Initial Development of Depletion Capability in the GPU-Based Monte Carlo Code PRAGMA

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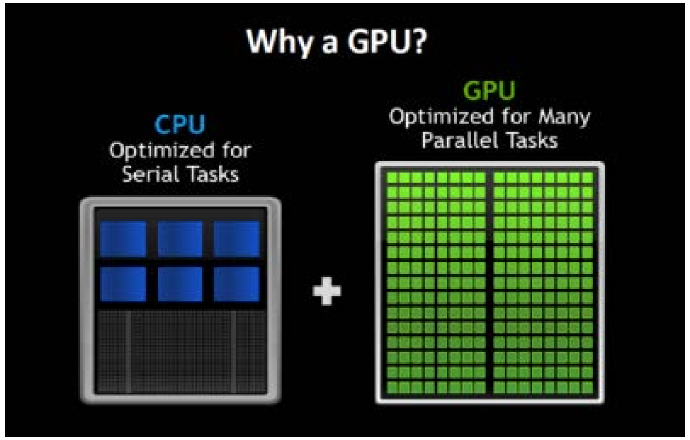
Contents

- **PRAGMA Power Reactor Analysis using GPU-based Monte Carlo Algorithm**



- **Funded by KHNP through K-CLOUD project.**

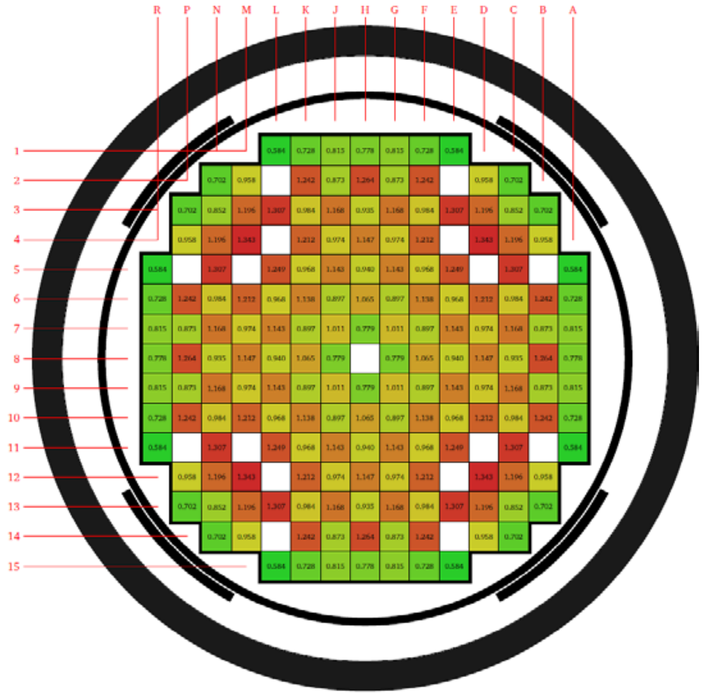
- **Language : CUDA C++**
- **Objectives of the PRAGMA code**
  - Apply dedicated optimizations for power reactor analysis.
  - Employ massive number of particles – at least over 10^8 per cycle – to eliminate inter-cycle correlation and reduce the number of active cycles.
  - Enable efficient simulation in feasible time scale on small cluster equipped with consumer-grade GPUs.

GeForce RTX 2080 Ti ($999)
13,450 GFLOPS FP32
420.2 GFLOPS FP64
11 GB (616.0 GB/s GDDR6)

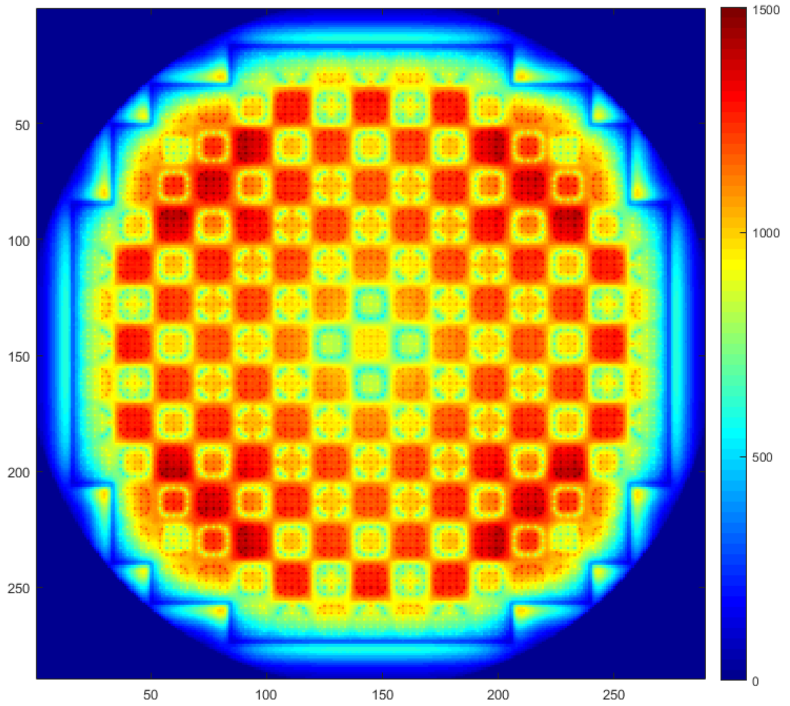
Tesla V100 ($10,664)
14,028 GFLOPS FP32
7,014 GFLOPS FP64
16 GB (900GB/s HBM2)

- **Calculation Condition**
  - 100 million particles / cycle
  - 100 active cycles
  - Execution time < 15 minutes

Detector Measurement Map



Thermal Flux



Comparison with Detector Signal

(RMS: 1.98% / Max : 3.36%)

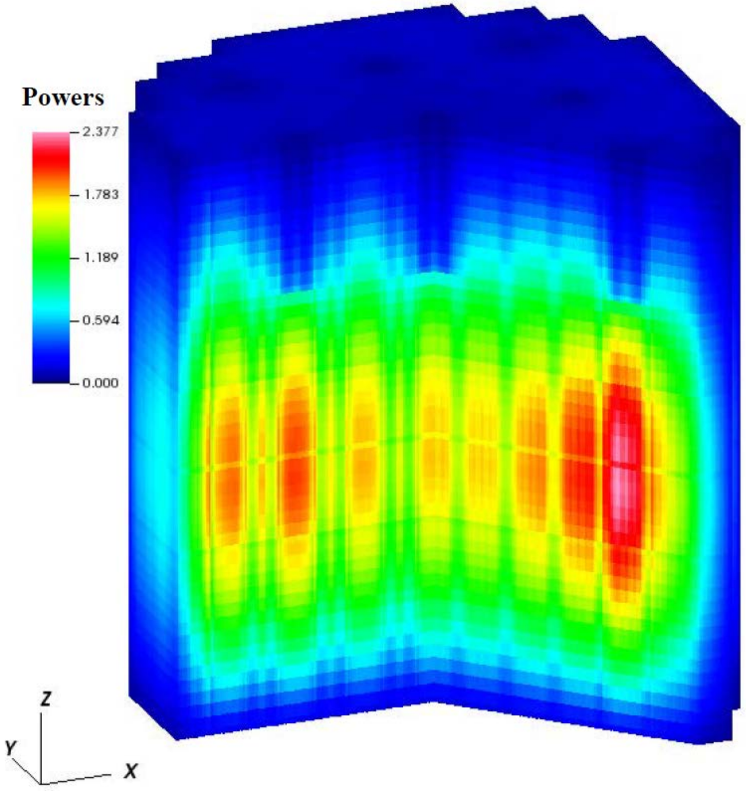
0.779 0.788 **1.11%**	1.011 1.040 **2.89%**					
1.065 1.084 **1.80%**	0.897 0.908 **1.24%**	1.138 1.161 **2.00%**				
0.940 0.937 **-0.31%**	1.143 1.166 **2.02%**	0.968 0.983 **1.50%**	1.249 1.266 **1.33%**			
1.147 1.163 **1.36%**	0.974 0.964 **-0.99%**	1.212 1.214 **0.18%**		1.343 1.311 **-2.40%**		
0.935 0.932 **-0.32%**	1.168 1.195 **2.34%**	0.984 0.970 **-1.45%**	1.301 1.357 **3.36%**	1.196 1.182 **-1.19%**	0.852 0.836 **-1.83%**	
1.264 1.255 **-0.68%**	0.873 0.856 **-1.92%**	1.242 1.253 **0.90%**		0.958 0.930 **-2.92%**	0.702 0.688 **-2.00%**	
0.778 0.758 **-2.60%**	0.815 0.790 **-3.10%**	0.728 0.707 **-2.87%**	0.584 0.578 **-1.11%**			Detector PRAGMA **Rel. Err.**

- **Comparison with KENO-VI**
  - Quarter Core (KENO-VI) vs Full Core (PRAGMA)

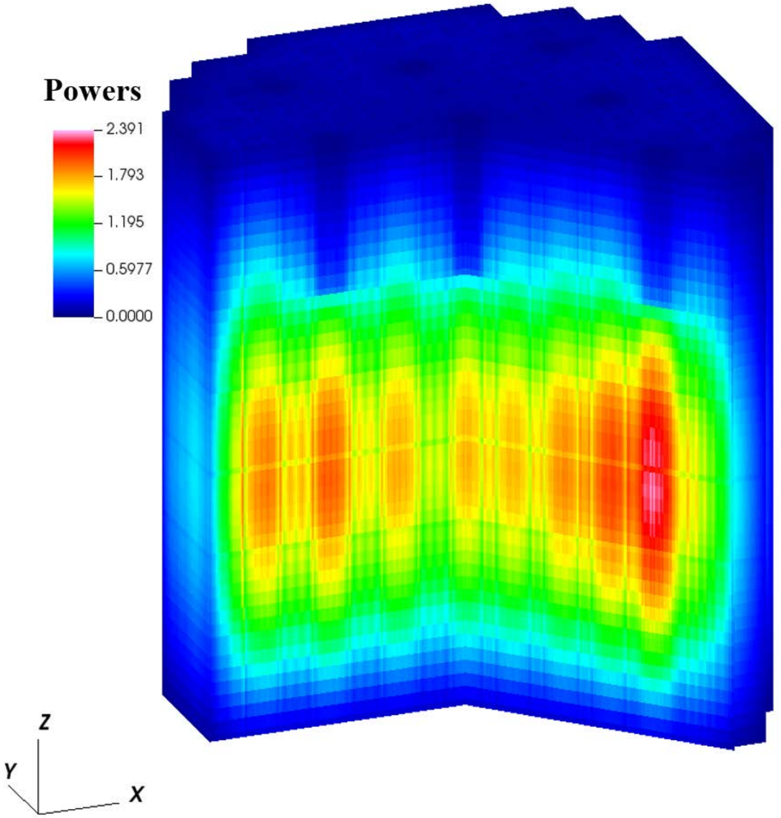
	KENO-VI	PRAGMA
k_{eff}	1.000072 (0.2)	1.000126 (0.2)
Average 3D Power Uncertainty	0.209%	0.425%
Maximum 3D Power Uncertainty	1.630% (< 1.0) 0.414% (> 1.0)	8.907% (< 1.0) 0.629% (> 1.0)
# of particles / cycle	10M	100M
# of active cycles	9500	1000
Runtime	29 days	2.08 hours

