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Verifying Burnup Calculations on Unstructured Mesh

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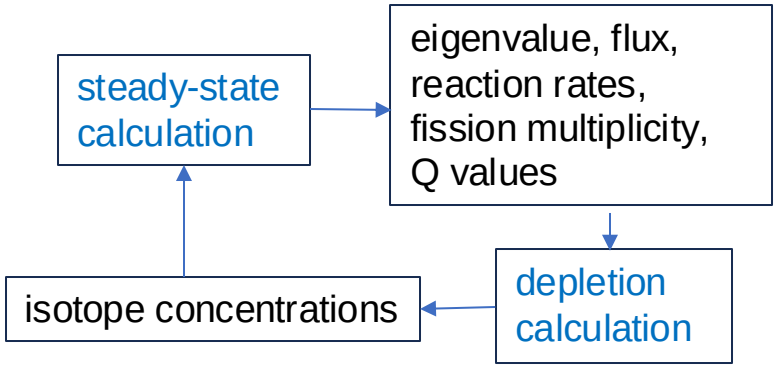
Outline

- Introduction:
  - MCNP6 Burnup Feature
  - MCNP6 Unstructured Mesh Feature
- Verify MCNP burnup calculations on unstructured mesh models
  - Unstructured Mesh (UM) geometry models VS Constructive Solid Geometry (CSG) models.
- ACTIUM
  - Coupling MCNP & CINDER2008 in AARE
- Conclusions and future works

MCNP6 Depletion/Burnup Feature

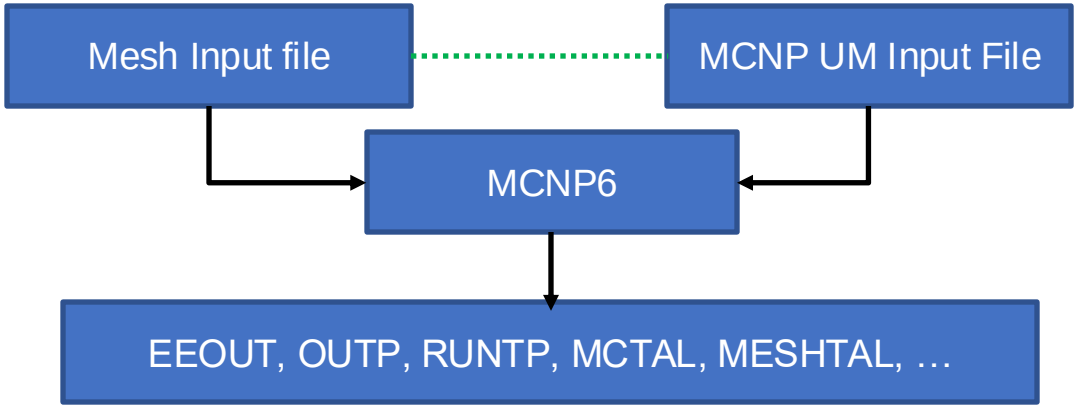
- Only for KCODE problems
- BURN card (MCNP internally links to CINDER90)
  - MCNP for steady-state flux calculations
  - CINDER90 for nuclide depletion calculations
- Limitations:
  - poor numerical stability
  - severely out-of-date data
  - not for fixed source problems



two iterations at each time-step

MCNP Unstructured Mesh (UM) Feature

- Particle transport on unstructured meshes



Mesh Input File Format:
- Abaqus Input [6.0 - 6.3 versions]
- HDF5 [6.3 version]

EEOUT (Element Edit OUTput) File Format:
- Flat File [6.0 - 6.3 versions]
- HDF5 [6.3 version]

High Fidelity Results at Elements

Burnup & Unstructured Mesh Verification

- MCNP burnup calculations on unstructured meshes are needed for advanced reactors design analysis.
  - MCNP UM calculations provide high-fidelity results that can be easily mapped to other finite element analysis codes for Multiphysics calculations.
  - MCNP burnup calculations on constructive solid geometries (CSG) were validated for many reactor applications.
  - No V&V (verification & validation) work on MCNP burnup calculations on unstructured meshes.
- Verification Approach:
  - Create equivalent MCNP CSG and UM input files.
  - Run MCNP CSG & UM calculations to compare calculation results.

