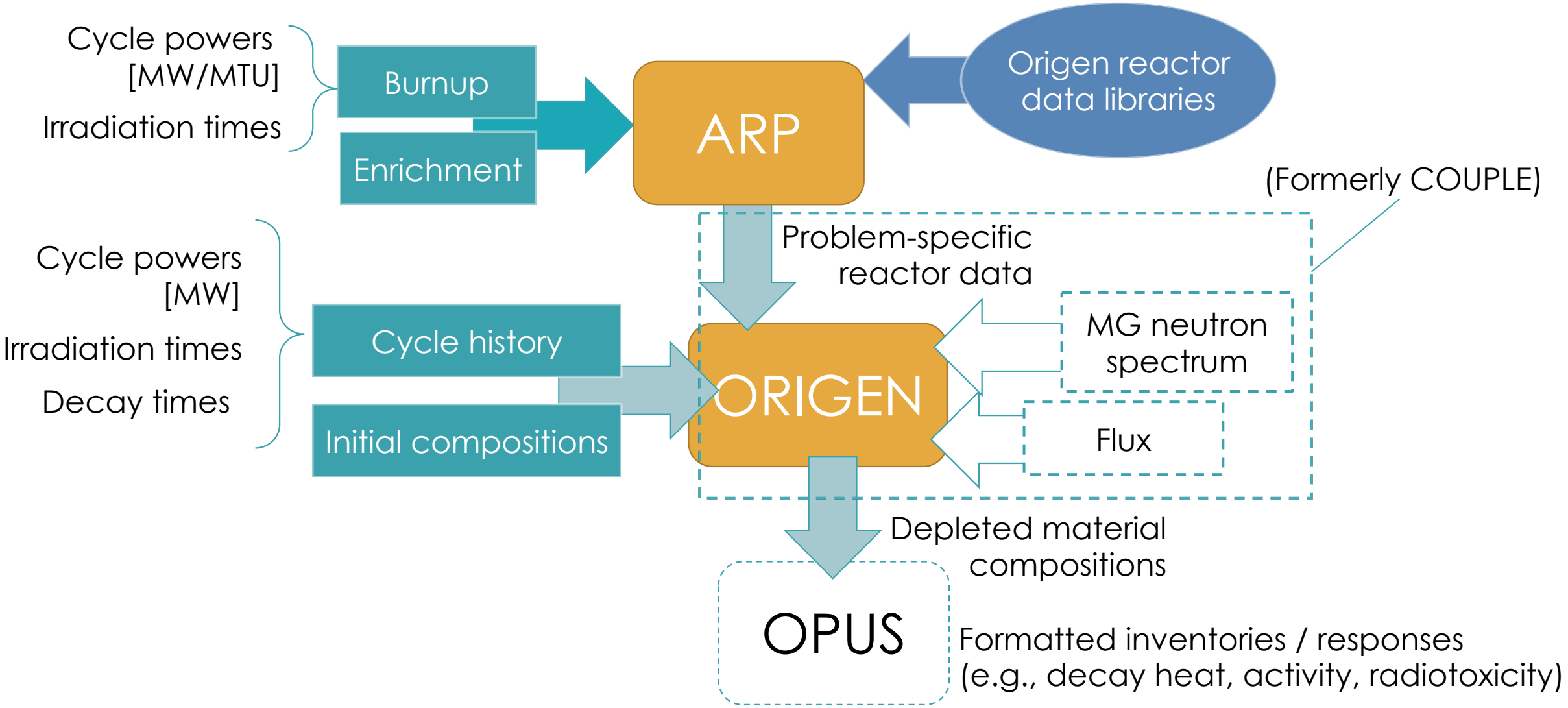
Key Capabilities

- Calculation of isotopics and source terms
  - nuclide concentrations (atoms and mass)
  - activities
  - decay heat
  - radiation emission rates and spectra (neutron and gamma)
  - radiotoxicity
- Application Environments
  - operating reactors
  - spent fuel storage/handling
  - structural material activation (in-core, ex-core)
  - fuel cycle analysis (material feed and removal processing)
- Methods and data enable comprehensive isotopic characterization of fuel over a large time scale (milliseconds to billions of years)

Evolution of ORIGEN capabilities

- **SCALE 5.1 (2006)**
  - Included graphical user interface, new ORIGEN libraries for different reactor types
- **SCALE 6.0 (2009)**
  - Included new base cross section libraries (ENDF/B-VI) & updated gamma ray libraries, retained all previous reactor libraries
- **SCALE 6.1 (2011)**
  - Included ENDF/B-VII decay data, expanded nuclides, energy-dependent fission yields
  - Replaced the old 3-group libraries with 238-group data from JEFF/A-3.0
- **SCALE 6.2 (2016)**
  - Completely rewritten modular ORIGEN source code, dynamic memory allocations
  - New CRAM solver
  - Rewritten, streamlined input format
  - Endian-agnostic binary f71 and f33 formats
  - Integrated alpha and beta sources & spectra
  - ORIGEN API to allow embedding depletion calculation in other codes

ORIGEN depletion calculation flow (standalone)



Further Reading

ISOTOPIC DEPLETION AND DECAY METHODS AND ANALYSIS CAPABILITIES IN SCALE

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The calculation of fuel isotopic compositions is essential to support design, safety analysis, and licensing of many components of the nuclear fuel cycle—from reactor physics and severe accident analysis to back-end fuel cycle issues, including spent-fuel storage and transportation, reprocessing, and radioactive waste management. Versions of the ORIGEN code, developed by Oak Ridge National Laboratory, have been used worldwide for isotopic depletion and decay analysis for more than three decades. The supported version of ORIGEN, maintained as the depletion analysis module for SCALE 6, performs detailed time-dependent isotopic generation and depletion for 1946 nuclides for reactor fuel and activation analysis. Stand-alone ORIGEN calculations can be performed using cross-section libraries developed for a wide range of reactor types and fuel designs used worldwide, including light water reactors UO_2 and MOX, CANDU, VVER 440 and 1000, RBMK, and graphite reactors. Alternatively, within SCALE 6, ORIGEN can be automatically coupled to two-dimensional discrete ordi-

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radiation source spectra,

I. INTRODUCTION

The calculation of fuel isotopic compositions and radiological properties is essential to support design, safety analysis, and licensing in many areas of the nuclear fuel cycle—from reactor physics to back-end fuel cycle issues, including spent-fuel storage and transportation, radioactive waste management, and increasingly, safeguards for spent nuclear fuel. Nuclear fuel cycle analysis requires codes and nuclear data that can accurately calcu-

late isotopic composition
scales: from seconds after f
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ORIGEN has been de
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decay module of the Sta

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A method for including external feed in depletion calculations with CRAM and implementation into ORIGEN ☆

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ABSTRACT

A method for including external feed with polynomial time dependence in depletion calculations with the Chebyshev Rational Approximation Method (CRAM) is presented and the implementation of CRAM to the ORIGEN module of the SCALE suite is described. In addition to being able to handle time-dependent feed rates, the new solver also adds the capability to perform adjoint calculations. Results obtained with the new CRAM solver and the original depletion solver of ORIGEN are compared to high precision reference calculations, which shows the new solver to be orders of magnitude more accurate. Furthermore, in most cases, the new solver is up to several times faster due to not requiring similar substepping as the original one.

1. Introduction

Calculating changes in the isotopic composition of nuclear fuel or other materials under irradiation or during decay is essential for a wide range of design, operational, and licensing analyses in applications ranging from reactor physics to waste management and safeguards. These applications require methods and codes that enable changes in compositions to be accurately and reliably calculated for widely different initial compositions, neutron spectra, flux levels, and time scales from seconds after fission to tens of thousands of years after fuel discharge. The number of nuclides to be accounted for also varies by application, but often it is either necessary or desirable to consider a large systems consisting of a thousand or more nuclides with widely varying decay constants and up to tens of thousands of possible transitions between them. Although external feed (i.e., the continuous introduction of material into the observed system from outside) is not relevant in the most typical applications of decay and depletion calculations, modeling it is necessary to easily and robustly handle certain systems. Examples of such systems include liquid fueled reactors and storage and reprocessing facilities, where the in-flow of material affects reactivity, decay heat, and activity loads.

In the SCALE nuclear systems modeling and simulation suite (Oak Ridge National Laboratory, 2011), all decay and depletion calculations are handled by ORIGEN (Gauld et al., 2011). The original depletion solver of ORIGEN uses a secular equilibrium approximation and the Bateman solution of linear chains for handling short-lived nuclides, and a power series approximation of the matrix exponential of a reduced coefficient matrix for long-lived nuclides. While the linear chains and matrix exponential can be solved accurately when independent, accounting for the effects of long-lived nuclides on the short-lived ones and vice versa requires additional approximations and leads to a loss of accuracy for some nuclides in the hybrid method. This method has usually been referred to as the matrix exponential method or the ORIGEN method. However, as a part of the SCALE modernization campaign, the ORIGEN code now has more than one solver. To make a distinction between these solvers, the original method of solution is referred to as MATREX.

While the MATREX solver has continued to perform adequately, there has also been significant development in depletion algorithms. CRAM (Pusa and Leppänen, 2010) is perhaps the most promising of the new methods. It has been shown to yield very accurate results while still being among the fastest methods for solving the decay and depletion of large systems of nuclides (e.g.,

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Validation of new depletion capabilities and ENDF/B-VII data libraries in SCALE

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ABSTRACT

New isotopic depletion capabilities and ENDF/B-VII data libraries have been implemented in the recent release 6.1 of SCALE, a comprehensive modeling and simulation suite for nuclear safety analysis and design developed and maintained by Oak Ridge National Laboratory. An assessment of the effect of the new developments on the code performance is the subject of this paper. The analysis is focused on evaluating the code performance in predicting isotopic compositions in spent nuclear fuel by using an extensive, measured isotopic assay database. The analysis results obtained using the latest ENDF/B-VII cross-section data and different resonance processing methods in SCALE are compared to the results of previous validation studies that used ENDF/B-V data. The performance of SCALE depletion capabilities with respect to other computational systems is assessed based on recent published results that were obtained using ENDF/B-VII libraries.

1. Introduction

New isotopic depletion and decay analysis capabilities have been implemented in the most recent release of SCALE, a comprehensive modeling and simulation suite for nuclear safety analysis and design developed and maintained by Oak Ridge National Laboratory (ORNL). The SCALE 6.1 release (RSICC Computer Code Collection, 2011) includes improved ENDF/B-VII cross-section data for neutron transport calculations. In addition, extensive updates have been made to data for ORIGEN, the isotopic depletion and decay module in SCALE, including addition of ENDF/B-VII nuclear decay data, multigroup neutron activation cross-section data, energy-dependent neutron branching between ground and isomeric product states, and energy-dependent fission product yields (Gauld et al., 2011a). An assessment of the effect of these developments on the code performance is the subject of this paper. The analysis is focused on evaluating the accuracy of code predictions for isotopic compositions using an extensive measured isotopic assay database that contains data obtained from destructive analysis of spent nuclear fuel.

Quantifying and evaluating the bias and uncertainties in the calculated isotopic compositions of spent nuclear fuel is essential for validating the accuracy of the codes and nuclear data used for safety and licensing calculations. Nuclear fuel being discharged from commercial reactors has achieved progressively higher burnup through the use of higher enrichments, improved assembly designs, and more efficient fuel management strategies. The continuous change in the characteristics of spent fuel being discharged by the nuclear industry requires a continuous reassessment of the bias and uncertainties associated with code predictions. To accomplish this, a comprehensive experimental database is needed to cover the increased domains of fuel enrichment, burnup, and cooling time of relevance to spent fuel analyses, including radionuclide inventories and activities, decay heat, and radiation source terms.

Over the past decade there has been an increased international recognition of the need for expanded, high quality experimental data to validate spent fuel calculations. The Nuclear Science Committee of the Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) decided in 2006 to establish a new Expert Group on Assay Data of Spent Nuclear Fuel (EGADSNF) to compile and document a comprehensive database of assay data and update the OECD/NEA web-based Spent Fuel Isotopic Composition Database (SFCOMPO). The extended and updated database, with contributions from many NEA member countries, is intended to support analyses and safety evaluations for the nuclear fuel cycle and back-end nuclear facilities related to fuel handling, dry spent fuel storage installations, pool storage, fuel reprocessing facilities, and waste repositories (OECD/NEA, 2011). The related activities at ORNL included efforts to compile and document radiochemical assay data from publicly available sources and international commercial experimental programs for use in validating calculated isotopic compositions in spent fuel. These data have been applied to validate the depletion capabilities in SCALE using ENDF/B-V-based cross-section libraries, as documented in a series of validation reports (Ilas et al., 2010a,b; Mertyurek et al., 2010; Ilas and Gauld, 2011) and other publications (Ilas and Gauld, 2008, 2009; Radulescu et al., 2009). More recently, the database

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Megapower

- Not your typical superhero, coming soon!
  - DC Comics

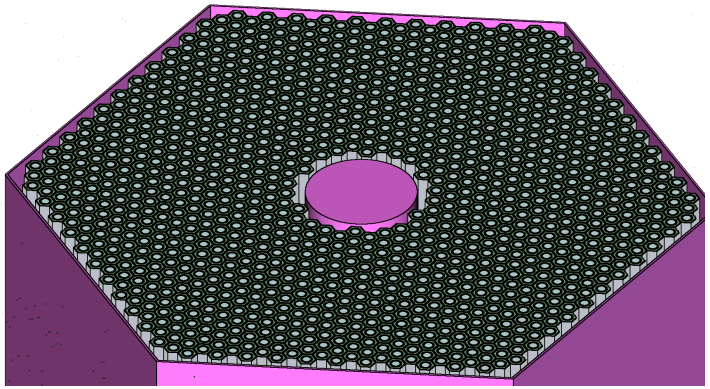
https://superheroes.fandom.com/wiki/List_of_DC_Comics_Characters