Calculation Summary

KENO-VI Fission Power



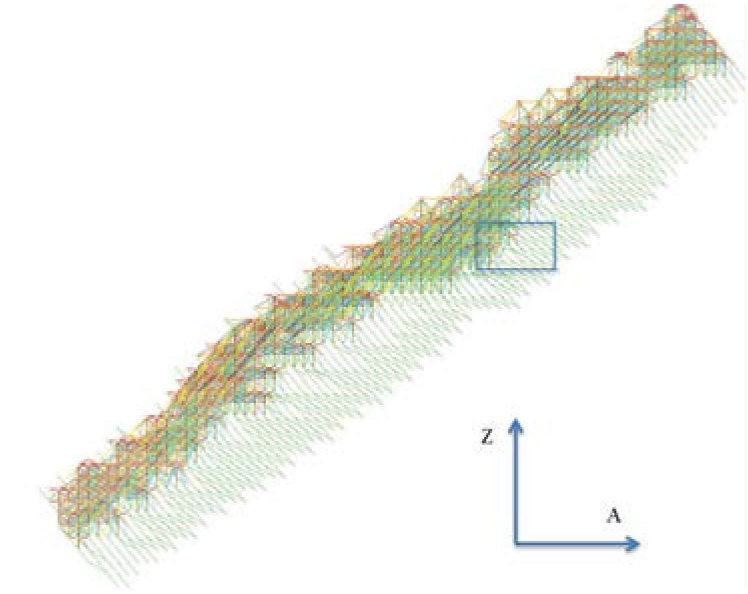
PRAGMA Fission Power

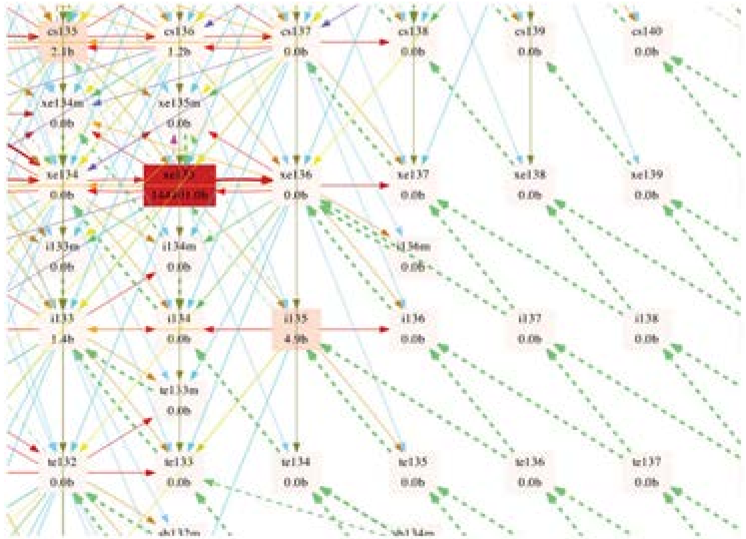


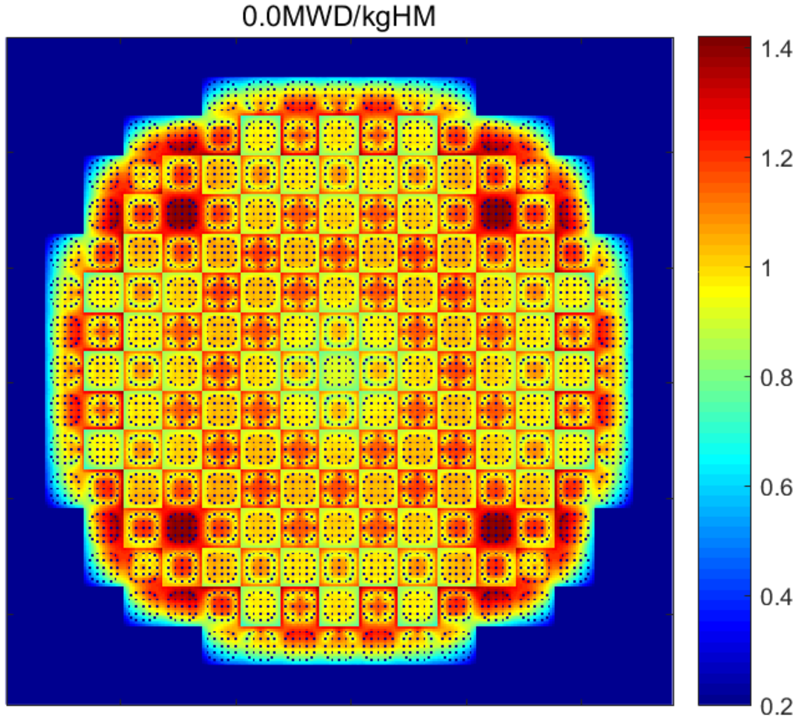
Next Stage?

- **Cycle Depletion for Power Reactors with PRAGMA**
  - Minimize increase of calculation time.
  - Memory and performance optimization for GPU
  - Need to tackle memory burden.

$$\frac{dN_i}{dt} = -\left(\lambda_i + \overline{\sigma_i \phi}\right) N_i + \sum_j \left(\lambda_{ji} + \overline{\sigma_{ji} \phi}\right) N_j$$



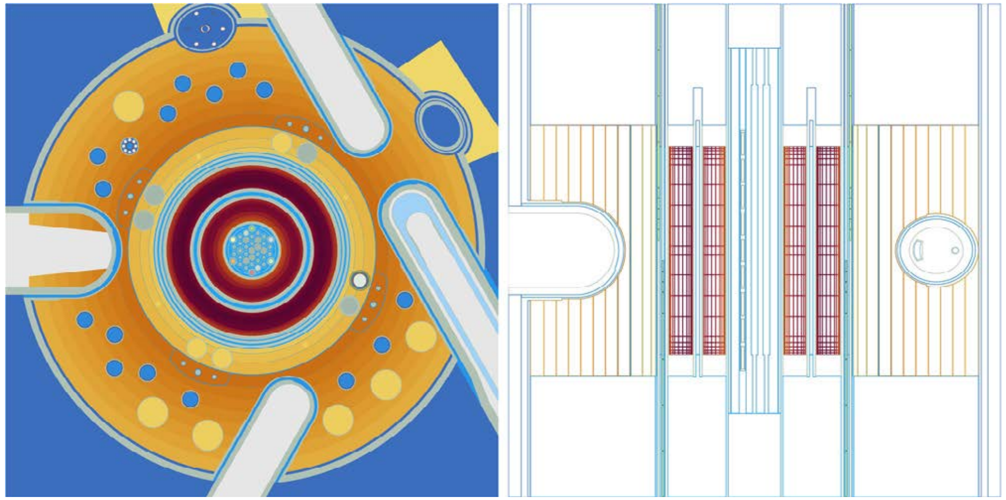




Burnup Tally

- Conventional Methods
- Limitations

- **Online Tally**
  - McCARD at SNU
  - Several types of reaction rates are directly tallied during neutron tracking
    - E.g.) absorption, (n, 2n), (n, 3n), fission, capture, (n, p) and (n, α)
  - Those reaction rates are tallied in **every neutron track for every nuclide**.
- **Fine Group Spectrum Tally**
  - Shift Monte Carlo Code* at ORNL
  - Fine group spectra are tallied for each depletion region.
  - **43,000 energy bins** per depletion region are used to produce one-group reaction rates.



$$\frac{dN_i}{dt} = -\left(\lambda_i + \overline{\sigma_i \phi}\right) N_i + \sum_j \left(\lambda_{ji} + \overline{\sigma_{ji} \phi}\right) N_j$$

Energy bounds [eV]	Number of equilethargy bins
2.0×10^7 - 1.0×10^7	1000
1.0×10^7 - 1.0×10^6	1000
1.0×10^6 - 1.0×10^5	4000
1.0×10^5 - 1.0×10^4	4000
1.0×10^4 - 1.0×10^3	10000
1.0×10^3 - 1.0×10^2	10000
1.0×10^2 - 1.0×10^1	4000
1.0×10^1 - 1.0×10^0	4000
1.0×10^0 - 1.0×10^{-1}	1000
1.0×10^{-1} - 1.0×10^{-2}	1000
1.0×10^{-2} - 1.0×10^{-3}	1000
1.0×10^{-3} - 1.0×10^{-4}	1000
1.0×10^{-4} - 1.0×10^{-5}	1000

*G. G. Davidson, et al., "Nuclide Depletion Capabilities in the Shift Monte Carlo Code," Ann. Nucl. Energy 114, pp. 259 – 276 (2018)

Target Problem and Available GPU VRAM

- Target problem : APR1400 full core
  - Total 3,650,832 tally cells
  - About 11,000,000 depletion regions
- **Maximum available GPU VRAM for burnup tally : 100 GB**

GPU VRAM

Model	VRAM (GB)
NVIDIA GeForce GTX 1080	8
NVIDIA GeForce RTX 2080 Ti	11
NVIDIA GeForce RTX 3090	24

Online Tally

- For each depletion regions, about **2500 reaction types** (ENDF/B-VII.1) are tallied.
- The amount of required memory : 2,500×11,000,000×8 bytes = **205 GB** → **Overflow!**
- **Performance degradation** heavily imposed on GPU due to massive **random access**.