Verification

Two Test Problems

- Two test problems are taken from the International Handbook of Evaluation Criticality Safety Benchmark Experiments.
  - **Godiva**: HEU-MET-FAST-001; Bare HEU sphere
  - **GodivaR**: HEU-MET-FAST-004; HEU sphere reflected by water

- CUBIT (Sandia National Laboratory's automated mesh generation toolkit) is used to create unstructured mesh models.
  - Linear hexahedral (6-face 8-node) elements

Unstructured Mesh Models

- **Godiva** (HEU-MET-FAST-001):
  - Highly Enriched Uranium (HEU) bare sphere
  - Metallic uranium with 93.71 wt. % U-235 with a radius of 8.7407 cm
  - Meshed Volume: 99.58% of HEU
  - Number of elements: 7,168

- **GodivR** (HEU-MET-FAST-004):
  - HEU sphere refracted by water
  - 97.67 wt. % U-235 with a radius of 6.55 cm
  - Reflected by a sphere of water that has a radius of 33.47 cm surrounding it
  - Meshed Volume: 99.9% of HEU and 99.8% of H2O
  - Number of elements: 127,688 HEU and 125,928 H2O

MCNP Input Setup

- **KCODE** card
  - 10,000 neutrons/cycle; total of 250 cycles; discard the first 50 cycles
  - use default for other options
- **BURN** card
  - fissile material will be depleted
  - 60 days of burnup (time steps: 1,1,1,1,1,55)
  - 1 MW power
  - use default for other options

Results: Keffective Value

- Godiva (HEU-MET-FAST-001):
  - CSG: 1.000395 ±0.00073
  - UM: 0.998231 ± 0.000703.
  - Benchmark: 1.000 ± 0.001
  - Meshed Volume: **99.58% of HEU**

- GodivR (HEU-MET-FAST-004):
  - CSG: 0.999 ±0.0006
  - UM: 0.999 ±0.0005
  - Benchmark: 0.9985 ± 0.0011
  - Meshed Volume: **99.9% of HEU and 99.8% of H2O**

Results: Isotope Compositions

- Isotopes Compositions of the fissile material after the final burnup time

- Discrepancies between the UM & CSG models are observed for the other transuranic isotopes produced upon burnup

  – Th^{230}, Pa^{231}, $U^{233,236,237,239}$, $Np^{237,238,239}$ and $Pu^{238,239,240}$

Fuel Initial Compositions

-Godiva

Uranium	Composition
U-235	93.77%
U-238	5.21%
U-234	1.03%

-GodivR

Uranium	Composition
U-235	97.69%
U-238	0.993%
U-234	1.115%
U-236	0.199%

BURN: Time steps of 1-day, 1-day, 1-day, 1-day, 1-day, and 55-days for a total of 60 days burnup. With 10,000 neutrons/cycle for 250 total cycles.

Comparing the fuel composition after Burn

- Godiva
  - CSG

		Initial	60 days	
zaid	mass (g)	atom fr.	atom fr.	% change
92235	21640.0	0.93770	0.93770	0.02132
92238	246.0	0.05207	0.05207	0.07681
92234	222.7	0.01025	0.01025	0.09756

  - UM

		Initial	60 days	
zaid	mass (g)	atom fr.	atom fr.	% change
92235	21640.0	0.93770	0.9369	0.02132
92238	246.0	0.05207	0.05275	0.07682
92234	222.7	0.01025	0.01021	0.09756

- GodivR
  - CSG

		Initial	60 days	
zaid	mass (g)	atom fr.	atom fr.	% change
92235	21640.0	0.97690	0.976400	0.05118
92234	246.0	0.01115	0.011170	0.17937
92238	222.7	0.00993	0.009945	0.20151
92236	44.32	0.00199	0.002436	22.28915

  - UM

		Initial	60 days	
zaid	mass (g)	atom fr.	atom fr.	% change
92235	21640.0	0.97690	0.976400	0.05118
92234	246.0	0.01115	0.011170	0.17937
92238	222.7	0.00993	0.009945	0.20151
92236	44.32	0.00199	0.002436	22.28915

The same change is observed for the initial fuel isotopes in both CSG and UM.