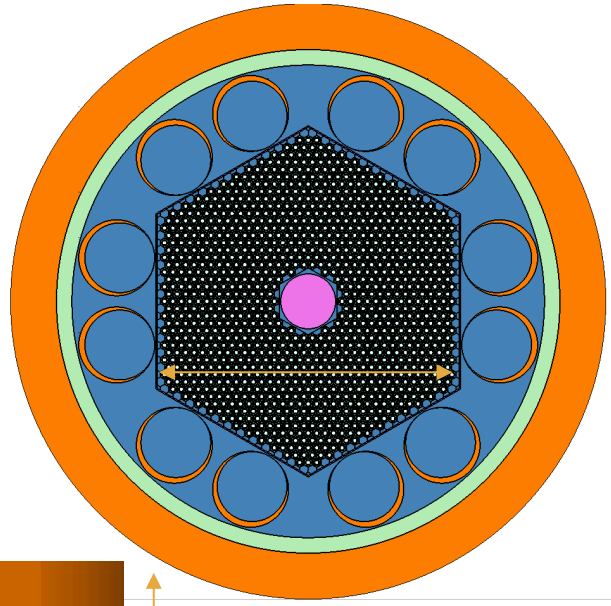
Tutorial Outline

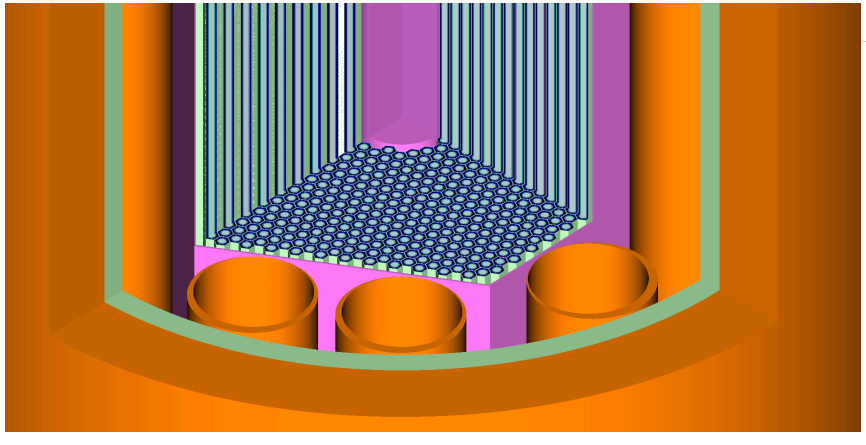
- Overview of the Megapower design concept
- Decay source generation with Origen
- Activation source generation with Origen
- Dose calculation with MAVRIC

Megapower microreactor concept

- 5 MWt core designed for remote deployment
- 1134 annular hexagonal UO_2 pins
  - 19.75% enrichment
- 12 rotatable B_4C control drums
- Heat rejection via "heat pipes" with a Brayton cycle







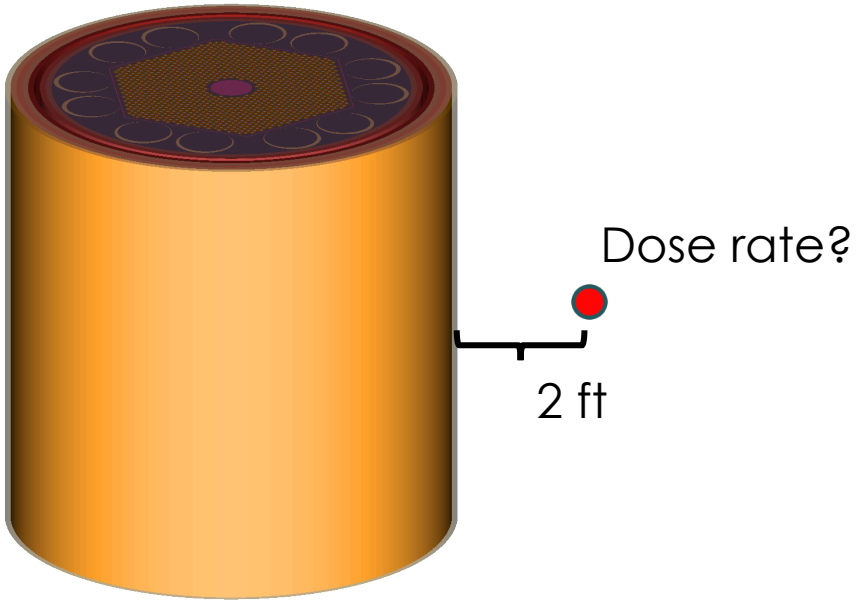
~1 m core diameter

1.5 m active height

Sterbentz, J. W. et al., "*Preliminary Assessment of Two Alternative Core Design Concepts for the Special Purpose Reactor*", INL, May 2018, INL/EXT-17-43212

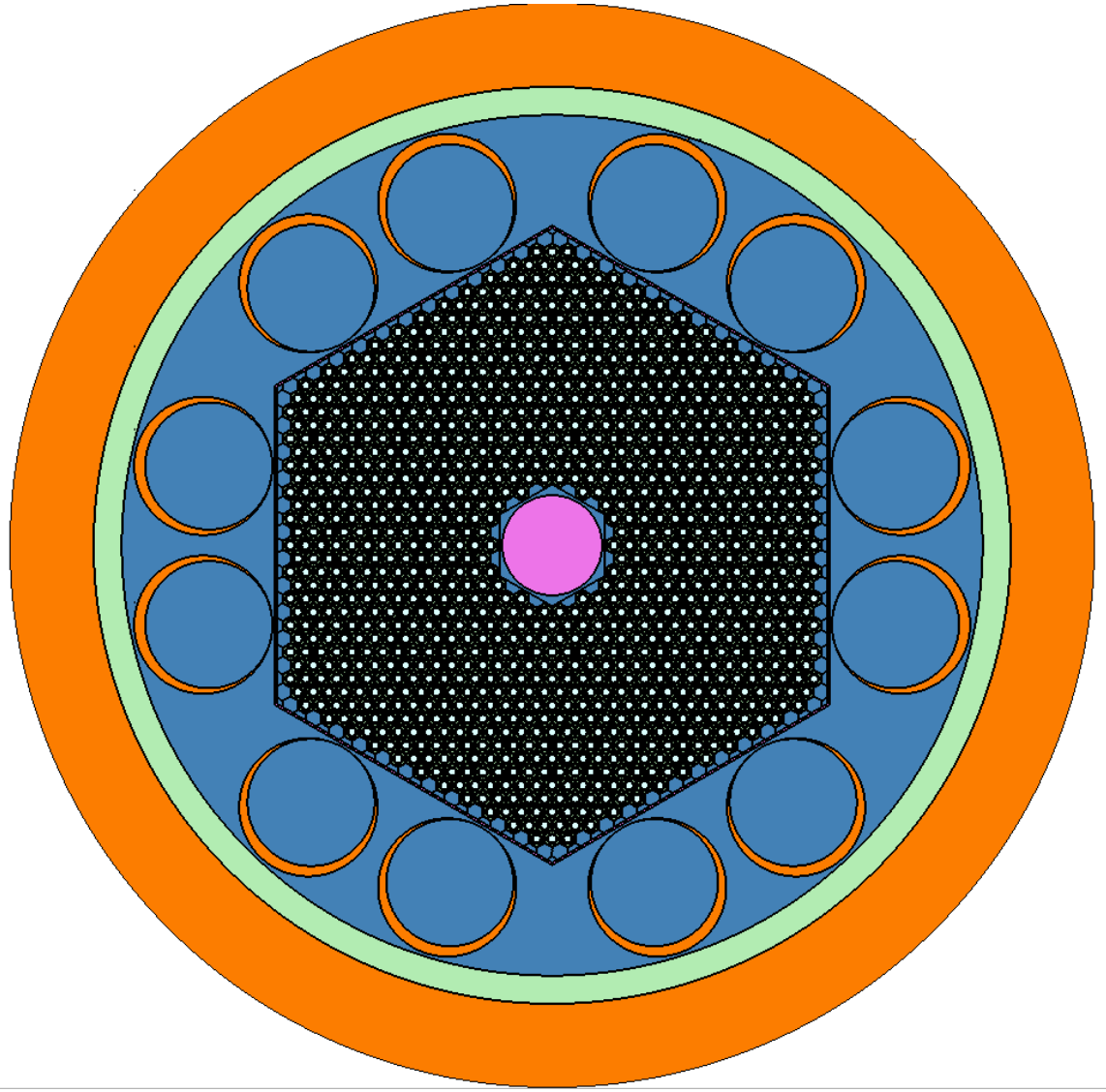
Goal: Calculate the external shutdown dose rate

Calculate the dose rate at a point radially 2 ft away from the beltline of the core 1 month after shutdown!



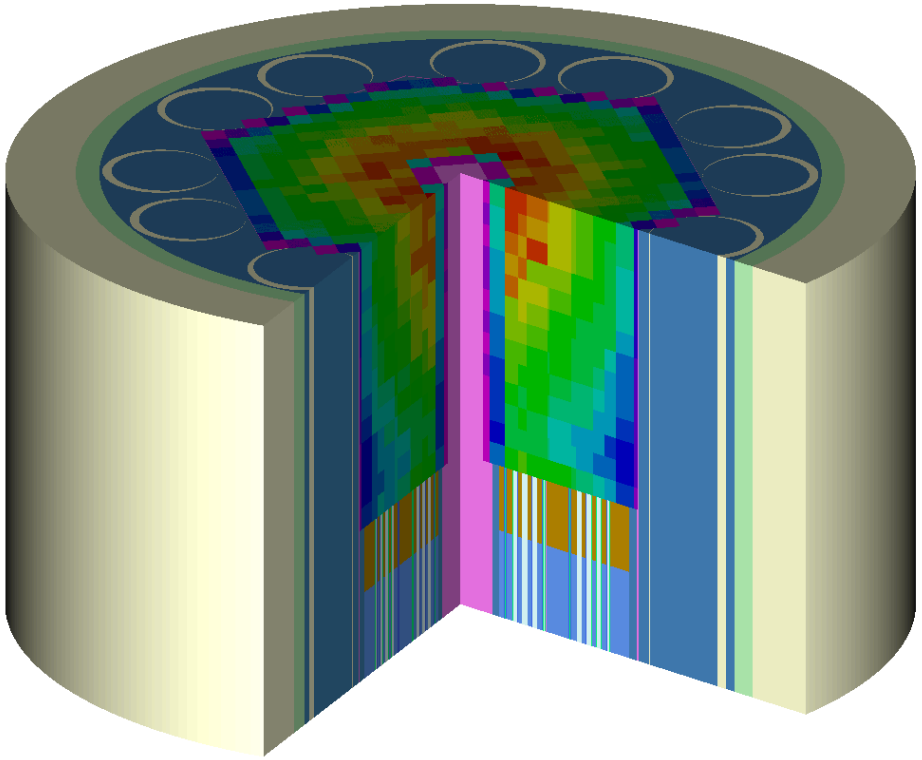
CSAS Model

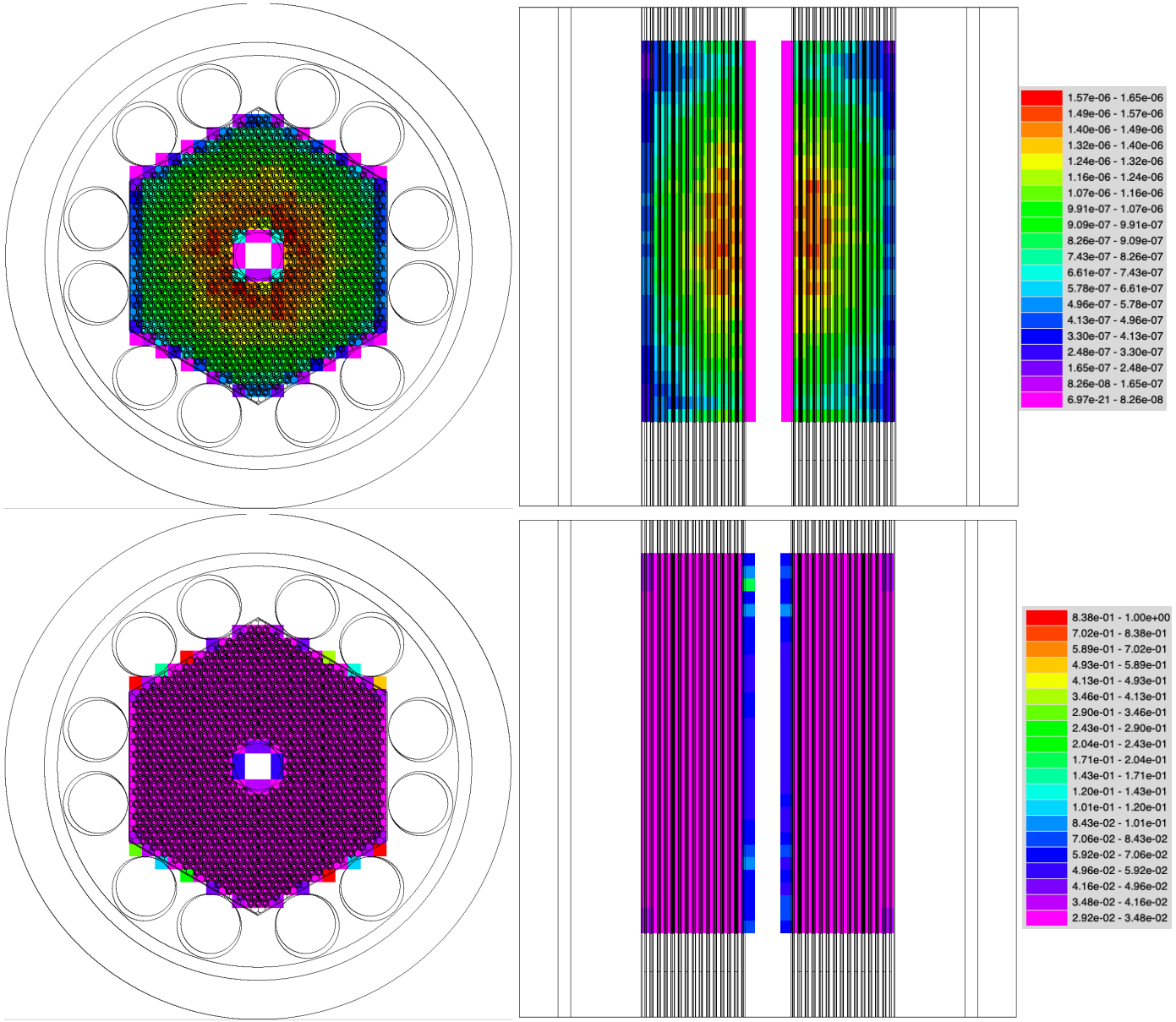
- Have materials and geometry
- Calculates a few things
  - k_{eff}, flux, fission source distribution



