EFFICIENT COUPLED TRANSPORT-DEPLETION SEQUENCE USING HYBRID MONTE CARLO-REDUCED ORDER SCHEMES

Approved by:

Dr. Dan Kotlyar
Nuclear and Radiological Engineering
*Georgia Institute of Technology*

Dr. Bojan Petrovic
Nuclear and Radiological Engineering
*Georgia Institute of Technology*

Dr. Anna Erickson
Nuclear and Radiological Engineering
*Georgia Institute of Technology*

Dr. Paul Romano
Computational Physical Sciences
*Argonne National Laboratory*

Dr. G. Ivan Maldonado
Nuclear Engineering
*University of Tennessee - Knoxville*

Date Approved: November 25, 2020
[We] see more and further than our predecessors, not because we have keener vision or greater height, but because we are lifted up and borne aloft by their gigantic stature.

*John of Salisbury, 1159*
To Leeza, the family that has shaped us, and the family we will build together
ACKNOWLEDGEMENTS

I am grateful for my Ph.D. committee, who has provided guidance and prompting remarks from the beginning of this journey. And for Dr. Kotlyar in particular, who has allowed me the academic and research freedom to pursue interesting concepts and projects throughout my graduate studies. I am truly thankful for his invaluable stream of advice, expertise, insight, and mentorship.

I would be remiss if I did not mention my fantastic labmates who have made this journey truly memorable. Stefano, Jim, Vedant, Naiki, Matt, and Coral, thank you for the inspiring conversations, collaborations, and amusement. I wish you all the absolute best going forward.

Without the 20+ years of support, encouragement, and prodding from my family, I would not have made it to where I am today, nor as the man I have become. To Mom, Dad, Steve, Gramma, Grappa, Oma, and Opa, from the bottom of my heart, thank you.

And finally, to dear Leeza, where can I begin. Thank you for joining me on this incredible and terrifying and exhilarating journey to grad school and in marriage. Thank you for being supportive of my studies, pushing me to be better than I was the day before, and being an absolute goof with me when we both need a good laugh.
# TABLE OF CONTENTS

Acknowlegments ........................................... v
List of Tables ........................................... ix
List of Figures ........................................... x
Abbreviations, Notation, and Useful Terms ....................... xiv
Summary ................................................... xv

Chapter 1: Introduction ........................................ 1
  1.1 Fundamentals of Depletion Theory .......................... 2
  1.2 Solution Methods ........................................ 6
    1.2.1 Linear and non-linear chains .......................... 7
    1.2.2 Matrix-based solutions ............................... 8
  1.3 Time-integration and coupling methods ...................... 11
    1.3.1 Predictor and predictor-corrector ..................... 12
    1.3.2 Higher-order schemes ............................... 13
    1.3.3 Iterative solutions ................................. 15
  1.4 Challenges and Issues .................................... 16
    1.4.1 Statistical uncertainties ............................ 16
    1.4.2 Stability ........................................... 16
  1.5 Objectives and goals .................................... 18

Chapter 2: Substep hybrid depletion scheme ...................... 21
  2.1 Substep depletion ........................................ 21
    2.1.1 Constant reaction rates ............................. 21
    2.1.2 Piecewise constant reaction rates .................... 23
  2.2 Hybrid methods ......................................... 24
  2.3 Hybrid depletion with mixed-fidelity transport ............ 24
  2.4 Custom depletion framework ................................ 27
    2.4.1 Geometry modeling ................................... 28
    2.4.2 Transport solver interfaces ........................... 30
    2.4.3 Depletion backend ................................... 32
  2.5 Conclusion ............................................. 33

Chapter 3: The Spatial Flux Variation Method .................... 34
  3.1 Derivation ............................................. 34
  3.2 Use of the fission matrix ................................ 36
    3.2.1 Real vs. complex eigenvalues ......................... 38
    3.2.2 Obtaining the adjoint ................................ 39
LIST OF TABLES

1.1 Weights for extrapolating / interpolating reaction rates in Equation 1.14 . . 15

4.1 Isotopes considered as highest contributors to total absorption . . . . . . . . 52
4.2 Transport time and penalties associated with individual modeling aspects . . 66
4.3 Figure of merit and components for UO₂ pin . . . . . . . . . . . . . . . . . . . 68

5.1 Fission product yields for ²³⁵U from ENDF/B VII.1 [48] . . . . . . . . . . . . . . . 82
5.2 Break down of the timing penalties for the supercell . . . . . . . . . . . . . 86
5.3 Summary of supercell results and figure of merit . . . . . . . . . . . . . . . 87

A.1 Thermal-spectrum neutron capture to ground ratios . . . . . . . . . . . . . . . . 103

C.1 Fuel pin compositions for UO₂ pin . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 105
C.2 Simulation properties for UO₂ pin problem . . . . . . . . . . . . . . . . . . . . . . 105

D.1 Polynomial coefficients for coolant density profile . . . . . . . . . . . . . . . . . . 106
D.2 Fuel compositions for supercell model . . . . . . . . . . . . . . . . . . . . . . . . 106
D.3 Plenum and reflector compositions . . . . . . . . . . . . . . . . . . . . . . . . . . . . 108
D.4 Zircaloy-4 cladding compositions for supercell . . . . . . . . . . . . . . . . . . . 109
D.5 Composition for air in instrumentation tube . . . . . . . . . . . . . . . . . . . . 109
**LIST OF FIGURES**

1.1 $^{235}\text{U}$ fission product yields for a subset of products ............................... 6
1.2 Sample depletion chain .................................................................................. 8
1.3 Sample depletion system from Figure 1.2 cast as linear chains ..................... 8
1.4 Structure of a depletion matrix for a toy LWR problem ............................... 10
1.5 Flux solution for beginning-of-life and three consecutive points in time for an initially symmetric fuel pin .............................................................. 18

2.1 Depiction of a mixed-fidelity substep depletion scheme .............................. 25
2.2 Change in PWR microscopic cross sections since BOL ............................... 26
2.3 Depiction of depth-first search used to find and differentiate materials .... 29
2.4 Three-point example stack used to store microscopic cross sections in the custom framework ................................................................. 33

3.1 Fission matrix for 3-D fuel pin with axial reflectors ..................................... 38
3.2 Real and imaginary components of eigenvalues obtained from fission matrix in Figure 3.1 ................................................................. 39
3.3 BOS and EOS fluxes from Serpent for SFV verification .............................. 44
3.4 Absolute error in predicted flux (left) and distributions (right) for 5, 25, and 50 day steps ................................................................. 44
3.5 Mean (left) and variance (right) of difference in SFV flux prediction for increasing number of modes ................................................................. 45
3.6 Contour plot of higher order forward (left) and adjoint (right) fission source modes ........................................... 46

3.7 Select modes of the forward fission source ............................................ 47

4.1 UO$_2$ pin reference multiplication factors and agreement with framework ........................................... 53

4.2 Scalar flux produced by the framework reference (top) and relative difference to Serpent predictor-corrector (bottom) ........................................... 54

4.3 Relative difference in framework reference flux for select early depletion steps ........................................... 54

4.4 Relative difference in framework reference $^{135}$Xe concentration for select early depletion steps ........................................... 55

4.5 Agreement in select isotopics between Serpent and framework UO$_2$ references 55

4.6 Difference in UO$_2$ pin multiplication factor using hybrid depletion scheme ........................................... 56

4.7 MARD in UO$_2$ pin compositions for key isotopes, computing using hybrid depletion scheme ........................................... 57

4.8 MARD in UO$_2$ pin scalar flux at coarse and substep level using hybrid scheme ........................................... 58

4.9 Error in UO$_2$ pin multiplication factor with predictor scheme ........................................... 59

4.10 UO$_2$ scalar fluxes for predictor (top) and hybrid (bottom) depletion schemes ........................................... 60

4.11 MARD in top contribution isotopes for UO$_2$ pin for with predictor (left) and hybrid (right) schemes ........................................... 60

4.12 Error in $k$ using LE/LI (left) and hybrid framework (right) ........................................... 61

4.13 MARD in top contributing isotopes for UO$_2$ pin for LE/LI (left) and hybrid (right) schemes ........................................... 62

4.14 Axial offset in UO$_2$ pin for all four cases ........................................... 63

4.15 Transport CPU time for all four UO$_2$ pin cases ........................................... 67

4.16 Ratio of hybrid scheme FOM to predictor and LE/LI FOMs ........................................... 69
5.1 Quarter-symmetric XY-plane for supercell problem .................................. 73
5.2 Convergence of the SFV prediction for supercell mode .............................. 75
5.3 Accuracy of SFV prediction on super cell and effect of axial discretization on prediction ................................................................. 76
5.4 Convergence in mean absolute relative difference (MARD) in EOS Serpent flux and predicted SFV flux with variable number of modes .............................. 77
5.5 Serpent reference flux for the supercell .................................................. 77
5.6 Serpent reference $k$ (left) and difference obtained by the framework reference (right) ................................................................. 78
5.7 Mean absolute relative atom density difference between supercell and framework references for isotopes with the largest difference (left) and for key isotopes (right) ................................. 79
5.8 Difference in multiplication factor estimated by hybrid method compared for framework reference .................................................. 80
5.9 Mean absolute relative difference in scalar fluxes obtained by the hybrid scheme ................................................................. 80
5.10 Mean absolute relative difference in isotopics obtained using hybrid method compared to framework reference .................................................. 81
5.11 Distribution of end-of-life $^{235}$U atom density differences with increasing step sizes produced using the hybrid depletion scheme .............................. 82
5.12 $\Delta k$ obtained by Serpent predictor (left) and hybrid (right) depletion schemes ................................................................. 83
5.13 Axial flux distribution for node E using the Serpent predictor (top) and hybrid (bottom) depletion schemes .................................................. 84
5.14 Difference in $k$ using LE/LI (left) and hybrid (right) depletion schemes ... 84
5.15 Normalized axial flux distributions for node E using LE/LI and hybrid depletion schemes .................................................. 85
5.16 Mean absolute relative difference in top contributing isotopes for LE/LI (left) and hybrid (right) depletion schemes .................................................. 86
5.17 Figure of merit ratios for hybrid depletion scheme applied to supercell model .......................................................... 87

D.1 Coolant density profile for supercell model .......................................................... 107
### Abbreviations, Notation, and Useful Terms

<table>
<thead>
<tr>
<th>Term</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>BOL</strong></td>
<td>Beginning of life</td>
</tr>
<tr>
<td><strong>BOS</strong></td>
<td>Beginning of (coarse) step</td>
</tr>
<tr>
<td>Coarse step</td>
<td>Larger time interval separating two high-fidelity transport solutions</td>
</tr>
<tr>
<td><strong>CRAM</strong></td>
<td>Chebyshev rational approximation method</td>
</tr>
<tr>
<td><strong>EOL</strong></td>
<td>End of life</td>
</tr>
<tr>
<td><strong>EOS</strong></td>
<td>End of (coarse) step</td>
</tr>
<tr>
<td><strong>FOM</strong></td>
<td>Figure of merit</td>
</tr>
<tr>
<td><strong>IPF</strong></td>
<td>Incomplete partial factorization form of CRAM</td>
</tr>
<tr>
<td><strong>LE/LI</strong></td>
<td>Linear extrapolation / linear interpolation depletion scheme</td>
</tr>
<tr>
<td><strong>LWR</strong></td>
<td>Light water reactor</td>
</tr>
<tr>
<td><strong>MARD</strong></td>
<td>Mean absolute relative difference</td>
</tr>
<tr>
<td><strong>ODE</strong></td>
<td>Ordinary differential equation</td>
</tr>
<tr>
<td><strong>pcm</strong></td>
<td>Per cent mille or $10^{-5} \Delta k/k$</td>
</tr>
<tr>
<td><strong>PWR</strong></td>
<td>Pressurized water reactor</td>
</tr>
<tr>
<td><strong>RMSD</strong></td>
<td>Root mean squared difference</td>
</tr>
<tr>
<td><strong>SFV</strong></td>
<td>Spatial flux variation</td>
</tr>
<tr>
<td><strong>Substep</strong></td>
<td>Smaller increment inside a coarse step</td>
</tr>
<tr>
<td><strong>Transmutation</strong></td>
<td>Particle-induced isotopic changes of the form $X + an \rightarrow {Y_i} + bn$</td>
</tr>
<tr>
<td><strong>ZAI</strong></td>
<td>Isotope identifier by number of protons (Z), atomic number (A) and metastable state (I)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_i$</td>
<td>Concentration of atoms for isotope $i$, given as number per volume. Also used to reflect a total number of atoms in a control volume.</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Scalar neutron flux</td>
</tr>
<tr>
<td>$\Psi$</td>
<td>Angular neutron flux</td>
</tr>
<tr>
<td>$\psi_m$</td>
<td>Mode $m$ of the higher-order angular flux</td>
</tr>
<tr>
<td>$\psi^i_m$</td>
<td>Mode $m$ of the higher-order angular adjoint flux</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Microscopic cross section</td>
</tr>
<tr>
<td>$\Sigma$</td>
<td>Macroscopic cross section</td>
</tr>
</tbody>
</table>
SUMMARY

In order to determine the lifetime of a nuclear application, one must model and understand the variation in power distributions and important safety parameters over months to years of operation. These behaviors are obtained through a depletion study, modeling the interaction between power production and isotopic evolution. The operational period is divided into discrete time intervals and the simulation is split between a neutronics solution, producing a neutron flux profile given a set of compositions, and a depletion solution, producing new compositions at a later time given this flux profile. Through this process, trade-offs are made between stability and accuracy, and the potentially prohibitively large computational requirements necessary to use smaller time intervals.

This work introduces a novel method for efficiently improving the accuracy of this coupled sequence, obtaining better accuracy than existing methods in less time. The novelty of this work is the linkage of expensive high-fidelity Monte Carlo methods with faster reduced-order codes in a hybrid depletion scheme. These reduced-order solutions are interspersed between the high-fidelity solutions, and the compositions are updated with a finer temporal discretization. By modeling the compositions with this fine scale, the accuracy of the overall sequence is improved with limited computational expense compared to not using the reduced-order solutions.

A new reduced-order method has been developed for this research that predicts the change in scalar neutron flux across a depletion step using linear perturbation theory. A custom software library has been developed to interface with transport codes and perform the depletion routines external to any code. This library is used to model a stability-limited test case, demonstrating the improved stability and accuracy of the method. The benefits of this hybrid scheme persist when applied to a 3-D collection of fuel assemblies, indicating this scheme has exceptional practical benefits.
CHAPTER 1
INTRODUCTION

When developing innovative engineering devices, from automobiles to cell phones to nuclear reactors, eventually one must ask the question: how long will the concept remain operational? Such systems eventually require some external source of energy to replace and replenish the exhausted fuel supply and continue running. The estimation of remaining fuel in a car or charge in a battery and the performance of the device over time are key quantities to understand, predict, and optimize the longevity of such a device. All things exist in time, and we wish to be able to understand the behavior of concepts and applications through time, aided by modeling and simulation tools.

In nuclear applications, specifically fission reactors, the distance between refueling is typically called a fuel cycle, and may span one to two years. A reactor is loaded with fuel in some fixed arrangement, which is consumed over time. Heavier atoms are fissioned by neutrons, producing lighter isotopes and releasing energy. The rate at which fissionable isotopes are removed and produced over time can provide insight into how long a reactor can operate before it must be refueled.

When fuel is removed from a reactor, due to reloading or full shutdown events, this spent fuel is often placed in some wet repository in order to cool down, both thermally and radioactively. Correct knowledge of the compositions can lead to optimal storage design, such that the heat generated through radioactive decay can be adequately mitigated. Furthermore, non-proliferation discussions require a precise understanding of the concentration and production of key isotopes.

This process of transmuting isotopes through nuclear reactions is commonly referred to as depletion or burnup, and is the primary subject of this work. Many analysis tools used in industry and academia are capable of modeling both the power distribution and the
isotopic evolution, including but not limited to MCNP, MC21, Serpent, and OpenMC [1, 2, 3, 4]. The power distribution is obtained by solving the neutron transport equation with a number of techniques, while the later is usually handled with a dedicated depletion solver. Providing power distribution and reactions to the depletion enables the modeling of isotopic evolution, producing updated compositions for the transport solver. The interplay between transport solutions and isotopic compositions requires very careful attention, as will be discussed in great detail throughout this work.

The depletion system presents a tightly-coupled system of equations that, if not properly handled, can result in mis-predictions in the operational cycle length that can accumulate to tens of days. This mis-prediction can have economic consequences, as fuel that is not fully burned could be removed from the core. Depending on how the transport-depletion system is solved, the obtained solution may over-estimate the power peaking profiles, as is often seen in stability analysis [5, 6, 7, 8]. Here, specific points in space may see much greater neutron flux than their neighbors, producing far more energy and heat. Local spikes in heat production can drive decisions on fuel loading, safety margins, and other balance of plant features in order to maintain fuel integrity.

The following sections will formally introduce the topic of depletion theory, solution methods, and issues with the state-of-the-art. At the culmination of this review, the motivation and objectives for this work will be presented.

1.1 Fundamentals of Depletion Theory

The core of depletion theory involves determining isotopic compositions through some simulated period of time. The simplest example would be a two isotope system, where the parent isotope \( A \) undergoes spontaneous radioactive decay to produce a stable, non-decaying product isotope \( B \). After one half-life, \( t_{1/2} \), half of the parent isotope has decayed and produced an equal quantity of the product. Assuming only \( N_{A,0} \) atoms of isotope \( A \)
exist initially, the system can be expressed as

\[
\begin{aligned}
\frac{d}{dt}N_A(t) &= -\lambda_A N_A(t) \\
N_A(0) &= N_{A,0} \\
N_B(0) &= 0 \\
N_B(t) + N_A(t) &= N_{A,0}
\end{aligned}
\]  

for \( t > 0 \). \( \lambda_A = \ln(2)/t_{1/2} \) is the decay constant in units of decays per time for isotope A. Equation 1.1 has an analytic solution

\[
\begin{aligned}
N_A(t) &= N_{A,0} \exp(-\lambda_A t) \\
N_B(t) &= N_{A,0} (1 - \exp(-\lambda_A t))
\end{aligned}
\]  

In reality, the system of equations is more complicated and can require modeling thousands of isotopes with far more complicated decay and transmutation paths. Isotopes are destroyed and produced not only by radioactive decay, but also due to particle interactions. Uranium 235 can produce uranium 236 by capturing a neutron and releasing a gamma ray photon. Similarly, isotopes can produce lighter elements through \((n, \alpha)\), or \((n, Xn)\) reactions, where a \(^3\)He \(\alpha\)-particle or \(X\) neutrons are ejected from the compound nucleus formed during the interaction with the incident neutron. All of these reactions include some energy change, depending on the mass difference between the initial and final states.

When these reaction modes are cast into a system of equations, the Bateman equations [9] are produced. These equations describe the time rate of change across all isotopes of interest by all transmutation modes, radioactive decay and induced by incident particles.
For a single product isotope $j$, the rate of change can be written as

$$\frac{d}{dt}N_j(t) = -N_j(t)\left[\lambda_j + RR_{j,\text{abs}}(t)\right] + \sum_i N_i(t)\left[\lambda_{i,j} + \sum_r \beta_{i,j,r} RR_{i,r}(t)\right].$$

(1.3)

Here, $\lambda_{i,j}$ is the rate at which isotope $i$ spontaneously decays to isotope $j$, $RR_{i,r}$ is the microscopic reaction rate of reaction $r$ of isotope $i$, and $\beta_{i,j,r}$ is the fractional yield by which isotope $j$ is produced from reaction $r$ of isotope $i$. In practical cases, Equation 1.3 is solved for all “burnable” materials, or materials that undergo significant depletion. Structural materials such as pressure vessel and grid plates are typically not included in this calculation.

Reaction rates are integral quantities, calculated as

$$RR_{i,r}(t) = \frac{1}{V_i} \int_0^\infty \int_{V_i} \sigma_{i,r}\phi(F, E, t) \, d^3r \, dE,$$

(1.4)

where $\phi$ is the incident particle scalar flux in volume $V_i$, and $\sigma$ is the microscopic reaction cross section. This work considers neutron induced reactions only, but photon induced transmutation is also possible. The collection of all pathways by which isotopes decay and transmute will be referred to as the depletion chain through this work.