Comparing the products after Burn: Godiva

- Over only 60 days of burnup, significant difference is observed for certain isotopes.
- Difference is growing iteratively.
- Will continue to grow with more burn up.
- Burn steps 1,1,1,1,1,55 days

Atomic Fraction

Isotope	UM	CSG	% Difference
Th-230	4.76E-09	4.76E-09	0
Th-232	3.73E-10	3.83E-10	2.76618
Pa-231	1.79E-10	1.81E-10	0.720222
U-233	**2.10E-08**	**2.25E-08**	**6.408545**
U-234	1.03E-02	1.03E-02	0
U-235	9.38E-01	9.38E-01	0
U-236	1.32E-04	1.32E-04	0.075529
U-237	8.96E-08	9.01E-08	0.610162
U-238	5.21E-02	5.21E-02	0
U-239	1.89E-09	1.89E-09	0.052826
Np-237	4.57E-07	4.60E-07	0.565709
Np-239	2.73E-07	2.73E-07	0
Pu-239	4.54E-06	4.54E-06	0.022022
Pu-240	2.23E-10	2.24E-10	0.134228

Comparing the products after Burn: GodivR

- Over only 60 days of burnup, significant difference is observed for certain isotopes.
- Difference is growing iteratively.
- Will continue to grow with more burn up.
- Burn steps 1,1,1,1,1,55 days

Atomic Fraction

Isotope	UM	CSG	% Difference
Th-230	5.17E-09	5.17E-09	0
Th-232	6.80E-10	6.90E-10	1.42132
Pa-231	2.14E-10	2.15E-10	0.558399
U-233	3.96E-08	4.07E-08	2.656173
U-234	1.12E-02	1.12E-02	0
U-235	9.76E-01	9.76E-01	0
U-236	2.44E-03	2.44E-03	0
U-237	2.73E-07	2.78E-07	1.690647
U-238	9.95E-03	9.95E-03	0.010054
U-239	1.62E-09	1.58E-09	2.213789
Np-237	1.32E-06	1.34E-06	1.494768
Np-239	1.22E-10	1.24E-10	1.856336
Pu-239	2.34E-07	2.28E-07	2.232925
Pu-238	9.33E-10	9.48E-10	1.572393
Pu-239	3.87E-06	3.79E-06	1.977848
Pu-240	2.15E-09	2.11E-09	1.994302

Considerations, observations

- 1 Time step review (60 days) GodivR
- Comparing CSG and UM

- The biggest difference is observed for Th-232.
- Missing the initial smaller time step increments.

-Such as 1 day, 5 day
-Not accounting accurately for shorter lived isotopes.

Atomic Fraction

Isotope	UM	CSG	% Difference
Th-230	5.17E-09	5.17E-09	0
Th-232	7.19E-10	6.94E-10	3.66099741
Pa-231	2.23E-10	2.20E-10	1.4084507
U-233	4.20E-08	4.12E-08	2.0651118
U-234	1.12E-02	1.12E-02	0
U-235	9.76E-01	9.76E-01	0
U-236	2.44E-03	2.44E-03	0.0410509
U-237	2.69E-07	2.66E-07	1.08940646
U-238	9.95E-03	9.95E-03	0.01005429
U-239	1.59E-09	1.56E-09	1.98336532
Np-237	1.30E-06	1.28E-06	1.09119252
Np-239	1.19E-10	1.19E-10	0.25210084
Pu-239	2.30E-07	2.26E-07	1.90349712
Pu-238	8.98E-10	8.99E-10	0.18903592
Pu-239	3.83E-06	3.75E-06	1.94511058
Pu-240	2.12E-09	2.10E-09	1.0952381

Considerations, things to note

- Burn time steps 60 days vs 1, 1, 1, 1, 1, 55 days (GodivR)
- CSG, difference in UM is also observed.
- Dependent on your burn time step set up.

