MOCUM Verification with a Heterogeneous MOX Whole Core C5G7 Benchmark Problem

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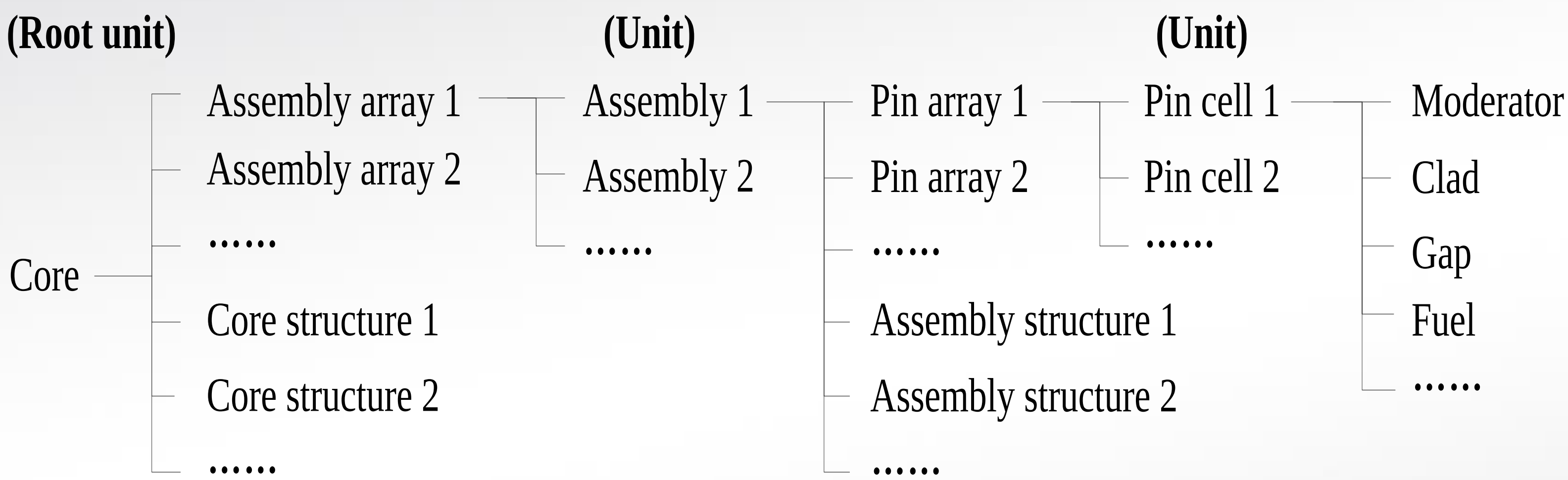
Overview

- MOCUM
- Past research works
- Research objective/significance
- Methodology
  - benchmark description,
  - Single UO_2 test assembly,
  - Whole core benchmark model
- Result and discussion
- Conclusion
- Future work

MOCUM Code

MOCUM [1-4]: <u>M</u>ethod of <u>C</u>haracteristics <u>U</u>nstructured <u>M</u>eshing

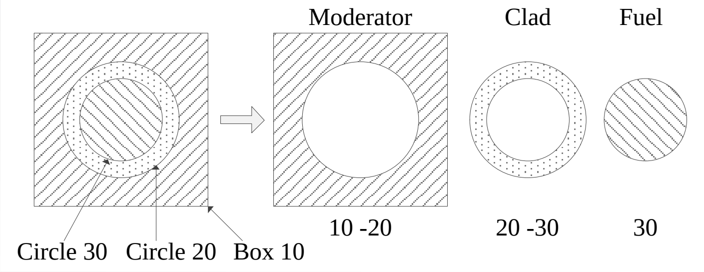


Hierarchical tree structure for organizing and storing the CSG objects.

1) Yang, Xue, Rajan Borse, and Nader Satvat. “MOCUM solutions and sensitivity study for C5G7 benchmark.” *Annals of Nuclear Energy* (2016): In Press.
2) Yang, Xue, and Nader Satvat. "MOCUM solutions to the 2-D hexagonal HTTR benchmark problems." *Annals of Nuclear Energy* 56 (2013): 102-108.
3) Yang, Xue, and Nader Satvat. "MOCUM: A two-dimensional method of characteristics code based on constructive solid geometry and unstructured meshing for general geometries." *Annals of Nuclear Energy* 46 (2012): 20-28.
4) Yang, Xue and Nader Satvat. “MOCUM: A two-dimensional method of characteristics code based on unstructured meshing for general geometries.” Paper presented at International Conference on the Physics of Reactors 2012, *PHYSOR 2012: Advances in Reactor Physics*, v 1, p 502-516, Knoxville, TN, April 15-20, 2012.

MOCUM Geometry Processor

- The Computational Geometry Algorithms Library (CGAL) [7].
- Geometry object organization
  - Primitives: circle, box, hexagon, polygons;
  - Units: box or hexagon
    - Contains several primitives;
    - Material regions are defined by Boolean operation
  - Arrays: rectangular or hexagonal
    - Special primitive
    - Can Participate Boolean operation
    - One unit can contain other units by using the array command

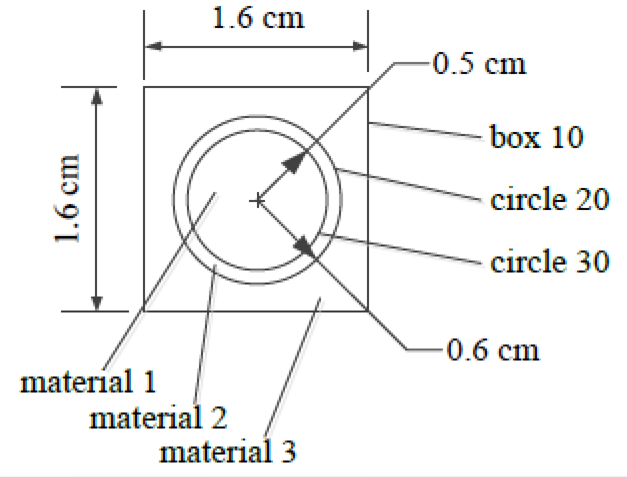


A unit cell composed by three CSG objects [6]

```
unit 1
box 10 0 1.6 0 1.6
circle 20 0.8 0.8 0.6
circle 30 0.8 0.8 0.5
media 3 10 -20
media 2 20 -30
media 1 30
boundary 10
```

```
unit 2
box 10 0 1.6 0 1.6
circle 20 0.8 0.8 0.6
circle 30 0.8 0.8 0.5
media 3 10 -20
media 2 20 -30
media 4 30
boundary 10
```

```
unit 0
box 10 0 6.4 0 6.4
array 111 box 4 4 lowerleft 0 0
1 1 1 1
1 2 1 1
1 1 2 1
1 1 1 1
media 0 111
boundary 10
@end
```



Unit cell example [8]

5. http://www.cgal.org/
6. Xue Yang, ‘user manual for MOCUM v.1.0.0’, school of nuclear engineering, Purdue University. August, 2012.

