# Pebble fuel source term generation

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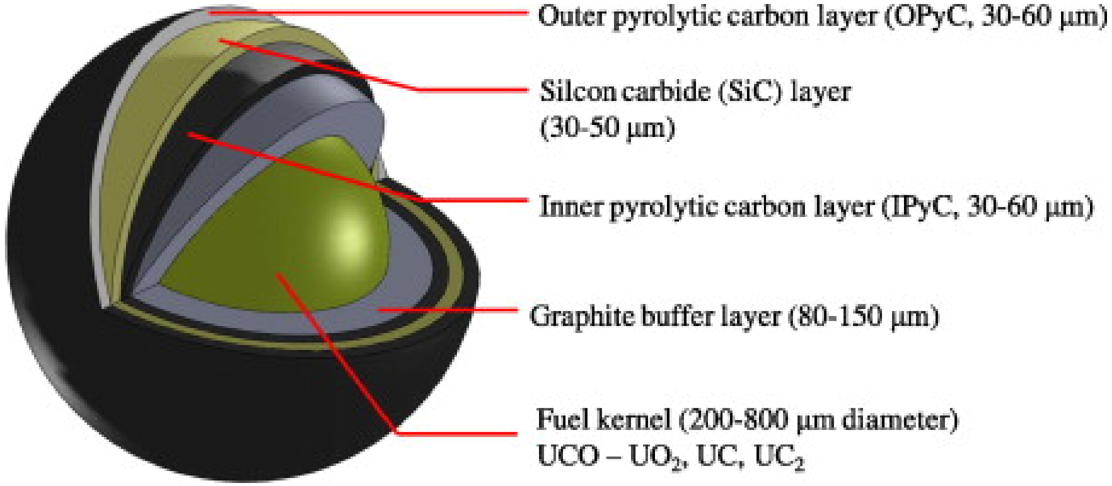
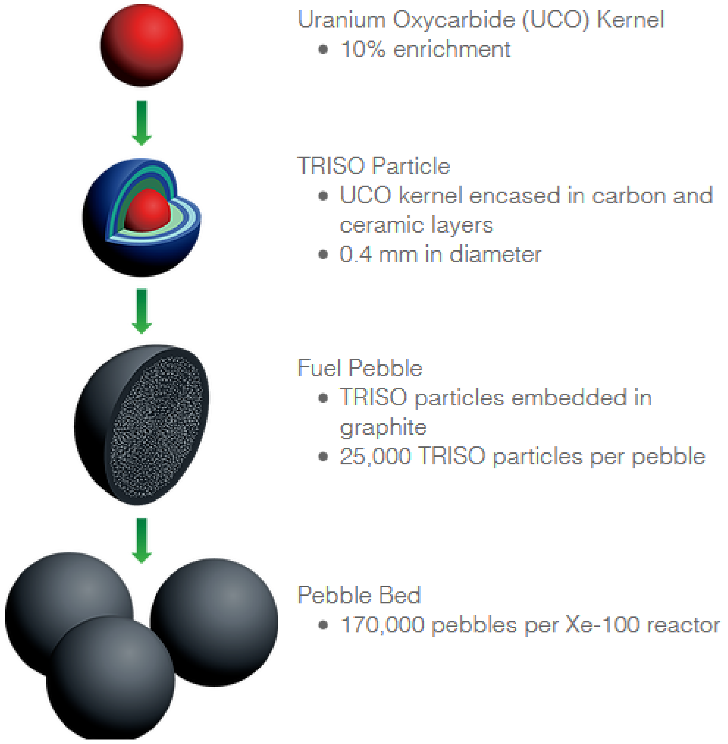
# Overview

- Introduction to TRISO fuel and pebble-based reactor systems
- Modeling strategy
  - How can we model flowing-pebble systems using SCALE?
  - How does this compare to prior approaches for PBR modeling?
  - What level of detail is required to capture the relevant physics?
- Physics observations of the PBR-400 core
  - Relevant parameters for ORIGEN library development

# TRISO-based fuels

- TRISO particle
  - TRISO: portmanteau for **tri**structural **iso**tropic
  - Kernel – 1.5 g U; 250 μm radius
  - Porous carbon buffer layer
  - 3 coatings to contain fission products
- TRISO pebble
  - Contains 14,500 TRISO particles
  - 25 mm radius
  - 5 mm graphite outer shell



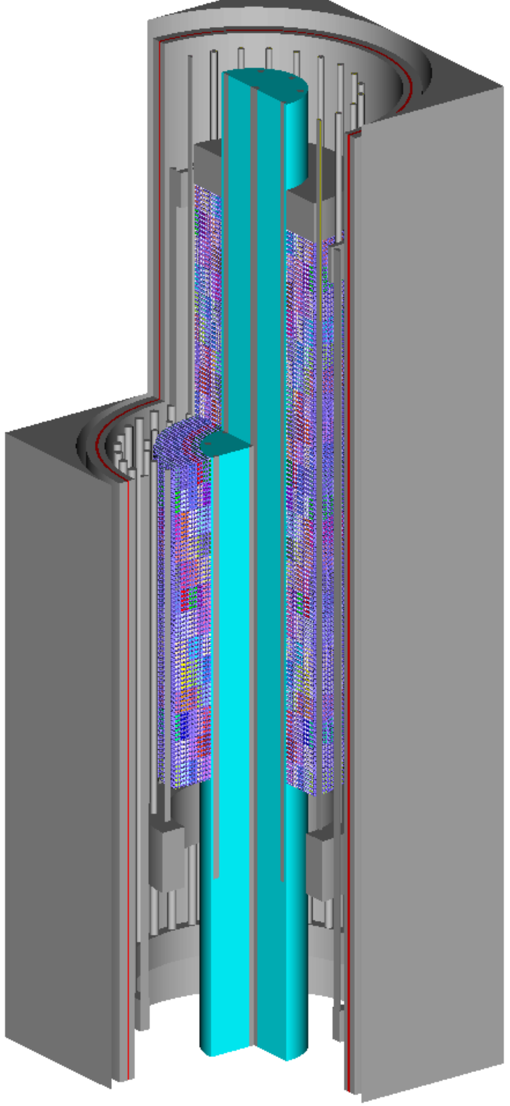




**TRISO pebble**
(U.S. Department of Energy)

Figures: Courtesy of M. P. Baker, et al., *J. Nucl. Materials* 432, pp.395-406, 2013; X-Energy website

# PBMR-400

- 400 MWt
- Helium coolant
  - 9 MPa (1300 psi)
  - 500 C inlet / 900 C outlet
- 452,000 TRISO pebbles in an annular core with graphite reflectors
  - 2.0 inner diameter / 3.7 m outer diameter
  - 11 m height
- 92,000 MWd/MTU target burnup
- Two cases evaluated
  - **Startup core:** 1/3 fuel pebbles, 2/3 graphite "dummy" pebbles
  - **Equilibrium core:** 110 material zones with pre-specified material compositions (100% fuel)



PBMR-400 SCALE geometry
(S. Skutnik, ORNL)

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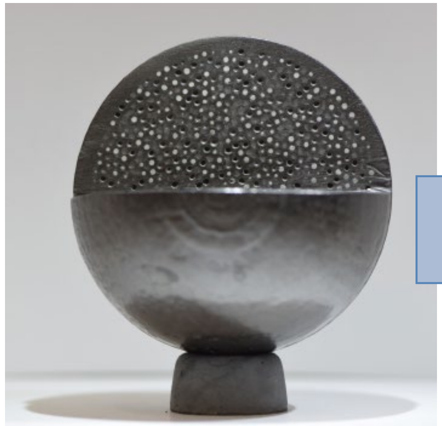
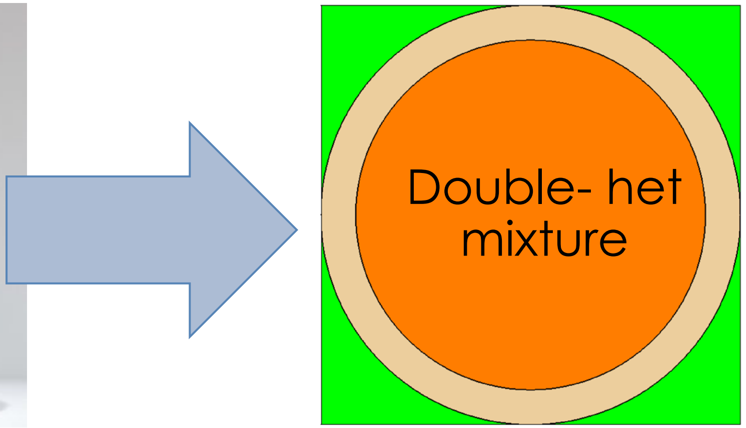
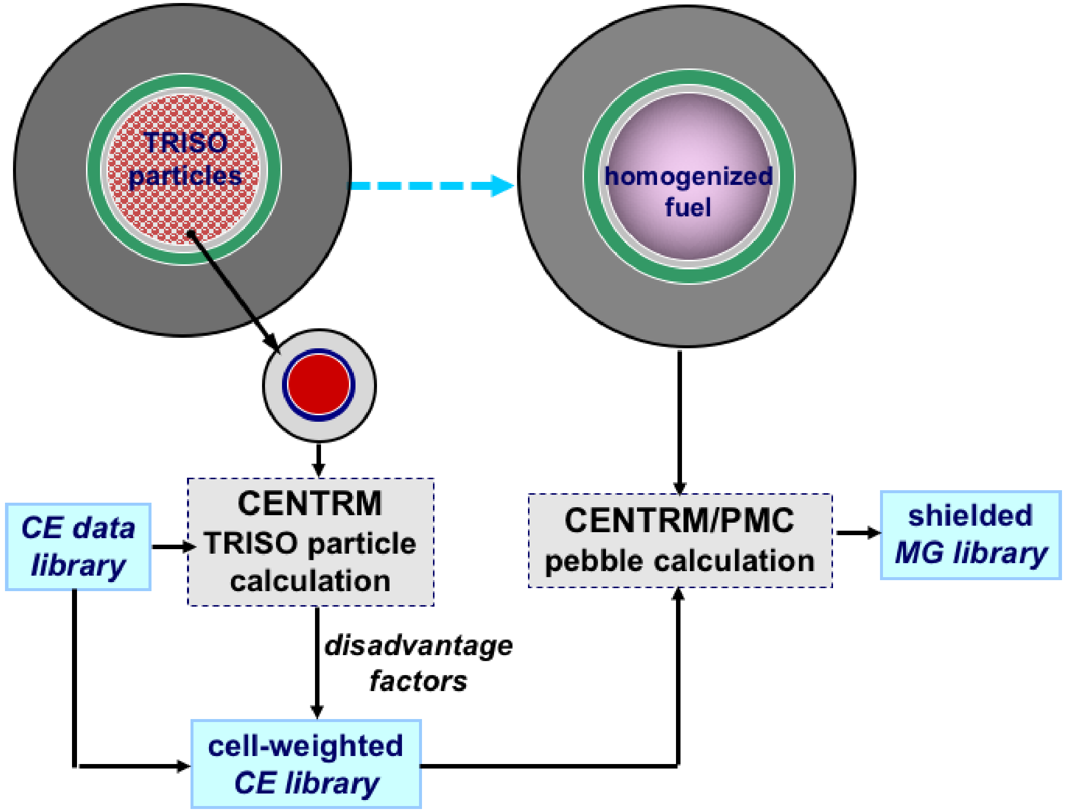
# Modeling strategy for pebble-based reactors

