Burning fuel for cheap! Transport independent depletion in OpenMC

Oleksandr Yardas [1]
Paul Romano [2] Madicken Munk [3] Kathryn Huff [1]

[1]University of Illinois Urbana-Champaign

[2]Argonne National Laboratory

[3]Oregon State University

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Outline

Simulating a nuclear reactor is expensive!

- Seven dimensions: space (3), energy (1) angle (2), time (1)
- Low-error → computationally-intensive methods

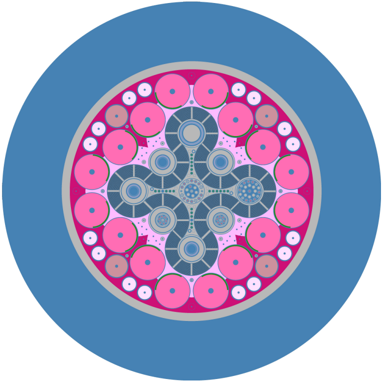


Figure 1: OpenMC model of the ATR Reactor, from [4]. The blue cross shape contains the fuel. The Pink circles on the otuside are control drums.

Fission Chain Reaction

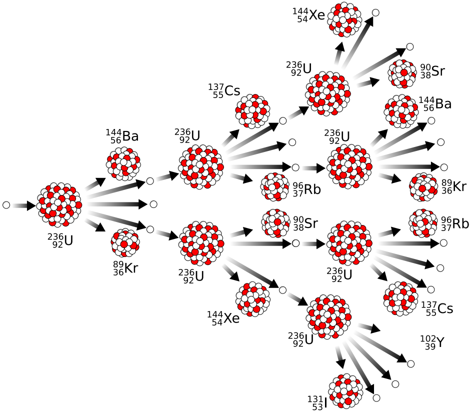


Figure 2: Diagram of a fission chain reaction, from [1].

Depletion

Concentration of nuclides in a reactor are constantly changing due to fission, neutron capture, and decay.

Why do we care?

- Strong coupling between depletion and transport
  - Neutron poisions → affects neutron economy
  - ↓ U, ↑ Pu → Change in fission neutron energy distribution
- Fission product decay heat → affects fuel reprocessing/disposal

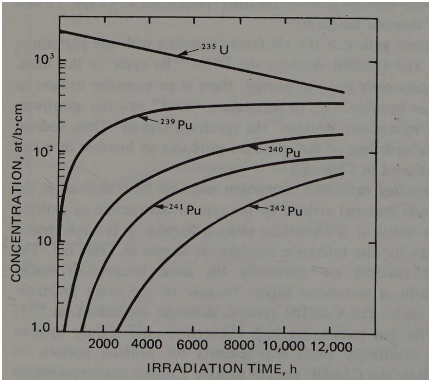
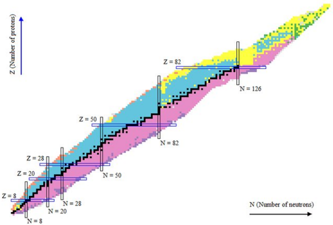


Figure 3: Buildup of plutionium isotopes with a burnup for a typical LWR fuel composition. Reproduced from Figure 6-2 in [6].

Depletion makes everything *more* expensive

- Depletion calculation track thousands of nuclides
- Nonuniform neutron density in reactor → each fuel element is a unique material (recall the ATR, Fig 1)
- Axial discretization can add additional orders of magnitude of complexity



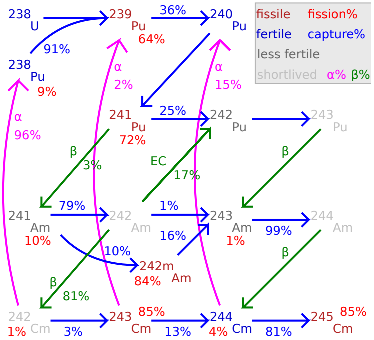


Figure 5: Example of the complicated web of production and transmutation reactions. From [3]

Outline

1. Motivation
   - The Computer Problem
   - Nuclear Basics
2. Methods
   - Modeling Depletion
   - Code Additions
   - Model Problem
3. Results
4. Conclusion