CSAS Results, default

- Looks good!
  - 1.00242 +or- 0.00049

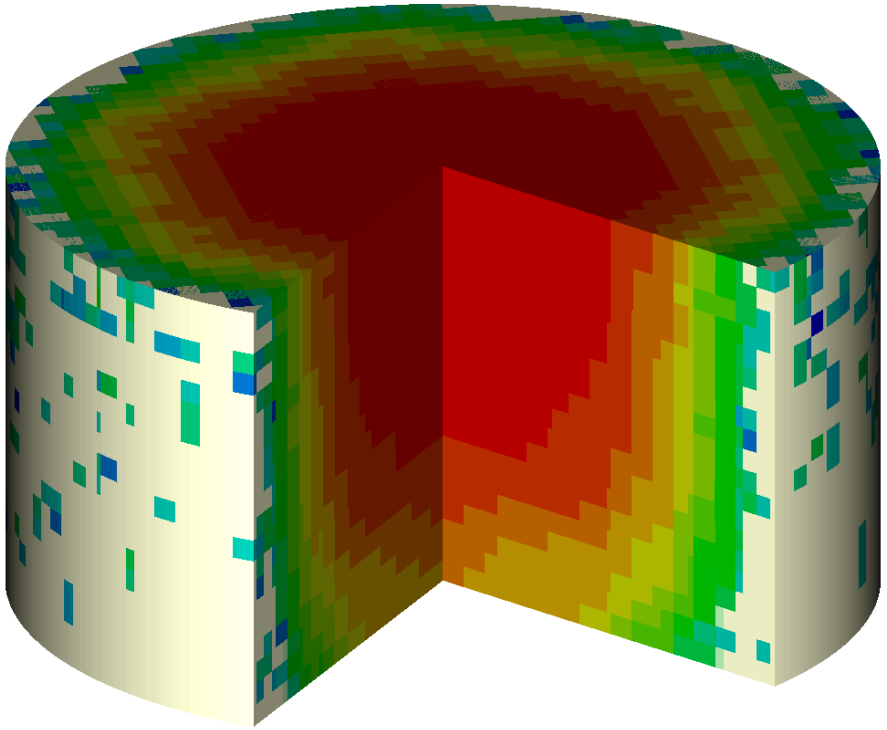


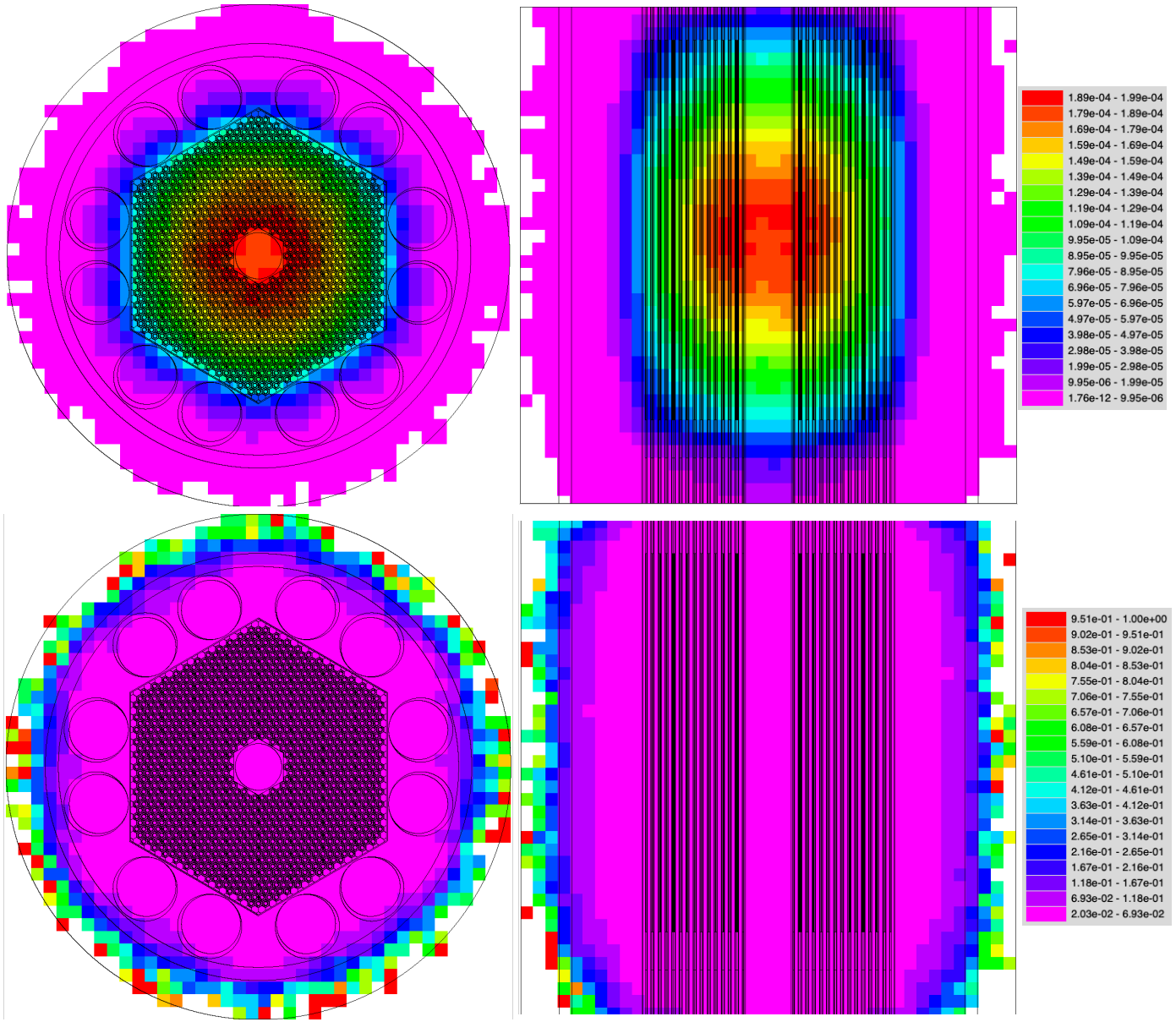


Fission Source Distribution

CSAS Results, default

- Or, is it?