The fractional yield term $\beta_{i,j,r}$ covers many transmutation paths, namely branching ratios and fission yields. For some capture reactions, there are two possible reaction targets, each with a fractional chance of production. $^{241}\text{Am}$ will produce ground state $^{242}\text{Am}$ with sub-14 MeV neutrons for nearly 90% of capture reactions and metastable $^{242}\text{Am}$ the remaining 10%. As each of these products have different decay and transmutation paths, their production must be well quantified. A set of thermal-spectrum branching coefficients is provided in Table A.1 and will be used throughout this work.

Fission yield data are used to determine the production of lighter isotopes from fission.

---

1Other sources may express this term as a product of the total decay constant $\lambda_i$ and a fractional decay yield $\gamma_{i,j}$.
events. The mechanisms are not deterministic, and therefore a distribution of fission products is typically provided with nuclear data libraries at a few discrete energies. One must make a distinction between independent and cumulative fission yields. The former refers to a path by which the product is directly formed from the parent, while the latter includes all secondary decay and transmutation paths. Cumulative yields are used when information on some isotopes is not necessary or not provided, as can be used to approximate the inclusion of the missing isotopes.

In some cases, it may be desirable to model tens or hundreds of isotopes, rather than the thousands that may arise throughout depletion. When select isotopes are removed from the depletion chain, their contributions must still be captured in order to maintain a mass balance. Here, one may choose to create and use a set of cumulative fission product yields to account for isotopes that have been excluded.

Figure 1.1 presents a subset of independent fission yields for $^{235}$U reflecting thermal, epithermal, and fast spectrum problems. The subset of products was chosen to efficiently model the depletion of light water reactors [10] and contains less than 200 fission products. Using a full evaluated nuclear data library, one would easily see 1000 or more fission products, each with a unique energy distribution. Figure 1.1 is provided to explain both the distinct set of energies at which these yields are typically provided and general trends in the energy dependence.

As an aside, some next generation fission reactor concepts involve an external feed for in-line refueling and/or removal of some fission products. Concepts like the molten salt reactor that involve a liquid, flowing fuel may also have to model the movement of isotopes between neighboring control volumes. This could change Equation 1.3 into a non-homogeneous set of equations with the addition of an external isotopic source (or sink) term. An alternative approach, proposed in [11], is to modify the decay constants $\lambda$ to represent this behavior while maintaining the homogeneity of the system. Modeling these systems is very interesting as it provides a field for new technical and academic research,
1.2 Solution Methods

The challenge now becomes arranging the nuclear data and reactions rates such that a solution to Equation 1.3 can be found for all isotopes $j$ in all materials of the modeled problem. There are two families of solutions, that will be briefly introduced here: linear and non-linear chains, and matrix-based solutions.

Much of the discussion in this and following sections will refer to isotopic concentrations in a single material, and the solution of future concentrations. Depletion solvers typically update concentrations for all materials of interest in parallel with the number of materials distributed first across several parallel instances (e.g., MPI ranks) and further across individual threads. For simplicity, discussion will center on a single material with the calculation performed in serial.
1.2.1 Linear and non-linear chains

The typical depletion chain is highly non-linear and in some cases cyclical, as there exist many pathways for a single isotope to be produced by or removed from the problem. By traversing this depletion chain and solving modified versions of Equations 1.1 and 1.3 to smaller problems, one can obtain an analytic or near analytic solution. The most common such approach is transmutation trajectory analysis (TTA) [12].

TTA casts the Bateman equations into linear chains following isotopes with initial non-zero concentrations at root nodes. For each progeny of these root isotopes, the following steps are taken. First, the concentration of the parent isotope is updated with \( N_1(t) = e^{-\lambda_1 t} N_1(0) \). Second, it is determined if the linear chain should continue from this node or terminate. Continuation depends on the product isotope having additional progeny and a cutoff criteria to prevent chains of infinite length. This process repeats for all progeny of the root nodes, and then successively for the next level of isotopes.

The explanation of the TTA solution method is aided by a demonstration system in Figure 1.2. For the sake of demonstration, isotope \( A \) will be denoted as a root node with non-zero initial concentration. Following each transmutation path, the linearized version of this system presented in Figure 1.3 can be produced. Terminated chains are indicated by \( \times \), or else the chain \( A \leftrightarrow B \) would continue for an infinite length. Similarly, following the chain \( A \rightarrow B \rightarrow A \rightarrow B \rightarrow C \) encounters isotope \( C \) for the second time but with a different concentration of parent isotope \( B \) and thus the net update of \( C \) may be sufficiently low that any future edges \( B \rightarrow C \) need not be considered.

Along each edge of the graph, the concentrations of the parent and progeny isotopes are updated based on the relevant nuclear data and reaction rates, with initial conditions reflecting the current concentrations. These concentrations may be updated multiple times, as isotopes appear as both parents and progeny throughout the chain.

The benefit of the TTA is that one can obtain analytic or near-analytic solutions, especially for simple models. However, the solution can become computationally expensive
when solving realistic burnup problems. In cases where the depletion chain can become cyclical, as in the case of $A \leftrightarrow B$ or with multiple intermediate isotopes $X \rightarrow Y \rightarrow \cdots \rightarrow X$, some determinations must be made about when to terminate the trajectory. This cutoff can be determined by some threshold concentration, as successive solutions of $e^{-\lambda_i t} N_i(0)$ for the cyclical $AB$ chain will lead to decreasing initial conditions, or a maximum trajectory length. Readers are referred to [12, 13] for further discussion on the TTA method.

### 1.2.2 Matrix-based solutions

Recently, solution methods have been introduced that rely on matrix solutions rather than linear and non-linear chains. The MC21 Monte Carlo code [2] relies on a variable-coefficient ordinary differential equation solver, while the Serpent andnd the code would become a bit more complicated, but we’ve attempted to market this project as a way to get publication quality plots with ease. Having MPL handle this upstream would be great, but I think we can shoulder the burden in a few select cases. OpenMC Monte Carlo codes [3, 4] employ
a matrix exponential. Both of these techniques involve casting Equation 1.3 as a matrix system

\[
\begin{align*}
\frac{d}{dt} \vec{N}(t) &= A(t) \vec{N}(t) \quad \text{for } t > 0 \\
\vec{N}(0) &= \vec{N}_0,
\end{align*}
\]  

(1.5)

where \( \vec{N} \) is a vector of nuclide concentrations, and \( A \) is referred to as the depletion matrix. Matrix element \( A_{i,j} \) is the net rate by which isotope \( j \) is produced by isotope \( i \). The diagonal elements \( i = j \) denote the net production rate of isotope \( i \) by all pathways and are typically negative since the reaction rates \( \sum_r R_{r,i} \) and decay constant \( \lambda_i \) that make up the main diagonal describe removal rates.

This matrix is a function of time in that updated compositions \( \vec{N}(t) \) will lead to updated reaction rates, altering the contents of the depletion matrix. This tightly coupled system is traditionally solved with a quasi-static approach, described in Section 1.3. For now, discussion will focus on a fixed depletion matrix for a given time interval.

Figure 1.4 presents a sample depletion matrix that one might experience in a typical fission reactor. The indices correspond to increasing isotope ZAI identifier, where \( Z \) is the number of protons, \( A \) the atomic number, and \( I \) an indicator of ground or meta-stable states. The right-most columns corresponds to the production of fission products, while the near-diagonal elements indicate non-fission transmutations. Reactions like \( (n,\alpha) \) and \( (n,\gamma) \) create products that are similar in atomic mass, and thus the products are close to the main diagonal.

The general matrix exponential solution seeks a solution of the form

\[
\vec{N}(t) = \exp(A(t)t) \vec{N}_0.
\]  

(1.6)

The matrix is highly sparse, as indicated in Figure 1.4, with negative eigenvalues ranging from \( \Delta t \times 10^{\pm 15} \), leading to a challenging numeric problem. Classical approaches like the Padé approximation for computing the exponential of a matrix have been shown to break
down when applied to the depletion matrix \cite{14, 15}, leading to application and development of the Chebyshev rational approximation method (CRAM) \cite{15}.

The Chebyshev rational approximation method finds the best rational approximant $\hat{r}_{k,k}(x)$ for the matrix exponential, such that

$$\vec{N}(t) = \exp(At) \vec{N}_0 \approx \hat{r}_{k,k}(At) \vec{N}_0.$$  \hfill (1.7)

As introduced by Pusa and Leppänen, the traditional form of CRAM uses rational functions

$$\hat{r}_{k,k}(x) = \alpha_0 + \text{Re} \left( \sum_{i=1}^{k/2} \frac{\alpha_i}{x - \theta_i} \right)$$ \hfill (1.8)

where coefficients $\theta_i$ are the poles of the approximant $\hat{r}_{k,k}$, and $\alpha_i$ are the residues of $\theta_i$.

Pusa later presented the incomplete partial factorization (IPF) formulation of CRAM \cite{16}, using

$$\hat{r}_{k,k}(x) = \alpha_0 \prod_{i=1}^{k/2} \left( 1 + 2\text{Re} \left( \frac{\tilde{\alpha}_i}{x - \theta_i} \right) \right)$$ \hfill (1.9)

where $\tilde{\alpha}_i$ are residues of a factorized rational function. Both expressions in Equations 1.8
and 1.9 refer to approximations of order $k$, with coefficients prepared in [16] for orders four through 48. Implementation details are provided in Appendix B.

Several studies have been done introducing and comparing solutions to the Bateman equations. Conclusions made in [13, 15, 17] are summarized below.

1. The accuracy and computational time of TTA is highly dependent on termination criteria.

2. For non-decay steps—less than a few years—CRAM and TTA are in good agreement.

3. CRAM is orders of magnitude faster than TTA, with IPF CRAM faster still.

4. CRAM suffers with short-lived isotopes, and when only modeling radioactive decay.

5. IPF CRAM can obtain agreement with TTA for decay systems with sufficient order$^{2}$. Due to its improved numerical stability and accuracy, the 16th-order IPF representation of CRAM will be used in this work.

1.3 Time-integration and coupling methods

The Bateman equations are intrinsically tied to both compositions and reaction rates, as discussed previously. As compositions evolve over time, the solution to the transport equation and reaction rates will evolve as well. On the depletion side, this coupling is contained through the depletion matrix $A(t)$, with updated reaction rates representing changing neutron energy spectra and other local information.

This poses a modeling challenge as solving the neutron transport equation is far more challenging than a series of coupled ordinary differential equations. Several transport codes have been introduced in this work, and all rely on fixed compositions at a given point in time. This section will describe classical and modern time-integration schemes for solving

$^{2}$16th-order IPF CRAM was found to be highly accurate for decay steps of one million years [16]
the truly coupled transport and depletion system. Each scheme will be presented given initial reaction rates $RR_i$ and isotopic compositions $\vec{N}_i$, and tasked with finding $\vec{N}_{i+1}$ after a step size $\Delta t = t_{i+1} - t_i > 0$. Furthermore, these schemes will use some constant power across the interval $t \in [t_i, t_{i+1})$.

1.3.1 Predictor and predictor-corrector

The most straight-forward approach is the forward Euler or predictor scheme. This can be represented nearly identically to Equation 1.5, using a fixed depletion matrix $A_i$ generated using beginning-of-step (BOS) reaction rates $RR_i$. If one chooses to use a matrix exponential solution, the end-of-step (EOS) compositions are obtained simply as

$$\vec{N}_{i+1} = \exp (A_i \Delta t) \vec{N}_i.$$  \hspace{1cm} (1.10)

While this is the easiest solution scheme, the predictor has been shown to be problematic and, for some problems, highly unstable. This will be discussed more in Section 1.4.

As an improvement, predictor-corrector schemes were developed that use an intermediate correct step. Let $F(\vec{N}(t))$ denote a solution to the transport equation that provides updated reaction rates given compositions at time $t$. Using the discrete time intervals $\{t_i\}$, one can imagine this function directly producing the depletion matrix $F(\vec{N}_i) \rightarrow A_i$. The constant extrapolation / linear interpolation predictor-corrector scheme, as coined in [18], can be described as

$$\vec{N}_{i+1}^p = \exp (A_i \Delta t) \vec{N}_i$$

$$A_{i+1}^p \leftarrow F(\vec{N}_{i+1}^p)$$

$$\vec{N}_{i+1} = \exp \left( \frac{\Delta t}{2} (A_i + A_{i+1}^p) \right) \vec{N}_i.$$  \hspace{1cm} (1.11)

These predicted concentrations $\vec{N}_{i+1}^p$ are used to obtain a new set of reaction rates, which are averaged (or linearly interpolated) with the BOS reaction rates.
The inclusion of the corrector step has been shown to increase convergence with respect to EOS isotopics from $O(\Delta t)$ to $O(\Delta t^2)$ [14]. However, the fundamental issue with these and other such quasi-static time-integration schemes is that the reaction rates are updated at increments of $\Delta t$. Some schemes like the mid-point predictor corrector use reaction rates at $t_{i+1/2}$ but then still use a constant corrected matrix across the interval $\Delta t$ or $\Delta t/2$. While this may hold in the limit of small $\Delta t$, a balance must be struck between transport solutions $F(\vec{N}(t))$ and accurate isotopic modeling.

1.3.2 Higher-order schemes

Higher-order schemes draw from the vast literature on solving time-dependent systems. These schemes seek to extend the step size and reduce the number of potentially expensive transport solutions without introducing excessive inaccuracies. The current state-of-the-art will be summarized here, though readers are recommended to follow references for additional information.

*Runge-Kutta family*

The application of a Runge-Kutta scheme is well-known way to solve a system of ODEs. Of these, the most well known is the fourth-order, often referred to as RK4. Given an initial value problem of the form

$$\begin{align*}
\frac{dy(t)}{dt} &= f(y,t) \text{ for } t > t_i \\
y(t_i) &= y_i,
\end{align*}$$

(1.12)
the RK4 solution scheme follows as

\[
\begin{align*}
    x_1 &= f(y_i, t) \\
    x_2 &= f(y_i + \frac{\Delta t}{2} x_1, t + \frac{\Delta t}{2}) \\
    x_3 &= f(y_i + \frac{\Delta t}{2} x_2, t + \frac{\Delta t}{2}) \\
    x_4 &= f(y + \Delta t x_3, t + \Delta t) \\
    y_{i+1} &= y_i + \frac{1}{6} (x_1 + 2x_2 + 2x_3 + x_4)
\end{align*}
\]  

(1.13)

The Bateman equations are of the form \( \frac{d}{dt} y(t) = f(y, t)y \), and therefore the RK4 scheme must be adapted slightly for this application. Josey, Forget, and Smith introduced such a variation as the extended predictor-corrector RK4 (EPC-RK4) scheme, demonstrating that this scheme is well suited for depletion analysis [14].

**Solutions utilizing previous time points**

Isotalo and Aarnio proposed extrapolating and interpolating the reaction rates using one previous transport solution [18]. This allows the reaction rates to be modeled as constant, linear, or quadratic functions of time by weighting previous, current, and predicted reaction rates with

\[
RR = \omega_{i-1} RR_{i-1} + \omega_i RR_i + \omega_{i+1} RR^p_{i+1}.
\]  

(1.14)

The various weights depend on the length of the current time step \( \Delta t_i \) but also the previous step \( \Delta t_{i-1} \), and are reproduced in Table 1.1.

Obtaining the EOS concentrations with this family of higher-order schemes is very similar to the predictor-corrector from Section 1.3.1. Indeed, that presentation is identical with a constant extrapolation on reaction rates for the predictor step and linear interpolation on the corrector step. The inclusion of the previous step allows the depletion matrix for the predictor and corrector step to contain additional temporal information, and has been shown to improve the accuracy of the coupled solution [18].
Table 1.1: Weights for extrapolating / interpolating reaction rates in Equation 1.14. From [18]

<table>
<thead>
<tr>
<th></th>
<th>$\omega_{i-1}$</th>
<th>$\omega_{i}$</th>
<th>$\omega_{i+1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant extrapolation</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Linear extrapolation</td>
<td>$-\frac{\Delta t_i}{2\Delta t_{i-1}}$</td>
<td>$1 + \frac{\Delta t_i}{2\Delta t_{i-1}}$</td>
<td>0</td>
</tr>
<tr>
<td>Linear interpolation</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>Quadratic interpolation</td>
<td>$-\frac{\Delta t_i^2}{6\Delta t_{i-1}(\Delta t_i+\Delta t_{i-1})}$</td>
<td>$\frac{1}{2} + \frac{\Delta t_i}{6\Delta t_{i-1}}$</td>
<td>$\frac{1}{2} - \frac{\Delta t_i}{6(\Delta t_i+\Delta t_{i+1})}$</td>
</tr>
</tbody>
</table>

1.3.3 Iterative solutions

Many of the schemes presented to this point adopt an explicit Euler approach, wherein data from the beginning of step is used to deplete. Explicit Euler schemes are known to be conditionally stable, and thus impose strict requirements on the time step, else unstable solutions may be obtained. The stochastic implicit Euler (SIE) method proposed by Dufek, Kotlyar and Shwageraus [19] seeks to use the EOS reaction rates to deplete the BOS concentrations

$$\vec{N}_{i+1} = \exp \left( f(N_{i+1}) \Delta t \right) \vec{N}_i.$$  \hspace{1cm} (1.15)

As these reaction rates are not known, the SIE method employs a Robbins-Monro iteration [20]

$$\phi_{i+1}^{(n+1)} = \frac{1}{n} \sum_{j=1}^{n} \hat{G}(\phi_{i+1}^{(j)})$$  \hspace{1cm} (1.16)

where $\hat{G}(\phi_{i+1}^{(j)})$ is a stochastic function (i.e., the Monte Carlo solution) that uses the $j$-th iterate of the EOS concentrations to approximate the scalar flux and reaction rates of the current iteration. This iteration continually updates the EOS flux and reaction rates, approximating an implicit solution to Equation 1.15.

The SIE method is stable in the limit of infinite iterations $n$, but each evaluation of $\hat{G}$ requires an additional transport solution. While previously mentioned schemes use between one and four intermediate transport solutions per time step, analysis in [19, 21] indicate that one may need ten or more iterations for a stable SIE solution.
1.4 Challenges and Issues

A wide pool of research has been devoted to the study of these and more depletion schemes. Key issues will be summarized from the existing literature, which will be useful to help frame discussions and motivations for this work.

1.4.1 Statistical uncertainties

When coupling a depletion solution to a Monte Carlo transport solver, one must contend with systematic uncertainties that are present in the reaction rates. Obviously if the Monte Carlo solution is poorly converged, then subsequent depletion solutions will be inaccurate regardless of time-integration scheme. This is less an issue of coupling methodology, but is worth mentioning in passing.

Additionally, the propagation of statistical uncertainties on reaction rates through depletion is a non-trivial task. This would allow the EOS concentrations to have an associated uncertainty and uncertainty on quantities like $k$ and tallied fluxes to reflect the total history of the simulation rather than a single steady state calculation. Currently, no Monte Carlo codes in the literature report the ability to use such uncertainties throughout the transport solution.

A standard approach to propagate uncertainties is to repeat the entire simulation with unique random number seeds to measure expected properties (concentrations, $k$, tallies, etc.) and the associated variance. These issues are known in the field of Monte Carlo and depletion coupling, and will not be addressed in this work.

1.4.2 Stability

It is well known that forward Euler schemes in general are numerically conditionally stable, requiring a time step to be below some characteristic size or else unstable solutions can be obtained. For depletion analysis, these instabilities can be made manifest through spatial
oscillations in neutron fluxes and large errors in multiplication factor.

This is most easily demonstrated by simulating some mono-dimensional problem with symmetric properties (e.g., initial compositions, power, coolant density). Should the problem be declared in a certain manner, one can expect some symmetry in the time-dependent solution. This could be constant flux and concentrations in the case of reflective boundary conditions, or some symmetric wave function for vacuum boundary conditions. However, as discussed in [5, 6, 7, 8], symmetric solutions are not obtained for sufficiently large step sizes.

