Recoverable Energy per Fission Discrepancies in NEA FHR Benchmark Depletion Studies

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Background

- Renewed interest in molten salt coolants in push for Generation IV reactors

- Lack of experimental and reactor physics data related to molten salt *cooled* reactors motivates code-to-code V&V and benchmarking

- NEA Benchmark exercise created to improve confidence in modelling reactor physics of advanced systems and obtaining data for V&V purposes

FHR Benchmark Overview

- Voluntary benchmark under the NEA Nuclear Science Committee covering a plate-type Fluoride-salt High Temperature Reactor (FHR)

ID	Organization	Participants	Method	Code	Library	Energy structure
CVREZ	Research Centre Rez, Czech Republic	Evžen Losa	MC	SERPENT2	ENDF/B-VII.0	CE
GT ANL	Georgia Institute of Technology, USA Argonne National Laboratory	Bojan Petrovic Jonathon Faulkner Kyle Ramey	MC MC	SCALE6.2.4 SERPENT2	ENDF/B-VII.1 ENDF/B-VII.0	CE, (MG?) CE
VCU	Virginia Commonwealth University, USA	Zeyun Wu Mohamed Elhareef	MC	SERPENT2	ENDF/B-VII.0	CE
BNL	Brookhaven National Laboratory, USA	Cihang Lu Lap-Yen Cheng	MC	SERPENT2	ENDF/B-VII.0 VII.1, VIII.0	CE
MAC	McMaster University, Canada	Javier Gonzalez David Novog	MC	OpenMC	ENDF/B-VII.1	CE
UIUC	University of Illinois at Urbana-Champaign, USA	Madicken Munk Luke Seifert Oleksander Yardas Gwendolyn Chee	MC	OpenMC	ENDF/B-VII.1	CE
CAM-BU	University of Cambridge, UK Bangor University, UK	Eugene Shwageraus Alejandra De Lara Marat Margulis	DET	WIMS	JEFF-3.1.2	MG 172
FER	University of Zagreb, Croatia	Davor Grgić	MC	SCALE6.2.4	ENDF/B-VII.1	CE
NEA	Nuclear Energy Agency, France	Ian Hill				

*Authors and contributors of this paper highlighted in red

For exact specifications: “Benchmark Specifications for the Fluoride-salt High-temperature Reactor (FHR) Physics Calculations”

FHR Benchmark Overview

- Phased approach to benchmark
  - Phase I – 2D/3D Fuel assembly (current)
  - Phase II – Full core 3D depletion
  - Phase III – Full core with feedback and multicycle analysis
- Challenges due to complex fuel and assembly geometry
  - TRISO particles → Fuel Planks → Hexagonal Fuel Assembly → Whole Core
  - Problem geometry can be considered “Triply Heterogenous”
- Consistent results between codes is non-trivial
  - Geometry simplifications and challenges
  - Particle tracking bottlenecks simulations in certain codes
  - Periodic BCs
  - Deterministic vs. Monte Carlo
  - $S(\alpha,\beta)$ and graphite cross sections
  - Discrete burnable poison depletion
  - Depletion

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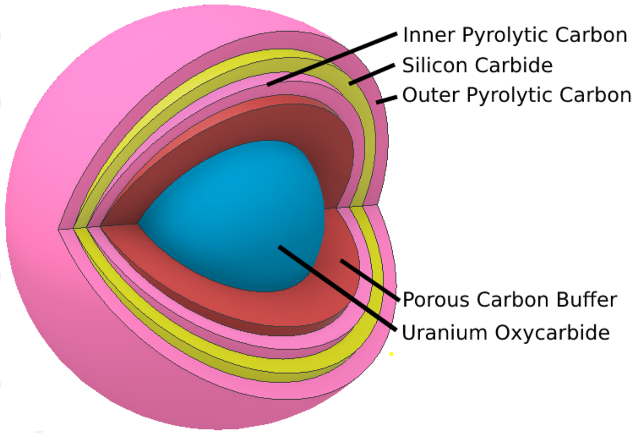
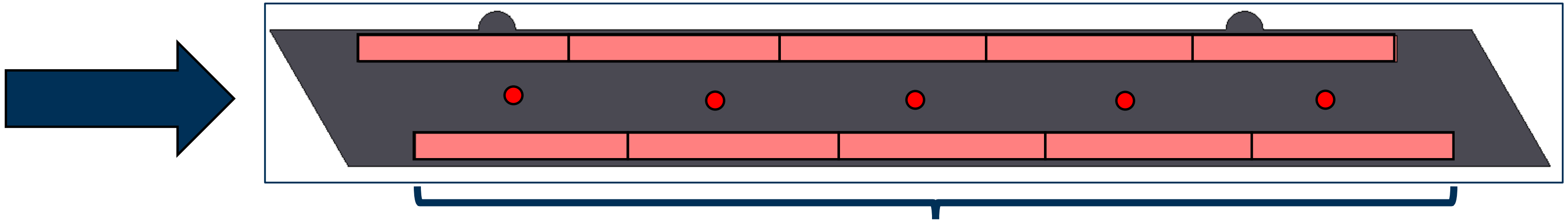
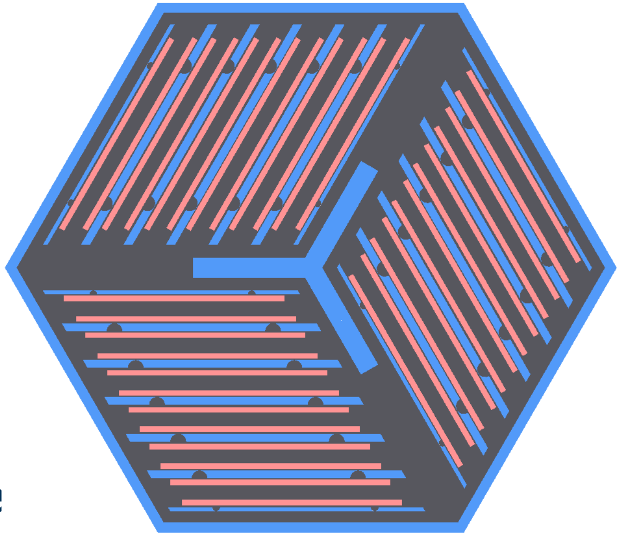
AHTR Style Fuel Assembly Setup and Design

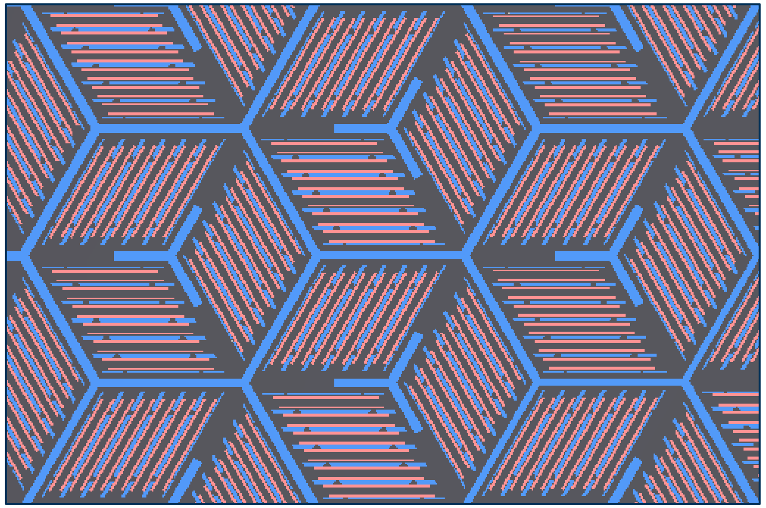




Particle Placement Zone
Even placement of a 210x4 array of TRISO Particles
Discrete Europium burnable poisons represented by ●

- Fuel "Planks" formed by adding TRISO particles in two 210x4 arrays on each plank
- Planks are placed in rows of 6 with FLiBe coolant flowing between planks
- Each assembly contains central Y-shaped control blade
- Assemblies are arranged by placing three separate "thirds" of fuel planks in 120° rotational symmetry





