Using Serpent 2 as a cross section generation tool for the OSCAR-4 code system

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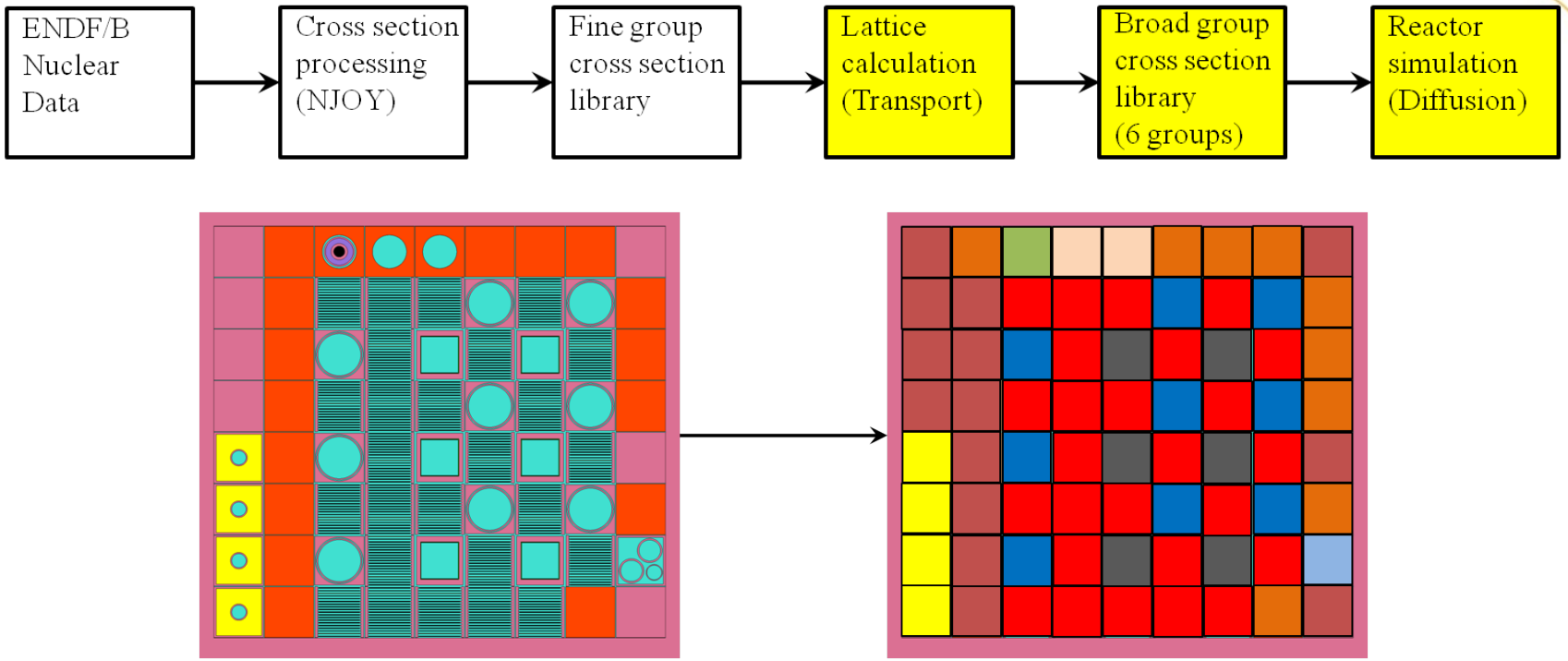
Overview

Intoduction



- Homogenization – Space: Cells to nodes (single homogenized material per assembly)
- Homogenization – Energy: Point wise or group wise data to broad group library (6 energy groups)

Homogenization and Diffusion

$$-\nabla \cdot \mathrm{D}(\mathbf{r})\nabla\hat{\phi}(\mathbf{r},\mathrm{E}) + \overline{\Sigma}_{\mathrm{a}}(\mathbf{r},\mathrm{E})\hat{\phi}(\mathbf{r},\mathrm{E}) = \hat{\mathrm{S}}(\mathbf{r},\mathrm{E}) \tag{1}$$

