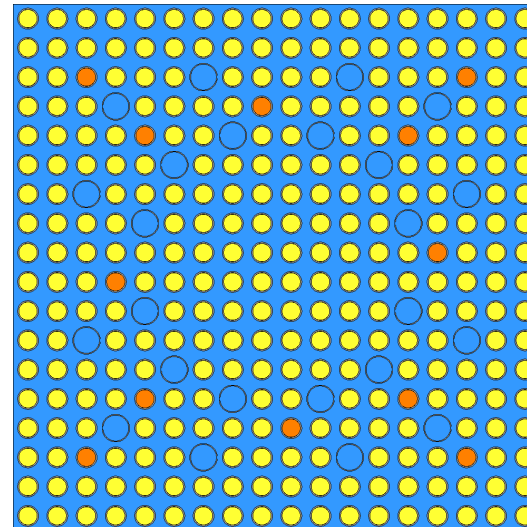
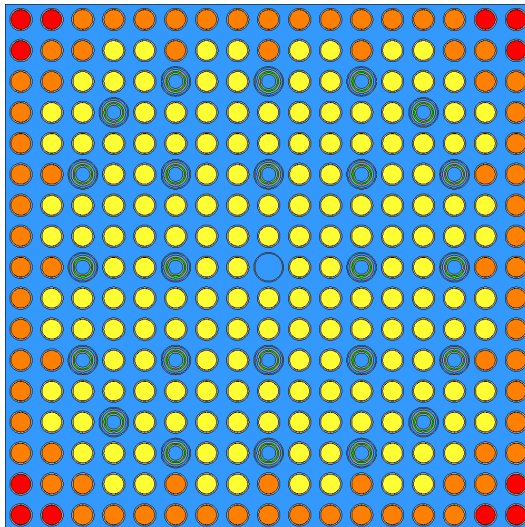


# Generation of pin level multi-dimensional XS tables with Serpent 2

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Reactor Physics and Dynamic Group (RPD)



# Agenda

- Pin power reconstruction
  - Using Serpent 2 for pin power reconstruction constant generation
  - Serpent 2 support in GenPMAXS
  - Selected verification cases
  
- Pin level cross section generation
  - General approach and pin level homogenization corrections
  - Serpent 2 support in createXSlib
  - Selected verification cases
  - Impact on homogenization corrections on Serpent 2 performance
  
- Conclusions and outlook

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## Pin power reconstruction with Serpent 2

- Employing pin powers → cpd card

$$p_{pin,i} = \kappa \Sigma_f \overline{\Phi} f_i$$

- Employing group-wise form functions → new **ppw card**

$$p_{pin,i} = \sum_g \overline{\kappa} \overline{\Sigma_{fg}} \overline{\Phi}_g f_{g,i}$$

- PPW card syntax:     set ppw <universe> <lattice>

## Serpent 2 support in GenPMAXS

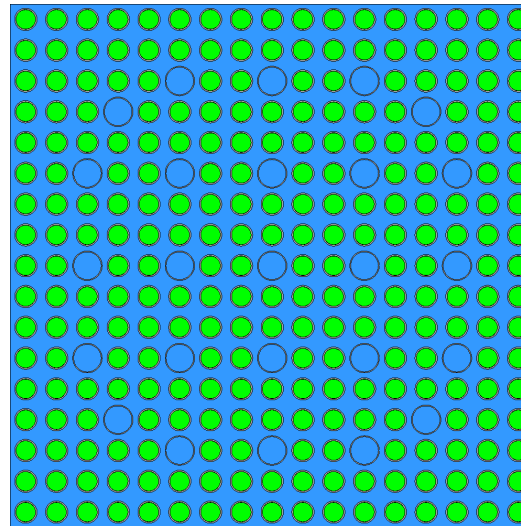
- Verification cases to be done with U.S. NRC reactor simulator PARCS v3.0
- GenPMAXS tool to generate PMAX-type multi-dimensional cross section tables for PARCS
- Extension of GenPMAXS to support Serpent 2 (based on partial Serpent 1 support)
- GenPMAXS Serpent 2 features:
  - general nodal few-group constants,
  - group-wise form functions,
  - reflector ADF and
  - 1D interface discontinuity factors
- Serpent 2 support should be available through U.S. NRC CAMP program starting with GenPMAXS v6.2 release

# Agenda

- Pin power reconstruction
  - Using Serpent 2 for pin power reconstruction constant generation
  - Serpent 2 support in GenPMAXS
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  - Impact on homogenization corrections on Serpent 2 performance
  
- Conclusions and outlook

# Pin power reconstruction – HZP case 1 (1/3)

- Serpent 2: 100,000,000 histories in 500 active cycles  
 2g cross sections (0.625 eV boundary)



UOX fuel  
assembly of PWR  
MOX/UOX  
benchmark

UOX 0.15 GWd/tU

Code	$k_{inf}$	Rel. Diff. [pcm]
Serpent 2 CE	1.124230±0.00005	-
PARCS 2g NEM	1.1242304	0.04