Fine Group Spectrum Tally

- According to Shift, **43,000 energy groups** are tallied for each depletion regions.
- The amount of required memory : 43,000×11,000,000×8 bytes = **3.5 TB** → **Impossible!**

➢ **Workaround Required!**

Multilevel Spectral Collapse

- Concept
- Assembly-wise MSC
- Pin-wise MSC

- **How to Accurately Evaluate Reaction Rates with Less Information?**
  - Two spectra in different level of geometries can be utilized.
  - Finer granularity for larger system and coarser for smaller system (depletion region)
  - ➢ Multilevel spectral collapse (MSC)

g-th group

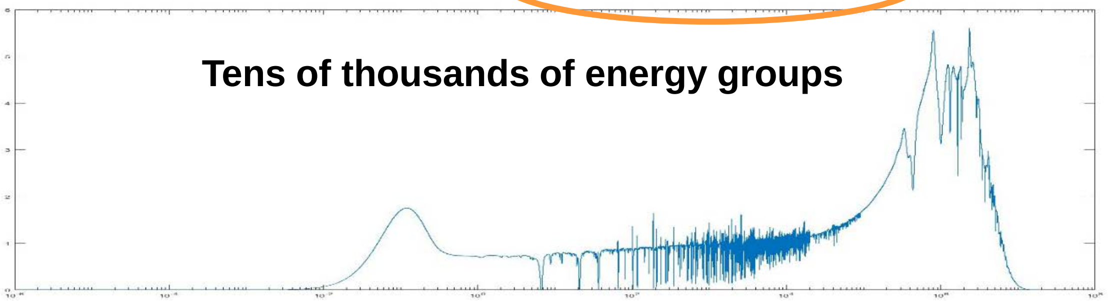
Energy grid of fine group spectrum

G-th group

Energy grid of coarse group spectrum

- **Procedure for One Group Collapse**

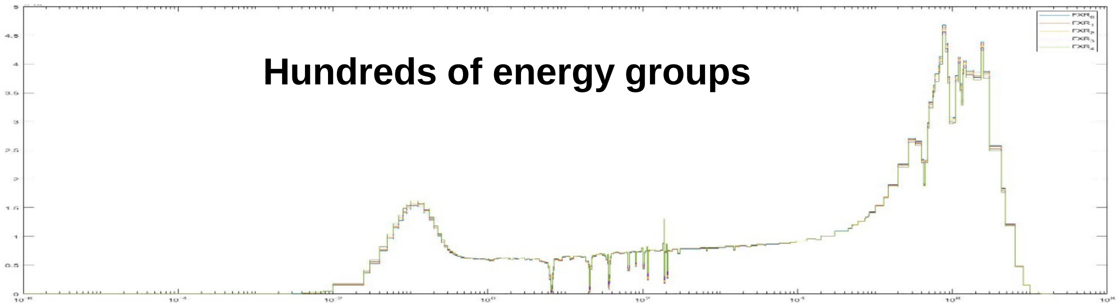
Fine spectrum of background geometry → **What to choose?**



$\varphi_g \Delta E_g$ →

$$\sigma_G(T) = \frac{\sum_{g \in G} \varphi_g \Delta E_g \sigma_g(T)}{\sum_{g \in G} \varphi_g \Delta E_g}$$

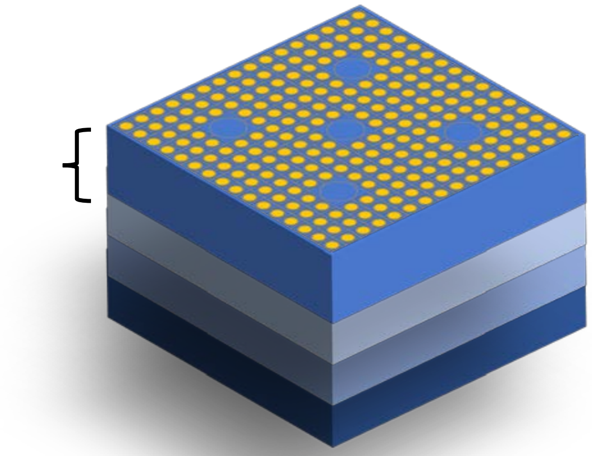
Coarse spectrum of depletion region

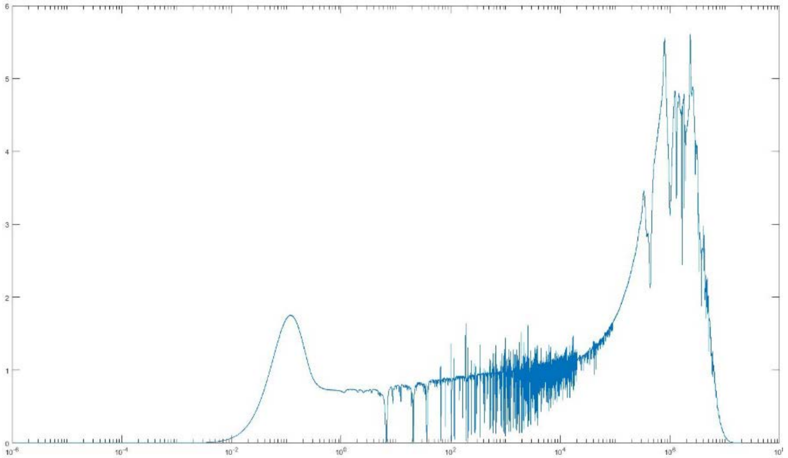


$\sigma_G(T)$ →

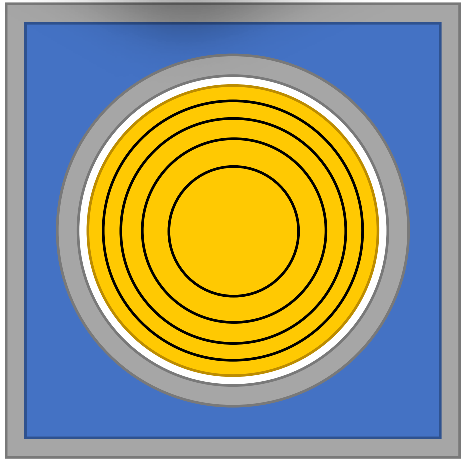
$$\overline{\sigma\phi} = \sum_G \sigma_G(T)\phi_G$$

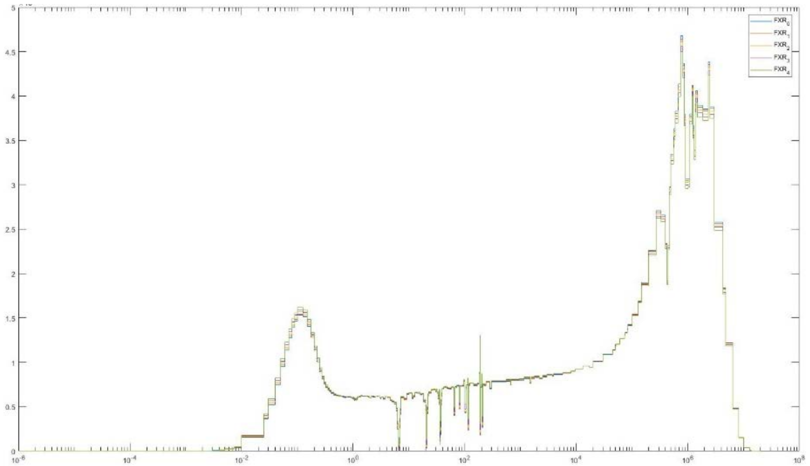
- **Axial Assembly Segment as Background Geometry**





$$\varphi_g \Delta E_g \rightarrow \sigma_G(T) = \frac{\sum_{g \in G} \varphi_g \Delta E_g \sigma_g(T)}{\sum_{g \in G} \varphi_g \Delta E_g}$$



