Cross section generation with Polaris and Sampler for LWR modeling

P. Rouxelin, G. Delipei, M. Avramova, K. Ivanov

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Objective

- Give an overview of some of the activities carried on with SCALE at North Carolina State University
- Present and discuss current struggles

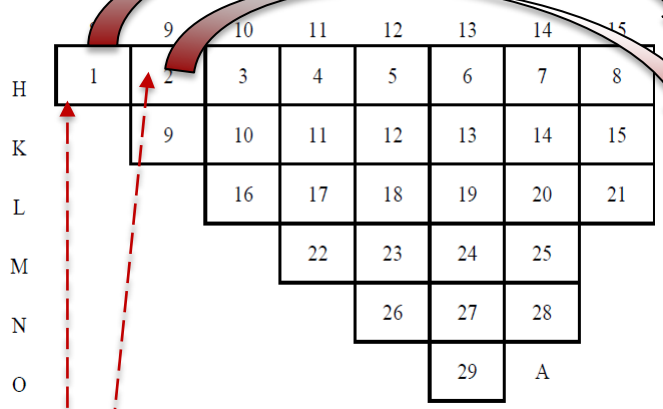
Outline

- Description of Data Management sequence developed at NCSU
  - Polaris assembly construction
  - Data generation and verification
  - Conversion to PMAXS
- Sample of results on TMI-1 core model
  - Correlation between Sampler's elemental perturbation factors on core metrics
- Discussion on reflector modeling in Polaris and effect in core results

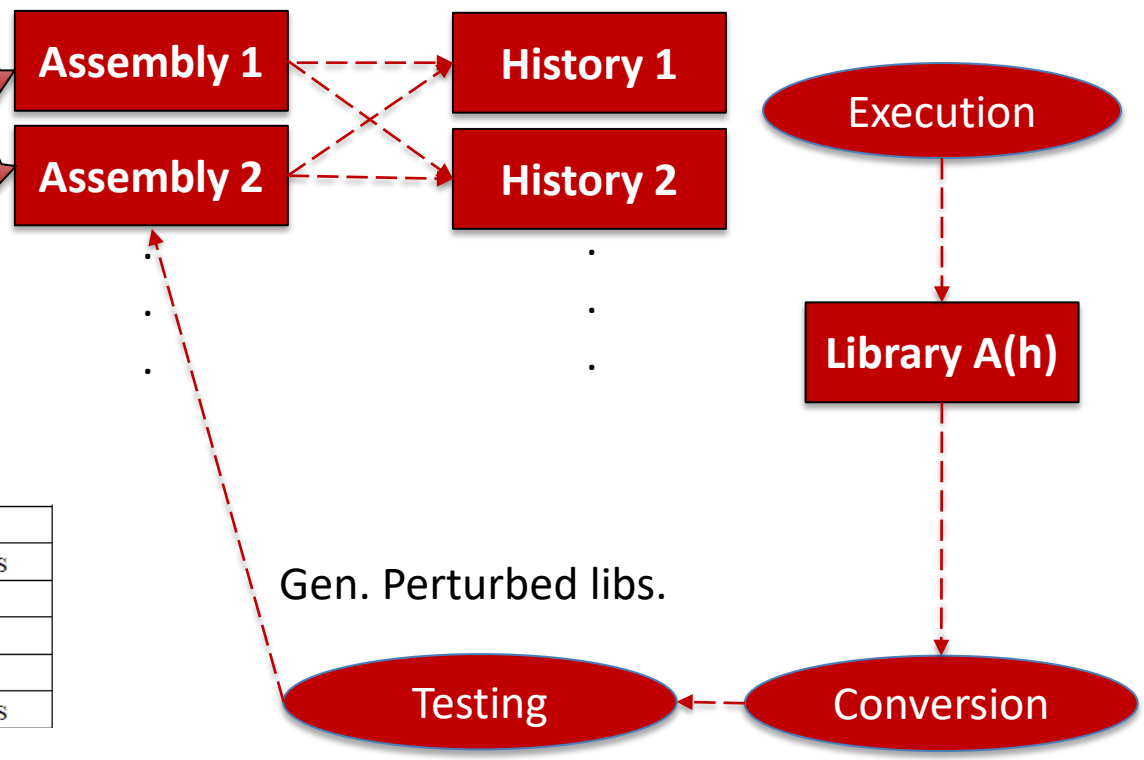
Generic process to generate libraries

Generation of cross section libraries for nodal calculations usually requires multiple Polaris inputs