# Pin power reconstruction – HZP case 1 (2/3)

10.0	2.2	0.4	-0.5	-0.7	-0.9	-1.0	-1.0	-0.9	-1.0	-1.0	-0.7	-0.8	-0.5	0.3	2.2	9.9
2.3	0.9	-0.2	-0.5	-1.2	1.0	-1.5	-1.3	0.9	-1.3	-1.3	1.1	-1.2	-0.5	-0.1	0.8	2.1
0.3	-0.1	-0.8	1.2	0.6	0.0	1.0	1.0	0.0	1.0	1.0	0.0	0.7	1.2	-0.9	-0.1	0.3
-0.4	-0.5	1.3	0.0	0.5	1.0	-1.5	-1.5	1.0	-1.4	-1.4	0.9	0.5	0.0	1.2	-0.5	-0.5
-0.7	-1.2	0.7	0.4	-1.9	0.9	-1.5	-1.4	1.0	-1.5	-1.5	0.8	-1.8	0.3	0.6	-1.2	-0.7
-0.8	1.0	0.0	1.0	0.9	0.0	1.0	1.0	0.0	1.0	1.0	0.0	0.8	0.9	0.0	0.9	-0.8
-0.9	-1.3	0.9	-1.5	-1.5	1.0	-1.5	-1.4	1.1	-1.3	-1.5	1.0	-1.6	-1.5	1.0	-1.4	-0.9
-1.0	-1.3	1.1	-1.4	-1.5	1.0	-1.3	-1.4	1.1	-1.3	-1.4	1.0	-1.5	-1.5	1.0	-1.4	-0.9
-0.8	0.9	0.0	1.0	1.0	0.0	1.1	1.1	0.0	1.0	1.1	0.0	1.0	0.9	0.0	1.1	-0.8
-1.0	-1.3	1.0	-1.4	-1.4	0.9	-1.3	-1.4	1.1	-1.3	-1.4	1.0	-1.5	-1.5	1.0	-1.3	-1.0
-1.0	-1.3	0.9	-1.4	-1.4	0.9	-1.5	-1.4	1.0	-1.4	-1.4	0.9	-1.5	-1.5	1.0	-1.3	-1.1
-0.8	0.9	0.0	1.0	0.9	0.0	0.8	1.1	0.0	1.0	0.9	0.0	0.9	1.0	0.0	1.0	-0.8
-0.7	-1.2	0.7	0.4	-1.8	0.9	-1.5	-1.4	1.0	-1.4	-1.5	0.9	-1.8	0.5	0.5	-1.1	-0.7
-0.4	-0.4	1.2	0.0	0.5	1.0	-1.4	-1.5	1.0	-1.4	-1.6	0.9	0.4	0.0	1.2	-0.6	-0.4
0.3	-0.1	-0.8	1.2	0.7	0.0	1.0	1.0	0.0	1.1	1.1	0.0	0.6	1.2	-0.8	-0.1	0.4
2.3	0.9	-0.1	-0.5	-1.1	1.0	-1.3	-1.2	1.0	-1.3	-1.3	1.0	-1.1	-0.5	-0.1	0.9	2.2
10.0	2.3	0.3	-0.5	-0.8	-0.7	-1.0	-1.0	-0.8	-0.9	-0.9	-0.8	-0.6	-0.5	0.3	2.3	10.0

PARCS pin power reconstruction relationship for pin cell i:

$$p_{pin,i} = \sum_g \bar{\kappa} \bar{\Sigma}_{fg} \underbrace{\bar{\Phi}_g f_{g,i}}_{\Phi_{g,i}}$$

Serpent 2 pin power relationship for pin cell i:

$$p_{pin,i} = \sum_g \kappa_i \Sigma_{fg,i} \Phi_{g,i} \\ = \kappa_i \Sigma_{f,i} \Phi_i$$