Figure 1.5 presents an example of these instabilities with a five day step predictor scheme applied to an axially symmetric fuel pin. The flux has a reported uncertainty of less than one percent in each node and is initially symmetric within this uncertainty. As with the discussions in Section 1.4.1, these uncertainties do not reflect the propagation of uncertainty through depletion.

The axial flux distribution becomes highly peaked later on in the simulation and oscillates between consecutive steps. The curves for days 85 and 95 are nearly overlain. If one were to obtain flux or power profiles with these shapes in a production design, one might expect to see similarly peaked temperature profiles which must be controlled through increased cladding thicknesses, exotic materials, or other mitigation strategies.

One would be justified in believing that the issues stem from the Monte Carlo solution and associated statistical properties. Indeed, work by Cosgrove, Shwageraus, and Parks indicates that neutron clustering can be a driver for oscillations [22]. However, this is likely not the sole cause of the instabilities, as such oscillations appear when a deterministic transport solution is used. Densmore, Gill, and Griesheimer applied stability analysis to a 1-D diffusion problem and were able to derive a stability criteria that, if exceeded, resulted in oscillating solutions [8]. Instead, these instabilities are a by-product of the time integration scheme exceeding some stable step size. This conclusion is empirically confirmed in [5, 6, 7].
While the predictor scheme is the subject of most if not all of the previous stability analyses, there is no reason to believe it alone is subject to these oscillations. With the exception of the SIE method with many iterations, all the previous schemes are some higher-order explicit Euler scheme and could be subject to similar instabilities. The restricting step size would likely be larger with such schemes, but detailed analysis has yet to be produced. Analysis in [5, 6, 7] suggests that, for a predictor-corrector scheme, the oscillations could be present in the predictor and corrector step, yet averaged when forming the depletion matrix used to deplete across the time step.

1.5 Objectives and goals

Through this chapter, the theoretical and practical basis for understanding depletion theory has been presented. It is a phenomena that is fundamental to understanding the behavior of nuclear applications over time, and has been studied and improved with decades of mathematical analysis. Several production-grade analysis tools have incorporated isotopic depletion solvers directly into or alongside a transport solver [2, 4, 23, 24, 25, 26].
The common trade-off presented in these studies is the desire to achieve high-fidelity results with reasonable computational resources (e.g., time and/or computing units). Take too large of a depletion step and one may experience instabilities or the accuracy may suffer more subtly, but the results may be available much faster [5, 6, 7, 8, 22]. To counter these penalties, improved solution techniques are being developed to either improve the underlying mathematics of the solution phase [15, 16, 27], or leverage more transport solutions per step with the hope of increasing the depletion step size [14, 18, 28].

This work introduces a first-of-a-kind hybrid transport-depletion coupling scheme, where a high-fidelity transport solution is linked with a reduced-order code to reduce computational time without losing sufficient accuracy. In doing so, one may find that a solution that requires \( N \) high-fidelity transport solutions can be obtained using \( M \ll N \) high-fidelity and \( R \) reduced-order solutions. Ideally, the reduced-order code is orders of magnitude faster than the high-fidelity tool, allowing the result to be obtained in less time. Such a reduced-order code also allows smaller time steps to be taken, which can lead to more stable and accurate depletion solutions [6, 7, 8].

This hybrid depletion scheme is realized using a custom coupling framework responsible for interfacing with transport codes and performing depletion. The Serpent [3] Monte Carlo code will be used as the high-fidelity solver of choice, but the framework has general interfaces that could be used to link additional codes. A novel reduced-order transport method has been developed for this work, capable of predicting the change in scalar neutron flux using perturbation theory.

This dissertation is arranged as follows. Chapter 2 presents the concept of substep depletion and how this can be extended to the hybrid coupling scheme that is the subject of this work. Chapter 3 derives the aforementioned reduced-order transport solution and presents some verification results. Chapter 4 applies the hybrid depletion scheme to a single fuel pin, including sensitivity studies and convergence analysis. Chapter 5 applies the scheme to a multi-dimensional, heterogeneous problem, providing evidence of the merit of
this scheme to engineering-scale problems. Finally, Chapter 6 summarizes the methodologies and results herein, with suggestions for follow-on work and improvements.
CHAPTER 2
SUBSTEP HYBRID DEPLETION SCHEME

This chapter will introduce a depletion scheme that couples high-fidelity and reduced-order transport solutions in a substep manner. Individually, substep depletion and hybrid transport schemes exist in the literature, and will be discussed in Sections 2.1 and 2.2, respectively. The substep hybrid depletion scheme will be introduced in detail in Section 2.3. Finally, the custom depletion framework that was written to implement this method will be discussed in Section 2.4.

2.1 Substep depletion

The general principle of substep depletion is to update the compositions at a finer time scale without running additional transport simulations. A time interval \( t \in [t_i, t_{i+1}] \) is divided into \( S \) intervals, not necessarily of equal size. New compositions are obtained at the intermediate points until the interval is completed, where a new transport simulation is performed. This process repeats until all intervals have been exhausted and the simulation has modeled the entire window of interest.

This method can also be extended to a predictor-corrector scheme quite easily, using corrected reaction rates for the second march through the depletion interval. Furthermore, since a depletion system is solved at each substep, one might desire to update the reaction rates as well. Two approaches for handling the substep reaction rates will be discussed in the following subsections.

2.1.1 Constant reaction rates

The most straight-forward substep approach would be to simply hold the depletion matrix \( A \) constant across the entire interval, but to deplete with smaller time steps \( \Delta t_s \). When
using CRAM or another matrix exponential routine and with equally sized substeps $\Delta t_s = \Delta t / S$, the incremental compositions can be obtained with

$$\vec{N}_{s+1} = \exp(\mathbf{A}t / S)\vec{N}_s$$

(2.1)

given the BOS compositions $\vec{N}_0$. This does not exclude other techniques for solving the Bateman equations in a substep manner, but the matrix exponential will be the focus as it is used in this work.

The EOS compositions can therefore be expressed as

$$\vec{N}_S = \exp(\mathbf{A}t / S)\vec{N}_{S-1} = (\exp(\mathbf{A}t / S))^2 \vec{N}_{S-2} = \cdots = (\exp(\mathbf{A}t / S))^S \vec{N}_0,$$

(2.2)

consistent with the scaling and squaring approach for matrix exponentials [29]. Isotalo and Pusa applied this constant reaction rate substep procedure using CRAM [30], and discovered the following key insights.

First, this method has a small additional burden. The main cost of the CRAM routine is solving sparse linear systems of the form $(\mathbf{A} - \theta \mathbf{I})^{-1} \vec{b} = \vec{x}$ with intermediate vectors $\vec{b}$ and $\vec{x}$. Due to its structure and sparsity, $LU$ decomposition is well suited for solving these linear systems, as described in [27]. If the depletion matrix is constant across the interval, the decompositions of $\mathbf{A}$ need not be recomputed at each substep.

Second, this method captures short-lived isotopes with greater accuracy. The depletion system can contain isotopes that decay very quickly; $^{135}$Xe and its metastable isomer have half-lives of approximately nine hours and fifteen minutes respectively. By taking smaller depletion steps, the destruction of these transient isotopes is captured in earlier steps.

While the substeps can be advantageous, this approach alone is not enough. The largest source of error is not due to the solution of $\frac{d}{dt} \vec{N} = \mathbf{A} \vec{N}_0$, but the physics surrounding the problem. The authors of [30] did not make any claims regarding improved stability of this substepping approach. As discussed throughout this work, the reaction rates are
tightly coupled to the compositions. A further improvement, discussed next, is to update the reaction rates through the substeps.

2.1.2 Piecewise constant reaction rates

Isotalo and Aarnio proposed projecting the reaction rates in time to update the depletion matrix at each substep [28]. This equates to assuming the reaction rates are piecewise constant inside each substep, and can be found with

\[ RR_s = \frac{1}{t_s - t_{s-1}} \int_{s-1}^{s} RR(t) \] (2.3)

for \( 1 \leq s \leq S \). The primary benefit of this approach is that the reactions rates can be updated with finer temporal resolution without extra transport simulations. All that is required is to determine an appropriate fitting for \( RR(t) \).

As proposed in [18], one could use information from the previous time step \( i - 1 \) to create linear or quadratic models of reaction rates for all isotopes. Additionally, isotopes can be treated with different fitting models, such as a quadratic model for gadolinium [31]. Such an approach would require restructuring the depletion system to model the transmutation of some isotopes separately, but has demonstrated good improvements over the standard predictor-corrector method.

When implemented in conjunction with a higher-order time integration scheme, like the linear extrapolation / linear interpolation (LE/LI) form [18], larger step sizes are achievable. That research, as well as further work by Josey [14], demonstrated that a factor of four increase in step size could be obtained without sacrificing accuracy. At a first approximation, this translates to a reduction in simulation time by between two and four times, as some of the higher-order schemes require two transport simulations per depletion step.
2.2 Hybrid methods

The concept of hybrid methods typically refers to coupling a Monte Carlo solution to a reduced-order solution with the intent of speeding up the overall sequence. One such example would be accelerating the fission source convergence; since the distribution of fission sites is not known \textit{a priori}, a non-negligible amount of computational time is spent converging upon this fission source. After some number of inactive batches, the simulation moves to the active sequence, wherein reaction rates and other quantities of interest are computed.

In order to reduce the impact of the inactive batches, hybrid schemes have been developed that use finite-difference diffusion \cite{32} and discrete ordinates \cite{33} schemes to accelerate the source convergence. Some work has been done to improve thermal-hydraulic coupling by incorporating a hybrid diffusion-Monte Carlo scheme \cite{34}. Following a thorough literature review and to the best of the author’s knowledge, no such scheme has been applied to a depletion problem.

2.3 Hybrid depletion with mixed-fidelity transport

A method for using a reduced-order transport solution to improve a depletion simulation is presented. Unlike previously discussed hybrid methods, the reduced-order solution will be performed at substeps and used to capture the spatial and temporal evolution in reaction rates. In principle, a reduced-order solution could also be used to accelerate the Monte Carlo solution at each time step. This is not the scope of this work.

Consider a single coarse step \(i\) between two high-fidelity transport solutions at times \(t_i\) and \(t_{i+1}\). These are depicted by the larger orange circles in Figure 2.1. The interval \(t \in [t_i, t_{i+1}]\) is divided into an integer number of substeps, not necessarily of the same length. After depleting out to the first substep and obtaining compositions \(N_{i,1}\), a reduced-order solution is performed to obtain a new set of reaction rates. These reaction rates are
used to deplete to the next interval, be that another substep or the beginning of the next coarse step. Figure 2.1 contains three sub substeps, denoting two reduced-order solutions in blue.

![Figure 2.1: Depiction of a mixed-fidelity substep depletion scheme](image)

While Figure 2.1 indicates that the scalar flux is obtained at each step, it is really the isotopic reaction rates that are of interest for depletion. These quantities are readily attainable with most Monte Carlo simulations, as continuous energy cross sections are present for all isotopes. However, some reduced-order schemes may spatially homogenize discrete regions and not have need for isotopic cross sections.

As a remedy, the proposed scheme reconstructs the reaction rates with the substep flux $\phi_{i,j}$ and a projection of the microscopic cross sections. The simplest of which is polynomial extrapolation, wherein cross sections are stored at previous points and then projected to the substeps using constant, linear, or quadratic fitting. The use of polynomial fitting is similar to the higher-order methods of [14, 18]. The difference is that, rather than extrapolate the reaction rates directly, the substep flux and the projected cross sections are combined to create the reaction rates.

This projection will degrade if the cross sections are over-extrapolated, similar to existing limits on depletion time steps. Figure 2.2 presents the relative change against the beginning-of-life (BOL) microscopic cross sections in a pressurized water reactor (PWR) fuel pin depleted out to 60 days using a realistic thermal power. Values at zero days are not included, as their relative change against the BOL is identically zero.

However, the initial values indicate a sharp change of a few to several percent across
the first depletion step, while the changes are smooth for later time steps. This figure demonstrates why taking some small initial steps is advantageous both for building up a fission product inventory, but also for improving extrapolation of cross sections.

![Graph showing change in PWR microscopic cross sections since BOL. Values are marked every five days](image)

**Figure 2.2**: Change in PWR microscopic cross sections since BOL. Values are marked every five days.

The hybrid substep depletion scheme is presented in Algorithm 1 for an arbitrary number of coarse steps $C$, each with a potentially different number of substeps $\{S_i\}_{i=0}^{C-1}$. The functions HF and RO indicate the high-fidelity and reduced-order flux solutions. As the names imply, the STORE and EXTRAP functions are responsible for storing microscopic cross sections provided by the high-fidelity solution, and then extrapolating these out to a future point in time. Finally, the DEPLETE function provides updated compositions for all materials at the next substep and coarse step given previous fluxes and cross sections.

As it is written, the scheme allows for each coarse step to have a different number of equidistant substeps. This could be beneficial for the initial stage of a simulation where not enough cross sections have been loaded to perform the extrapolation. Additionally, one could take fewer or no substeps at the beginning in order to ensure the cross sections reflect the sharp changes in neutron spectra as fission products are built up.

The process presented in Algorithm 1 goes beyond existing substep methods. With the
Algorithm 1 Substep depletion with mixed-fidelity transport solutions

Require: \(\{N_0\}\)  \(\triangleright\) Initial compositions

1: \(t \leftarrow 0\)

2: for \(i \leftarrow 0, C - 1\) do \(\triangleright\) Loop over coarse steps \(C\)

3: \(\phi_{i,0}, k_i, \sigma_{i,0} \leftarrow \text{HF}(N_{i,0})\)

4: \(\text{STORE}(\sigma_{i,0})\)

5: \(\Delta \leftarrow (t_{i+1} - t_i)/S_i\)

6: for \(j \leftarrow 1, S_i - 1\) do \(\triangleright\) Substep loop

7: \(N_{i,j} \leftarrow \text{DEPLETE}(N_{i,j-1}, \phi_{i,j-1}, \sigma_{i,j-1}, \Delta)\)

8: \(t \leftarrow t + \Delta\)

9: \(\sigma_{i,j} \leftarrow \text{EXTRAP}(t)\)

10: \(\phi_{i,j} \leftarrow \text{RO}(N_{i,j})\)

11: end for

12: \(N_{i+1,0} \leftarrow \text{DEPLETE}(N_{i,S_i-1}, \phi_{i,S_i-1}, \sigma_{i,S_i-1}, \Delta)\)

13: \(t \leftarrow t + \Delta\)

14: end for

15: \(\phi_C, k_C \leftarrow \text{HF}(N_{C,0})\) \(\triangleright\) Final transport solution

inclusion of a reduced-order solution at the substep level, the influence of changing compositions can influence the reaction rates, rather than projecting reaction rates over time with extrapolation and interpolation. This projection reduces the influence of surrounding materials and does not ensure the reaction rates reflect the most recent compositions. While the proposed scheme does rely on projecting the microscopic cross sections, the flux solution provided at the substeps \(\phi_{i,j}\) is closely tied to the updated isotopics and includes the effect of neighboring materials.

2.4 Custom depletion framework

A Python package was developed in order to implement and test the hybrid coupling scheme, as no such tool exists in the field. When developing this framework, emphasis was placed on abstraction and extensibility. By carefully abstracting away functionality from monolithic blocks into classes with succinct purposes and interfaces, the framework can easily be extended in the future. A brief discussion is warranted to explain the utilities to aid discussions in later chapters.
2.4.1 Geometry modeling

The package supports modeling common light water reactor (LWR) components, including right cylinder pins with annular regions, Cartesian lattices in the x-y plane, and vertical lattices in the z direction. Using these utilities, users can model pincells, fuel assemblies, or a supercell of adjacent fuel assemblies. While a full core solution including reactor pressure vessel, baffles, and other support material is out of the scope of this package, it is possible to build the active fuel region containing hundreds of fuel assemblies, each with some degree of axial discretization. The traditional combinatorial solid geometry (CSG) used by Monte Carlo codes is not directly provided, as the package does not seek to be a general transport modeling utility.

A common practice when depleting large problems, or problems with strong spatial flux gradients, is to divide burnable materials into axial and/or radial segments. Rather than have the user create thousands of identical burnable materials, each placed in a unique location, codes like Serpent and OpenMC [3, 35] can automate the division of the materials. A similar utility is provided in the framework, wherein a depth-first search is performed to find all burnable materials, copying and replacing repeated burnable materials.

This search is also used to find the ordering of all burnable materials, enabling a consistent map of compositions, fluxes, and reaction rates across transport and depletion. Figure 2.3 presents a visual representation of this search and is explained below to provide insight into the geometry capabilities of the framework.

The geometry is presented as two adjacent and identical fuel pins in Figure 2.3a, each containing the same fuel and moderator. Only a single instance of the pin has been created, stored inside a $1 \times 2$ Cartesian lattice. The Cartesian lattice has no knowledge of the contents of the pin, only that is is a pin, hence the hatching patterns at the top of both trees in Figure 2.3.

When the user requests that all burnable materials be differentiated, the search begins at the root universe. This universe begins searching through any constituent universes, fuel
Figure 2.3: Depiction of depth-first search used to find and differentiate materials. Left and right images depict a sample geometry before and after the search was applied and new burnable materials automatically copied. Numbers indicate the ordering of the descent pin A first, and descends one level deeper to find any contained universes or materials. In Figure 2.3a, the first descent is step 0 from the left most position to the shared pin instance.

A pin is considered to be a terminating node, as it does not contain universes, only materials taking up some space between concentric circles. An understanding of the materials and their outer radii are used to define the geometry of the fuel pin, depicted as orange fuel surrounded by blue moderating material. The search finds the fuel and moderator with edges 1 and 2, noting the existence of the fuel before withdrawing from the material search.

The Cartesian lattice then descends into the next contained universe, the right pin A, and performs the same search with descent 3. Step 4 finds the same fuel for a second time and the shared moderator is found in step 5. Having discovered the same fuel, Pin A creates a copy of the fuel in the same radial position as before and returns Pin B: an identical pin representation except with new burnable materials. The lattice observes that the universe returned is a copy and replaces the universe at this lattice position, storing Pin B in place of the second Pin A. After the successful traversal, two similar fuel pins exist in the lattice with and identical geometry and referencing the same non-burnable materials.
This type of searching is also performed when ordering burnable materials and creating the geometry model for the transport solver of choice. By storing the problem in a tree-like fashion, simple search routines can be used to explore the geometry without having to develop surface tracking routines. Furthermore, one can place lattices of fuel pins inside vertical stacks to create a 3-D fuel assembly, and into further XY lattices for a 2- or 3-D model up to a full reactor core.

2.4.2 Transport solver interfaces

The key aspects of the framework are two abstract interfaces for generic high-fidelity and reduced-order transport codes. These interfaces perform no computational benefits, instead serving as base classes for useful interfaces. With this approach, it would be much easier to incorporate additional transport solvers without having to rework the entire computational sequence. Developers need not worry about storing reaction cross sections or even exporting result data to disk, as these are handled by other classes in the framework. Instead, transport interfaces must be able to

1. initialize a solver-specific representation of the materials and geometry;
2. update material information given post-depletion burnable material definitions;
3. execute a transport solution; and
4. return back to the framework results including, at a minimum, scalar fluxes.

Reduced-order solvers and the depletion backend communicate what physics are necessary to the high-fidelity solver, which in turn should be aware of what physics are supported (e.g., spatial homogenization to obtain few-group macroscopic cross sections, fission matrix, collapsing of microscopic cross sections). This allows the framework to ensure compatibility between solvers that may have been developed independently. In the event the high-fidelity solver does not support some of the physics required, the framework safely terminates before any expensive work has been completed.
Discussion on the chosen reduced-order solver and interface will be delayed until Section 3.5, but the interface to the Serpent Monte Carlo code [3], the chosen high-fidelity code, will be discussed here.