Modeling Depletion

Governing Equation:

$$\begin{aligned}\frac{dN_i}{dt} = \sum_{j=1}^{n} \overbrace{N_j(t)\int_0^\infty f_{j\to i}(E)\sigma_j(E)\phi(E,t)dE}^{\text{Production of } i \text{ from } j} + \sum_{j=1}^{n} \overbrace{N_j(t)\lambda_{j\to i}}^{\text{Decay of } j \text{ into } i} \\ \underbrace{- N_i(t)\int_0^\infty \sigma_i(E)\phi(E,t)dE}_{\text{Consumption of } i} \underbrace{- N_i(t)\sum_{j=1}^{n}\lambda_{i\to j}}_{\text{Decay of } i},\end{aligned} \tag{1}$$

where

$N_i(t) \equiv$ density of nuclide i at time t [cm^{-3}]

$\sigma_i(E) \equiv$ transmutation cross section for nuclide i at energy E and time t [cm^2]

$\phi(E,t) \equiv$ neutron flux at energy E and time t [n cm^{-2} s^{-1}]

$f_{j\to i}(E) \equiv$ fraction of transmutation reactions in nuclide j that produce nuclide i

$\lambda_{j\to i} \equiv$ decay constant for decay modes in nuclide j that produce nuclide i [s^{-1}]

$n \equiv$ total number of nuclides.

Neutron transport software of choice: OpenMC

- Monte carlo neutron particle transport code [9]
- Open source, community developed!!
- C++ core: neutron transport
- Python API: creating input, processing output, **depletion module**
- Depletion dependencies: NumPy (arrays), H5Py (output file processing), Matplotlib (plotting), SciPy (sparse matrices), uncertainties (uncertainty propogation)

Depletion algorithm

What do we need to solve Equation 1?

- $N_i(0)$, n $\rightarrow$ Given by the problem's initial conditions (e.g. Westinghouse PWR using 5% enriched fuel at BOL)
- $\sigma_i(E)$, $f_{j\rightarrow i}$, $\lambda_{j\rightarrow i}$ $\rightarrow$ Material properties (data stored in memory for speed)
- $\phi(E,t)$ $\rightarrow$ Concentration of neutrons in the reactor; requires a neutron transport simulation
- t $\rightarrow$ time steppers (called *integrators* in the depletion module)

Simplified Algorithm

1. Run an OpenMC simulation to obtain $\phi(E,t_h)$
2. Plug in $\phi(E,t_h)$, $N_i(t_h)$, $\sigma_i(E)$, $f_{j\rightarrow i}$, $\lambda_{j\rightarrow i}$ to obtain production and consumption terms in Equation 1
3. Solve Equation 1 for $N_i(t_{h+1})$ (Chebyshev rational approximation method [8])
4. Update material compositions using $N_i(t_{h+1})$
5. Repeat for all time steps t_h for $h \in [0,H]$

Can we make this cheaper?

1. Assume *static* fluxes $\rightarrow$ decouple transport from depletion.
2. Use a discrete energy grid $\rightarrow$ Integrals in Equation 1 become sums over energy groups g (simple + fast to evaluate)

MicroXS

- Stores $\sigma_{i,g}$
- Indexed by nuclide, reaction, energy group

get_microxs_and_flux()

- Run an OpenMC simulation to obtain $\sigma_{i,g}$ and ϕ_g for all nuclides
- Can get $\sigma_{i,g},;\phi_g$ for as many materials/domains as desired

IndependentOperator

- Drop in replacement for Operator class
- Performs step 2 in the Simplified algorithm for energy-discretezed value ϕ_g and $\sigma_{i,g}$

Model Problem

- Single Pressurized Water Reactor (PWR) pincell
- 4.25% enriched fuel
- Reflective boundary conditions

Three cases:

1. Transport-coupled depletion (base truth)
2. Transport-independent depletion
3. Transport-independent depletion w/ recalculated cross sections (sanity check)

Ten time steps, two different Δt:

1. 3-day (Xe 135 poisioning limit)
2. 30-day (long timestep approximation)

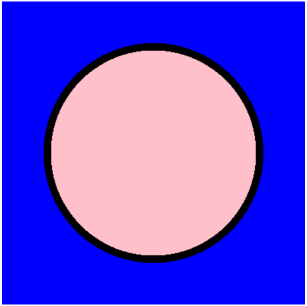


Figure 6: Slice plot of the pincell model in the xy-plane. Blue = water, black = cladding, pink = fuel