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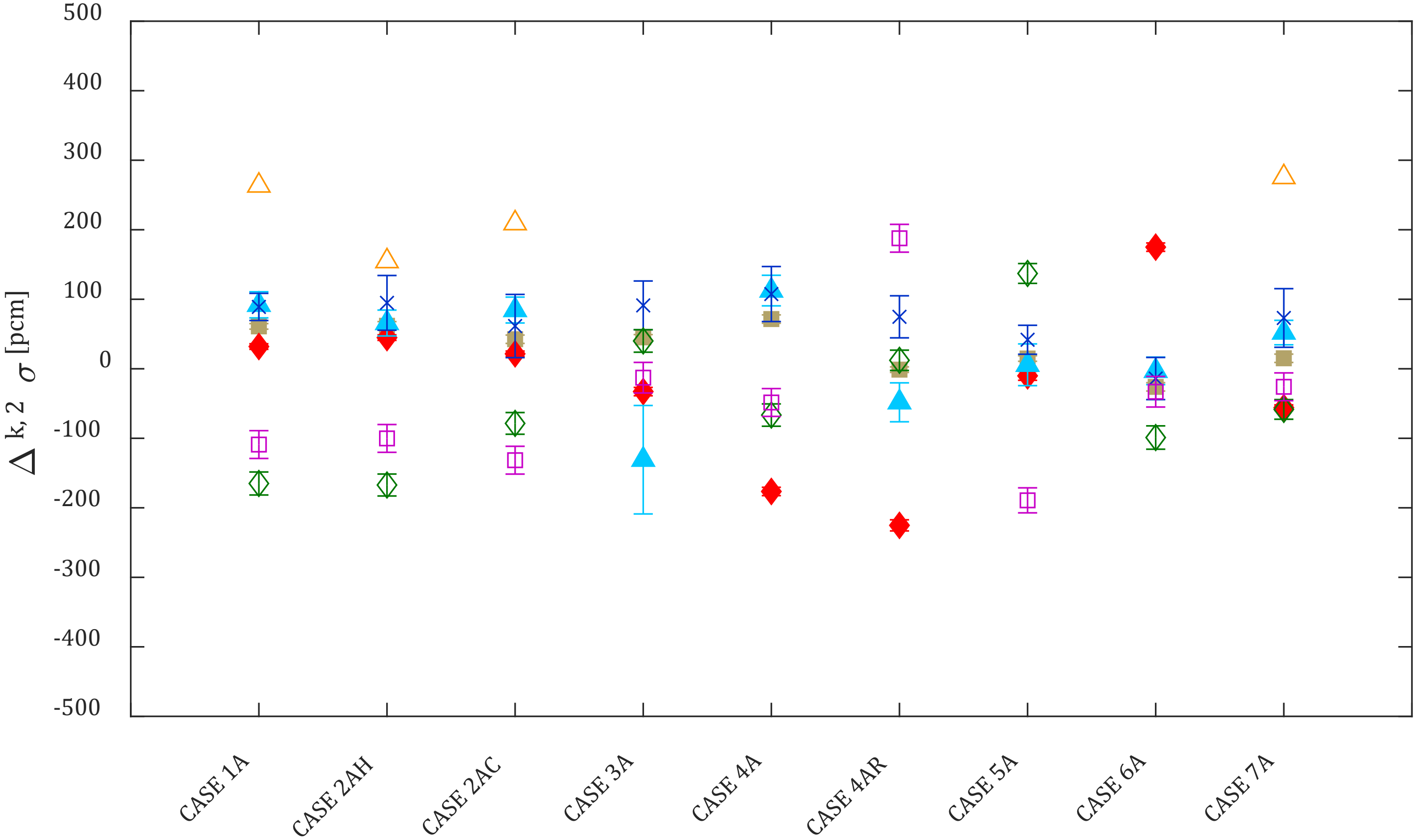
Motivation

- Code-to-code 2D eigenvalue comparisons yield very good results!
- Monte Carlo agrees well, even deterministic within 200-300 pcm of the average

Δk Results from 2D Cases 7 Participants
2 Monte Carlo and 1 Deterministic codes shown



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Motivation

- Depletion calculations bring more difficulties!

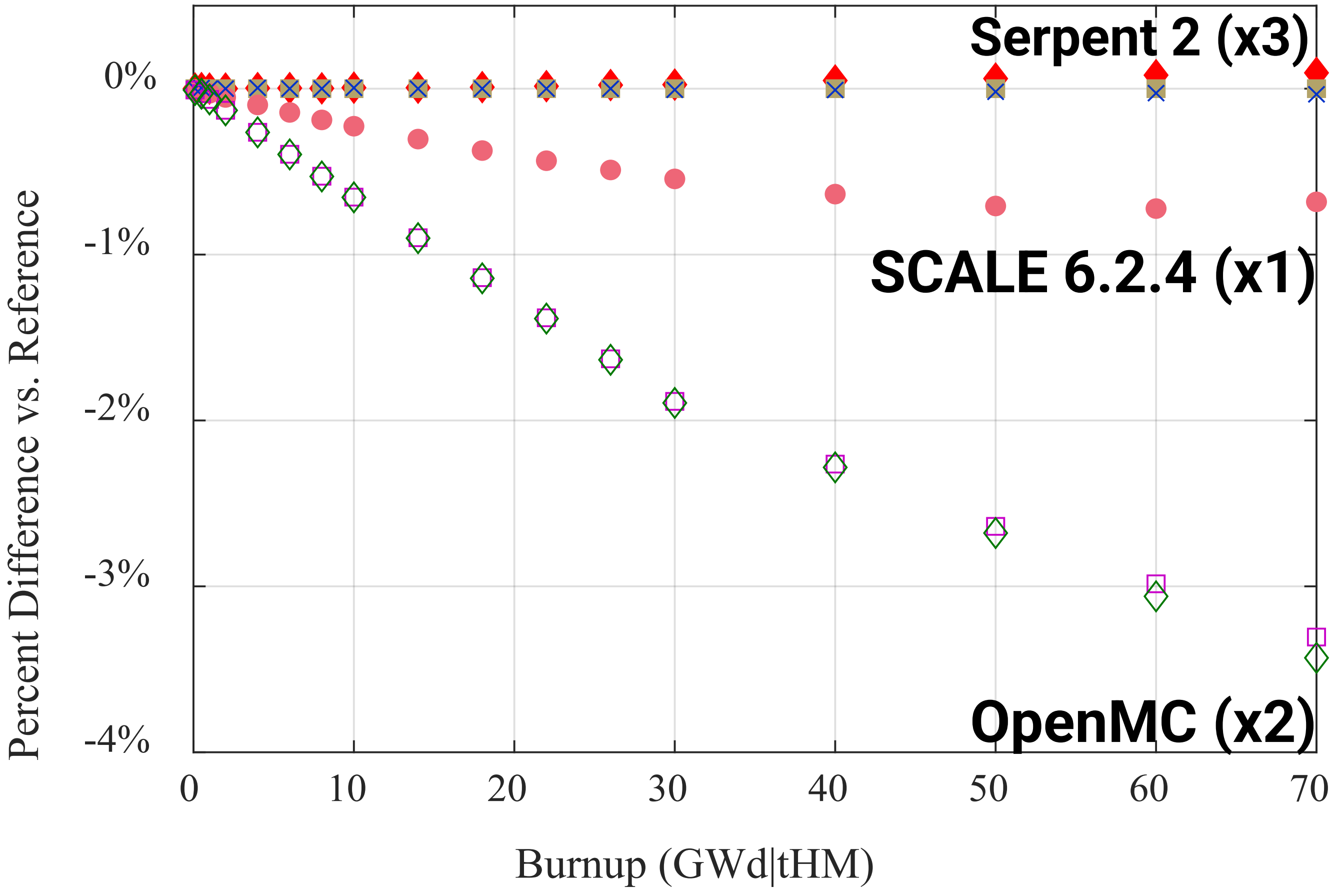
Uranium 235 Agreements (Compared to GT - Serpent 2 Result[1])

- Serpent 2 – Code agreement among Serpent 2 users
- SCALE[2] 0.75 EOL % Diff.
- OpenMC[2] 3.25 EOL % Diff