Relative pin power errors PARCS vs. Serpent 2 in per cent

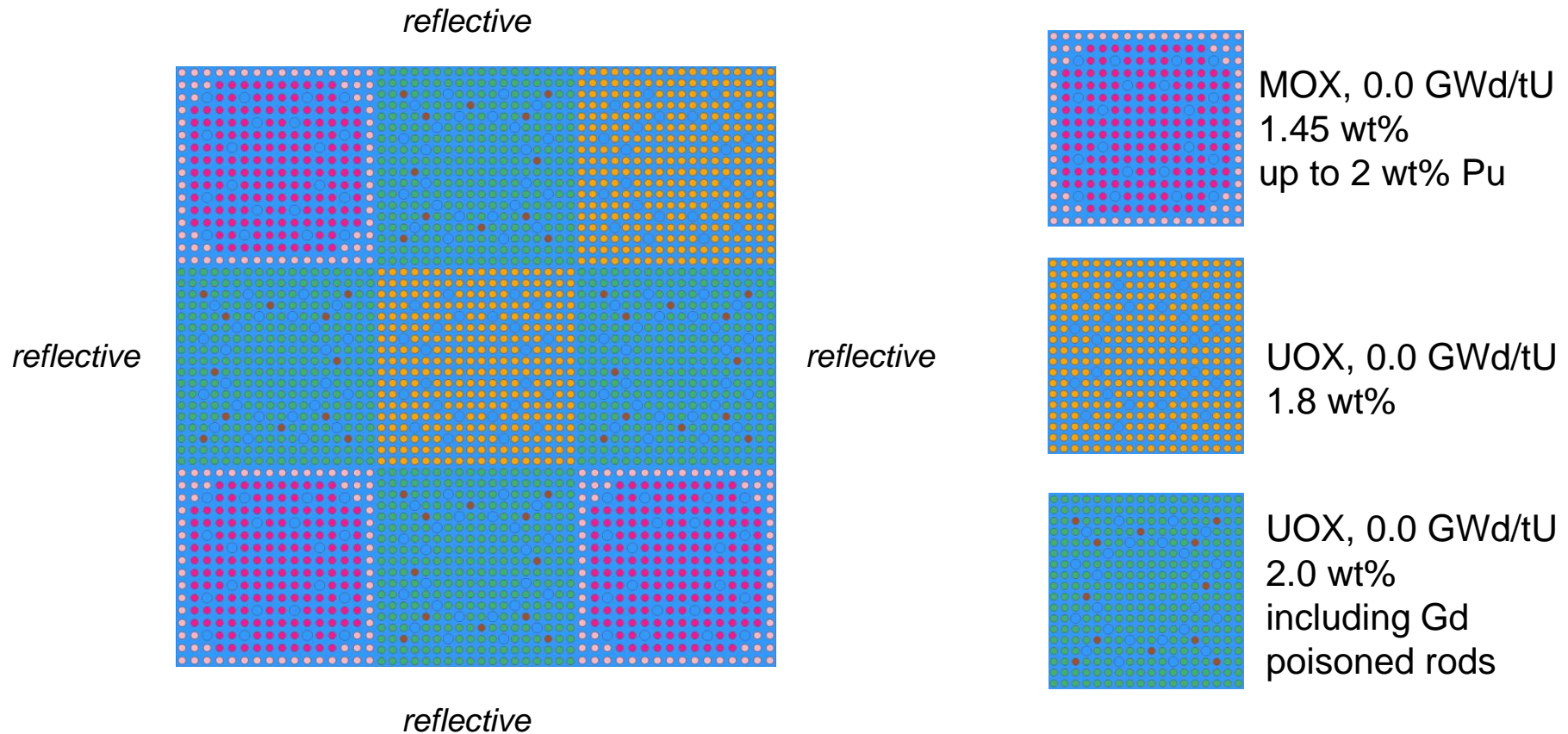


# Pin power reconstruction – HZP case 1 (3/3)

5.53	1.52	0.52	-0.07	-0.25	-0.38	-0.51	-0.48	-0.54	-0.49	-0.53	-0.20	-0.30	-0.03	0.43	1.37	5.39
1.49	0.78	0.12	0.00	-0.55	0.54	-0.90	-0.65	0.52	-0.66	-0.73	0.74	-0.43	-0.18	0.12	0.73	1.35
0.42	0.25	-0.21	0.83	0.36	0.00	0.60	0.40	0.00	0.52	0.54	0.00	0.48	0.74	-0.25	0.24	0.49
0.06	-0.10	0.84	0.00	0.31	0.52	-0.89	-0.95	0.38	-0.95	-0.87	0.41	0.25	0.00	0.80	-0.10	-0.04
-0.21	-0.43	0.47	0.12	-1.07	0.33	-1.00	-0.86	0.27	-1.05	-1.09	0.40	-1.02	0.07	0.34	-0.55	-0.15
-0.26	0.68	0.00	0.45	0.34	0.00	0.31	0.20	0.00	0.25	0.29	0.00	0.26	0.39	0.00	0.55	-0.30
-0.40	-0.48	0.33	-0.93	-1.05	0.24	-1.07	-1.15	0.20	-1.03	-1.18	0.31	-1.09	-0.88	0.46	-0.82	-0.41
-0.41	-0.68	0.59	-0.88	-1.03	0.23	-0.92	-1.12	0.22	-1.03	-1.05	0.14	-1.01	-0.95	0.47	-0.87	-0.38
-0.31	0.52	0.00	0.36	0.38	0.00	0.20	0.13	0.00	0.19	0.30	0.00	0.19	0.26	0.00	0.58	-0.51
-0.46	-0.69	0.47	-0.83	-0.88	0.21	-1.10	-1.11	0.26	-1.07	-1.09	0.25	-1.08	-0.93	0.44	-0.70	-0.53
-0.43	-0.57	0.47	-0.83	-0.83	0.23	-0.99	-1.01	0.17	-1.07	-1.08	0.24	-1.00	-0.82	0.53	-0.72	-0.65
-0.33	0.39	0.00	0.58	0.45	0.00	0.18	0.38	0.00	0.27	0.26	0.00	0.35	0.56	0.00	0.62	-0.31
-0.18	-0.49	0.48	0.20	-1.04	0.42	-0.91	-0.99	0.42	-0.93	-0.97	0.36	-1.08	0.31	0.38	-0.49	-0.22
0.06	0.03	0.87	0.00	0.44	0.51	-0.82	-0.82	0.51	-0.86	-0.99	0.37	0.27	0.00	0.84	-0.14	0.03
0.51	0.23	-0.17	0.85	0.53	0.00	0.54	0.52	0.00	0.54	0.57	0.00	0.43	0.73	-0.18	0.19	0.51
1.54	0.78	0.18	0.02	-0.39	0.67	-0.65	-0.56	0.51	-0.66	-0.58	0.64	-0.45	-0.06	0.22	0.80	1.46
5.62	1.58	0.45	0.03	-0.31	-0.26	-0.48	-0.49	-0.30	-0.43	-0.31	-0.35	-0.14	-0.06	0.40	1.51	5.52

