Knolls Atomic Power Laboratory

MC21

BETTIS LABORATORY

Integrated Decay Source Capability for Large-Scale Monte Carlo Radiation Transport Calculations

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Motivation

- Many types of transport analyses used a source-term based on the decay of radionuclides
  - Shutdown reactor shielding, detector response, and decay heat
- Transport solvers must model spatial and energy distribution of decay source
  - Many MC codes require user-defined decay source definitions.
    - Even with scripts, defining sources can be tedious
  - Other MC codes include built-in decay energy spectra but are targeted towards localized activation calculations
    - Not well suited for large-scale reactor calculations

Overview

- Describe a new method for sampling decay radiation in continuous-energy MC calculations.
  - New method accounts for the spatial and energy distribution of decay radiation
    - uses composition information from the MC model, along with ENDF-format decay data
  - Able to handle models with many radioactive nuclides distributed among large numbers of compositions.
    - Such as depleting 3-D models of nuclear reactors
  - This talk will describe the data processing and sampling algorithms and provide numerical results.

Decay Data

- ENDF-Format Decay Data
  - Sub-library 4, File 8, MT=457
  - Includes decay constant, branching fractions, radiation yield(s), and energy spectra for decay radiation.
    - ENDF/B-VII.1 – data for 3817 nuclides (1988 with spectra)
    - JEFF-3.1.1 – data for 3852 nuclides (1521 with spectra)
    - Secondary spectra may be discrete or continuous.
  - Data available for multiple secondary radiations
    - Gamma rays, x-rays, neutrons, alpha, etc.
  - Data available for a variety of decay modes
    - β^-, EC/β^+, internal transition, spontaneous fission

Decay Data Processing

- Reorganize data to facilitate decay source sampling
  - Secondary distributions converted to ACE law 4 format.
  - Yield and energy release separated into 3 categories
    - Neutron, photon, charged particle (local energy deposition)
- Complications arise when processing data
  - Accounting for compound decay modes (e.g., (β^-,n))
    - Single emission spectrum does not distinguish between multiple decay sequences for a single decay mode.
  - Ensuring conservation of energy
    - Overall energy release values for some decay modes do not agree with averages computed from the secondary energy spectra.

Decay Data Processing (II)

- Complications arise when processing data (continued)
  - Quality of the decay data
    - Some data set are incomplete or inconsistent with other references
    - ENDF/B-VII.1 uses continuous spectrum representation for ~30 nuclides (e.g., ^{87}Br) when discrete data is given by other references such as ENSDF and the Table of Isotopes.
    - ENDF/B-VII.1 only includes spontaneous fission spectra for ^{252}Cf. JEFF-3.1.1 provided spontaneous fission neutron and photon spectrum for most transuranics.

- Additional details and observations in full paper

Sampling Algorithm

- During MC simulation, initial position, energy, and direction of decay radiation is sampled
  - Based on relative concentration of radionuclides by composition and decay properties of the radionuclides
  - Decay source algorithm uses sequential approach for sampling decay-radiation state using conditional probabilities
    - Sample radiation type based on total activity by type.
    - Sample position based on composition activity for rad. Type.
    - Sample decay nuclide based on selected composition
    - Sample decay mode based on selected decay nuclide
    - Sample energy and direction based on selected decay mode

Radiation Type Sampling

- For radiation type t, the decay emission rate in each composition c is

$$A_{t,c} = V_c \cdot \sum_{i=1}^{M_c} N_{c,i}\, \lambda_i\, y_{t,i},$$

A = Activity (particles/sec)
V = Volume
N = Number density

M = Num. Radionuclides
λ = Decay constant
y = Decay yield

- Relative probability that a decay source particle will be emitted with type t

$$p_t = \frac{A_t}{A_{\text{total}}} = \frac{\sum_{c'=1}^{C} A_{t,c'}}{\sum_{t} \sum_{c'=1}^{C} A_{t,c'}}.$$