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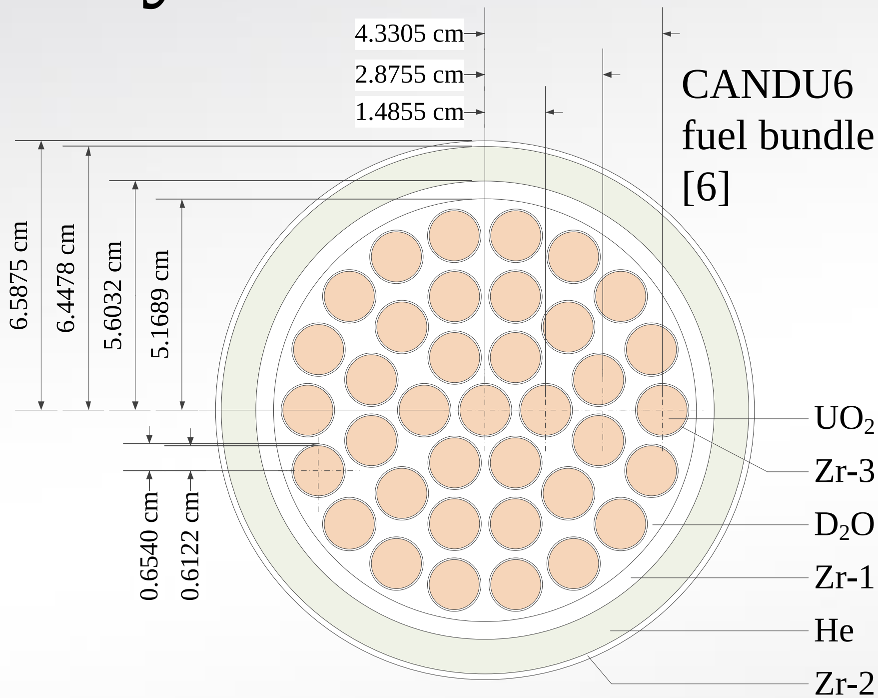
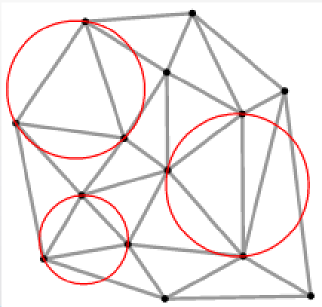
MOCUM Geometry Processor

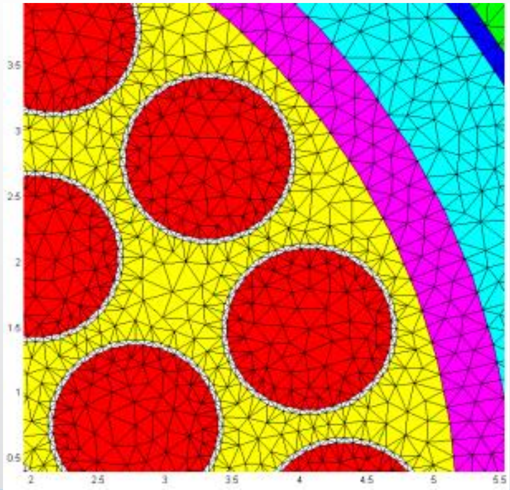
- Geometry object organization
  - All material regions are represented by CGAL “polygon with holes”.
- Delaunay triangulation with constrains
  - Circumscribing circle of any triangle contains no vertex of other triangles in its interior.
  - No thin triangle produced
  - Triangle size is controlled by a single variable limiting the side length of all triangles.
- The mesh file will be generated for plotting and subsequent MOC calculation.



CANDU6 fuel bundle [6]

Delaunay triangulation example. http://doc.cgal.org/latest/Triangulation_2/ [8]





A magnified view of the unstructured meshing of a CANDU fuel bundle [6]

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MOCUM Flux Solver

- MOC based program
- Ray tracing using neighbor information
  - Find one intersecting mesh
  - Walk along the neutron trajectory
- Parallel computing
  - OpenMP nested loops for energy group and azimuthal angle
  - Max number of threads = energy groups * azimuthal angles

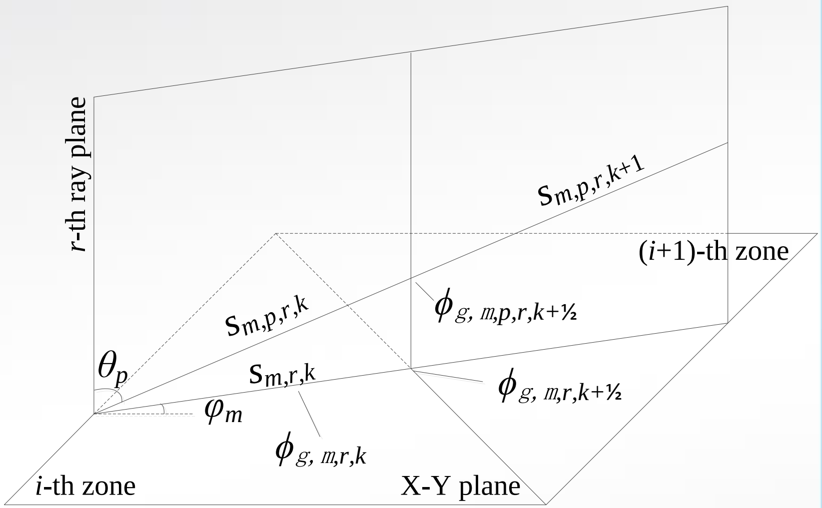
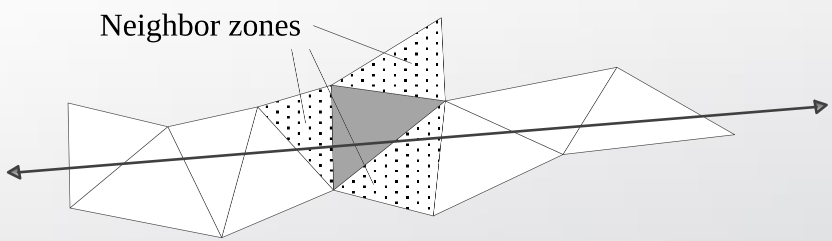