Relative pin power errors Serpent 2 PPR  
vs. Serpent 2 in per cent

# Pin power reconstruction – HZP case 2 (1/3)



Fuel assemblies design based on AREVA fuel for KONVOI PWR

# Pin power reconstruction – HZP case 2 (2/3)

- Serpent 2:
  - 2E+9 histories in 500 active cycles
  - 2g cross sections (0.625 eV boundary)

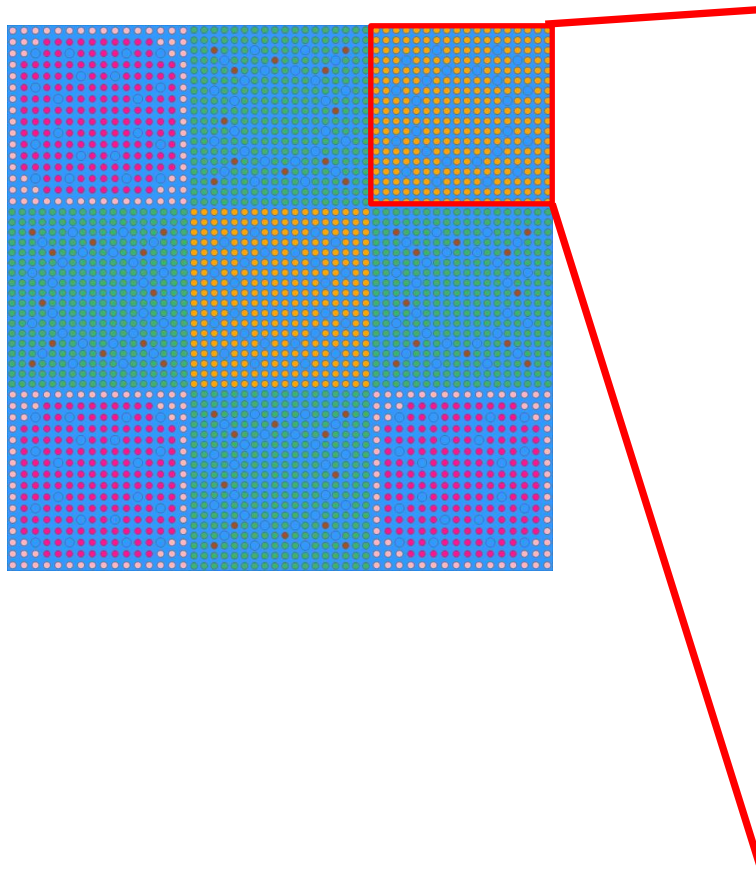
Code	$k_{inf}$	Rel. Diff. [pcm]
Serpent 2 CE	0.961211±0.00003	-
PARCS 2g NEM	0.960741	47.0

Serpent 2 CE PARCS 2g Rel. Diff. [%]
--

1.5441	0.5843	0.4224
1.5386	0.5904	0.4326
<b>-0.36</b>	<b>1.04</b>	<b>2.41</b>
0.8849	0.7056	0.5845
0.8845	0.7123	0.5904
<b>-0.04</b>	<b>0.96</b>	<b>1.01</b>
1.8449	0.8848	1.5445
1.8281	0.8845	1.5386
<b>-0.91</b>	<b>-0.04</b>	<b>-0.38</b>