- Sample t based on p_t
  - If decay source is combined with other (fixed) sources, an additional sampling step is required to determine the source type

Composition Sampling

- Birth location (and composition) is determined using rejection sampling.
  - Candidate birth positions are sampled uniformly over the volume containing all decay sources
  - The composition number, c, is determined for the candidate position and used to determine the composition activity $A_{t,c}$
  - Candidate position is randomly accepted with probability equal to the relative activity for the composition.

$$p_{t,c}^{\text{reject}} = 1 - \frac{A_{t,c}/V_c}{\max_{c'}\left(A_{t,c'}/V_{c'}\right)},$$

$\max_{c'}\left(A_{t,c'}/V_{c'}\right)$ is the maximum decay emission rate density over all compositions

  - Rejected birth positions are resampled from the uniform volumetric distribution.

Nuclide/Decay Mode Sampling

- Once a birth location has been sampled, the parent nuclide is sampled in proportion to the relative emission rate for all nuclides in the sampled composition

$$p_{t,i} = \frac{N_{c,i}\,\lambda_i\,y_{t,i}}{\sum_{i'=1}^{M_c} N_{c,i'}\,\lambda_{i'}\,y_{t,i'}}$$

- Similarly, decay mode is sampled in proportion to the relative emission rate for each mode that emits the given radiation type

$$p_{t,m} = \frac{y_{t,i,m}}{\sum_{m'=1}^{M_i} y_{t,i,m'}}$$

Note that the radiation yield value, y, includes the mode branching fraction

Energy/Direction Sampling

- Once location, nuclide, and decay mode have been determined, the energy and direction of the source particle are set.
  - Birth energy is sampled from the LAW 4 secondary energy distribution.
    - Uses existing sampling routines for MC code
  - Source direction is sampled isotropically

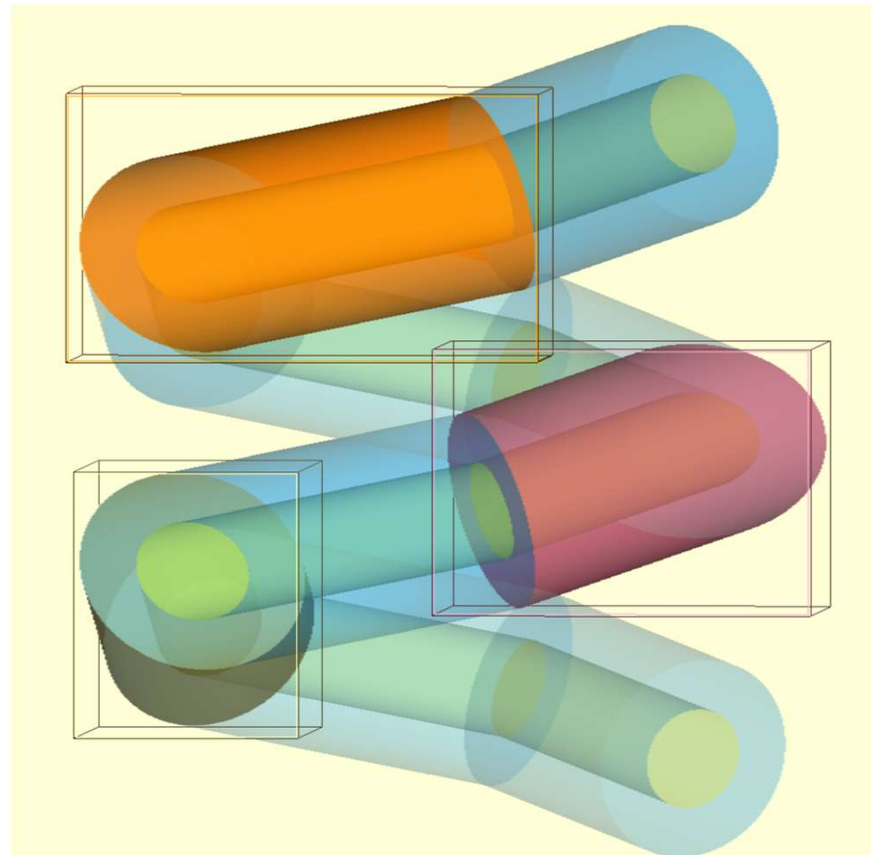
Implementation and Testing

- Integrated decay source capability was implemented in MC21
  - Continuous-energy MC radiation transport code
  - Processing of raw ENDF-format decay data performed by NDEX, an in-house data processing code