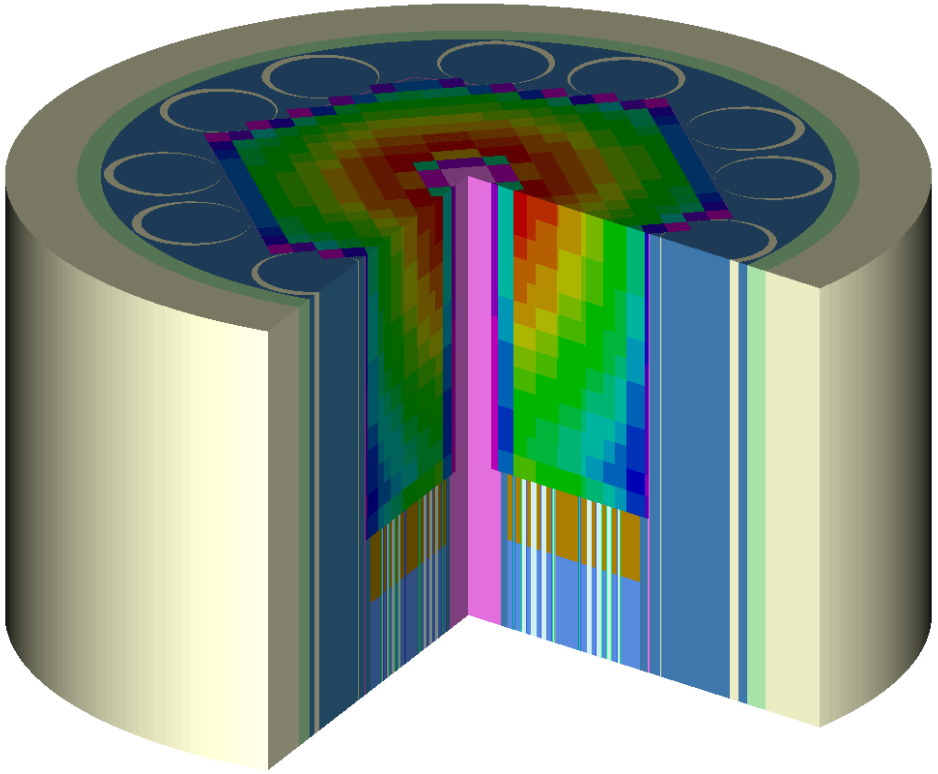


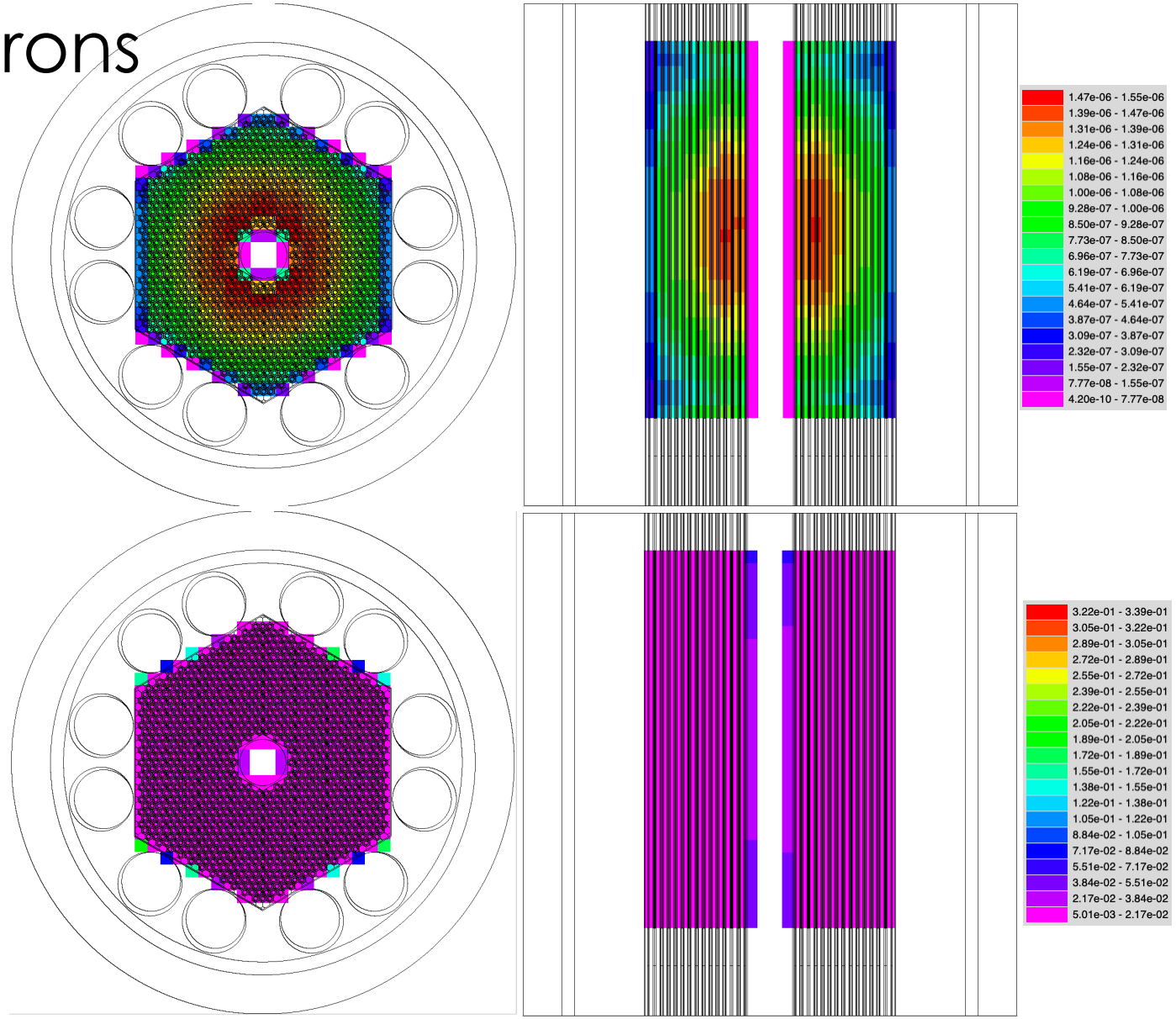


Flux Distribution

CSAS Results, more neutrons

- Better converged source!
  - 1.00218 +or- 0.00009

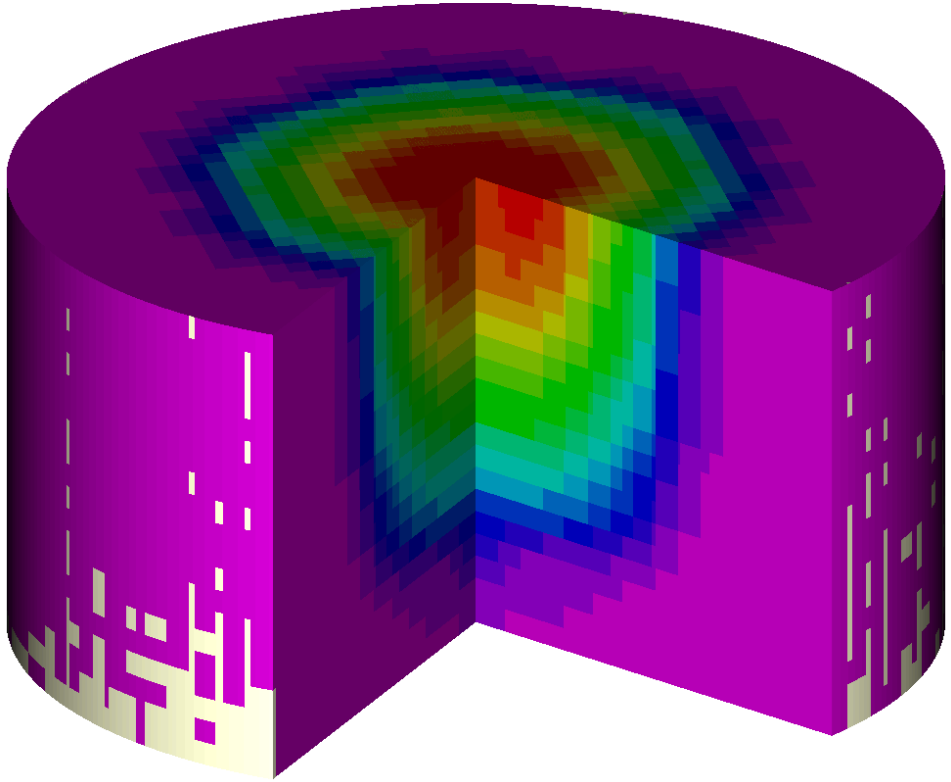


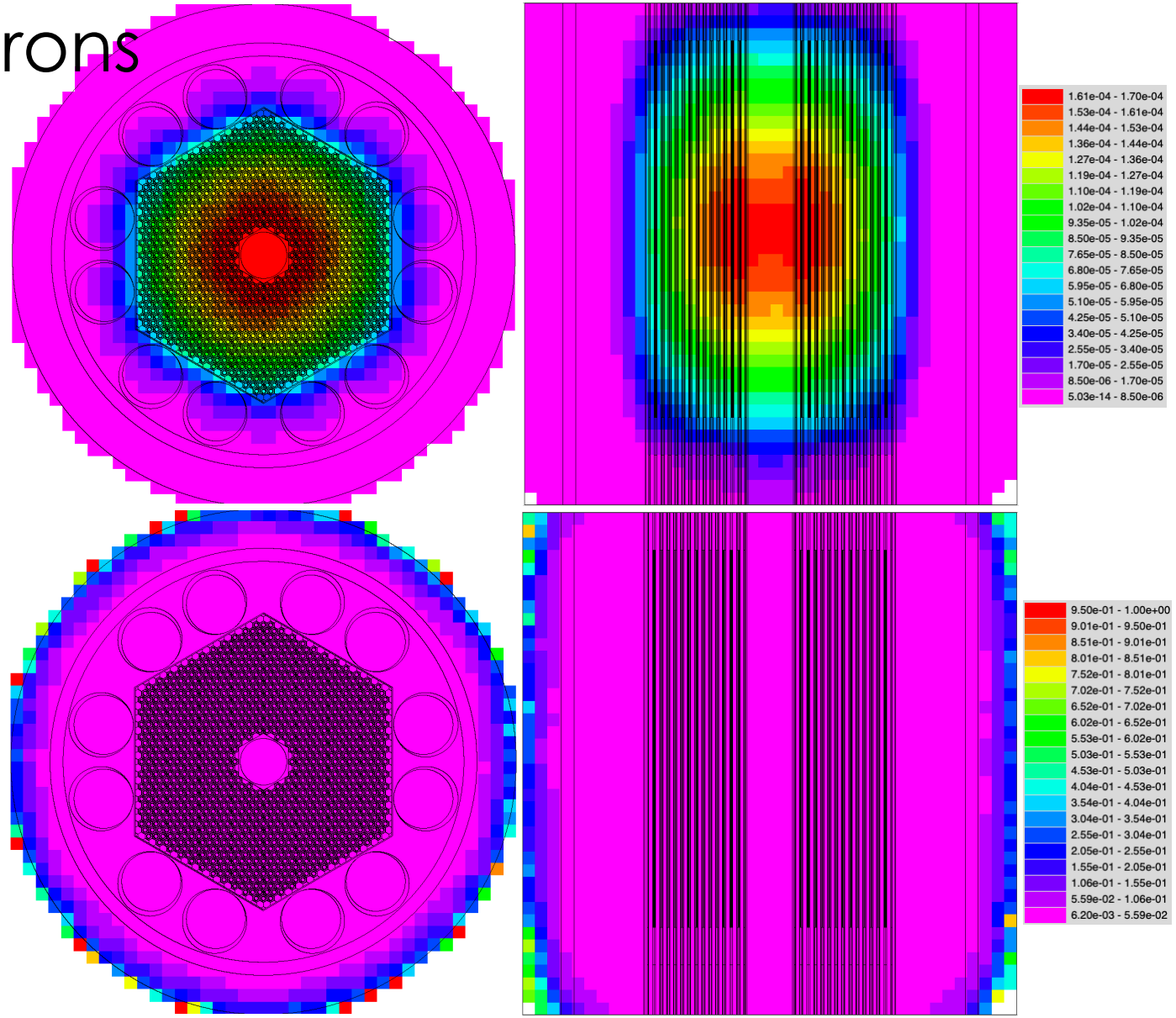


Fission Source Distribution

CSAS Results, more neutrons

- Flux is better too!

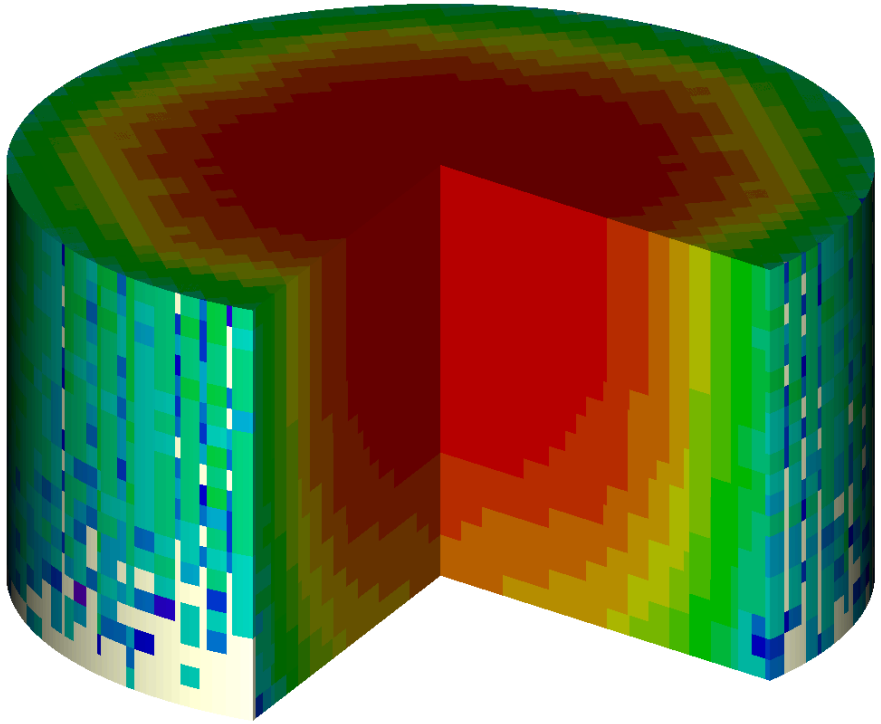


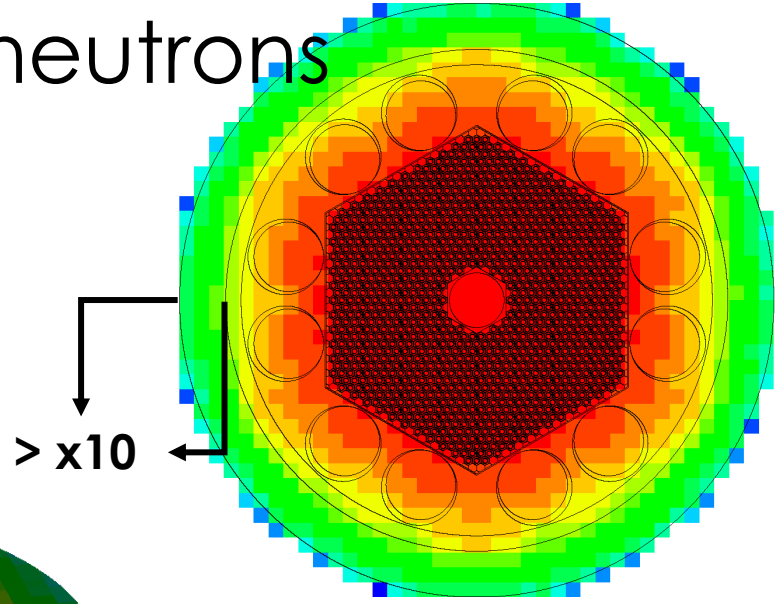


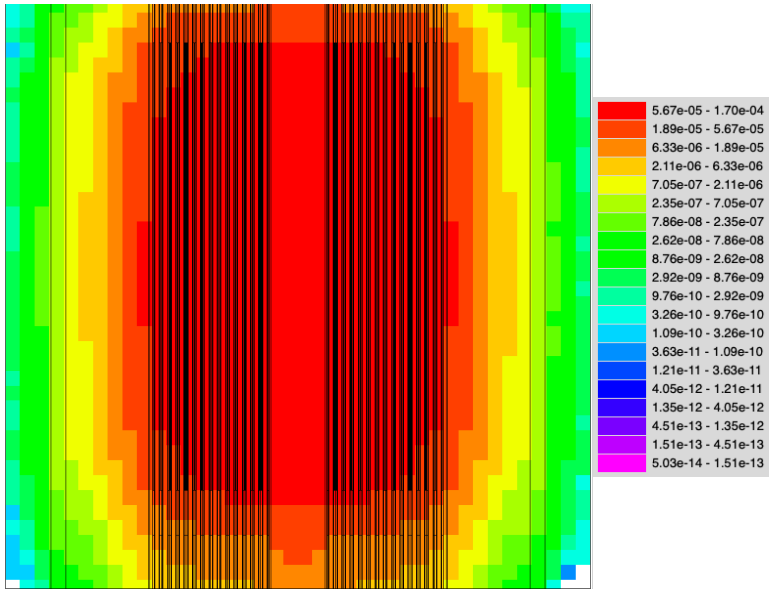
Flux Distribution

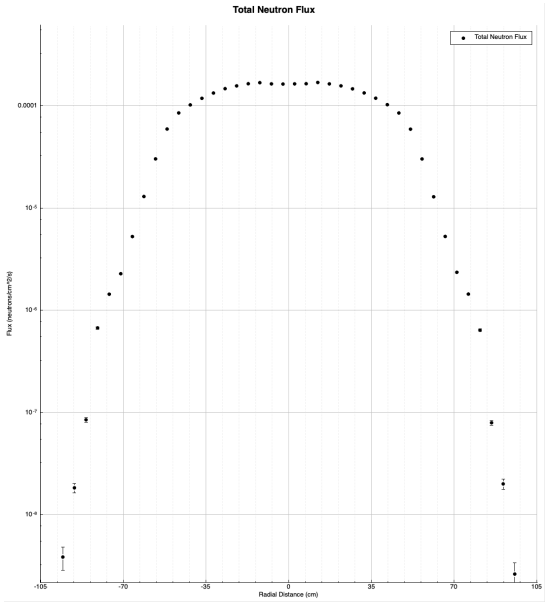
CSAS Results, more neutrons

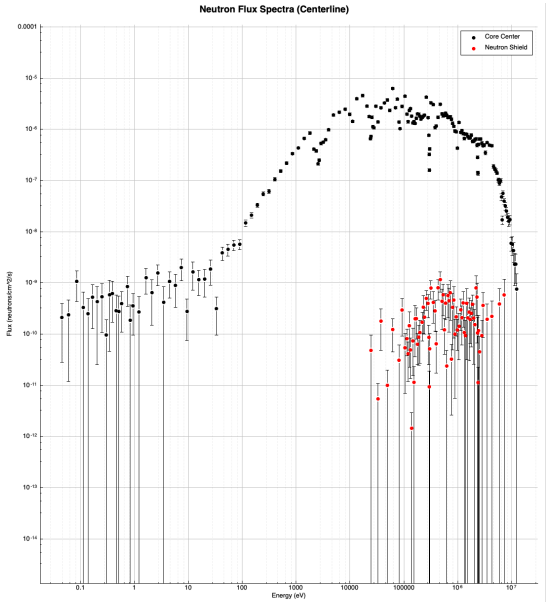
- Good enough?







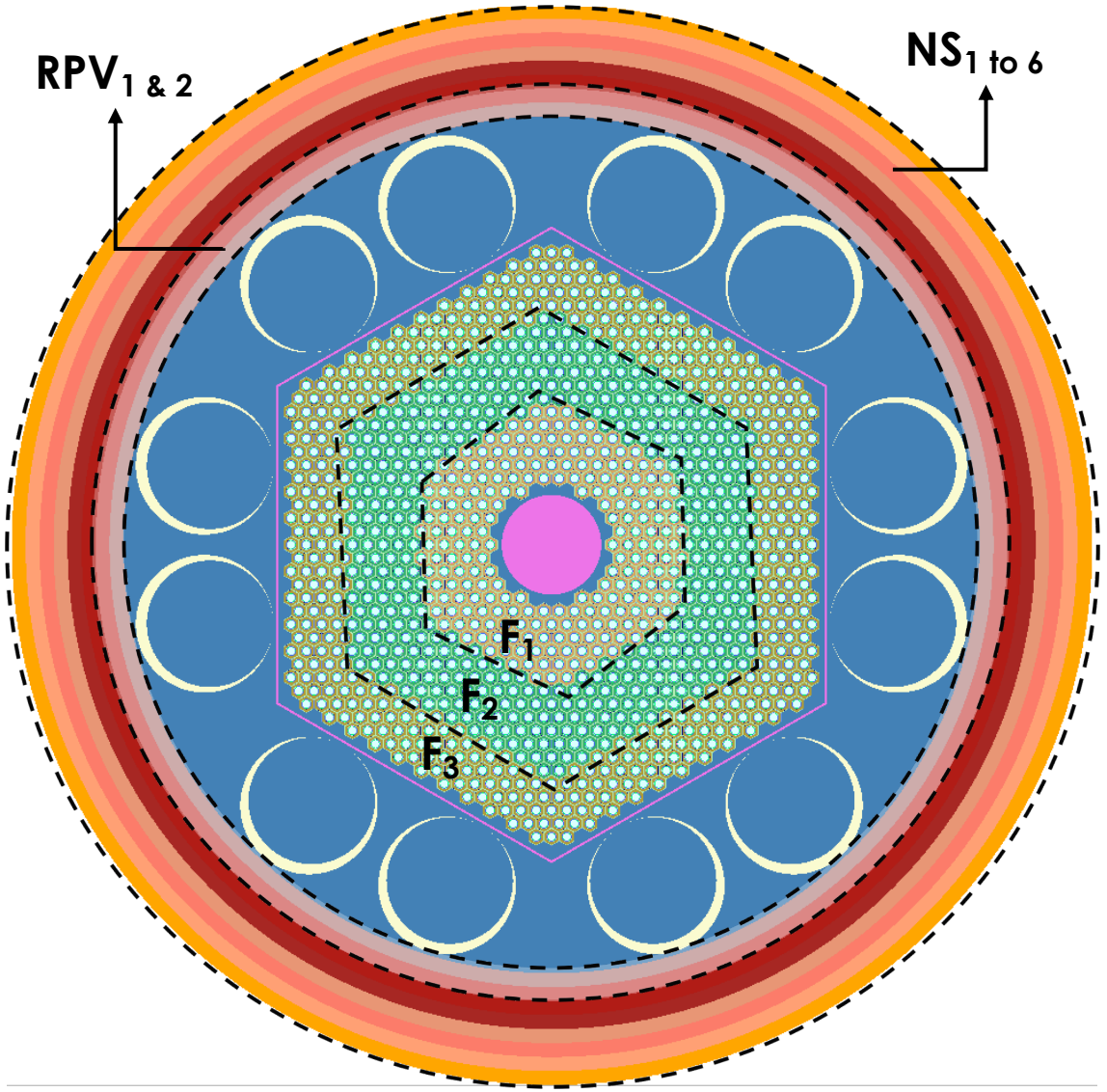




Flux Distribution (Log Scale)