- Homogenization
  - Replace heterogeneous detail with a single material per assembly
  - Homogenized cross sections used in diffusion
- Why use diffusion for core simulations?
  - Accuracy vs. speed
  - Faster to solve as a result of no angular dependence
  - Core consists mostly of fuel immersed in moderator – diffusive
- How diffusion can be improved: Equivalence theory

Equivalence Theory

$$\int_{\mathrm{S}} \mathrm{dA} \cdot \mathrm{J}(\mathbf{r}) + \int_{\mathrm{V}} \mathrm{d}\mathbf{r} \Sigma_{\mathrm{a}}(\mathbf{r}) \phi(\mathbf{r}) = \int_{\mathrm{v}} \mathrm{d}\mathbf{r} \mathrm{S}(\mathbf{r}) \tag{2}$$

$$-\mathrm{D} \int_{\mathrm{S}} \mathrm{dA} \cdot \nabla \hat{\phi}(\mathbf{r}) + \overline{\Sigma}_{\mathrm{a}} \int_{\mathrm{V}} \mathrm{d}\mathbf{r} \hat{\phi}(\mathbf{r}) = \int_{\mathrm{v}} \mathrm{d}\mathbf{r} \hat{\mathrm{S}}(\mathbf{r}) \tag{3}$$

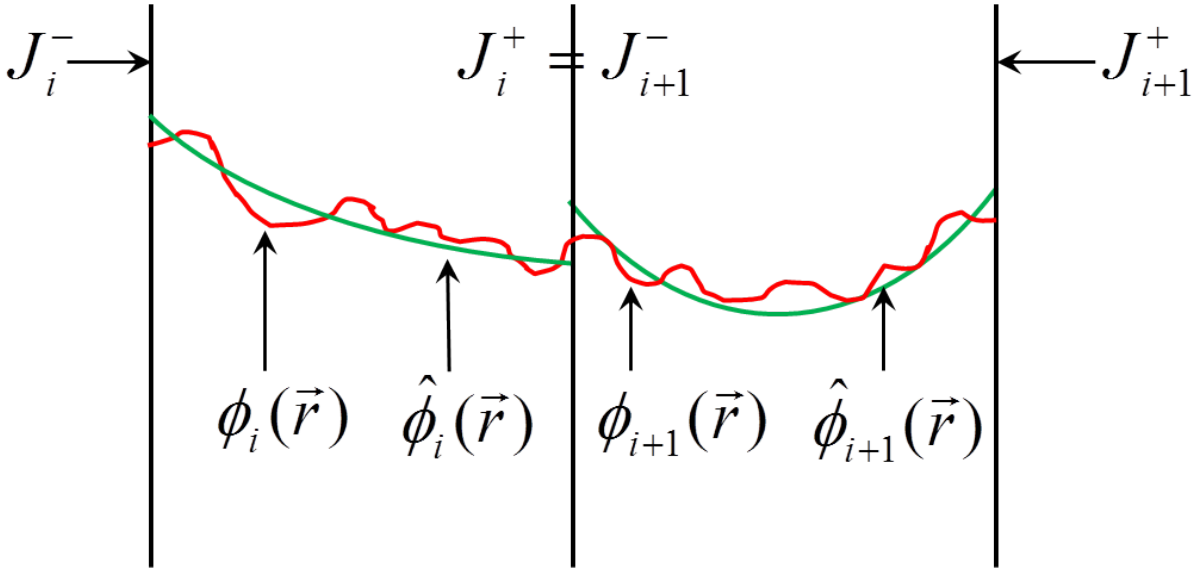
$$\overline{\Sigma}_{\mathrm{a}} = \frac{\int_{\mathrm{V}} \mathrm{d}\mathbf{r}\, \Sigma_{\mathrm{a}}(\mathbf{r}) \phi(\mathbf{r})}{\int_{\mathrm{V}} \mathrm{d}\mathbf{r}\, \phi(\mathbf{r})} \tag{4}$$

- To preserve the reaction rates – preserve the transport currents/leakages:

$$\int_{\mathrm{S}} \mathrm{dA} \cdot \mathrm{J}(\mathbf{r}) = -\mathrm{D} \int_{\mathrm{S}} \mathrm{dA} \cdot \nabla \hat{\phi}(\mathbf{r}) \tag{5}$$