Normalized nodal powers as predicted by Serpent 2 and PARCS

# Pin power reconstruction – HZP case 2 (3/3)



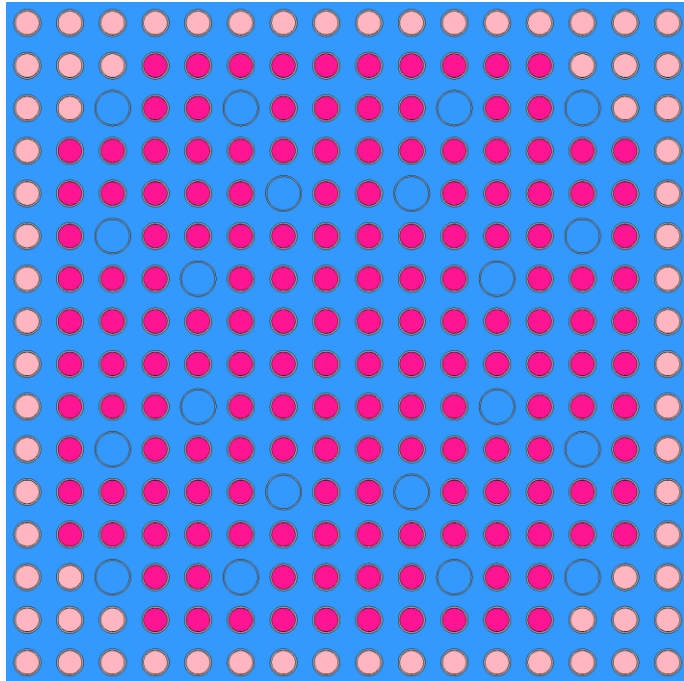
23.27	6.91	6.89	5.59	4.62	3.60	2.70	3.06	3.66	3.66	3.36	2.90	3.39	4.93	5.62	6.53	6.60	6.15
6.92	6.95	5.74	4.64	4.22	2.31	0.37	2.08	3.63	3.43	2.12	0.63	2.23	4.00	5.04	6.10	6.71	6.87
7.62	6.48	4.07	1.43	2.10	-0.40	0.00	-0.63	1.91	2.29	-0.42	0.00	0.44	1.86	1.55	4.36	6.12	6.64
6.83	5.25	1.63	0.00	-0.73	-0.80	-2.42	-1.95	0.91	0.68	-1.74	-2.29	-0.04	-0.59	0.00	1.72	5.09	6.42
5.71	4.63	2.12	-0.67	-0.51	-2.41	-2.86	0.00	-0.76	-1.01	0.00	-2.75	-2.19	-0.33	-0.37	2.64	4.72	5.83
4.32	2.70	-0.05	-0.58	-2.07	0.00	-2.04	-0.77	1.51	1.20	-0.75	-1.80	0.00	-2.12	0.09	0.56	3.51	5.02
3.41	1.02	0.00	-2.39	-2.74	-2.33	0.98	2.97	3.83	3.78	2.71	1.35	-2.04	-2.29	-1.80	0.00	1.91	4.84
3.92	2.56	-0.43	-2.00	0.00	-1.17	2.42	4.04	5.22	5.13	4.47	2.76	-0.85	0.00	-1.40	0.52	3.60	5.15
4.14	3.48	1.82	0.54	-1.16	1.41	3.47	5.04	5.72	6.21	5.18	3.80	1.87	-0.59	1.22	3.32	4.93	5.95
3.80	3.44	2.07	0.28	-1.13	1.21	3.70	5.15	5.88	5.58	5.02	3.76	1.66	-0.32	1.80	3.83	5.16	6.30
3.16	2.07	-0.57	-2.22	0.00	-1.23	2.26	4.29	4.69	5.01	4.44	3.04	-0.59	0.00	0.05	2.81	4.52	5.71
2.84	0.25	0.00	-2.68	-3.10	-2.32	0.42	2.45	3.45	3.83	2.83	1.32	-1.87	-2.45	-0.10	0.00	3.32	5.25
3.44	2.45	-0.68	-0.83	-2.65	0.00	-2.67	-0.98	1.18	1.37	-1.13	-2.04	0.00	-2.11	-1.99	-0.05	1.34	4.62
5.00	3.79	1.12	-1.24	-0.88	-2.45	-3.24	0.00	-1.16	-1.17	0.00	-3.16	-2.42	-1.40	-2.21	-0.71	2.80	5.11
6.25	4.60	1.08	0.00	-1.15	-0.85	-2.56	-1.78	0.65	0.53	-2.13	-2.78	-0.66	-1.36	0.00	0.80	4.06	5.55
7.06	5.88	3.98	1.17	1.65	-0.25	0.00	-0.55	2.18	2.38	-0.54	0.00	-0.29	1.16	1.13	3.62	5.51	6.79
6.62	6.68	5.51	4.81	4.02	2.59	0.91	2.73	3.77	3.81	2.77	0.75	3.02	4.06	4.63	5.76	6.73	7.31
23.87	6.75	6.33	5.78	5.18	4.63	3.62	4.18	4.64	4.69	4.32	3.96	4.15	5.02	6.06	6.38	7.16	7.45

Relative pin power errors PARCS vs. Serpent 2 in per cent

# Agenda

- Pin power reconstruction
  - Using Serpent 2 for pin power reconstruction constant generation
  - Serpent 2 support in GenPMAXS
  - Selected verification cases
  
- Pin level cross section generation
  - General approach and pin level homogenization corrections
  - Serpent 2 support in createXSlib
  - Selected verification cases
  - Impact on homogenization corrections on Serpent 2 performance
  
- Conclusions and outlook

# General pin level cross section generation approach



16x16-20 MOX  
0.0 GWd/tU

Pin level XS in  
Serpent 2 have issue  
with kinetics  
parameters

- Infinite lattice calculations per pin cell type
- Few-group constants per pin cell type generated based on finite lattice calculation for fuel assembly (*standard method*)
- Few-group constants per pin cell type and position generated based on finite lattice calculation for fuel assembly
- Few-group constants per pin cell type and position generated together with homogenization corrections based on finite lattice calculation for fuel assembly