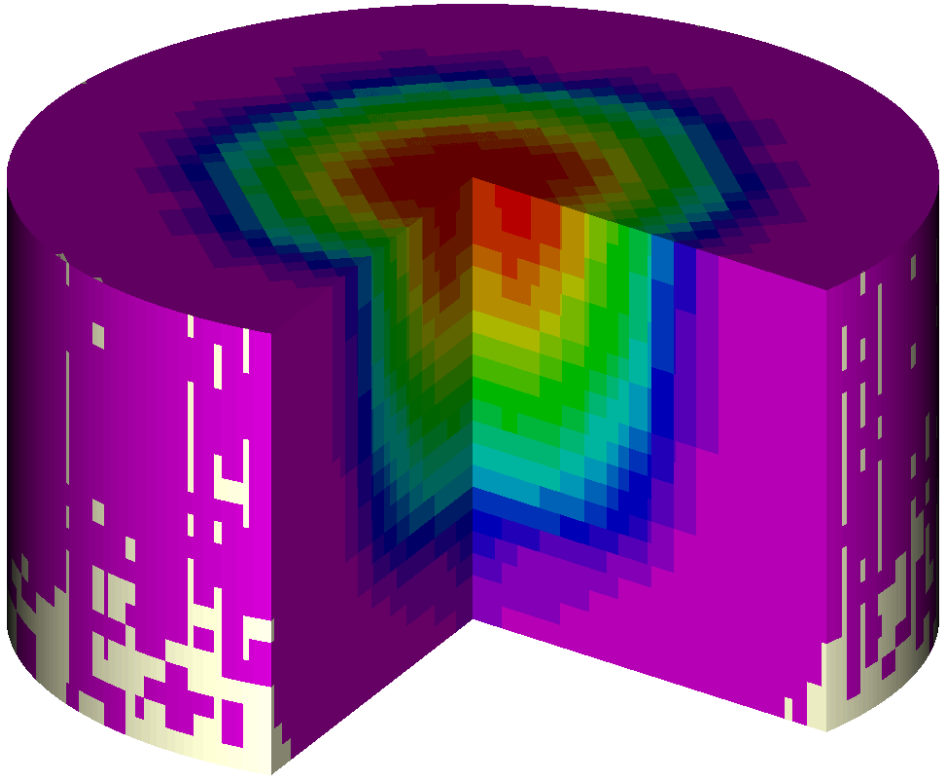
TRITON Model

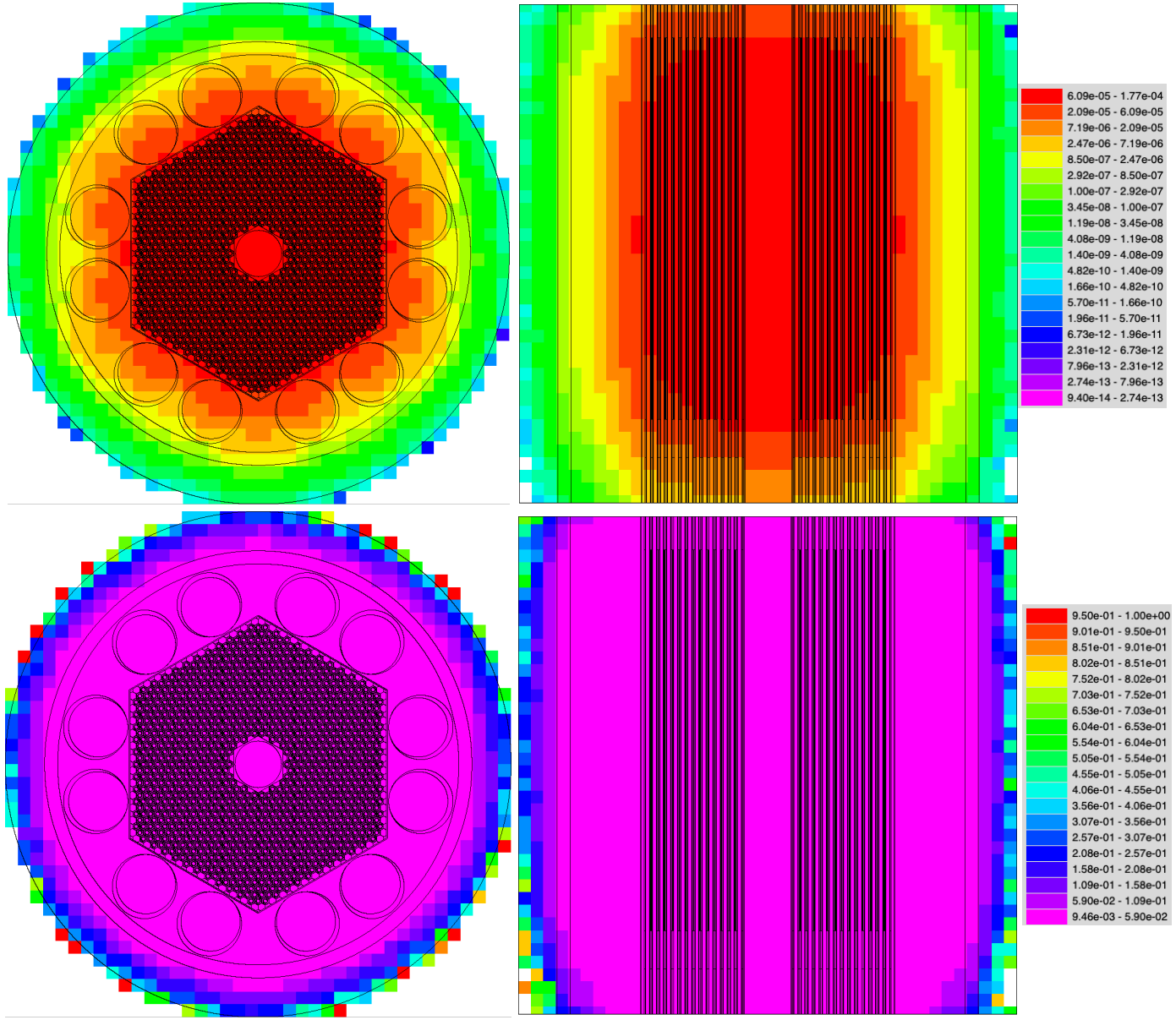
- Discretized materials
  - Fuel, RPV, neutron shield
- Calculates a lot of things
  - k_{eff}, flux, power, concentrations, decay heat and sources, etc.



TRITON Results

- Looks familiar!

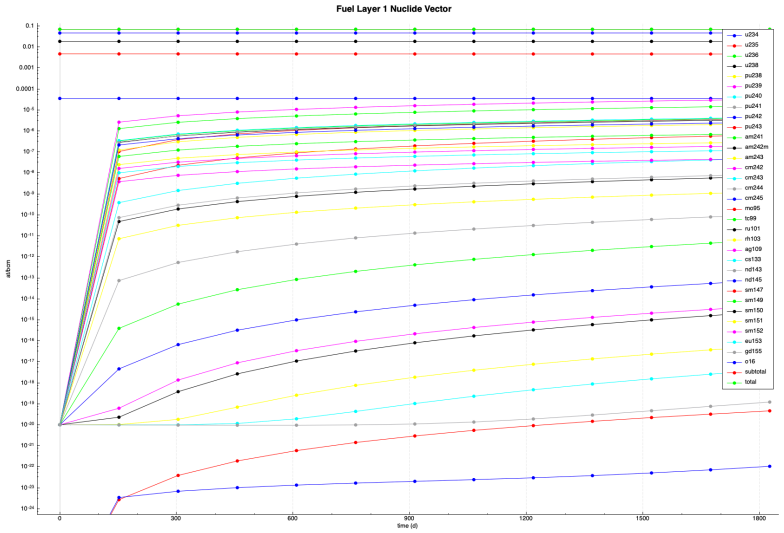


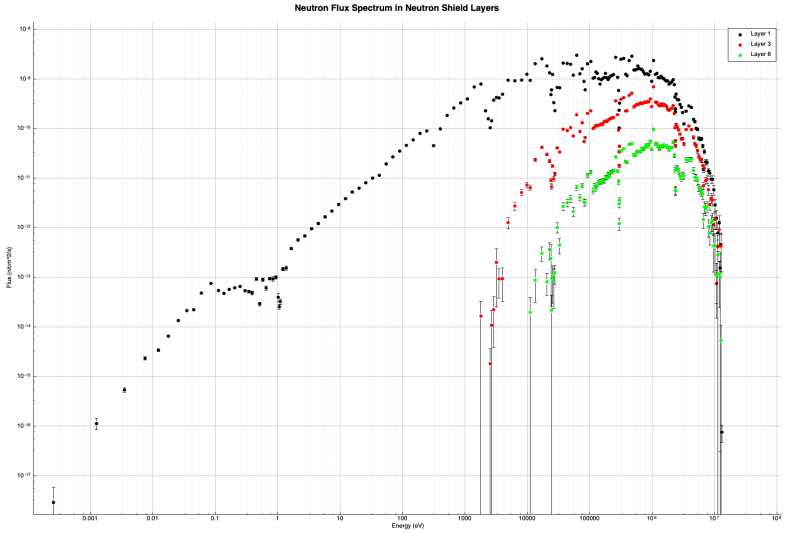


EOL, Flux Distribution (Log Scale)

TRITON Results

- Good enough?





Time (days)	Burnup (GWd/MTIHM)	k_{eff}	Total Neutron Flux (n/cm²/s)							
			R_{f1}	R_{f2}	R_{f3}	RPV_1	RPV_2	NS_1	NS_3	NS_6
0	0	1.0019	4.6e+13	3.7e+13	2.6e+13	3.4e+11	1.8e+11	4.6e+10	6.7e+09	7.9e+08
380	0.417	1.0017	4.6e+13	3.7e+13	2.6e+13	3.4e+11	1.8e+11	4.5e+10	6.8e+09	7.9e+08
685	0.750	1.0010	4.6e+13	3.7e+13	2.6e+13	3.4e+11	1.8e+11	4.5e+10	6.8e+09	7.9e+08
989	1.083	1.0005	4.6e+13	3.8e+13	2.6e+13	3.4e+11	1.8e+11	4.5e+10	6.7e+09	7.9e+08
1750	1.917	0.9994	4.6e+13	3.8e+13	2.6e+13	3.5e+11	1.8e+11	4.6e+10	6.7e+09	7.9e+08

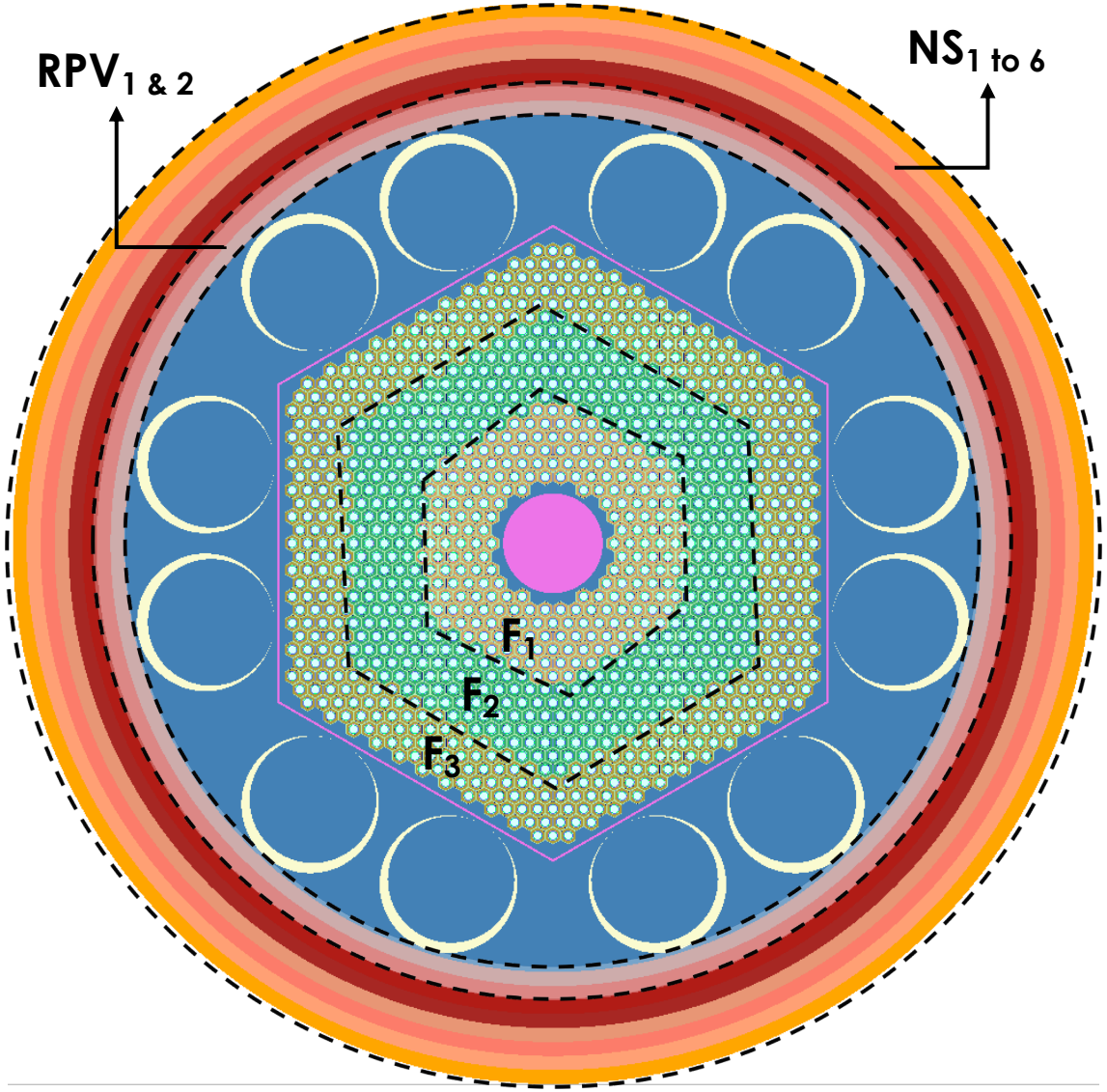
Generating the source term with Origen

Need to find:

1. Decay source term of fuel regions (F_1, F_2, and F_3)
2. Activation of RPV (RPV_1 & RPV_2)
3. Activation of neutron shield ($NS_{1\ to\ 6}$)

Procedure:

- Use the MG flux tally from CSAS to produce a one-group reaction library in Origen
- Deplete each region **by flux** to get the activation / decay source term



Origen input structure

```
'SCALE comment
=origen
 % ORIGEN comment
 bounds{ … }
 solver{ … }
 options{ … }
case(A){
  time=[31 365] % days
  …
}
case(B){
  …
}
% more cases?
end
```

- Origen inputs are organized into **cases**
- Each **case block** represents a single irradiation or decay cycle
- Material compositions can be passed from one case to the next

Each cycle (irradiation or decay) is a case block with time, powers, and (optionally) library & materials

Global problem configuration blocks

Multiple cases can be chained together to represent an irradiation history

SON syntax basics

- Origen 6.2 uses SON (Standard Object Notation) syntax for input

`[ arrays ]`	Consist of one or more numbered entries in brackets e.g., `time=[ 10 20 30 … ]`
`{ blocks }`	Contain keys and arrays within curly braces e.g., `case(caseLabel){ … }`

Specifying problem materials

```
=origen
case{
  …
  % create a material with 1 kg
  % of 3% enriched LEU
  mat{
    units=GRAMS
    iso=[u238=970.0E3 u235=3.0E4 o=123.1E3]
  }
  …
} % end case
end
```

Can specify individual isotope masses as key/value pairs

Can specify materials explicitly or load from a prior case

Valid units include grams, gram-atoms / moles and curies

Specifying only elemental symbol uses natural abundances for each isotope

Note: First case must **always** specify materials!

