Cross section generation with Polaris and Sampler for LWR modeling

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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.

<table>
<thead>
<tr>
<th>Assembly</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.00 w/o</td>
</tr>
<tr>
<td>2</td>
<td>4.95 w/o</td>
</tr>
<tr>
<td>3</td>
<td>5.00 w/o</td>
</tr>
<tr>
<td>4</td>
<td>4.95 w/o</td>
</tr>
<tr>
<td>5</td>
<td>4.40 w/o</td>
</tr>
</tbody>
</table>

- Assembly 1
- Assembly 2
- History 1
- History 2
- Library A(h)
- Execution
- Testing
- Conversion

Gen. Perturbed libs.
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**
- **Assembly Type A_i**
- **A_i Pin Layout**
  - For i = 1, ..., A

- **Assembly A_i**
- **History h_j**
  - For j = 1, ..., H

- **235U %**
- **UOx Density**
- **Material Definition**
- **Pin Configuration**
  - Fuel Pellet Radius
  - Cladding Radius
Template format – Nominal

```
if assembly == '400_gd_0_bp_0'
    pinLayout = \n    I\n    1 \n    1 \n    1 \n    2 \n    1 \n    1 \n    1 \n    1 \n    1 \n    1 \n    1 \n    1 \n    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_0_bp_1': {'UOX412': {'nom': '5.00', 'std': '0.000746'}, 'UOXgd': {'nom': '5.00', '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

```plaintext
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'}},
    '500_gd_4_bp_1': {'UOX412': {'nom': '5.00', 'std': '0.000746'}, 'UOXgd': {'nom': '5.00', 'std': '0.0010'}},
    '500_gd_8_bp_1': {'UOX412': {'nom': '5.00', 'std': '0.000746'}, 'UOXgd': {'nom': '5.00', '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:

No "distribution block" in template

```plaintext
end branch
end sequence
read variable[UOX412]
distribution = normal
cases = cl end
value = 4.00
stdev = 0.000746
end variable
read variable[UOXgd]
distribution = normal
cases = cl end
value = 4.00
stdev = 0.0010
end variable
read variable[Gd203]
distribution = normal
```
The sequence produces $H$ histories for $A$ assemblies and $N$ perturbations:

- 8 histories
- 11 assemblies
- 100 perturbations
- 2 reflectors
- ~9,000 samples
- 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.
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?
Frequency of ray spacing errors

Cases tested

Loss rate ~47%

For TMI fuel assemblies: ~20% loss rate

Cases successful
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

![Diagram]

M samples generated with Sampler

N samples effectively run

Feed samples from backup pool to run pool until N = 100 successful runs
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)

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

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%**.

<table>
<thead>
<tr>
<th>br</th>
<th>material</th>
<th>order</th>
<th>K-eff</th>
<th>RMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>no</td>
<td>ss</td>
<td>NA</td>
<td>0.99484</td>
<td>8.49%</td>
</tr>
<tr>
<td>no</td>
<td>struct</td>
<td>NA</td>
<td>0.99496</td>
<td>8.17%</td>
</tr>
<tr>
<td>no</td>
<td>tube</td>
<td>NA</td>
<td>0.99698</td>
<td>1.37%</td>
</tr>
<tr>
<td>yes</td>
<td>ss</td>
<td>yes</td>
<td>0.99471</td>
<td>8.98%</td>
</tr>
<tr>
<td>yes</td>
<td>struct</td>
<td>yes</td>
<td>0.99479</td>
<td>8.76%</td>
</tr>
<tr>
<td>yes</td>
<td>tube</td>
<td>yes</td>
<td>0.99689</td>
<td>1.43%</td>
</tr>
<tr>
<td>yes</td>
<td>ss</td>
<td>no</td>
<td>0.99446</td>
<td>9.95%</td>
</tr>
<tr>
<td>yes</td>
<td>struct</td>
<td>no</td>
<td>0.99459</td>
<td>9.55%</td>
</tr>
<tr>
<td>yes</td>
<td>tube</td>
<td>no</td>
<td>0.99533</td>
<td>6.37%</td>
</tr>
</tbody>
</table>
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 $^{238}\text{U}$
• Additionally, sensitivity of nodal core results with respect to nominal cross section were studied:
  – Most sensitive parameter is the ADF at the fuel/reflecter interface
  – This ADF is strongly dependent itself on the type of material used for the shroud in Polaris