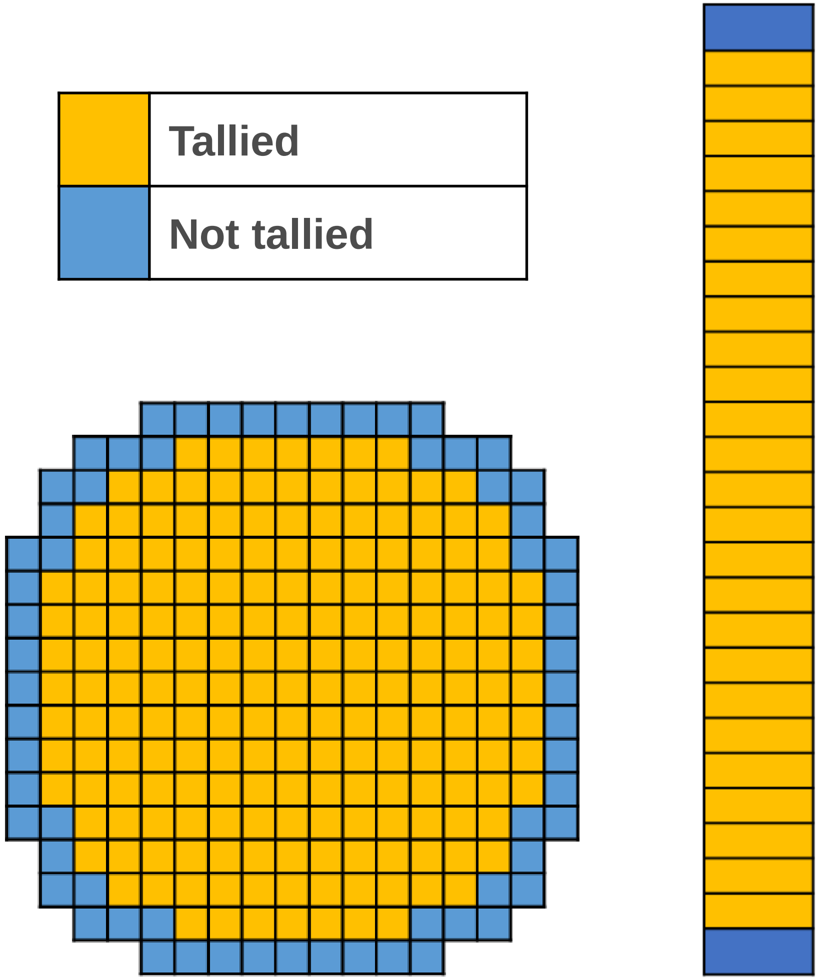


$$\sigma_G(T) \rightarrow \overline{\sigma\phi} = \sum_G \sigma_G(T)\phi_G$$

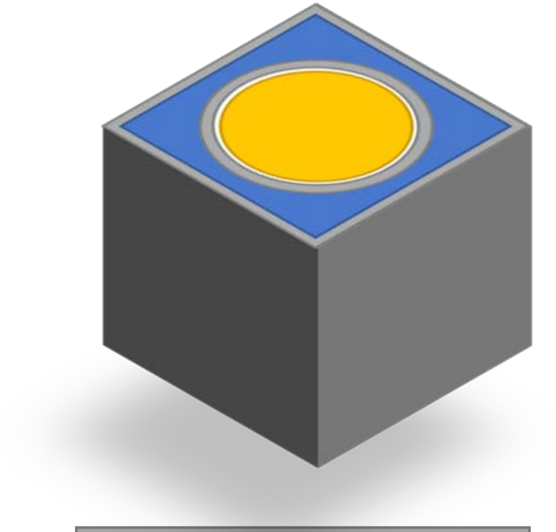
ENGINEERING

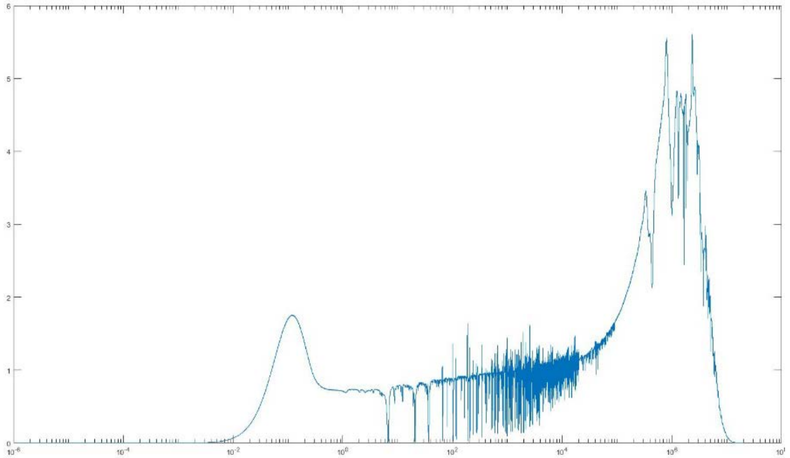
Assembly-wise MSC

- **Memory Requirements**
  - **For the fine spectrum,**
    - 241 fuel assemblies
    - 36 axial planes
    - 43,000 energy bins
    - ➢ 241 segments/plane × 36 planes × 56,000 bins/segment×8 bytes/bin = 3.6 GB
  - **For the coarse spectrum for each depletion domain,**
    - 11,000,000 depletion domains
    - 500 energy bins
    - ➢ 11,000,000 domains × 500 bins/domain × 8 bytes/bin = 41 GB
  - ➢ **About 45 GB required in total → Quite feasible**

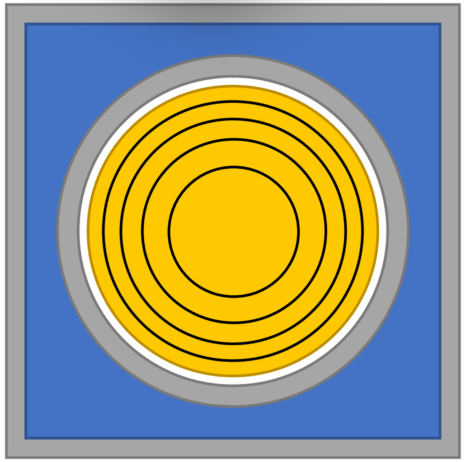


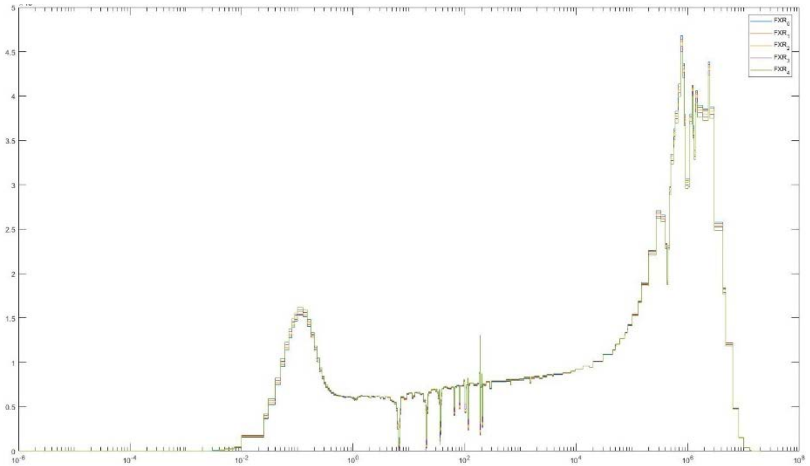
- **Radial Pin as Background Geometry**





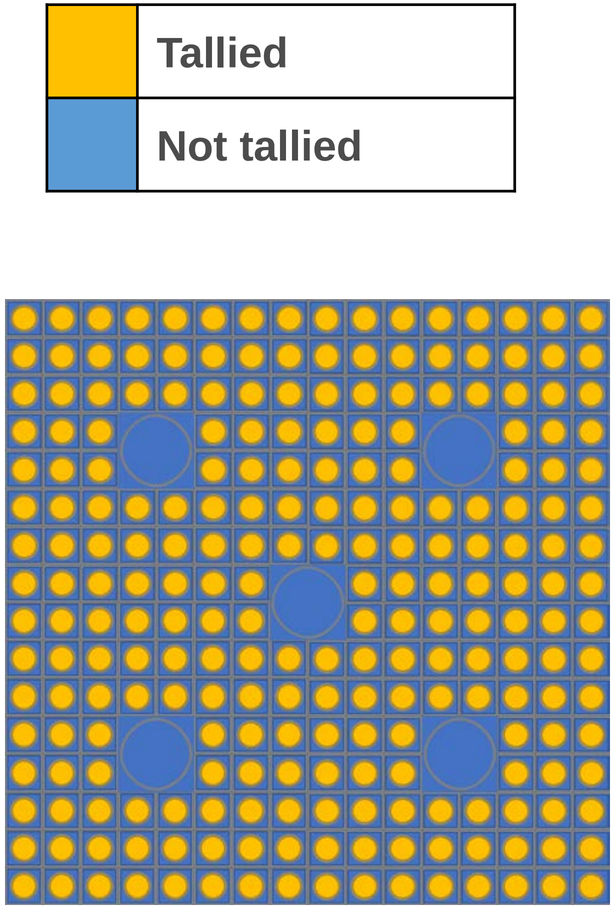
$$\varphi_g \Delta E_g \;\rightarrow\; \sigma_G(T) = \frac{\sum_{g\in G} \varphi_g \Delta E_g \sigma_g(T)}{\sum_{g\in G} \varphi_g \Delta E_g}$$

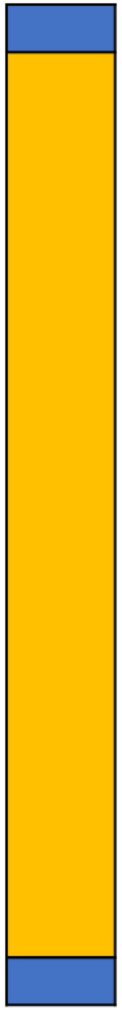




$$\sigma_G(T) \;\rightarrow\; \overline{\sigma\phi} = \sum_G \sigma_G(T)\phi_G$$

- **Memory Requirements**
  - **For the fine spectrum,**
    - 241 assemblies
    - 236 pins/assembly
    - 43,000 energy bins
    - ➢ 241 assemblies × 236 pins/assembly × 56,000 bins/pin×8 bytes/bin = 20 GB
    - ➢ Considering axial mesh, 20 GB × 36 = 720 GB (Overflow)
  - **For the coarse spectrum for each depletion domain**
    - 11,000,000 depletion domains
    - 500 energy bins
    - ➢ 11,000,000 domains × 500 bins/domain × 8 bytes/bin = 41 GB
  - ➢ **About 61 GB required in total → Yet feasible**