# Self-shielding calculations for doubly-heterogeneous fuel with CENTRM / XSPROC in SCALE

- Creation of an "effective" fuel mixture for MG calculations
  - Basically two self-shielding calculations
  - Simple user input in cell block for self-shielding
  - Creates one mixture to be placed in geometry model





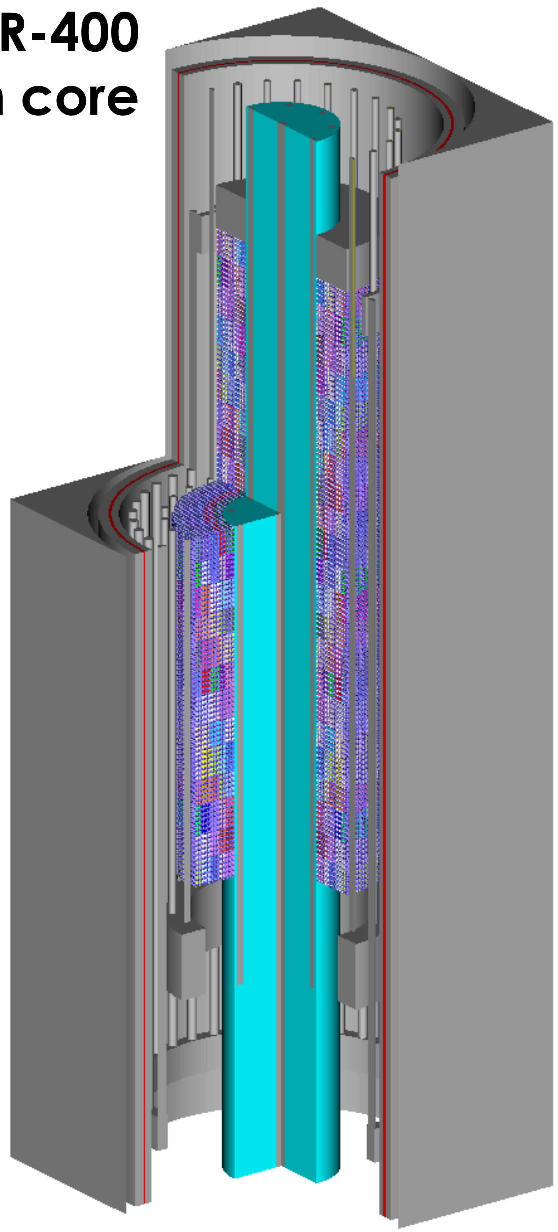

**Double-het computational procedure for a pebble fuel component with SCALE**

# HTGR analysis with SCALE: Overview

- **Main goals**
  - Evaluate neutronic characteristics
  - Generate individual pebble inventory within a core zone/batch (e.g., difference between fresh vs. once-through pebble in a single core zone)
  - Generate discharge pebble inventory/decay heat with sensitivity/uncertainty analysis

- Limitations / caveats
  - Goal is to construct an **equilibrium** core inventory; not trying to perform transient / reload analysis

**PBMR-400 equilibrium core**



How do we do this for moving / reloading pebbles?

# Strategy for LWRs

- What level of TRITON model fidelity is required to generate a reasonable 1-group xs database (ORIGEN reactor library) for rapid **LWR** inventory calculations?

Increasing fidelity

a. 3D full-core with plant-specific loading pattern
b. 3D full-core with equilibrium loading pattern
c. 3D core subset
d. 3D single assembly
e. 2D core subset
f. 2D single assembly
g. 2D single pin
h. 0D infinitely homogeneous mixture

Requires plant-specific knowledge

Assembly position matters → Imposes additional assumptions or requires too much information!

Has trouble with local variations (control elements, water holes, channel box)

Has trouble if **any** geometry is important

- For LWRs, using 2D single assembly models to generate the 1-group xs database appears sufficient!
  - **verification** confirms ORIGAMI reproduces TRITON results with same (simple) operating history
  - **validation** against spent fuel inventory and decay heat measurements confirms the overall approach is adequate
    - code results generally within experimental uncertainty bands
    - <1% error in decay heat, <5% error in important nuclides, <15% error in others

# Strategy for HTGRs

- What level of TRITON model fidelity is required to generate a reasonable 1-group xs database for rapid **HTGR** inventory calculations?
  a. 3D full-core with plant-specific pebble loading & discharge strategy
  b. 3D full-core with equilibrium pebble distribution
  c. 2D core slice with equilibrium pebble distribution
  d. 1D single pebble with "buffer" for neighbor effects
  e. 1D single pebble
  f. 0D infinitely homogeneous mixture

Requires plant-specific knowledge (a)

Computationally expensive (a, b)

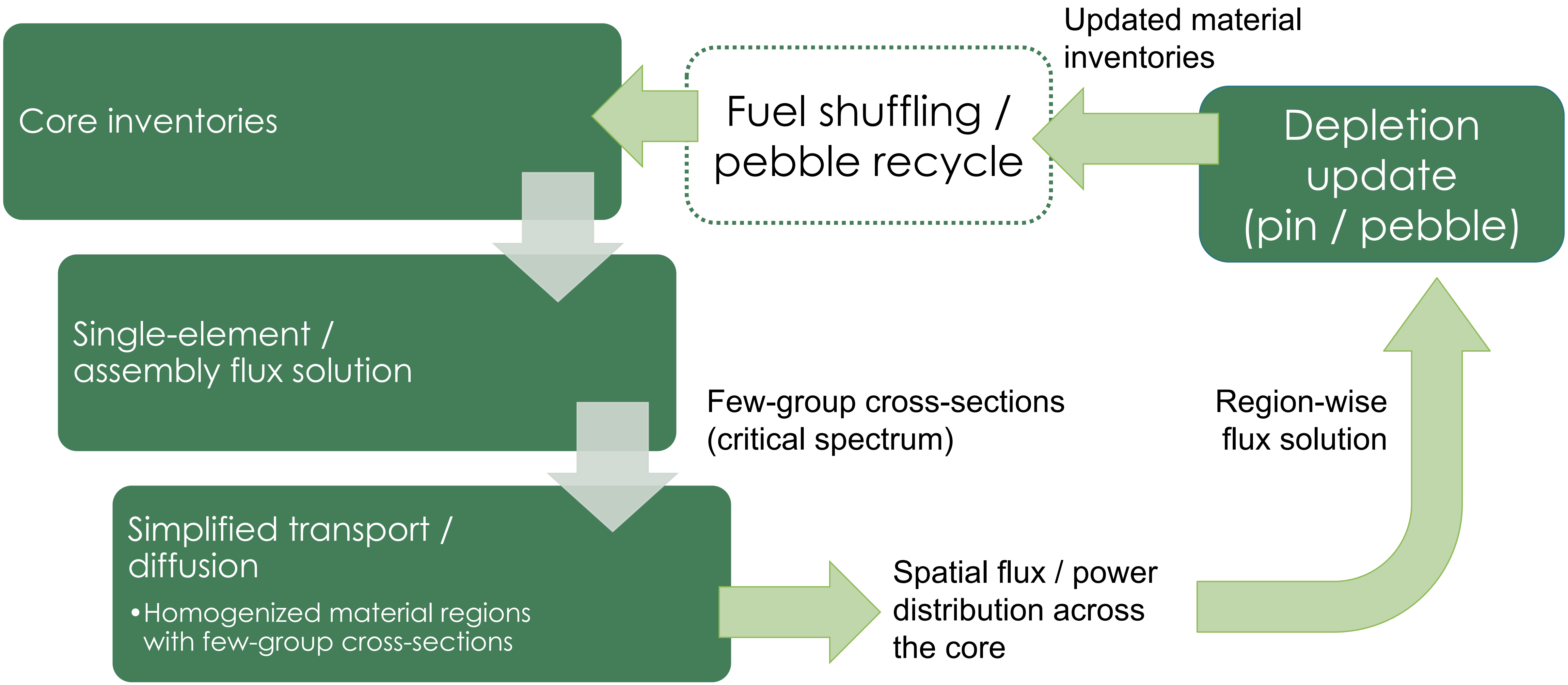
Previously investigated in other work; difficult to optimize buffer (d)

Does not account for reflectors (e, f)

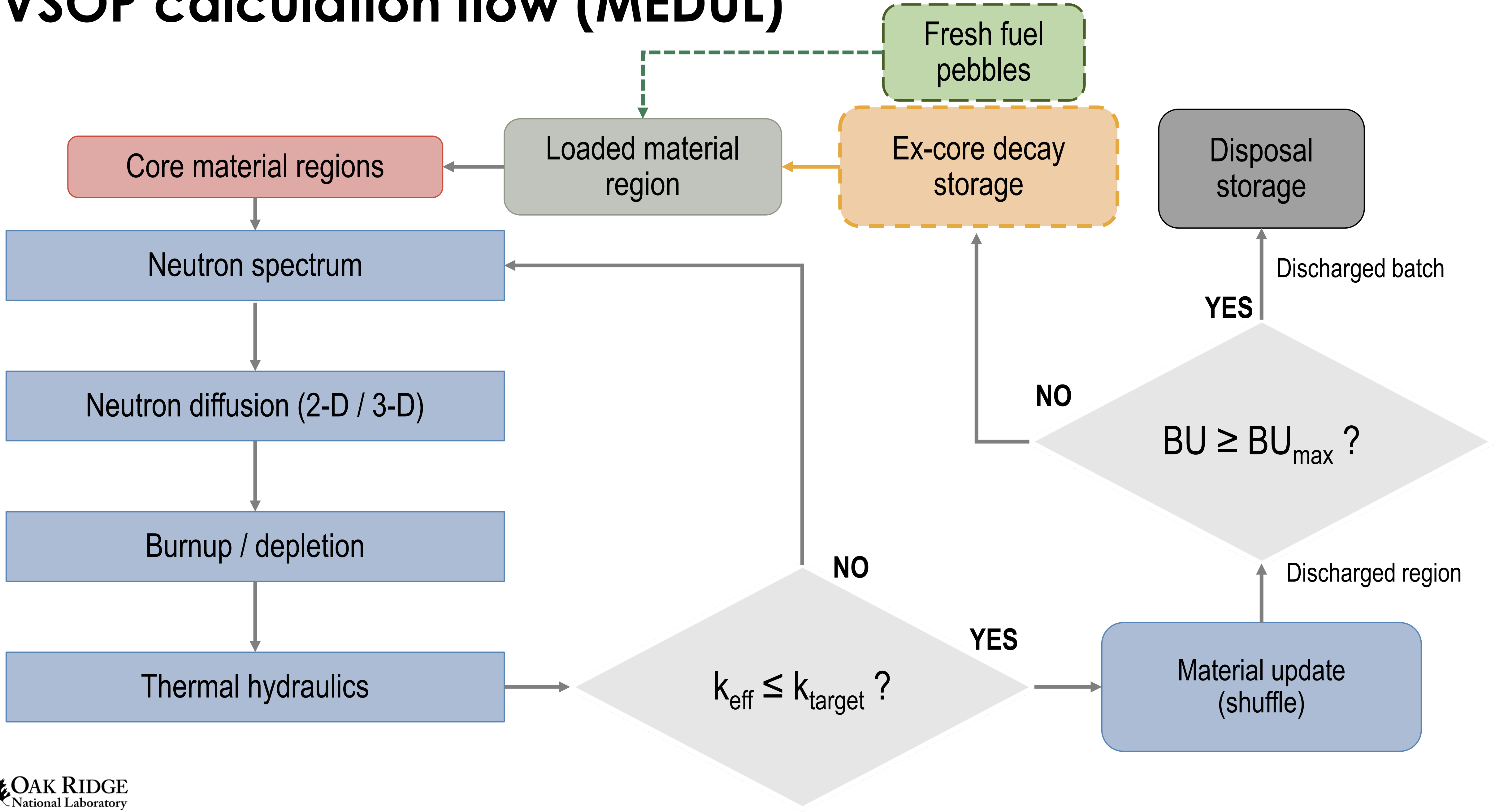
Used to understand sensitivity to model fidelity (b, c, e)