[1]GT Serpent 2 results chosen as reference for practical purposes

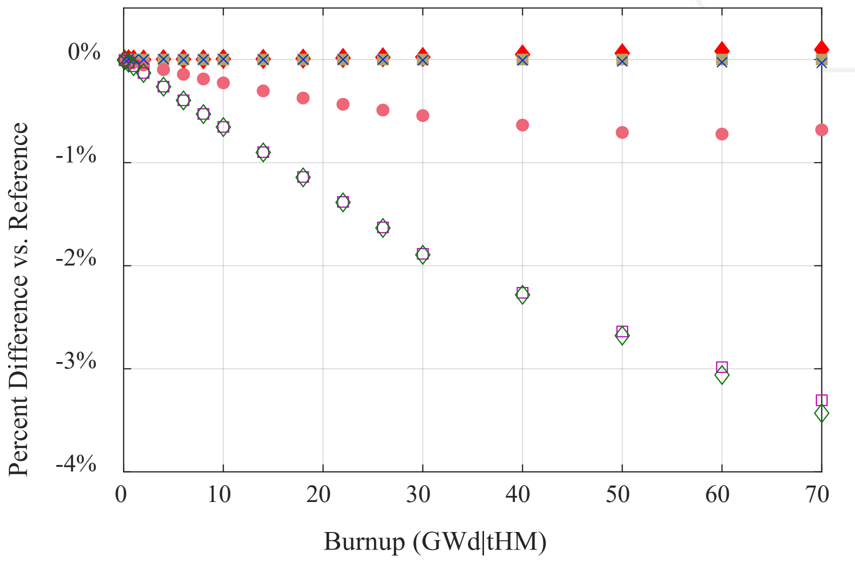
[2]Note that discrepancy amongst results does NOT imply better or worse results/performance!

Uranium 235 Concentration % Difference vs. GT Serpent 2 Result (No Burnable Poison)



Motivation

- Should 3 production level Monte Carlo codes using the same nuclear data yield such different results?
- What are the implications for V&V and benchmarking?
- What are the most accurate depletion assumptions and how can we correct for it?



Motivation and Purpose

1. Quantify and assess depletion differences across different codes.
2. Resolve said differences …
3. … and attempt to correct for differences to match most accurate method of depletion available – coupled neutron-gamma simulations
4. Set standard for future benchmark calculations and intra-code comparisons

Known Depletion Differences and Impacts

- Recoverable energy per fission
  - Large impact on ALL isotopes. Essentially changes burnup normalization
- Depletion Algorithm (Predictor vs. Predictor-Corrector)
- Unresolved Resonance Probability Tables
  - Different treatment in each code, relatively low impact for the epithermal FHR
- Fission product yield interpolation (Thermal ↔ Fast ↔ Fusion)
- Branching ratios
  - Energy dependent? 1 group, 2 group, 252 group?
- Depletion chain size
  - Tradeoff of computation expense and accuracy
- XS libraries

For Serpent 2 energy per fission description see:
Tuominen et al. “New energy deposition treatment in the Serpent 2 Monte Carlo transport code”

For an extensive evaluation of these parameters in OpenMC and Serpent see:
Paul K. Romano, Colin J. Josey, Andrew E. Johnson, Jingang Liang, “*Depletion capabilities in the OpenMC Monte Carlo particle transport code*” Annals of Nuclear Energy, Volume 152, 2021.

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Recoverable Energy E_R

- All implementations are reasonable but there is no completely agreed upon way to treat recoverable energy
- Neutron-gamma is most accurate, but very expensive at production level

- Serpent 2
  - Assumes an E_R value of 202.27 MeV for Uranium-235 – scale other isotopes based on Q values

$$E_R = 202.27\ MeV \times \frac{Q_i}{Q_{235}}$$

- OpenMC
  - User friendly way to change recoverable energy in input on an isotope-by-isotope basis

- SCALE 6.2.4
  - E_R dependent on fission and capture cross section and heating values
  - Attempts to include effects of heating from gamma through a capture cross section

$$P(t) = \sum_i \left(\sigma_{f,i}\kappa_{f,i} + \sigma_{c,i}\kappa_{c,i}\right)\mathrm{N_i(t)}\Phi$$

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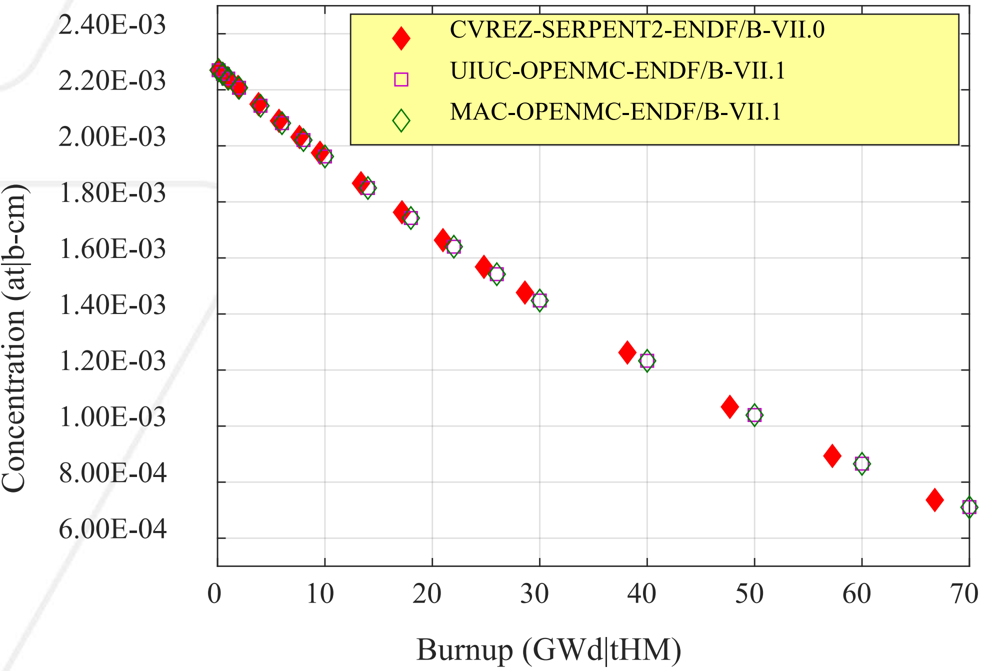
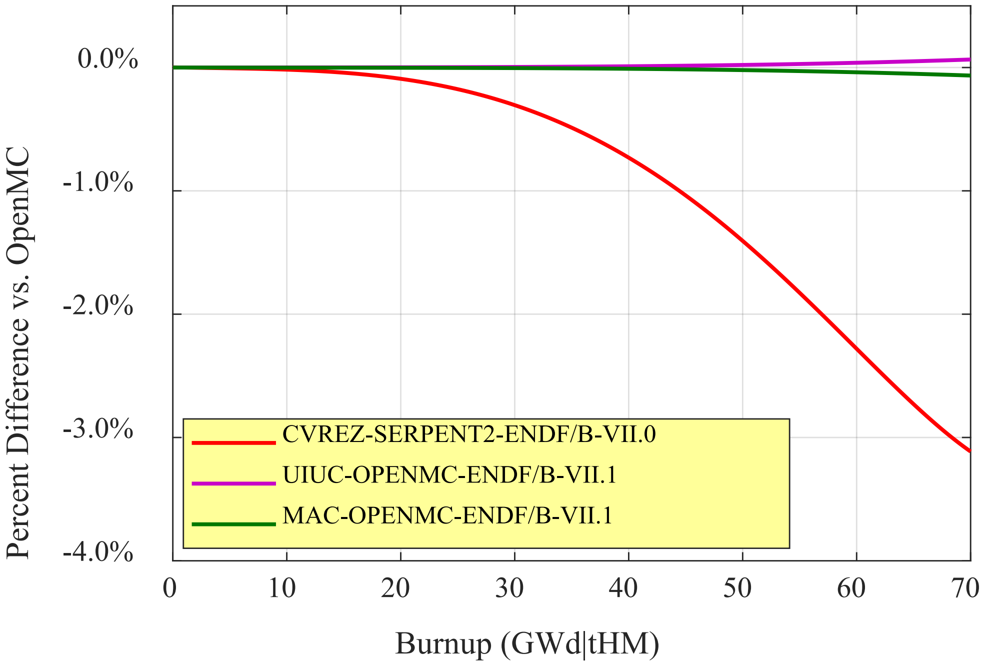
Recoverable Energy per Fission Corrections

