Generation and Application of Interface Discontinuity Factors in the Reactor Simulator DYN3D

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Institute for Neutron Physics and Reactor Technology

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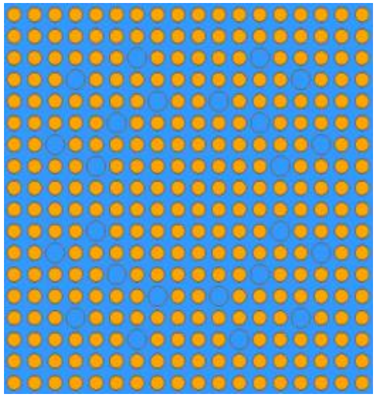

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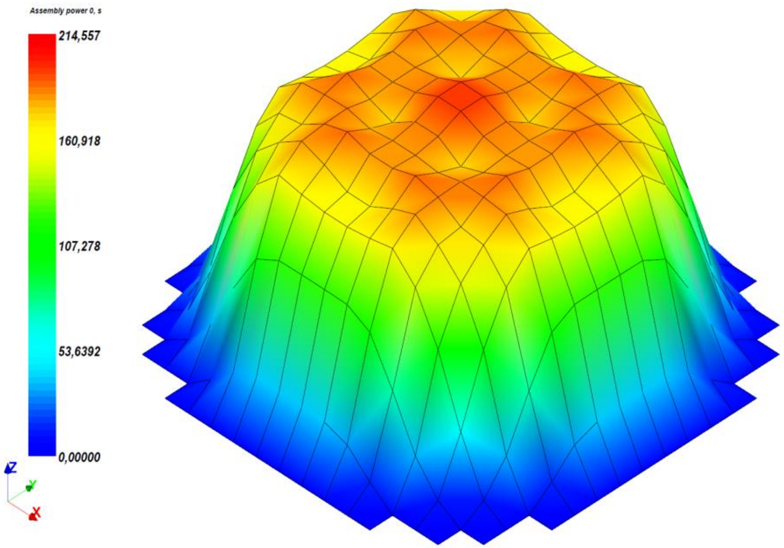
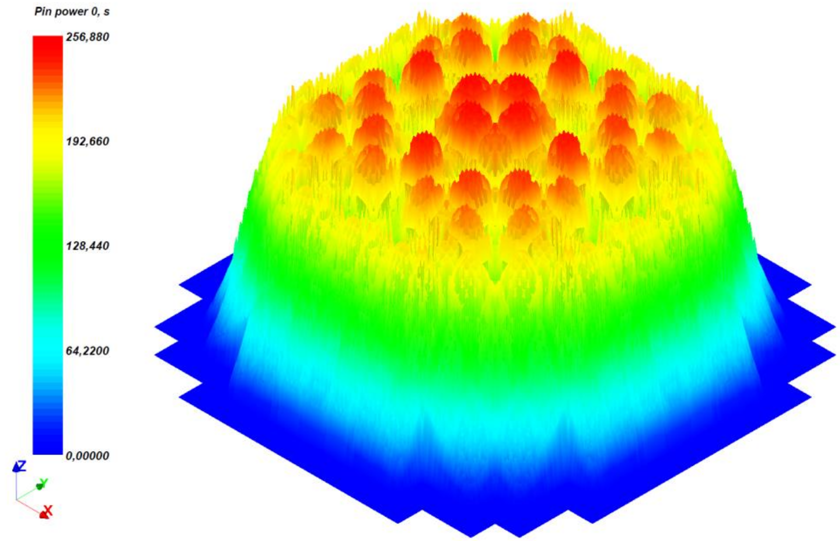
Upcoming pin-by-pin multi-physics simulations in need of accurate few-group constants



Fuel assembly / channel resolution coupled NK – TH simulation



Fuel pin / sub-channel resolution coupled NK – TH simulation

Discussion for pin-by-pin diffusion only

Multi-physics simulations done with DYNSUB.
OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark core under HFP conditions.