- Using SCALE/TRITON 3D full-core at equilibrium (b) is equivalent to prior approaches like VSOP, but with:
  – ENDF/B-VII.1+ modern nuclear data
  – Complete SCALE/ORIGEN nuclide set instead of VSOP limited set
  – SCALE high-fidelity full-core Monte Carlo transport instead of VSOP diffusion

# VSOP workflow shares several features of conventional 2-step LWR core analyses



# VSOP calculation flow (MEDUL)



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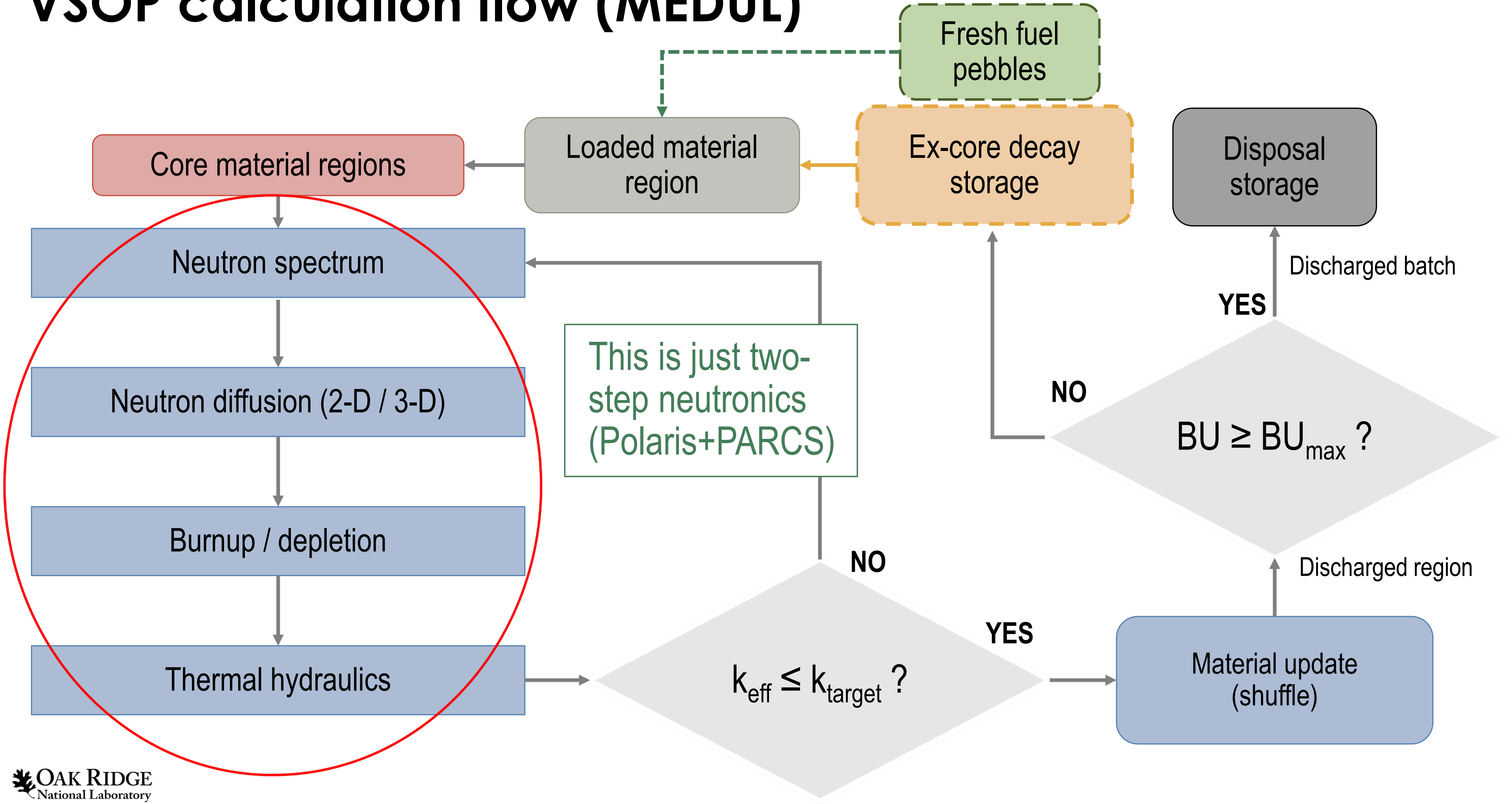

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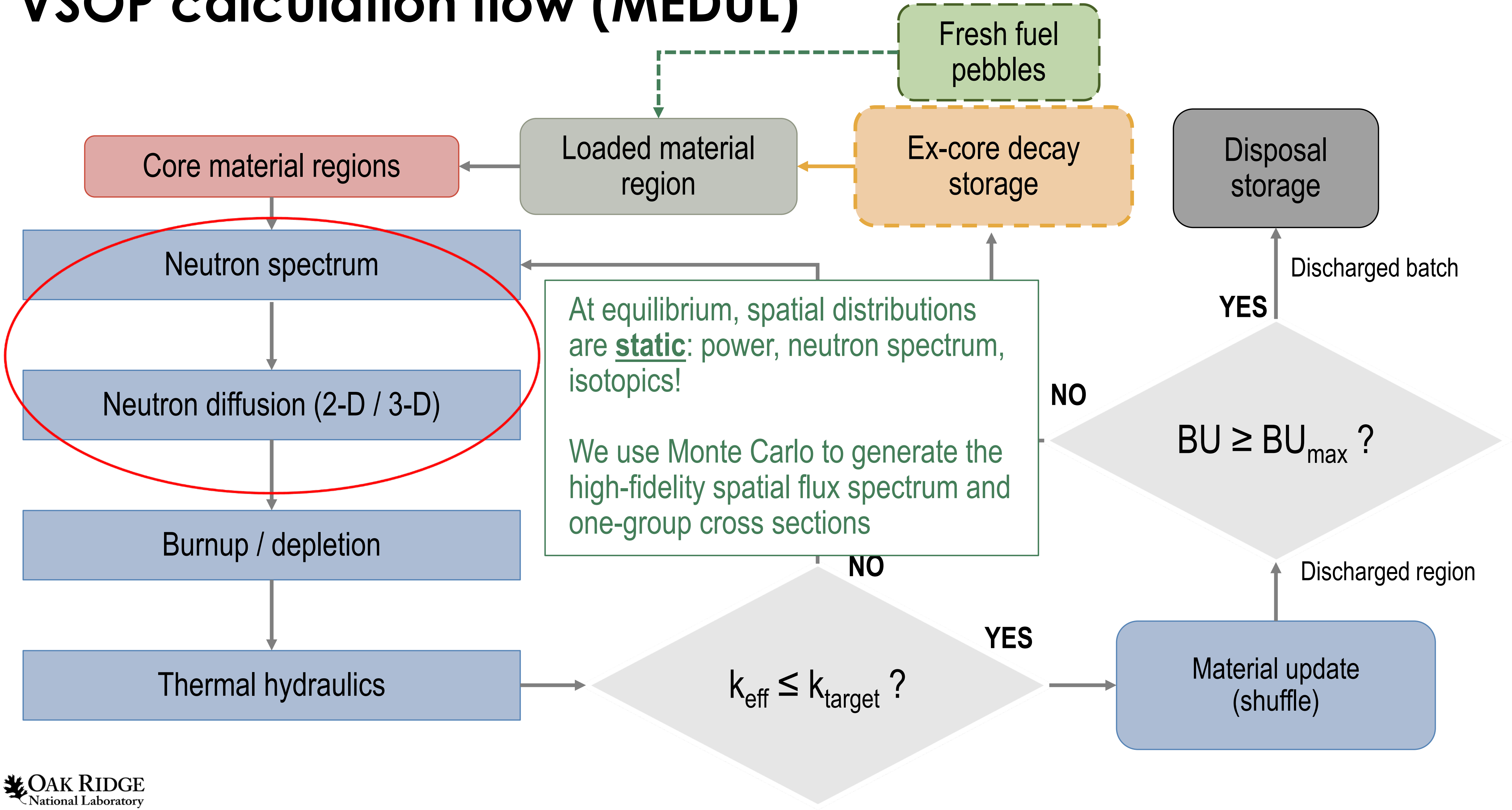
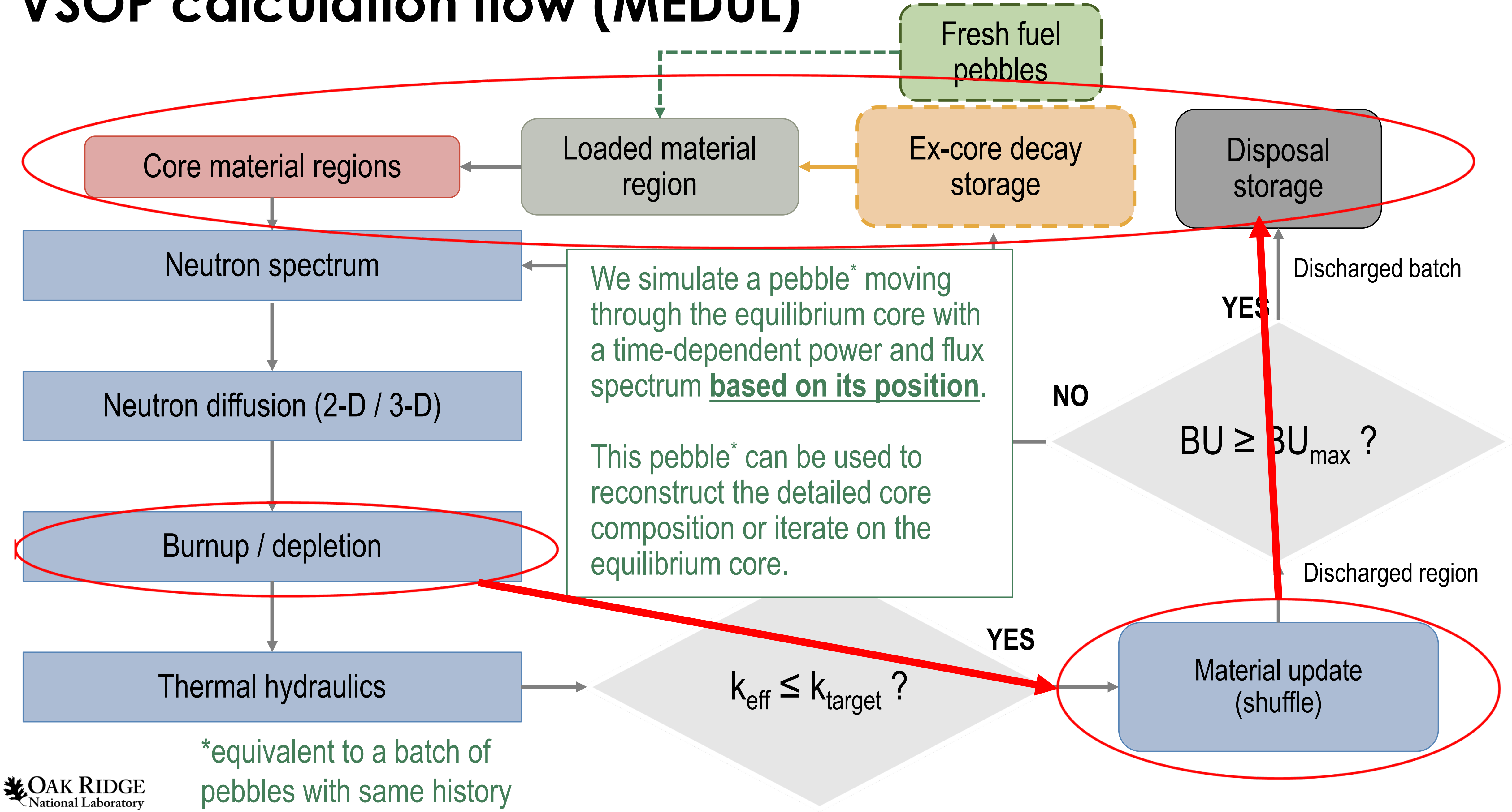