- Method 1 – Serpent 2 users modified the burnup rate to match OpenMC default settings. Replicates "fix" when there is no way to change ER
- New burnup steps chosen based on difference between OpenMC and Serpent Uranium-235 ER (~202 MeV vs. 196 MeV)
- Use of either post-processed line fitting or new modified input burnup rates
- Result now matches for first half but diverges as burnsteps increase

Uranium 235 - Post process line fit to lagged burnup steps (No Burnable Poison)

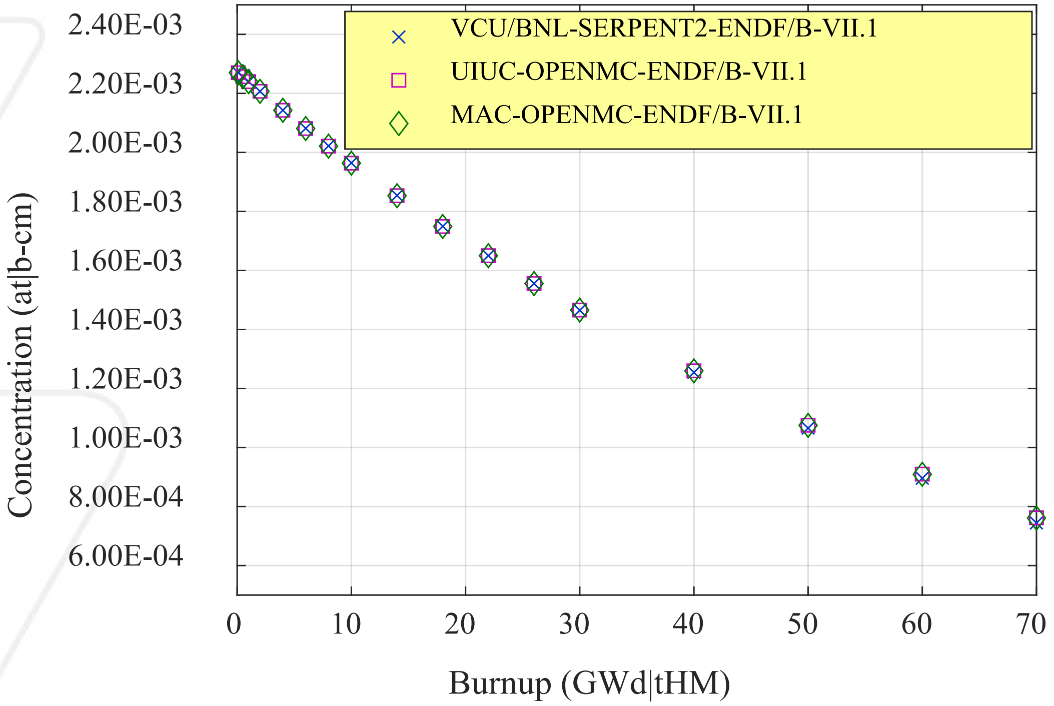


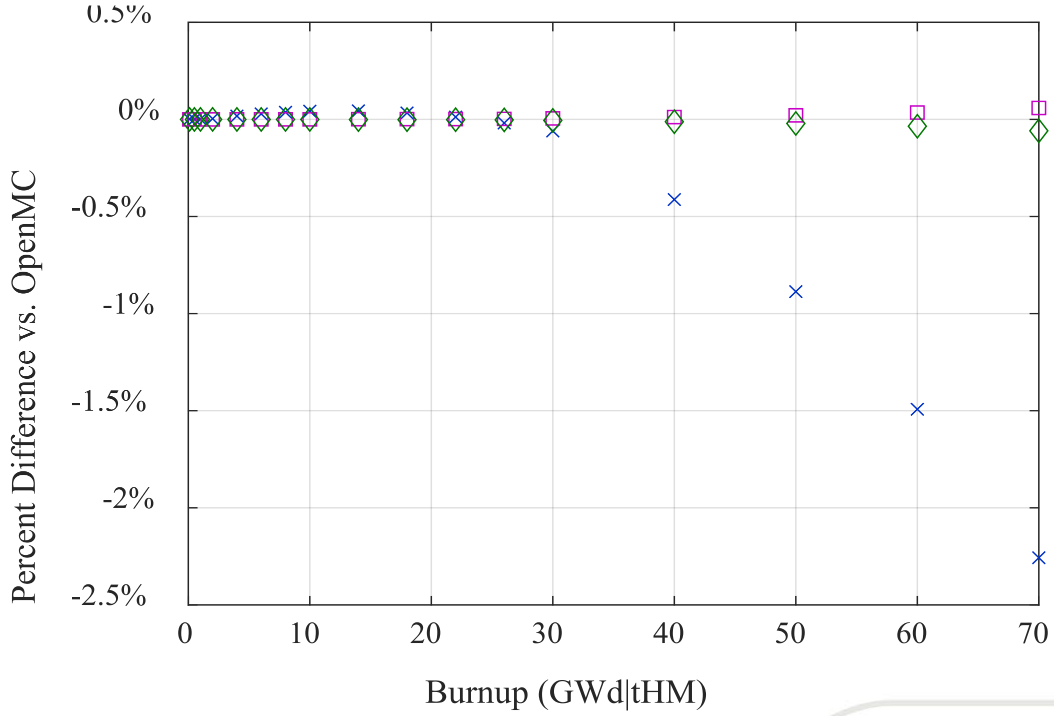


Recoverable Energy per Fission Corrections

- Change of burnup profile in input to reflect difference in recoverable energy
- Result again matches for first half of cycle but then diverges

Uranium 235 – Modified input burnup correction (With Discrete Europium Burnable Poison)





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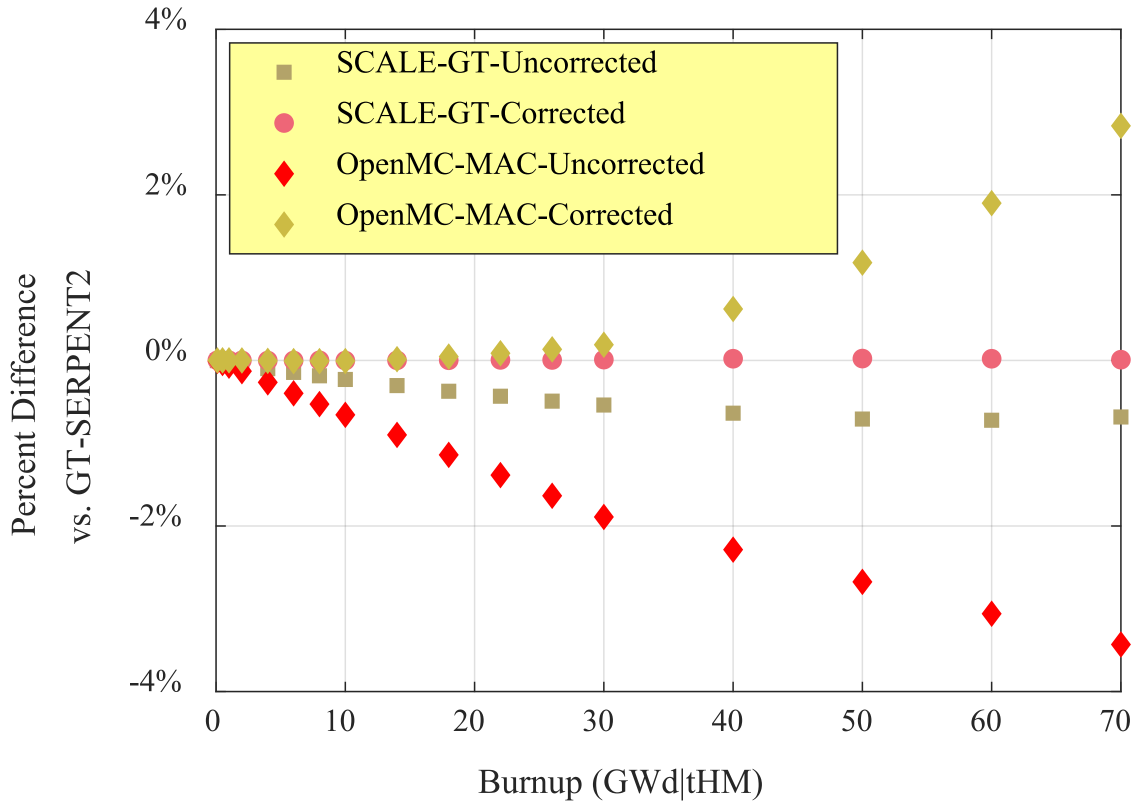
Recoverable Energy per Fission Corrections

- Method 2 – OpenMC and SCALE users modified recoverable energy through input (OpenMC) or by modifying source code (SCALE)
- ER for ALL fissionable isotopes changed to Serpent 2 default values.
- SCALE result now nearly perfectly matches Serpent 2 result
- OpenMC result now disagrees just as much as before we made corrections?