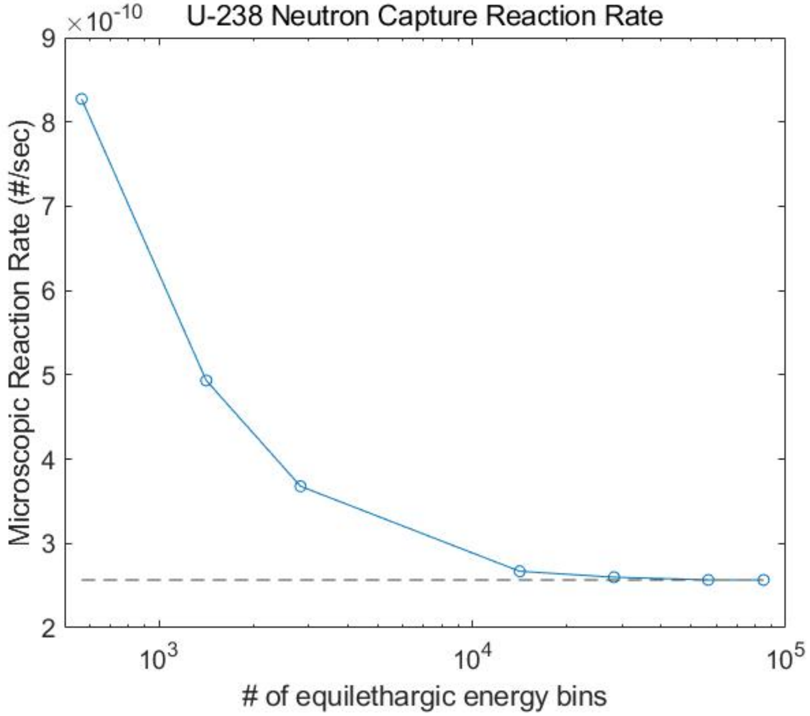
Evaluation on 2D Problems

- Fine Group Spectrum Tally
- Assembly-wise MSC
- Pin-wise MSC

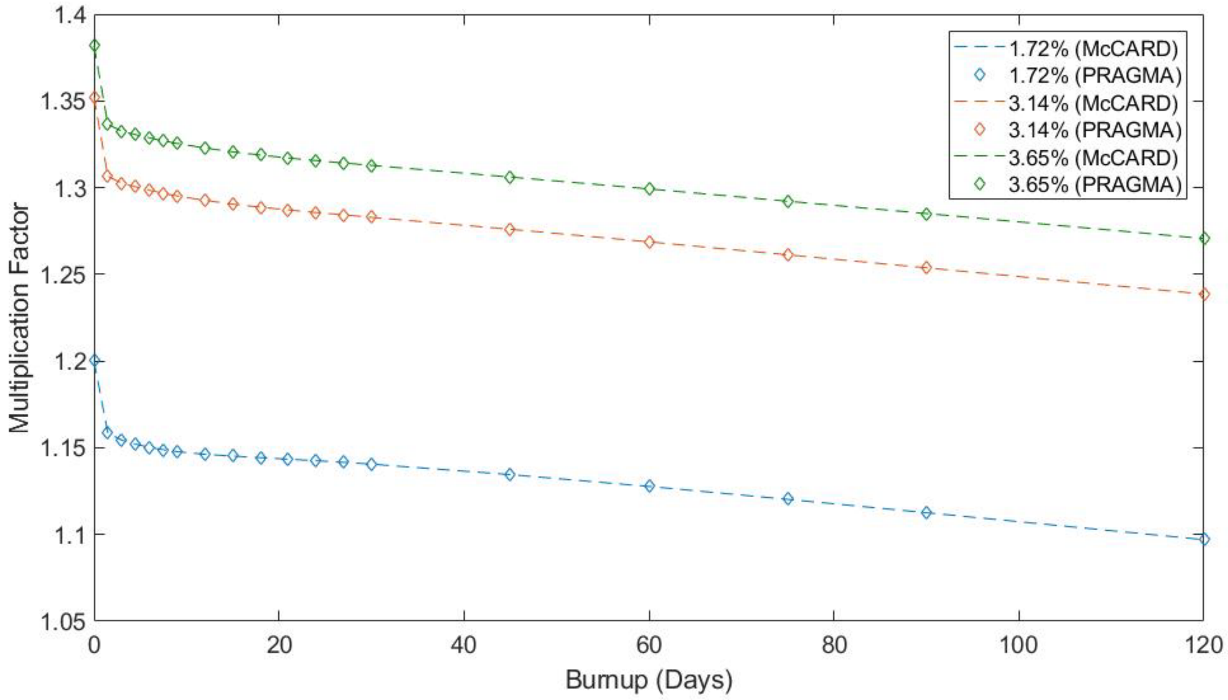
- **Comparison with Online Reaction Rate Tally (McCARD)**
  - On single pin and single region problem
  - Reference : McCARD / STD : ~ 2pcm

(yellow)	Fuel
(blue)	Moderator
(gray)	Cladding

Sensitivity of reaction rate on energy grid granularity

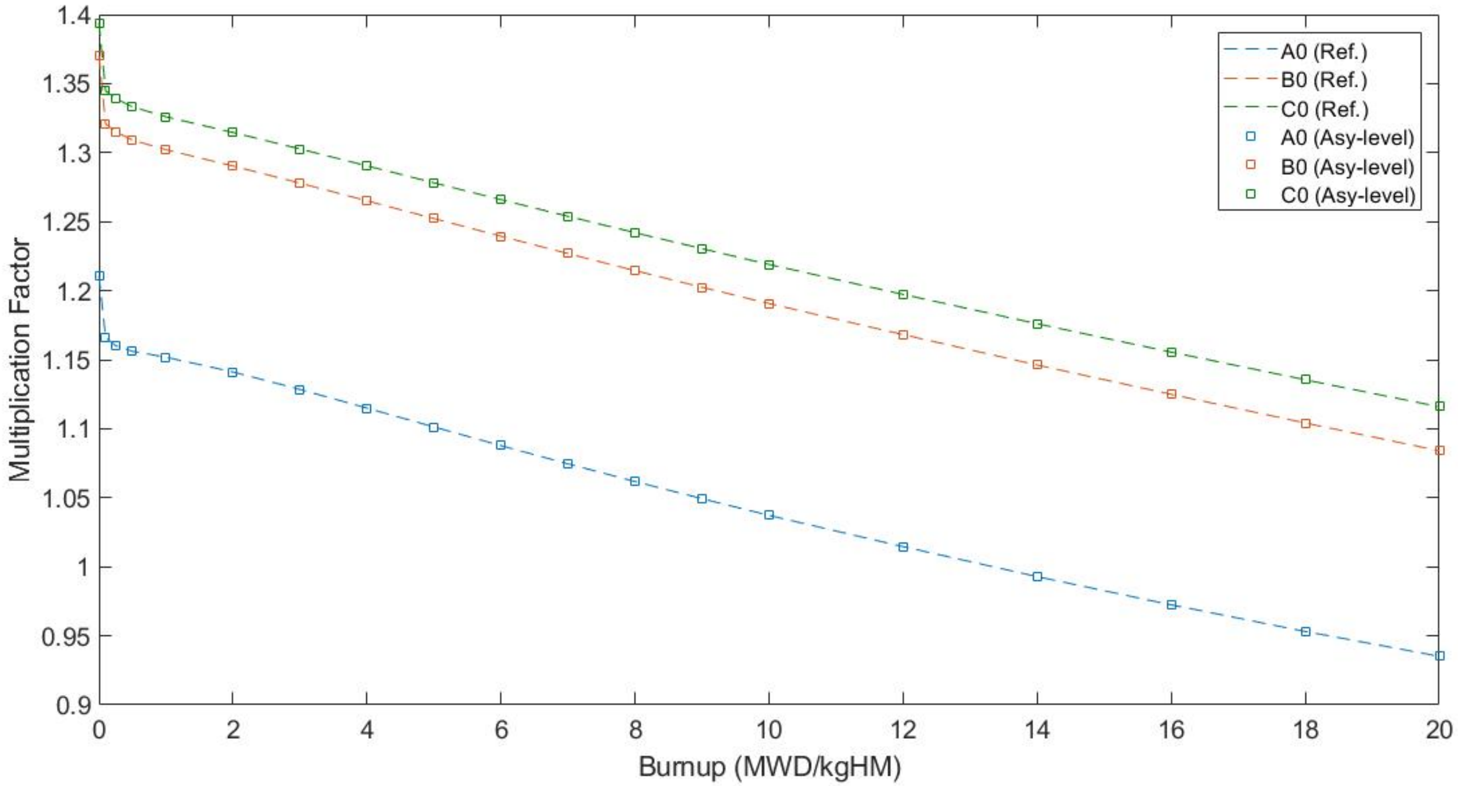


Eigenvalue comparison with McCARD



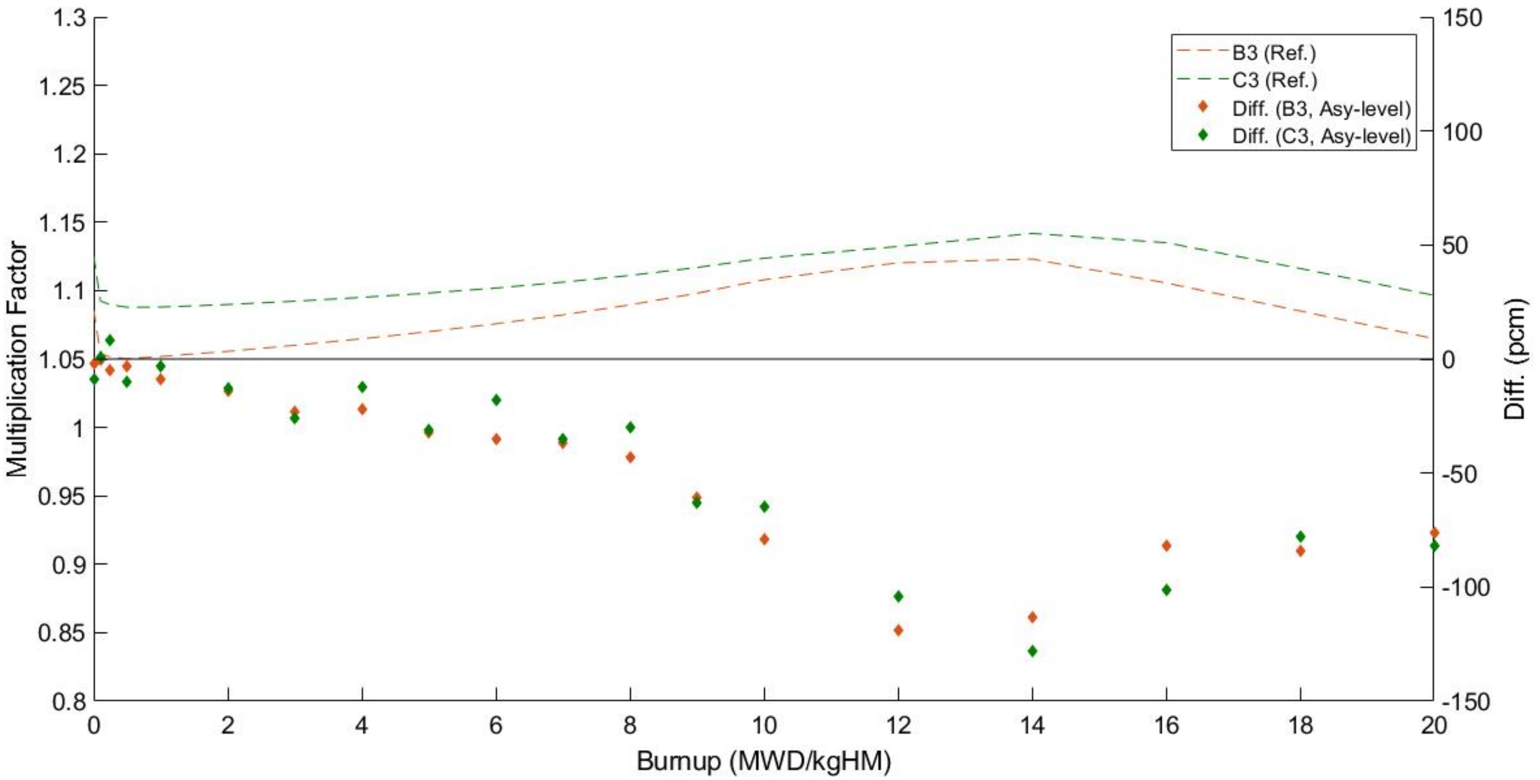
- **Accuracy Evaluation on APR1400 2D 0-type Assemblies**
  - 1000 active cycles with 1 million histories per cycle (STD ~ 2 pcm)
  - Reference : fine group spectrum tally for all depletion regions