At equilibrium, spatial distributions are **static**: power, neutron spectrum, isotopics!

We use Monte Carlo to generate the high-fidelity spatial flux spectrum and one-group cross sections

# VSOP calculation flow (MEDUL)




We simulate a pebble* moving through the equilibrium core with a time-dependent power and flux spectrum **based on its position**.

This pebble* can be used to reconstruct the detailed core composition or iterate on the equilibrium core.

*equivalent to a batch of pebbles with same history

# Iterative procedure for developing equilibrium core compositions

Determine **average burnup** of each pebble batch within a zone (axial / radial)

Deplete each **batch** within zone to its respective burnup

- Origen library based on region-wise flux from core transport

Average zone compositions

- Weighted sum of batches

Calculate core power distribution & flux shape by zone

- Generate ORIGEN library for each zone

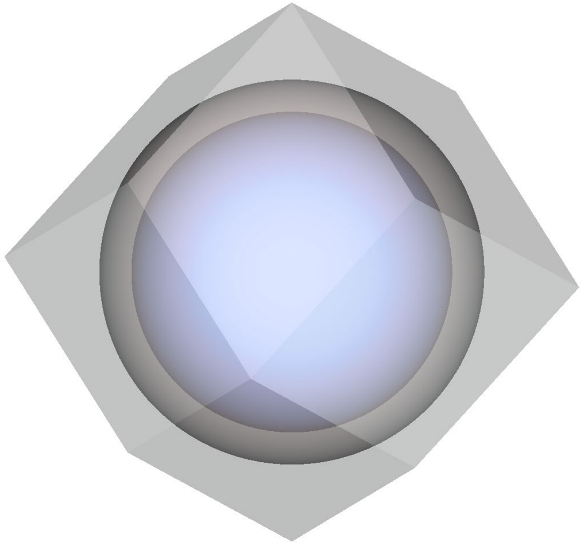
Repeat on initial guess inventories until $k_{eff}$ converges; depleted compositions represent approximate "equilibrium"

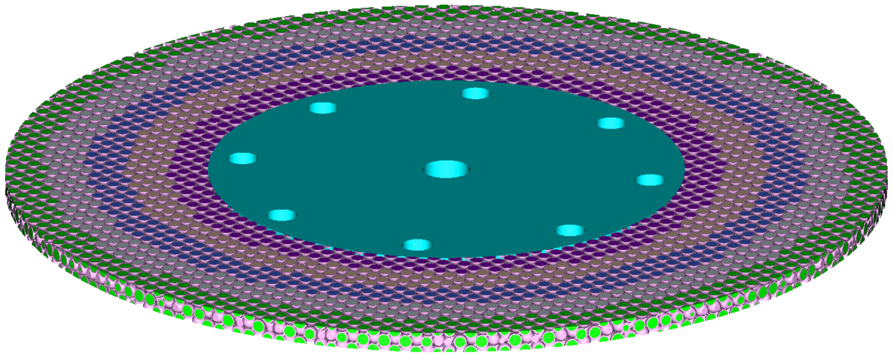
# ORIGEN library analysis strategy

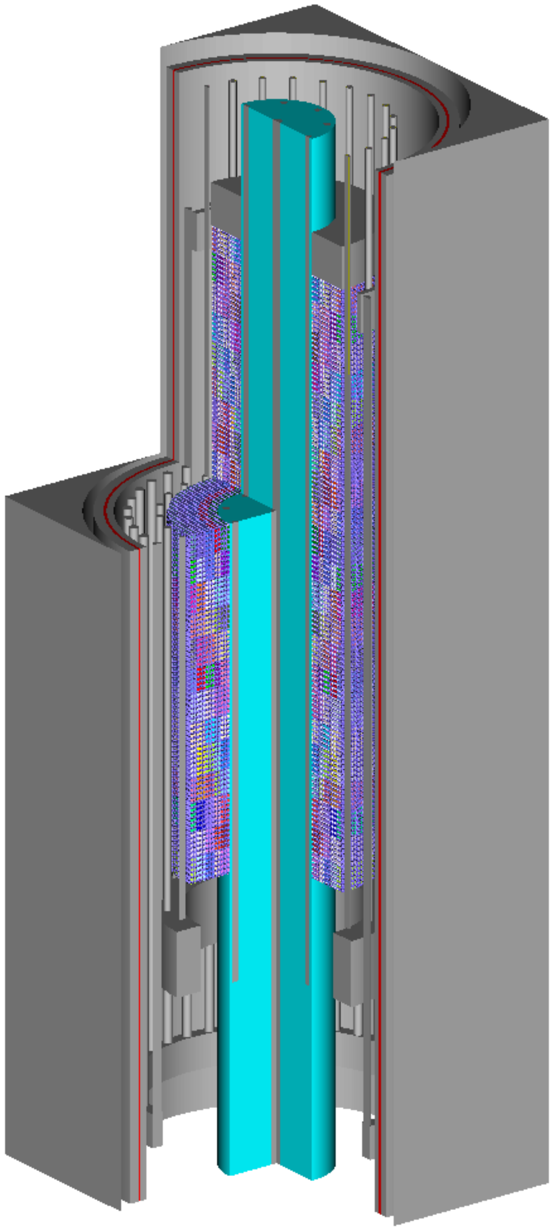
Evaluate PBMR-400 cross-sections & isotopic responses at different levels of model fidelity

Lower fidelity
Lower computational cost

High fidelity
High computational cost









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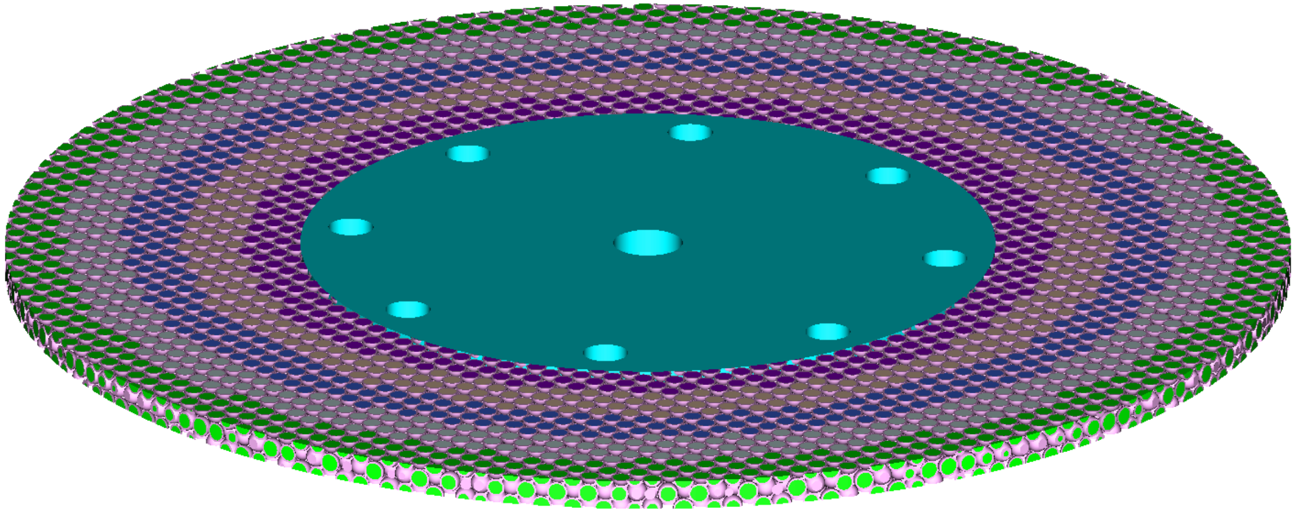
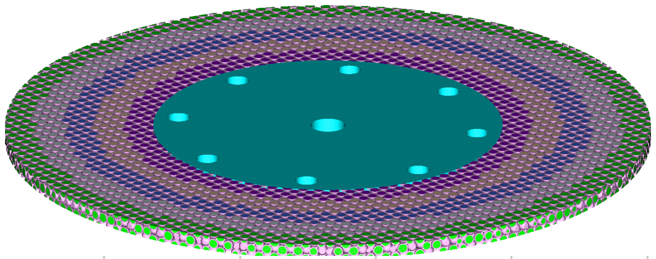
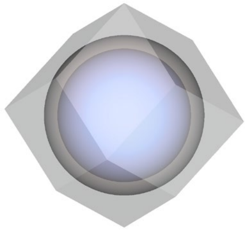
# ORIGEN library development: "reflected plane" model