Figure 27: [illegible]-1 – definition of fuel assembly types



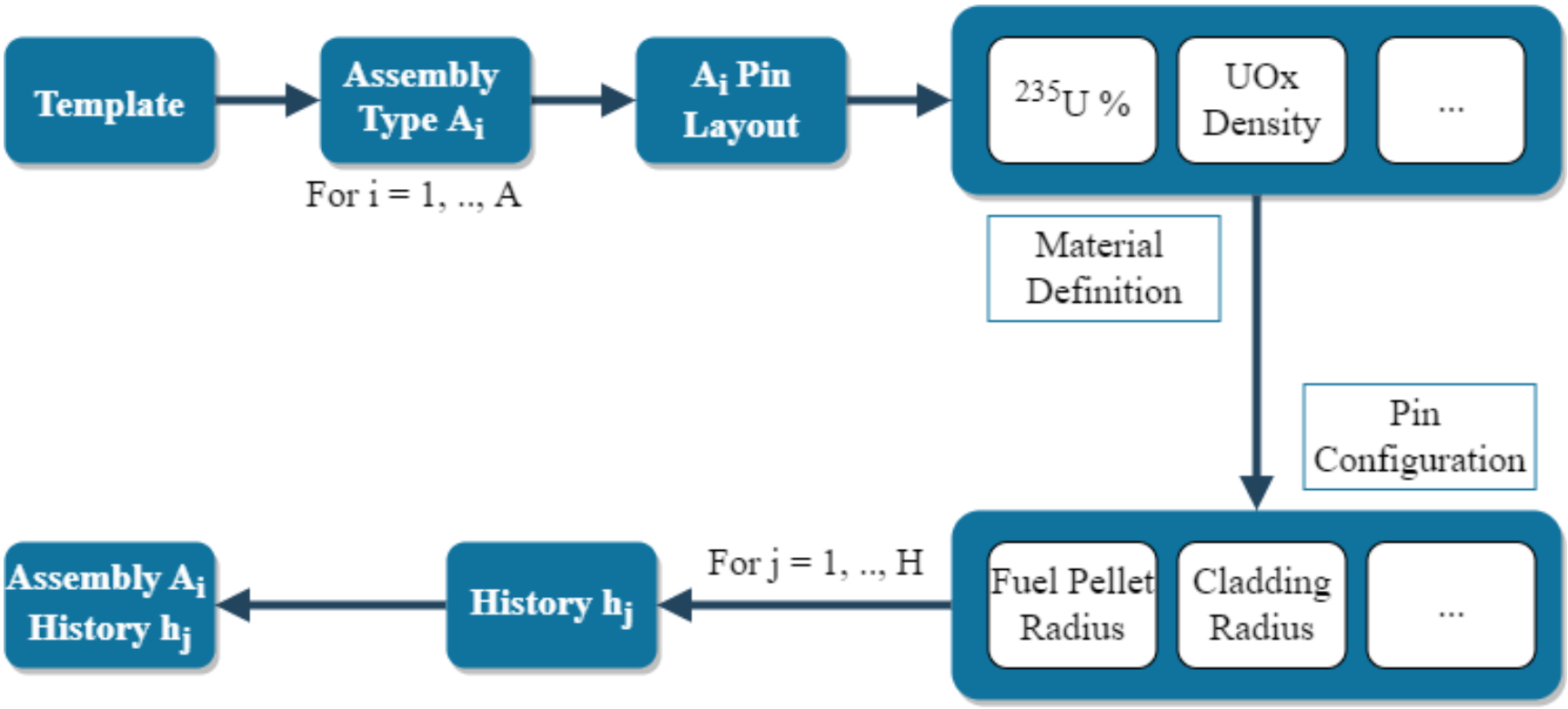
Assembly	Characteristics		
1	4.00 w/o	No BP	No Gd pins
2	4.95 w/o	3.5 % BP	4 Gd pins
3	5.00 w/o	No BP	4 Gd pins
4	4.95 w/o	3.5 % BP	4 Gd pins
5	4.40 w/o	No BP	No Gd pins



Generic process to generate libraries

- Process is error-prone, redundant
- It is heterogeneous: the conversion of t16 libraries is not handled by SCALE utilities
- Depending on computational power, the libraries cannot be generated simultaneously (typically 10,000 simultaneous jobs)
- The idea is to develop a “data management” sequence to handle workload, input creation, execution, library conversion input and library conversion execution