- Method was tested on two types of realistic calculations involving decay sources
  - Activated coolant pipe shielding example
  - PWR decay heating example

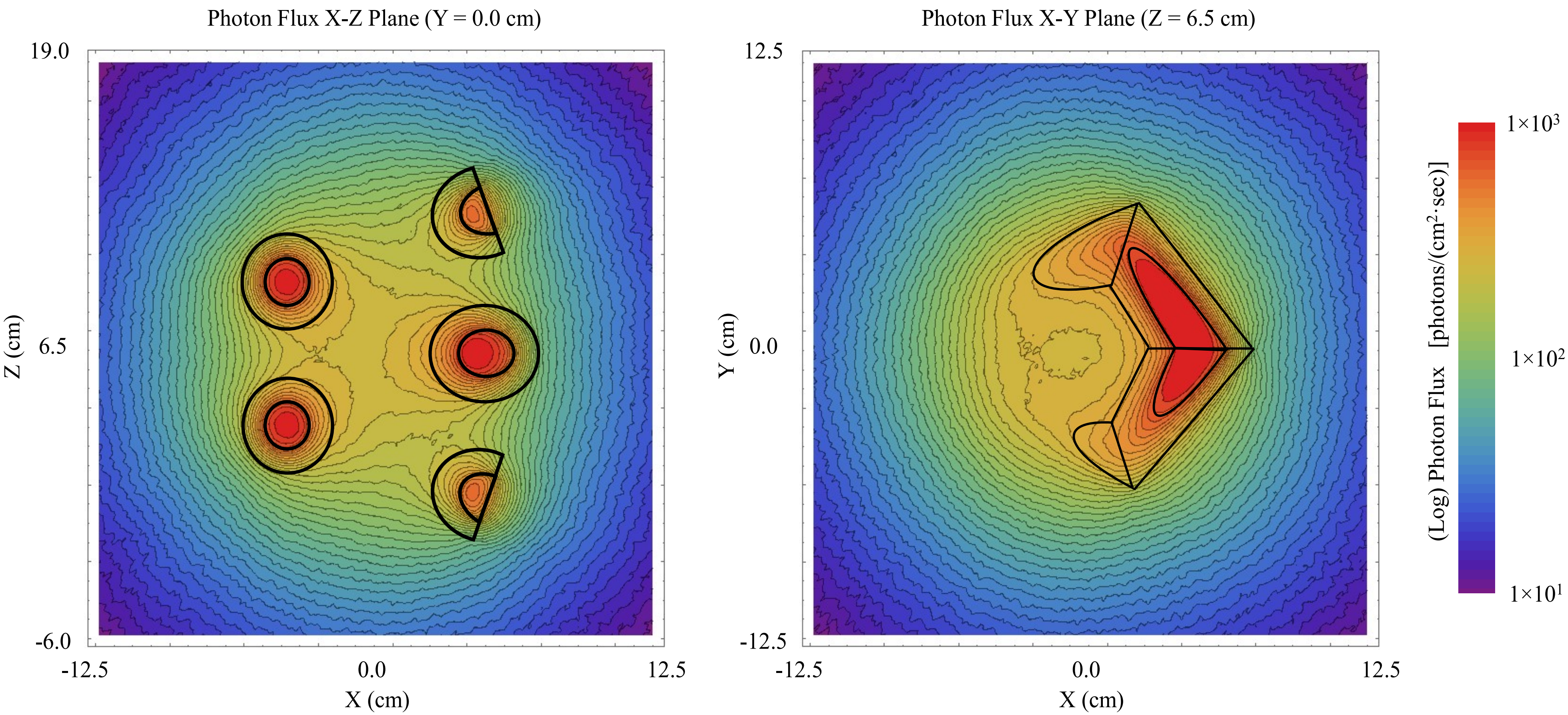
Activated Coolant in Pipe

- Helical 4 cm diameter steel pipe filled with water, with
  - ^{16}N: 3.5×10^6 Bq/cm^3
  - ^{17}N: 150 Bq/cm^3
  - Similar to levels seen in commercial LWRs