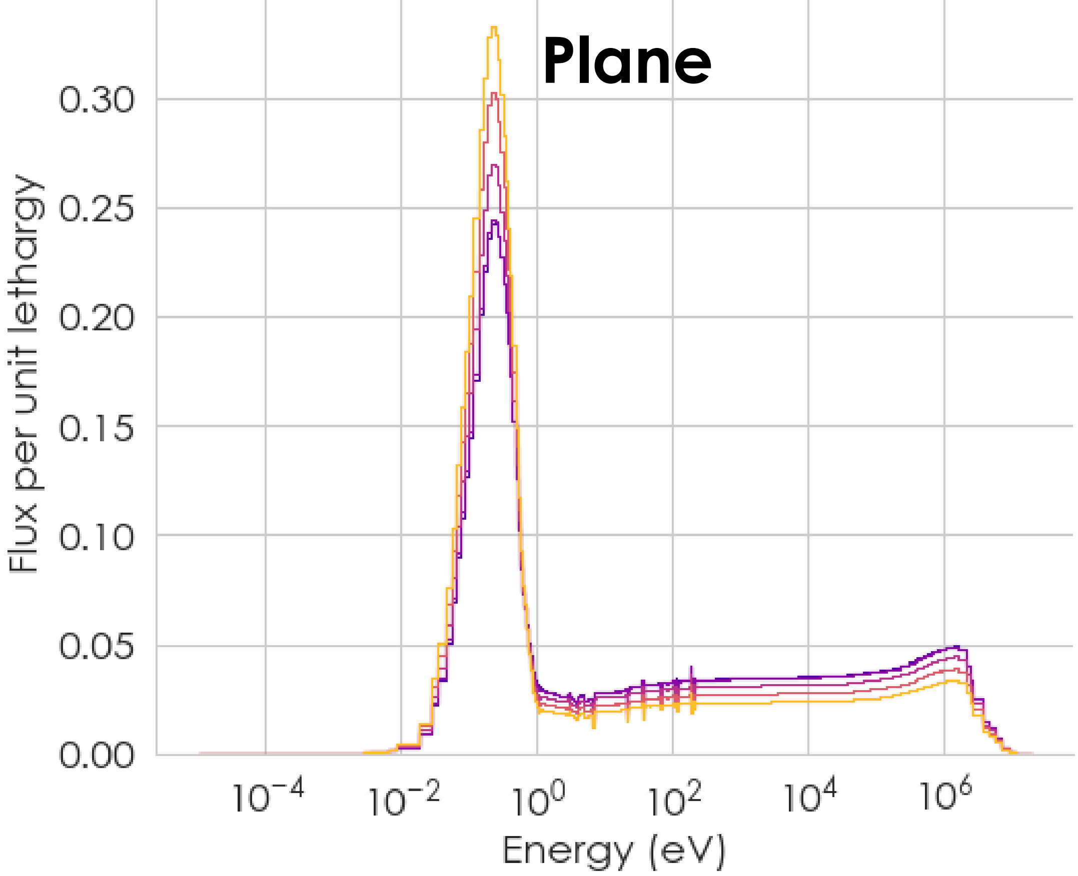
- Accounts for important radial effects
  - Proximity to reflector
  - Effects of nearest neighbor pebbles
- Can easily be tuned for different axial zones

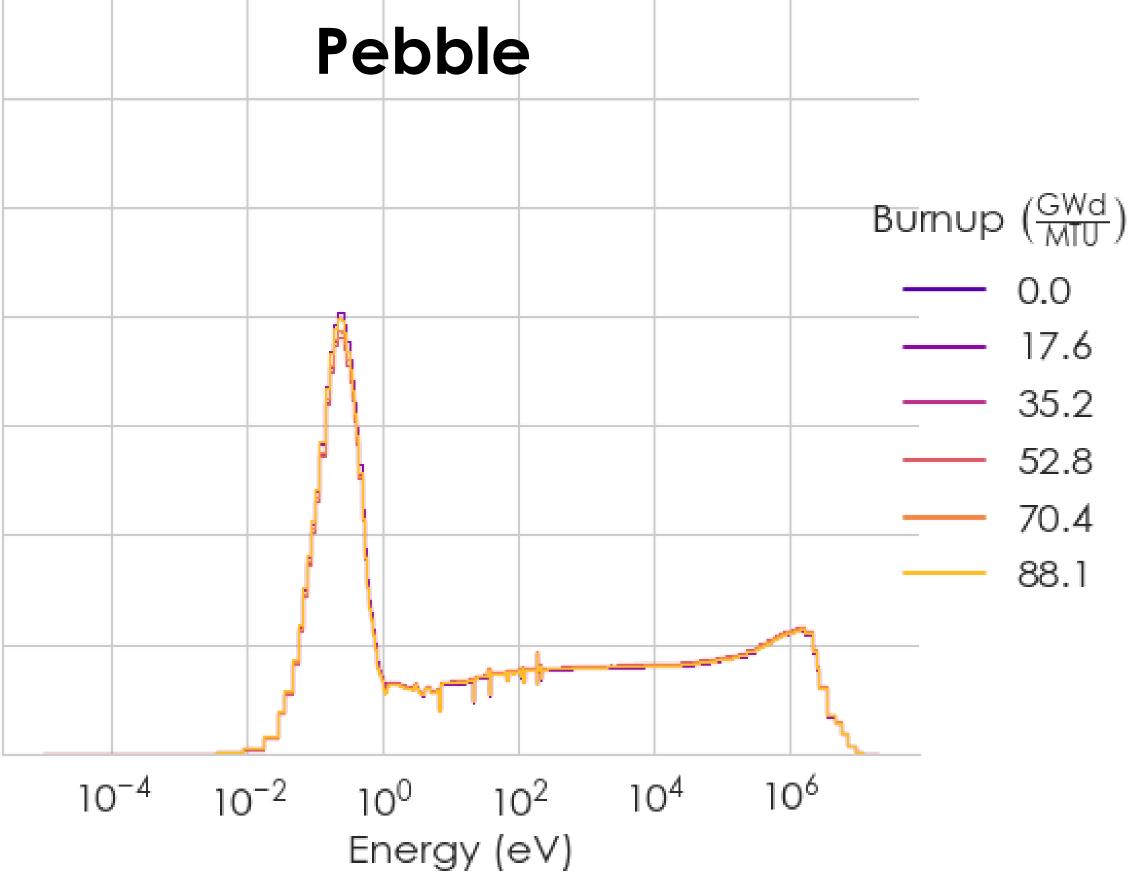


# Plane model captures important neighbor effects





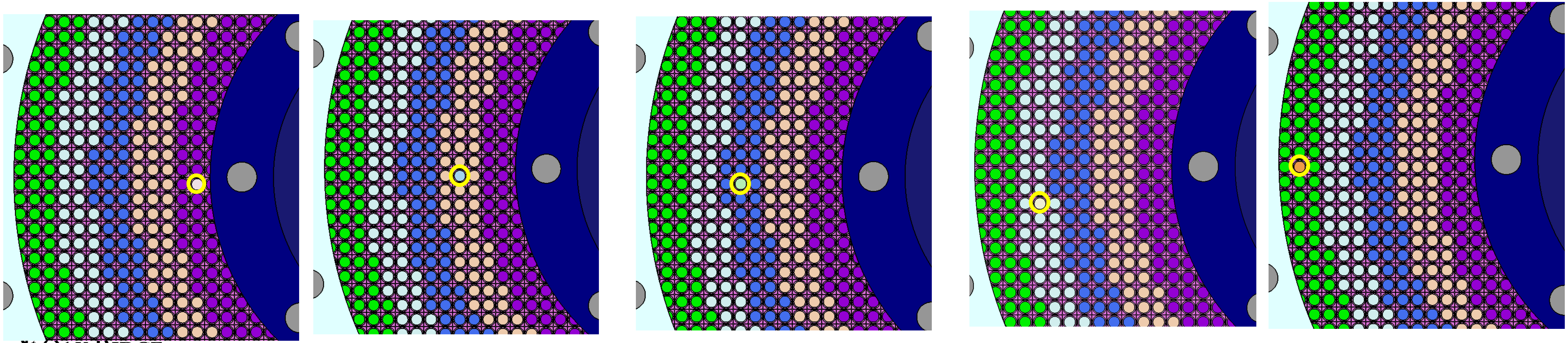


# ORIGEN library generation based on 5 spectral zones

- Five separate cases constructed starting with a fresh pebble surrounded by non-depleting neighbors with compositions derived from PBMR-400 benchmark inventory ND-Set3
- Pebble depleted to discharge burnup surrounded by invariant neighbors

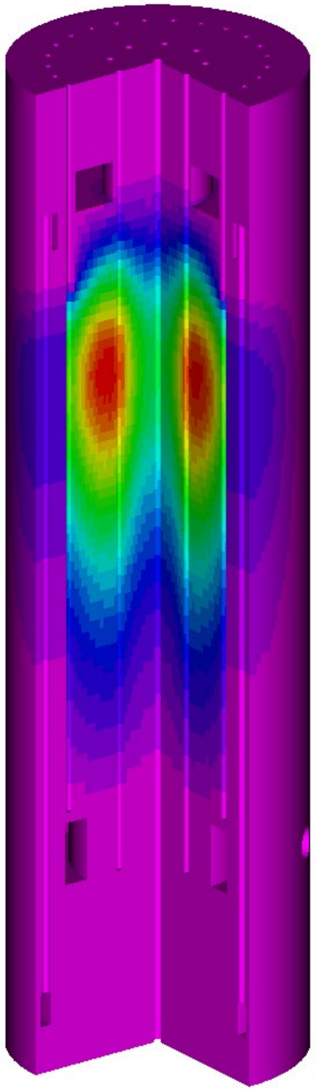
**rzone=1** **rzone=2** **rzone=3** **rzone=4** **rzone=5**



# Physics observations for the PBMR-400 core

# Temperature feedback (1/2)

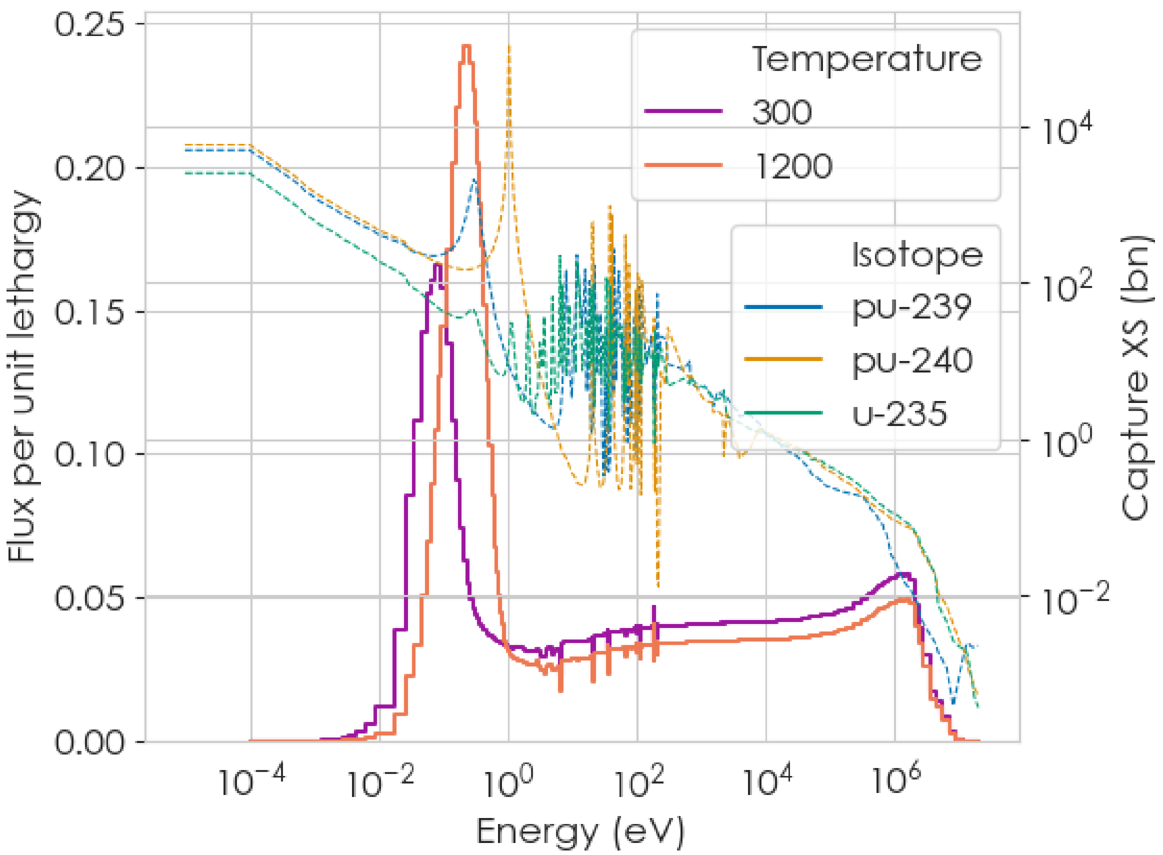
- Estimation of specific reactivity feedback components (e.g., temperature reactivity coefficients of fuel, moderator) requires detailed thermal hydraulic analysis of core
- **Strong coupling** between neutronics & thermal hydraulics
- **Approach:** Using system isotherms
  - All system materials adjusted to a fixed temperature
    - e.g., 300, 600, 900, 1200 K
  - Does not afford specific isolation of moderator / fuel temperature coefficients