**Serpent interface**

The Serpent interface is responsible for building the initial model of the problem, including geometry and necessary tallies, executing Serpent, and processing the coarse step results. The serpentTools Python package [36] is used to obtain fluxes, multiplication factor, homogenized macroscopic cross sections, and other required data. A modified Serpent version was developed that allows the user to update compositions through text files while cross section data and model representation are retained in memory. This modification means that, at the beginning of each coarse step, Serpent does not have to restart fully from scratch. Instead, Serpent reads this data file, updates compositions of burnable materials, and then proceeds into the transport solution.\(^1\)

As discussed in Section 1.1 and shown in Figure 1.1, fission yields are an energy-dependent property, while ultimately a single effective yield is used to populate the depletion matrix. As of version 2.1.31, Serpent does not readily provide a single set of fission yields to the end user, nor is a single set stored in memory. Therefore the effective yields must be obtained through a weighting or interpolation scheme, but the literature is inconclusive on the matter.

The ENDF-6 format dictates that linear interpolation should be used based on incident neutron energy [37], but this is difficult if not impossible to obtain without direct access to the transport routines. SCALE 6.1 computes the average neutron energy causing fission from the flux-weighted fission cross sections and interpolates based on this average energy [38]. Similar approaches are performed in Serpent [23] and OpenMC [35].

\(^1\)This interface was developed with inspiration and guidance from Jaakko Leppänen and Ville Valtavirta, developers of the Serpent Monte Carlo code. The author is very grateful for this assistance.
would entail tallying the average energy of fission for a specific nuclide as

$$\bar{E} = \frac{\int_0^{\infty} E \sigma_f(E) \phi(E) dE}{\int_0^{\infty} \sigma_f(E) \phi(E) dE}$$

(2.4)

and then interpolating based on this average energy $\bar{E}$. However, as of Serpent 2.1.31 (used
in this work), no such energy-weighted tally is provided. Therefore, the decision was made
to use only the fission product yields provided at 0.0253 eV, or the thermal spectrum yields.

2.4.3 Depletion backend

Using the current compositions and reaction rates across all materials, the package uses the
incomplete partial factorization (IPF) formulation of CRAM to update compositions [15,
16]. The depletion solution is performed in parallel across unique processes using the
`multiprocessing` library\(^2\), included in the standard library.

The implementation and some data structures are inspired by the OpenMC depletion
module [35], and heavily relies on the NumPy and SciPy Python packages [39, 40]. This
implementation has been verified against the Serpent internal depletion solver in previous
work by the author [41].

Users are able to specify the fitting order (e.g., constant, linear, quadratic) and number
of points used in the fit. While it is possible to project using all previous cross sections,
using one or two previous points has been shown to be sufficient [18, 41]. This reduced
memory requirements and allows the cross sections to be stored in a fixed-length stack,
shown in Figure 2.4. Previous points are loaded following the high-fidelity transport solu-
tion as they arrive, and sufficiently old cross sections are removed when the stack would
exceed capacity. Limits are also placed to avoid constructing a fit whose order exceeds the
number of stored points, e.g., linear fit with a single data point.

\(^2\)Documentation: https://docs.python.org/3/library/multiprocessing.html
Figure 2.4: Three-point example stack used to store microscopic cross sections in the custom framework. Cross sections $\sigma_i$ are provided at times $t_i$ from the high-fidelity solver. The depicted stack contains space for three sets of cross sections, and $\sigma_0$ is discarded once $\sigma_3$ is pushed on to the stack.

2.5 Conclusion

A hybrid substep depletion scheme has been presented, employing high-fidelity and reduced-order transport simulations. By using the most up-to-date compositions to obtain the substep flux, materials can be depleted using reaction rates that better reflect the spatial and temporal state of the problem. The hybrid scheme is presented first in a general manner, as any two well-matched codes could be used as either solver. To use the updated reaction rates, it is beneficial if both tools are capable of producing isotopic reaction rates, homogenized across each burnable region. However, in the event this is not possible, one can store and project microscopic cross sections from the high-fidelity solution.

A custom framework was discussed, including the interface for the Serpent Monte Carlo code, the high-fidelity code chosen for this work. For the curious, the framework has been released in its entirely to the public\(^3\). The next chapter will be devoted to the reduced-order solver developed for this work: a perturbation-theory based prediction that relies on no additional transport solutions.

\(^3\)https://github.com/CORE-GATECH-GROUP/hydep
A perturbation-theory-based reduced-order transport prediction was developed for this work. The motivation and derivation for the method is presented in Section 3.1. The derivation follows work by Carney et al. regarding the fission matrix [42] and its applications to neutron transport. Therefore a brief primer on the fission matrix is provided in Section 3.2. Additional changes and assumptions beyond the existing work are discussed in Section 3.3. Initial verification results are presented in Section 3.4. Finally, Section 3.5 narrows the scope and application of the method to a reduced-order solver appropriate for substep depletion.

Much of the content and discussion from this chapter has been published in *Nuclear Science and Engineering* [41].

### 3.1 Derivation

The goal of the spatial flux variation (SFV) method is to predict the change in neutron flux between two states. These states can refer to geometric changes, such as the inclusion of control mechanism, or material changes, as in the case of depletion. The latter will be the focus of this work, where the change in flux between the beginning-of-step (BOS) and end-of-step (EOS) will be computed by examining the variation in properties across a depletion step.

The method begins by expressing the BOS neutron transport equation in operator form as

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

(3.1)

where $\mathcal{L}$ and $\mathcal{M}$ are the neutron loss and production integral-differential operators, $\Psi$ is
the neutron flux, and \( \lambda \equiv 1/k_{\text{eff}} \) is the fundamental eigenvalue of the system. Operators \( \mathcal{L} \) and \( \mathcal{M} \) and flux \( \Psi \) can be continuous in space, energy, and angle, however this notation will be neglected.

The EOS state, denoted by superscript \( (1) \), is cast as a linear-perturbation from the BOS state

\[
\mathcal{L}^{(1)}\Psi^{(1)} = \lambda^{(1)}\mathcal{M}^{(1)}\Psi^{(1)}
\]

(3.2)

Equation 3.2 is expanded, discarding second- and third-order terms

\[
\mathcal{L}^{(0)}\Psi^{(0)} + L^{(0)}\delta\Psi + \delta\mathcal{L}\Psi^{(0)} = \lambda^{(0)}\mathcal{M}^{(0)}\Psi^{(0)} + \lambda^{(0)}\mathcal{M}^{(0)}\delta\Psi + \lambda^{(0)}\delta\mathcal{M}\Psi^{(0)} + \delta\lambda\mathcal{M}^{(0)}\Psi^{(0)}.
\]

(3.3)

The change in neutron flux \( \delta\Psi \) is obtained using a linear combination of basis functions \( \psi_m \)

\[
\delta\Psi = \sum_{m=1}^{M} a_m \psi_m
\]

(3.4)

chosen to satisfy the bi-orthogonality relation

\[
\langle \psi_n^\dagger, \mathcal{M}^{(0)}\psi_m \rangle = \delta_{n,m} \langle \psi_n^\dagger, \mathcal{M}^{(0)}\psi_m \rangle.
\]

(3.5)

with adjoint basis functions \( \psi_n^\dagger \). Applying Equations 3.1 and 3.4 to Equation 3.3 yields

\[
\delta\mathcal{L}\Psi^{(0)} + \mathcal{L}^{(0)}\sum_{m=1}^{M} a_m \psi_m = \lambda^{(0)}\mathcal{M}^{(0)}\sum_{m=1}^{M} a_m \psi_m + \lambda^{(0)}\delta\mathcal{M}\Psi^{(0)} + \delta\lambda\mathcal{M}^{(0)}\Psi^{(0)}.
\]

(3.6)

Expansion coefficients \( a_m \) are obtained by left-multiplying \( \psi_n^\dagger \) with Equation 3.6 and
taking the inner product

\[ a_m = \frac{\langle \psi_m^\dagger, (\delta L - \lambda^{(0)} \delta M) \Psi^{(0)} \rangle - \delta \lambda \langle \psi_m^\dagger, M^{(0)} \Psi^{(0)} \rangle}{(\lambda^{(0)} - \lambda_m) \langle \psi_m^\dagger, M^{(0)} \psi_m \rangle}, \]  

(3.7)

where the bi-orthogonality relation from Equation 3.5 has been used. Having obtained the expansion coefficients \( a_m \), one can reconstruct the EOS flux with

\[ \Psi^{(1)} = \Psi^{(0)} + \delta \Psi = \Psi^{(0)} + \sum_{m=1}^{M} a_m \psi_m. \]  

(3.8)

A method for predicting \( \delta \lambda \) involving the change in flux \( \delta \Psi \) is presented in [42]. As this is the target of the prediction and not known \textit{a priori}, an approximation must be made. This approximation is discussed in Section 3.3.

The task is now to determine sufficient basis functions such that coefficients \( a_m \) can be used to determine \( \Psi^{(1)} = \Psi^{(0)} + \delta \Psi \) using Equation 3.4. Carney et al. originally proposed using higher order modes of the forward and adjoint flux, \( \Psi_m \) and \( \Psi_m^\dagger \), respectively [42]. These could be computed using the corresponding modes of forward and adjoint fission sources \( S_m \) and \( S_m^\dagger \), computed using the fission matrix. A brief background on the fission matrix will be presented next, and readers are referred to [42, 43, 44] for more exhaustive discussion and applications.

3.2 Use of the fission matrix

The fission source is a common expression in neutron transport methods, as it allows the k-eigenvalue form the transport equation to be written as

\[ \mathcal{L} \Psi(\vec{r}, E, \hat{\Omega}) = \frac{\chi(\vec{r}, E)}{4\pi k} S(\vec{r}). \]  

(3.9)
The fission source

\[ S(\vec{r}) = \int \int dE' d\hat{\Omega} \nu(E, \vec{r}) \Sigma_f(E, \vec{r}) \Psi(E, \vec{r}, \hat{\Omega}) \]  (3.10)

describes the production of neutrons from fission, independent of energy and angle, across the domain.

The fission source is also attainable using the fission matrix, \( \mathbf{F} \in \mathbb{R}^{n \times n} \), with elements

\[ F_{i,j} = \int_{\vec{r} \in V_j} d\vec{r} \int_{\vec{r}_0 \in V_j} d\vec{r}_0 \frac{S(\vec{r}_0)}{S_j} H(\vec{r}_0 \rightarrow \vec{r}), \]  (3.11)

where

\[ S_j = \int_{\vec{r} \in V_j} d\vec{r} S(\vec{r}) \]  (3.12)

is the fission source inside domain \( j \). Element \( F_{i,j} \) describes the expected number of neutrons born from fission in region \( j \) due to a fission in region \( i \). The Green’s function \( H(\vec{r}_0 \rightarrow \vec{r}) \) is defined in [43], describing the transfer of fission neutrons from \( \vec{r}_0 \rightarrow \vec{r} \).

The following eigensystem relates the fission source and fission matrix

\[ \tilde{S}_m = \frac{1}{k_m} \mathbf{F} \tilde{S}_m \]  (3.13)

where \( \{k_m\} \) are \( k \)-eigenvalues of the higher-order transport equations

\[ \mathcal{L} \Psi_m = \frac{1}{k_m} \mathcal{M} \Psi_m. \]  (3.14)

By solving Equation 3.13, one can obtain some or all of the modes of the fission source, and then obtain the corresponding flux modes \( \Psi_m \) with

\[ \mathcal{L} \Psi_m(\vec{r}, E, \hat{\Omega}) = \frac{\chi(\vec{r}, E)}{4\pi k} S_m(\vec{r}). \]  (3.15)
Equation 3.15 is simply Equation 3.9 with the $m$-th mode of the fission source. Care should be taken to adequately sample the discrete fission source obtained from Equation 3.13 when obtaining these flux modes.

### 3.2.1 Real vs. complex eigenvalues

Figure 3.1 displays the fission matrix for a 360 cm long fuel pin, homogeneous in the axial dimension, with 20 cm of axial reflectors. The meshing for the fission matrix is defined by 100 equal volume axial discretizations. This specific fuel pin has constant axial properties (fuel enrichments, temperatures, and densities) and the resulting fission matrix is very nearly symmetric. There are some asymmetric elements farther from the main diagonal, but the magnitudes of these values are on the order of the statistical uncertainty.

![Figure 3.1: Fission matrix for 3-D fuel pin with axial reflectors](image)

The fission matrix will be square but is is not guaranteed to be symmetric, even for symmetric problems, due to the inherent statistical uncertainty of the Monte Carlo process. Therefore the eigenvalues and eigenvectors may have imaginary components. Eigenvalues from the matrix given in Figure 3.1 are provided in Figure 3.2 to provide two observations: the imaginary components are zero until the higher order modes, and their magnitude is
small relative to the magnitude of the real components.

![Figure 3.2: Real and imaginary components of eigenvalues obtained from fission matrix in Figure 3.1. Absolute values are applied to the imaginary components to present the complex conjugate pairs](image)

Carney et al. observed that the magnitude of the imaginary components decreases as the number of neutron histories is increased in the Monte Carlo simulation [42]. Based on these findings, the authors stated this provides strong evidence, but not a rigorous proof, that the $k$ eigenvalues for reactor systems are positive and real valued. Similar observations have been found by the author and for the remainder of this work, only the real eigenvalues and eigenvectors of the fission matrix will be considered.

### 3.2.2 Obtaining the adjoint

The adjoint fission matrix is defined as

$$ F_{ij}^\dagger = \int_{\vec{r} \in V_j} d\vec{r} \int_{\vec{r}_0 \in V_j} d\vec{r}_0 \frac{S_{ij}^\dagger(\vec{r}_0)}{S_{jj}^\dagger} H(\vec{r} \rightarrow \vec{r}_0). \quad (3.16) $$


In this formalism, the modes of the fission source $\vec{S}_m$ and $\vec{S}_m^\dagger$ can be obtained with the following eigenvalue problems

$$\vec{S}_m^\dagger = \frac{1}{k_m} F^\dagger \vec{S}_m^\dagger \quad (3.17)$$

$$\mathcal{L}^\dagger \Psi_m^\dagger = \frac{1}{k_m} M^\dagger \Psi_m^\dagger. \quad (3.18)$$

Carney et al. demonstrated that, for a sufficiently fine spatial discretization, the adjoint fission matrix converges to the transpose of the forward. This allows the modes of the forward and adjoint fission source to be extracted as right and left eigenvectors of the fission matrix. Furthermore, the eigenvalues $k_m$ and $k_m^\dagger$ are identical, as they correspond to the same eigensystem.

$\delta \lambda$ can be approximated by left multiplying Equation 3.2 and the BOS adjoint transport equation

$$\mathcal{L}^{(0)i\dagger} \Phi^{(0)i\dagger} = \lambda^{(0)} M^{(0)i\dagger} \Phi^{(0)i\dagger} \quad (3.19)$$

by $\psi_0^\dagger$ and subtracting the two expressions. The equivalence of $\lambda^{(0)}$ and $\lambda^{(0)i\dagger}$ has been used.

Solving for $\delta \lambda = \lambda^{(1)} - \lambda^{(0)}$ yields

$$\delta \lambda = \frac{\left< \psi_0^\dagger, \left( \delta \mathcal{L} - \lambda^{(0)} \delta M \right) \Psi^{(1)} \right>}{\left< \psi_0^\dagger, M^{(1)} \Psi^{(1)} \right>}. \quad (3.20)$$

Since $\Psi^{(1)}$ is the target of the analysis, which in turn relies on $\delta \lambda$, a first-order assumption can be made to replace the end-of-step flux with the beginning-of-step flux

$$\delta \lambda \approx \frac{\left< \psi_0^\dagger, \left( \delta \mathcal{L} - \lambda^{(0)} \delta M \right) \Psi^{(0)} \right>}{\left< \psi_0^\dagger, M^{(1)} \Psi^{(0)} \right>}. \quad (3.21)$$
3.3 Extensions for depletion

Having obtained the higher order fission source modes, the next step is to obtain the corresponding higher order flux modes $\Psi_m$ and $\Psi_m^\dagger$. Using the modes of the forward fission source $S_m$, Equation 3.9 can be used to obtain the forward flux modes with some modifications to existing Monte Carlo transport routines, as discussed in [42]. Unfortunately, tallying the transposed scattering kernel is necessary to obtain $\Psi_m^\dagger$ with $S_m^\dagger$, and is a non-trivial task.

Work by the author in [41] chose instead to use the forward and adjoint fission source modes as proxies for the higher-order flux modes. The primary motivation is that the higher-order forward and adjoint fission source modes are attainable directly from the fission matrix as described in Equations 3.13 and 3.17. The higher-order $\kappa$ eigenvalues can be directly mapped to the $\lambda$ eigenvalues. This approximation was found to be sufficiently accurate across large changes in the spatial neutron flux [41] and will be presented in Section 3.4.

Changes in neutron loss and production operators $\delta\mathcal{L}$ and $\delta\mathcal{M}$ were approximated as changes in macroscopic absorption and neutron production cross sections $\Delta\Sigma_a$ and $\Delta\nu\Sigma_f$, respectively. These cross sections are homogenized across non-overlapping spatial domains identical to those that make up the fission source and flux nodes. In doing this, loss due to neutron streaming and scattering is neglected.

Using a one-group formulation, neutrons are not removed from the phase space through scattering, as they exist in the same position and energy momentarily after a scattering event. The loss to streaming can be recovered by a similar perturbation-theory approach to the boundaries of each node, but was shown to be a non-substantial source of error in previous work [41].

It should be pointed out that the work in the previous sections has been aimed at predicting the change in angular flux $\Psi$, potentially continuous in energy and angle. For the
purposes of depletion, however, one needs the one-group reaction rates and thus all angular- and energy-dependence will be integrated out. The outcome of the spatial flux variation method is then the change in scalar flux $\delta \phi$ that will help approximate $\phi^{(1)} = \phi^{(0)} + \delta \phi$.

To summarize, the method must compute

1. higher-order fission source modes and eigenvalues from the fission source,
2. $\delta L$ and $\delta M$ with $\Delta \Sigma_a$ and $\Delta \nu \Sigma_f$,
3. $\delta \lambda$ with Equation 3.21,
4. expansion coefficients $a_m$ with Equation 3.7, and
to predict the EOS flux $\phi^{(1)} = \phi^{(0)} + \delta \phi$ with Equation 3.4.

### 3.4 Application to a 3-D pincell

This section summarized conclusions from [41], where this prediction was originally performed and verified. Important aspects of the problem are included in Section 3.4.1, but readers are referred to the previous reference for complete details.

#### 3.4.1 Test methodology

A 3-D pressurized water reactor (PWR) pin with axially varying coolant density was modeled and depleted with the Serpent Monte Carlo code [3]. The pin was divided into 10 equal volume axial segments for depletion and spatial homogenization. Five depletion schedules were used, each starting with ten single day steps, then depleting out to day 60 using steps size of one, five, ten, 25, and 50 days. The SFV method was tasked with obtaining the scalar flux at day 60 using the exact beginning-of-step (BOS) and end-of-step (EOS) macroscopic cross sections. The BOS flux was normalized to a unit volume integral prior to the prediction, since the eigenvectors of the fission matrix are normalized to an arbitrary scale and do not reflect the system power.
The fission matrix was computed using 100 axial layers in order to converge the fundamental adjoint fission source. To align with the spatial discretization of the flux and cross sections, the higher-order modes were averaged across ten consecutive nodes of equal volume. This was done as a first pass verification, and is not repeated in future analysis.

The SFV method has been implemented as a set of Fortran subroutines, with exposed Python bindings. This allows the prediction to be performed orders of magnitude faster than a pure-Python equivalent, but be usable from the custom depletion framework used in this work. The source code for this package has been released for public use and integration\(^1\).

### 3.4.2 Verification results

The reference Serpent fluxes are plotted for the penultimate and final time step in Figure 3.3. The EOS point in calendar time is day 60, and is consistent across all cases, while the BOS is one depletion step away, e.g., day 35 using 25 day step sizes, day 10 with 50 days, and day 59 with single day steps. Therefore one should not expect agreement in the BOS fluxes as they correspond to different points in calendar time. All five EOS fluxes should agree in principle, but the effect of the depletion step size is clearly seen.