- Tedious to manually define source distribution
- With new decay source, simply add ^{16}N and ^{17}N to the water compositions
  - No additional input required



Activated Coolant Photon Flux

Photon flux from ^{16}N decay using 1×10^8 source histories

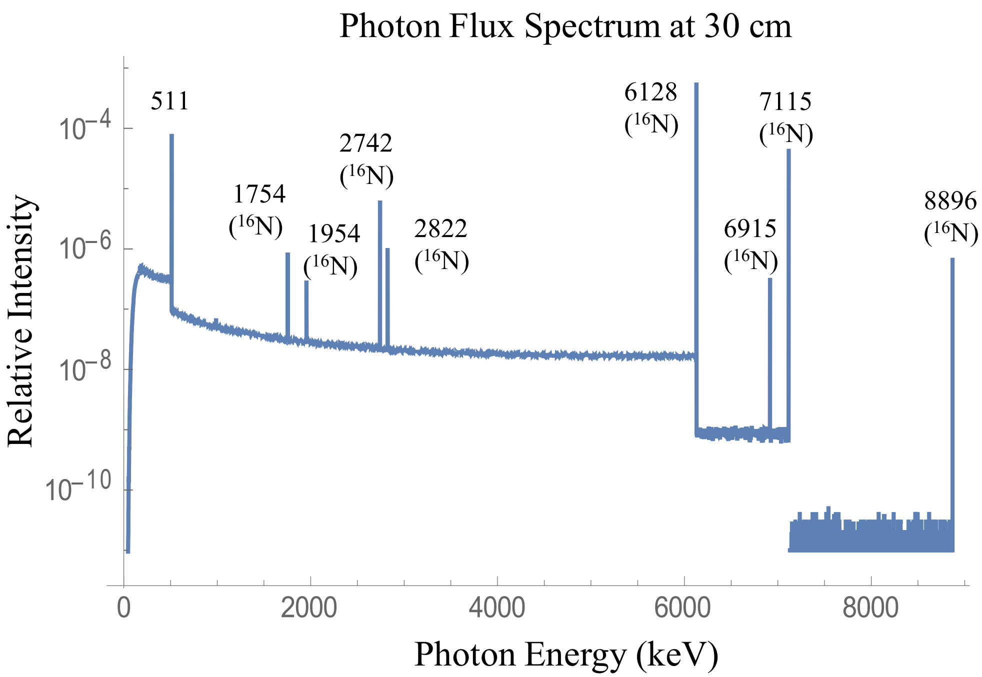


- Material attenuation through pipe wall and geometric attenuation in air.