Production XS  
libraries with  
critical spectrum  
correction

# Super-homogenization factors

- in case of zero currents across cell boundaries, SPH factors are the inverse of an ADF/CDF
- SPH factors are defined as for diffusion

$$\mu = \frac{\bar{\Phi}_{het}}{\bar{\Phi}_{hom}}$$

- They have to be obtained by an iterative procedure using the lower order formulation of the homogeneous system (DYN3D, COBAYA3k), based on the following expressions

$$\begin{aligned}\tilde{\Sigma} &= \mu \Sigma \\ \tilde{\Sigma} \bar{\Phi}_{hom} &= \Sigma \bar{\Phi}_{het}\end{aligned}$$

## GET interface discontinuity factors

- GET discontinuity factors are defined as ratio of average heterogeneous and homogeneous neutron fluxes on each surface  $S$  of a node for diffusion

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

- Heterogeneous neutron surface fluxes can be obtained from lattice calculation
- The method of obtaining the homogeneous surface fluxes depends on and has to be consistent with spatial discretization of reactor simulator used



## BBH interface discontinuity factors

- BBH discontinuity factors are defined to preserve surface averaged partial currents
- Factors are applied to surface averaged partial currents, only for diffusion as the low order operator BBH factors can also be formulated in terms of surface fluxes
- BBH factors are of the generic form for diffusion:

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

- The method of obtaining the partial currents depends on and has to be consistent with spatial discretization of reactor simulator used

# COBAYA3k: Interface discontinuity factors

- COBAYA3k employs FMFD method, an exact formula to compute GET IDF can be derived

$$f = \frac{\bar{\Phi}_{het}^s}{\bar{\Phi}_{hom}^s} = \frac{\bar{\Phi}_{het}^s}{\bar{\Phi}_{het} - \frac{J_{het} h}{2 D}}$$

- The corresponding exact formula for flux discontinuity factor form of the BBH IDF

$$f = 2 \frac{J_{het}^+ + J_{het}^-}{\bar{\Phi}_{het} - \frac{J_{het} h}{2 D}}$$

## DYN3D: Interface discontinuity factors

- Surface fluxes are **NOT** part of a **NEM solution**
- Expression for the transverse integrated, average neutron flux in direction  $u$

$$\Phi_g^i(u) = \sum_{k=0}^2 c_{g,k}^{i,u} h_k\left(\frac{u}{a_u}\right) + d_{g,+u}^i e^{B u} + d_{g,-u}^i e^{-B u}$$

with node index  $i$ , polynomial basis  $h_k$  and node length in direction  $u$   $a_u$ .

- Transverse integrated diffusion equation:

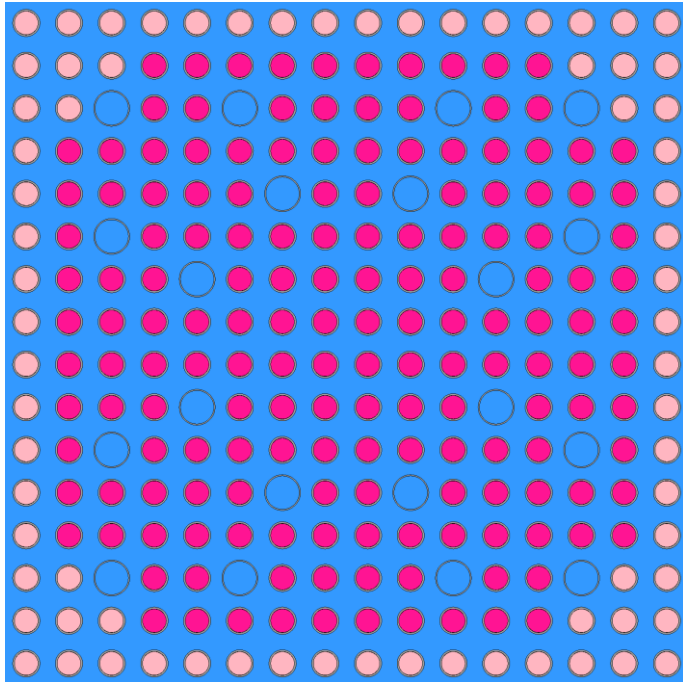
$$-D_g^i \frac{d^2}{du^2} \Phi_g^i(u) + \Sigma_R^i \Phi_g^i(u) = S_g(u) - L_g^{het}(u)$$

- Boundary conditions:

$$J_g^{het,s} = -D_g^i \frac{d}{du} \Phi_g^i(u) \Big|_{u = u_s}$$

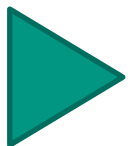
$$\bar{\Phi}_{g,het} = c_{g,0}^{i,u} + \frac{2}{B \cdot a} \sinh\left(B \cdot \frac{a}{2}\right) (d_{g,+u}^i + d_{g,-u}^i)$$

# Pin level homogenization corrections with Serpent 2



16x16-20 MOX  
0.0 GWd/tU

- SPH factors:  
pin cell average fluxes from group constant generation
- GET and BBH IDF:  
net pin cell surface currents, pin cell surface fluxes, pin cell average fluxes and pin cell surface partial currents  
→ ADF card
- System of Python scripts to translate Serpent models for nodal XS into different classes of pin level XS models