Automatized sequence to generate PMAXS - workflow



Template format – Nominal

```
=polaris_6.3
system PWR
lib mg="v7-56"

% -------------------- OPTIONS --------------------
  opt FG  0  0.1  0.5  1  2  4  6  8  10  12.5  15  17.5  20  25  30
  opt PRINT XFile16=true
  opt DEPL TrackingSet="complete"
% -------------------- GEOMETRY --------------------
  geom MyPin : ASSM 15 1.4427 sym=SE
  hgap 0.085 : COOL.1
  pinmap

%                    ---------- MATERIALS ----------

  comp Euo2      : UOX #{UOX412}
  mat FUEL.1     : Euo2 dens=#{UOXDens}

  comp Euo2Gd    : UOX #{UOXgd}
  comp gad       : WT GD2O3=#{Gd2O3}  Euo2Gd=-100
  mat FUEL.2     : gad dens=#{gadDens} % theoretical density of Gd2O3 =

  mat CLAD.1     : ZIRC4 dens=6.56

  mat GAP.1      : FILLGAS

  comp SS304L    : WT C=0.015 Mn=1.0 Si=0.5 Cr=17.5 Ni=10.5 P=0.02 Mo=2
  mat CR_304L.1  : SS304L dens=7.8

  mat CR_CNTL.1  : AIC dens=10.1586 % density from TMI
```

```
if assembly == '400_gd_0_bp_0'
  pinLayout = \n\
I\n\
1 1\n\
1 1 2\n\
1 1 1 1\n\
1 1 1 1 2\n\
1 1 2 1 1 1\n\
1 1 1 1 1 1 1\n\
1 1 1 1 1 1 1 1\n'
```

```
fuelAssemblies = {\
'400_gd_0_bp_0':{'UOX412':{'nom':'4.00','std':'0.000746'},'UOXgd':{'nom':'4.00','std':'0.0010'}
'440_gd_0_bp_0':{'UOX412':{'nom':'4.40','std':'0.000746'},'UOXgd':{'nom':'4.40','std':'0.0010'}
'485_gd_4_bp_0':{'UOX412':{'nom':'4.85','std':'0.000746'},'UOXgd':{'nom':'4.85','std':'0.0010'}
'495_gd_4_bp_0':{'UOX412':{'nom':'4.95','std':'0.000746'},'UOXgd':{'nom':'4.95','std':'0.0010'}
'495_gd_8_bp_0':{'UOX412':{'nom':'4.95','std':'0.000746'},'UOXgd':{'nom':'4.95','std':'0.0010'}
'500_gd_0_bp_0':{'UOX412':{'nom':'5.00','std':'0.000746'},'UOXgd':{'nom':'5.00','std':'0.0010'}
'500_gd_4_bp_0':{'UOX412':{'nom':'5.00','std':'0.000746'},'UOXgd':{'nom':'5.00','std':'0.0010'}
'500_gd_8_bp_0':{'UOX412':{'nom':'5.00','std':'0.000746'},'UOXgd':{'nom':'5.00','std':'0.0010'}
'495_gd_0_bp_1':{'UOX412':{'nom':'4.95','std':'0.000746'},'UOXgd':{'nom':'4.95','std':'0.0010'}
'495_gd_4_bp_1':{'UOX412':{'nom':'4.95','std':'0.000746'},'UOXgd':{'nom':'4.95','std':'0.0010'}
'500_gd_4_bp_1':{'UOX412':{'nom':'5.00','std':'0.000746'},'UOXgd':{'nom':'5.00','std':'0.0010'}
```

Template Format – Perturbations

```
fuelAssemblies = {\
'400_gd_0_bp_0':{'UOX412':{'nom':'4.00','std':'0.000746'},'UOXgd':{'nom':'4.00','std':'0.0010'}
'440_gd_0_bp_0':{'UOX412':{'nom':'4.40','std':'0.000746'},'UOXgd':{'nom':'4.40','std':'0.0010'}
'485_gd_4_bp_0':{'UOX412':{'nom':'4.85','std':'0.000746'},'UOXgd':{'nom':'4.85','std':'0.0010'}
'495_gd_4_bp_0':{'UOX412':{'nom':'4.95','std':'0.000746'},'UOXgd':{'nom':'4.95','std':'0.0010'}
'495_gd_8_bp_0':{'UOX412':{'nom':'4.95','std':'0.000746'},'UOXgd':{'nom':'4.95','std':'0.0010'}
'500_gd_0_bp_0':{'UOX412':{'nom':'5.00','std':'0.000746'},'UOXgd':{'nom':'5.00','std':'0.0010'}
'500_gd_4_bp_0':{'UOX412':{'nom':'5.00','std':'0.000746'},'UOXgd':{'nom':'5.00','std':'0.0010'}
'500_gd_8_bp_0':{'UOX412':{'nom':'5.00','std':'0.000746'},'UOXgd':{'nom':'5.00','std':'0.0010'}
'495_gd_0_bp_1':{'UOX412':{'nom':'4.95','std':'0.000746'},'UOXgd':{'nom':'4.95','std':'0.0010'}
'495_gd_4_bp_1':{'UOX412':{'nom':'4.95','std':'0.000746'},'UOXgd':{'nom':'4.95','std':'0.0010'}
'500_gd_4_bp_1':{'UOX412':{'nom':'5.00','std':'0.000746'},'UOXgd':{'nom':'5.00','std':'0.0010'}
```

After building from template

```
end branch
end sequence
read variable[UOX412]
distribution = normal
cases = c1 end
value =4.00
stddev =0.000746
end variable

read variable[UOXgd]
distribution = normal
cases = c1 end
value =4.00
stddev =0.0010
end variable

read variable[Gd2O3]
distribution = normal
```