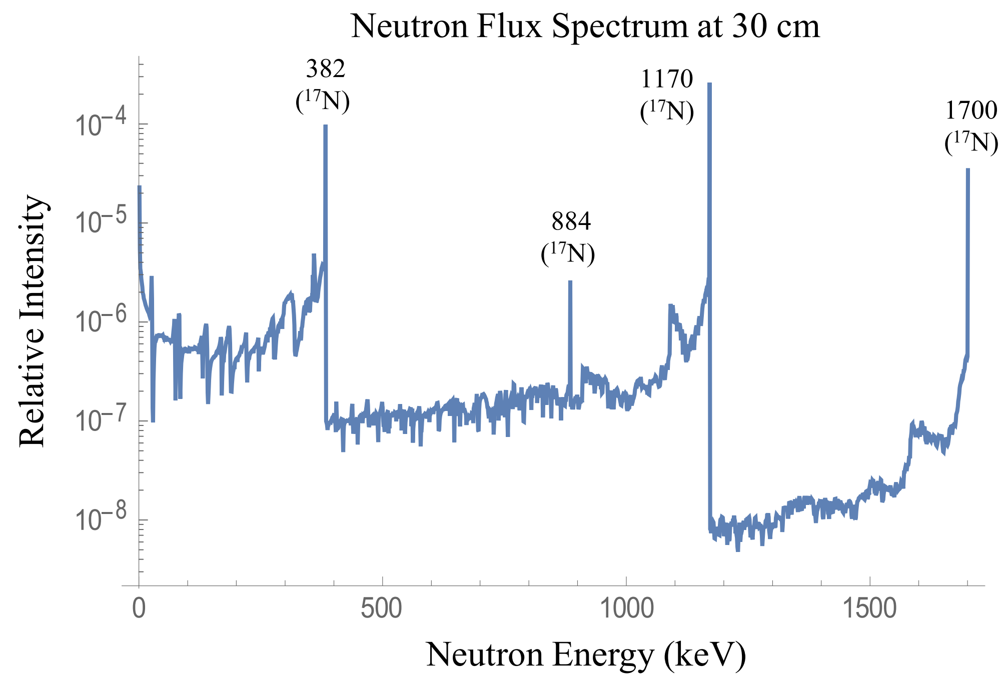
Activated Coolant Decay Spectrum

Decay Source Spectrum 30cm from Center of the Pipe

Photon



Neutron

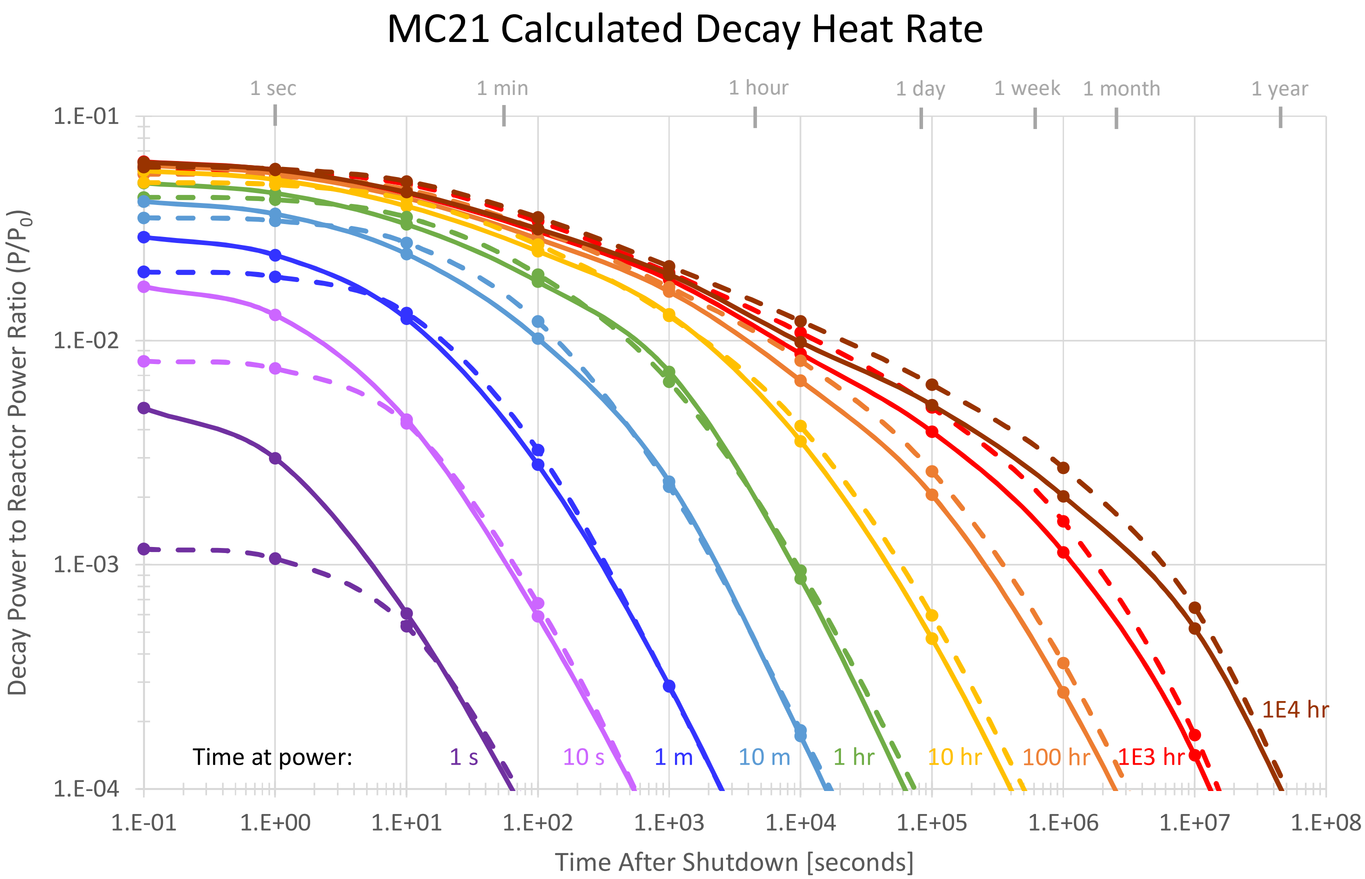


- Emission lines correspond to ^{16}N and ^{17}N.

Decay Heat – Pin Cell

- MC21 was used to test the decay power of a PWR unit-cell as a function of irradiation time and shutdown time.
- Unit-cell is based on H.B. Robinson fuel element spec.
  - Reflecting boundary conditions used to create an infinite lattice.
  - 1351 depletable nuclides in fuel (1169 with xs or decay data)
- Cell was depleted at power density of 30 MW/MTU
  - For periods of 1 second to 10,000 hours (1.14 years)
  - MC transport: 120 batches (20 discard) of 15,000 histories
- Shutdown depletion calculations following at-power calc.
  - 9 zero power depletions, from 0.1 seconds to 3.17 years shutdown
  - All calculations used built-in MC21 (BDF) depletion solver