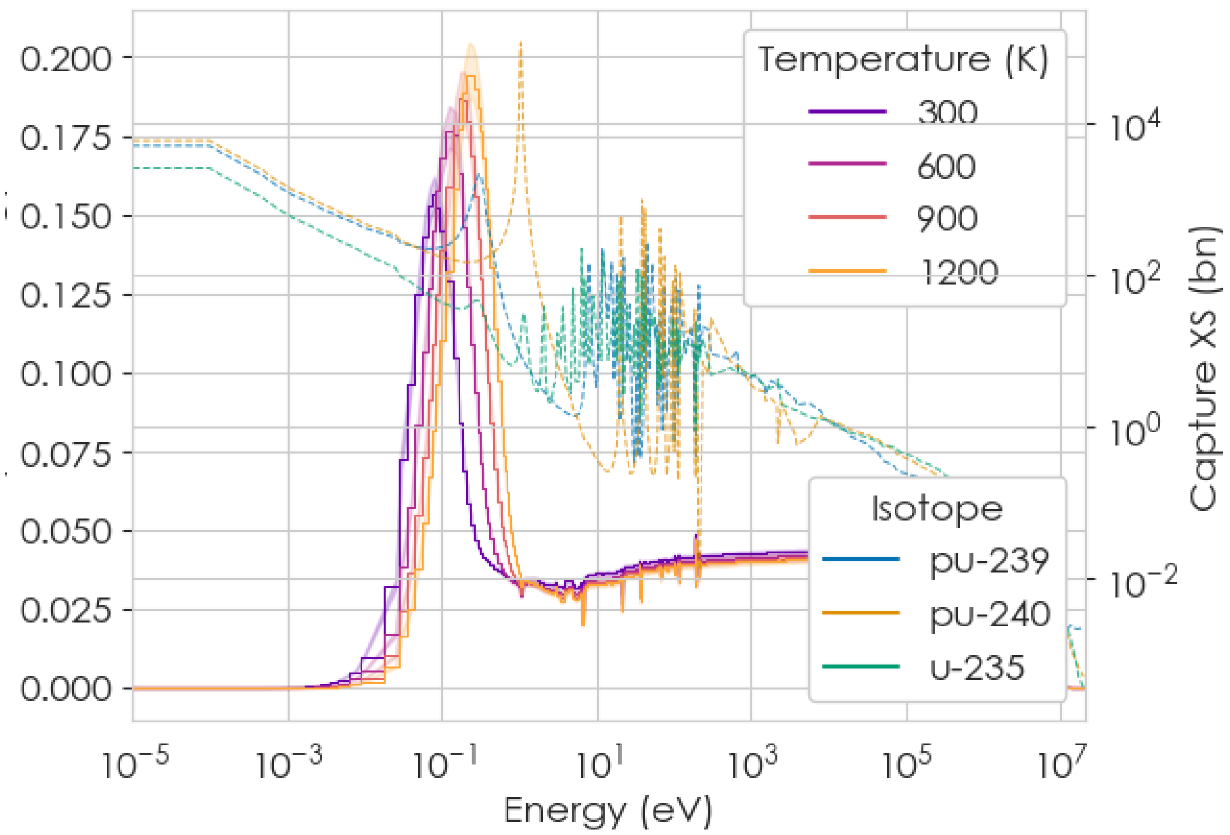
PBMR-400 total neutron flux, from SCALE/Shift 3D Monte Carlo Calculation

# Temperature feedback (2/2)

**Fresh core**

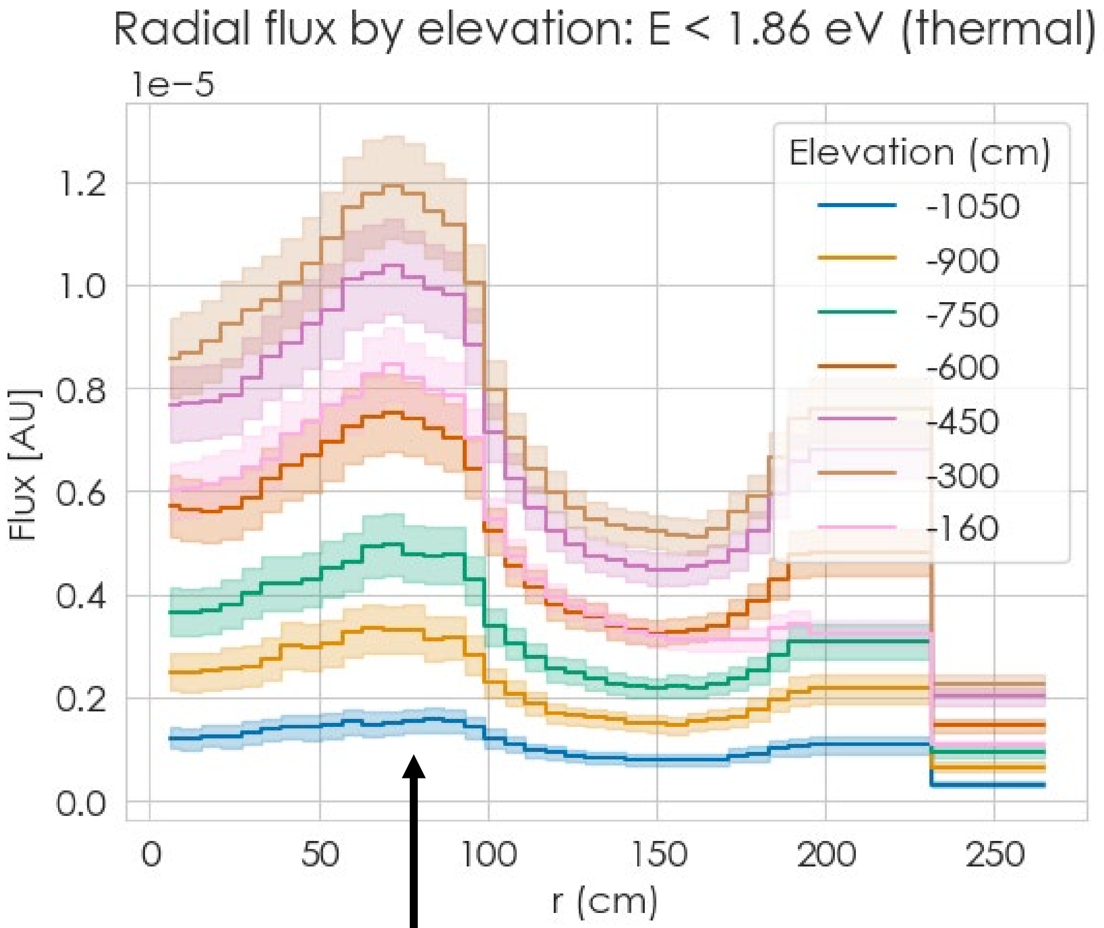


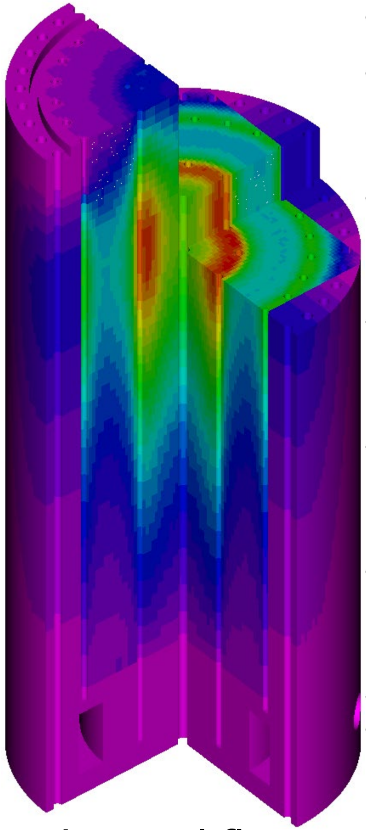

**Equilibrium core**



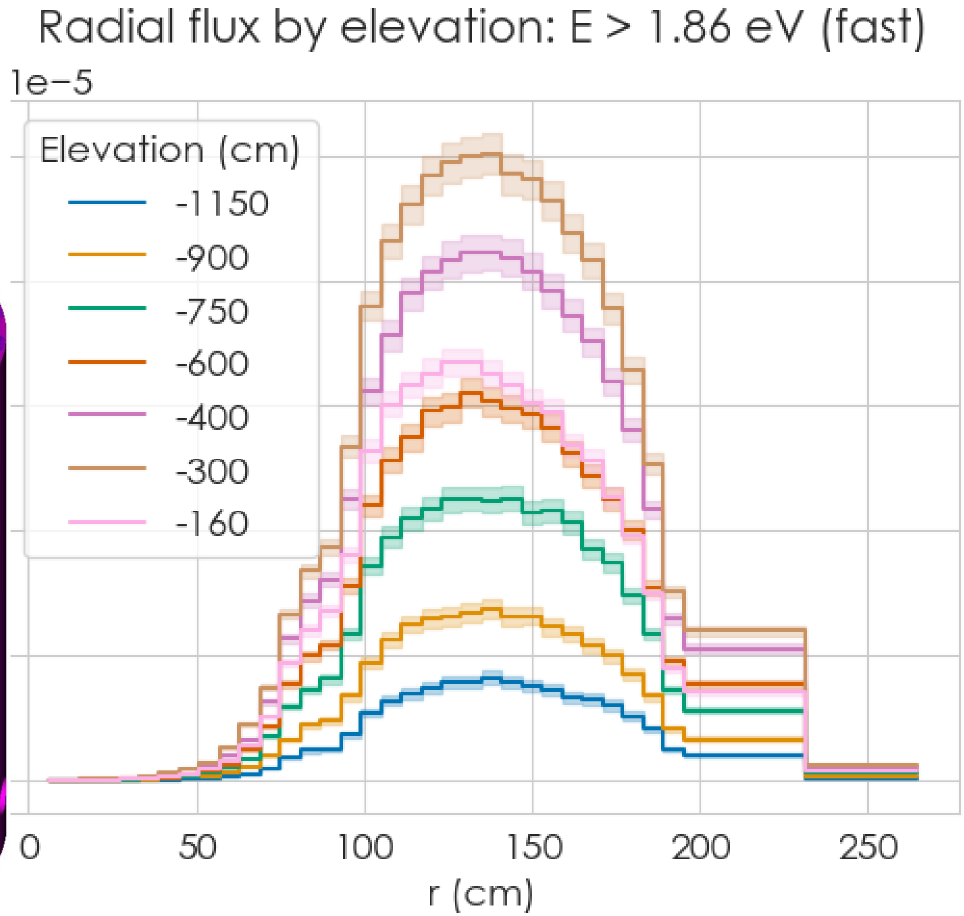

Strong temperature-driven spectral shifts, especially toward $^{239}$Pu low-lying resonance