- Allow $\hat{\phi}(\mathbf{r})$ to be discontinuous on the node interfaces
- Discontinuity factor: $f_{\mathrm{i}} = \frac{\phi_{\mathrm{i}}}{\hat{\phi}_{\mathrm{i}}}$, on interface i
- Simultaneously preserve the average reaction rates and transport leakages

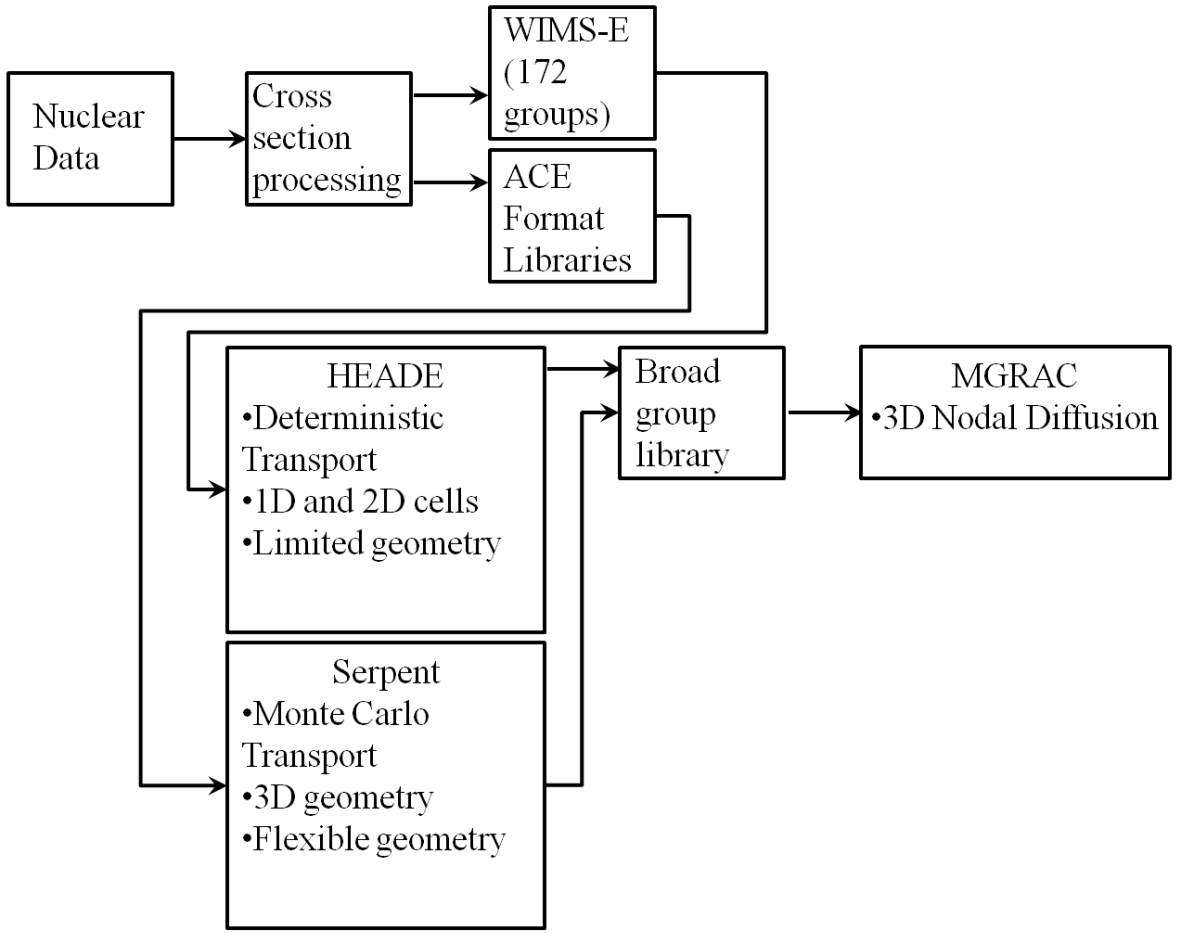
Equivalence Theory



$$\hat{\phi}_i^+ f_i^+ = \hat{\phi}_{i+1}^- f_i^- \tag{6}$$

$$f_i^+ = \frac{\phi_i^+}{\hat{\phi}_i^+}, f_i^- = \frac{\phi_{i+1}^-}{\hat{\phi}_{i+1}^-} \tag{7}$$