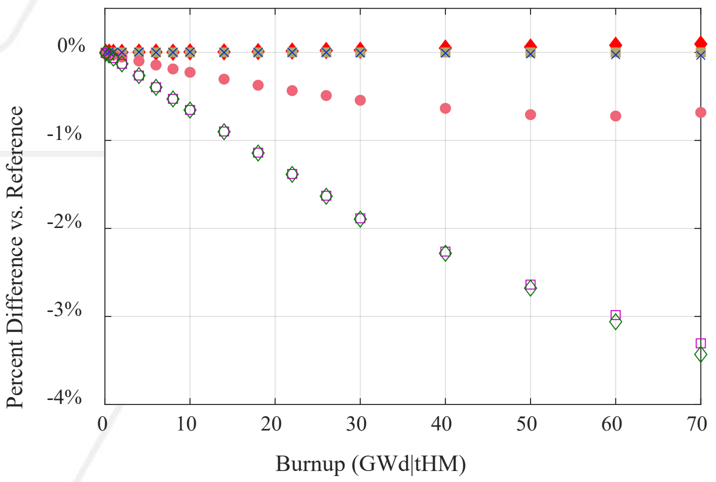
Before and After Corrections (No Burnable Poisons)



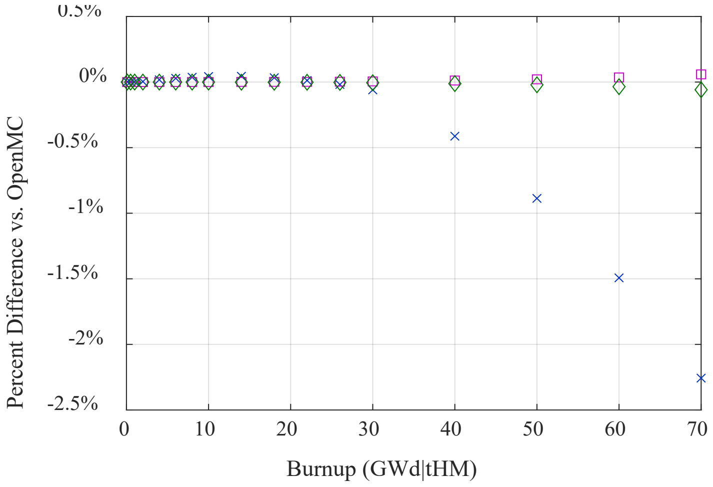
Predictor Corrector Corrections

- Differences are not fully resolved quite yet….
- Solution comparison is noticeably low until burnup steps get larger in ALL OpenMC cases so far
- SCALE cases show very good agreement once corrected

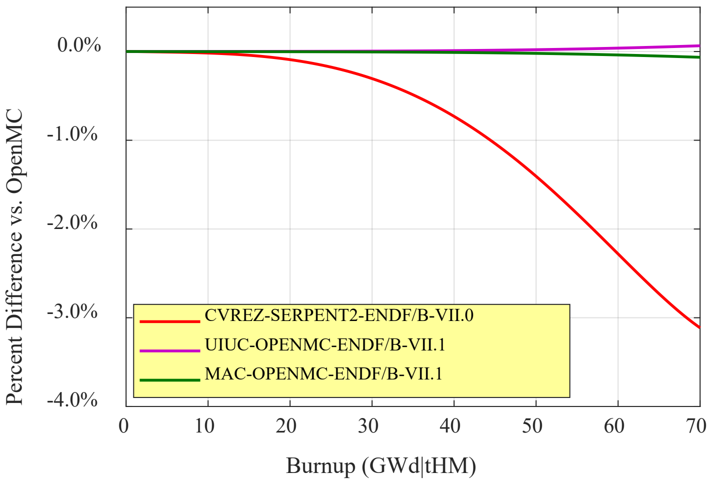
Pre-corrections (With BP)



Post-Correction (With BP)



Post-Correction (No BP)



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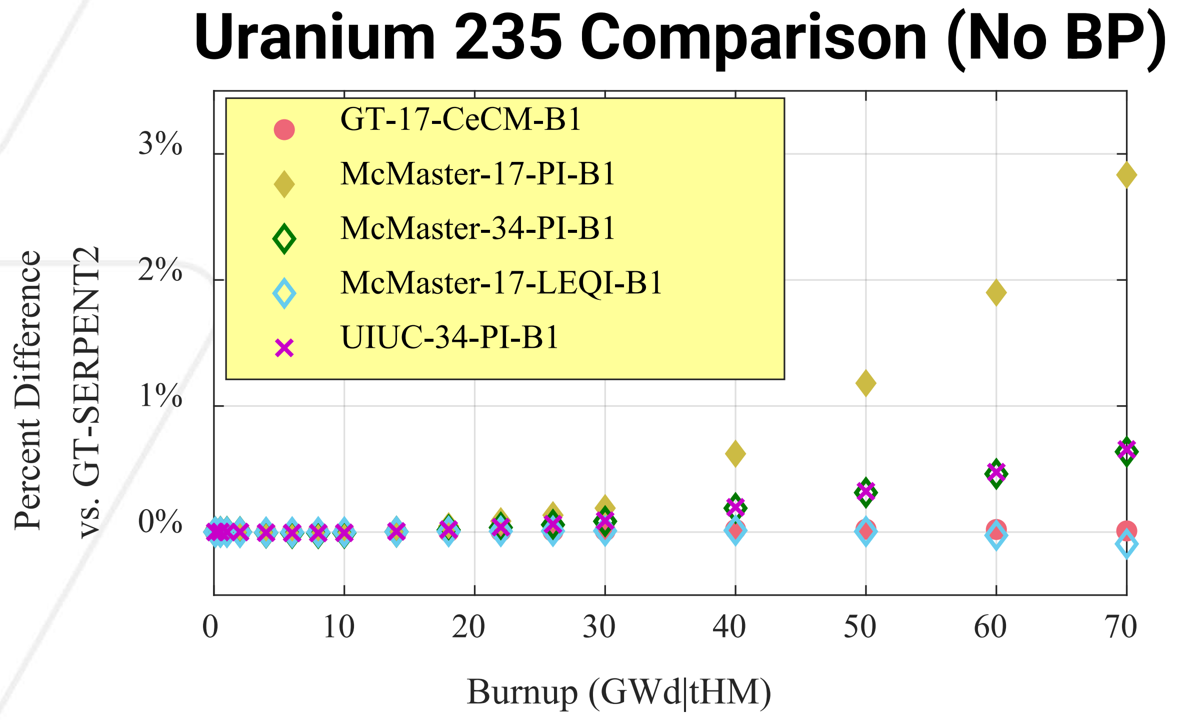
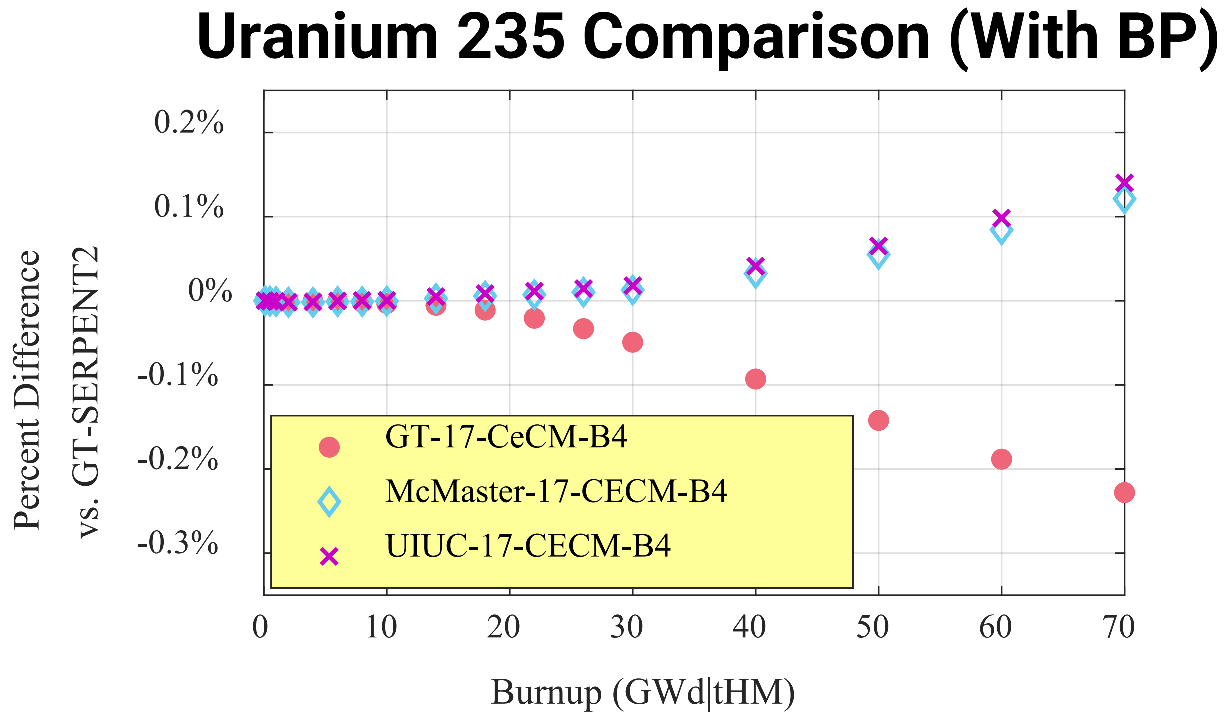
Predictor Corrector Corrections

