ORNL/TM-2016/57

Status Report on NEAMS PROTEUS/ORIGEN Integration



W. A. Wieselquist

February 18, 2016

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Reactor and Nuclear Systems Division

Status Report on NEAMS PROTEUS/ORIGEN Integration

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ACRONYMS

1D, 2D, 3D	one-, two-, three-dimensional
API	application programming interface
ATR	Advanced Test Reactor
CFD	computational fluid dynamics
CRAM	Chebyshev Rational Approximation Method
HDF5	Hierarchical Data Format, Version 5
MOC	method of characteristics
NEAMS	Nuclear Energy Advanced Modeling and Simulation
ODE	ordinary differential equation
ORIGEN	Oak Ridge Isotope Generation and Depletion Code
SAM	Sodium-cooled fast reactor Analysis Module
SFR	sodium-cooled fast reactor
SGAPI	Sub-Group API

ABSTRACT

The US Department of Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program has contributed significantly to the development of the PROTEUS neutron transport code at Argonne National Laboratory and to the Oak Ridge Isotope Generation and Depletion Code (ORIGEN) depletion/decay code at Oak Ridge National Laboratory. PROTEUS's key capability is the efficient and scalable (up to hundreds of thousands of cores) neutron transport solver on general, unstructured, three-dimensional finite-element-type meshes. The scalability and mesh generality enable the transfer of neutron and power distributions to other codes in the NEAMS toolkit for advanced multiphysics analysis. Recently, ORIGEN has received considerable modernization to provide the high-performance depletion/decay capability within the NEAMS toolkit. This work presents a description of the initial integration of ORIGEN in PROTEUS, mainly performed during FY 2015, with minor updates in FY 2016.

1. INTRODUCTION

The US Department of Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program has contributed significantly to the development of the PROTEUS neutron transport code at Argonne National Laboratory and to the Oak Ridge Isotope Generation and Depletion Code (ORIGEN) at Oak Ridge National Laboratory. This work presents a description of the initial integration of ORIGEN in PROTEUS.

The following sections serve to familiarize the reader with the PROTEUS-SN solver and ORIGEN and to introduce the basic variables and input where appropriate.

1.1 PROTEUS-SN

PROTEUS is actually a suite of neutron transport algorithms [2] able to solve neutron and gamma transport problems on large, unstructured finite element meshes. It includes the following solvers:

- S_N solver,
- P_N solver,
- general three-dimensional (3D) method of characteristics (MOC), and
- an experimental 2D/1D method based on MOC in 2D and P_N in a 1D axial geometry with special constraints of an "extruded" geometry/mesh, such that the domain is divided into axial "slices."

Like most of the current applications in NEAMS, this work utilizes the S_N solver, which is referred to as PROTEUS-SN. It is the most mature and scalable solver and thus is the workhorse for full system simulations (SHARP), which coupled PROTEUS to Nek 5000 (computational fluid dynamics) and Diablo (structural mechanics) through MOAB, as shown in Figure 1.