Three energy group structures: One group (single energy), 8 group, 40 group

Outline

Run time

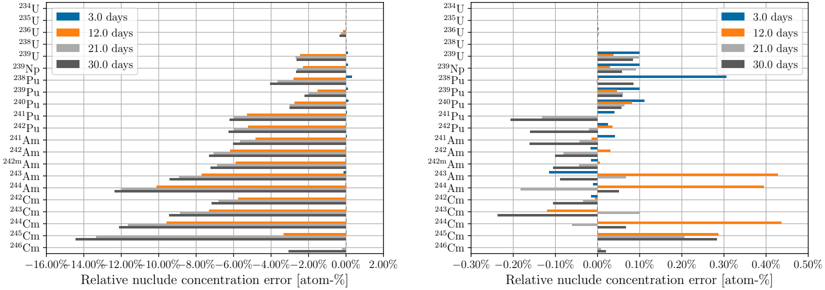
Explicit run time data was not collected, but based on the file timestamps, we can estimate how long each case took to complete on a cluster

Table 1: Comparison of average total runtimes

Case	Runtime scale	Notes
1	hours	
2	minutes	Does not include the initial simulation to obatin ϕ_g and $\sigma_{i,g}$
3	hours	Cross section data had to be loaded in at each timestep, s this case took the longest amount of time

Case 2 is *very* fast!

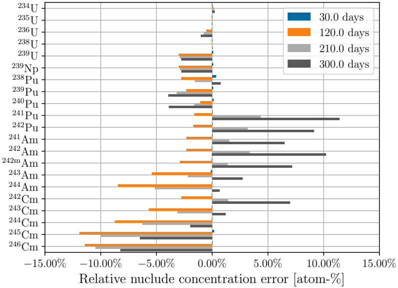
One-group actinides (3-day time steps)



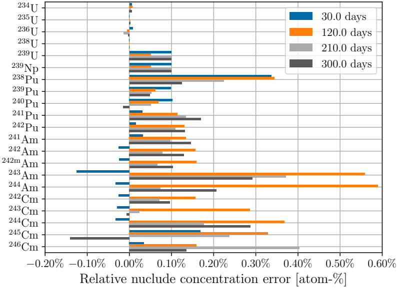
(a) (b)

Figure 7: Actinide concentration error relative to Case 1 using 3-day time steps at 3, 12, 21, and 30 days of depletion for (a) constant cross sections (Case 2); (b) updating cross sections (Case 3).

One-group actinides (30-day time steps)



(a)



(b)

Figure 8: Actinide concentration error relative to Case 1 using 30-day time steps at 30, 120, 210, and 300 months of depletion for (a) constant cross sections (Case 2); (b) updating cross sections (Case 3).

Overprediction of (n, γ) reaction rates on ^{240}Pu

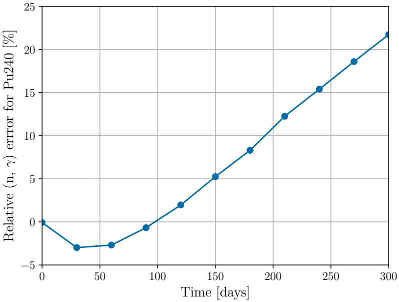


Figure 9: Relative ^{240}Pu (n, γ) reaction rate error using constant cross sections and 30-day time steps.

Fission products (3-day time steps)

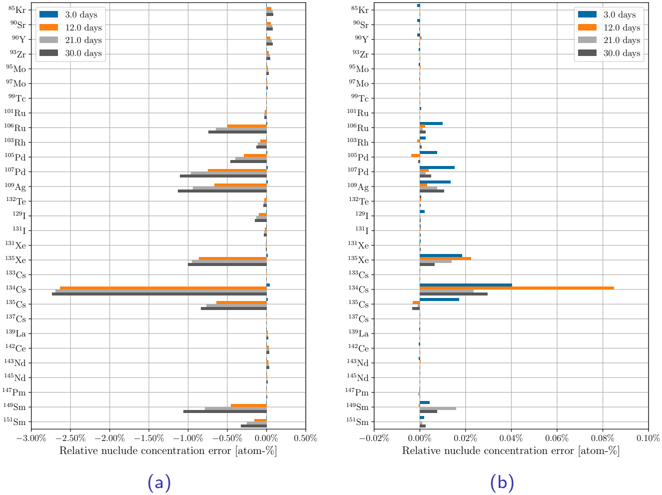
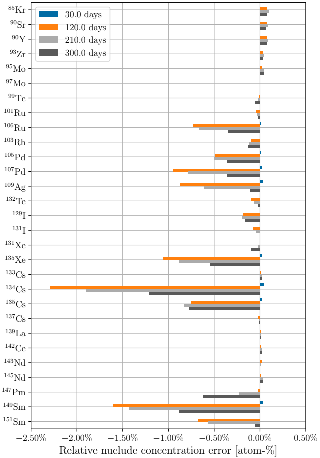
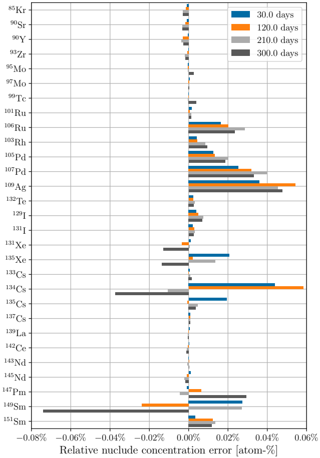