- SCALE – uses a predictor corrector scheme dubbed “Ce/CM”
- OpenMC – originally used just pure predictor without corrector.
  - “CE/CM” and LE/QI predictor corrector schemes now investigated
  - Normal predictor with twice shorter timesteps also investigated
- Normal predictor with shorter burnup steps shows good improvement
- Both SCALE and OpenMC with predictor-corrector schemes now show excellent agreement





Coupled Neutron Gamma

- How do these approaches compare to the most accurate method available?
- OpenMC coupled neutron-gamma calculation now performed (with predictor corrector scheme)
- SCALE default settings also used which naturally attempts to correct for gamma energy through capture Q value
- Result for OpenMC AND SCALE expected to now deviate from Serpent 2
- How comparable are SCALE neutron-only and OpenMC neutron-gamma?

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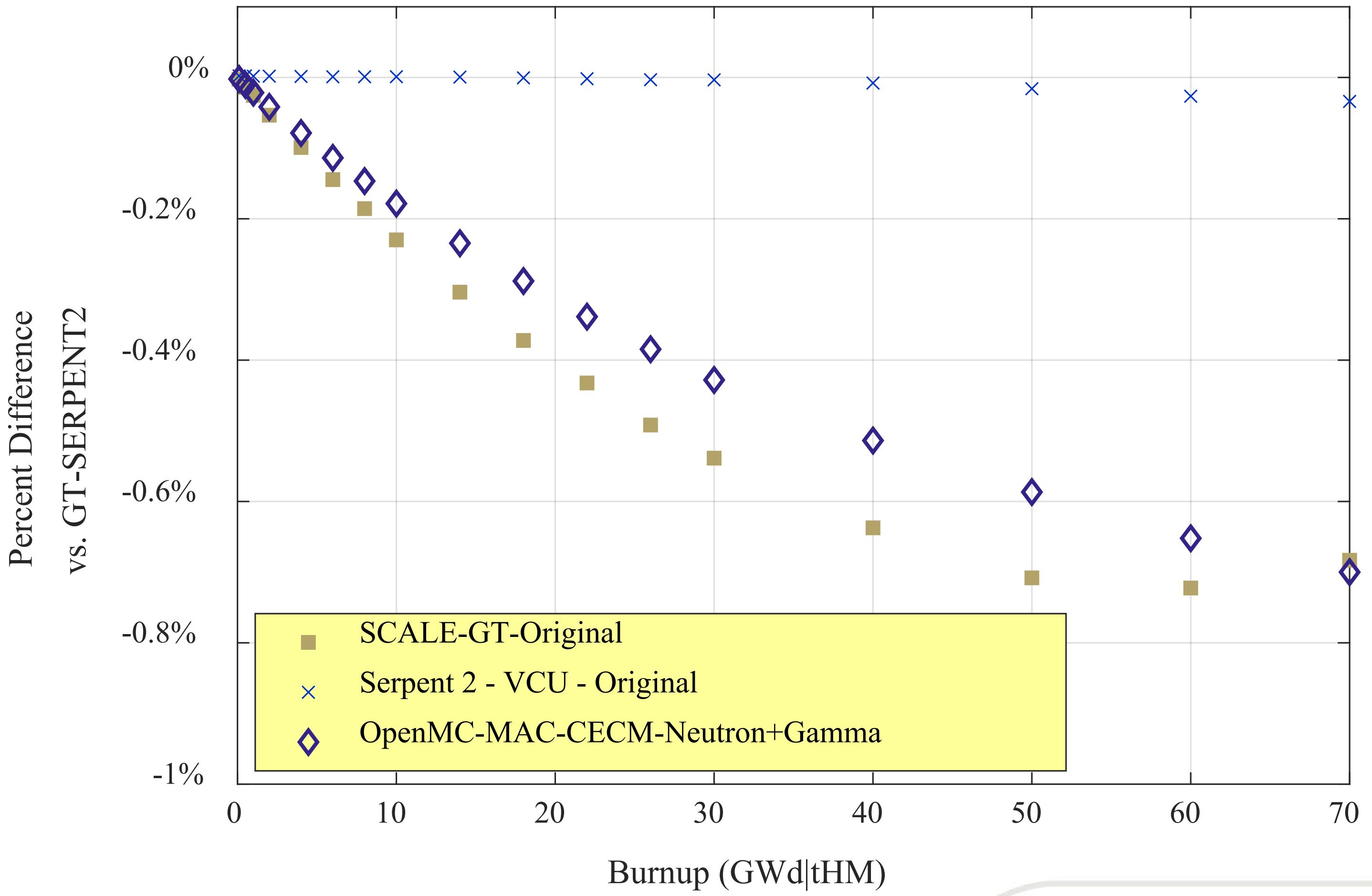
Coupled Neutron Gamma