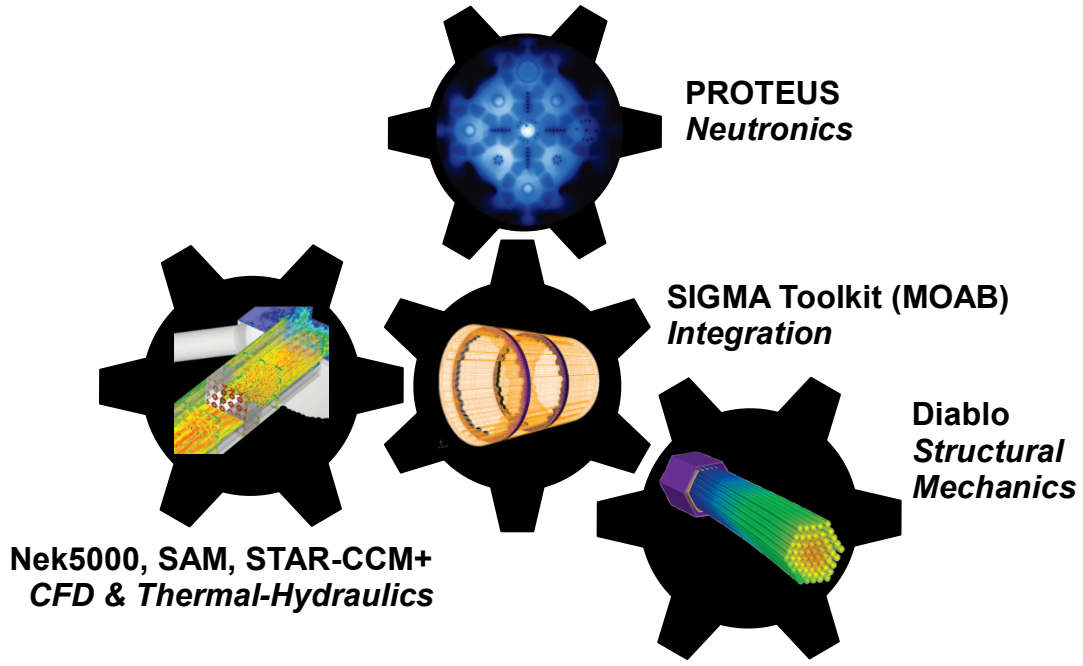


Figure 1. SHARP Framework for Reactor Physics.

A useful property of PROTEUS is the ability to produce Hierarchical Data Format Version 5 (HDF5) files containing the mesh and neutron and power distribution that can be natively imported in VisIt, a tool for high-performance visualization [4] using the "UNIC" plugin (the former name of PROTEUS). Figure 2 shows an example of a mesh generated for the Advanced Test Reactor (ATR), with scalar flux plots shown in Figure 3 (3D) and Figure 4 (2D overhead view).

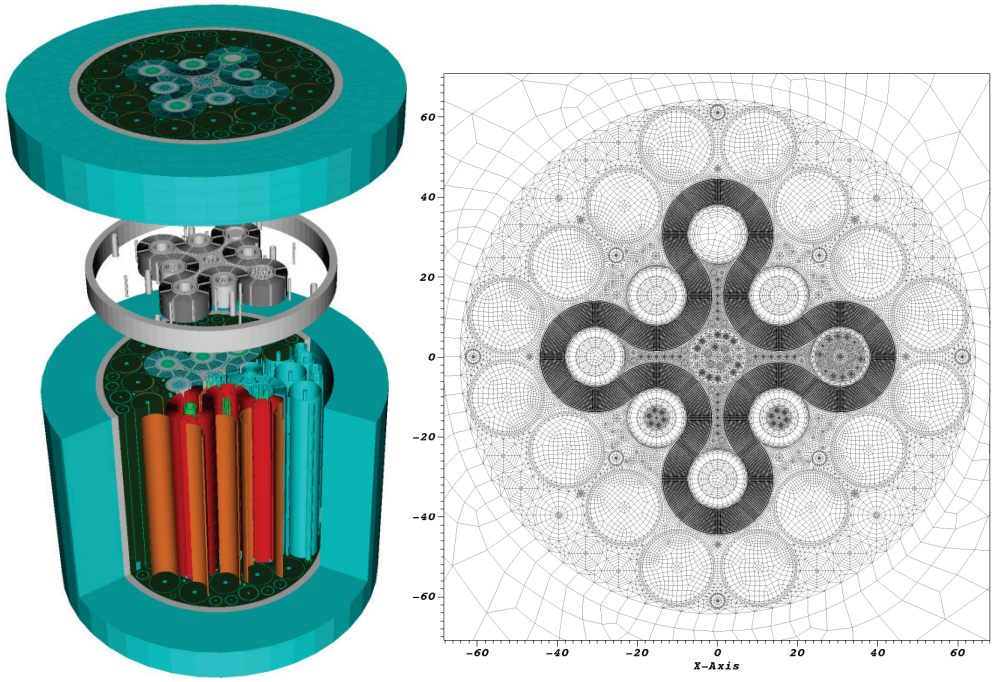


Figure 2. Visualization of 3D geometry and mesh used to analyze the Advanced Test Reactor with PROTEUS-SN.