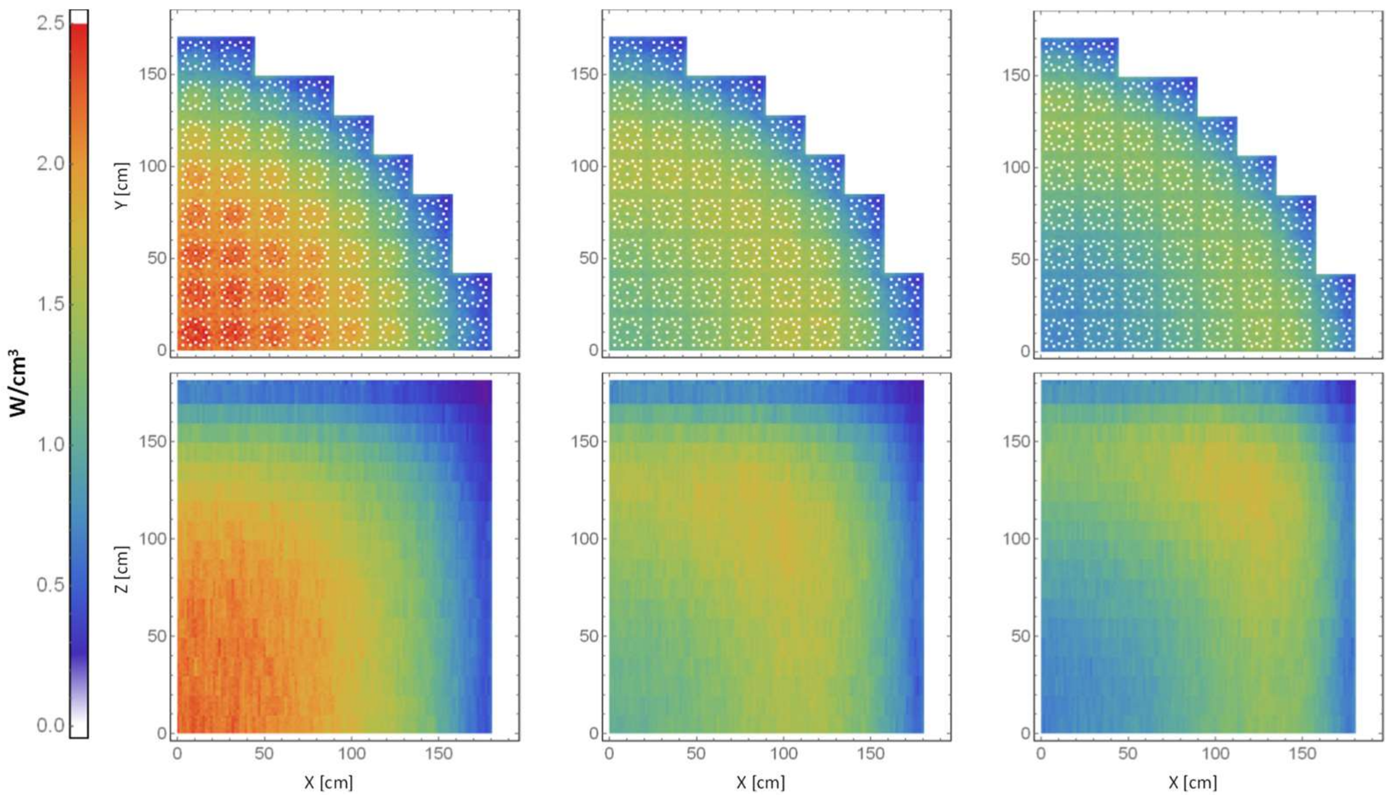
Decay Heat – Pin Cell (Results)



- Decay heating results are compared with an empirical correlation from Todreas and Kazimi
  - Including both fission product and activation products
- MC21 results agree well for shutdown times > 10 seconds
  - MC21 overpredicts decay heat for at-power times less than 1 minute

- Average run time on 224 processors:
  - 1.25 minutes for MC radiation transport
  - 0.1 – 0.2 seconds per depletion calculation