Interface discontinuity factors

- Generalized Equivalence theory (GET) flux discontinuity factors

$$f_{GET}^{s} = \frac{\phi_s^{het}}{\phi_s^{hom}}$$

- Black-box homogenization (BBH) current discontinuity factors

$$f_{\pm BBH}^{\;s} = \frac{J_{\pm s}^{\;het}}{J_{\pm s}^{\;hom}}$$

In case of the diffusion approximation can be written as flux discontinuity factor:

$$f_{BBH}^{s} = 2\,\frac{J_{-s}^{\;het} + J_{+s}^{\;het}}{\phi_s^{hom}}$$

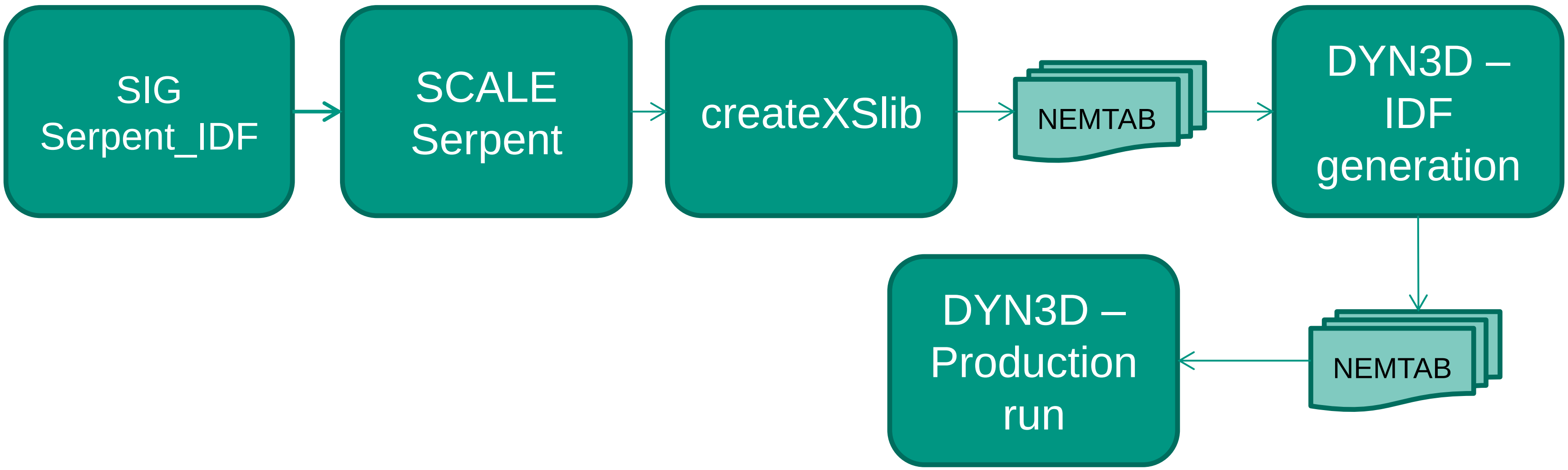
Energy group indices were omitted for simplicity

