Reduced-order flux predictions for depletion

Andrew Johnson

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Outline

Background

- Solution to transport equation tightly coupled to compositions
- Many interesting phenomena are time dependent
- Depletion studies how compositions evolve over days to centuries
- Cutting edge MC codes support depletion in-line
  - Serpent, MC21, OpenMC

Background

- Typical two stage approach:
  1. Solve transport
  2. Freeze flux or power and deplete across some Δt
- Longer steps $\rightarrow$ fewer transport solutions
- Shorter steps $\rightarrow$ capture time-dependent behavior

How to best capture time-dependence with practical run time?

Solution schemes

- Basic Euler methods: predictor, predictor-corrector
- Sub-step methods: deplete with smaller time steps without transport
- Higher order methods: projection, extrapolation / interpolation
- Iterative methods

Solution Schemes

- More recent schemes cast time-dependence onto reaction rates
  - Higher order methods, iterative methods
  - Substep depletion
- Issues with stability, oscillations

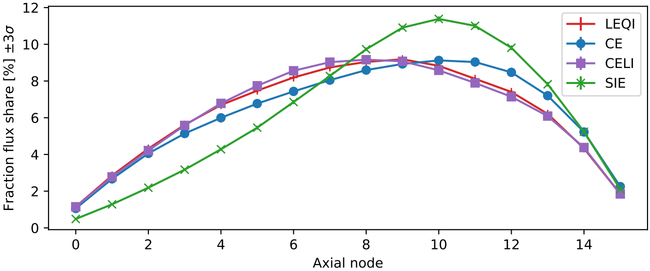

Figure: EOL Flux share for fuel assembly using one day steps[1]

[1] Johnson and Kotlyar, PHYSOR 2018

Solution Schemes

- Most schemes isolate physics of each node / region
- Neighboring materials do not communicate
- Spectral changes are indirectly lost or misrepresented through extrapolation

Possible to re-capture spectral information without re-running full-transport?

Reduced Order Methods

- Trade some levels of accuracy for speed
- Monte Carlo $\rightarrow$ nodal diffusion
- CFD $\rightarrow$ subchannel
- Can we apply this for depletion?
- Better approximate how reaction rates and/or powers change?

Spatial Flux Variation (SFV)

- Predict how flux changes due to changes in compositions[2]
- Ability to emulate a transport solution using perturbation theory
- Require k_{eff}, beginning- and end-of-step macroscopic cross sections
- Require modes of forward and adjoint flux
- Derivation relies upon work by Carney et. al[3]

[2] Johnson and Kotlyar (2019) Nuclear Science and Engineering. doi:10.1080/00295639.2019.1661171

[3] Carney, Brown, Kiedrowski, and Martin (2013) LA-UR-13-27078

Derivation

- Represent beginning-of-step (BOS) transport equation as

$$\mathcal{L}^{(0)}\Psi^{(0)} = \lambda^{(0)}\mathcal{M}^{(0)}\Psi^{(0)} \tag{1}$$

- Represent end-of-step (EOS) solution as perturbation of BOS

$$\begin{split}\left(\mathcal{L}^{(0)} + \delta\mathcal{L}\right)\left(\Psi^{(0)} + \delta\Psi\right) = \\ \left(\lambda^{(0)} + \delta\lambda\right)\left(\mathcal{M}^{(0)} + \delta\mathcal{M}\right)\left(\Psi^{(0)} + \delta\Psi\right)\end{split} \tag{2}$$

- Expand $\delta\Psi$ into sum of complete and biorthogonal basis functions

$$\delta\Psi = \sum_{m=1}^{\infty} a_m\psi_m \approx \sum_{m=1}^{M} a_m\psi_m \tag{3}$$

Derivation

- Basis functions ψ_m and adjoint $\psi_m^\dagger$ satisfy

$$\mathcal{L}^{(0)}\psi_m = \lambda_m \mathcal{M}^{(0)}\psi_m \tag{4}$$

- Expand EOS solution and neglect second and third order perturbations
- Left multiply by adjoint mode $\psi_n^\dagger$ and use orthogonality to obtain

$$a_m = \frac{\left\langle \psi_m^\dagger, \left(\delta\mathcal{L} - \lambda^{(0)}\delta\mathcal{M}\right)\Psi^{(0)} \right\rangle - \delta\lambda \left\langle \psi_m^\dagger, \mathcal{M}^{(0)}\Psi^{(0)} \right\rangle}{\left(\lambda^{(0)} - \lambda_m\right)\left\langle \psi_m^\dagger, \mathcal{M}^{(0)}\Psi^{(0)} \right\rangle} \tag{5}$$