## Adapted ADF card:

```
set adf <universe> <bc_west> <bc_south> <bc_east> <bc_north>
```

## Serpent 2 support in createXSlib

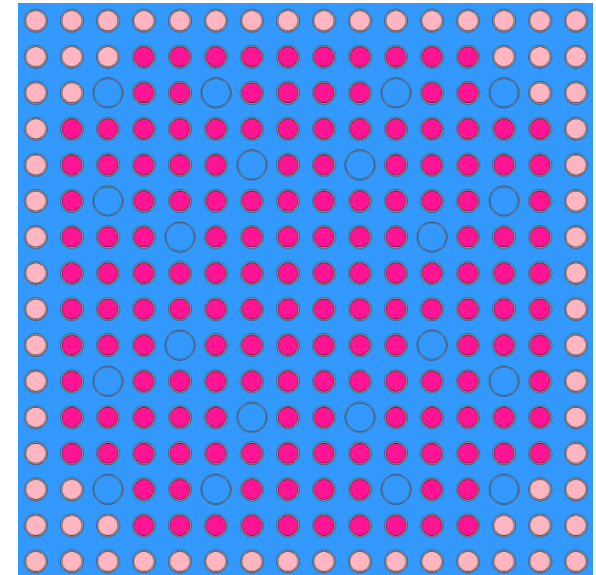
- Verification cases to be done with reactor simulators DYN3D and COBAYA3k
- createXSlib is KIT INR inhouse tool to generate multi-dimensional NEMTAB cross sections tables for DYN3D and COBAYA3's solvers COBAYA3k and ANDES
- createXSlib Serpent 2 features:
  - General nodal and pin-by-pin few-group constants
  - Reflector ADF
  - GET and BBH IDF
  - SPH factors (DYN3D only)

# Agenda

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- Pin level cross section generation
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  - Serpent 2 support in createXSlib
  - **Selected verification cases**
  - Impact on homogenization corrections on Serpent 2 performance
  
- Conclusions and outlook

# Assessment of different pin level XS generation methods (1/3)

- Serpent 2: 2E+9 histories in 500 active cycles  
2g cross sections (0.625 eV boundary)
- Serpent 2 output translated with createXSlib, achievable accuracy tested with DYN3D and COBAYA3k
- XS tables generated per pin type (3M),  
per pin type and position (32M),  
per pin type and position with IDF (IDF) and  
per pin type and position with SPH (SPH)



16x16-20 MOX  
0.0 GWd/tU

MOX fuel  
assembly for  
AREVA KONVOI  
PWR

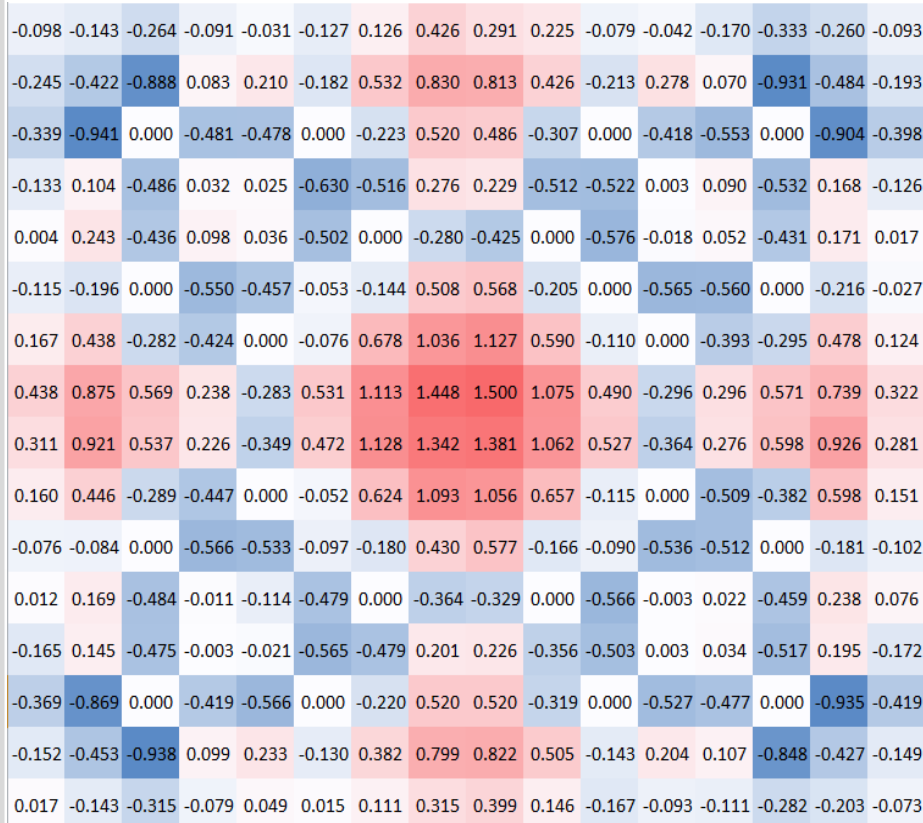
# Assessment of different pin level XS generation methods (2/3)