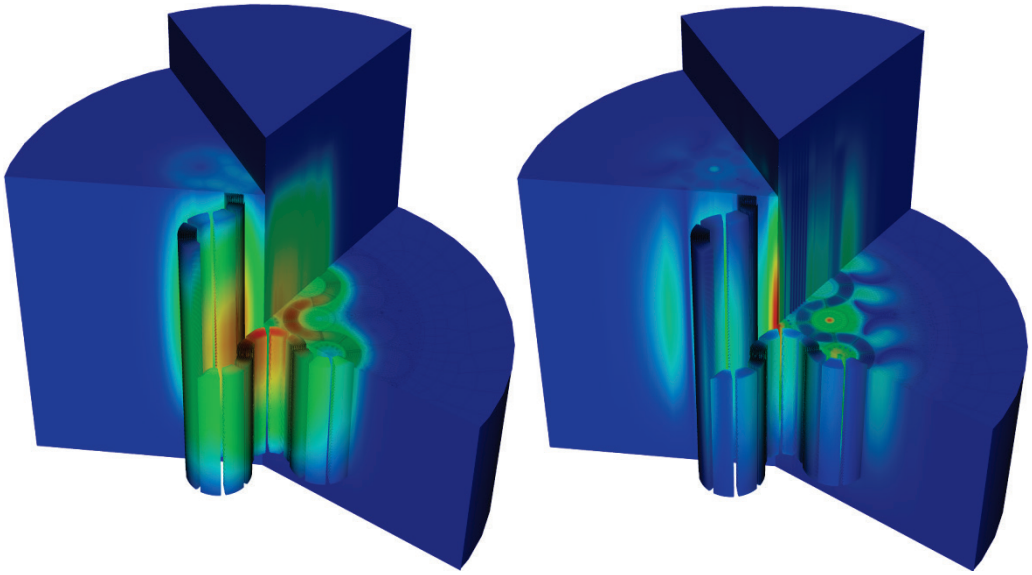


Figure 3. Advanced Test Reactor fast (left) and thermal (right) flux calculated by PROTEUS-SN.

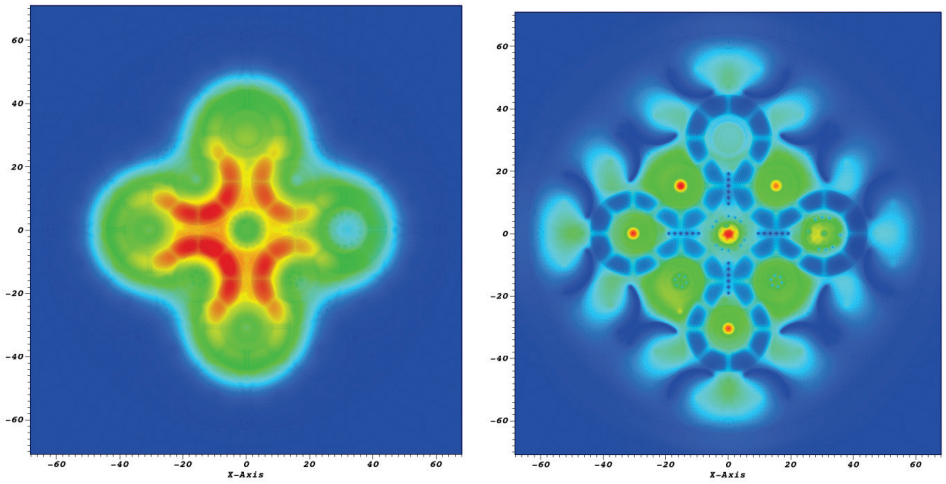


Figure 4. Advanced Test Reactor fast (left) and thermal (right) flux calculated by PROTEUS-SN for a 2D calculation.