The OSCAR-4 code system



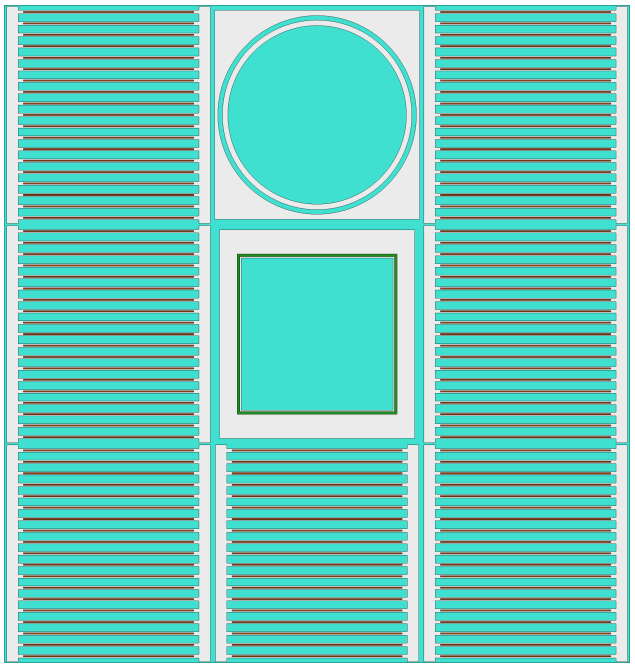
Part 1: Verification for a colorset environment

Verification test: Motivation

- Equivalence theory requires additional homogenized parameters apart from cross sections
- For a single assembly calculation, Serpent produced the expected results
- Anomalous results were produced with multiple assemblies in a lattice structure
- Suspected incorrect leakages and/or reaction rates when using lattices

Problem description

- 2D 3x3 colorset problem
- Vacuum boundary conditions radially
- Reflective boundary conditions axially



MCNP reference calculation parameters

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- KCODE calculation:
- FMESH tallies used for reaction rates and node average fluxes
- F2 tallies for side fluxes and F1 tallies for currents
- All tallies used EMESH to generate 6-group values with group structure: 1.4E-07, 6.25E-07, 4.0E-06, 0.00553084, 0.82085, 20.0
- No additional variance reduction

Serpent calculation parameters

- Serpent v2.1.15 with local modifications used
- Generated 6-group values with group structure: 1.4E-07, 6.25E-07, 4.0E-06, 0.00553084, 0.82085, 20.0
- Tracking options:
  - Default tracking options
  - Delta-tracking only

Serpent: Default tracking options

	sf : 0.69 *c* : 15.48	*sf* : 1.82 *c* : 16.49	*sf* : 2.21 *c* : 15.82	
sf : 1.73 *c* : 1.23	*f* : 0.79 *r* : 0.12	*f* : 0.51 *r* : 0.13	*f* : 0.74 *r* : 0.33	*sf* : 1.00 *c* : 1.00
sf : 1.32 *c* : 0.73	*f* : 1.04 *r* : 0.14	*f* : 0.36 *r* : 0.18	*f* : 0.65 *r* : 0.18	*sf* : 1.38 *c* : 0.94
sf : 1.30 *c* : 0.54	*f* : 0.95 *r* : 0.15	*f* : 0.57 *r* : 0.18	*f* : 0.61 *r* : 0.22	*sf* : 1.55 *c* : 0.64
	sf : 0.91 *c* : 14.78	*sf* : 1.05 *c* : 14.70	*sf* : 0.96 *c* : 14.75	