Loading materials from a saved file

```
=origen
case{
  …
  % Load from position 2 on saved f71 file
  mat{
    load{ file="origen_saved.f71" pos=2 }
  } % end mat
  …
} % end case
end
```

Specifying irradiation powers: the POWER array

```
=origen
case{
  …
  mat{
    units=GRAMS
    iso=[u238=970.0E3 u235=3.0E4 o=123.1E3]
  }
  % 10 steps at 35 MW each
  % 14,000 MWd/MTU total cycle burnup
  power=[ 10R 35.0 ]
  time=[ 8I 10 400.0 ]
} % end case
end
```

10 steps of all the same power (35 MW); can be different powers for each time interval

times = # powers
(Origen supplies t_0 by default)

<u>Note:</u> Powers are in **total MW** (not MW/MTU)

Depletion / activation by user-specified flux spectrum

```
=origen
case{
  …
  lib {
    update {
      resource {
        reaction="origen.rev03.jeff200g"
        decay=decay
        yield=yields
      }
    neutron { flux=[Φ(E1) Φ(E2) … Φ(EN)] }
    save {
       title="Fuel Layer 1"
       file="megapower_Fuel_Layer1.f33"
    }
    extend=no
  }
  flux = [Φ(t1) Φ(t2) … Φ(ti)]
  time{
    t = [t1 t2 … ti]
    units=seconds
}
```

Generates an updated one-group reaction library for activation

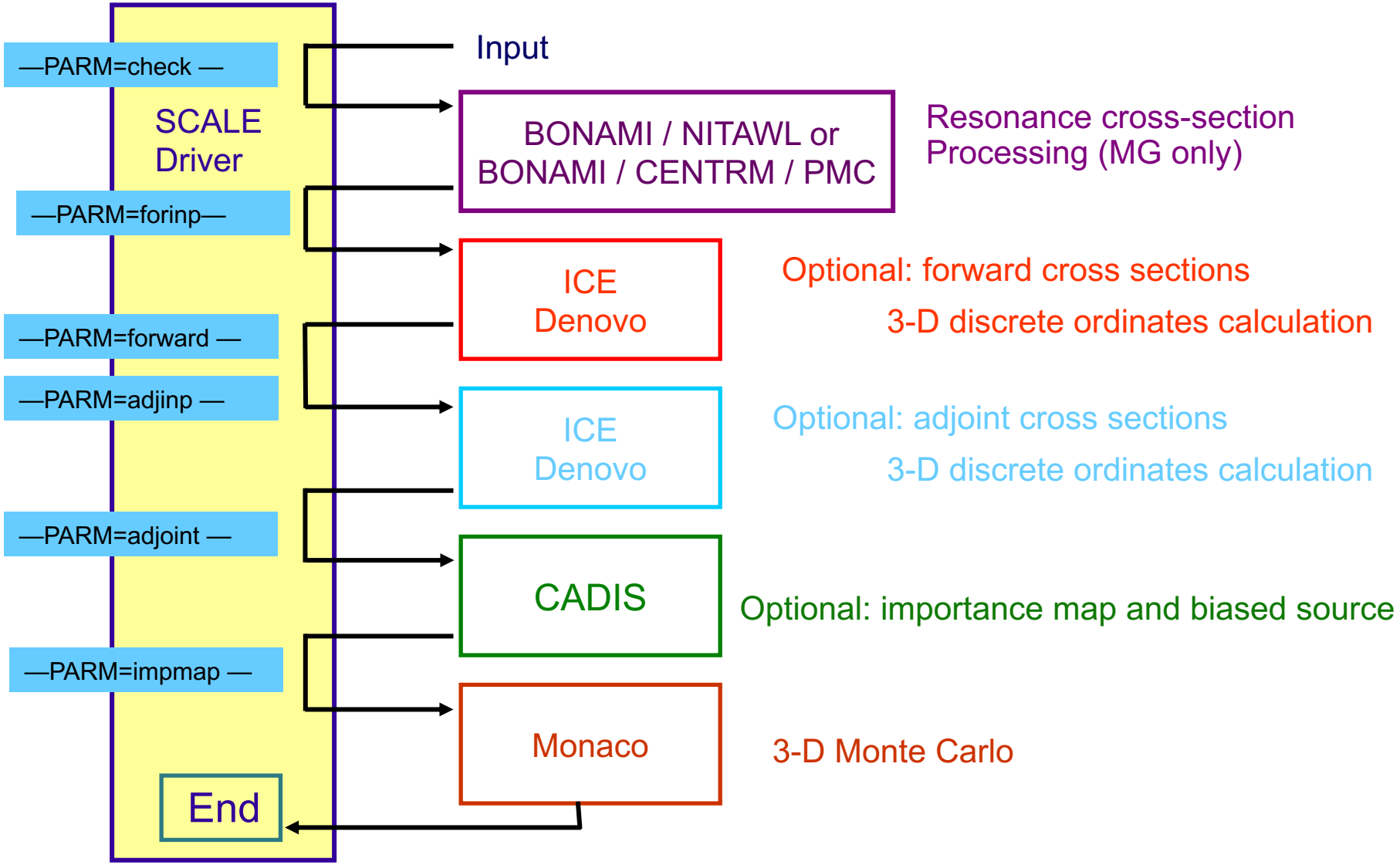
…from an existing AMPX multi-group reaction library

…and Origen decay & fission yield resources

User-provided neutron flux weighting spectrum used for collapsing to one-group

Scalar flux intensity (n/cm^2-s) for each time interval

MAVRIC Sequence



MAVRIC Input

- Material Compositions
- Geometry
  - regions made of intersections of:
    - solids, arrays, volumes (same as KENO-VI)
- Definitions
  - locations, response functions, grid geometries, distributions
- Sources
  - spatial, energy, direction
- Tallies
  - region tallies, point detectors, mesh tallies
- Basic Calculational Parameters
- Variance Reduction Parameters

```
=mavric    parm=keyword
Some title for this problem
v7.1-28n19g

read compositon
   ...
end composition
read celldata
   ...
end celldata

read geometry
   ...
end geometry
read array
   ...
end array
read volume
   ...
end volume
read plot
   ...
end plot
```

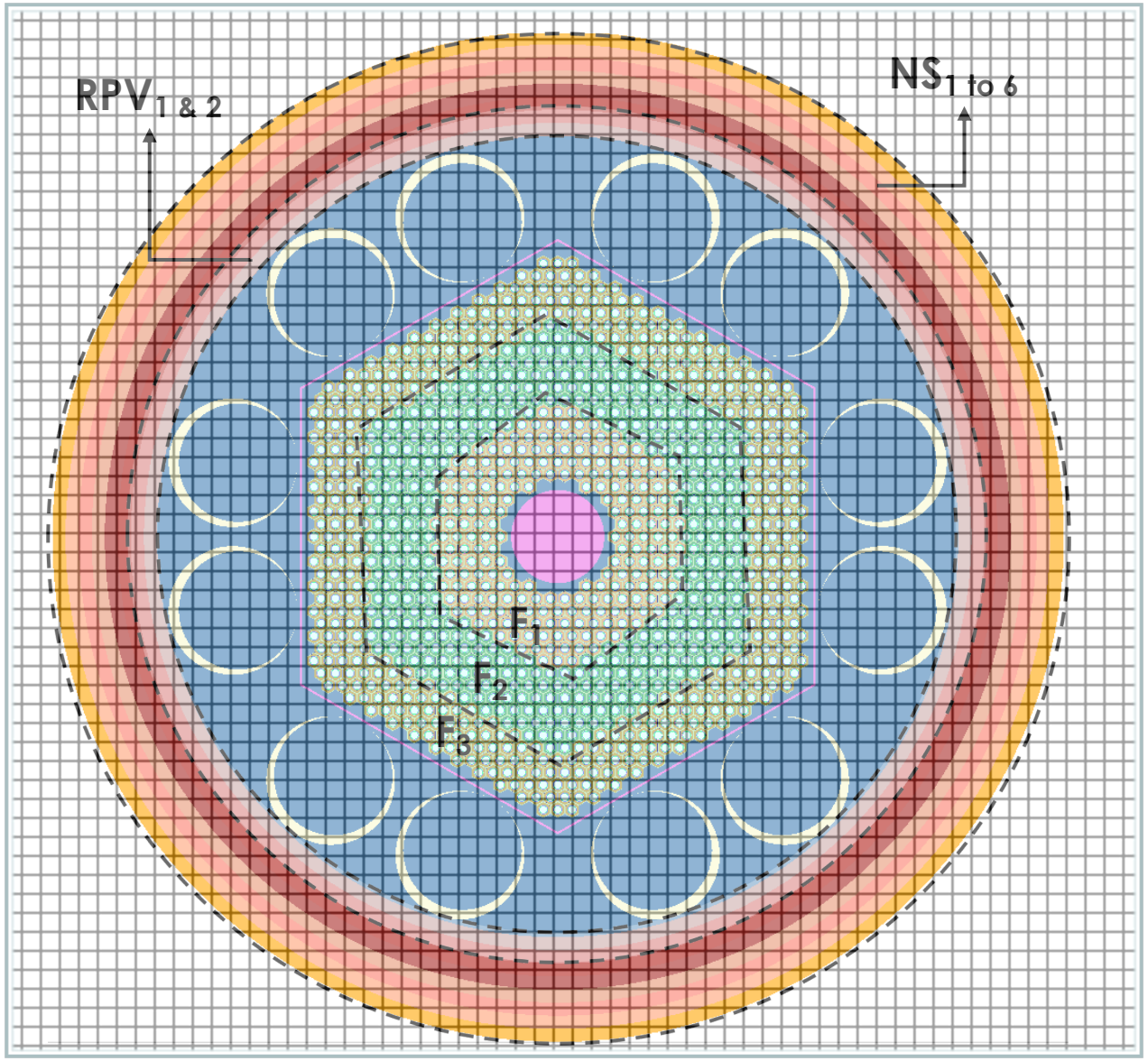
```
read definitions
   ...
end definitions
read sources
   ...
end sources
read tallies
   ...
end tallies

read parameters
   ...
end parameters
read biasing
   ...
end biasing
read importanceMap
   ...
end importanceMap

end data
end
```

MAVRIC Model

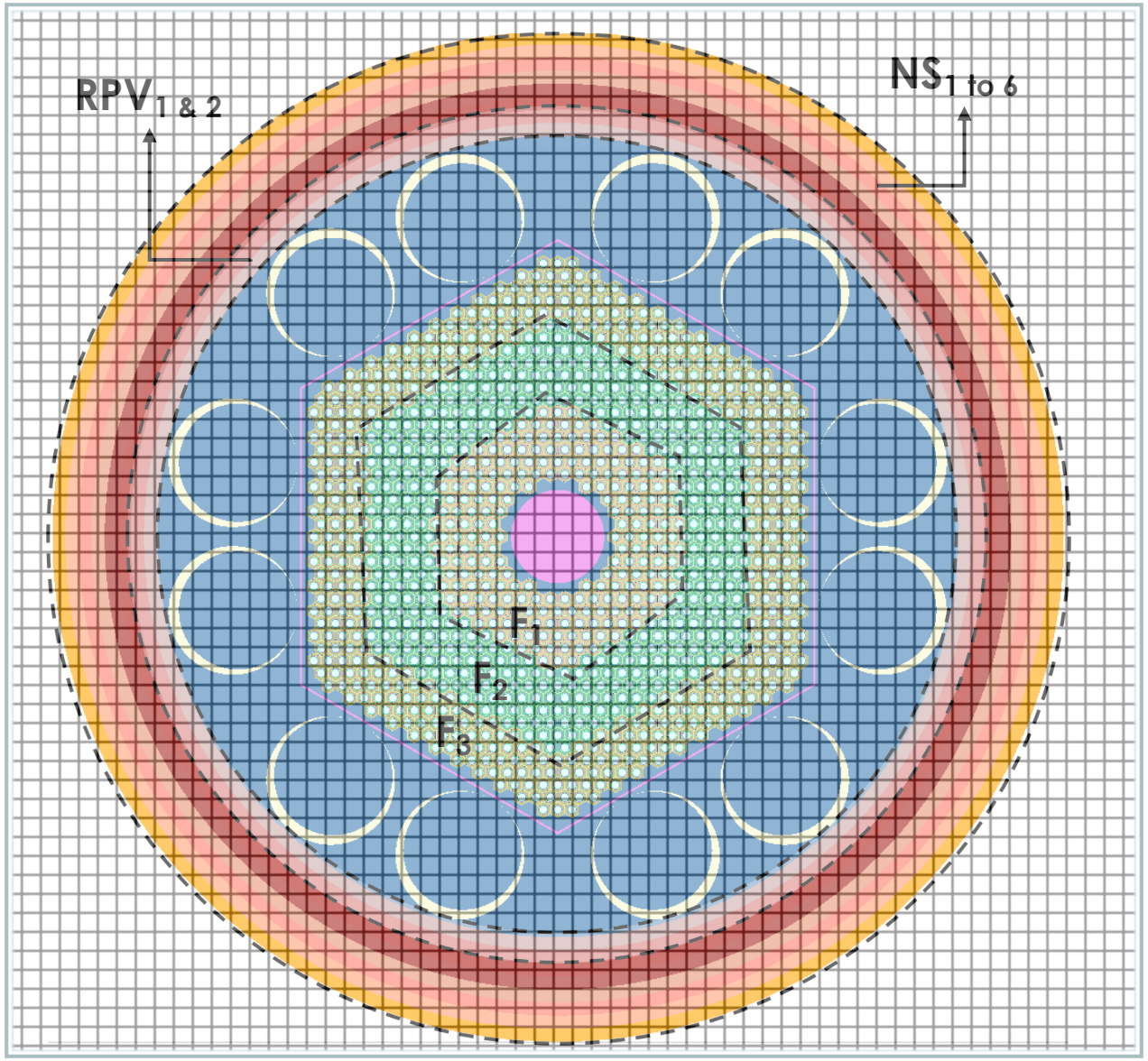
- Discretized materials
  - fuel, RPV, neutron shield
- Fission source
  - interfacing CSAS
- Decay and activation sources
  - interfacing ORIGEN
- Variance reduction
- Tallies with responses