While the 50 day step flux is not the converged flux observed with smaller step sizes, the SFV method seeks to predict the state reflected by the provided cross sections. As the cross sections are directly provided by Serpent at this incorrect state, the predicted flux will not correspond to fluxes produced by smaller step sizes. Instead, it will be the task of the hybrid depletion sequence to obtain accurate macroscopic cross sections that better reflect the true state of the problem.

The difference in the predicted flux shape for all cases and distributions of select cases are plotted in Figure 3.4. As seen in Figure 3.3, the EOS flux for smaller step sizes can be close to converged, and therefore would be coincident if plotted together. The differences are visible in the left plot, indicating agreement to within a few percent. Larger differences

\[^1\text{https://github.com/CORE-GATECH-GROUP/sfv}\]
Figure 3.3: BOS and EOS fluxes from Serpent for SFV verification

correspond with larger changes in reference flux and cross sections, as seen in Figure 3.3
for 25 and 50 day steps specifically.

Figure 3.4: Absolute error in predicted flux (left) and distributions (right) for 5, 25, and 50
day steps

A counter-intuitive conclusion from Figure 3.4 is that the prediction performs poorly
for single day steps. The error with these small step sizes is attributed to small changes
in the macroscopic cross sections between the two states. As $\Delta \Sigma_a$ and $\Delta \nu \Sigma_f$ approach
Figure 3.5: Mean (left) and variance (right) of difference in SFV flux prediction for increasing number of modes.

zero, the change in loss and production operators $\delta L$ and $\delta M$ also tend to zero. The term $\delta L - \lambda^{(0)} \delta M$ appears when computing the expansion coefficients (Equation 3.7) and $\delta \lambda$ (Equation 3.21). If the change between the two states is sufficiently small, the expansion coefficients will go to zero, leading to the solution $\phi^{(1)} \rightarrow \phi^{(0)}$.

3.4.3 Effect of higher-order modes

Results presented up to this point used ten modes of the forward and adjoint fission sources. This was chosen on an ad hoc basis, but the choice is explained through the following convergence study. Each step size was re-analyzed using 1, 5, 20, 50, and 100 modes of the fission matrix. The absolute relative difference was computed for all axial nodes, with the mean and variance plotted in Figure 3.5.

Using 50 day depletion steps, increasing the number of modes marginally improves the prediction. Referring back to the $k_m$ eigenvalues from Figure 3.2, the higher-order eigenvalues were nearly two orders of magnitude less than the fundamental eigenvalue. As $k_m \rightarrow 0$, $\lambda_m \rightarrow \infty$, and expansion coefficient $a_m$, acting as the weight for the higher-order flux mode, goes to zero, as Equation 3.7 contains $\lambda^{(0)} - \lambda_m$ in the denominator. Figure 3.6 presents all available modes of the forward and adjoint fission source, with select modes of the forward source in Figure 3.7. For this specific case, the higher order modes of the
fission source contribute less information back to the problem, indicating that some number can safely be discarded.

Convergence studies like the one presented in Figure 3.5 will be applied for models used in this work. By reducing the number of eigenvalues and higher-order fission source modes, the overall memory footprint of the method can be reduced. The computational cost is also reduced, as some of the internal routines must loop over each of the modes.

### 3.5 Integration with substep depletion

The spatial flux variation method was chosen as the primary reduced-order solver for this work. In order to be compatible with the custom framework introduced in Section 2.4, some additional actions must be taken.

First, the high-fidelity solver must be capable of producing the fission matrix, discretized across burnable regions. As these regions are not likely to appear in a regular arrangement, e.g., a fuel assembly that includes guide pins and instrumentation tubes, the fission matrix should be attainable across arbitrary spatial domains. The Serpent Monte Carlo
Figure 3.7: Select modes of the forward fission source

code is capable of binning the fission matrix in Cartesian lattices, but also on a universe-based binning. This allows a consistent indexing across modes of the fission source, scalar flux tallies, and microscopic cross sections.

Up to this point, the EOS macroscopic cross sections have been exactly known when applying the SFV method. However, this requires a transport solution at the EOS, implying the true flux solution is already known. The macroscopic cross sections will instead be reconstructed at the substep level.

Given the new compositions $N_{i,j}$ and microscopic cross sections extrapolated to the substep point $\sigma_{i,j}$, macroscopic quantities are created by summing over atom densities and the appropriate reaction cross section. The average number of neutrons produced per fission $\nu$ in each burnable region is obtained at each coarse step and extrapolated using similar extrapolation as the microscopic cross sections. Since the SFV and depletion routines need these data at the same point in calendar time, the results of the most recent extrapolation are retained for re-use.

Since the forward and adjoint fission source modes are eigenvectors of the fission matrix, their magnitudes are arbitrarily normalized and may not reflect the power of the sys-
tem. As a result, the substep flux predicted by the SFV method \( \tilde{\phi} \) must be scaled to the correct magnitude by computing a constant \( c \) such that

\[
\phi = c \tilde{\phi}
\] (3.22)

reflects the correct.

The fission energy production in each region can be computed using Q-values quantifying the energy produced per fission for an individual isotope, updated compositions, and extrapolated microscopic cross sections, as dictated by the following relation

\[
\tilde{P} = \tilde{\phi} \kappa \Sigma_f,
\] (3.23)

with \( \kappa \Sigma_f \) being the sum of products of isotopic fission Q-values, compositions, and fission cross sections. The scaling constant \( c \) can be computed by normalizing to the system power \( P \) using

\[
c = \frac{PV}{\sum_i \tilde{P}_i V_i}
\] (3.24)

where \( V_i \) is the volume of each burnable region, and \( V = \sum_i V_i \).

According to this model, all fission energy is considered to be deposited at the fission site. This is a simplification, as a few percent of the energy is deposited by fission neutrons and gamma rays interacting with materials [45]. This is the default option in Serpent and OpenMC, unless additional heating data are provided [35, 45]. The properly normalized scalar fluxes \( \phi \) are then used to deplete materials along the substeps. Compositions at the next substep can be used to rebuild \( \Sigma_a \) and \( \nu \Sigma_f \) necessary for the next prediction, repeating until all substeps are exhausted.
3.6 Conclusion

A method for predicting the change in scalar neutron flux using perturbation-theory has been presented. The end-of-step (EOS) flux shape is obtained without having to run a transport solution, instead using the EOS macroscopic absorption and neutron fission production cross sections. The beginning-of-step (BOS) transport solution is more expensive due to the computation of the fission matrix, requiring 10-15% more computational time. However, this allows the reduction of at least one transport simulation, reducing the total BOS and EOS simulation time by 45% for a 3-D PWR pin.

The SFV method is well suited for the reduced-order solver in this work. Average time to perform the prediction is on the order of milliseconds, and rebuilding absorption and fission cross sections is straightforward given the new compositions and projected microscopic cross sections. The remaining chapters will focus on applying the SFV method in the full hybrid depletion sequence.
This chapter will discuss the verification of the framework, responsible for building Serpent inputs and for depleting materials, with and without the hybrid depletion scheme. The chosen model is discussed in Section 4.1. Verification is distributed across several sections, each with a specific purpose. Section 4.2 compares the coupled framework solution, without hybrid substeps, against Serpent. The substep procedure with reduced-order solutions is tested in Section 4.3, demonstrating the accuracy of the hybrid depletion scheme. The hybrid scheme is compared against existing depletion schemes across Sections 4.4 to 4.7, examining stability, accuracy, and a figure of merit. Concluding remarks are made in Section 4.8.

The methodology and results presented in this chapter follow a paper submitted for publication in *Annals of Nuclear Energy* [46].

### 4.1 Description

A 3–D PWR fuel pin with constant axial properties was first studied. Fresh fuel consisted of 4.45 w.t.% UO$_2$ spanning 360 cm, Compositions and properties are described in detail in Appendix C. The fuel pin was discretized into 100 equivolume axial layers in order to converge the fundamental mode of the adjoint fission source. Using 250 thousand particles per cycle, with 250 active and 200 inactive cycles, the max uncertainty in the nodal scalar flux was less than 1%.

The fuel pin was depleted with a constant power of 636.226 kW, producing a power density around 0.04 kW/gU, for a total of 310 days. Ten single day depletion steps were used to build up fission product inventory, and to provide sufficiently stable cross sections for extrapolation. The remaining 300 day period was divided into equal step size intervals.
with five, ten, and 20 day depletion steps.

Two reference solutions were generated: a Serpent reference using the predictor-corrector depletion scheme and a framework reference using no reduced-order substeps. Both solutions used single day depletion steps for the entire irradiation period. A reflective boundary condition was placed at the axial mid-point and only the upper half of the fuel pin was modeled in these references. Since this model is known to have stability issues—see [5, 8] for examples—the reference solutions were obtained using a stable and symmetric solution by design. This symmetry also allowed the reference solutions to be generated using half the number of total histories without any increased uncertainty in scalar fluxes. When comparing to these references, the axial fluxes and isotopic compositions are mirrored across the midpoint to obtain a truly symmetric reference solution.

The hybrid solutions used single day substeps and cross sections were extrapolated using three-point linear fitting. This extrapolation proved to be sufficient for time steps of up to 50 days for a similar fuel pin and power [41]. Additionally, 25 higher order fission sources modes were used when rebuilding the reduced-order flux. These parameters were chosen to configure the framework for the highest accuracy. Factoring in the additional storage requirements and time spent depleting with single day substeps could yield more optimal settings, potentially at the cost of accuracy.

4.1.1 Error metrics

As each case begins with ten single day depletion steps before using larger step sizes, the first ten days will be excluded from the comparisons. The difference in multiplication factor

$$\Delta k \ [pcm] = \frac{k' - k}{k} \times 10^5$$

will be presented to compare a global quantity. The mean absolute relative difference (MARD) in the nodal scalar flux will be used to measure local accuracy against the reference solutions.
Isotopes that make up 99.99% of the macroscopic absorption cross section according to \( \Sigma_a = \sum_n N_n \sigma_{a,n} \) will be compared across all cases. These isotopes are contained in Table 4.1, corresponding to the most important isotopes for this model. The difference for each isotope will be computed per node, and the MARD will be computed from these differences. In some figures, the mean relative difference will be presented as a line graph, surrounded by a shaded region denoting ± one standard deviation.

**Table 4.1: Isotopes considered as highest contributors to total absorption**

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Mass Number</th>
<th>Mass Number</th>
<th>Mass Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ce</td>
<td>141</td>
<td>Cs</td>
<td>135</td>
</tr>
<tr>
<td>Eu</td>
<td>153</td>
<td>Eu</td>
<td>157</td>
</tr>
<tr>
<td>I</td>
<td>131</td>
<td>Kr</td>
<td>139</td>
</tr>
<tr>
<td>Mo</td>
<td>99</td>
<td>Nd</td>
<td>145</td>
</tr>
<tr>
<td>Nd</td>
<td>147</td>
<td>Np</td>
<td>239</td>
</tr>
<tr>
<td>O</td>
<td>16</td>
<td>Pd</td>
<td>147</td>
</tr>
<tr>
<td>Pm</td>
<td>148</td>
<td>Pm</td>
<td>151</td>
</tr>
<tr>
<td>Pr</td>
<td>143</td>
<td>Pu</td>
<td>240</td>
</tr>
<tr>
<td>Rh</td>
<td>103</td>
<td>Rh</td>
<td>101</td>
</tr>
<tr>
<td>Ru</td>
<td>103</td>
<td>Sm</td>
<td>150</td>
</tr>
<tr>
<td>Sm</td>
<td>151</td>
<td>Sm</td>
<td>153</td>
</tr>
<tr>
<td>Tc</td>
<td>99</td>
<td>Te</td>
<td>129</td>
</tr>
<tr>
<td>U</td>
<td>234</td>
<td>U</td>
<td>236</td>
</tr>
<tr>
<td>Xe</td>
<td>133</td>
<td>Xe</td>
<td>93</td>
</tr>
</tbody>
</table>

### 4.2 Verification of depletion framework

Before comparing the accuracy of the hybrid depletion scheme, the underlying transport-depletion solution will be compared against Serpent. This will allow differences in data handling, depletion solver, and fission yield treatment to be isolated from the hybrid methods in Section 4.3. Figure 4.1 presents the multiplication factor provided by Serpent and the relative difference in the framework solution. The maximum uncertainty on \( k \) and \( \Delta k \) across all time points was 12 pcm. The dashed lines on the right indicate ± two standard deviations from the reference solution, indicating that most framework values are within or near two standard deviations from the Serpent reference.
Figure 4.1: Reference estimate of $k$ from Serpent (left) and relative difference with framework solution (right)

The framework flux solution and relative difference to the Serpent flux is given in Figure 4.2. The maximum relative difference of 15% is produced after the first depletion step, detailed in Figure 4.3 and is dominated by the production of the initial fission products, demonstrated by the initially large difference in $^{135}$Xe density after the first depletion step in Figure 4.4. After a few days, however, the flux and xenon densities are more closely aligned and the systems reach a similar equilibrium state.

For a more granular comparison, the accuracy of isotopic compositions across all 50 nodes is performed. Figure 4.5 presents the MARD for isotopes with the largest difference and select isotopes commonly examined in depletion studies. Since the framework and Serpent use different models for fission yields, it is understandable that fission products would have a larger difference. The difference in $^{127m}$Te is due to differences in the Serpent decay library, ENDF/B VII.0. There, $^{127}$Sb undergoes $\beta^-$ decay to ground state $^{127}$Te with a branching ratio of 0.95, rather than the 0.84 used in the framework’s library (ENDF/B VII.1). Despite these differences, the framework solution will be considered an adequate reference solution when examining the hybrid depletion scheme.
Figure 4.2: Scalar flux produced by the framework reference (top) and relative difference to Serpent predictor-corrector (bottom). As the reference solutions are mirrored across $z = 180$, the scalar flux and difference are only plotted for the upper half.

Figure 4.3: Relative difference in framework reference flux for select early depletion steps.
Figure 4.4: Relative difference in framework reference $^{135}$Xe concentration for select early depletion steps.

Figure 4.5: Mean absolute relative difference in isotopes with largest difference across all points (left) and select isotopes (right). Values obtained from symmetric reference solutions.
4.3 Hybrid scheme results

Previous sections have demonstrated the accuracy of the spatial flux variation method (Section 3.4) and the depletion routines (Section 4.2) separately. The following section presents results across the entire irradiation period using the hybrid scheme with various coarse step sizes.

Figure 4.6 presents the difference in $k_{eff}$ as reported by Serpent at the coarse steps. The red lines indicate the ± twice the uncertainty on the framework reference. Each reported multiplication factor is within two standard deviations from this reference.

![Graph showing difference in $k_{eff}$](image)

Figure 4.6: Difference in UO$_2$ pin multiplication factor using hybrid depletion scheme

Figure 4.7 contains the difference in key actinides and fission products, and is useful for diagnosing sources of differences in the hybrid solution. Examining the 20 day step case, the difference trends upward until day 30, after which the mean difference begins to decrease for most isotopes. A new Serpent simulation is performed at day 30, producing a new set of microscopic reaction cross sections.

Until this point, the extrapolation was performed using cross sections generated at days eight through ten. All three curves have a similar increasing trend in difference starting at day ten, until the next high fidelity transport solution: day 15, 20, and 30 for five, ten,
Figure 4.7: MARD in UO$_2$ pin compositions for key isotopes, computing using hybrid depletion scheme

and 20 day coarse steps. Once the updated microscopic cross sections are provided for the extrapolation, the difference begins to tend down until around day 120. This initial increase then decrease indicates that the extrapolated microscopic cross sections, used for reaction rates and the substep SFV prediction, do not fully capture the changes in this initial period.

The later spikes observed in $^{235}$U, $^{239}$Np, and some fission products are related to the accuracy of the transport solution. Figure 4.8 presents the MARD between the coarse step and substep flux produced in the hybrid solution against the symmetric framework reference. Shaded regions indicate $\pm$ one standard deviation across the 100 axial nodes. While the majority of the five and ten day fluxes are at or below 5% difference, there are larger spikes using the 20 day step, aligning with isotopic spikes from Figure 4.7.

Almost all of the spikes are preceded by a gradual increase in MARD until the next Serpent solution, further indicating that, for this problem, a 20 day coarse step pushes or exceeds the limits of cross section extrapolation and/or the SFV prediction. Despite
these shortcomings, it will be demonstrated in later sections that the hybrid solution is more stable, and thus accurate, than existing scheme when applied to this stability-limited problem.

Figure 4.8: MARD in UO$_2$ pin scalar flux at coarse and substep level using hybrid scheme

4.4 Comparison to existing methods

To put these differences into a sensible frame of reference, the fuel pin was depleted with identical step sizes in Serpent using two depletion schemes. Comparisons will be made against the predictor in Section 4.4.1. Section 4.4.2 will compare the hybrid depletion scheme to the linear extrapolation / linear interpolation scheme introduced by Isotalo and Aarnio [18].
4.4.1 Predictor

The implementation of the hybrid scheme is similar in kind to the predictor, as both use a single transport solution per coarse step. However, the predictor has well documented issues with accuracy and stability for this problem [5, 7, 8].

Figure 4.9 presents the difference in $k$ using five and ten day steps. As these differences are substantial, a predictor case with 20 day steps was not performed and will be left from the analysis. Oscillations in the axial flux distribution are clearly visible in Figure 4.10. For comparison, the flux distribution is plotted using the hybrid framework with 20 day coarse steps. A more detailed discussion on stability for all cases is included in Section 4.5, but the improved stability of the hybrid scheme is evident from this figure.

These oscillations drive large differences in the compositions for the predictor scheme, presented in Figure 4.11. Here, the mean absolute relative difference for each isotope in Table 4.1 is computed across all time steps and axial nodes. The maximum MARD exceeds 20%, with a slight descent toward the end of the irradiation period. For contrast, the same difference is computed for the hybrid scheme using similar coarse step sizes and does not register above 2%.
Figure 4.10: UO$_2$ scalar fluxes for predictor (top) and hybrid (bottom) depletion schemes

Figure 4.11: MARD in top contribution isotopes for UO$_2$ pin for with predictor (left) and hybrid (right) schemes
4.4.2 Linear extrapolation / linear interpolation

With the established research on the shortcomings of the predictor method, especially for spatially large models where oscillations are more likely, and the myriad of more advanced depletion schemes, comparing against only the predictor may not be the best metric. Comparing against the LE/LI method is not as equivalent of a comparison as the predictor, as the hybrid scheme uses only one Monte Carlo solution per coarse step, while the LE/LI method employs a second for a corrector step. However, both cases use information from a previous step to perform some polynomial fitting in time.

Figure 4.12 demonstrates that this additional information greatly improves the prediction on $k$ compared to the predictor alone. Larger deviations on the order of hundreds of pcm are still observed using a 20 day step, but there is a clear improvement as the depletion step size is reduced. The difference in $k$ at EOL was $9 \pm 9$ pcm using LE/LI with five day steps, while the hybrid with 20 days yielded an EOL $\Delta k$ of $14 \pm 10$ pcm. As seen in the right figure and Figure 4.6, the hybrid scheme maintains excellent agreement on $k$ throughout the simulation, independent of step size.

Figure 4.13 demonstrates that the LE/LI method is a much better predictor of isotopics than the predictor scheme. Contrasted with this observation are the results produced by the hybrid scheme, with a lumped MARD across similar isotopes that is consistent across
coarse step size. Aside from a few spikes in the 20 day coarse step case discussed above, this lumped difference is consistently at or below 1% using the hybrid scheme.

4.5 Stability

As this problem has initially symmetric conditions and no changes are made throughout the simulation, one can expect a symmetric axial flux profile over time. A simple metric to measure the symmetry is the axial offset, defined in this work as

\[
AO \equiv \frac{\sum_{l=N/2+1}^{N} \phi_l}{\sum_{l=1}^{N} \phi_l} - 0.5
\]  

Using this metric, a positive axial offset of \(x\) denotes a 100\(x\) percentage point deviation from symmetry; the upper half of the problem contains \(50 \times (1 + 100x)\)\% of the flux. Oscillatory behavior is also reflected with this metric, since alternative positive and negative offsets indicate the majority of the scalar flux is located in the upper and then lower sections of the model.