Assembly type	Enrichment (wt%)
A0	1.72
B0	3.14
C0	3.64 / 3.14

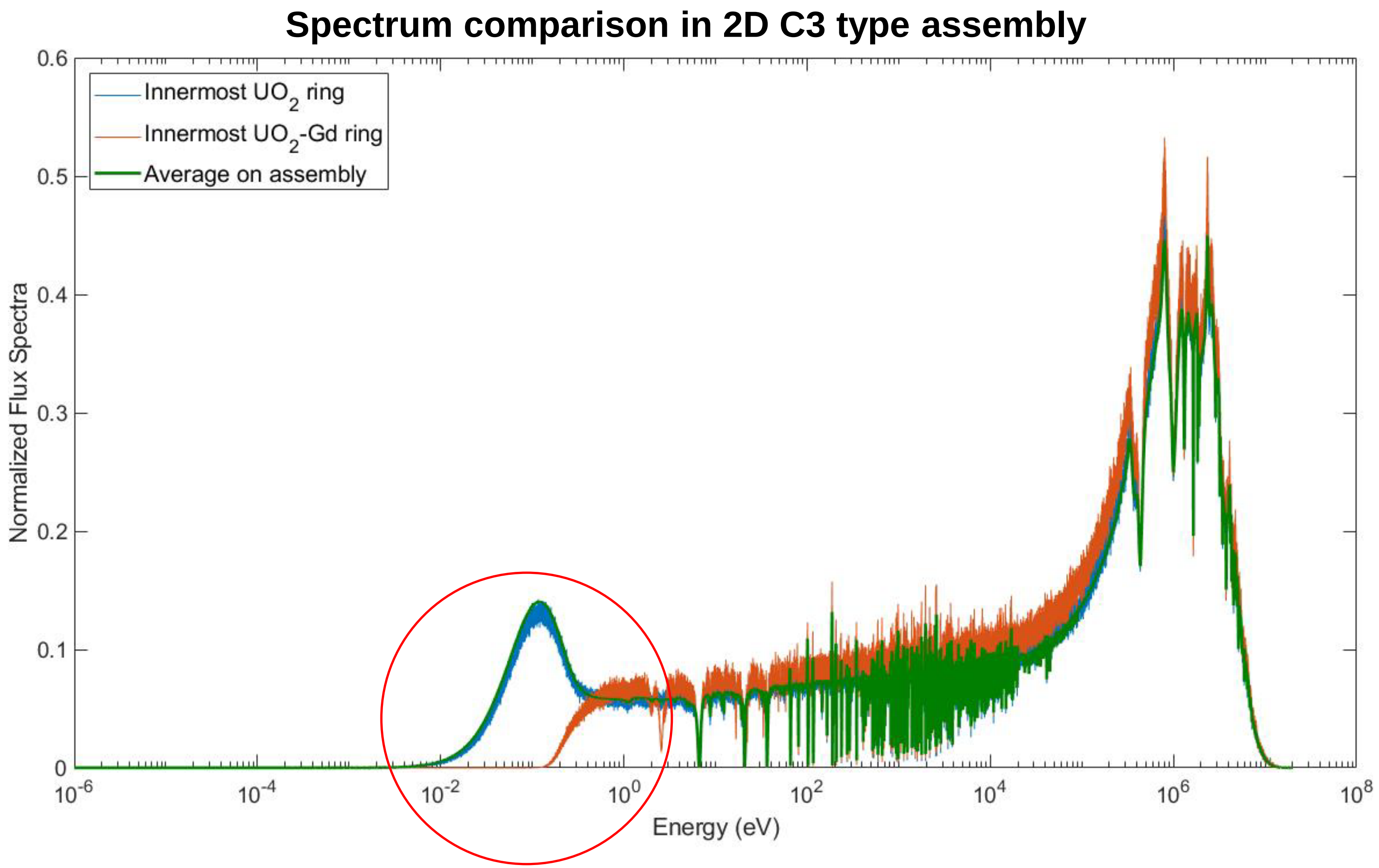


- **Accuracy Evaluation on APR1400 2D 3-type Assemblies**
  - 1000 active cycles with 1 million histories per cycle (STD ~ 2 pcm)
  - Reference : fine group spectrum tally for every depletion region

Assembly type	Enrichment (wt%)	# of Gd pins
B3	3.14 / 2.64	16
C3	3.64 / 3.14	

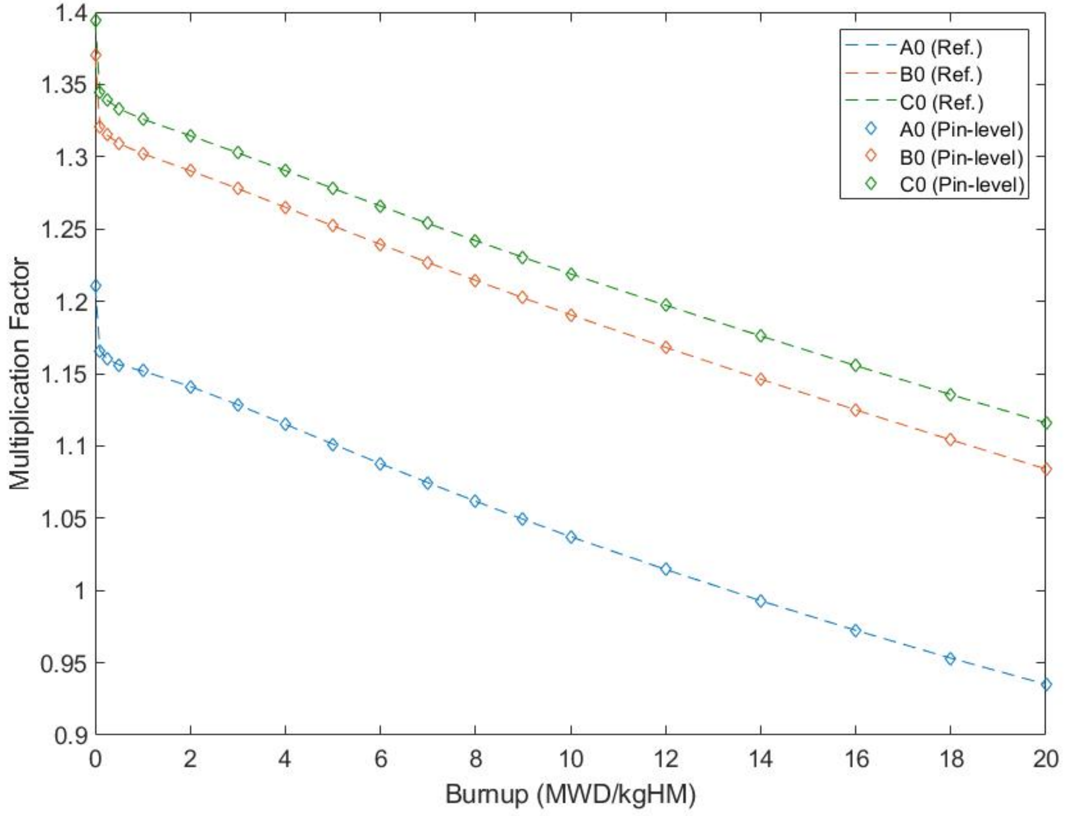


- **Spectral Difference among UO_2, UO_2-Gd Fuel Pins and Average on Assembly**

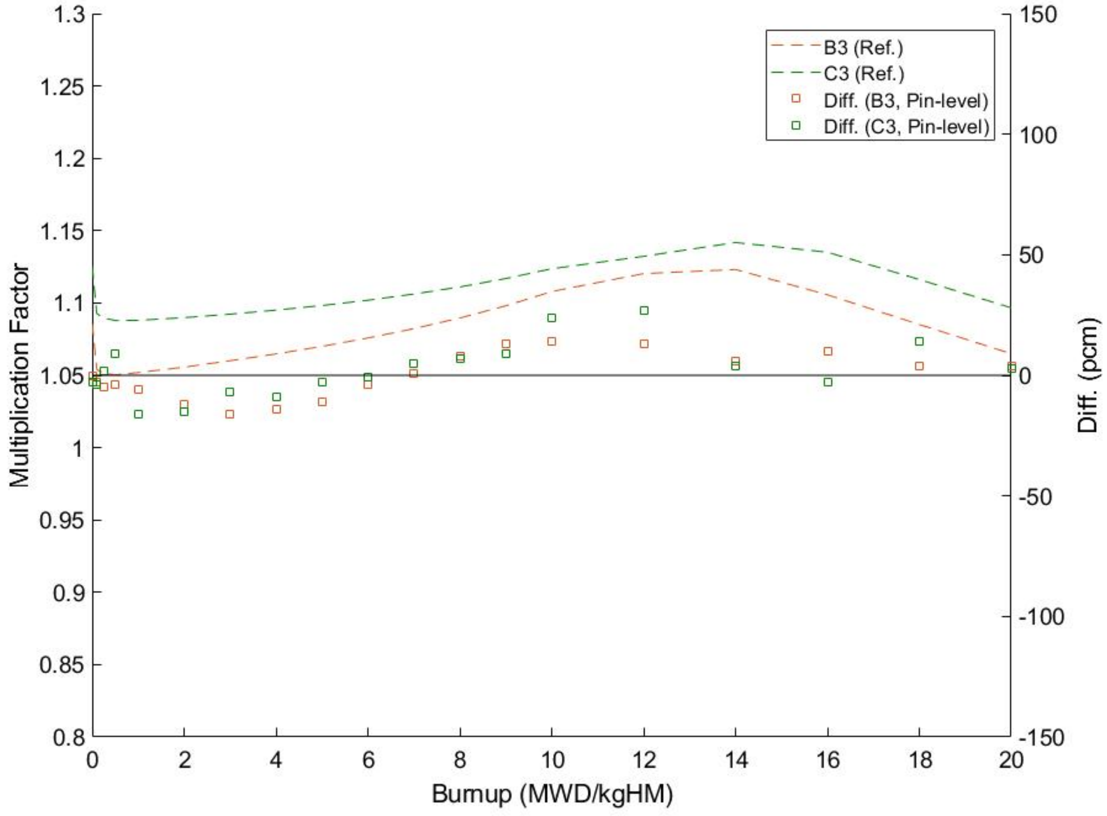


- **Accuracy Evaluation of Pin-wise MSC**
  - Same problems and conditions as previous