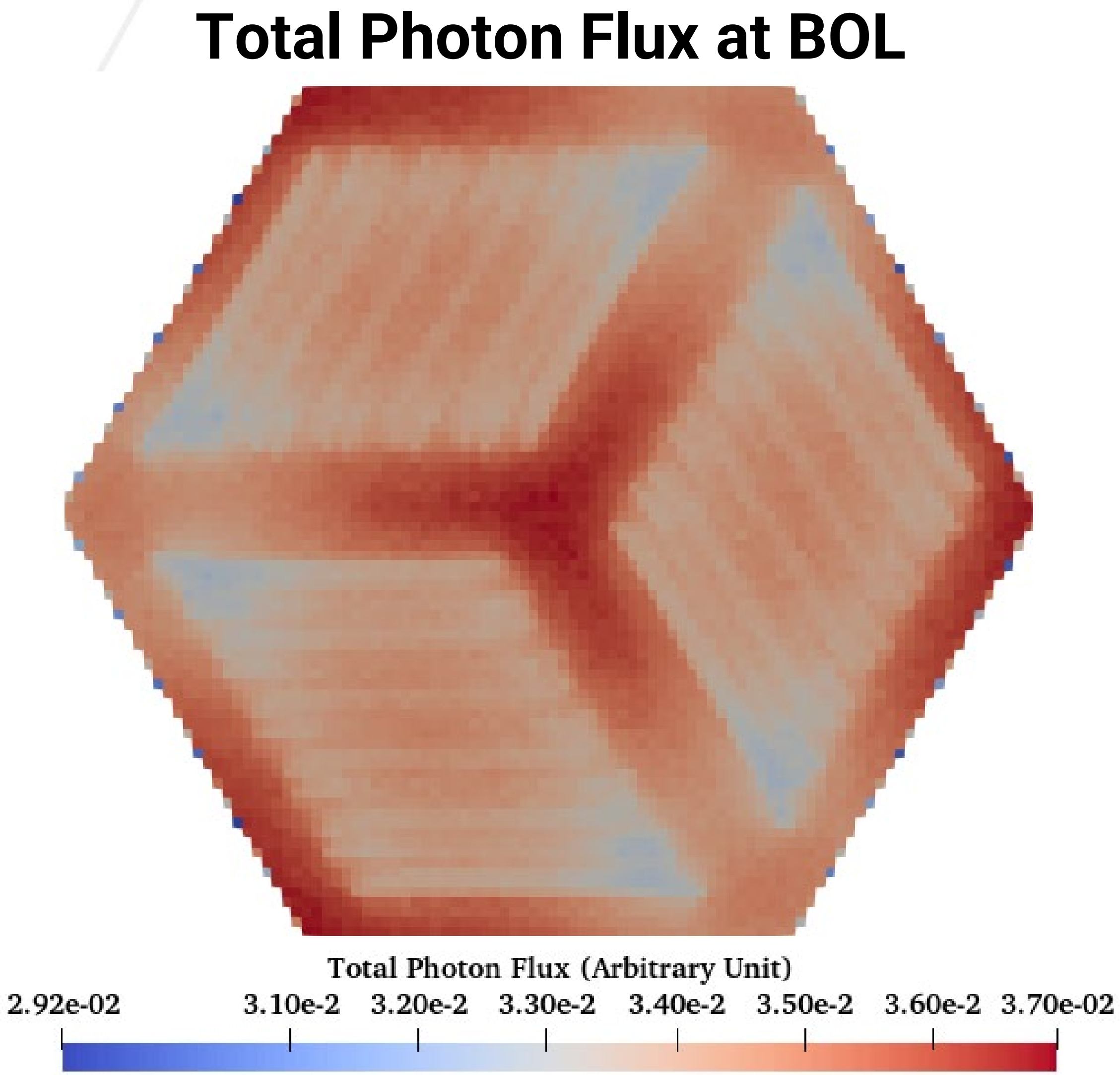
- SCALE approximation performs quite well – trends well with OpenMC results
- Lack of gamma heating causes a large source of error in cores with such large fractions of graphite
- Differences between OpenMC neutron-gamma and Serpent 2 default depletion are nearly linear due to change in burnup normalization

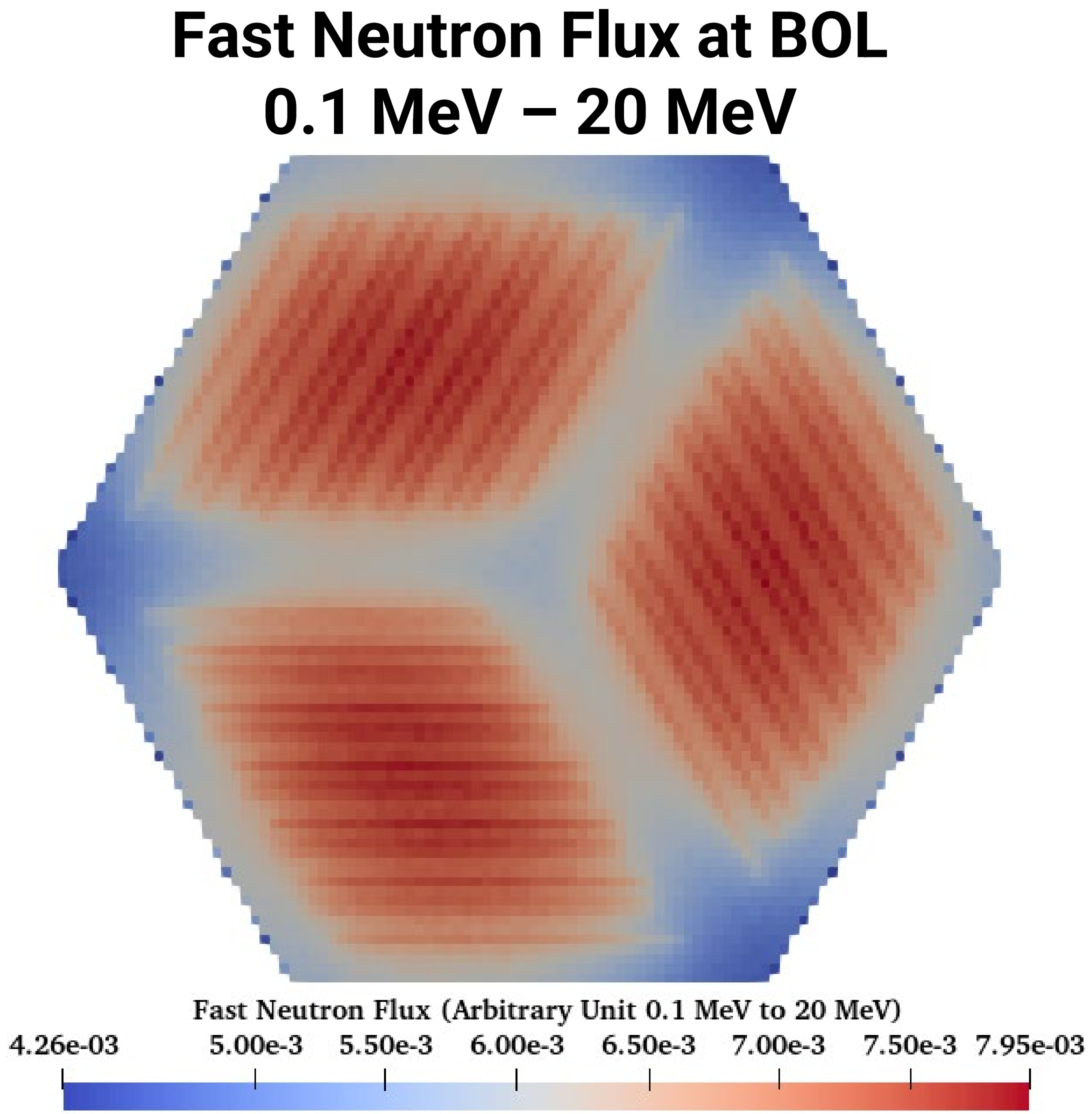
Uranium-235 Neutron-Gamma Results Compared to Serpent 2 Neutron Only Reference Soln.