Illustration of the MOC spatial discretization [6]



Fast ray tracing scheme using neighbor information [6]

Past research works

1. In 2012, Yang and Satvat verified the capabilities and accuracy of MOCUM code by using it to solve different benchmark set [5]. These include:

   - BWR lattice with adjacent gadolinium burnable poison pins, (The percentage error between MOCUM and Reference DRAGON results was 0.12% for the multiplication factor, maximum relative error for pin power is 0.15%).

   - CANDU-6 type annular cell, (The percentage error between MOCUM and Reference DRAGON results was -0.13% for the multiplication factor, pin power maximum relative error per ring was 0.31%).

2. In 2013, Yang and Satvat solved a two dimensional (2-D) hexagonal High Temperature Test Reactor (HTTR) using MOCUM code [4]. (The *k*eff from MOCUM for the three different cases tried i.e. case 1, case 2, and case 3 are 0.8962, 1.00395, and 1.09113 respectively).

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Research objective/Significance

- The objective of this research is to use the MOCUM program to solve the whole core, highly heterogeneous MOX benchmark problem, so as to determine its efficiency in solving complicated reactor benchmarks
- Results in previous research works have shown the accuracy of MOCUM in solving reactor problems. Some of these models are the BWR lattice, CANDU-6 fuel bundle, plate-type fast reactor, VHTR hexagonal fuel, etc. [3]. However, the capability of MOCUM in solving the complex MOX C5G7 benchmark problem that represents a real reactor core has not been fully tested. Successfully carrying out this work will further establish the high-level of accuracy and efficiency of the MOCUM code.

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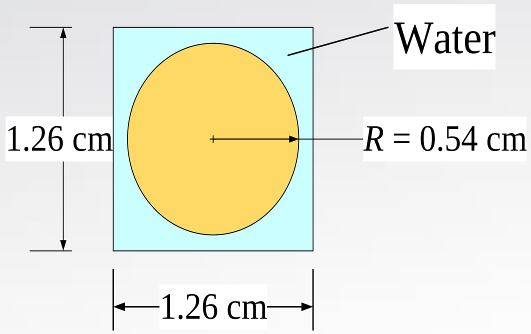
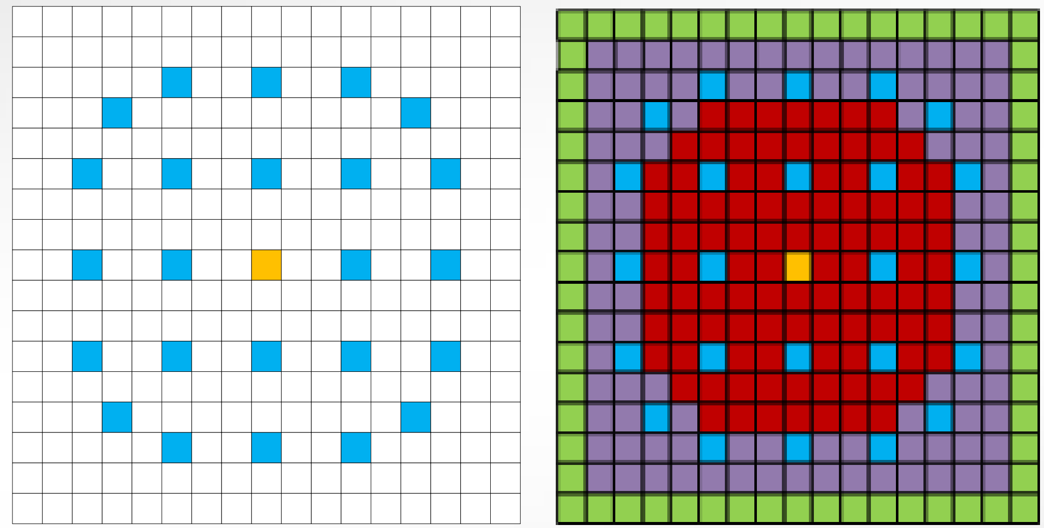
Methodology (benchmark description)

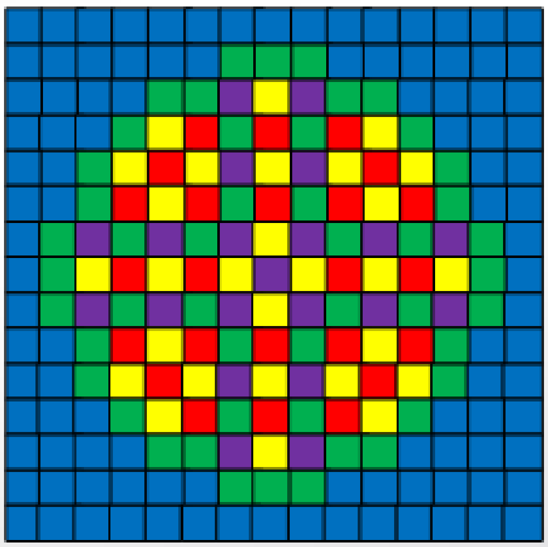


Layout of all unit cells [8]



Fuel assembly configuration. Left: UO_2 assembly; Right: MOX assembly. [2]

Legend:- Green: 4.3% MOX fuel; Violet: 7.0% MOX fuel; Red: 8.7% MOX fuel; Blue: Control rod; Orange: Fission chamber.