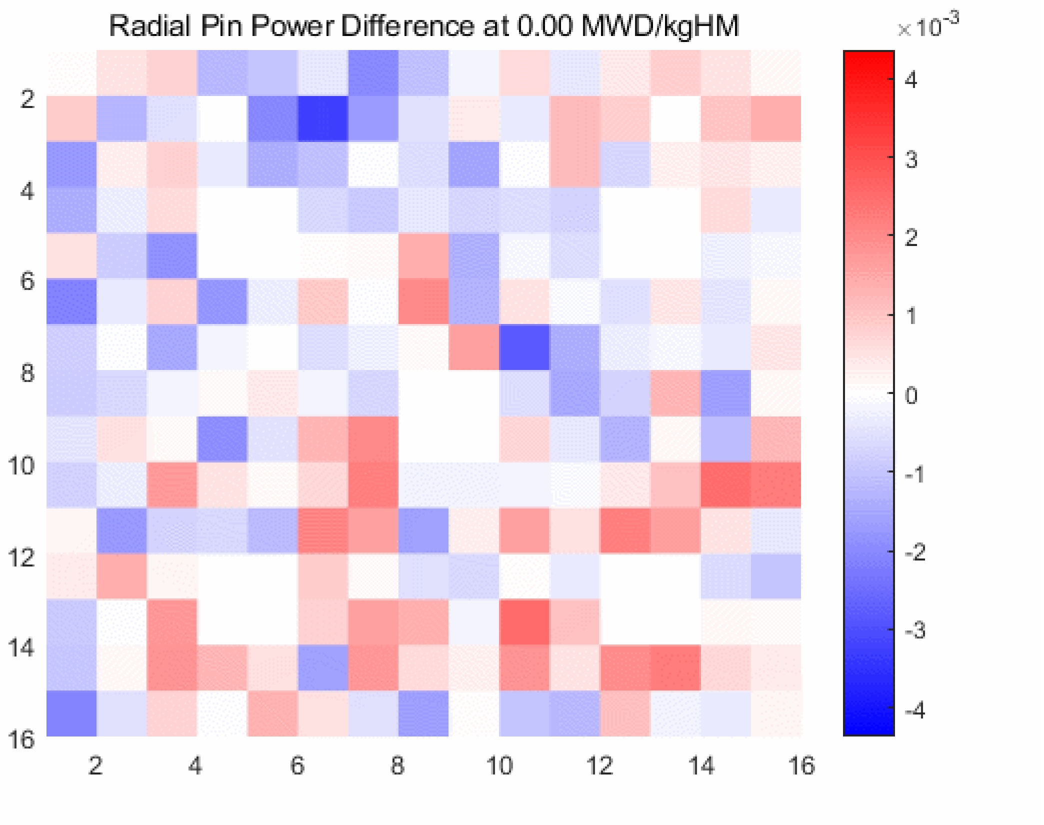
APR1400 2D 0-type assemblies

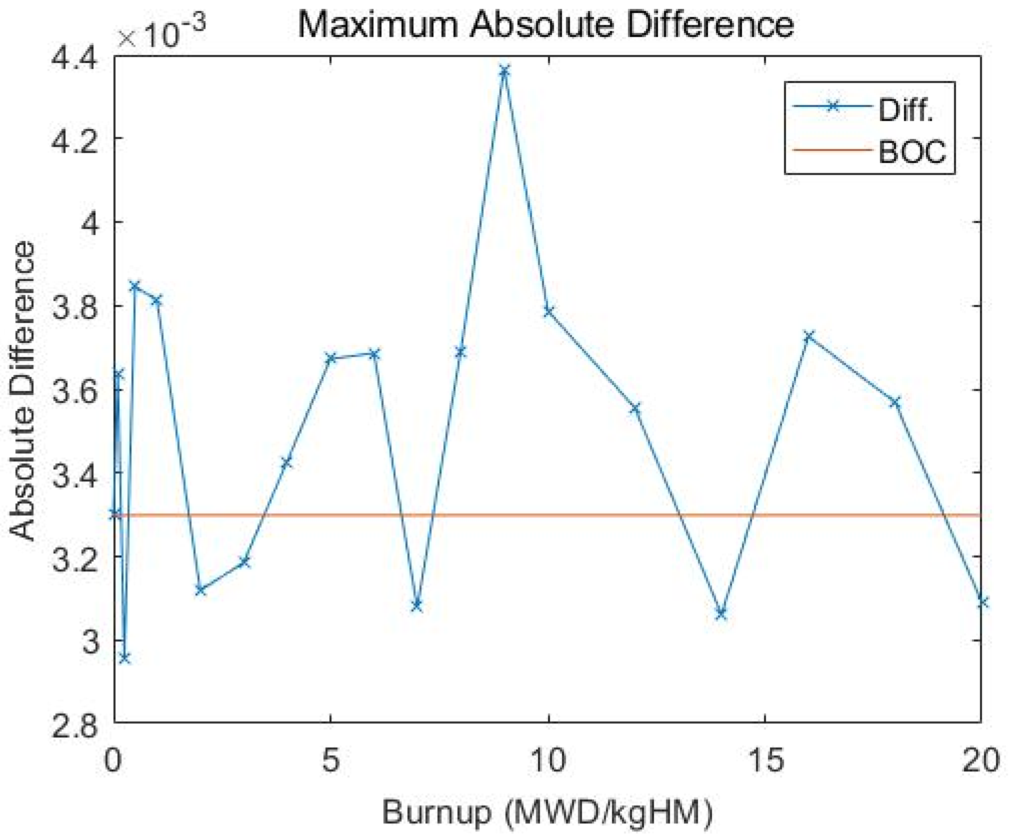


APR1400 2D 3-type assemblies



- **Pin Power Distribution Evaluation**
  - **APR1400 2D C3 assembly, STD ~ 7 pcm**