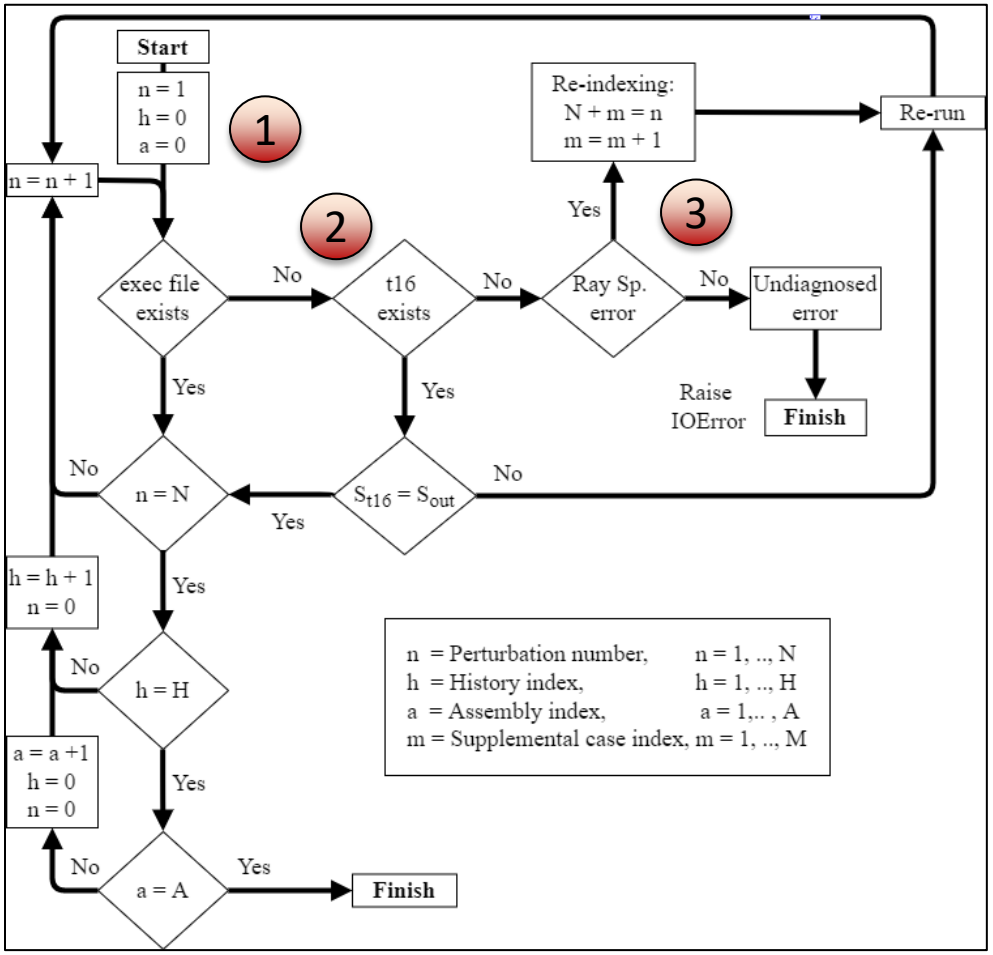
No "distribution block" in template

```
end branch

end
```

```
=sampler
 read parameters
 run_cases=no
perturb_xs=yes
perturb_yields=yes
perturb_decay=no
library="v7-56"
first_sample=1
n_samples=109
end parameters
read case[c1]
sequence=polaris_6.3
system PWR
lib mg="v7-56"
```

Data management sequence



The sequence produces H histories for A assemblies and N perturbations

1

8 histories
11 assemblies
100 perturbations
2 reflectors

~9,000 samples

2

Restart capabilities implemented

Cases may fail due to ray spacing errors. In that case, an additional sample is added, and case is re-indexed and re-run

3

Handling ray spacing errors

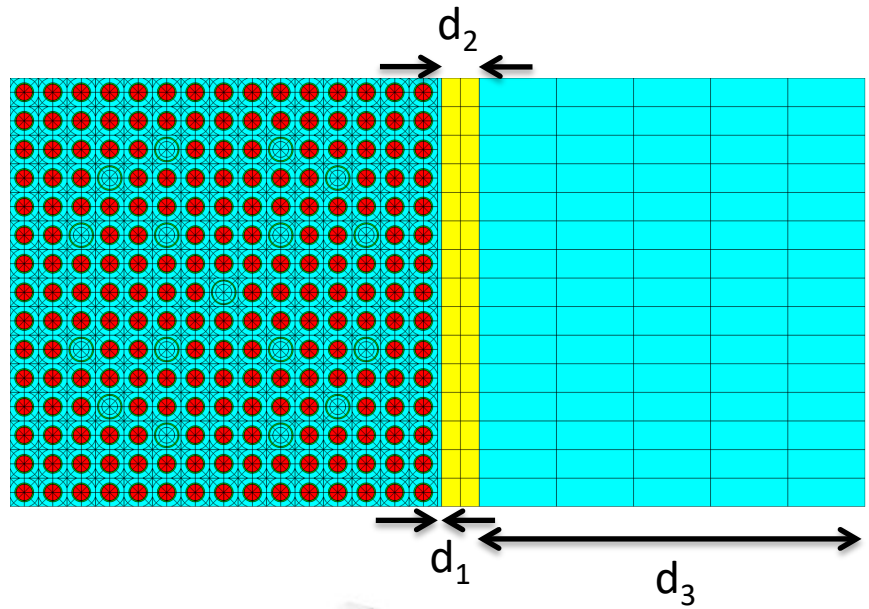
- If manufacturing uncertainties are implemented, geometrical parameters may be varied
  - Pin dimensions, Assembly size, half gap etc.
- Certain configurations induce ray spacing errors in Polaris
- Mitigation:
  - Discretization?
  - Ray space tolerance?