# Flux shape shows a top-weighted distribution due to pebble loading & depletion



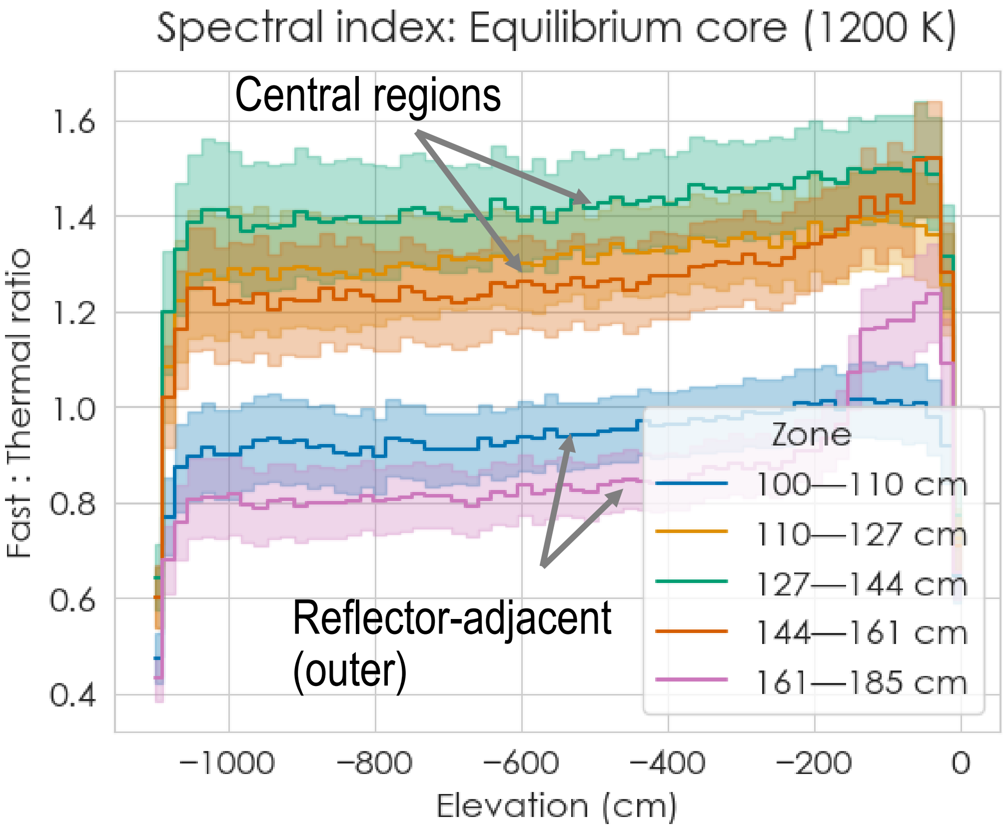
thermal flux



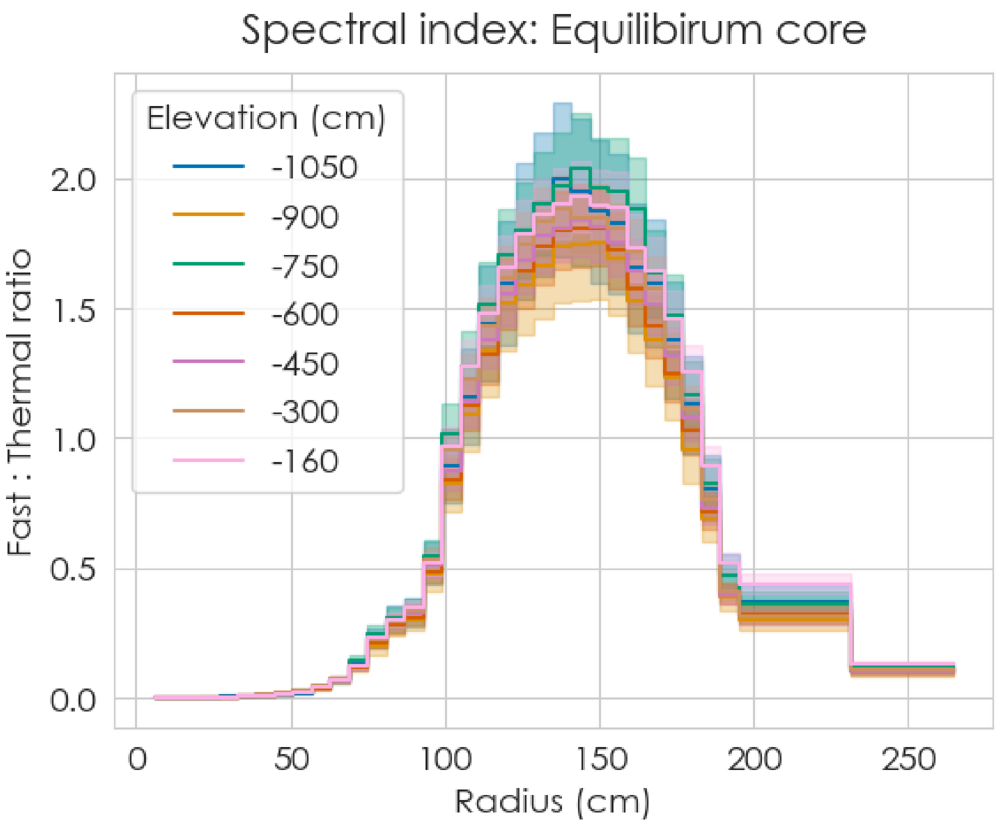

Strong power peaking effects observed near graphite reflector regions (esp. interior)