Legend:- yellow: controlled MOX assembly (24); purple: controlled UO_2 assembly (21); red: uncontrolled MOX assembly (28); green: uncontrolled UO_2 assembly (48).

Core Configuration of the MOX whole core. [2]

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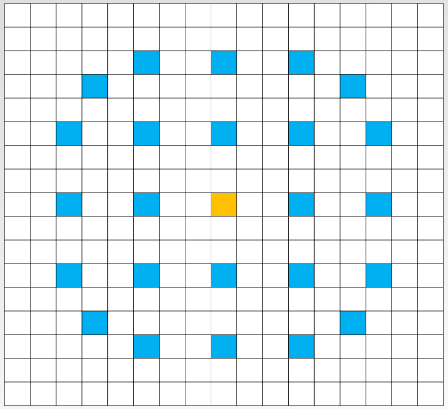
MOCUM Input structure

MOCUM

Input geometry file is divided into sections,

- geometry card section starts with @geo-def and ends with @end. Consists of several number of units to fully specify the geometry.
- The triangulation option specify the mesh input data. Starts with @geo-opt and ends with @end. Produce a temporary. core_diagnosis file. MOCUM-UM produces a mesh file with name inputname.mesh , containing the vertex coordinates and neighbor information.
- The macroscopic cross-section, read by MOCUM-MOC card starts at @xs and ends with @end. Provides information about the number groups, number of materials and the material compositions.
- MOC parameters section; the last part of the input structure in MOCUM. Starts @solver and ends with @end. Information such as the merge flux, plot distribution, azimuthal angles, number of threads, ray density, polar angle, convergence criterion and boundary conditions are specify here.

Single UO_2 test assembly



UO_2 Fuel assembly;

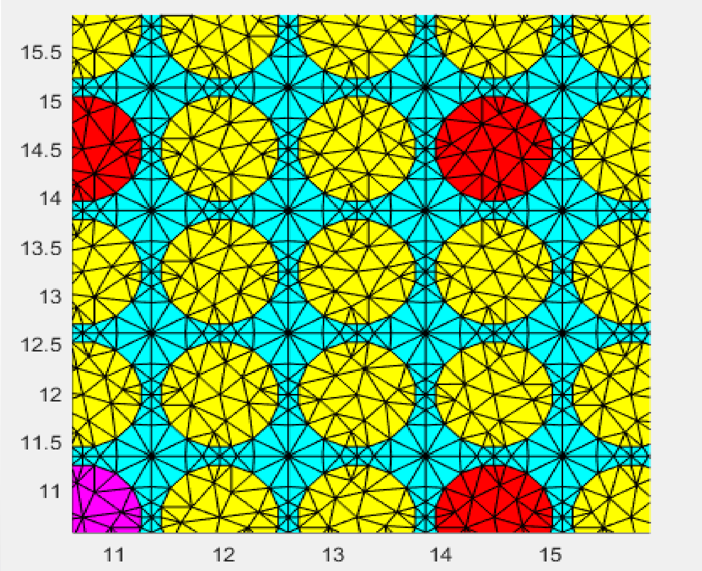
MOCUM k_{eff}, percentage error, and runtime.

MOCUM – Eigenvalue (k_{eff})	0.3877
MCNP6 Eigenvalue (k_{eff})	0.3874 $\pm$ 0.00038
Relative Difference	0.077%
Runtime in MOCUM (mins)	4.65

Optimum MOC parameters used for single UO_2 test assembly calculation.

Pin Pitch	1.26 cm
Fuel Pin / Guide tube / Control Rod Radius	0.54 cm
Assembly Pitch	21.42 cm
Shape Criterion	0.125
Circle-Side	16
Number of Energy groups	7
Number of threads for parallel computing	21
Number of Materials	8
Number of Azimuthal Angles	48
Number of Polar Angles	3
Ray Density	200 cm^{-1}
Convergence Criterion	1e-8
Number of Threads for Azimuthal Angle Parallelization	12

Dual Intel Xeon E5-2699 v3



magnified view of the unstructured meshes of the UO_2 assembly (units: cm)

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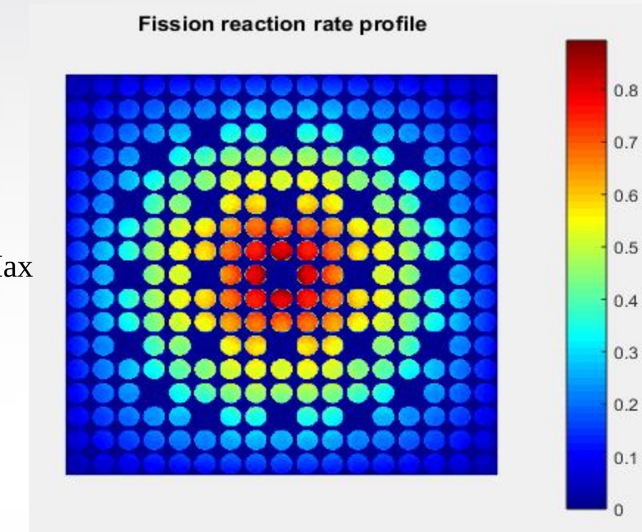
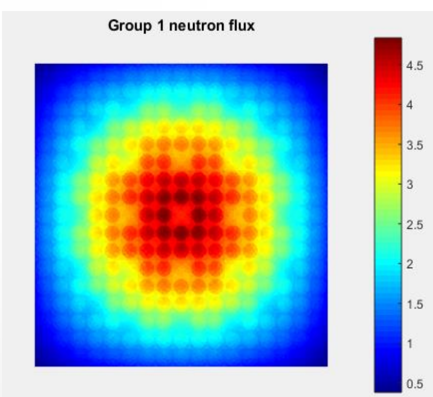
UO_2 fission reaction rates