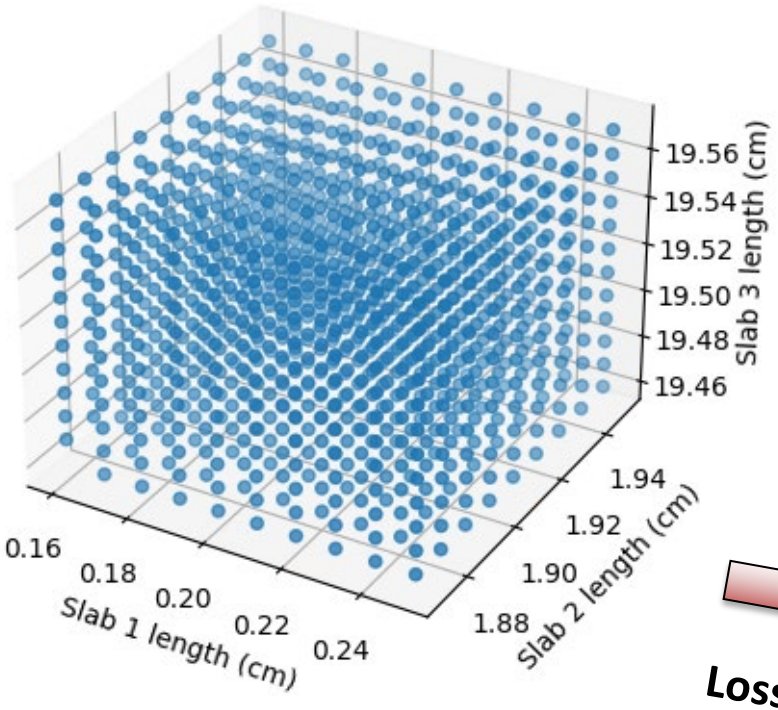
```
terminate called after throwing an instance of 'nemesis::assertion
  what():  Ray did not end on problem boundary.

Program received signal SIGABRT: Process abort signal.

Backtrace for this error:
#0  0x2AAABDDC82E7
#1  0x2AAABDDC88EE
#2  0x2AAABE84F3FF
#3  0x2AAABE84F387
#4  0x2AAABE850A77
#5  0x2AAABEC46A44
#6  0x2AAABEC44BE5
#7  0x2AAABEC44C12
#8  0x2AAABEC44E85
#9  0x2AAAABE5D33C
#10  0x2AAAAAFA80FF
#11  0x2AAAAAD32AC7
#12  0x2AAAAAD39ACA
#13  0x404A05 in MAIN__ at Polaris.f90:?
```