Additional capabilities of PROTEUS-SN include the capability to solve both fixed-source and eigenvalue problems in forward and adjoint modes. The principal solution of the PROTEUS-SN code is the multigroup angular flux at all finite element vertices. For the purposes of coupling to depletion, a larger region called a "block" or "material" is defined, which is a collection of finite elements that have the same cross-section data. The material-average scalar flux is defined as

$$\Phi_m^g = \frac{1}{\sum_{e \in m} V_e} \sum_{e \in m} V_e \sum_{k \in e} f_k \sum_n w_n \Psi_{kn}^g, \tag{1}$$

where the weights w_n are the angular cubature weights for direction index n and angular flux Ψ_{kn}^{g}, at finite element vertex k with integration weight f_k, for a finite element e, with volume V_e, for all elements in material/block m.

The PROTEUS code has three ways to determine multigroup cross sections [3].

1. a static set of cross sections can be read from a standard ISOTXS binary library file,
2. a static set of cross sections can be read from a special ANLXS text file and converted to ISOTXS, or
3. the Sub-Group API (SGAPI) in SHARP can be used for on-the-fly cross-section calculations.

1.2 ORIGEN

ORIGEN has been used to model nuclide transmutation for over 40 years. It has the capability to generate source terms for accident analyses, characterize used fuel (including activity, decay heat, radiation emission rates, and radiotoxicity), activate structural materials, and perform fuel cycle analysis studies [5,6]. This wide range of applications is possible because the guiding principle has been to explicitly simulate all decay and neutron reaction pathways using the best available data and to rigorously validate the result vs experiment. ORIGEN has been subject to hundreds of validation cases [7] using measured data from the destructive isotopic assay of spent fuel, decay heat of spent fuel, gamma spectra resulting from burst fission, and neutron spectra resulting from spontaneous fission and *(α,n)* reactions.

An active modernization has taken place over the last few years [8], and the ORIGEN depletion/decay module has received extensive improvement, including an application programming interface (API) for both C++ and Fortran with modern object-oriented design and various solver enhancements. This paper highlights the API capabilities that are currently available for embedding ORIGEN depletion calculations in other codes [9].

1.2.1 Overview

The fundamental purpose of ORIGEN and the new API is to solve the following system of ordinary differential equations (ODEs) describing the depletion/decay phenomena:

$$\frac{d\vec{n}_m}{dt} = (\boldsymbol{A}_{\phi m}\Phi_m + \boldsymbol{A}_{\lambda})\vec{n}_m(t) + \vec{S}_m(t), \tag{2}$$

where

- m is a material index,
- $\vec{n}_m$ is the nuclide number density vector for material m (*atoms/barn-cm*),
- $\boldsymbol{A}_{\phi m}$ is the transition matrix for the reaction transitions (*barns* or cm^2),
- Φ_m is the scalar flux magnitude ($1/cm^2 s$),
- $\boldsymbol{A}_{\lambda}$ is the transition matrix for decay transitions (*1/s*), and
- $\vec{S}_m$ is an external source.

The ORIGEN API solves the above system of ODEs for large systems (thousands of nuclides/tens of thousands of transitions). In traditional coupling to neutron transport codes, a quasi-static approximation is used to approximate the evolution of the system with time, where

- the steady-state, transport eigen-problem or fixed-source problem is solved at time *points*, (with appropriate problem-dependent self-shielding of cross sections) and

- the depletion equations of Eq. (2) are solved over each time *step*.

In typical coupled transport/depletion simulations, the a fixed amount of initial material is present in each depletable zone and the external source $\vec{S}_m(t)$ (i.e., feed of material into the volume) is zero.