Percentage error relative to MCNP reference

Serpent: Delta-tracking only

	sf : 1.10 *c* : 1.05	*sf* : 1.84 *c* : 1.60	*sf* : 1.19 *c* : 1.29	
sf : 2.00 *c* : 1.24	*f* : 0.79 *r* : 0.11	*f* : 0.53 *r* : 0.14	*f* : 0.74 *r* : 0.35	*sf* : 0.82 *c* : 0.94
sf : 1.19 *c* : 0.77	*f* : 1.07 *r* : 0.18	*f* : 0.36 *r* : 0.26	*f* : 0.67 *r* : 0.19	*sf* : 1.26 *c* : 0.91
sf : 1.06 *c* : 0.58	*f* : 0.91 *r* : 0.18	*f* : 0.55 *r* : 0.18	*f* : 0.62 *r* : 0.20	*sf* : 1.63 *c* : 0.61
	sf : 0.99 *c* : 0.42	*sf* : 1.14 *c* : 0.36	*sf* : 1.50 *c* : 0.41	

Percentage error relative to MCNP reference

Summary of Part 1

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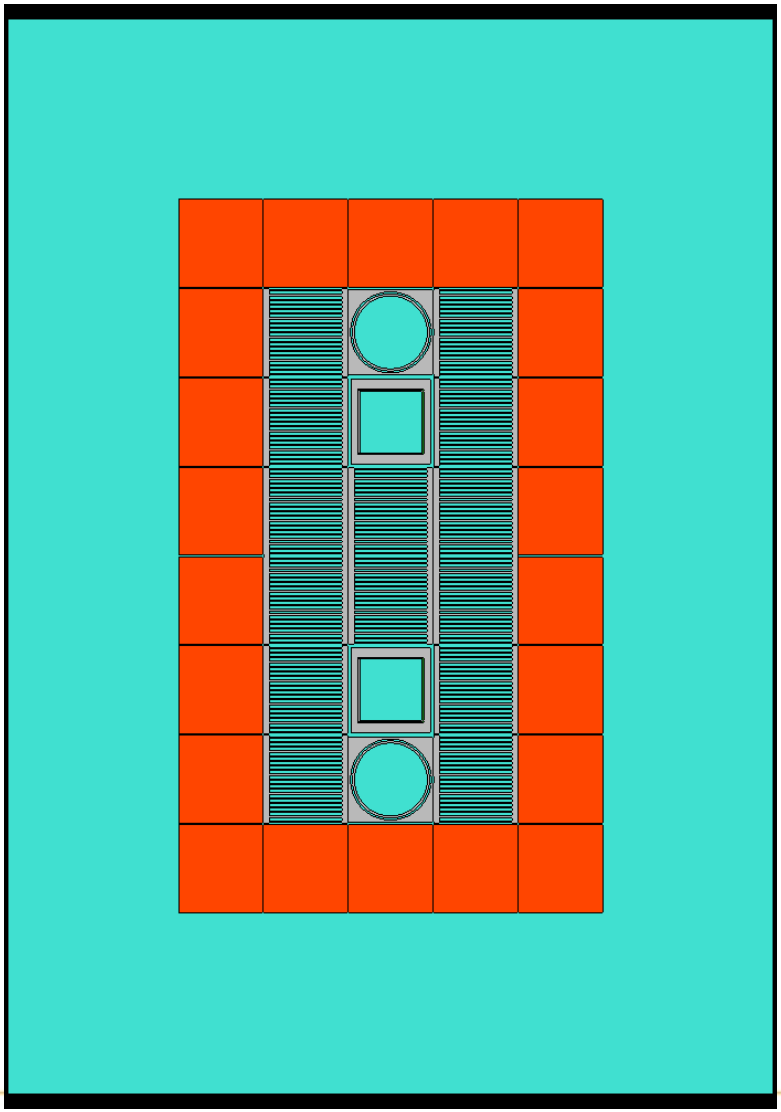
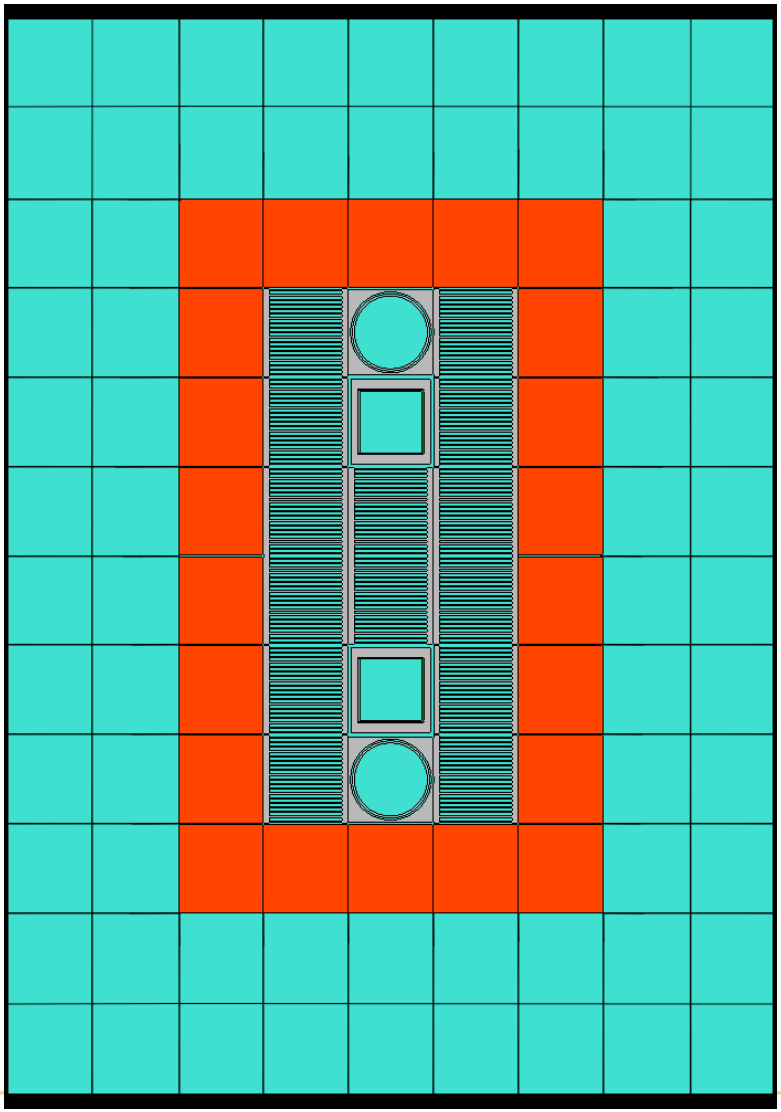
- Two tracking options were evaluated – default and pure delta-tracking
- Serpent v2.1.15 with delta-tracking only produces currents with highest accuracy
- Pure delta-tracking significantly increases simulation time