Calculation route for interface discontinuity factors

- New explicit iterative solver to evaluate ϕ_s^{hom} consistent with DYN3D

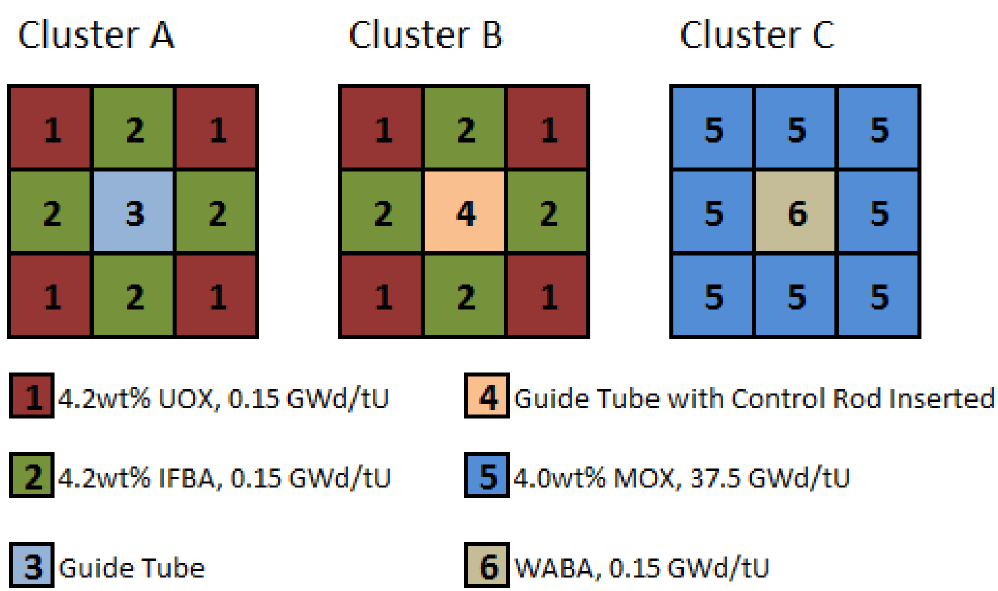
$$-D_g{}^i \frac{d^2}{du^2}\Phi_g^i(u) + \Sigma_{R,g}{}^i\Phi_g^i(u) = S_{g,i}(u) - L_{g,i}{}^{het}(u)$$

- Boundary conditions: $\vec{J}_{g,i}{}^{het}$ and $\overline{\Phi_g^i}^{het}$



Selected Verification cases – 3x3 pin clusters (1/3)

- Definition of fuel pins based on taken from OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark
- Serpent 2.1.15 with ENDF/B-VII point wise XS at 600 K
- 2E+09 histories simulated with Serpent



Selected Verification cases – 3x3 pin clusters (2/3)

3x3 Pin Cluster A Eigenvalue Comparison

Code	k-inf	Absolute difference [pcm]
Serpent CE	1.09266±0.000043	-
DYN3D 2g	1.094381	172.1
DYN3D 4g	1.093542	88.2
DYN3D 8g	1.093038	37.8
DYN3D 2g GET IDF	1.092631	-2.9
DYN3D 4g GET IDF	1.092630	-3.0
DYN3D 8g GET IDF	1.092629	-3.1
DYN3D 2g BBH IDF	1.092631	-2.9
DYN3D 4g BBH IDF	1.092630	-3.0
DYN3D 8g BBH IDF	1.092629	-3.1

3x3 Pin Cluster C Eigenvalue Comparison

Code	k-inf	Absolute difference [pcm]
Serpent CE	0.972880±0.000041	-
DYN3D 2g	0.974442	156.2
DYN3D 4g	0.973113	31.3
DYN3D 8g	0.972997	11.7
DYN3D 2g GET IDF	0.972894	1.4
DYN3D 4g GET IDF	0.972898	1.8
DYN3D 8g GET IDF	0.972900	2.0
DYN3D 2g BBH IDF	0.972894	1.4
DYN3D 4g BBH IDF	0.972898	1.8
DYN3D 8g BBH IDF	0.972900	2.0

3x3 Pin Cluster B Eigenvalue Comparison

Code	k-inf	Abolute difference [pcm]
Serpent CE	0.713814±0.000046	-
DYN3D 2g	0.667408	-4640.6
DYN3D 4g	0.647620	-6619.4
DYN3D 8g	0.642787	-7102.7
DYN3D 2g GET IDF	0.713834	2.0
DYN3D 4g GET IDF	0.713817	0.3
DYN3D 8g GET IDF	0.713732	-8.2
DYN3D 2g BBH IDF	0.713834	2.0
DYN3D 4g BBH IDF	0.713817	0.3
DYN3D 8g BBH IDF	0.713732	-8.2