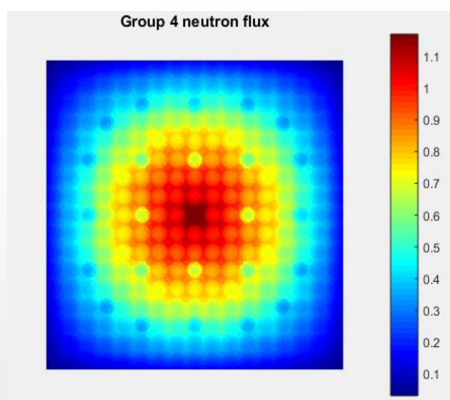
Percentage relative error; pin fission rates between MOCUM and MCNP6 for the UO_2 assembly

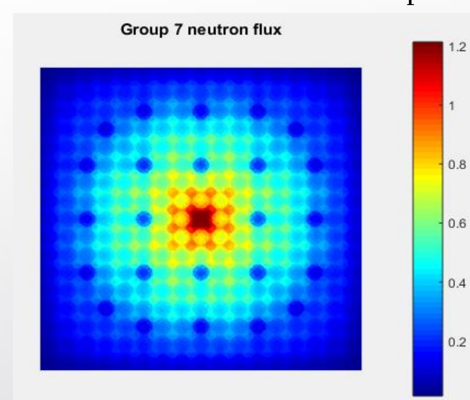
-0.1%	-0.1%	-0.1%	0.0%	-0.1%	-0.1%	0.0%	-0.1%	-0.1%	
	-0.5%	0.4%	0.2%	0.6%	0.0%	-0.4%	-0.3%	-0.8%	Max
		0.3%	-0.2%	0.1%	0.4%	-0.8%	-0.7%	0.2%	
			0.0%	0.0%	0.0%	0.0%	-0.4%	-0.2%	
				-0.6%	0.0%	0.1%	-0.7%	-0.1%	
					0.0%	0.4%	0.4%	0.3%	
						2.2%	0.4%	0.4%	
							1.1%	-0.7%	
								-0.2%	



Fission reaction rate profile (UO_2 assembly)







MOCUM Neutron flux profiles (Energy group 1, 4, 7)

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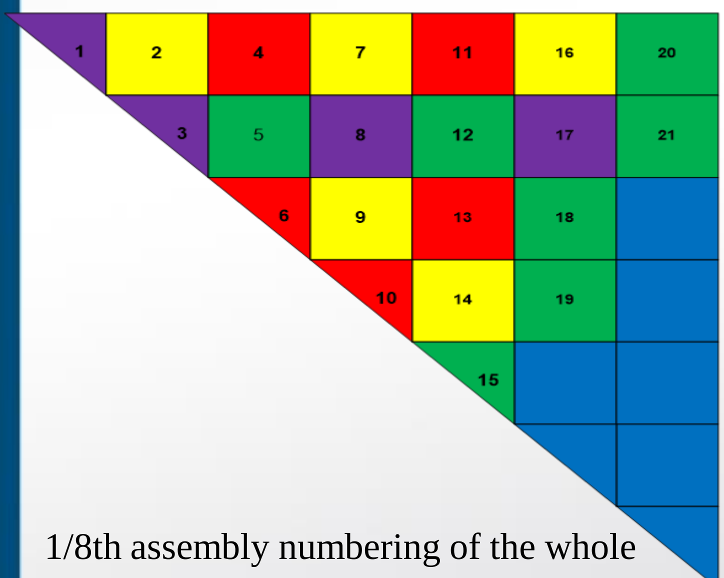
Whole-core benchmark model

MOCUM parameters used for whole-core model

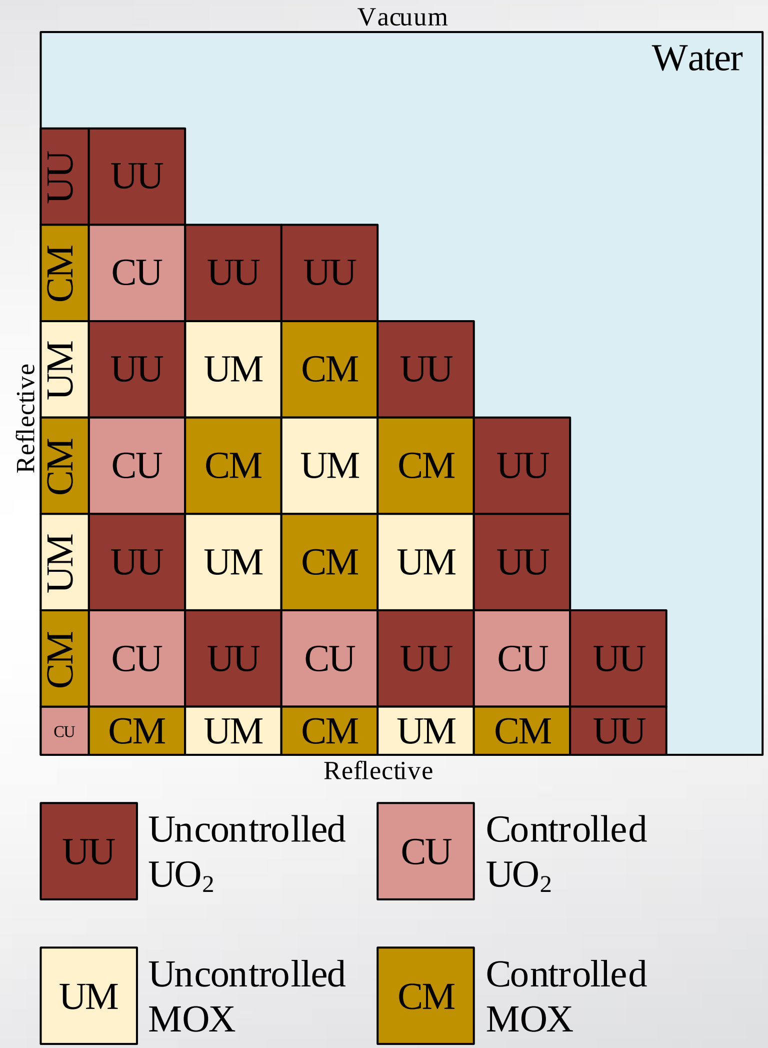
Number of meshes in one fourth core	1648581
Average mesh size	$0.0157 cm^2$
Number of Energy Groups	7
Number of threads for parallel computing	48
Number of Materials	8
Number of Azimuthal angles	48
Number of polar angles	3
Ray Density	$100 cm^{-1}$
Convergence Criterion	10^{-8}



1/8th assembly numbering of the whole core

Whole-core materials composition:

1. UO_2 Fuel,
2. 4.3% MOX fuel,
3. 7.0% MOX fuel,
4. 8.7% MOX fuel,
5. Control rods,
6. Guide tubes,
7. Fission chamber,
8. Moderator.



quarter core loading arrangement.