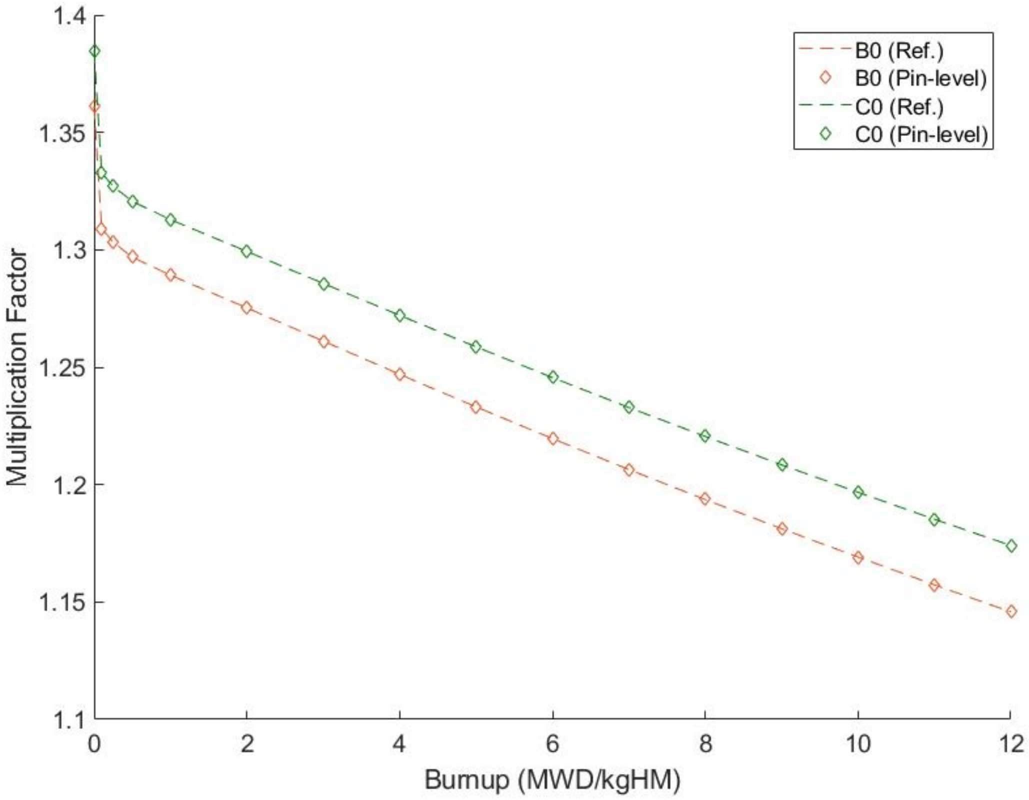


Evaluation on 3D Problem

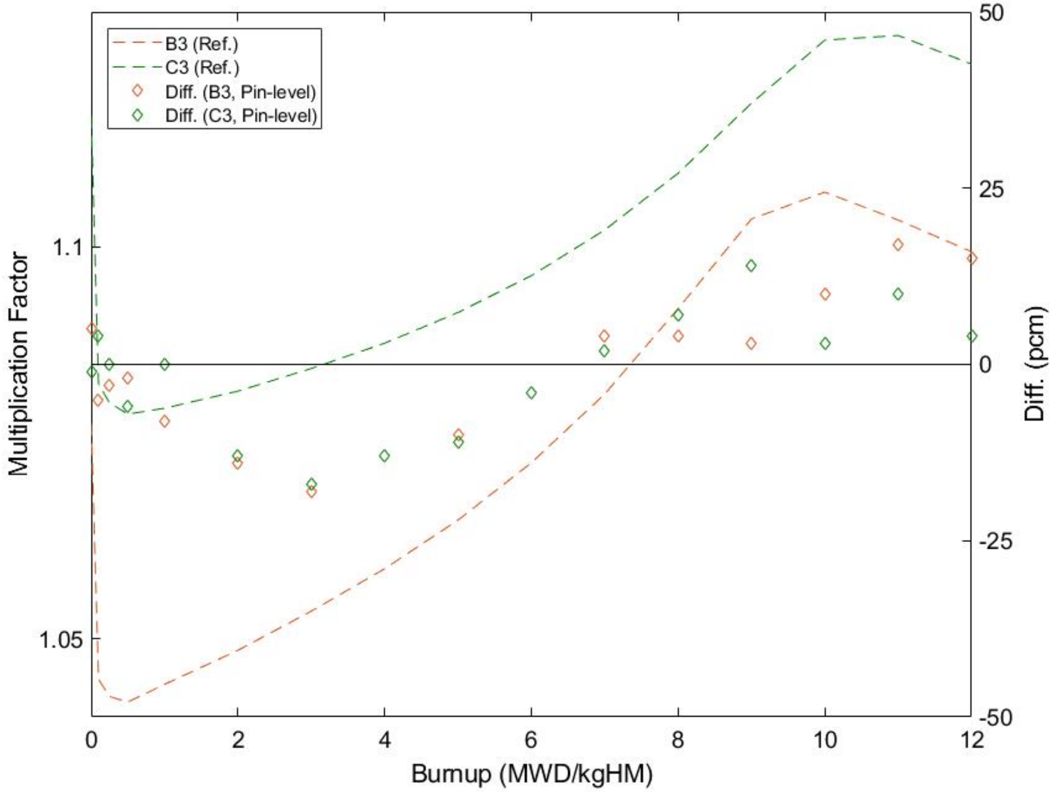
- Examination on Eigenvalue
- Examination on Axial Power

- **Pin-wise MSC on 3D Assembly Problems**
  - 250 active cycles with 4 million histories per cycle
  - Reference : fine group spectrum tally for every depletion region

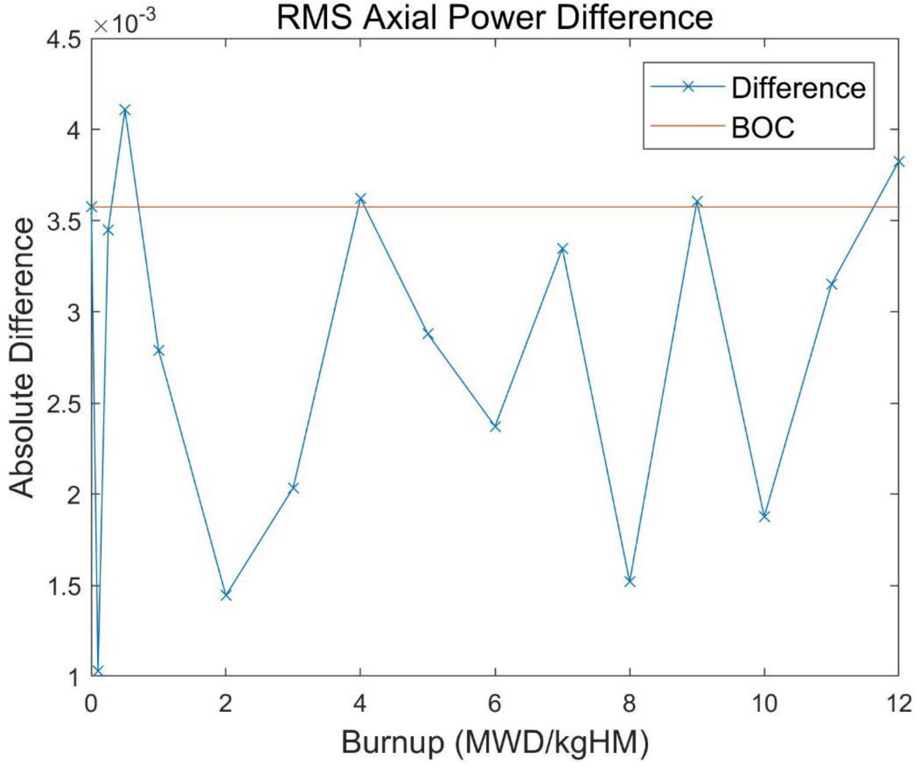
APR1400 3D 0-type assemblies

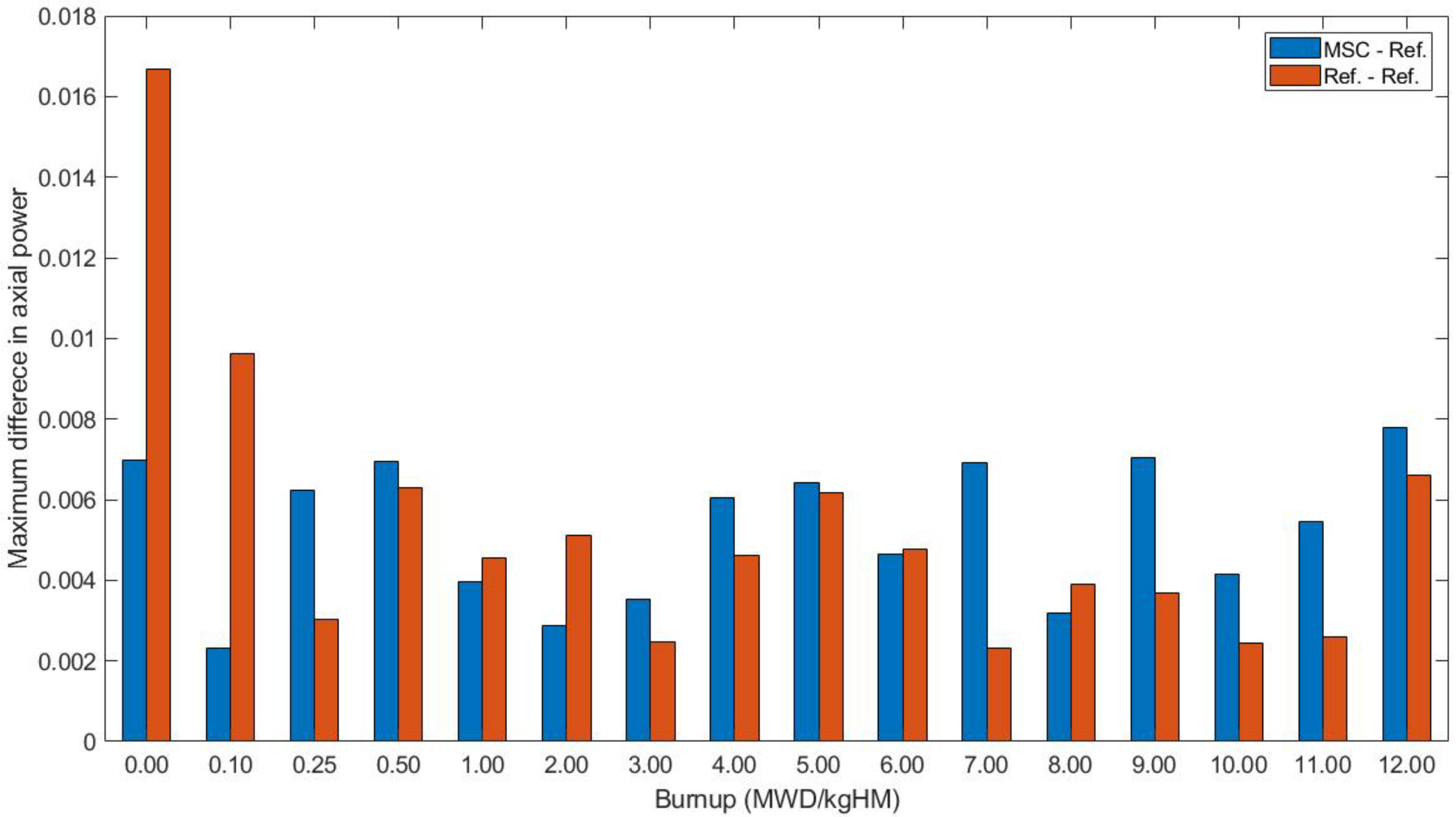


APR1400 3D 3-type assemblies



- **Axial Power Difference on Burnup**





Conclusion & Future Plan

- **Initial Development of Depletion Capability in PRAGMA**
  - **Confirmed the traditional tally methods are not feasible in our target architecture.**
  - **Developed an alternative, MSC, which employs multilevel spectra.**
    - The assembly-wise scheme requires much less memory consumption but shows inaccurate results in the burnable absorbers.
    - The pin-wise scheme needs quite large memory capacity, yet it shows good agreement in the eigenvalue and fission power.
  - **The pin-level scheme is applied for every 3D assembly problem and axial heterogeneity is not large as expected.**
- **Remaining Instability Issues in 3D Problems**
  - **Xenon equilibrium module cannot completely suppress the uncertainty from MC calculations.**
  - **Instability caused by the uncertainty triggers axial power oscillation in later burnup stages.**
  - **It requires more elaborate methods to resolve.**

- **Online Tally for Specific Reaction Types**
  - **Considered to improve accuracy in Gd-bearing problems.**
  - **Several reaction rates of Gd nuclides and significant fissile will be tallied online to enhance accuracy.**
- **Optimization**
  - **GPU porting of hotspots, such as group collapse and CRAM**
  - **Memory reduction for stable execution**
- **Whole-core Cycle Depletion**