GodivR CSG comparison of Burn

Isotope	60 day	time steps	% Difference
Th-230	5.17E-09	5.17E-09	0
Th-232	6.94E-10	6.90E-10	0.623640
Pa-231	2.20E-10	2.15E-10	2.419730
U-233	4.12E-08	4.07E-08	1.229710
U-234	1.12E-02	1.12E-02	0
U-235	9.76E-01	9.76E-01	0
U-236	2.44E-03	2.44E-03	0
U-237	2.66E-07	2.78E-07	4.244604
U-238	9.95E-03	9.95E-03	0.000000
U-239	1.56E-09	1.58E-09	1.138520
Np-237	1.28E-06	1.34E-06	4.110613
Np-239	1.19E-10	1.24E-10	3.954802
Pu-239	2.26E-07	2.28E-07	1.094571
Pu-238	8.99E-10	9.48E-10	5.097087
Pu-239	3.75E-06	3.79E-06	1.028481
Pu-240	2.10E-09	2.11E-09	0.284900

ACTIUM

Alternative Approach: ACTIUM

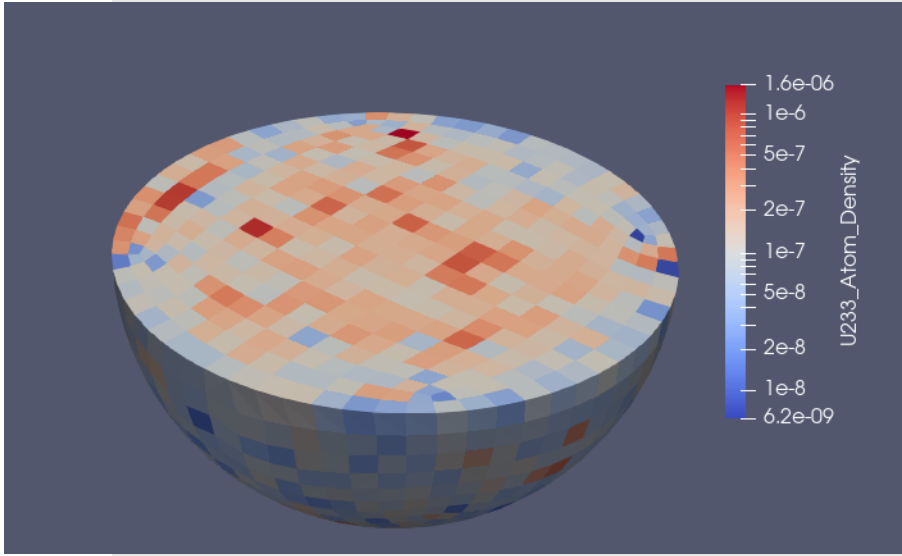
- The ACTIUM code was developed for coupling CINDER2008 as a part of the Activation in Accelerator Radiation Environments (AARE) package with MCNP6 and produce transmuted quantities per time step on an unstructured mesh.
  - ACTIUM is a Python code developed at LANL.
  - ACTIUM uses the latest ENDF/B VIII.0 cross section libraries for the transmutation calculations.

- The ACTIUM code was updated to handle HDF5 EEOUT files created by MCNP6.3.
  - This allows for post processing of the results with ParaView.

Closer look at ACTIUM

- Advantage:
  - Perform burnup at elements
  - Writes an HDF5/XDMF file with atomic composition at elements
  - Visualization in ParaView
  - ENDF/B VIII.0 cross section

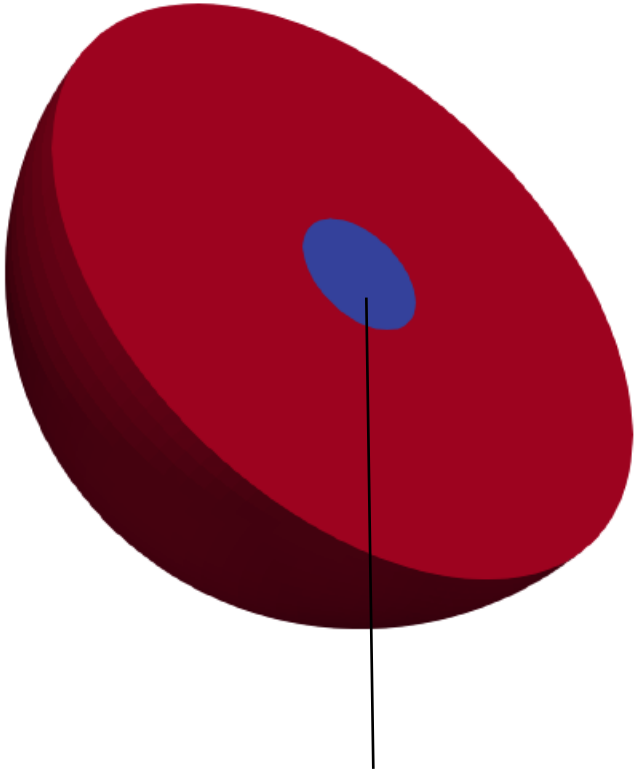
- Limitations:
  - Poor performance for models with large number of elements
  - One time step only