Number of fuel assemblies in 1/4th core - 37

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Results (k_{eff} & assembly power)

MOCUM – Eigenvalue (k_{eff})	1.12593
MCNP6 – Eigenvalue (k_{eff})	1.12621
Relative Difference	-0.025%
MOCUM Runtime (hours)	8.67
MCNP6 Runtime (days)	7

*k*eff results between MOCUM and MCNP6 for whole-core

MCNP6 assembly results after normalization

0.12	0.65	0.55	0.62	0.46	0.53	0.48
0.00	0.57	1.70	1.02	1.39	0.79	0.75
0.00	0.00	0.50	1.02	0.78	0.97	0.00
0.00	0.00	0.00	0.32	0.82	0.72	0.00
0.00	0.00	0.00	0.00	0.36	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00

*Data marked in yellow signify the region of the 1/8th core symmetry

MOCUM assembly results after normalization

0.11	0.64	0.54	0.62	0.46	0.53	0.49
0.00	0.56	1.69	1.01	1.39	0.79	0.75
0.00	0.00	0.50	1.02	0.78	0.98	0.00
0.00	0.00	0.00	0.32	0.83	0.73	0.00
0.00	0.00	0.00	0.00	0.37	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00

Percentage relative error; assembly fission rates between MOCUM and MCNP6 for whole-core (%)

-1.79	-1.26	-0.82	-0.56	-0.19	0.09	0.34
0.00	-1.04	-0.59	-0.41	0.04	0.22	0.62
0.00	0.00	-0.38	0.00	0.38	0.76	0.00
0.00	0.00	0.00	0.33	0.88	1.18	0.00
0.00	0.00	0.00	0.00	1.22	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00

*Data marked in blue signify the region of the 1/8th core symmetry

Max rel. diff assembly = -1.79%
Max pin power MOCUM = 2.21
Max pin power MCNP6 = 2.23
Max rel. diff. pin power = -2.53%

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Results (Fission rates for Assembly 5 pins)

1.35	1.37	1.40	1.42	1.44	1.46	1.45	1.45	1.46	1.44	1.44	1.44	1.41	1.39	1.36	1.34	1.31
1.51	1.56	1.61	1.66	1.71	1.79	1.73	1.73	1.79	1.72	1.71	1.77	1.68	1.63	1.57	1.51	1.46
1.60	1.68	1.78	1.92	1.98	0.00	1.97	1.97	0.00	1.96	1.95	0.00	1.94	1.88	1.73	1.63	1.55
1.66	1.77	1.96	0.00	2.09	2.09	1.99	1.99	2.07	1.98	1.97	2.06	2.05	0.00	1.90	1.71	1.60
1.70	1.84	2.05	2.12	2.08	2.15	2.06	2.05	2.14	2.04	2.03	2.11	2.03	2.06	1.98	1.77	1.63
1.73	1.94	0.00	2.14	2.17	0.00	2.18	2.18	0.00	2.17	2.15	0.00	2.11	2.07	0.00	1.86	1.65
1.73	1.89	2.07	2.05	2.09	2.19	2.12	2.12	2.20	2.10	2.09	2.15	2.03	1.98	1.99	1.80	1.64
1.74	1.90	2.08	2.06	2.10	2.21	2.13	2.13	2.22	2.12	2.10	2.16	2.03	1.98	1.99	1.80	1.64
1.76	1.98	0.00	2.15	2.19	0.00	2.23	2.23	0.00	2.21	2.19	0.00	2.12	2.06	0.00	1.87	1.65
1.76	1.91	2.09	2.07	2.11	2.22	2.13	2.13	2.22	2.12	2.09	2.15	2.03	1.97	1.98	1.79	1.64
1.77	1.92	2.10	2.07	2.10	2.21	2.12	2.12	2.20	2.10	2.08	2.14	2.02	1.97	1.97	1.78	1.63
1.78	1.99	0.00	2.17	2.19	0.00	2.19	2.19	0.00	2.16	2.14	0.00	2.09	2.05	0.00	1.83	1.62
1.77	1.90	2.10	2.16	2.12	2.18	2.07	2.06	2.14	2.04	2.02	2.09	2.01	2.03	1.94	1.74	1.59
1.75	1.85	2.03	0.00	2.13	2.13	2.01	2.00	2.07	1.97	1.96	2.04	2.02	0.00	1.86	1.67	1.55
1.72	1.77	1.86	1.98	2.03	0.00	1.99	1.98	0.00	1.95	1.93	0.00	1.90	1.83	1.68	1.57	1.49
1.66	1.67	1.69	1.73	1.76	1.83	1.75	1.74	1.79	1.71	1.69	1.73	1.64	1.58	1.52	1.46	1.40
1.55	1.51	1.49	1.48	1.48	1.49	1.47	1.46	1.45	1.43	1.41	1.41	1.38	1.34	1.31	1.28	1.25

*yellow the max pin power remarkgion

Results

(% rel. diff. between MOCUM and MCNP6)