Decay Heat – 1/8 Core

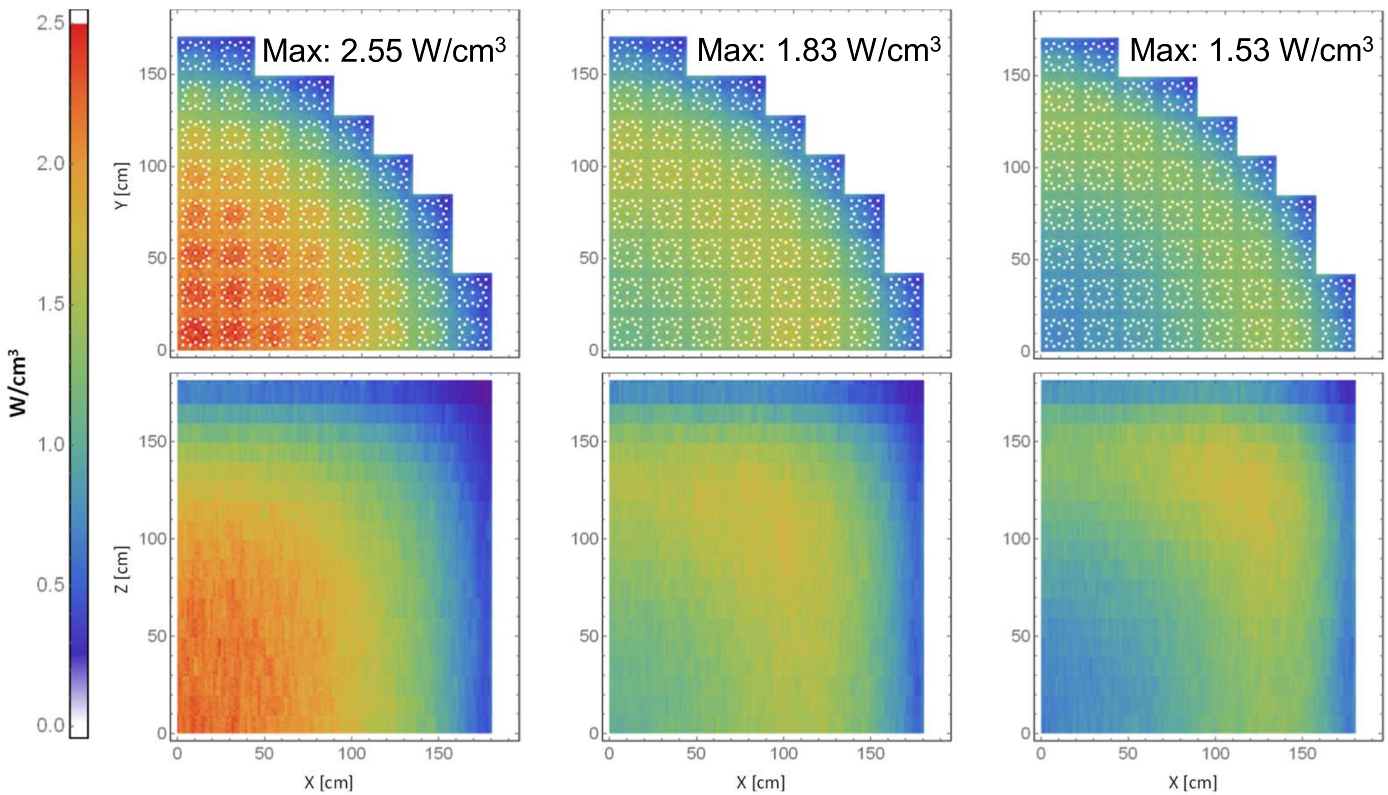


a) 5,844 power hours b) 11,688 power hours c) 15,432 power hours

- 3D H.B. Robinson PWR Model
  - ¼ core radial
  - ½ core axial
  - 192,888 unique depletable comps.
  - 1,169 nuclides in each composition.
  - 11.32 GB/node
- Running Strategy
  - 328 MW power
  - 3 operating cycles
  - 22 depletion steps
    - 16 at power
    - 6 shutdown

- 600 batches (100 discard) of 100,000 neutrons each.
- ~1 hour per at-power timestep on 384 processors.

Decay Heat – 1/8 Core (II)



a) 5,844 power hours
b) 11,688 power hours
c) 15,432 power hours

- Decay heat density at radial (z = 0) and axial (y = 0) core mid-plane 1 hour after shutdown for each cycle.

- Cycle 1
  - Decay heat is highly peaked in the center of the core
- Cycles 2-3
  - Decay heat moves upward and outward in core.
  - Peak local heating density decreases through life.
- Total decay heat remains constant over all cycles
  - 4.23±0.27 MW

Conclusions

- An integrated decay source capability for continuous-energy MC has been developed and tested on several realistic models.
- Decay source method uses:
  - Rejection sampling based on nuclide inventories to generate decay emission sites.
  - Radiation energies sampled from nuclide and decay-mode specific distributions in the ENDF decay sub-libraries.
- Method produces decay source as accurate as the underlying nuclide inventories and decay data.
  - Eliminates the need to generate decay sources by hand or with an external script, simplifying shielding, spectroscopy, and shutdown source calculations.

QUESTIONS?