- Use a_m to predict $\delta\Psi$ and obtain $\Psi^{(1)}$

Implementation

- Predicted flux produced from routine is scalar flux, one group $\phi^{(1)}$
  - Equations are general, but ϕ is needed for depletion
- Approximate $\delta\mathcal{L}$, $\delta\mathcal{M}$ with changes in macroscopic cross sections, $\delta\mathcal{L} \approx \Sigma_a^{(1)} - \Sigma_a^{(0)}$, $\delta\mathcal{M} \approx \nu\Sigma_f^{(1)} - \nu\Sigma_f^{(0)}$
- Approximate higher order modes of the flux with modes from fission matrix

Test Problem

- Demonstrate the SFV method on a PWR pin
- Use exact EOS macroscopic cross sections
- Data generated with SERPENT 2.1.30
- Axially-varying moderator density
- Five different step sizes: 1, 5, 10, 25, 50 days
- Task with predicting the EOS flux across final step
  - From day 59→60, 50→60, etc

Accuracy of SFV Prediction

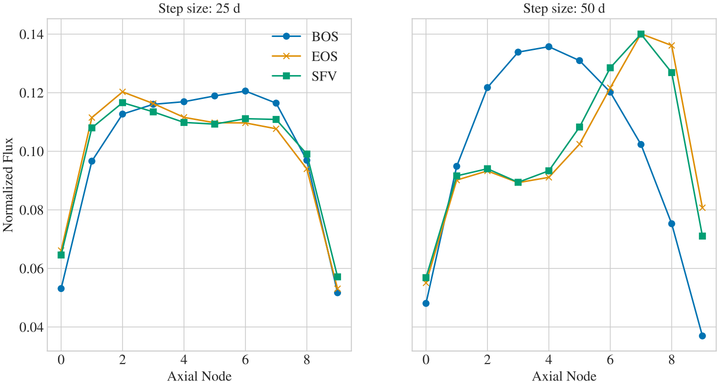

Figure: Predicted flux across 25 and 50 day step size using exact macroscopic cross sections

Custom Depletion Framework

- Ideally obtain EOS $\Sigma^{(1)}$ without rerunning transport simulation
- Model microscopic cross sections $\sigma(t)$ as low-order polynomial

$$\Sigma_r(t+\Delta t) = \sum_i N_i^{(1)} \sigma_r(t+\Delta t) \tag{6}$$

- Write an external depletion program to compute EOS densities, Σ
  - Use Serpent as transport solver
  - Extract σ, fission yields, other nuclear data
  - Deplete using IPF CRAM[4]
  - Extrapolate microscopic cross sections using low-order polynomials
- Goal is to emulate inclusion of SFV prediction into transport + burnup routine