Frequency of ray spacing errors

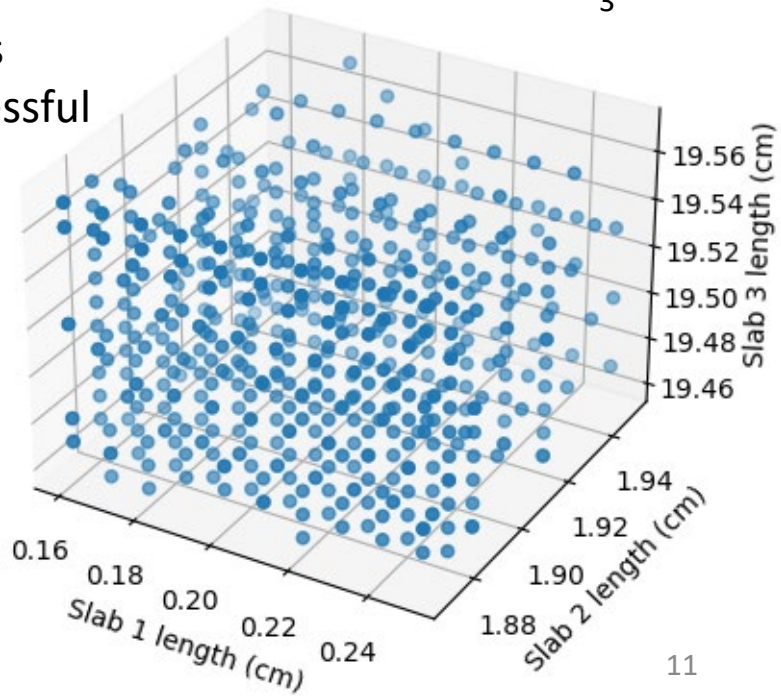




Cases tested

Loss rate ~47%

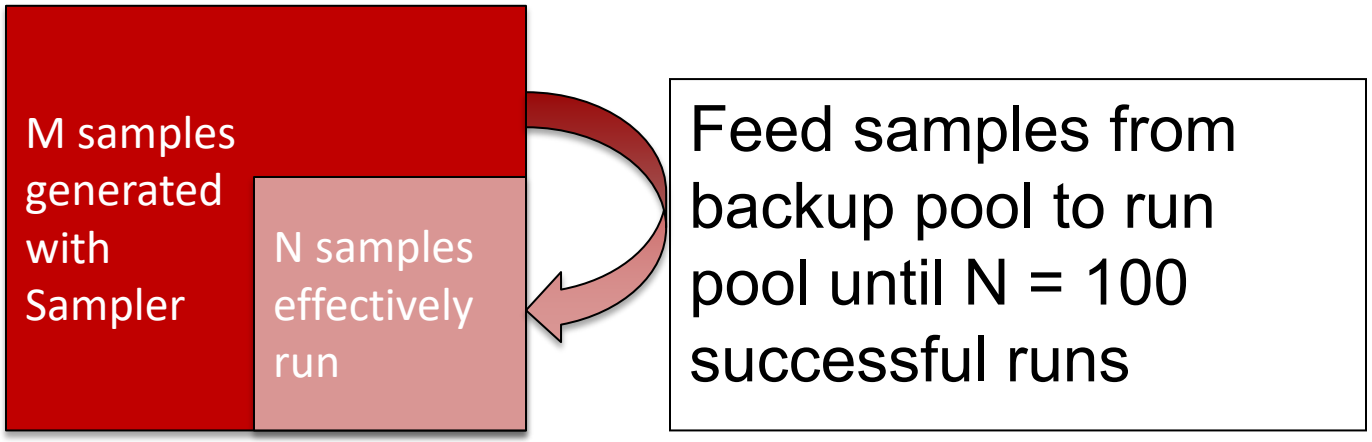
Cases successful



For TMI fuel assemblies: ~20% loss rate

Remediation adopted for ray spacing errors

- If number of samples large enough (> 500), ignore the failed cases
  - re-index cases to facilitate post-processing
- Otherwise, generate backup files with Sampler
  - This solution is adopted in the Data Management Sequence



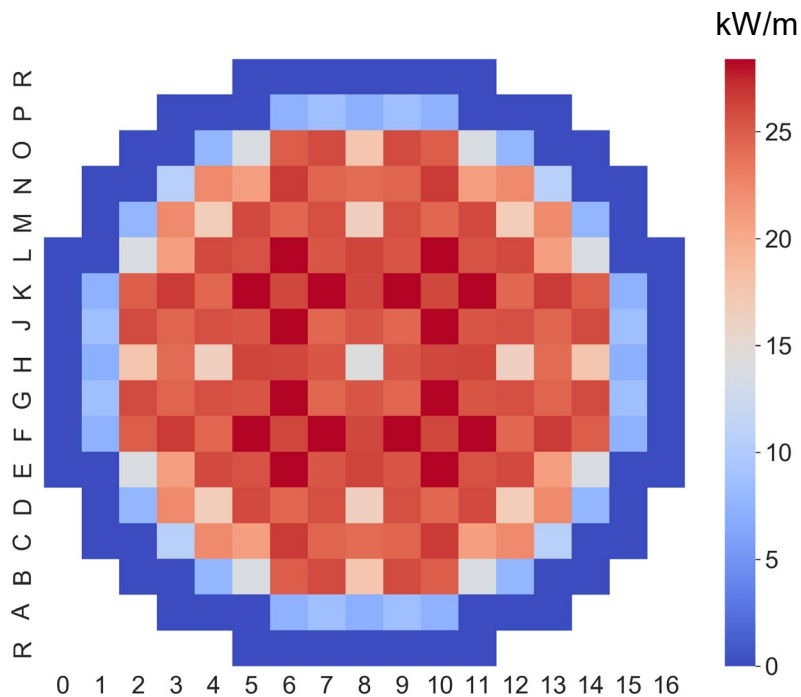
Cross section conversion

- After the generation of the t16 with Polaris, the libraries are converted into PMAXS for PARCS calculations
- The GenPMAXS inputs for t16-to-PMAXS conversion are automatically constructed from the Polaris inputs
- GenPMAXS is executed automatically by the sequence after generating the GenPMAXS inputs

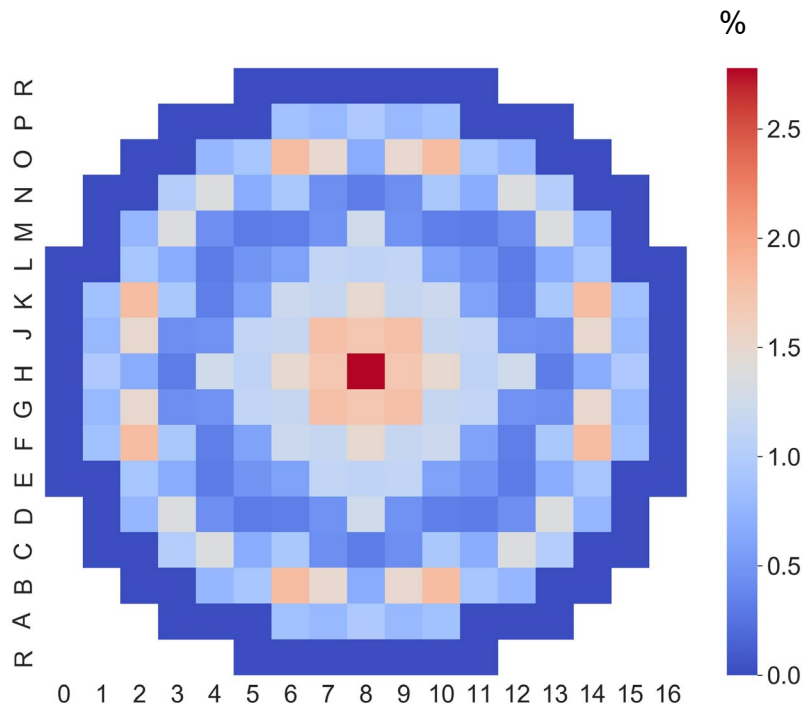
Effectively, the sequence generates 9,000 PMAXS libraries from 2 Polaris templates (fuel assembly, reflector)