Part 2: 2D Core investigations

Concept Core Description



Concept Core Description



Fully Equivalent Model

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- All component cross sections generated using Serpent v2.1.15 with delta-tracking only
- Component cross sections are position dependent and unique for each component
- Discontinuity factors on component interfaces are calculated using a full 2D core model

Fully Equivalent Model

- Reference power distribution, no approximations

	1	2	3	4	5	6	7	8	9
A									
B									
C									
D				597.5		597.5			
E				648.0		648.0			
F				870.0	769.5	870.0			

- Reference $k_{eff} = 1.10886$
- MGRAC $k_{eff} = 1.10885$

Model Without Discontinuity Factors

- No equivalence parameters with position dependent cross sections

	1	2	3	4	5	6	7	8	9
A									
B									
C									
D				4.3		4.3			
E				3.1		3.1			
F				-5.5	-1.0	-5.5			

- Reference $k_{eff} = 1.10886$
- MGRAC $k_{eff} = 1.12541 (1326.20 pcm)$
- Maximum relative error percentage = 5.5%

Limitations in current implementation

- Position dependent, burnup dependent cross sections and equivalence parameters
- Requires full core transport solutions at every burnup step: Not feasible

- Replace reference fuel with ”ideal” fuel
- Fuel generated in an infinite environment
- Current implementation of the cross section generation tool does not support burnup dependent parameters
- Generate the fuel parameters with HEADE
- Break full core equivalence