[4] Pusa (2016) Nuclear Science and Engineering. doi: 10.13182/NSE15-26

Validating CRAM Solver

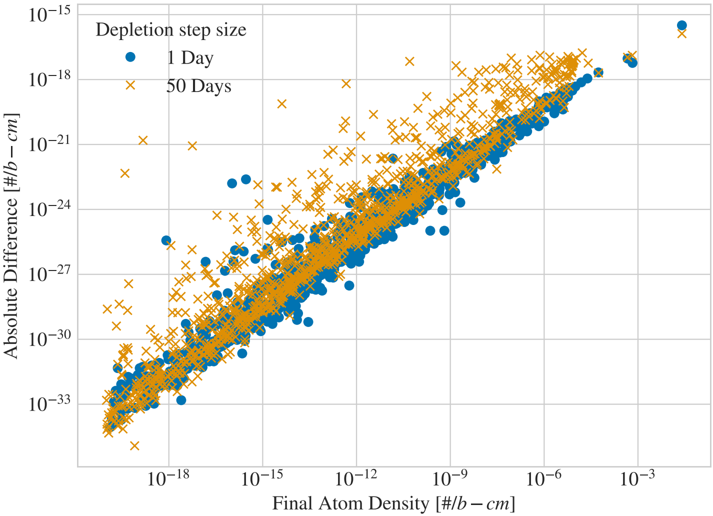

Figure: Error using custom CRAM solver with Serpent depletion matrix

Accuracy of cross section extrapolation

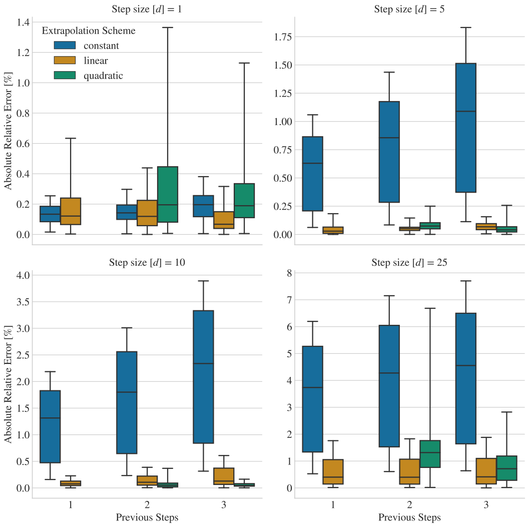

Figure: Distribution in extrapolation errors for step sizes and orders

Flux Prediction with Custom Depletion Framework

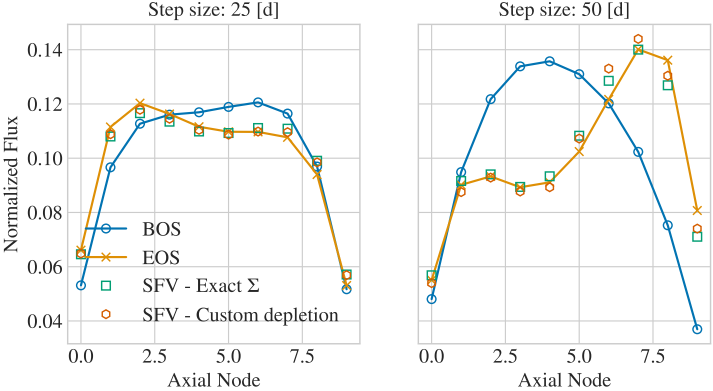

Figure: Predicted fluxes with and without depletion framework

Figure of Merit

- How beneficial is this approach?
- Define figure of merit to be

$$FOM \equiv \frac{SF}{RMS^2} \tag{7}$$

- Fission matrix has non-negligible cost $SF \approx 1.15$x
  - But avoid an entire transport solution
- Compare as if BOS flux taken to be EOS flux, e.g. $SF \equiv 2$

Figure of Merit

Table: Tabulated RMS percent error and FOM for comparing SFV predicted flux

	BOS Fluxes		SFV		
Step side [d]	RMS	FOM	RMS	FOM	SFV / BOS
1	0.016	2261.8	0.030	6797.5	3.005
5	0.013	6852.0	0.017	10551.2	1.540
10	0.014	2315.4	0.029	9247.4	3.994
25	0.036	228.0	0.094	1322.1	5.799
50	0.052	16.1	0.353	635.1	39.447

Conclusion

- Introduced the SFV method for predicting changes in spatial flux
- Verified against Serpent for a PWR pin
  - Accurate to within few percent
  - Captures $\geq 100\%$ changes in flux
- Employed a custom depletion framework to predict EOS macroscopic cross sections
- Demonstrate this as a potential reduced order flux prediction

Future Work

- Re-deplete using predicted flux in substep method
- Improve assumptions on $\delta\mathcal{L}$, $\delta\mathcal{M}$, $\delta\lambda$
- Alternative reduced order flux predictions e.g. diffusion
- Larger, more complicated problems

Serpent + External Depletion

- Serpent was and is used in conjunction with other external depletion programs
  1. Run Serpent; Get depletion data; Terminate
  2. External depletion → new compositions
  3. Reload Serpent with new compositions
  4. Repeat
- Require user-modified source code to avoid redundant transport solution

For larger problems, Step 3 is costly

Proposal: Depletion interface

- Similar in function to TH interface, but compositions not temperatures
- Avoid modifying Serpent source to ungracefully terminate
- Keep model, cross sections in memory
- Yield depletion matrix, microscopic cross section outputs
- Wait for new compositions before new transport
- Profit?