Neutron and Photon Flux

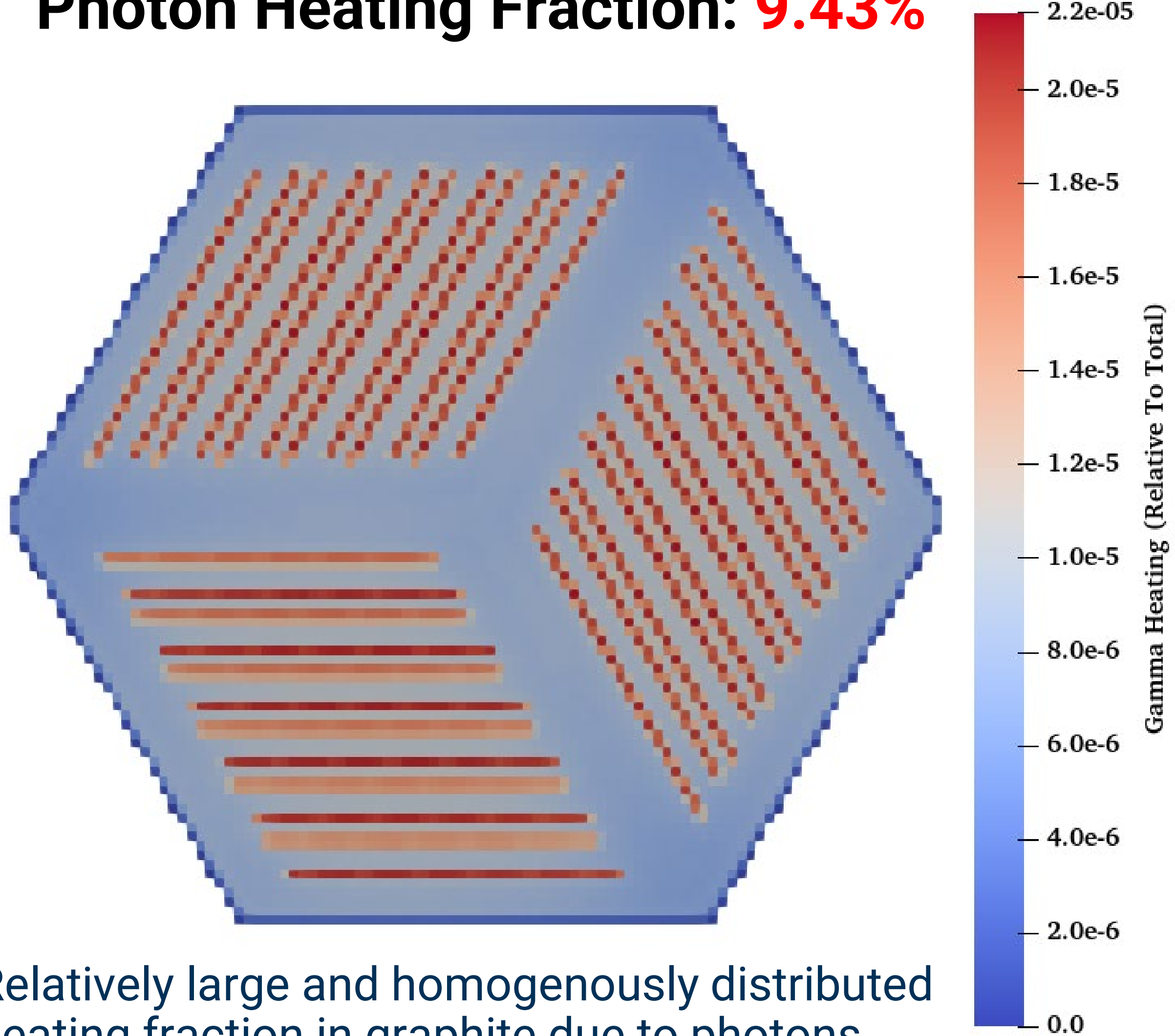
- Photon flux peaks in graphite, causing significant non-fuel energy deposition





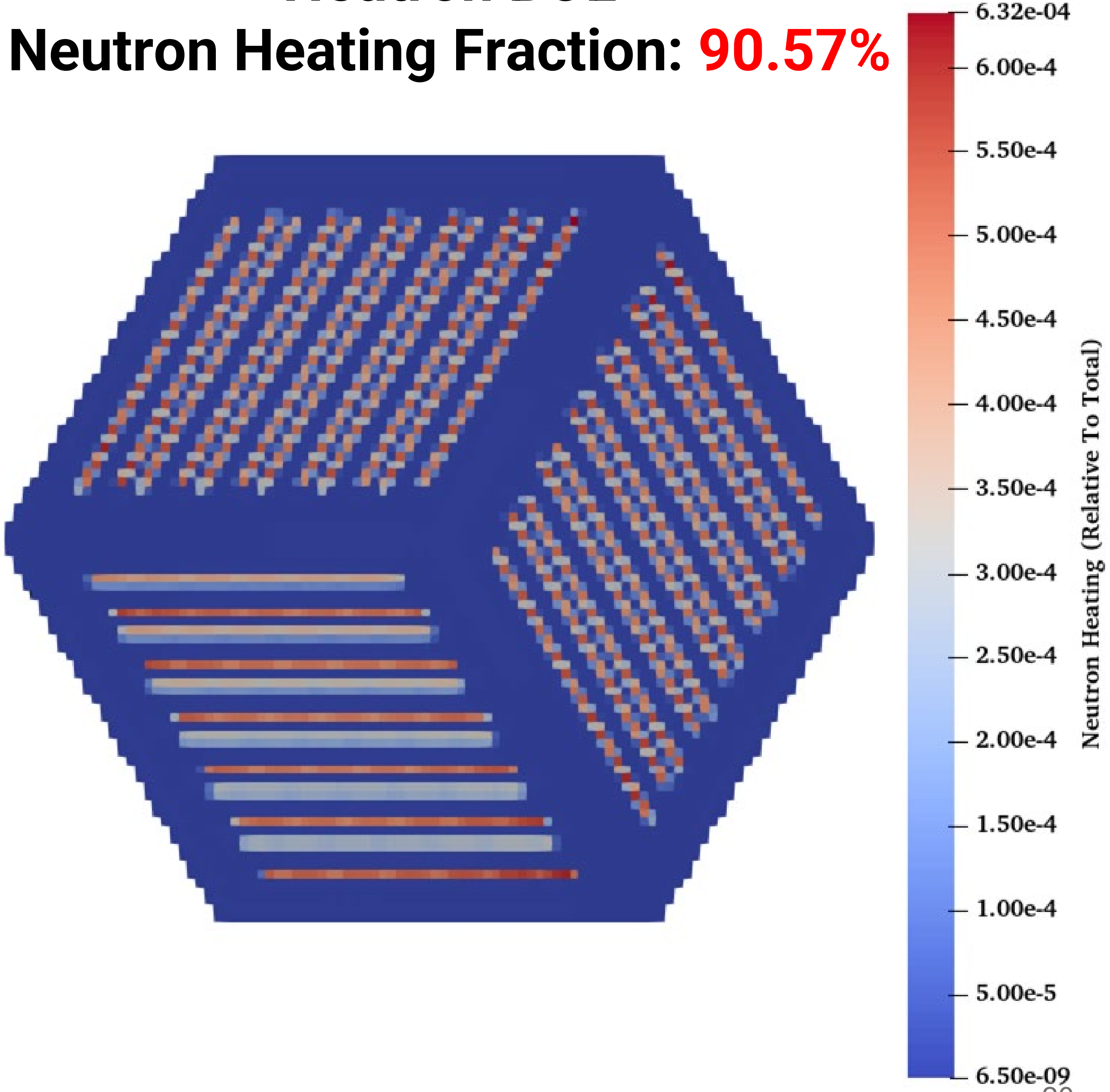
True Energy Deposition in FHR

Photon + Electron + Positron BOL
Photon Heating Fraction: 9.43%



Relatively large and homogenously distributed heating fraction in graphite due to photons

Neutron BOL
Neutron Heating Fraction: 90.57%



Conclusions and Future Work

- Depletion benchmark with large initial differences – eventually resolved
- Recoverable energy actually causes a significant amount of discrepancy
- SCALE scheme based on capture energy deposition is quite comparable to neutron-gamma simulations with relatively low implementation difficulty – even with a highly heterogenous geometry
- Time integration scheme causes more error than initially expected for even Uranium-235
  - See full paper for more data on comparison of select isotopes

<u>Future work</u>

- How does SCALE's method compare in full core calculations
  - Effect of non-homogenous photon flux in graphite
- More comprehensive comparison of other isotopes
  - See paper for comparison of some select isotopes – not included here due to time
- Room for future investigation of burnable poison cases
- Future work planned for Serpent 2 neutron-gamma comparisons

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Thank you for your attention!
Questions?

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