-1.06	**-1.01**	**-0.99**	**-1.00**	**-0.91**	**-0.88**	**-0.88**	**-0.83**	**-0.88**	**-0.81**	**-0.85**	**-0.85**	**-0.82**	**-0.79**	**-0.86**	**-0.84**	**-0.80**
-1.06	-0.98	-1.01	-0.98	-0.88	-0.98	-0.93	-0.84	-0.86	-0.80	-0.78	-0.90	-0.78	-0.77	-0.81	-0.80	-0.81
-1.00	-0.99	-0.96	-0.97	-0.93	0.00	-0.89	-0.85	0.00	-0.85	-0.82	0.00	-0.80	-0.81	-0.76	-0.80	-0.82
-0.96	-0.93	-0.96	0.00	-0.89	-0.87	-0.79	-0.77	-0.78	-0.79	-0.76	-0.73	-0.80	0.00	-0.70	-0.70	-0.72
-0.95	-0.92	-0.93	-0.84	-0.77	-0.82	-0.76	-0.70	-0.80	-0.74	-0.75	-0.75	-0.68	-0.74	-0.67	-0.64	-0.75
-0.90	-0.94	0.00	-0.91	-0.83	0.00	-0.84	-0.80	0.00	-0.74	-0.75	0.00	-0.71	-0.70	0.00	-0.72	-0.67
-0.92	-0.81	-0.85	-0.78	-0.75	-0.78	-0.73	-0.68	-0.77	-0.70	-0.69	-0.73	-0.68	-0.66	-0.70	-0.66	-0.67
-0.88	-0.77	-0.86	-0.74	-0.74	-0.81	-0.70	-0.72	-0.80	-0.69	-0.64	-0.70	-0.65	-0.61	-0.71	-0.68	-0.63
-0.81	-0.88	0.00	-0.84	-0.87	0.00	-0.77	-0.74	-0.86	-0.75	-0.71	0.00	-0.65	-0.68	0.00	-0.68	-0.70
-0.88	-0.76	-0.83	-0.71	-0.75	-0.80	-0.69	-0.63	-0.74	-0.68	-0.65	-0.69	-0.59	-0.61	-0.67	-0.63	-0.66
-0.82	-0.82	-0.80	-0.72	-0.67	-0.70	-0.68	-0.63	-0.72	-0.66	-0.62	-0.65	-0.61	-0.65	-0.71	-0.61	-0.60
-0.81	-0.81	0.00	-0.79	-0.71	0.00	-0.70	-0.69	0.00	-0.70	-0.65	0.00	-0.70	-0.67	0.00	-0.66	-0.57
-0.84	-0.73	-0.76	-0.75	-0.66	-0.73	-0.62	-0.65	-0.71	-0.62	-0.61	-0.67	-0.60	-0.61	-0.65	-0.57	-0.60
-0.75	-0.77	-0.80	0.00	-0.71	-0.73	-0.63	-0.65	-0.73	-0.65	-0.63	-0.68	-0.68	0.00	-0.68	-0.59	-0.57
-0.74	-0.78	-0.70	-0.73	-0.70	0.00	-0.69	-0.69	0.00	-0.68	-0.67	0.00	-0.59	-0.62	-0.61	-0.57	-0.55
-0.77	-0.75	-0.73	-0.72	-0.65	-0.67	-0.63	-0.63	-0.71	-0.68	-0.66	-0.58	-0.57	-0.56	-0.60	-0.55	-0.59
-0.80	-0.82	-0.73	-0.71	-0.67	-0.72	-0.66	-0.68	-0.62	-0.58	-0.60	-0.63	-0.64	-0.61	-0.61	-0.54	-0.51

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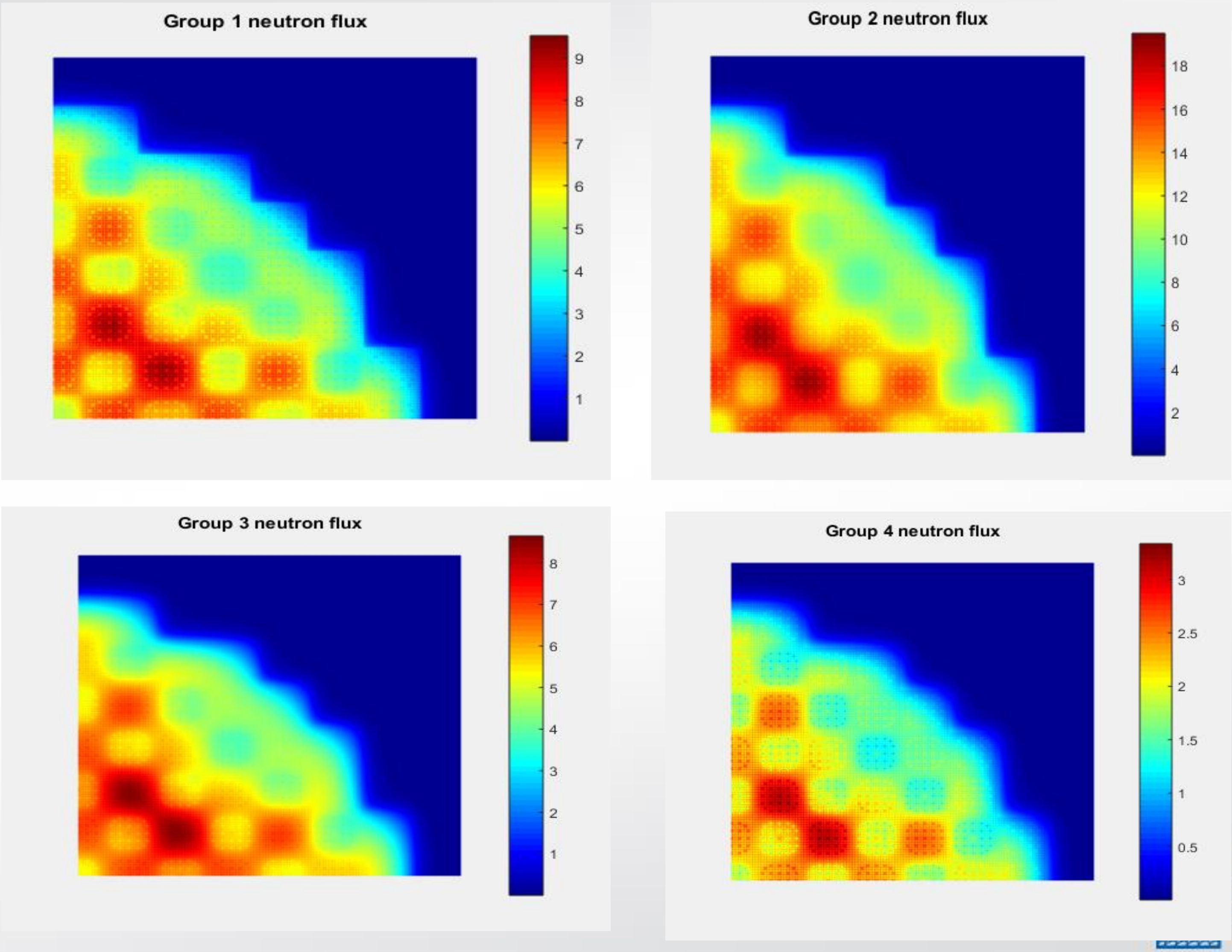
Results (neutron flux profile)



Neutron flux profile for whole-core. Group 1-4.