Atom Density for U-233 after 60 day burn period for Godiva using MCNP Actium

Benefit of ACTIUM approach:

- ACTIUM provides the material composition at elements
- CSG provides the average result on the cell.
- Current UM capabilities of MCNP provide the average result of the Pseudo-cell.

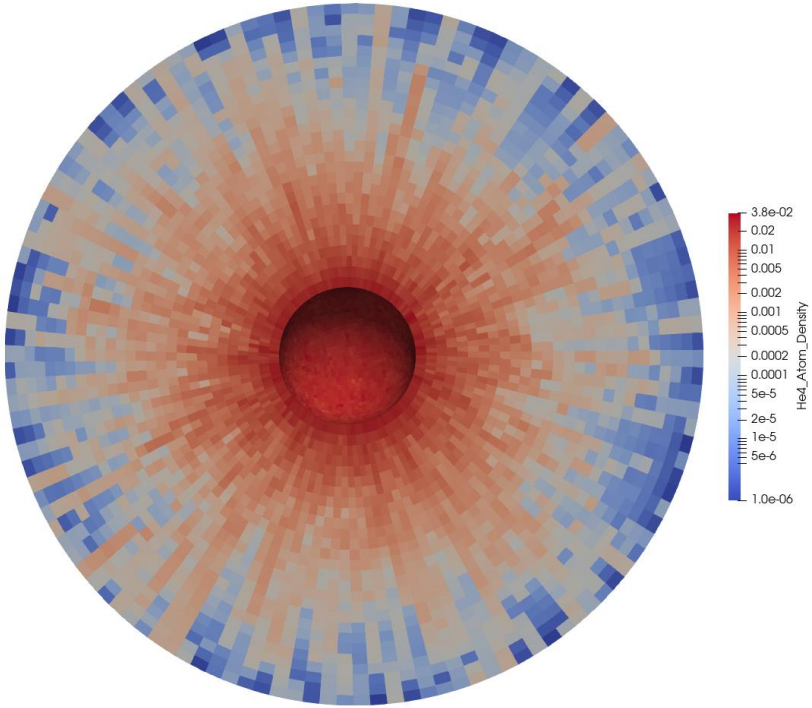


U-233 Atom Density (2.25E-08) post burn
(HEU in blue) –for GodivR
(H2O in red)

Benefit of ACTIUM approach:

- UM can interrogate individual sections within a cell.
- Closer look at each isotope.

- $^{4}_{2}He$, alpha from decay and activation resulting from neutron capture.



Atom Density for $^{4}_{2}He$ after 60 day burn period for GodivR (H2O region) using ACTIUM (MCNP/CINDER2008)

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Conclusions & Future Work

MCNP6, which internally links to CINDER90, does not output material compositions at elements for unstructured mesh calculations.

ACTIUM (MCNP/CINDER2008) can be used for depletion calculations on unstructured mesh and output material compositions at elements.

- Very poor performance for large number of elements when using ACTIUM. Example: 150k elements took over a week to run.

Future work:

- Refactor ACTIUM to fix performance.
- Integrate CINDER2024 in ACTIUM.

References

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[2] Josey, “The Status of Accelerator Transmutation Modelling within the MCNP Code”, LA-UR-24-22232, Los Alamos National Laboratory (2024).

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[4] Gonzalez et al., “MCNP6.3 Unstructured Mesh Verification: GodivR and CANDU Models”, LA-UR-22-33091, Los Alamos National Laboratory (2022).