Uncertainties on core level – PARCS/CTF

Perturbed cross sections were used to build a TMI core model

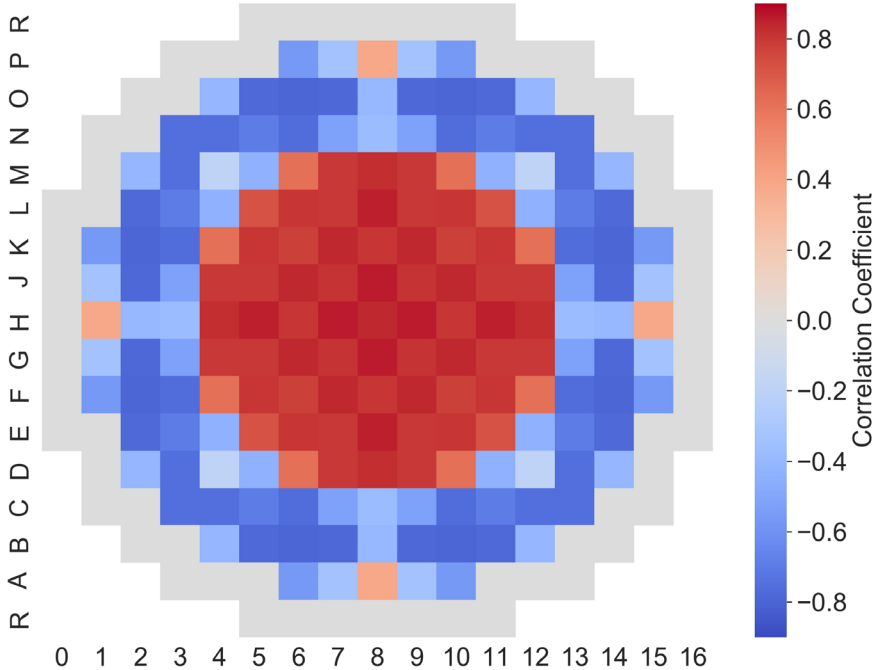


Maximum axial linear power

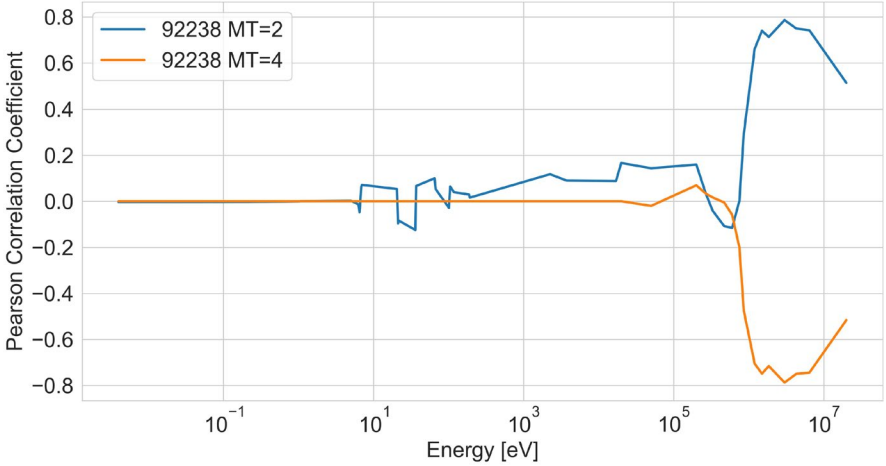


Uncertainty of maximum axial linear power

Uncertainties on core level – PARCS/CTF



Max. Spearman correlation coefficient of maximum axial linear power and ^{238}U elastic scattering



Group-wise spearman correlation coefficient of ^{238}U elastic/inelastic scattering and maximum linear power

Reflector modeling in Polaris (WB1)