Figure 10: (a) constant cross sections (Case 2); (b) updating cross sections (Case 3).

Fission products (30-day time steps)



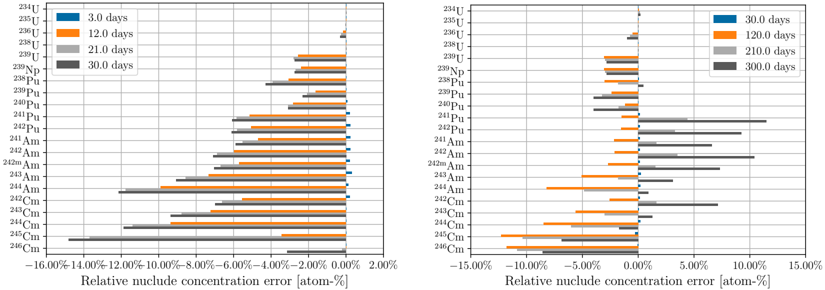
(a)



(b)

Figure 11: (a) constant cross sections (Case 2); (b) updating cross sections (Case 3).

8-group actinides



(a) (b)

Figure 12: (a) 3-day time steps; (b) 30-day time steps

40-group actinides

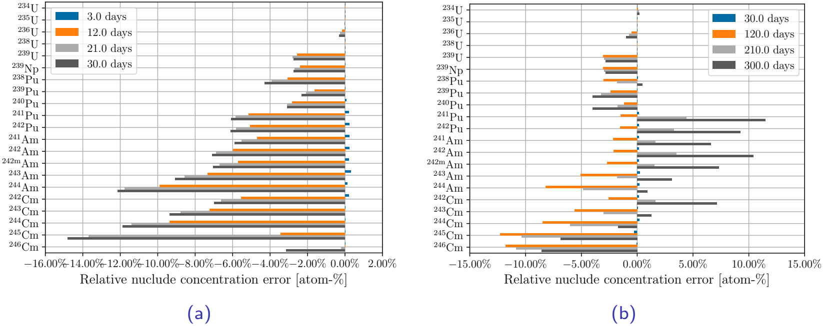


Figure 13: (a) 3-day time steps; (b) 30-day time steps

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- Transport-independent depletion provide orders of magnitude of speedup for low to moderate errors in nuclide concentration.

Conclusion

- Depletion calculations are expensive!
- Static, energy-discretized fluxes and cross sections yield low errors for abundant nuclides, moderate errors for trace nuclides
- Transport-independent depletion provide orders of magnitude of speedup for low to moderate errors in nuclide concentration.
- Energy group structure does not matter for simple models

Technical Gaps and future work

- Full core model
- Multiple materials/depletion zones

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Application to fusion systems

- Proposed fusion energy facilities have a source rate high enough to activate materials, low enough to avoid significant composition change via depletion
- Activated nuclides decay and relase high energy photons after long after reactor shutdown
- Computing this dose is an important quantity for saftey and liscensing

Transport-independent depletion was used in the workflow to calculate the shutdown dose rate in [7]

Application to fuel cycles

- Depletion determines how loaded fuel compositin affect spent fuel compositions and related fuel cycle metrics.
- Global fuel cycle accounts for hundreds of reactors at once $\rightarrow$ impractical to run transport-coupled depletion to get spent fuel compositions
- A common approach is to use "recipes" that are based on depletion calculations for a specific reactor.

Transport-independent depletion was used in Cyclus [5], an open source fuel cycle simulator, to provide real-time fuel depletion capabilities that is reactor-agnostic [2].