The axial offsets for all four examined cases (reference, hybrid, predictor, LE/LI) are provided in Figure 4.14. As demonstrated in Figure 4.10, the predictor scheme demonstrates strong axial flux oscillations, echoing conclusions in previous stability research [5,
Figure 4.14: Axial offset in UO$_2$ pin for all four cases. Step size legend applies to all figures.

8]. Using smaller steps sizes with both the predictor-corrector and LE/LI schemes, one observes more stable solutions. The LE/LI scheme does experience some oscillations, even with five day depletion steps. Conversely, for much of the simulations, the solution obtained by the hybrid case is as stable as the reference case. There is some asymmetry growing near day 90, coincident with differences in fission products seen in previous figures.

4.6 Simulation time

It has been established in the previous sections that the hybrid framework combined with the spatial flux variation (SFV) method can obtain an accurate prediction of flux, multiplication factor, and local isotopics. This accuracy comes at a cost of additional reduced-order transport solutions, and a more expensive high-fidelity Serpent simulation. The total trans-
port time would be the sum of time spent in the high-fidelity and reduced-order solutions.

However, the high-fidelity Serpent simulation is burdened with computing more data than is strictly necessary for the SFV prediction, as it must also compute data for depletion, namely local scalar fluxes, fission yields, and microscopic reaction cross sections. Therefore simply comparing the total times is not adequate, as the simulation time from the framework is inflated by these structures, as well as the SFV data.

4.6.1 Penalty due to depletion data

In order to perform the depletion, microscopic reaction cross sections, and scalar fluxes must be computed in Serpent and returned to the framework. These are provided by flux tallies and the `set mdep` parameter to compute microscopic reaction cross sections in each designated universe. When the burnable materials are defined through the Serpent interface, Serpent automatically creates internal data structures and tallies to compute these exact properties, as they are necessary for Serpent’s own depletion routines. As of the time of this writing however, these quantities are not readily provided to the end user without substantial modifications. Therefore an additional penalty is observed when using the hybrid framework to create duplicate tallies that are more readily accessible.

4.6.2 Penalty due to reduced-order solver data

The previous slowdown could be wholly removed if the hybrid depletion scheme presented in this work was integrated at a source code level. One would still have to compute some additional data necessary for the reduced-order transport solver to achieve the benefits presented in this work. For the spatial flux variation (SFV) method, this includes computing the fission matrix and homogenized macroscopic cross sections across each universe containing burnable materials. For larger problems this penalty will likely increase, and will be studied in the following chapter as well.
4.6.3 Computing the total and individual penalties

Since the depletion penalty could be removed entirely, it is desirable to compute just the penalty associated with computed data for the SFV method. To determine the individual penalties, the total Serpent transport time was compared across the predictor cases, the framework reference, and the hybrid solutions. Comparing the predictor and framework references will determine the cost to obtain the microscopic reaction cross sections necessary for depletion. Comparing the hybrid simulation times and the framework reference will determine the cost of including the fission matrix and spatial homogenization routines necessary for the SFV prediction.

The penalties associated with each case are

\[ T_F = T_P \times (1 + P_D) \]  \hspace{1cm} (4.3a)
\[ T_{SFV} = T_F \times (1 + P_{SFV}) \]  \hspace{1cm} (4.3b)

where \( T_P, T_F, \) and \( T_{SFV} \) correspond to the average transport times for the predictor cases, framework reference, and SFV hybrid cases. The time spent in the framework reference will be doubled since the symmetric model uses half the number of total histories. The corresponding penalties \( P_D \) and \( P_{SFV} \) are the additional costs of obtaining depletion data and SFV data, respectively, from Serpent.

One can compare the base time to the SFV case with

\[ T_{SFV} = T_P (1 + P_D) (1 + P_{SFV}) \]  \hspace{1cm} (4.4)

If one was to integrate the SFV solution and a hybrid depletion solver directly into a compatible transport and depletion sequence, the depletion penalty could be removed. The penalty of computing the data only for the SFV method would be \((1 + P_S)\). Therefore, when comparing simulation times from the hybrid framework, the SFV cases will be rep-
represented as
\[
\hat{T}_S = T_P (1 + P_{SFV}) = \frac{T_S}{1 + P_D}
\] (4.5)

where \(T_S\) is the time spent in the Serpent high-fidelity solution. Time spent in the reduced-order solver will not be modified.

The average run time and associated penalties are included in Table 4.2, indicating that a 108% increase in simulation time can be removed by better access to depletion data. Including the fission matrix and routines to produce homogenized macroscopic cross sections in each node adds a 8.85% increase.

Table 4.2: Transport time and penalties associated with individual modeling aspects

<table>
<thead>
<tr>
<th>Case</th>
<th>Time [CPU h]</th>
<th>Penalty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>5.2443</td>
<td>-</td>
</tr>
<tr>
<td>Depletion</td>
<td>10.9274</td>
<td>1.0837</td>
</tr>
<tr>
<td>SFV</td>
<td>11.8944</td>
<td>0.0885</td>
</tr>
</tbody>
</table>

4.7 Figure of merit

The following figure of merit (FOM) will be used to weigh the accuracy and expediency of each depletion scheme and step size:

\[
FOM = \left[ T \times \sqrt{\frac{1}{N} \sum_{n=1}^{N} \left( \theta_n - \hat{\theta}_n \right)^2} \right]^{-1}
\] (4.6)

Here, the simulation time \(T\) is multiplied by the root mean square deviation (RMSD) in end-of-life (EOL) isotopics when compared to the reference case \(\hat{\theta}\). The RMSD is taken across all axial nodes and isotopes in Table 4.1.

When comparing simulation times, only the time inside a transport simulation is used. This neglects time to initialize the model and deplete materials, as these are fundamentally different between the Serpent runs and those using the custom framework. The CPU time,
or the product of wall clock time and number of processors, is presented in Figure 4.15.

![Figure 4.15: Transport CPU time for all four UO$_2$ pin cases](image)

Table 4.3 summarizes the conclusions across all cases and quantities of interest. The simulation times for the hybrid scheme have been modified to present the penalty due only to the reduced-order solutions (on the order of milliseconds) and a high-fidelity Serpent solution that only includes the SFV data. The hybrid scheme required a Monte Carlo solution that required $\approx 9\%$ more simulation time than the standard predictor due to the calculation of the fission matrix and spatial homogenization. However, the inclusion of reduced order substeps leads to greatly increased accuracy in EOL $k$ and isotopics.

Figure 4.16 presents the ratio

$$R_{\text{scheme,step}} = \frac{FOM_{\text{hybrid,step}}}{FOM_{\text{scheme,step}}}$$

for the predictor and LE/LI schemes. For all cases, the ratio is greater than unity, indicating this hybrid scheme has a consistent benefit. The error in $k$ and isotopics is consistent for the predictor for both five and ten day steps, leading to a decrease in FOM ratios due to the less expensive simulation required by the predictor.
4.8 Conclusion

The hybrid depletion scheme has been tested against a symmetric 3–D UO$_2$ pincell. By employing the SFV reduced-order solution at the substep level, the hybrid scheme obtained a global multiplication factor that was within 20 pcm of the reference solution throughout the 310-day irradiation period. This agreement was within 2 standard deviations from the reference across all step sizes and calendar days.

Furthermore, local isotopics and scalar flux were captured with good agreement. Key isotopes such as $^{235}$U, $^{239}$Pu, and $^{145}$Nd experienced mean absolute relative differences (MARD) of a few percent or much less. In some cases, the hybrid solution experienced an increase between 2-3% using 20 day coarse steps up to day 30, where the next set of microscopic cross sections were obtained. Following this point, the differences in $^{239}$Pu and $^{125}$Nd, as well as $^{135}$Xe and $^{149}$Sm diminished. The overall behavior of $^{135}$Xe, $^{149}$Sm, and $^{239}$Np, especially for 20 day coarse steps, resulted in spikes of greater than 5% before dropping at the next high-fidelity transport solutions. These results indicate the linear extrapolation of microscopic reaction cross sections may not be sufficient for all isotopes across such a step, given that the five and ten day coarse step simulations provide a lower MARD.
Using five day coarse steps, the majority of the scalar fluxes yielded a MARD less than 5% compared to the framework reference. The maximum MARD increased as the coarse step size increased, exceeding 15% in some cases. In particular, the 20-day coarse step solution produced peaks in scalar flux difference that coincide with the differences in $^{135}$Xe, $^{149}$Sm, and $^{239}$Np.

The scalar flux solution obtained by the hybrid method is tied to the accuracy of the isotopes and the reduced-order solver, as reflected in Figure 4.8. Comparing to the framework reference, the difference in five and ten day flux solutions was almost consistently 1-2%. Some days experienced mean differences of 5%, with the 20-day coarse step experiencing mean differences of 15%. One could not meaningfully call a Monte Carlo simulation accurate with 12% MARD in scalar flux, but these results can be explained and improved.

First, the SFV reduced-order solver, even given the exact macroscopic cross sections across large depletion steps, is only accurate to a few percent: it is a first-order prediction and thus cannot be as accurate as a Monte Carlo solution. But the reduced-order solver as implemented in this work cannot have the exact macroscopic cross sections, as that implies the true flux solution is already known. If the reduced-order solution is improved, then the
end-of-step solution will be likely of higher-fidelity as well, since the fluxes used to deplete across the interval are closer to the real solution.

Finally, and most notably, the hybrid scheme does not contain a corrector step. The framework reference solution is a predictor scheme and still experiences a few percent difference in scalar flux compared to the predictor-corrector Serpent reference, both using single day depletion steps. The inclusion of a corrector step could allow larger coarse step sizes and, through the averaging of reaction rates, produce a solution that is less sensitive to the substep flux. A discussion on the use of higher-order schemes inside this hybrid depletion method will be provided in more detail in Section 6.4.2.

Despite the lack of a corrector step, the hybrid depletion scheme produces a far more stable solution than the predictor and linear extrapolation / linear interpolation schemes. The predictor scheme produced greater than 1000 pcm difference in the multiplication factor and large axial flux oscillations. While the LE/LI scheme did produce better results than the predictor, it also produced an asymmetric solution at larger time steps, and required smaller time steps than the hybrid scheme to obtain comparable accuracy.

Some discussion is merited in order to explain the orders of magnitude improvement the hybrid method could provide, as indicated by Table 4.3 and Figure 4.16. First, in taking the absolute difference between the reference densities and those produced by hybrid, predictor, and LE/LI schemes, the term \( \theta_n - \hat{\theta}_n \) will tend towards isotopes with larger densities. A 0.1\% difference in \(^{235}\text{U}\) that has an EOL density on the order of \(5 \times 10^{-4}\) atoms/b/cm is a similar or greater absolute difference than 100\% difference on atom density on the order of \(10^{-7}\) atoms/b/cm.

The presence of fission products and other trace elements that may contribute still to the 99.99\% of \(\Sigma_a\) in Table 4.1 will contribute little to this absolute difference, but will serve to reduce the arithmetic mean of the squared differences \( \frac{1}{N} \sum_{n}^{N} \left( \theta_n - \hat{\theta}_n \right)^2 \). While the FOM ratios may seem sensationaly large, they are in consistent with the data and results presented in this chapter. Furthermore, Table 4.3 indicates that the hybrid scheme with 20
day step sizes is nearly 10 times more accurate with respect to $k$ and isotopes, but requires nearly one quarter of the simulation time.
CHAPTER 5
VERIFICATION ON A SUPERCELL MODEL

To further demonstrate the benefits of this hybrid scheme, a more complicated problem has been chosen: a supercell of fuel assemblies with varying enrichments and thermal-hydraulic properties. The problem contains more heterogeneity and more dimensionsality than the pincell from Chapter 4 and emulates a more realistic reactor physics problem. However, the hybrid depletion scheme and the SFV method demonstrate similar promise and performance.

The supercell model is described in Section 5.1, with supplemental information in Appendix D. Verification of the spatial flux variation (SFV) and depletion framework as applied to this model are presented in Sections 5.2 and 5.3, respectively. Section 5.4 presents the results obtained by applying the hybrid depletion scheme to this work, comparing to Serpent predictor and linear extrapolation / linear interpolation (LE/LI) schemes in Section 5.5. The figure of merit for each scheme is given in Section 5.6, with concluding remarks in Section 5.7.

5.1 Description

The model is a 3x3 collections of typical PWR assemblies, surrounded by a homogenized steel and water reflector on all sides. To ease the computational burden, only an octant of the problem was explicitly modeled, unfolded to represent one quarter of the problem with reflected boundary conditions. Each assembly contains UO$_2$ fuel, enriched to one of three weight fractions in $^{235}$U: the center assembly is enriched to 3.4 wt%, assemblies directly adjacent are enriched to 2.4 wt% and the corner assemblies are enriched to 1.6 wt%. The assemblies and fuel compositions follow the Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) specification [47] and includes guide and instrumentation
Figure 5.1: Quarter-symmetric XY-plane for supercell problem. Right image is enlarged view of fuel region. Each assembly is divided into four sections and octant symmetry is used. Unique colors indicate unique materials. Red is the center 3.4 wt% fuel, orange and yellow the 2.4 wt% adjacent assemblies above and to the right of the center assembly. Green, brown, and purple are the 1.6 wt% in the upper right diagonal assembly. White denotes the air in the instrumentation tube. Overlain white letters indicate the alphabetic node numbering used to identify each section of the model in later figures.

The assemblies are divided into four radial zones and 100 axial layers to both capture spatial depletion effects and to better converge the adjoint fission source necessary for the spatial flux variation (SFV) prediction. Figure 5.1 displays the XY-plane of the problem, and highlights the radial discretization of the model.

The beginning-of-life power distribution obtained from Serpent was provided to a heat transfer solver to obtain an axially varying coolant density profile. A third-order polynomial defined the profile, and each axial layer used a constant density according to the evaluation at the axial midpoint. Each assembly used the same coolant density profile, with constant axial temperatures. Coefficients and visualizations of the profiles are provided in Appendix D.

As with the pincell model, two reference solutions will be produced: one with the
Serpent predictor-corrector and the other fully within the framework. Reference solutions were generated using single day depletion steps, but no further symmetry than the octant symmetry applied to all cases. The hybrid scheme will be similarly compared against the predictor and LE/LI methods using depletion steps of five, ten, and twenty days. The initial ten days were divided into ten single day depletion steps across all cases, after which larger depletion steps and substeps were used. As before, 20 day steps will be excluded from the predictor analysis. Each simulation was performed with 500 thousand particles per cycle, with 200 inactive and active cycles, with a total power density of 0.04 kW/gU equating to a system power of 39.1686 MW.

It would be ideal to apply this method to an irradiation period as long as or longer than in Chapter 4. Due to the computational burden of simulating this model and the resources available, only 110 days of irradiation are analyzed. Despite this shorter period, the trends presented by the hybrid depletion scheme do not indicate the method suffers on such a model. The impacts of this shorter depletion schedule will be discussed in Sections 5.3 and 5.4.

### 5.2 Verification of SFV predictions

Previous chapters have demonstrated the accuracy of the SFV prediction for simple geometries, and thus the method will be re-verified on the new 3-D supercell model. After depleting with ten single day depletion steps, two five, two ten, and one twenty day depletion step was used to simulated depletion out to day 60. Varying the number of axial layers and modes of the fission matrix used in the prediction will yield a convergence study on the ideal run conditions for larger simulations. For cases satisfying a depletion step of one, five, ten, twenty, and fifty days, the SFV method was applied using the exact beginning-and end-of-step data provided by Serpent.

Figure 5.2 displays the mean absolute relative difference (MARD) between the predicted end-of-step (EOS) flux and the reported value from Serpent. For context, the MARD
between the beginning- and end-of-step Serpent fluxes are also plotted. Inside this dataset are variable number of modes of the fission matrix and starting time point in time, as a ten day step is possible from day ten to twenty, and twenty to thirty. The figure indicates that the prediction is more accurate with a smaller step size, similar to conclusions from previous chapters. Additionally, the mean difference in the prediction is noticeably less than the mean change in the beginning- and end-of-step fluxes as reported by Serpent. As the difference between the two states increases due to a larger step size, the accuracy of the prediction suffers proportionally.

Inspecting Figure 5.2, one might believe that 20 axial layers is sufficient for a good prediction, as the difference in predicted flux is similar to the difference obtained using 100 axial layers across a 50 day step. Unfortunately, this is an artifact of using a single number to represent the accuracy of the predictions, despite the convenience of the outcome. Ex-
Figure 5.3: Accuracy of SFV prediction on super cell and effect of axial discretization on prediction. Fluxes have been normalized to a unit volume integral.

Analysing the predicted fluxes in Figure 5.3, the increased axial layers greatly improves the accuracy of the prediction.

The lines in Figure 5.3 represent the volume-normalized scalar flux in each of the six burnable regions (colors in Figure 5.1) across the axial layers. The scalar fluxes estimated by Serpent at days 10 and 60 are provided to show the change between the two states. The SFV prediction was generated using exact cross sections from Serpent at days 10 and 60 with 20 modes from the fission matrix. With 100 axial layers, the prediction is closer to the actual emulated EOS value at day 60. The improvement is due to a more converged fission source, similar to convergence shown in [41].

Using 100 axial layers, the number of modes used in the prediction was varied. Figure 5.4 indicates that using a larger set of forward and adjoint fission source modes leads to a less accurate solution than a smaller set.
Figure 5.4: Convergence in mean absolute relative difference (MARD) in EOS Serpent flux and predicted SFV flux with variable number of modes

Figure 5.5: Serpent reference flux for the supercell

5.3 Verification of depletion framework

As with Section 4.2, the framework will be verified against the Serpent reference in order to determine sources of error with the hybrid depletion scheme. Figure 5.5 presents the Serpent reference flux in Node E, the node with the highest scalar flux magnitude. Other nodes had similar profiles, but lower magnitudes.

The difference in multiplication factor achieved by the framework reference and Serpent reference is provided in Figure 5.6. As before, the uncertainty on $\Delta k$ does not include
the uncertainty propagated through depletion. Isotopic comparisons between the references are shown in Figure 5.7, and are similar to those seen in Figure 4.5. $^{127m}$Te had a similarly large difference, due to the differences in $\beta^-$ decay branching ratios used by Serpent and the framework, and have been excluded from the figure.

Compared to the previous model, the framework does achieve similar differences for isotopics, but with a marginally larger difference in $k$. From before, the maximum absolute difference across 310 days of irradiation was 32 ± 12 pcm. Figure 5.6 contains a maximum absolute difference of 43 ± 11 pcm with what appears to be a slight bias towards under predicting $k$. Over longer irradiation periods, the impact of the thermal fission yields used in the framework may become more clear. However, the agreement in $k$ and in the isotopics indicate that the framework will provide a valid solution against which the hybrid depletion scheme can be compared.

### 5.4 Hybrid depletion scheme

Having shown that the framework upon which the hybrid scheme is built provides a sufficiently accurate solution, the hybrid solution will again be presented. Figure 5.8 shows that
Figure 5.7: Mean absolute relative atom density difference between supercell and framework references for isotopes with the largest difference (left) and for key isotopes (right)

The multiplication factor obtained by the hybrid depletion scheme is within good agreement to the framework reference, with a maximum \( \Delta k \) of 20 \( \pm \) 10 pcm across all cases. The majority of the values are within two standard deviations to the framework reference.

The scalar flux obtained by the hybrid scheme is consistent with results seen in Figure 4.8 in Section 4.3. As a point of comparison, the largest errors of 15\% were observed around days 130 using 20 day coarse steps. Similar trends are apparent in the 20 day case, where the difference grows through the coarse step and is reduced following another Serpent transport solution. These new solutions provide more recent microscopic reaction cross sections, and indicate that linear extrapolation may not be completely sufficient for this problem.

The MARD in scalar fluxes are also consistent across the step size, indicating that any oscillations this model may experience either do not arise or have yet to arise for the hybrid scheme. A longer irradiation period would surely help demonstrate the suppression or removal of such phenomena, but, as will be seen in the following section, divergences in the scalar fluxes are produced by the predictor and LE/LI methods for identical step sizes.
Figure 5.8: Difference in multiplication factor estimated by hybrid method compared for framework reference. Red lines denote two standard deviations on framework reference.