Infinite Fuel Approximation

- Equivalence parameters for all non-fuel components, with fuel from an infinite environment (Serpent)

	1	2	3	4	5	6	7	8	9
A									
B									
C									
D				3.2		3.2			
E				-0.2		-0.2			
F				-1.7	-1.1	-1.7			

- Reference $k_{eff} = 1.10886$
- MGRAC $k_{eff} = 1.10168(-587.75pcm)$
- Maximum relative error percentage = 3.2%

Infinite Fuel Approximation – HEADE

- Equivalence parameters for all non-fuel components, with fuel from an infinite environment (HEADE)

	1	2	3	4	5	6	7	8	9
A									
B									
C									
D				1.4		1.4			
E				-1.3		-1.3			
F				-0.6	1.1	-0.6			

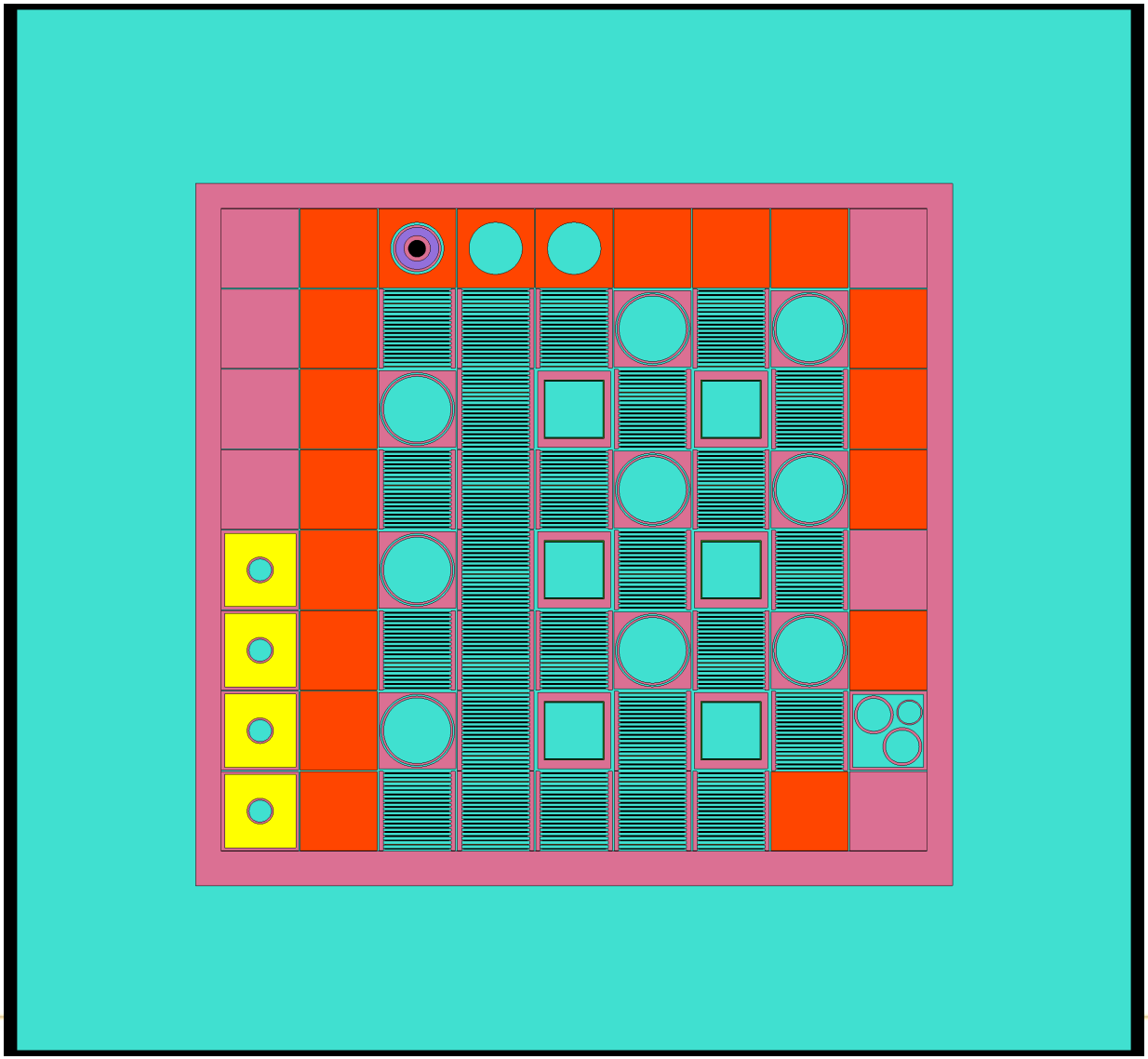
- Reference $k_{eff} = 1.10886$
- MGRAC $k_{eff} = 1.09725(-954.22pcm)$
- Maximum relative error percentage = 1.4%