1.2.2 Transition Representation

A visualization of the full transition matrix, $\boldsymbol{A} = \boldsymbol{A}_\phi + \boldsymbol{A}_\lambda$, for ~1200 fission products is shown in Figure 5; a zoomed-in view of Xe-135 is shown in Figure 6. Solid colored lines are used for reaction transitions, and dashed green lines are used for decay transitions.

The decay portion, $\boldsymbol{A}_\lambda$, of the transition matrix is given by row as

$$a_{\lambda,ii'} \stackrel{\text{def}}{=} \begin{cases} \gamma_{d,i\leftarrow i'}\lambda_{d,i'} & \text{for } i \neq i' \\ -\sum_d \lambda_{d,i} & \text{for } i = i' \end{cases} \tag{3}$$

where *d* indicates a decay mode, the top term (off-diagonal) represents gains of nuclide *i* due to decay mode *d*, and the bottom term (diagonal) represents the loss of nuclide *i* due to all decay modes. The decay portion is independent of material *m*.

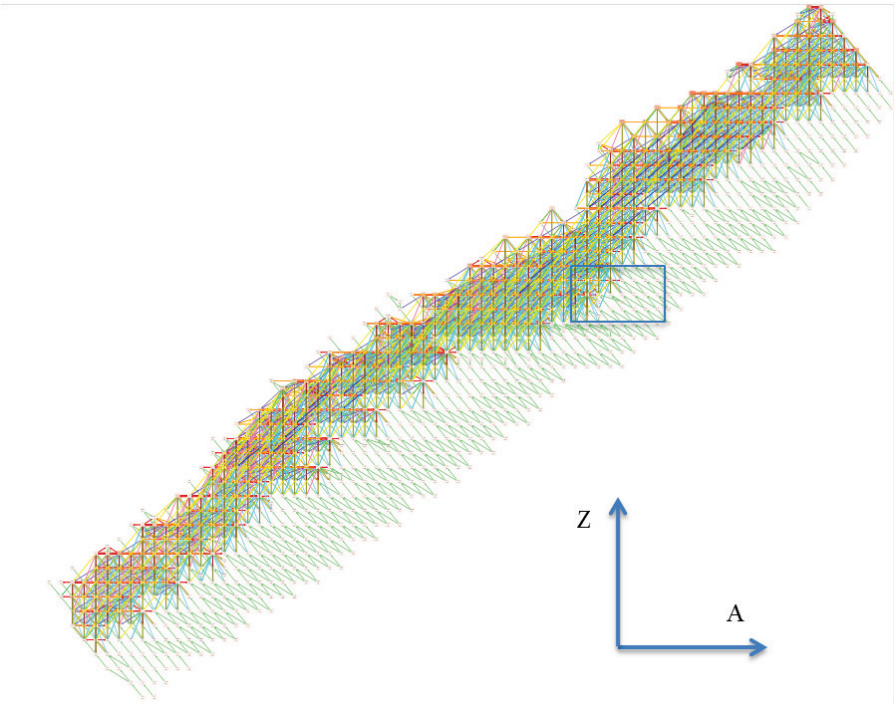


Figure 5. Visualization of the transition matrix for fission products.