Figure 5.9: Mean absolute relative difference in scalar fluxes obtained by the hybrid scheme.
Figure 5.10: Mean absolute relative difference in isotopics obtained using hybrid method compared to framework reference

Figure 5.10 presents differences in key isotopes for the hybrid scheme. The 20 day case again has similar profiles for the chosen isotopes as seen in Figure 4.7, where differences accumulate between days ten and thirty and descend after this new high-fidelity Serpent solution. Differences exist between this figure and isotopic comparisons in the UO$_2$ pin model (Figure 4.7) and are worth exploring. First, while the difference in $^{235}$U is less than 0.1%, both the mean and standard deviation on the differences are larger than for the pincell model.

At the final simulation point, the deviation in $^{235}$U is dominated by the upper third of the model, shown in Figure 5.11. There are two key competing factors driving this spread. Towards the top of the assembly where coolant density is lowest, the average neutron energy is higher due to the reduced moderation, and the microscopic reaction cross sections
Table 5.1: Fission product yields for $^{235}$U from ENDF/B VII.1 [48]

<table>
<thead>
<tr>
<th>Representative spectrum</th>
<th>Thermal</th>
<th>Epithermal</th>
<th>Fast</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{157}$Gd</td>
<td>$1.48 \times 10^{-9}$</td>
<td>$6.50 \times 10^{-10}$</td>
<td>$2.08 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{149}$Sm</td>
<td>$1.71 \times 10^{-12}$</td>
<td>$5.72 \times 10^{-13}$</td>
<td>$2.66 \times 10^{-8}$</td>
</tr>
<tr>
<td>$^{135}$Xe</td>
<td>$7.85 \times 10^{-4}$</td>
<td>$1.20 \times 10^{-3}$</td>
<td>$4.54 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

would reflect this harder spectrum. Similar trends are present for $^{238}$U and $^{239}$Pu, which are burned and bred, respectively, at faster rates with higher average neutron energies.

While the fission cross sections used in the framework are obtained from the transport solutions, the fission product yields used by the framework do not contain spectral information. As the thermal fission product yields in Table 5.1 indicate, the production of thermal poisons like $^{135}$Xe and $^{149}$Sm from fission decreases as the energy of incident neutron increases. The fission product yields for $^{238}$U follow a similar trend, while yields for $^{239}$Pu are essentially constant up to the fast yields.
5.5 Comparison to existing schemes

Figure 5.12 presents the difference in multiplication factor obtained by the Serpent predictor compared to the Serpent reference solution. Using five day steps, the differences produced by the predictor and the hybrid solution are very similar, indicating that this model is less prone to instabilities than the previous pincell model.

However, a depletion step of ten days introduces larger differences in $k$, driven by oscillating scalar flux distribution seen in Figure 5.13. For comparison, the hybrid solution using ten day coarse steps and single day substeps is plotted for the same node, demonstrating the improved stability of this method.

Figure 5.14 presents the difference in $k$ estimated using the LE/LI method [18], demonstrating that this method scales better than the standard predictor for increasing depletion step size. Similar to the hybrid method, the results using five and ten day steps are almost entirely within two standard deviations from the reference solution. A time step of 20 days, however, leads to similarly large differences in $k$ driven by a shift in the scalar flux distribution, presented in Figure 5.15. However, the hybrid method does not produce such a tilt using twenty day steps, and has a more agreeable estimate on $k$.

Comparing the accuracy of the isotopic prediction in Figure 5.16, the five and ten day
Figure 5.13: Axial flux distribution for node E using the Serpent predictor (top) and hybrid (bottom) depletion schemes

Figure 5.14: Difference in $k$ using LE/LI (left) and hybrid (right) depletion schemes. Step sizes for hybrid results refer to coarse step size
LE/LI and hybrid results are very similar. The large difference in scalar flux distribution observed with twenty day steps and the LE/LI scheme leads to a much larger lumped relative difference than obtained with the hybrid method. If trends from Figure 4.13 are expected to continue for this model, the lumped MARD for LE/LI will trend downwards over time, despite the fact that the same metric obtained by the hybrid depletion scheme is consistent across the chosen step sizes.

The peak leading up to day 30 using 20 day coarse steps is consistent with increasing differences in $^{135}$Xe, $^{149}$Sm, and $^{237}$Np from Figure 5.10. Similar trends were observed for the pincell model, where the concentration of these isotopes might be quite small at day 10, but also the accuracy of the cross section extrapolation degrades both the SFV flux prediction and reaction rate reconstruction.
Figure 5.16: Mean absolute relative difference in top contributing isotopes for LE/LI (left) and hybrid (right) depletion schemes

5.6 Figure of merit

Before assessing the figure of merit, the penalties for using the hybrid depletion scheme must be determined. The process will be similar to that in Section 4.6, comparing the simulation times of the framework and hybrid cases to the Serpent predictor simulation. Similar to what was shown in the pincell model, the additional routines necessary to perform the external depletion account for a large performance hit in the framework, given in Table 5.2.

As in Section 4.6, the figure of merit will be calculated for each depletion scheme and step size studied. The timing results for the hybrid method have been adjusted by a factor of $(1 + 2.57)^{-1}$ to remove the necessary penalty of calculating and retrieving the microscopic reaction cross sections through the depletion framework. Table 5.3 presents the important results from this chapter, ending with the figures of merit.

Table 5.2: Break down of the timing penalties for the supercell. Data are collected by comparing simulation times for Serpent predictor, framework reference, and hybrid method

<table>
<thead>
<tr>
<th></th>
<th>Time [CPU h]</th>
<th>Penalty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>17.22</td>
<td>-</td>
</tr>
<tr>
<td>Depletion</td>
<td>61.08</td>
<td>2.57</td>
</tr>
<tr>
<td>SFV</td>
<td>66.60</td>
<td>0.09</td>
</tr>
</tbody>
</table>
Table 5.3: Summary of supercell results and figure of merit

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Step size [d]</th>
<th>Time [CPU h]</th>
<th>$\Delta k$ [pcm]</th>
<th>Isotope RMSD</th>
<th>FOM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Predictor</td>
<td>5</td>
<td>533</td>
<td>7 ± 12</td>
<td>$3.7 \times 10^{-8}$</td>
<td>$1.37 \times 10^{12}$</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>356</td>
<td>154 ± 12</td>
<td>$3.53 \times 10^{-7}$</td>
<td>$2.25 \times 10^{10}$</td>
</tr>
<tr>
<td>LE/LI</td>
<td>5</td>
<td>917</td>
<td>11 ± 11</td>
<td>$2.55 \times 10^{-8}$</td>
<td>$1.68 \times 10^{12}$</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>628</td>
<td>9 ± 12</td>
<td>$4.33 \times 10^{-8}$</td>
<td>$8.51 \times 10^{11}$</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>474</td>
<td>518 ± 12</td>
<td>$2.31 \times 10^{-6}$</td>
<td>$3.95 \times 10^{10}$</td>
</tr>
<tr>
<td>Hybrid</td>
<td>5</td>
<td>576</td>
<td>$-13 \pm 11$</td>
<td>$3.53 \times 10^{-8}$</td>
<td>$1.4 \times 10^{12}$</td>
</tr>
<tr>
<td></td>
<td>10</td>
<td>392</td>
<td>15 ± 11</td>
<td>$8.04 \times 10^{-8}$</td>
<td>$3.94 \times 10^{11}$</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>300</td>
<td>27 ± 11</td>
<td>$1.68 \times 10^{-7}$</td>
<td>$1.18 \times 10^{11}$</td>
</tr>
</tbody>
</table>

Figure 5.17: Figure of merit ratios for hybrid depletion scheme applied to supercell model
5.7 Conclusion

To demonstrate that the hybrid depletion scheme can be applied to more practical problems, a collection of 3–D assemblies has been modeled. The increased heterogeneity through the distribution of enrichments and the axial coolant density profile are more representative of practical problems compared to the UO$_2$ pin cell from the previous chapter. Early analysis indicated that the spatial flux variation (SFV) method could indeed be applied to this model. The accuracy of the prediction is still dependent on the total change between the two statepoints (e.g., depletion step size) but was sufficiently accurate for the small substeps used in the hybrid depletion scheme.

The custom depletion framework was able to accurately model this more complicated problem, including enrichment zoning, axially varying coolant density profiles, octant symmetry, and a combination of fuel and reflector assemblies. These features indicate that one could use the framework to model the active region of a full core, up to cylindrical barrel and pressure vessel structures.

Across the 110 day irradiation period, the hybrid depletion scheme provided an estimate of $k$ that was within 30 pcm of the framework reference using five, ten, and twenty day depletion steps. Many of the values lie within 2 standard deviations from the reference, and the remaining few had overlapping uncertainties with this solution. There appear to be no indications of oscillations or diverging solutions based on this irradiation period, while the other depletion schemes did experience oscillatory flux solutions.

When comparing the isotopics produced by the hybrid scheme, the depletion step size had a larger step on the distribution of errors than the UO$_2$ pin. Fission products and some higher actinides experienced similar trends as the previous problem, where an initial increase in differences would be reduced following the next high-fidelity transport solution. As new microscopic reaction cross sections are provided after these solutions, changing the fitting order when extrapolating or applying nuclide-specific fitting options could further
improve these results.

Comparisons between the hybrid, predictor, and LE/LI schemes showed that the novel scheme presented in this work can be applied to this problem with sufficient benefits. While the LE/LI method with five and ten days was as or slightly more accurate than the hybrid method, the figures of merit indicate there is a beneficial trade-off between these methods, with FOM ratios between unity and 0.625 for these two step sizes.

For the largest time steps presented, ten days with predictor and 20 with LE/LI, the hybrid scheme demonstrated much greater benefits. This is due in large part to the additional stability of the method, as evidenced by plots of scalar flux distributions in Figures 5.13 and 5.15. Furthermore, the hybrid depletion scheme yielded far more consistent results, largely independent of the depletion step size.
CHAPTER 6
CONCLUSIONS

As organizations design new nuclear concepts, they inevitably must determine how long the utility will be operational. The cost of electricity produced at a nuclear power plant depends on, among a myriad of other factors, how often the plant must shutdown to reload and the efficiency with which the reactor can consume fuel. When depositing the depleted fuel, keen understanding of the isotopics can inform shielding and storage facilities to maximize safety as isotopes continue to emit heat and radiation.

These are all topics that an accurate transport and depletion solution can inform. The following sections will summarize the current state of coupled transport-depletion solutions, how the research presented in this work closes the technical gaps in this field, and suggestions on future work.

6.1 Summary of Monte Carlo and depletion coupling

Due to improved methods and increased computing abilities, researchers and engineers are applying Monte Carlo methods to determine the transport of neutrons to larger and more challenging problems. Coupling of Monte Carlo methods and thermal hydraulic codes is an avid area of research, due in part to the higher fidelity of the transport solution. Monte Carlo solutions are typically taken to be the reference solution for comparing deterministic transport and diffusion solutions, and hence are valuable for licensing, validating, and verifying nuclear analysis tools and concepts.

When a nuclear engineer or researcher then chooses to model the irradiation period of the fuel cycle, a depletion simulation is crucial. The accuracy of the transport solution is inherently tied to the certainty on the compositions that make up the model. As many transport codes do not support time-dependent compositions, such codes are often
linked to a depletion solver to model the isotopic evolution. If the accuracy of the entire transport-depletion sequence is to be preserved, especially for instability-prone problems, small depletion steps must be taken [5, 6, 7, 8].

In order to obtain accurate results in a timely fashion, some or all of the following actions can be taken:

1. Increase the computing power available, either by purchasing more power or increasing the allotted share for the simulation (in the case of a shared computing cluster).

2. Decrease the fidelity of the neutronics simulation, either by reducing the number of simulated particle histories or using a reduced cross section set (e.g. multi-group).

3. Reduce the number of neutronics simulations by extending the amount of simulated calendar time between state points.

4. Employ a higher-order depletion scheme that, at the cost of more transport solutions per depletion step, allows the overall number of depletion steps to be reduced (e.g. predictor-corrector).

The first action can bear a financial cost to the organization, and the remaining three actions can reduce the fidelity of the overall results, if done poorly.

Improved depletion methods like the predictor-corrector, linear extrapolation / linear (or quadratic) interpolation, and more advanced higher-order schemes have proven to improve the overall fidelity of the coupled transport-depletion system [14, 18]. These schemes rely on the assumption that, across a depletion step, the reaction rates for a single material are constant and decoupled from the problem. Beyond the predictor method however, these schemes employ multiple transport steps to correct for the time-dependence of the system.

6.2 Summary of the hybrid depletion scheme

This hybrid depletion scheme presented in this work is an innovative twist on items two and three above: the fidelity of some neutronics simulations are reduced, exchanged for
faster reduced-order simulations. This allows the time step between expensive Monte Carlo simulations to be extended, but still modeling the isotopic evolution with a fine temporal resolution.

The hybrid depletion scheme was fully presented in Chapter 2, guided by a discussion on the state-of-the-art in Chapter 1. This scheme leverages research on hybrid methods for accelerating Monte Carlo solutions [32, 33, 34] and the benefits of smaller depletion steps through substeps [28, 30] by linking a faster reduced-order transport solver at the sub-depletion step. By allowing compositions to be updated with small time scales, one could reduce or remove the production of well-reported oscillations without the burden of requiring many expensive Monte Carlo solutions.

A first-of-its-kind framework was written to facilitate this research, capable of modeling 3-D Cartesian reactor problems from pincells to collections of fuel assemblies. This framework contains abstract interfaces, through which generic high-fidelity and reduced-order codes can communicate with the framework. A dedicated depletion solver has similarly been implemented, enabling codes that do not contain depletion capabilities to be integrated, provided calculations of scalar fluxes, microscopic reaction rates can be obtained. Support for extrapolating microscopic cross sections and reconstructing reaction rates is also provided in the framework.

Dedicated interfaces for the Serpent Monte Carlo code [3] and spatial flux variation (SFV) method [41] are included in the library, acting as the chosen high-fidelity and reduced-order solvers for this work. The SFV method was developed and verified for this work, and is a unique manner by which to obtain a prediction of the scalar flux change without running another transport solution. The derivation and discussion for this method was presented in Chapter 3. The SFV method provides a fast prediction of the change in scalar flux between two time points, provided one can obtain the fission matrix and reconstruct the macroscopic cross sections at the end-of-step point.

Throughout Chapters 3 to 5, the SFV method was first applied using the exact macro-
scopic cross sections at the beginning and end time steps. This analysis demonstrated that the prediction can be applied for both simple problems (e.g., 3-D pincell) and more complicated and heterogeneous models. Scoping studies indicated that only a small percentage of the higher-order fission source modes were useful when performing the prediction, which is especially useful for larger problems.

This method is not without its limitations, namely the underlying first-order perturbation theory upon which the method is derived, and the ability to reconstruct macroscopic cross sections. While this prediction was found to be practical and useful for this work, further improvements are discussed in Section 6.4.1

Key insights were revealed when the presented scheme was applied to a 3–D UO$_2$ pincell in Chapter 4. First, step sizes of five, ten, and twenty days produced estimates on the multiplication factor within two standard deviations of the reference solution for the entire 310 day irradiation period. Comparisons to the basic predictor and the more advanced linear extrapolation / linear interpolation [18] (LE/LI) schemes demonstrate the increased stability of the hybrid method.

After applying the method further to a more heterogeneous problem, a 3–D collection of fuel assemblies, it was demonstrated that the benefits provided by the hybrid method persist for practical problems. The irradiation period was shorter due to extraneous factors, but the results provide strong evidence that the increased stability and accuracy provided by the hybrid scheme will not deteriorate.

Further evidence of the spatial instability of the predictor scheme was found, while the hybrid scheme presented no such oscillatory behavior. The LE/LI scheme was able to produce stable results, but the stability and accuracy degraded faster than the hybrid scheme for increasing step sizes. In the examined cases, the hybrid scheme was able to obtain similar accuracy as the higher order LE/LI scheme, but by taking 25–50% less computational time. The results presented in this work indicate that this hybrid depletion is an accurate, efficient, and stable method by which to solve the coupled transport-depletion sequence.
6.3 Further discussion on convergence

An interesting conclusion from Chapter 4 is the lack of a convergence towards a “correct” solution. Typically, one would examine the effect of decreasing the depletion step size until the gains in accuracy had ceased. This is most clearly evident comparing the relative differences in $k$ and isotopics against decreasing step size for the LE/LI method. Figures 4.12 and 4.13 demonstrate a clear trade-off between increased accuracy and decreased depletion step size.

Comparing the accuracy on $k$ and axial offsets produced by the hybrid method in Figures 4.6 and 4.14, there does not appear to be such a convergence, as all three chosen step sizes are similarly stable and accurate. Examining more local properties such as scalar flux or individual isotopics, decreasing from twenty to ten day steps does confer a definite gain in accuracy, but less so decreasing from ten to five days. Table 4.3 indicates the accuracy on $k$ between five and ten day steps is statistically identical, while the root mean squared difference on the end-of-life isotopics is very similar.

The use of reduced-order solutions with fine time steps seems to be more forgiving in problems that are known to be stability limited. One could potentially save two-thirds of the total simulation time and use twenty day steps compared to five day steps if only an accurate estimate on $k$ is required. This claim does not mean one should forgo a convergence study to ensure the depletion step size yields sufficiently accurate results, but that a much larger step size could be attainable without losses in stability and accuracy.

From the supercell model, the LE/LI method performed quite well for the shorter depletion step sizes. The root mean squared difference (RMSD) on end-of-life (EOL) isotopics was comparable to the hybrid method for similar steps. Even the predictor scheme, using five day depletion steps, achieved good agreement on $k$ and isotopics, indicating this model is not as prone to instabilities as the pincell. And yet, the hybrid depletion scheme was able to consistently provide a stable solution for the depletion step sizes chosen for this work.
These conclusions provide evidence that the hybrid depletion scheme presented in this work is far less sensitive to *coarse* step size, or the distance between high-fidelity transport solutions. When modeling a new system or concept, one would likely still have to undergo a convergence study to find the optimal coarse step size as is currently done. This convergence study may not have to go to nearly as fine a coarse step, providing to the diligent nuclear engineer solutions with similar accuracy faster.

6.4 Future work

6.4.1 Improvements to the spatial flux variation method

One of the innovations presented in this work is the spatial flux variation method, a technique for predicting changes in scalar neutron flux using perturbation theory. This technique has proven to be immensely valuable as a simple library, and was sufficiently accurate using two sets of one-group macroscopic cross sections and the fission matrix. This last item should serve as the starting point for future work, as the method transparently assumes the higher-order modes of the fission matrix can serve as proxies for higher-order neutron flux.

Consider the following example: a simple $3 \times 3$ collection of pincells, with the center fuel pin containing gadolinia burnable absorber. Such a problem has been previously used for depletion studies— see [7, 14] — as the central pin requires further spatial discretization in order to capture the sharp flux gradients towards the rim. Furthermore, the burnout of gadolinia often requires finer time steps at the beginning of the simulation as to properly account for depletion of gadolinium.

This problem was attempted using the hybrid method, but did not perform adequately due to the limitations of the SFV method. Because of the large concentration of thermal neutron poison gadolinium, the fission matrix falls by several orders of magnitudes in these regions, and is flat across the central pin. Conversely, while the scalar flux is indeed lower in the absorber compared to the surrounding fuel pins, it is surely not flat.
Furthermore, the work by Carney et al. that inspired the SFV method [42, 43] proposed the ability to estimate the change in the fundamental eigenvalue $\Delta \lambda$ between the two states. Alas, this estimation requires the difference in scalar flux $\Delta \phi$ that is the primary output of the prediction. One could perform an iterative procedure to further improve guesses on $\Delta \phi$ and $\Delta \lambda$ in order to predict not just the change in scalar flux but also the next multiplication factor $k^{(1)} \equiv \frac{1}{\lambda^{(1)}}$.

6.4.2 Higher-order depletion schemes

For problems with large numbers of burnable regions, simulating single day depletion steps may become taxing. Additionally, the reduced order transport solution, while hopefully much faster than a high fidelity solution, could become burdensome with this fine level of temporal discretization. It would be desirable then, to increase the substep size and use fewer depletion and reduced-order transport simulations, without sacrificing stability nor accuracy.