MAVRIC Model

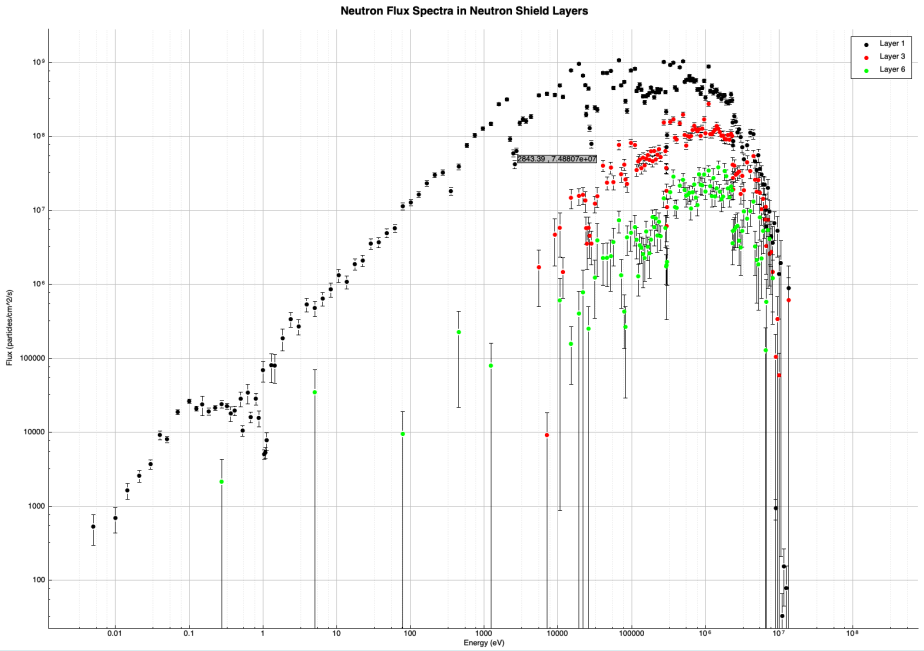
- Need to define:
  - gridGeometry, response, energyBounds, tallies
- Fission source
  - use thermal power
    (5 MW_t)/(200 MeV/fission)/
    (1.602e-13 J/MeV) = 1.56e17 fissions/sec

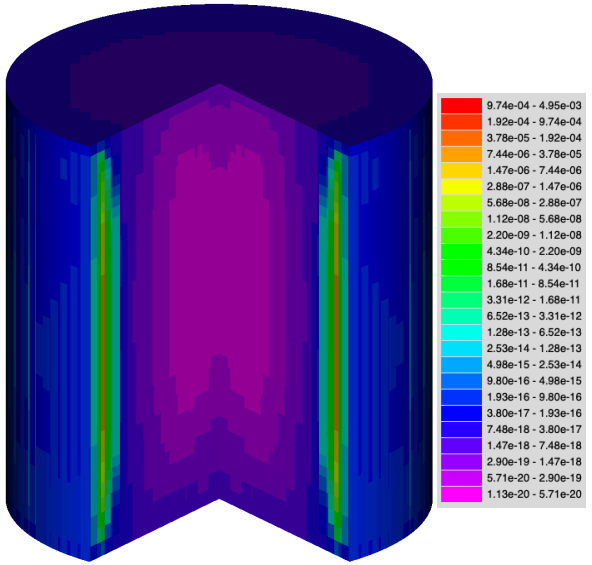
Fuel Region	Volume Fraction	Power Fraction
R_{f1}	0.194	0.260
R_{f2}	0.377	0.404
R_{f3}	0.429	0.336



MAVRIC Results

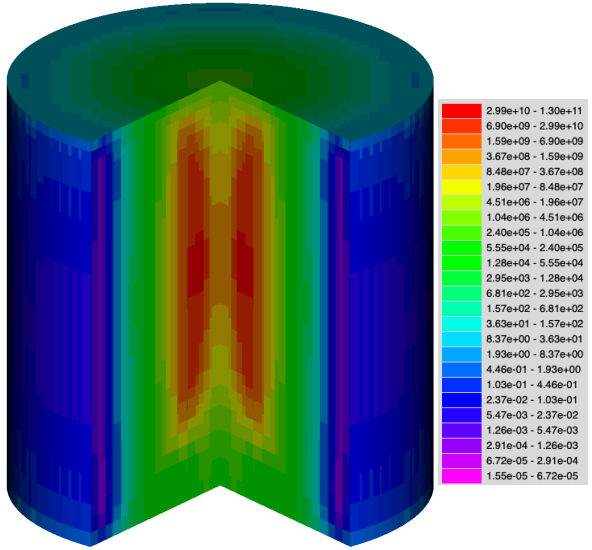
- Good enough?





Adjoint flux

Code	Total Neutron Flux (n/cm²/s)							
	R_{f1}	R_{f2}	R_{f3}	RPV_1	RPV_2	NS_1	NS_3	NS_6
TRITON	4.6e+13	3.7e+13	2.6e+13	3.4e+11	1.8e+11	4.6e+10	6.7e+09	7.9e+08
MAVRIC	4.6e+13	3.8e+13	2.6e+13	3.6e+11	1.9e+11	4.8e+10	7.6e+09	3.0e+09
MAVRIC-RPV (FW-CADIS)	-	-	-	3.9e+11	2.1e+11	-	-	-
MAVRIC-NS (FW-CADIS)	-	-	-	-	-	4.6e+10	7.6e+09	3.3e+09

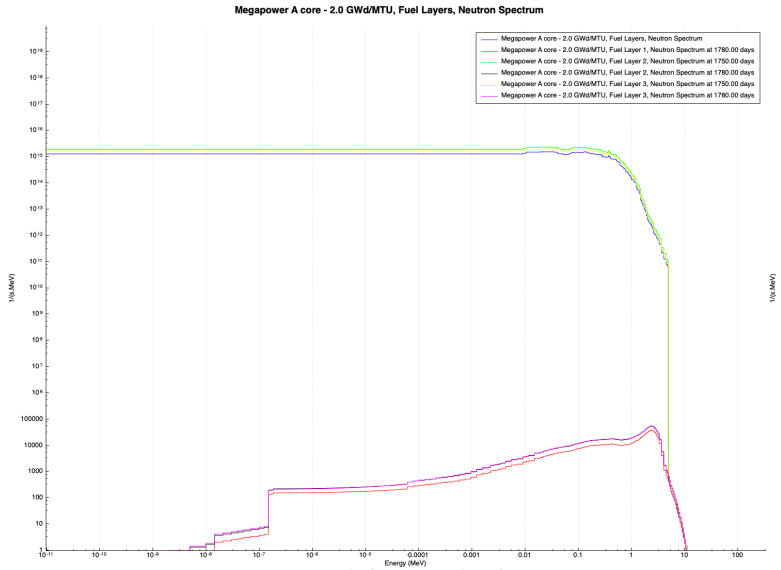


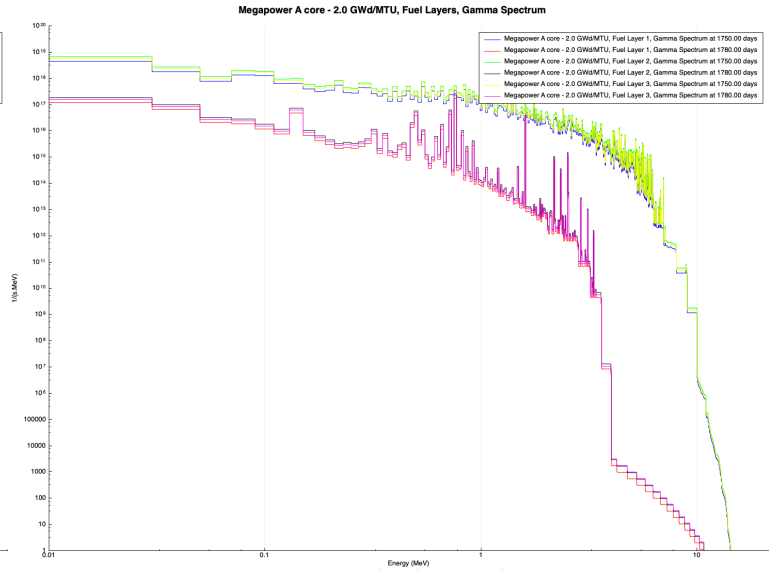
Importance

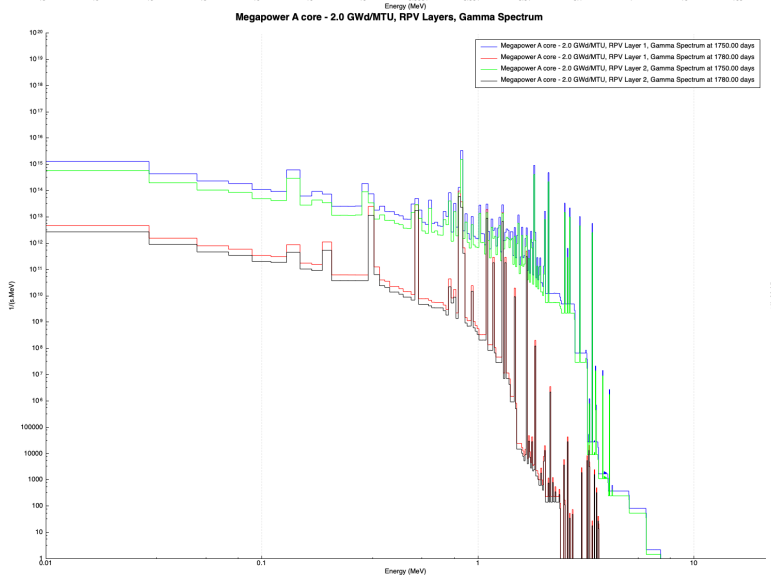
ORIGEN Sources

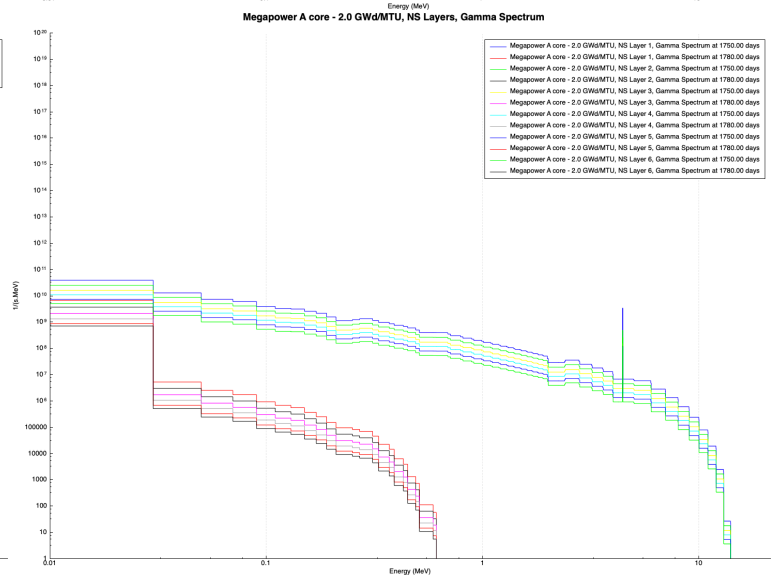
- Discretized materials
- Decay and activation sources
  - need power and flux
- 1-month cooldown after almost 5 years of operation
- Gamma emissions are dominant
  - Self-shielding will help

Fuel







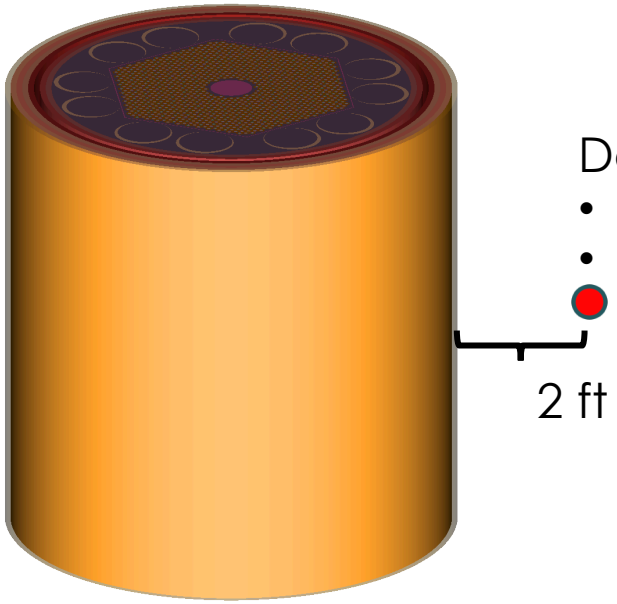


RPV

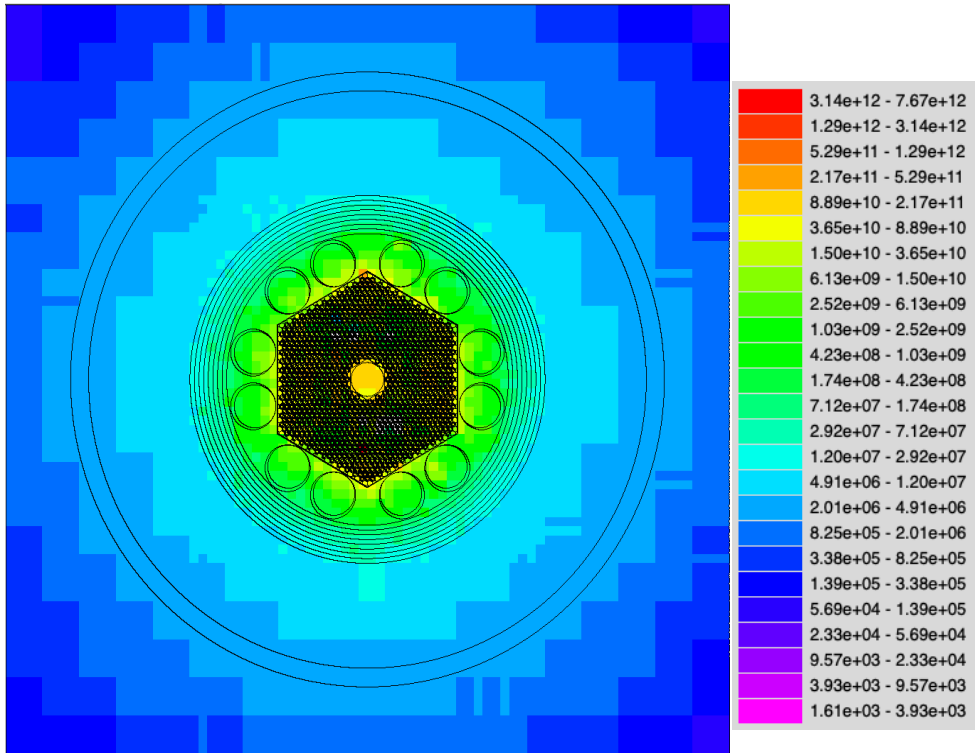
NS

Dose Results

- Dose rate is hopefully:
  - not lethal after some shielding
  - lower than regulated limits