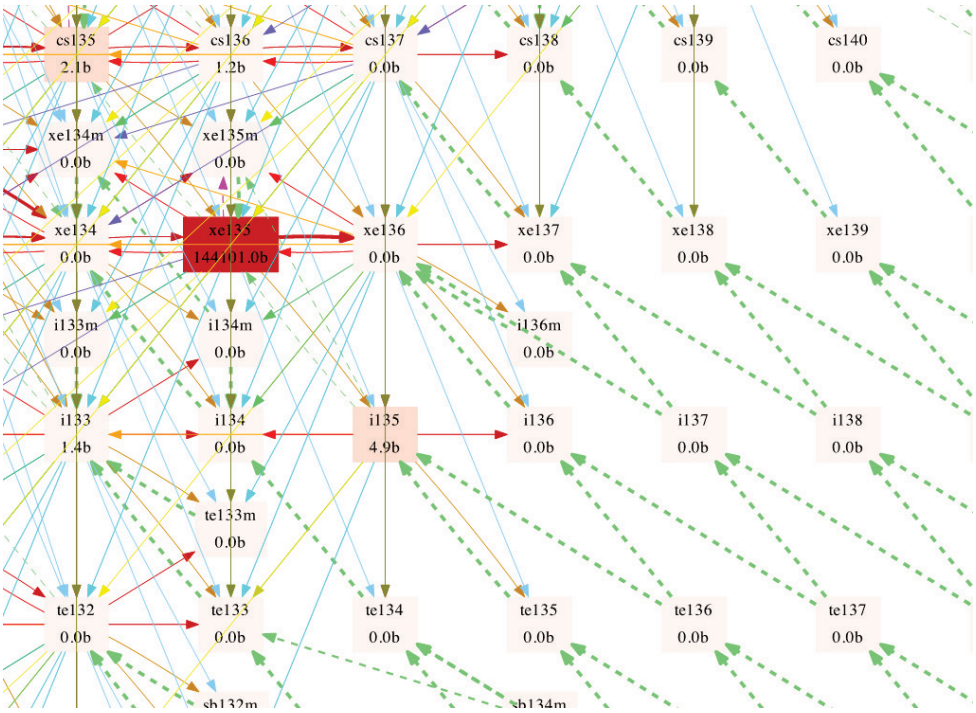


Figure 6. Visualization of the transition matrix zoomed in around Xe-135.

The reaction part is treated in essentially the same way, with the off-diagonal entries in the matrix $\boldsymbol{A}_{\phi m}$ defining the creation of nuclide i from reaction transitions of all other nuclides i'. The structure of each row of $\boldsymbol{A}_{\phi m}$ is

$$a_{\phi m,ii'} \stackrel{\text{def}}{=} \begin{cases} \gamma_{xm,i\leftarrow i'}\sigma_{xm,i'} & \text{for } i \neq i' \\ -\sum_{x} \sigma_{xm,i} & \text{for } i = i' \end{cases} \tag{4}$$

where the top term (off-diagonal) represents gains of nuclide i due to reaction type x and the bottom term (diagonal) represents the loss of nuclide i due to all reaction mechanisms. The gain term is convenient to represent in terms of "yield," $\gamma_{xm,i\leftarrow i'}$, and reaction cross section, $\sigma_{xm,i'}$.

The use of a "yield" γ is convenient for modeling not only fission (where it is a necessity) but also for modeling isomeric branching and by-product production. For example, in an isomeric-branching model in which the (n,γ) reaction cross section of U-234 is 1 barn and both U-235 (99%) and U-235m (1%) are produced, ORIGEN would have $\sigma_{(n,\gamma),U4} = 1\ barn$, $\gamma_{(n,\gamma),U5m\leftarrow U4} = 1\%$, and $\gamma_{(n,\gamma),U5\leftarrow U4} = 99\%$, indicating that 1% of the reactions go to the first metastable state of U-235 and 99% go directly to the ground state. Byproduct protons, deuterons, tritons, helions (He-3), and alphas emitted in reaction/decay transitions are tracked by ORIGEN explicitly with yield the multiplicity of the product; for example, an (n,α) reaction results in a gain term for the alpha by-product of $\gamma_{(n,\alpha),\alpha\leftarrow *} = 1$, and an $(n,2\alpha)$ reaction results in $\gamma_{(n,2\alpha),\alpha\leftarrow *} = 2$, with "*" indicating validity for any parent nuclide. In the case of fission and isomeric reaction transitions, the yield is dependent on the neutron spectrum. For by-products, the yield is a constant. ORIGEN contains an extensive multigroup reaction cross-section library based on JEFF/3.1-A with more than 12,000 cross sections for the following reactions: *(n,2n), (n,3n), (n,f), (n,nα), (n,n3α),*

(n,2nα), (n,3n α), (n,np), (n,n2α), (n,2n2α), (n,nd), (n,nt), (n,n ^{3}He), (n,nd2α), (n,nt2α), (n,4n), (n,g), (n,p), (n,d), (n,t), (n,^{3}He), (n,α), (n,2α), (n,3α), (n,2p), (n,pα), (n,t2α), (n,d2α), (n,n'). In typical activation problems, where self-shielding is not important, given a multigroup neutron flux spectrum, the JEFF library is sufficient to calculate the one-group cross sections and yields needed to perform transmutation calculations.