As discussed in Section 1.3.2, there exist a multitude of depletion schemes beyond the predictor discussed here. These schemes introduce a trade-off in more transport solutions per depletion step in exchange for increased accuracy. If one views the DEPLET function in lines 7 and 12 of Algorithm 1 as simply the solution of the Bateman equations by any integration scheme, it is possible to perform higher-order time-integration inside the hybrid depletion scheme.

Algorithm 2 provide details on how the CE/LI predictor-corrector variant could be implemented inside the main DEPLET function. A fourth-order Runge-Kutta scheme is presented in Algorithm 3 to serve as the inspiration for this future work. These two schemes have been implemented into the depletion framework, but with minimal testing against the models presented in this work.

While this is not the first work to introduce higher-order schemes for depletion, the use of the reduced-order transport solution provides a novelty not found in existing lit-
Algorithm 2 Constant extrapolation / linear interpolation (CE/LI) time integration using hybrid transport solutions

Require: $N_0, \phi_0, \sigma_0, t_0, \Delta$

1: $A_0 \leftarrow A(\phi_0, \sigma_0)$ \hspace{1cm} \triangleright Build BOS depletion matrix
2: $N_1^P \leftarrow \exp (\Delta A_0) N_0$
3: $\sigma_1^P \leftarrow \text{EXTRAP}(t_0 + \Delta)$
4: $\phi_1^P \leftarrow \text{RO}(N_1^P, \sigma_1^P)$
5: $A_1^P \leftarrow A(\phi_1^P, \sigma_1^P)$
6: $N_1 \leftarrow \exp \left( \frac{\Delta}{2} (A_0 + A_1^P) \right) N_0$
7: return $N_1$

Algorithm 3 Fourth order Runge-Kutta depletion scheme using hybrid transport solutions

Require: $N_0, \phi_0, \sigma_0, t_0, \Delta$

1: $A_0 \leftarrow A(\phi_0, \sigma_0)$
2: $N_1^P \leftarrow \exp \left( \frac{\Delta}{2} A_0 \right) N_0$
3: $\sigma_1 \leftarrow \text{EXTRAP}(t_0 + \frac{\Delta}{2})$
4: $\phi_1 \leftarrow \text{RO}(N_1^P, \sigma_1)$
5: $A_1 \leftarrow A(\phi_1, \sigma_1)$
6: $N_2 \leftarrow \exp \left( \frac{\Delta}{2} A_1 \right) N_0$
7: $\phi_2 \leftarrow \text{RO}(N_2, \sigma_1)$ \hspace{1cm} \triangleright Cross sections already provided at mid-point
8: $A_2 \leftarrow A(\phi_2, \sigma_1)$
9: $N_3 \leftarrow \exp \left( \Delta A_2 \right) N_0$
10: $\sigma_3 \leftarrow \text{EXTRAP}(t_0 + \Delta)$
11: $\phi_3 \leftarrow \text{RO}(N_3, \sigma_3)$
12: $A_3 \leftarrow A(\phi_3, \sigma_3)$
13: $\hat{A} \leftarrow \frac{1}{6} (A_0 + 2A_1 + 2A_2 + A_3)$
14: $N_{EOS} \leftarrow \exp \left( \Delta \hat{A} \right) N_0$
15: return $N_{EOS}$
erature. Provided the reduced-order scheme is sufficiently accurate and fast enough, one could achieve the additional accuracy for little to no extra computational time. This could be extremely desirable for schemes that require many transport solutions per time step, e.g., RK4, stochastic implicit Euler (SIE), commutator-free integration [19, 49], etc. One could develop variations on these schemes that rely on reduced-order transport solutions for the intermediate steps, e.g., $\phi^p_1$ from line 4.

Alternatively, one could perform a high-fidelity solution at the end-of-step (EOS) after marching through with the predictor scheme presented in this work. Rather than use this high-fidelity solution as the next beginning-of-step (BOS) solution, the newly obtained microscopic cross sections could be used to interpolated during a corrector step. This would be similar to a standard predictor-corrector or the higher-order linear and quadratic interpolation schemes proposed in [18], but with the added benefit of using reduced-order transport solutions at the substeps. Work presented here and in the literature has shown that the additional high-fidelity solutions do provide a tangible benefit [14, 18], which could further improve the stability and accuracy of the hybrid depletion scheme.

6.4.3 Alternative reduced-order solutions

The primary reduced-order transport solution used in this work was based on perturbation-theory and required the fission matrix to be computed at each coarse step. As not every high-fidelity transport code may provide the fission matrix, it would be useful to explore additional reduced-order codes.

Nodal diffusion

Due to their rapid simulation time and decades of development, nodal diffusion codes are a strong candidate. Here a nodal diffusion code refers to a code that has limited geometric understanding, treating assemblies or potentially pin cells as homogenized volumes. Much like the spatial flux variation method used in this work, integrating a nodal diffusion code
would require reconstructing macroscopic cross sections at the substep, but for a larger region that may include several burnable regions. Additionally, non-burnable materials like moderating and cooling fluids, and structural materials may also contained in one homogenized region.

Furthermore, one would have to reconstruct potentially every macroscopic cross section used to represent the region. This would include absorption and fission neutron production $\nu \Sigma_f$, but also multi-group scattering cross sections, and either a transport cross sections or diffusion coefficient. One may be able to make empirical arguments that the transport cross section or diffusion coefficient for some problems are less dependent on the fuel than moderating materials. Nonetheless, the reconstruction of macroscopic cross sections will be more involved than with the spatial flux variation (SFV) method.

Finally, the diffusion code of choice may be required to return pin or sub-pin level scalar fluxes to compute the microscopic reaction rates. This could be facilitated through the use of form factors relating the fine-resolution flux to the nodal flux provided by the diffusion code. The use of more elaborate reconstruction methods using expansion functions could be beneficial.

*Deterministic transport*

Nodal diffusion codes may be problematic when obtaining the local fluxes necessary for pin-level depletion as parts of the geometry have been homogenized. One could create a model that represents each pin cell as a homogenized region, but such small domains push the limits of diffusion theory. Additional reconstructions would still be necessary to compute properties for sub-pin regions, i.e., radial rings in a gadolinia pin.

The use of deterministic transport could be able to handle these small domains with greater accuracy than nodal diffusion. One still must update cross sections inside the sub-step like with the nodal diffusion and SFV method, but this would be limited to the burnable regions only.
6.4.4 Multi-physics coupling

There is a large push towards coupling transport solutions with additional physics, with thermal-hydraulic (TH) being arguably the dominant field of interest. Previously, if one was to perform coupled depletion-neutronics-TH analysis, the existing time step trade-off still exists: small enough for accuracy and stability, but large enough for reasonable computational times. Additionally, each point in calendar time now requires potentially many coupled neutronics-TH simulations.

The scheme presented in this work allows the simulated life of a problem to approach a time-continuous model, as fluxes and compositions are able to be computed with very fine temporal resolution. One could also compute TH quantities of interest (e.g., coolant and temperature profiles) using this fine time scale by coupling a TH solver at each substep. At the coarse step, one could iterate between continuous energy Monte Carlo and computational fluid dynamics to convergence. At each substep, reduced-order transport and TH solutions (e.g., hot-channel or equivalent model) could be performed.

The framework that was written for this research could be used to facilitate this coupling. Indeed, there is nothing that requires the high-fidelity and reduced-order solver interfaces to perform only neutron transport. So long as necessary depletion data can be retrieved from these coupled interfaces, the routines provided by the framework should facilitate the time-integration. Therefore additional solver interfaces could be developed to perform coupled transport-TH simulations before the framework depletes and advances in time.
Appendices
APPENDIX A
SUPPLEMENTARY NUCLEAR DATA

Table A.1 contains a set of branching ratios $\beta_{i,g}$ for $(n, \gamma)$ reactions. Parent isotopes are provided with the fraction of capture events that produce a ground state nuclide. These values are the default branching ratios used in Serpent, and can be found at http://serpent.vtt.fi/mediawiki/index.php/Default_isomeric_branching_ratios.
Table A.1: Thermal-spectrum neutron capture to ground ratios

|   | 23Na | 37Cl | 45Sc | 59Co | 72Ge | 74Ge | 76Ge | 76Se | 78Se | 80Se | 82Se | 82Se | 85Br | 87Br | 98Kr | 98Kr | 98Kr | 98Sr | 98Sr | 99Y | 99Y | 103Nb | 103Nb | 105Rh | 105Rh | 106Pd | 108Pd | 110Pd | 117Ag | 119Ag | 119Cd | 112Cd |
|---|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
|   | 0.232 00 | 0.880 90 | 0.556 00 | 0.444 00 | 0.501 20 | 0.666 00 | 0.400 50 | 0.740 90 | 0.117 80 | 0.845 40 | 0.140 20 | 0.768 70 | 0.091 40 | 0.970 40 | 0.603 10 | 0.333 00 | 0.183 90 | 0.879 10 | 0.253 00 | 0.198 80 | 0.997 90 | 0.749 60 | 0.310 10 | 0.961 00 | 0.997 80 | 0.952 70 | 0.977 90 | 0.850 00 | 0.989 80 | 0.954 00 | 0.994 50 | 0.868 50 |
|   | 114Cd | 116Cd | 113In | 112Sn | 116Sn | 118Sn | 120Sn | 122Sn | 124Sn | 126Sn | 121Sb | 120Te | 122Te | 124Te | 126Te | 129I | 131I | 124Xe | 126Xe | 128Xe | 130Xe | 132Xe | 133Xe | 134Xe | 133Cs | 134Cs | 135Cs | 132Ba | 130Ba | 132Ba | 134Ba |
|   | 0.881 20 | 0.666 00 | 0.419 10 | 0.725 30 | 0.956 80 | 0.979 40 | 0.987 50 | 0.011 20 | 0.037 50 | 0.301 80 | 0.936 90 | 0.887 10 | 0.644 80 | 0.991 20 | 0.868 90 | 0.413 00 | 0.983 90 | 0.830 00 | 0.869 10 | 0.892 30 | 0.916 40 | 0.886 70 | 0.960 00 | 0.985 30 | 0.907 00 | 0.996 00 | 0.984 00 | 0.887 10 | 0.917 50 | 0.926 30 |
APPENDIX B
NOTES FOR CHEBYSHEV RATIONAL APPROXIMATION METHOD

The routine for applying the incomplete partial factorization variation of CRAM was originally presented in [16]. A small typo exists in the algorithm presented, with the resolved version appearing outside of a publication in the OpenMC openmc.deplete library\(^1\) [4]. Algorithm 4 reproduces the algorithm for completeness.

**Algorithm 4** Implementation of the IPF form of CRAM [16]

<table>
<thead>
<tr>
<th>Require:</th>
<th>( \vec{N}_0, A, \Delta t )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \vec{\tilde{N}} \leftarrow \vec{N}_0 )</td>
<td></td>
</tr>
<tr>
<td>for ( n \leftarrow 1, k/2 ) do</td>
<td></td>
</tr>
<tr>
<td>( \vec{\tilde{N}} \leftarrow \vec{\tilde{N}} + 2 \text{Re} (\tilde{\alpha}_n (A \Delta t - \theta_n I)^{-1}) \vec{\tilde{N}} )</td>
<td></td>
</tr>
<tr>
<td>end for</td>
<td></td>
</tr>
<tr>
<td>return ( \alpha_0 \vec{\tilde{N}} )</td>
<td></td>
</tr>
</tbody>
</table>

The CRAM solvers used by both openmc.deplete and the custom framework presented in this work are built using sparse linear algebra solvers provided by the scipy.sparse package [40]. The solvers are indeed shared between the codes, originally written by Colin Josey for [14, 49] and then modified by the author in a later revision of OpenMC\(^2\).

---

\(^1\)https://docs.openmc.org/en/latest/methods/depletion.html#matrix-exponential

\(^2\)https://github.com/openmc-dev/openmc/pull/1356
APPENDIX C

UO₂ TEST PIN SPECIFICATIONS

Table C.1: Fuel pin compositions for UO₂ pin

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Atom density [atoms/b/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>¹⁶O</td>
<td>4.639 171 60 × 10⁻²</td>
</tr>
<tr>
<td>²³⁴U</td>
<td>9.342 261 00 × 10⁻⁶</td>
</tr>
<tr>
<td>²³⁵U</td>
<td>1.045 213 00 × 10⁻³</td>
</tr>
<tr>
<td>²³⁶U</td>
<td>4.787 577 60 × 10⁻⁶</td>
</tr>
<tr>
<td>²³⁸U</td>
<td>2.214 531 00 × 10⁻²</td>
</tr>
</tbody>
</table>

Density [g/cm³] 10.40

Table C.2: Simulation properties for UO₂ pin problem

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel radius</td>
<td>0.392 176</td>
<td>cm</td>
</tr>
<tr>
<td>Cladding outer radius</td>
<td>0.457 20</td>
<td>cm</td>
</tr>
<tr>
<td>Pin pitch</td>
<td>1.26</td>
<td>cm</td>
</tr>
<tr>
<td>Total power</td>
<td>6368</td>
<td>W</td>
</tr>
<tr>
<td>Height</td>
<td>360</td>
<td>cm</td>
</tr>
</tbody>
</table>
Coolant density coefficients and profile presented in Table D.1 and Figure D.1 were originally given as tabulated properties for a similar geometry by Stefano Terlizzi. The data were originally given across 20 equally spaced layers and have been fit to a third degree polynomial.

Table D.1: Polynomial coefficients for coolant density profile. When given axial height $z$ in cm, yields coolant density in $g/cm^3$

<table>
<thead>
<tr>
<th></th>
<th>$z^3$</th>
<th>$z^2$</th>
<th>$z$</th>
<th>Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$1.90224615 \times 10^{-9}$</td>
<td>$-1.01435388 \times 10^{-6}$</td>
<td>$-6.462708 \times 10^{-5}$</td>
<td>$7.65581437 \times 10^{-1}$</td>
</tr>
</tbody>
</table>

Table D.2: Fuel compositions for supercell model. Replicated from Tables 4, 5, and 8 from [47]

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Atom density [atoms/b/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3.4 wt% center</td>
</tr>
<tr>
<td>$^{16}\text{O}$</td>
<td>$4.6108 \times 10^{-2}$</td>
</tr>
<tr>
<td>$^{17}\text{O}$</td>
<td>$1.7564 \times 10^{-5}$</td>
</tr>
<tr>
<td>$^{234}\text{U}$</td>
<td>$6.4018 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{235}\text{U}$</td>
<td>$7.9681 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{238}\text{U}$</td>
<td>$2.2307 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

| Density [g/cm$^3$] | 10.31341 | 10.29748 | 10.31341 |
Figure D.1: Coolant density profile for supercell model. Coefficients given in Table D.1
Table D.3: Plenum and reflector compositions. Represents a 70/30% by weight mixing of steel and water

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Atom density [atoms/b/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1$H</td>
<td>$4.7165 \times 10^{-1}$</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>$2.3583 \times 10^{-1}$</td>
</tr>
<tr>
<td>$^{50}$Cr</td>
<td>$2.4673 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{52}$Cr</td>
<td>$4.758 \times 10^{-2}$</td>
</tr>
<tr>
<td>$^{53}$Cr</td>
<td>$5.3951 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{54}$Cr</td>
<td>$1.343 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{55}$Mn</td>
<td>$5.6687 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{54}$Fe</td>
<td>$1.1217 \times 10^{-2}$</td>
</tr>
<tr>
<td>$^{56}$Fe</td>
<td>$1.7738 \times 10^{-1}$</td>
</tr>
<tr>
<td>$^{57}$Fe</td>
<td>$4.2545 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{58}$Fe</td>
<td>$5.4149 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{58}$Ni</td>
<td>$1.7122 \times 10^{-2}$</td>
</tr>
<tr>
<td>$^{60}$Ni</td>
<td>$6.5978 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{61}$Ni</td>
<td>$2.8421 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{62}$Ni</td>
<td>$9.1398 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{64}$Ni</td>
<td>$2.329 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{90}$Zr</td>
<td>$5.9311 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{91}$Zr</td>
<td>$1.2934 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{92}$Zr</td>
<td>$1.977 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{94}$Zr</td>
<td>$2.0035 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{96}$Zr</td>
<td>$3.2278 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

**Density [g/cm$^3$]** 6.55
Table D.4: Zircaloy-4 cladding compositions for supercell. Reproduced from Table 16 [47]

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Atom density [atoms/b/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{16}$O</td>
<td>$3.07430 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{17}$O</td>
<td>$1.17110 \times 10^{-7}$</td>
</tr>
<tr>
<td>$^{50}$Cr</td>
<td>$3.29620 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{52}$Cr</td>
<td>$6.35640 \times 10^{-5}$</td>
</tr>
<tr>
<td>$^{53}$Cr</td>
<td>$7.20760 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{54}$Cr</td>
<td>$1.79410 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{54}$Fe</td>
<td>$8.66990 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{56}$Fe</td>
<td>$1.36100 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{57}$Fe</td>
<td>$3.14310 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{58}$Fe</td>
<td>$4.18290 \times 10^{-7}$</td>
</tr>
<tr>
<td>$^{90}$Zr</td>
<td>$2.18270 \times 10^{-2}$</td>
</tr>
<tr>
<td>$^{91}$Zr</td>
<td>$4.76010 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{92}$Zr</td>
<td>$7.27580 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{94}$Zr</td>
<td>$7.37340 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{96}$Zr</td>
<td>$1.18790 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{112}$Sn</td>
<td>$4.67350 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{114}$Sn</td>
<td>$3.17990 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{115}$Sn</td>
<td>$1.63810 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{116}$Sn</td>
<td>$7.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>$^{117}$Sn</td>
<td>$3.70 \times 10^{-5}$</td>
</tr>
<tr>
<td>$^{118}$Sn</td>
<td>$1.16690 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{119}$Sn</td>
<td>$4.13870 \times 10^{-5}$</td>
</tr>
<tr>
<td>$^{120}$Sn</td>
<td>$1.56970 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{122}$Sn</td>
<td>$2.23080 \times 10^{-5}$</td>
</tr>
<tr>
<td>$^{124}$Sn</td>
<td>$2.78970 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

**Density [g/cm$^3$]** | 6.55

Table D.5: Composition for air in instrumentation tube. Reproduced from Table 9 [47]

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Atom density [atoms/b/cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{16}$O</td>
<td>$5.2863 \times 10^{-6}$</td>
</tr>
<tr>
<td>$^{17}$O</td>
<td>$2.0137 \times 10^{-9}$</td>
</tr>
<tr>
<td>$^{14}$N</td>
<td>$1.9681 \times 10^{-5}$</td>
</tr>
<tr>
<td>$^{15}$N</td>
<td>$7.1899 \times 10^{-8}$</td>
</tr>
<tr>
<td>$^{12}$C</td>
<td>$6.7564 \times 10^{-9}$</td>
</tr>
<tr>
<td>$^{13}$C</td>
<td>$7.3076 \times 10^{-11}$</td>
</tr>
<tr>
<td>$^{36}$Ar</td>
<td>$7.8729 \times 10^{-10}$</td>
</tr>
<tr>
<td>$^{38}$Ar</td>
<td>$1.4844 \times 10^{-10}$</td>
</tr>
<tr>
<td>$^{40}$Ar</td>
<td>$2.3506 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

**Density [g/cm$^3$]** | 0.000616
REFERENCES


VITA

Andrew was born in Hillsboro, OR to Anthony and Ginger Johnson. After moving throughout the beautiful Pacific Northwest, he graduated from Stadium High School in Tacoma, WA in 2011. It was there his passion for nuclear energy was cemented, with much help from grandparents who seemed to be deeply and coincidentally connected to Pacific Northwest National Laboratory. Andrew obtained B.S. degrees in engineering and in physics from Northwest Nazarene University in Nampa, ID in 2015. It was there he met his wonderful wife Leeza before moving with her to the South for graduate school. At Georgia Institute of Technology, Andrew earned a M.S. in Nuclear and Radiological Engineering in May of 2018.