Microscopic group constants with Serpent

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Microscopic group constants

Why?

What?

What was wrong earlier?

How?

What you can and can’t do (currently)?

The motivation (for us)

Nodal neutronics solver Ants currently developed at VTT

$\Rightarrow$ Interest in developing better group constant models

$\Rightarrow$ Interest in applying nodal calculations beyond legacy applications at VTT

$\Rightarrow$ Interest in testing and enhancing the microscopic group constant calculation features of Serpent

Microscopic group constants

Spatial homogenization methodology

Macroscopic group constant for reaction x in energy group g homogenized for a universe in volume V as

$$\Sigma_{\mathrm{x},g} = \frac{\int_{E_g}^{E_g-1} \int_V \Sigma_{\mathrm{x}}(\mathrm{r},E)\phi(\mathrm{r},E)\,\mathrm{d}V\,\mathrm{d}E}{\int_{E_g}^{E_g-1} \int_V \phi(\mathrm{r},E)\,\mathrm{d}V\,\mathrm{d}E} \tag{1}$$

What if the atomic density of a single nuclide i is different in some $w \in V$? E.g. w is fuel and V is the fuel assembly.

$\Rightarrow$ Microscopic group constants $\overline{\sigma}^{i}_{\mathrm{x},g}$

Microscopic group constants I

The reaction rate

$$\overline{\sigma}^{i}_{\mathrm{x},g}\overline{N}^{i}\overline{\phi}_{g} = \frac{1}{\int_V \mathrm{d}V}\int_{E_g}^{E_g-1}\int_{w}\sigma^{i}_{\mathrm{x}}(\mathrm{r},E)N^{i}(r)\phi(\mathrm{r},E)\,\mathrm{d}V\,\mathrm{d}E \qquad (2)$$

is wanted to be preserved in the nodal code.

However, the nodal program only knows about V, not w.

Microscopic group constants II

$\Rightarrow$ Calculate the microscopic group constant for reaction x in energy group g homogenized for materials making up w for a universe in volume V as

$$\overline{\sigma}^{i}_{\mathrm{x},g} = \frac{1}{\overline{N}^{i}\overline{\phi}_{g}} \frac{1}{\int_V \mathrm{d}V} \int_{E_g}^{E_{g-1}} \int_{w} \sigma^{i}_{\mathrm{x}}(\mathrm{r},E) N^{i}(r) \phi(\mathrm{r},E)\, \mathrm{d}V\, \mathrm{d}E \qquad (3)$$

Microscopic group constants III

with the average number density given as

$$\overline{N}^i = \frac{1}{\int_V \mathrm{d}V} \int_w N^i(r)\,\mathrm{d}V \tag{4}$$

and the neutron flux given as

$$\overline{\phi}_g = \frac{1}{\int_V \mathrm{d}V} \int_V \phi(\mathrm{r}, E)\,\mathrm{d}V \tag{5}$$

Microscopic group constants IV

If the nuclide density $N^i(r)$ is zero everywhere in w, assume i is evenly distributed in w. Then $\overline{N}^i = 0$, $\overline{\phi}_g$ is as defined before, and

$$\overline{\sigma}^i_{\mathrm{x},g} = \frac{1}{\overline{\phi}_g} \frac{1}{\int_w \mathrm{d}V} \int_{E_g}^{E_g - 1} \int_w \sigma^i_{\mathrm{x}}(\mathrm{r}, E) \phi(\mathrm{r}, E) \, \mathrm{d}V \, \mathrm{d}E. \tag{6}$$

This is the case for example during the first corrector step in burnup calculations with fresh fuel.

Example use cases

Typically, microscopic group constants are needed in nodal calculations to capture the effect of historical depletion conditions being different than in the nominal group constant calculation.

- Poison calculations
  - Varying absorption group constant due to Xe-135, Sm-149 etc.
- Tracking of historical conditions without ad hoc corrections
  - Use for example deviation of Pu-239 density from nominal
- Activation of structural materials
  - Burnup calculation in non-fuel materials

Earlier implementations

The Serpent implementations of microscopic group constant calculation did not print all necessary values for nodal programs.

Additionally, the reaction rates were not preserved.

The poison group constants have not preserved the reaction rates.

They were erroneously calculated with Eq. (6), thus not taking into account the spatial distributions of the poison nuclides.

Example input and output

Simple Pu-239 depletion chain I

Square fuel assembly, with cross sectional area 462.4065332496 cm^2. Fuel volumes set with `set mvol`, only one fuel material `fuel` divided into burnup zones.

Calculate most relevant microscopic cross sections to model U-238 $\rightarrow$ Np-239 $\rightarrow$ Pu-239 chain with

Simple Pu-239 depletion chain II

```
set mdep 0 4.624065332496000e+02 1 fuel
922380 16 922380 18 922380 102
932390 16 932390 18 932390 102
942390 16 942390 18 942390 102
```

Extracts from *_mdx*.m output file:

Simple Pu-239 depletion chain III

```
dec = [
...
922380   4.91608E-18   6.84142E-13       4   9.99999E-01   902340   % U-238 alpha to Th-234
922380   4.91608E-18   6.84142E-13       6   5.46000E-07        0   % U-238 spontaneous fission
922380   4.91608E-18   6.84142E-13       4   9.99999E-01   902340   % U-238 alpha to Th-234
922380   4.91608E-18   6.84142E-13       6   5.46000E-07        0   % U-238 spontaneous fission
922390   4.92222E-04   7.39367E-14       1   1.00000E+00   932390   % U-239 beta- to Np-239
942390   9.10900E-13   8.40565E-13       4   6.00000E-04   922350   % Pu-239 alpha to U-235
942390   9.10900E-13   8.40565E-13       4   9.99400E-01   922351   % Pu-239 alpha to U-235m
942390   9.10900E-13   8.40565E-13       6   3.10000E-12        0   % Pu-239 spontaneous fission
...
];
```