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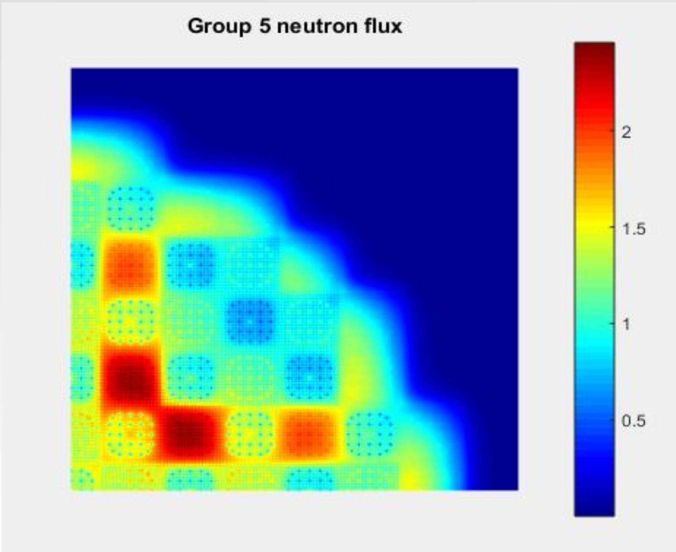
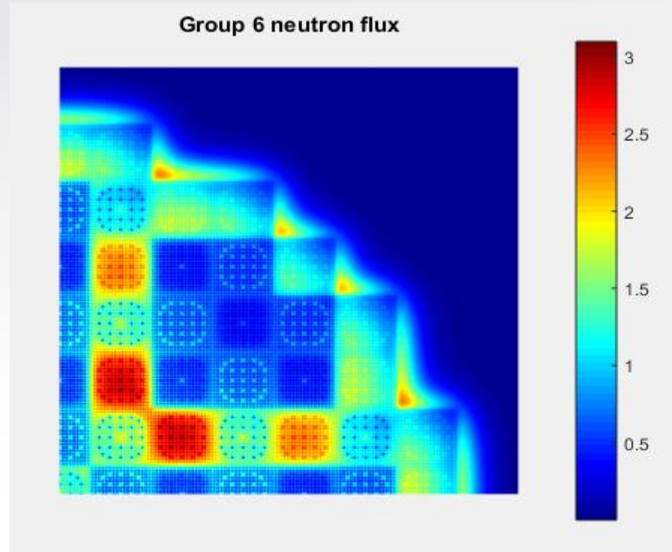
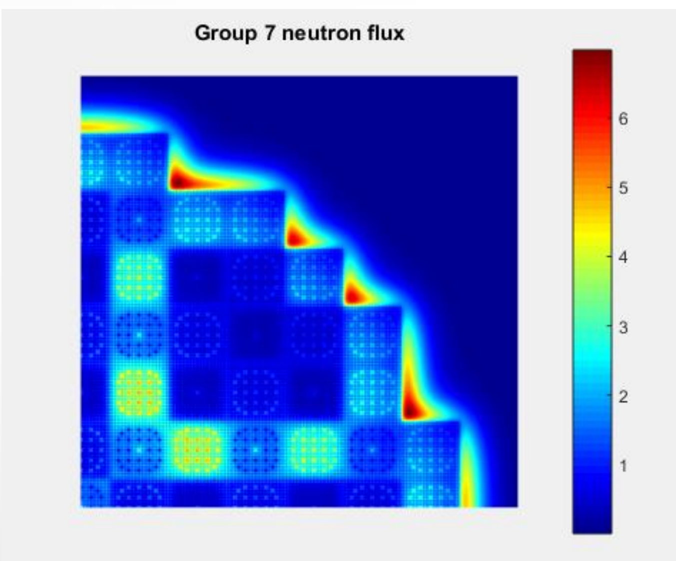
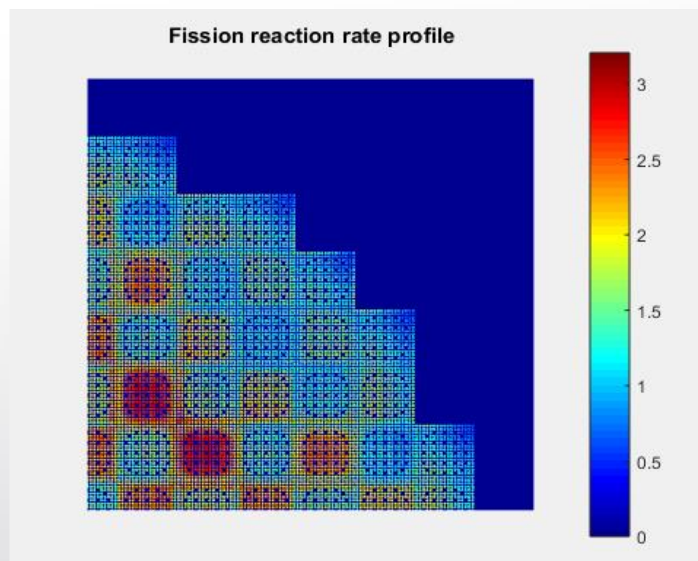
Results (neutron flux profile)





Neutron flux profile for whole-core. Group 5-7.





Fission reaction rate profile (whole-core)

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Conclusion

- MOCUM k_{eff} of the MOX whole core benchmark shows good agreement with the reference MCNP6 Monte Carlo results.
- The very accurate results obtained from MOCUM has shown that the computational tool is highly efficient in modelling and solving complicated and highly heterogenous benchmark problems that depicts realistic reactor design.

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Future work

- MOCUM capabilities should be increased for 3D geometry modelling of reactor benchmarks problems.

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