	MOX FA $k_{inf}$	Rel. Diff. Eigenvalue [pcm]	Max. Rel. pin power error [%]
Serpent 2 CE	1.08496±0.000030	-	-
DYN3D diff (3M)	1.087627	266.7	1.22
DYN3D sp3 (3M)	1.086733	177.3	1.50
COBAYA3k diff (3M)	1.084761	19.9	1.45
DYN3D diff (32M)	1.087578	261.8	0.49
DYN3D sp3 (32M)	1.086685	172.5	0.28
COBAYA3k diff (32M)	1.084710	25.0	0.60
DYN3D diff (IDF)	1.084950	1.0	0.05
DYN3D diff (SPH)	1.084951	0.9	0.01
COBAYA3k diff (IDF)	1.084950	1.0	0.02

Statistical  
uncertainty pin  
power below  
0.04%



# Assessment of different pin level XS generation methods (3/3)



Relative pin power errors DYN3D sp3 (3M)  
vs. Serpent 2 in per cent



Relative pin power errors DYN3D sp3 (32M)  
vs. Serpent 2 in per cent

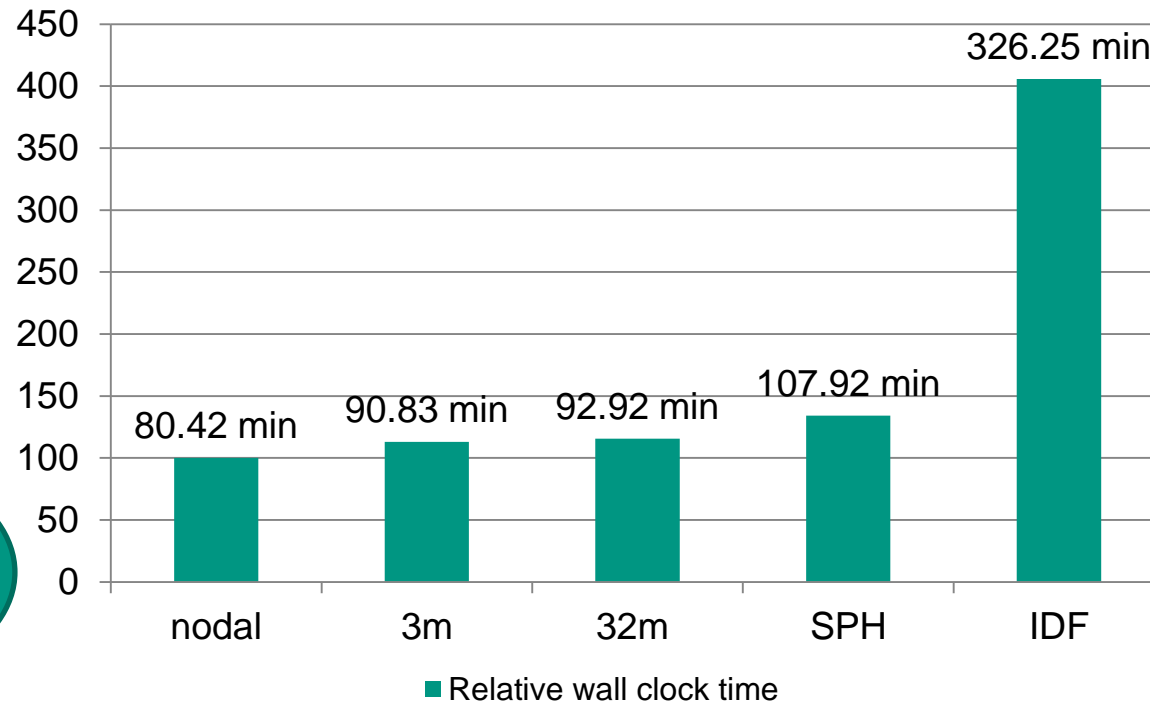
# Agenda

- Pin power reconstruction
  - Using Serpent 2 for pin power reconstruction constant generation
  - Serpent 2 support in GenPMAXS
  - Selected verification cases
  
- Pin level cross section generation
  - General approach and pin level homogenization corrections
  - Serpent 2 support in createXSlib
  - Selected verification cases
  - Impact on homogenization corrections on Serpent 2 performance
  
- Conclusions and outlook

# Performance impact of homogenization corrections

- Measurements for 16x16-20 MOX FA using for 16 MPI processes with 8 OpenMP threads each
- Thread affinity and proper page placement assured by batch system
- 2E+9 histories in 500 active cycles, 2g cross sections (0.625 eV boundary)

Results for KIT HC3, dual socket Intel Xeon E5540 compute nodes with 24GB memory



Nodal and 3m cases would yield sufficient results with less histories

# Agenda

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## Conclusions and Outlook

- Group-wise form functions may now be obtained with Serpent 2
- Accuracy of PPR systematically limited
- All pin-level cross section generation approaches are supported by Serpent 2
- For high accuracy solutions, one should employ pin level homogenization corrections
- Homogenization corrections lead to a (large) penalty in terms of computational resource, IDF: fourfold runtime increase compared to a nodal cross section generating model with same number of neutron histories
- Future work:
  - Kinetics parameters per pin cell
  - Performance optimization of IDF generation