# Fast : thermal flux ratio (spectral index) sensitive to radial zone; relatively invariant axially

## Axial

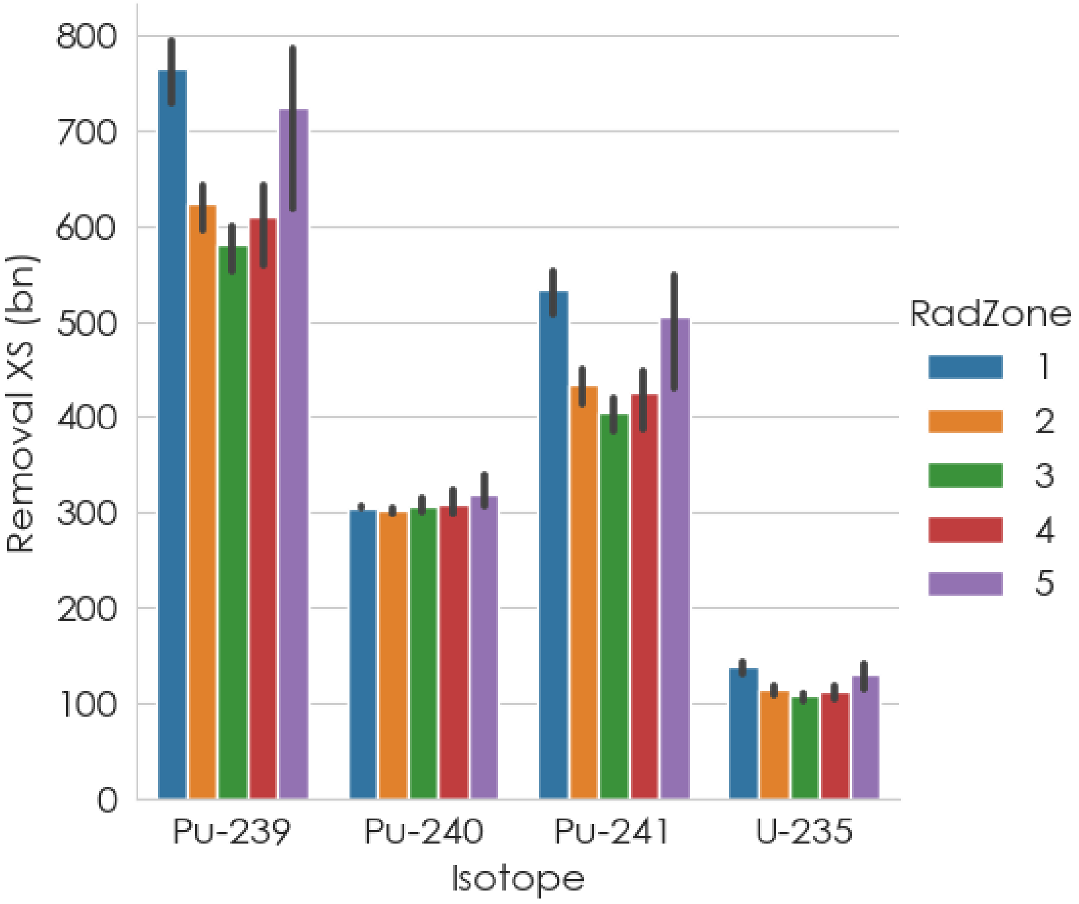


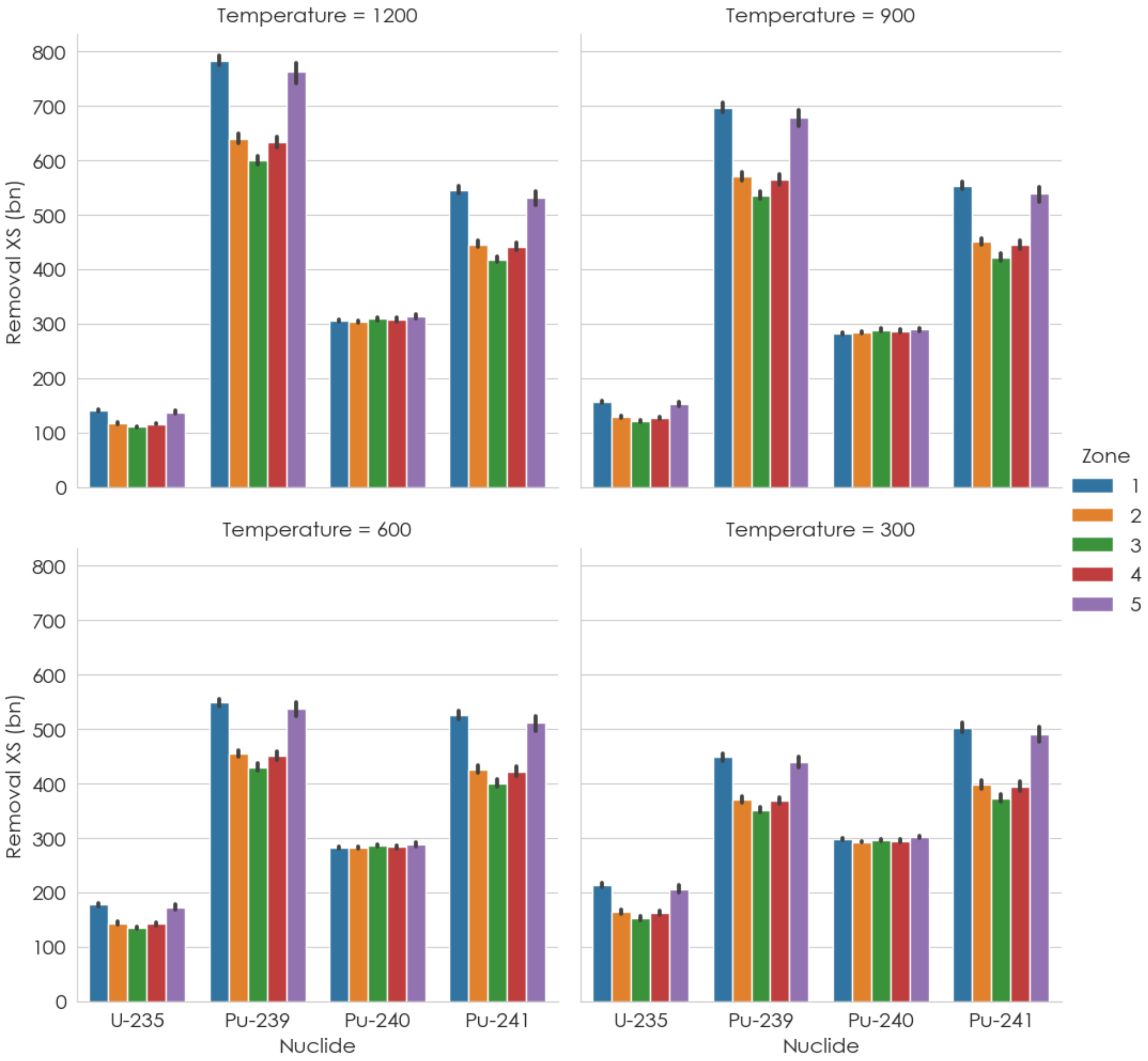

## Radial




Major spectral shifts primarily occur across **radial** zones; i.e., primarily need **radial** zone Origen libraries

# Radial, temperature effects drive differences in ORIGEN library 1-group cross-sections





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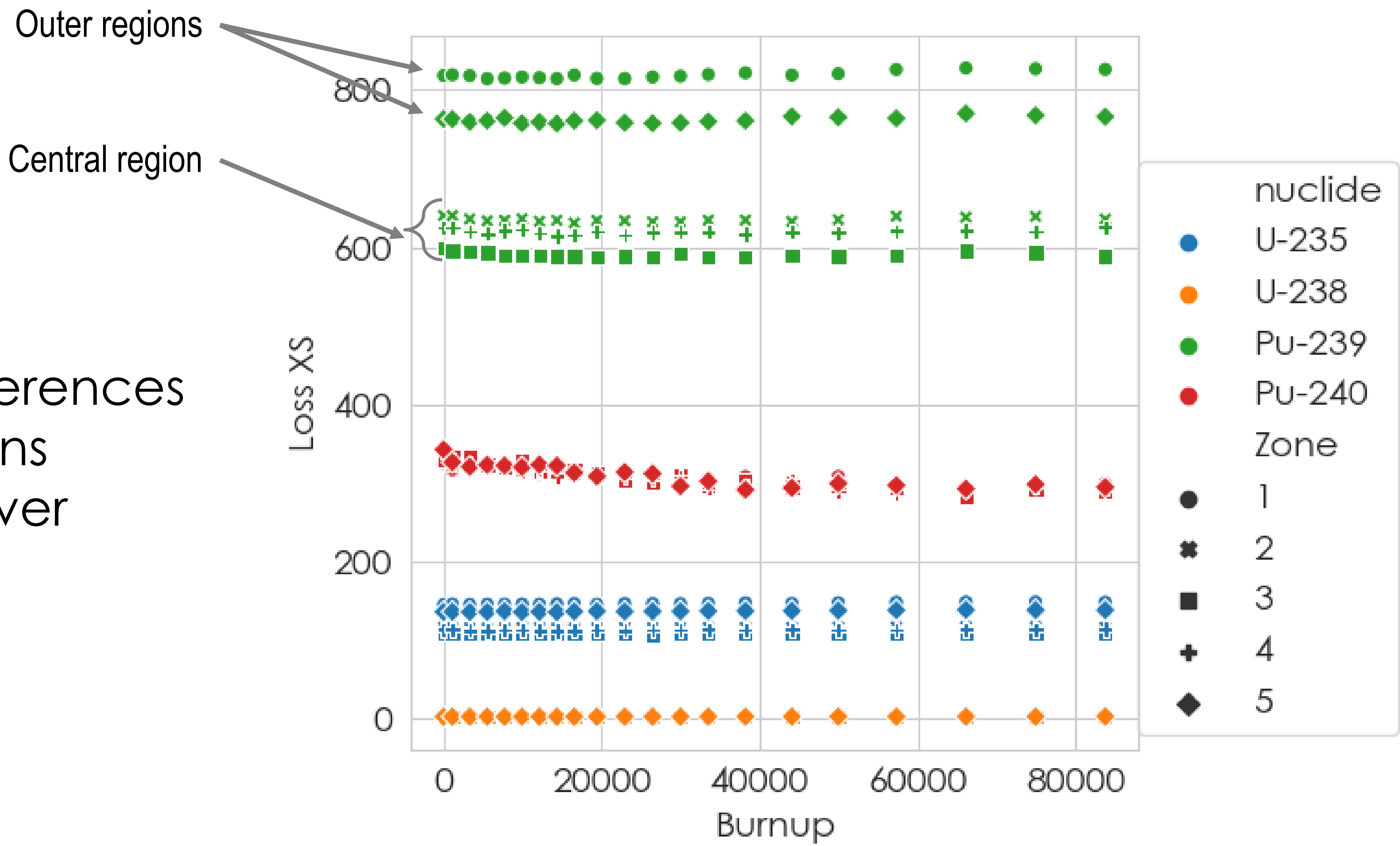
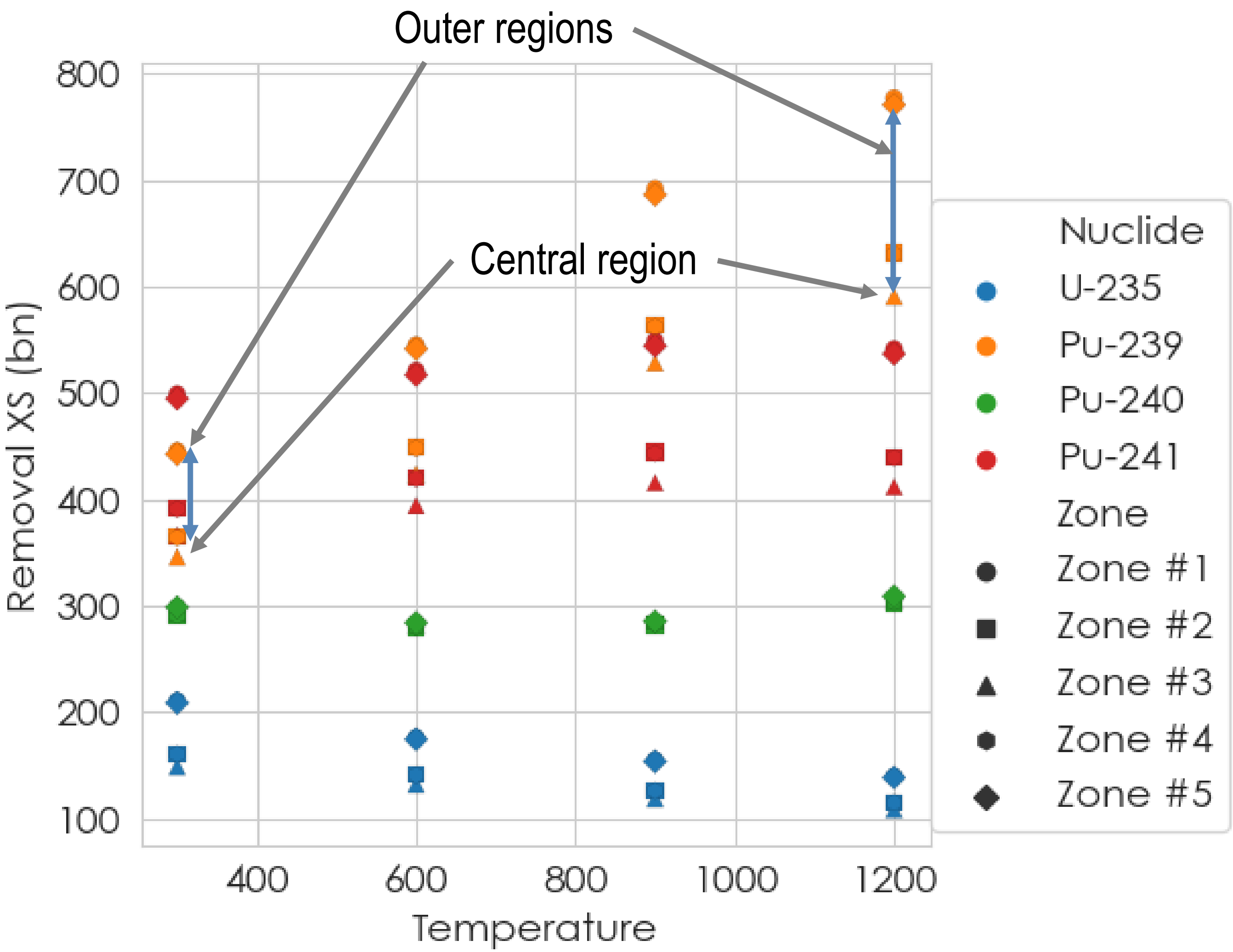
# Radial zone effects far more prevalent than burnup effects for pebble bed depletion

Spatial-driven differences in loss cross-sections relatively stable over burnup



# Temperature (system isotherm) shows a large, region-dependent effect on 1G removal XS

- Magnitude of XS differences due to radial location **increases with system temperature**
  - Gap between “inner” and “outer” regions grows with increasing temperature
  - Implies a covariant relationship between location & temperature





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# Conclusions

# Conclusions for pebble bed reactor ORIGEN library development

- Modeling pebble-based cores in SCALE
  - Mature cross-section processing capabilities for doubly-heterogeneous systems
  - Derive ORIGEN depletion libraries from spectral characteristics of the equilibrium core
    - Known “a priori“ or iteratively derived

**Further details:**
S. Skutnik, W. Wieselquist, “Assessment of ORIGEN Reactor Library Development for Pebble-Bed Reactors Based on the PBMR-400 Benchmark,” ORNL/TM-2020/1886, July 2021
*Available on osti.gov*

- For ORIGEN library generation
  - Burnup effects appear to be second-order, roughly linear in nature
  - Radial distance from the reflector is a first-order spectrum characteristic
    - Must be accounted for in library generation
  - Temperature (system isotherm) also a first-order effect
    - Shows covariance with radial position
    - Driven primarily by graphite (reflector) temperature