Except for 8g solution of cluster B DYN3D results lie within statistical uncertainty of Serpent reference

Selected Verification cases – 3x3 pin clusters (3/3)

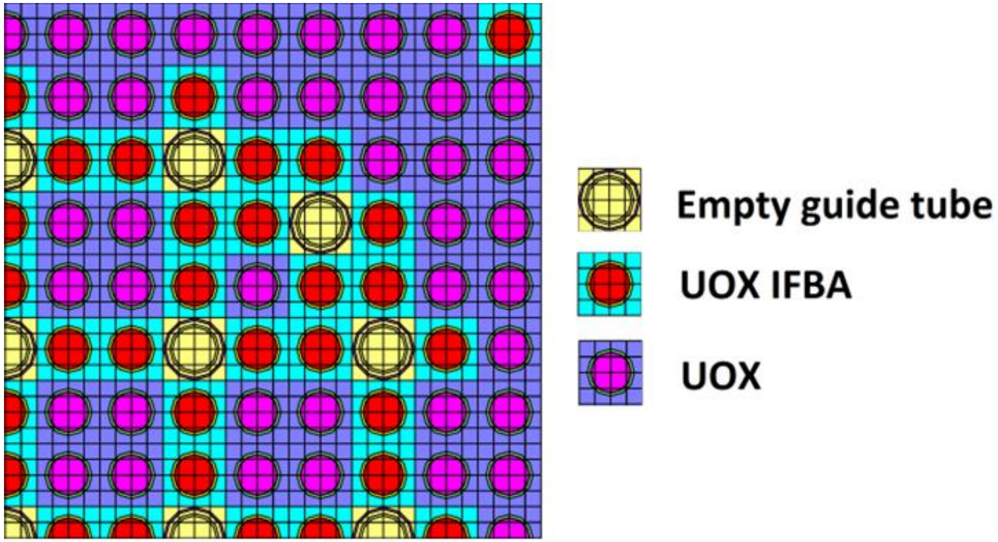
3x3 Pin Cluster Pin Power Maximum Difference in Per Cent

Code	Cluster A	Cluster B	Cluster C
DYN3D 2g	0.43	0.66	0.26
DYN3D 4g	0.38	0.73	0.31
DYN3D 8g	0.45	0.73	0.28
DYN3D 2g GET IDF	0.01	0.03	0.02
DYN3D 4g GET IDF	0.01	0.00	0.02
DYN3D 8g GET IDF	0.01	0.04	0.02
DYN3D 2g BBH IDF	0.01	0.03	0.02
DYN3D 4g BBH IDF	0.01	0.00	0.02
DYN3D 8g BBH IDF	0.01	0.04	0.02

All pin powers reproduced within statistical uncertainty of Serpent reference

Selected Verification cases – UOX fuel assembly (1/2)

- Definition of fuel assembly based on taken from OECD/NEA and U.S. NRC PWR MOX/UO2 core transient benchmark
- 0.15 GWd/tU burn-up 17x17-25 UOX assembly
- SCALE 6.1/TRITON (BONAMI / CENTRM / PMC / NEWT)
- 238g library based on ENDF/B-VII



Selected Verification cases – UOX fuel assembly (2/2)

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UOX Fuel Assembly Eigenvalue Comparison

Code	k-inf	Absolute difference [pcm]
SCALE 238g	1.1231457	-
DYN3D 4g (3M)	1.070184	-5296.17
DYN3D 4g (37M)	1.123647	50.13
DYN3D 4g (289M) GET IDF	1.123144	0.17
DYN3D 4g (289M) BBH IDF	1.123144	0.17