				-17.7	-14.5	-14.5	-13.4	-14.5	-14.4	-17.6				
		-20.7	-14.3	-9.0	-5.3	-5.5	-3.7	-5.5	-5.3	-8.9	-14.2	-20.6		
	-20.7	-10.4	-3.8	-1.2	-0.2	2.3	2.5	2.3	-0.2	-1.1	-3.8	-10.3	-20.6	
	-14.3	-3.8	2.3	3.4	5.5	6.9	11.3	7.0	5.6	3.5	2.4	-3.7	-14.2	
-17.7	-9.0	-1.2	3.4	7.0	8.2	11.0	11.3	11.0	8.2	7.1	3.5	-1.1	-8.9	-17.6
-14.5	-5.3	-0.2	5.5	8.1	11.6	12.4	14.3	12.4	11.6	8.2	5.6	-0.1	-5.2	-14.4
-14.5	-5.6	2.3	6.9	11.0	12.4	15.7	15.9	15.7	12.5	11.1	7.0	2.4	-5.4	-14.4
-13.4	-3.8	2.4	11.3	11.2	14.2	15.9	20.8	15.9	14.3	11.3	11.4	2.5	-3.7	-13.4
-14.5	-5.6	2.3	6.9	11.0	12.4	15.7	15.9	15.7	12.5	11.1	7.0	2.4	-5.4	-14.4
-14.5	-5.3	-0.2	5.5	8.1	11.6	12.4	14.2	12.4	11.6	8.2	5.6	-0.1	-5.2	-14.4
-17.7	-9.0	-1.2	3.4	7.0	8.2	11.0	11.2	11.0	8.2	7.1	3.5	-1.1	-8.9	-17.6
	-14.3	-3.8	2.3	3.4	5.5	6.9	11.3	7.0	5.6	3.5	2.4	-3.7	-14.2	
	-20.6	-10.4	-3.8	-1.2	-0.2	2.3	2.5	2.3	-0.2	-1.1	-3.8	-10.3	-20.6	
		-20.6	-14.3	-9.0	-5.3	-5.5	-3.7	-5.5	-5.3	-8.9	-14.2	-20.6		
				-17.6	-14.4	-14.5	-13.4	-14.5	-14.4	-17.6				

Rel. difference PARCS/MPACT of normalized assembly power using SS shroud in reflector in Polaris

Mean: 9.1%

Rel difference PARCS/MPACT of normalized assembly power using "Tube" shroud in reflector in Polaris

				1.5	-3.5	-4.9	-4.6	-4.8	-3.4	1.6				
		2.1	0.5	-2.4	-2.3	-4.3	-3.0	-4.2	-2.3	-2.3	0.5	2.1		
	2.1	-0.3	1.1	0.2	-1.4	-0.5	-0.8	-0.4	-1.3	0.3	1.2	-0.2	2.2	
	0.5	1.1	2.8	0.9	0.8	0.8	4.4	0.8	0.9	1.0	2.9	1.2	0.6	
1.5	-2.4	0.2	0.9	1.6	0.6	1.9	1.7	2.0	0.7	1.7	1.0	0.3	-2.3	1.6
-3.5	-2.3	-1.4	0.8	0.6	1.8	1.2	2.4	1.3	1.8	0.7	0.9	-1.3	-2.2	-3.4
-4.9	-4.3	-0.5	0.7	1.9	1.2	2.8	2.6	2.9	1.3	2.0	0.8	-0.4	-4.2	-4.8
-4.6	-3.0	-0.9	4.3	1.7	2.4	2.6	6.5	2.7	2.5	1.8	4.4	-0.8	-2.9	-4.5
-4.9	-4.3	-0.5	0.7	1.9	1.2	2.8	2.6	2.9	1.3	2.0	0.8	-0.4	-4.2	-4.8
-3.5	-2.3	-1.4	0.8	0.6	1.8	1.2	2.4	1.3	1.8	0.7	0.9	-1.3	-2.2	-3.4
1.5	-2.4	0.2	0.9	1.6	0.6	1.9	1.7	2.0	0.7	1.7	1.0	0.3	-2.3	1.6
	0.5	1.1	2.9	0.9	0.8	0.8	4.4	0.8	0.9	1.0	2.9	1.2	0.6	
	2.1	-0.3	1.1	0.3	-1.4	-0.5	-0.8	-0.4	-1.3	0.3	1.2	-0.2	2.2	
		2.1	0.5	-2.4	-2.3	-4.2	-3.0	-4.2	-2.2	-2.3	0.6	2.2		
				1.6	-3.4	-4.8	-4.6	-4.8	-3.4	1.6				

Mean: 1.9%

Sensitivity analysis on reflector modeling

- The PARCS results were compared with MPACT, KENO and Serpent for Watts Bar 1 reactor.
- The calculations were repeated using 4-group cross sections. The mean normalized power decreased to **1.3 %**

br	material	order	K-eff	RMS
no	ss	NA	0.99484	**8.49%**
no	struct	NA	0.99496	**8.17%**
no	tube	NA	0.99698	**1.37%**
yes	ss	yes	0.99471	**8.98%**
yes	struct	yes	0.99479	**8.76%**
yes	tube	yes	0.99689	**1.43%**
yes	ss	no	0.99446	**9.95%**
yes	struct	no	0.99459	**9.55%**
yes	tube	no	0.99533	**6.37%**

Conclusions

- A data management sequence was implemented to generate efficiently and robustly PMAXS libraries from Polaris
- The sequence relies on two Polaris templates – one fuel assembly and one reflector – to generate both nominal and perturbed libraries
- It handles history, burnup, and branch modeling
- Multiple LWR models were produced (WB1, TMI1, PB2, Koeberg).

Conclusions

- In addition, elemental perturbation factors from SCALE were correlated
  - To downstream FoM (e.g. maximum temperature in nodal core calculations)
- The correlations between elemental cross sections are usually weak, a few exceptions:
  - E.g. elastic scattering ^{238}U
- Additionally, sensitivity of nodal core results with respect to nominal cross section were studied:
  - Most sensitive parameter is the ADF at the fuel/reflector interface
  - This ADF is strongly dependent itself on the type of material used for the shroud in Polaris