Summary of Part 2

Approximation	k_{eff} error (pcm)	Power RMS error (%)
None	-	-
No Discontinuity Factors	1326.20	4.1
Infinite Fuel (Serpent)	-587.75	2.0
Infinite Fuel (HEADE)	-954.22	1.2

Part 3: Reactor applications – SAFARI-1

SAFARI-1 description



SAFARI-1 model description

- Full core 2D transport calculation used for homogenized cross section and equivalence parameters
- Two cases required for 3D model – Control rods inserted and extracted

Fully equivalent SAFARI-1 model

- Serpent: All rods in (ARI) k_{eff} = 1.04221
- MGRAC All rods in (ARI) k_{eff} = 1.04198
- 21.2 pcm difference is suspected to be a result of the currents in the reflector not being fully converged.

- Serpent: All rods out (ARO) k_{eff} = 1.30402
- MGRAC All rods out (ARO) k_{eff} = 1.30306
- Similar to the ARI case the difference (56.5 pcm) is suspected to be a result of currents not being fully converged in the reflector

Infinite fuel approximation – ARI

- Equivalence parameters for all non-fuel components (ARO case)
- Control rod equivalence parameters from ARI case
- Fuel parameters from an infinite environment (HEADE)

	1	2	3	4	5	6	7	8	9
A									
B			-0.04	-0.11	0.05		0.10		
C				-0.24		0.12		0.10	
D			-0.13	0.20	0.08		0.16		
E				-0.29		0.13		0.09	
F			-0.07	-0.17	0.09		0.14		
G				-0.16		0.07		0.06	
H			0.08	0.00	0.05	0.05	0.04		

- Serpent: All rods in (ARI) k_{eff} = 1.04221
- MGRAC All rods in (ARI) k_{eff} = 1.03639 (-538.82 pcm)

Infinite fuel approximation – ARO

- Equivalence parameters for all non-fuel components (ARO case)
- Fuel follower parameters from an infinite environment (HEADE)
- Fuel parameters from an infinite environment (HEADE)

	1	2	3	4	5	6	7	8	9
A									
B			-0.02	-0.06	0.03		0.06		
C				-0.07	-0.11	0.14	-0.08	0.06	
D			-0.04	-0.09	0.08		0.12		
E				-0.09	-0.15	0.14	-0.10	0.06	
F			-0.02	-0.08	0.10		0.11		
G				-0.03	-0.09	0.10	-0.08	0.05	
H			0.02	-0.01	0.05	0.01	0.03		

- Serpent: All rods out (ARO) k_{eff} = 1.30402
- MGRAC All rods out (ARO) k_{eff} = 1.30634 (136.19 pcm)

Summary of Part 3

All rods in case

Approximation	k_{eff} error (pcm)	Power RMS error (%)
None	21.1	0.02
Non-fuel components from ARO, Rods from ARI, Infinite Fuel (HEADE)	-538.82	0.13

All rods out case

Approximation	k_{eff} error (pcm)	Power RMS error (%)
None	56.5	0.01
Non-fuel components from ARO, Infinite Fuel (HEADE), Infinite Fuel Follower (HEADE)	136.19	0.08

Conclusions

- Equivalence obtained between MGRAC and Serpent when full core 2D models are used to generate homogenized parameters (k_{eff} within 60 pcm, rms power error within 0.02 %)
- Extending the 2D model to 3D induces further errors because of a lack of 3D equivalence parameters

Thank you

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