Depletion Theory

NEA OpenMC Course
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OpenMC

Depletion/activation

$$\frac{dN_i(t)}{dt} = \sum_j \underbrace{\left[\underbrace{f_{j\rightarrow i} \int_0^\infty dE\ \sigma_j(E,t)\phi(E,t)}_{\text{transmutation}} + \underbrace{\lambda_{j\rightarrow i}}_{\text{decay}} \right] N_j(t)}_{\text{Production of nuclide } i \text{ from nuclide } j}$$

$$- \underbrace{\left[\underbrace{\int_0^\infty dE\ \sigma_i(E,t)\phi(E,t)}_{\text{transmutation}} + \underbrace{\sum_j \lambda_{i\rightarrow j}}_{\text{decay}} \right] N_i(t)}_{\text{Loss of nuclide } i}$$

Depletion as a system of ODEs

$$\frac{d\mathbf{n}}{dt} = \mathbf{A}(\mathbf{n}, t)\mathbf{n}, \quad \mathbf{n}(0) = \mathbf{n}_0$$

where

$$\mathbf{n} = \begin{pmatrix} N_1 \\ N_2 \\ \vdots \\ N_n \end{pmatrix}, \quad \mathbf{n}_0 = \begin{pmatrix} N_{1,0} \\ N_{2,0} \\ \vdots \\ N_{n,0} \end{pmatrix}$$

Since transport solution only depends on **n**, we can write

$$\frac{d\mathbf{n}}{dt} = \mathbf{A}(\mathbf{n})\mathbf{n}$$

Solution for constant A

When **A** is constant, the solution is given by

$$\mathbf{n}(t) = \exp\left(\mathbf{A}t\right)\mathbf{n}_0$$

where

$$\exp(\mathbf{X}) = \sum_{k=0}^{\infty} \frac{\mathbf{X}^k}{k!}$$

Components of a depletion solver

Depletion solvers generally have three components:

1. A method for evaluating the burnup matrix (the *operator*)
   - Given **n**, evaluate **A**(**n**)
2. A method to advance the system in time (the *integrator*)
   - Given **A** and **n**(0), solve for d**n**/dt
3. A method for evaluating the matrix exponential (the *solver*)
   - Given constant **A** and t, evaluate exp(**A**t)

Predictor method

The simplest integration method is known as the “predictor” method or constant extrapolation. Let

$$\mathbf{n}_i \equiv \mathbf{n}(t_i)$$

$$\mathbf{n}_{i+1} \equiv \mathbf{n}(t_i + h)$$

The method is then as follows:

1. Evaluate $\mathbf{A}(\mathbf{n}_i)$
2. Deplete over the full step using those reaction rates

$$\mathbf{n}_{i+1} = \exp\left(h\mathbf{A}(\mathbf{n}_i)\right)\mathbf{n}_i\,.$$

Predictor method

- Requires one transport solution per step **(+)**
- Requires one matrix exponential per step **(+)**
- First-order accurate (shorter timesteps necessary) **(-)**

Other integration methods

- OpenMC gives you a wide choice of integrators with tradeoffs in accuracy, computational cost, and memory requirements
- Other than predictor, all requires at least **two** transport solutions and **two** matrix exponentials per timestep
- For all integration methods, OpenMC relies exclusively on the Chebyshev Rational Approximation Method (CRAM) for evaluating matrix exponentials

Further information

For more information on the theoretical background of depletion and comparisons of OpenMC with Serpent, see the journal paper by Romano et al.