-8.35	-8.98	-9.04	-8.73	-10.13	-11.88	-12.72	-11.13	-0.11
2.92	-4.26	-4.20	3.00	-4.89	-7.95	-10.84	-11.93	-11.13
0.00	6.89	7.27	0.00	8.91	5.45	-6.19	-10.84	-12.72
8.52	0.40	1.01	11.39	12.47	0.00	5.45	-7.95	-11.88
9.53	1.34	1.84	11.63	5.61	12.47	8.91	-4.89	-10.13
0.00	10.09	10.35	0.00	11.63	11.39	0.00	3.00	-8.73
10.25	1.88	1.93	10.35	1.84	1.01	7.27	-4.20	-9.04
10.35	1.95	1.88	10.09	1.34	0.40	6.89	-4.26	-8.98
0.00	10.35	10.25	0.00	9.53	8.52	0.00	2.92	-8.35

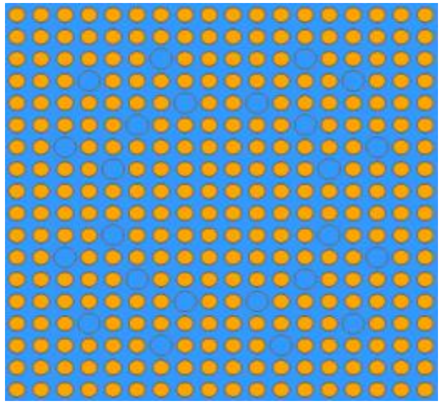
Relative Errors of DYN3D 4g (3M) Pin Powers in Per Cent Compared to SCALE Reference in 1/4th of the Fuel Assembly

-0.48	-0.41	-0.41	-0.52	-0.47	-0.55	-0.62	-0.67	0.74
0.52	-0.24	-0.25	0.49	-0.28	-0.53	-0.60	-0.68	-0.67
0.00	0.54	0.53	0.00	0.65	0.43	-0.44	-0.60	-0.62
0.54	-0.20	-0.21	0.49	0.73	0.00	0.43	-0.53	-0.55
0.59	-0.13	-0.16	0.58	-0.05	0.73	0.65	-0.28	-0.47
0.00	0.60	0.60	0.00	0.58	0.49	0.00	0.49	-0.52
0.62	-0.10	-0.10	0.60	-0.16	-0.21	0.53	-0.25	-0.41
0.64	-0.10	-0.10	0.60	-0.13	-0.20	0.54	-0.24	-0.41
0.00	0.64	0.62	0.00	0.59	0.54	0.00	0.52	-0.48

Relative Errors of DYN3D 4g (37M) Pin Powers in Per Cent Compared to SCALE Reference in 1/4th of the Fuel Assembly

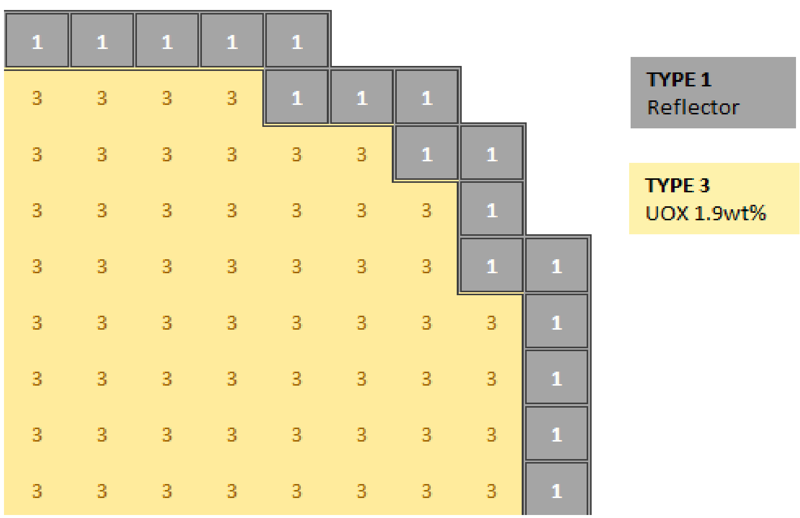
Employing IDF relative errors below 5e-05