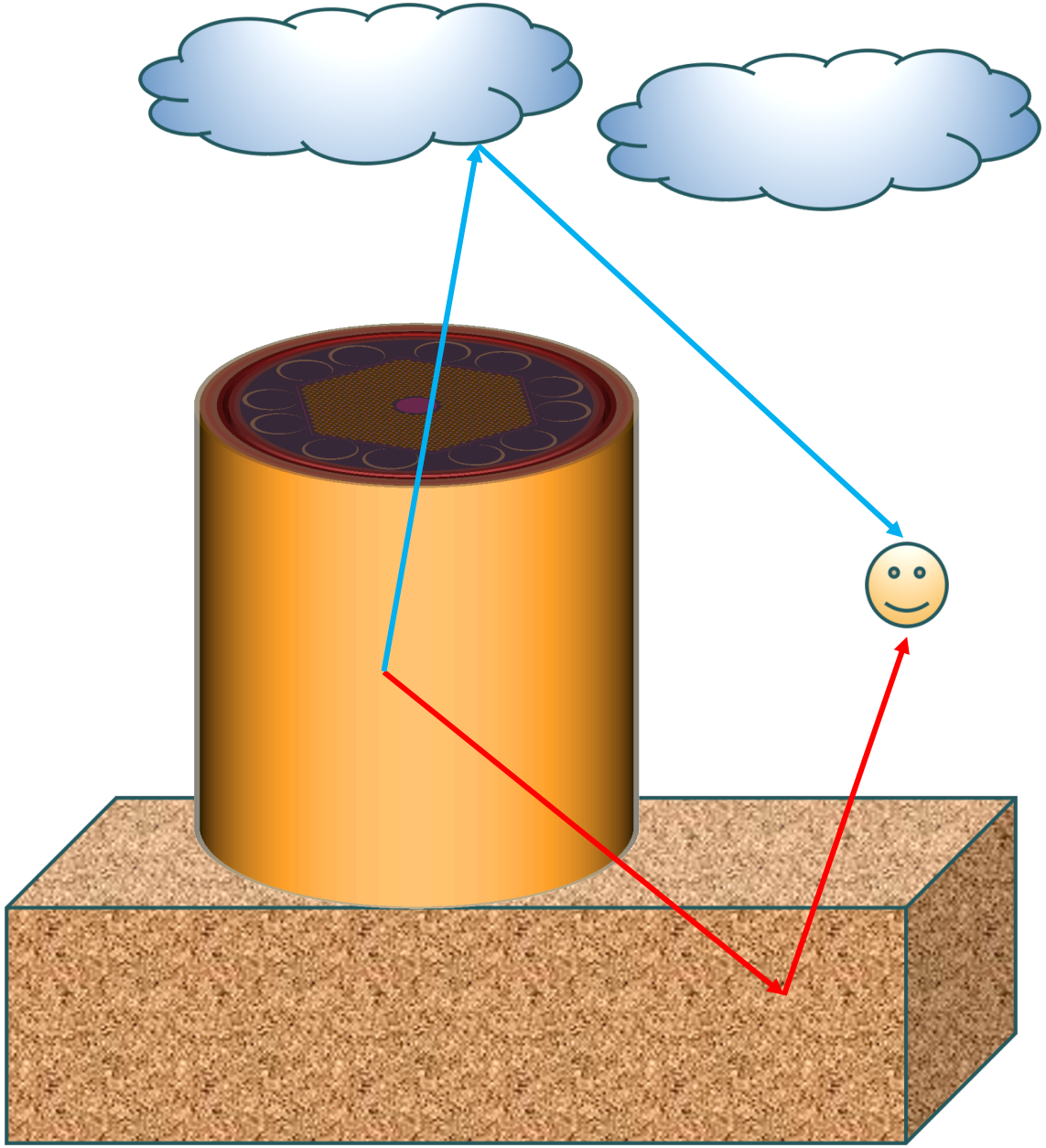
Dose rate: ~ 3 Mrem/hr
- all from gammas
- dominated by decay gammas
  - ~40% from RPV



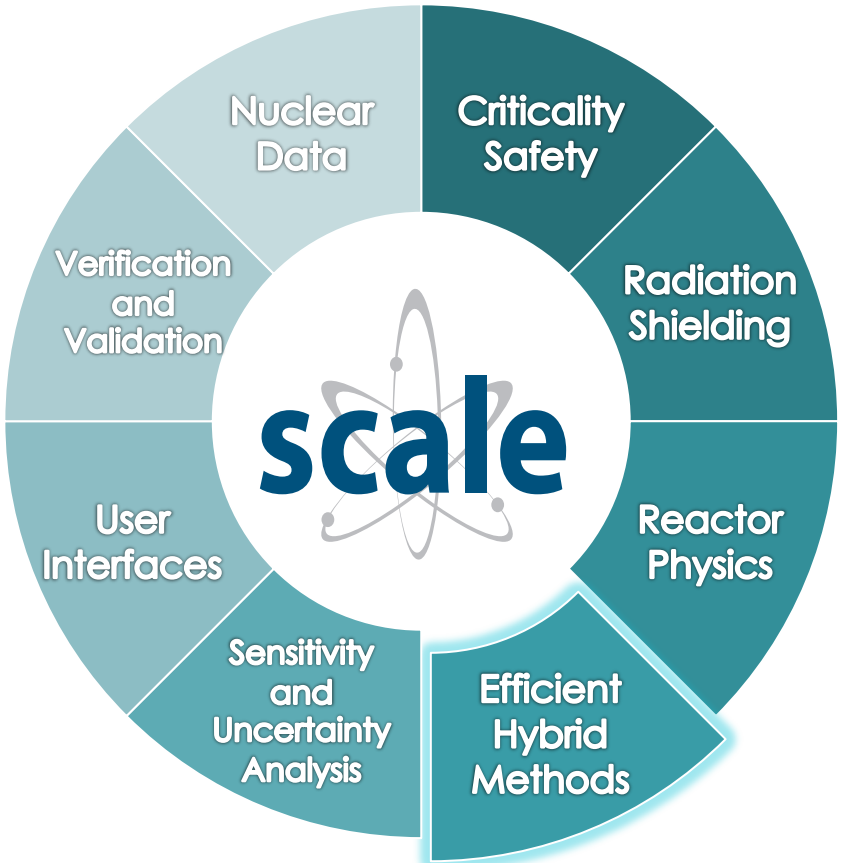
Gamma Flux Map

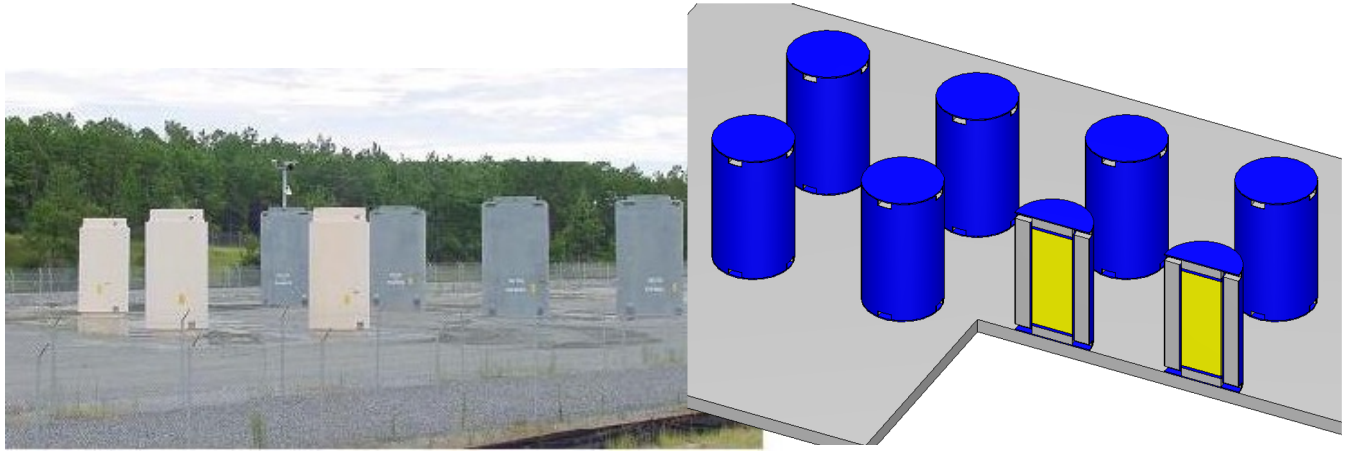
Summary

- Shielding calculations by using:
  - fission sources
  - decay and activation sources
  - fixed-sources
  - combination of any and all sources
  - built-in variance reduction methods
- What else is missing?
  - first-order approximation
  - surroundings, groundshine, and skyshine



SCALE has efficient hybrid methods





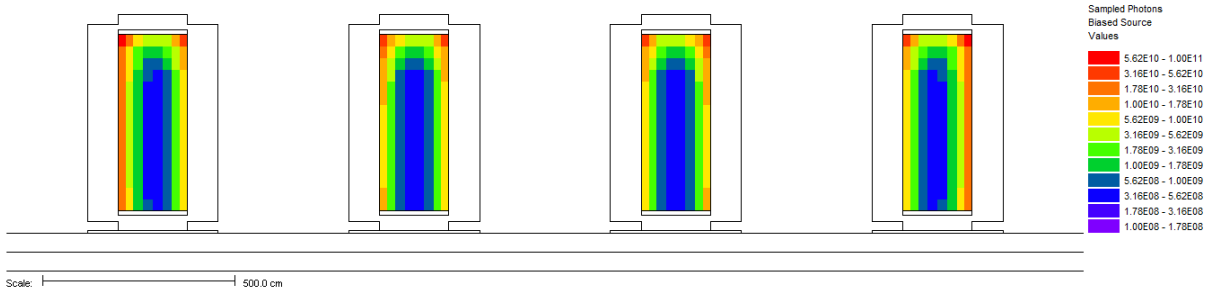
Dose analysis for used nuclear fuel storage

Dose Rate (rem/hr)

Relative Uncertainty

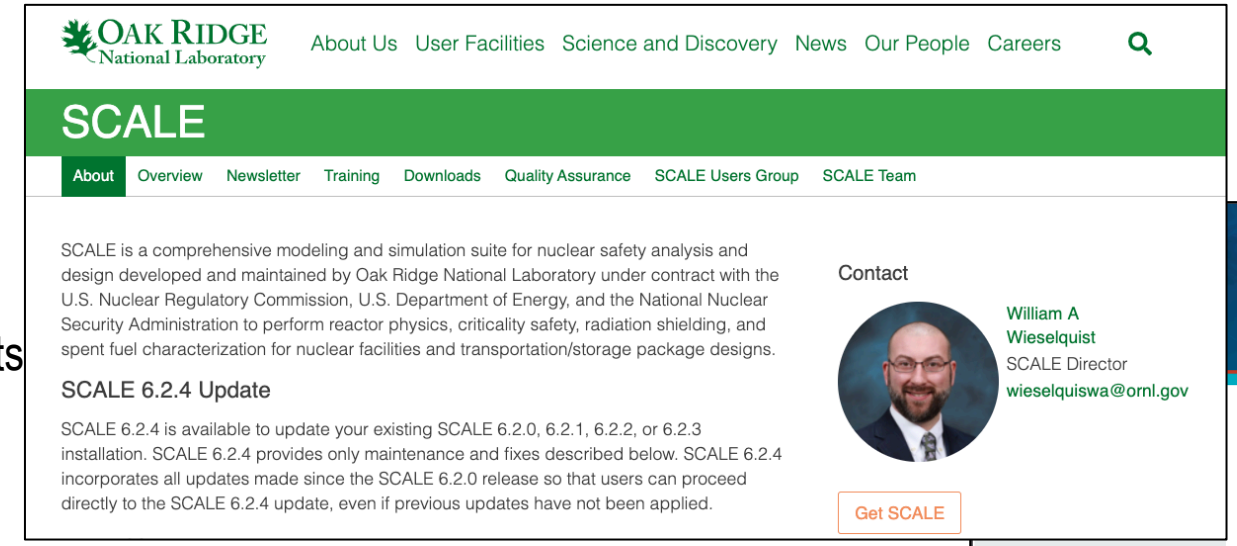
Analog

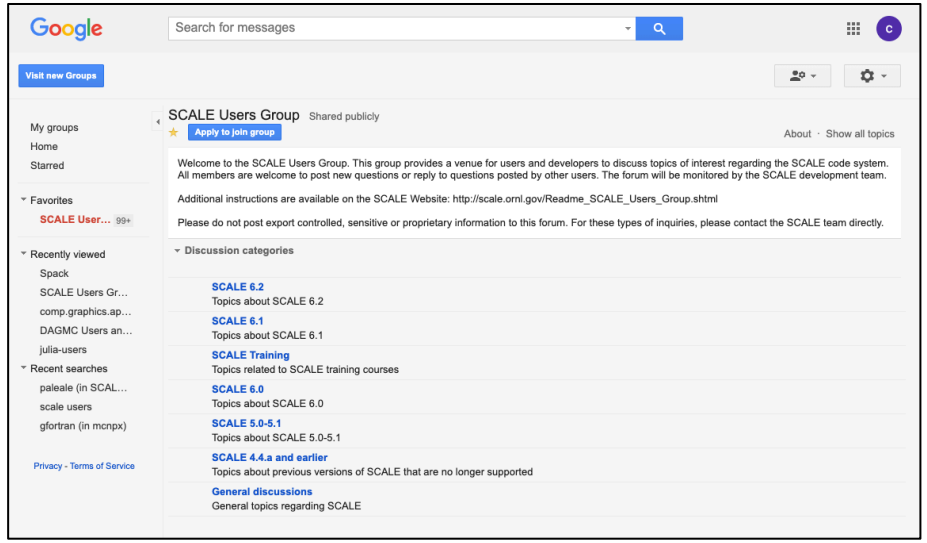
Hybrid (Same run time)



Need Help?

- SCALE Website
  scale.ornl.gov
  - Publications/Training
  - Validation and benchmark reports
  - Downloads
- SCALE Newsletter
- SCALE Users Group forum
- On-demand assistance
  scalehelp@ornl.gov
- Users Group Workshop
  scalemeetings.ornl.gov





Questions?

https://en.wikipedia.org/wiki/Question_(character)