Simple Pu-239 depletion chain IV

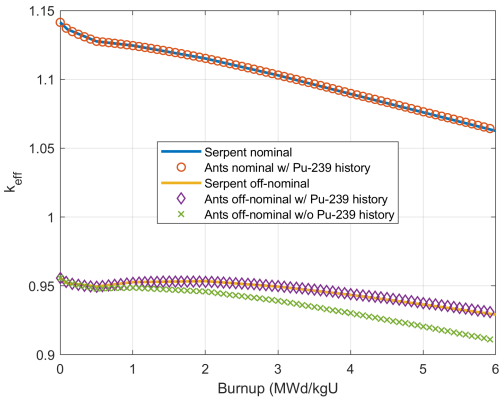
```
FLUX_0 = [   2.44339E+14  0.00000   6.56616E+13  0.00000  ];
```

```
XS_0 = [
922380   16   0   6.18131E-03 0.00000   5.62618E-03 0.00000   0.00000E+00 0.00000
922380   18   0   6.18131E-03 0.00000   1.20728E-01 0.00000   1.33493E-05 0.00000
922380  102   0   6.18131E-03 0.00000   8.55052E-01 0.00000   1.36076E+00 0.00000
932390   16   0   0.00000E+00 0.00000   1.36358E-03 0.00000   0.00000E+00 0.00000
932390   18   0   0.00000E+00 0.00000   6.88850E-01 0.00000   0.00000E+00 0.00000
932390  102   0   0.00000E+00 0.00000   1.43322E+01 0.00000   3.85740E+01 0.00000
942390   16   0   0.00000E+00 0.00000   1.89862E-03 0.00000   0.00000E+00 0.00000
942390   18   0   0.00000E+00 0.00000   9.89803E+00 0.00000   7.18132E+02 0.00000
942390  102   0   0.00000E+00 0.00000   5.67648E+00 0.00000   4.00660E+02 0.00000
];
```

Simple Pu-239 depletion chain V

Which is enough for us to construct a burnup matrix in a nodal solver.

Example with Serpent and Ants



- Single assembly calculation (not the previous example)
- Simplified U-238 $\rightarrow$ Pu-239 tracking
- DYN3D-like Pu-239 history parametrization
- Only the histories used in the group constant parametrization shown

set poi and set mdep example I

Poison calculation (again a new example, this time a VVER-440 fuel assembly) with

```
set poi 1 1.871394295037793e+02
```

Note the change of volume fraction of fuel to total volume of homogenized universe.

set poi and set mdep example II

Microscopic group constant calculation with

```
set mdep 0 1.871394295037793e+02 0
531350 102 541350 102 611490 102 621490 102
```

set poi and set mdep example III

After a simple burnup calculation:

res.m:

```
INF_XE135_MICRO_ABS =
1.2327e+02    1.1800e-03    1.2136e+06    4.9000e-04
1.2328e+02    1.1100e-03    1.1958e+06    4.1000e-04

INF_XE135_MACRO_ABS =
0             0             0             0
4.2342e-07    1.1100e-03    4.1069e-03    4.1000e-04
```

set poi and set mdep example IV

```
mdx1.m (XS_0):
541350   102   0   0.00000E+00 0.00000   1.23265E+02 0.00118   1.21359E+06 0.00049

mdx2.m (XS_0):
541350   102   0   3.43462E-09 0.00000   1.23280E+02 0.00111   1.19575E+06 0.00041
```

So after the second burnup, we can see that the microscopic depletion atomic density of Xe-135 (3.43462×10^{-9}) times the thermal microscopic (n, γ) cross section of Xe-135 (1.19575×10^{6}) equals the thermal macroscopic absorption cross section of Xe-135 (4.10695×10^{-3}) calculated with `set poi`.

Features and limitations

Current features

- Reaction cross sections for nuclide ZAI and ENDF MT pairs
- Possible to calculate cross sections separately for reaction product to be in ground/isomeric state
- Fission cross sections for weighting different fission yield tables
- Possible to calculate nufission and kappafission
- Prints decay table containing nuclide decay constants, decay energies, branching ratios etc.
- Prints fission yield tables
- Produces equivalent results with `set poi` calculation
- Multiple mdep regions in one group constant calculation universe

Current limitations

- No scattering or scattering production matrixes
- No diffusion coefficients of any kind
- No fission spectrums
- All results in infinite spectrum, no critical spectrum (`set fum`)

Some other changes in depletion

Other changes in depletion features

- Support for IPF CRAM with orders 16 and 48
  - Previously only PFD CRAM with orders $4, 6, \ldots, 16$ (default 14)
- Support decay/low flux burnup calculations with CRAM using user specified number of substeps
  - Previously TTA was always enforced (still default behavior)
- Substeps used also for constant extrapolation (CE) depletion calculations
  - Previously CE did not use substeps
  - Substeps affect the accuracy of CRAM
  - For example the first corrector of each burnup calculation
  - Only feature on this slide for which the default behavior is changed

Summary

Microscopic group constant calculation features enhanced

Microscopic group constants preserve reaction rates

Poison group constants preserve reaction rates

More options for depletion calculations

Microscopic group constants with Serpent

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