Thank you!

Questions?

Reference Fluxes

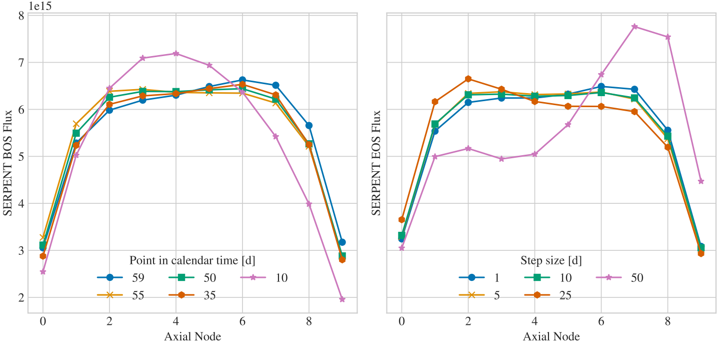

Figure: Beginning- and end-of-step fluxes from Serpent

Error in smaller step sizes

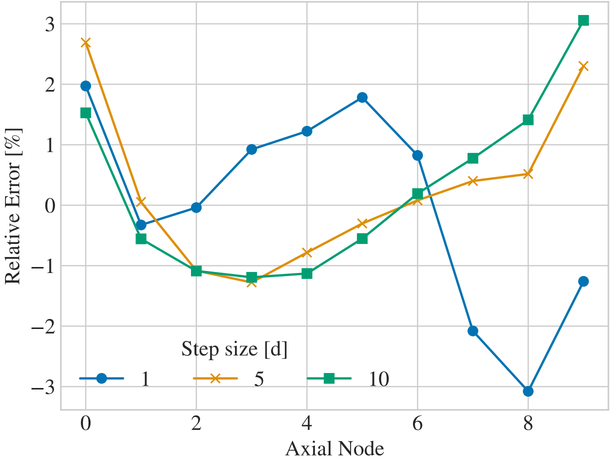

Figure: Error in predicted flux across 1, 5, and 10 day steps

Modes from the fission matrix

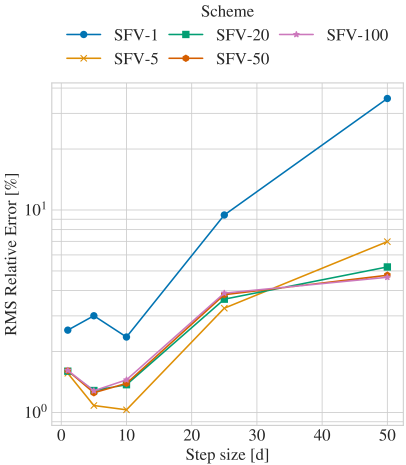

Figure: Error to one day step flux for increasing modes and step size

Validating CRAM Solver

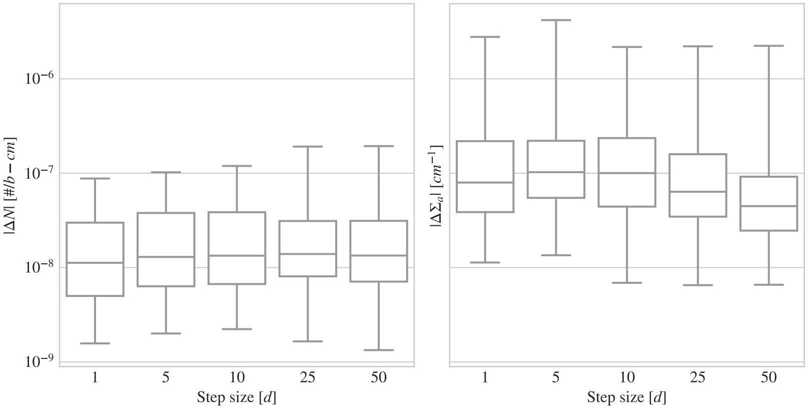

Figure: Distribution of errors in predicted densities, absorption cross section