PWR application (1/2)

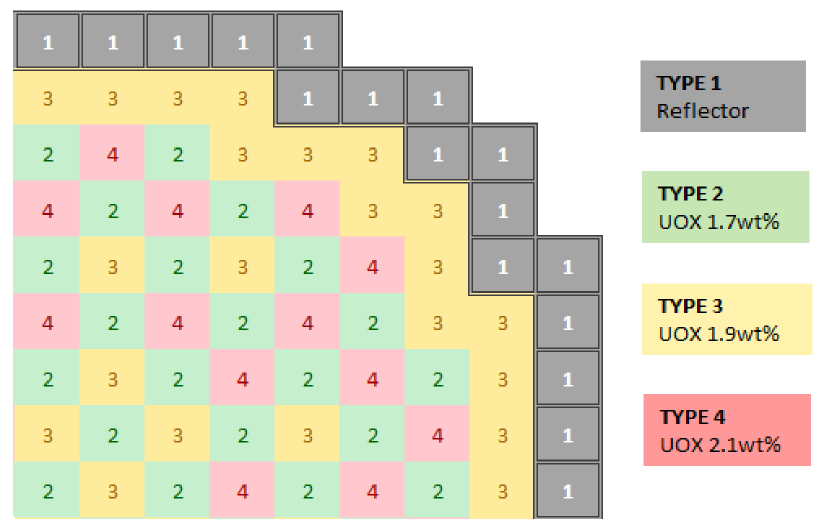


Fresh 18x18-24 UOX fuel assembly

- Serpent 2.1.15 reference calculation
- ENDF/B-VII
- 5e+09 histories in 500 active cycles



Quarter Core Fuel Loading Pattern for First Configuration



Quarter Core Fuel Loading Pattern for Second Configuration

PWR application (2/2)

PWR Configuration 1 Eigenvalue Comparison

Code	k-eff	Absolute difference [pcm]
Serpent CE	1.01673±0.000029	-
DYN3D 4g (3M)	1.023283	655.3
DYN3D 4g (1620M) GET IDF	1.017469	73.9
DYN3D 4g (1620M) BBH IDF	1.017469	73.9

PWR Configuration 2 Eigenvalue Comparison

Code	k-eff	Absolute difference [pcm]
Serpent CE	1.00211±0.000029	-
DYN3D 4g (7M)	1.008292	618.2
DYN3D 4g (2268M) GET IDF	1.007179	506.9
DYN3D 4g (2268M) BBH IDF	1.007179	506.9

-2.51	-2.66	-2.96	-3.63				
-0.22	-0.46	-0.71	-1.16	-2.40	-3.46		
0.33	0.28	0.03	-0.07	-0.55	-1.41	-3.46	
0.51	0.51	0.45	0.32	-0.21	-0.55	-2.40	
0.48	0.40	0.46	0.46	0.32	-0.07	-1.16	-3.63
0.27	0.30	0.36	0.46	0.45	0.03	-0.71	-2.96
0.16	0.14	0.30	0.40	0.51	0.28	-0.46	-2.66
0.01	0.16	0.27	0.48	0.51	0.33	-0.22	-2.51

Relative differences in nodal powers for PWR configuration 1 between DYN3D 4g (1620M) IDF and Serpent reference in per cent

Single fuel assemblies with conservative boundary conditions are insufficient super-cells

Conclusions and Outlook

- A calculation route for interface discontinuity factors for DYN3D‘s pin-by-pin simulations has been developed and verified
- Improvement of DYN3D pin-by-pin solution deemed too low for PWR application cases
- Propor choice of super-cells and corresponding cross section parameterization to be further improved
- Assess methodologies to evaluate SP3 interface discontinuity factors (recent publication by L. Yu et al. (Annals of Nuclear Energy))