Given the groupwise neutron spectrum ϕ_m^g, where *g* is the multigroup energy index, the one-group cross sections used by ORIGEN are calculated with standard flux weighting:

$$\sigma_{xm,i} = \frac{\sum_g \sigma_{xm,i}^g \phi_m^g}{\sum_g \phi_m^g} \tag{5}$$

For isomeric reaction branching, energy-dependent yields are calculated as

$$\gamma_{xm,i\leftarrow i'} = \frac{\sum_g \gamma_{x,i\leftarrow i'}^g \sigma_{x,i}^g \phi_m^g}{\sigma_{x,i}}, \tag{6}$$

where the multigroup yield term, $\gamma_{x,i\leftarrow i'}^g$, and weighting cross section, $\sigma_{x,i}^g$, are contained on the JEFF library and are independent of material. For fission yields, the average energy of fission is calculated and linear interpolation is performed on yields tabulated at one to three discrete energy points,

$$\gamma_{fm,i\leftarrow i'} = interp(E_{fm,i'}, \gamma_{f,i\leftarrow i}(E_1), \gamma_{f,i\leftarrow i}(E_2), \dots) \tag{7}$$

where the average energy of fission in actinide *i'*, which creates fission products *i*, is given as

$$E_{fm,i'} = \frac{\sum_g \bar{E}_g \sigma_{fm,i}^g \phi_m^g}{\sum_g \sigma_{fm,i}^g \phi_m^g}, \tag{8}$$

where $\bar{E}_g$ is some average energy for group *g* that depends only on the group structure.

1.2.3 Time Approximation

To resolve the no-linear dependence of the depletion/decay model in Eq. (2) on the evolution of the transport flux in time, the reaction transition matrix and flux magnitude are fixed at some known "average" value, $\bar{\boldsymbol{A}}_{\phi m,j}$ and $\bar{\Phi}_{m,j}$,

$$\begin{gathered} \frac{d\vec{n}_m}{dt} = \left(\bar{\boldsymbol{A}}_{\phi m,j}\bar{\Phi}_{m,j} + \boldsymbol{A}_\lambda\right)\vec{n}_m(t), \\ \text{over step } t_j \le t \le t_{j+1}, \\ \text{with initial condition } \vec{n}_m(t_j) = \vec{n}_{m,j}. \end{gathered} \tag{9}$$

where

- $\bar{\Phi}_{m,j}$ is the step-average material flux (*1/cm^{2}s*) and

- $\overline{\boldsymbol{A}}_{\phi m,j}$ is the step-average reaction transition matrix (*barns*).

The representation in Eq. (9) assumes that the flux magnitude, $\overline{\Phi}_{m,j} = \sum_g \Phi_{m,j}^g$, will be available as a result of the transport calculation, which produces multigroup fluxes $\Phi_{m,j}^g = \Phi_m^g(t_j)$ at each transport solution time. The simple "predictor" (or explicit) approximation used in the current PROTEUS/ORIGEN coupling assumes that $\overline{\Phi}_{m,j} = \Phi_{m,j}$ and $\overline{\boldsymbol{A}}_{\phi m,j} = \boldsymbol{A}_{\phi m,j}$ (i.e., the average is approximated as the standard beginning-of-step value).

2. IMPLEMENTATION

The current implementation relies on the ISOTXS multigroup cross-section library format for PROTEUS-SN's cross-section data. This leads to the following important limitations in the current ORIGEN coupling.

- The user must provide a mapping of (arbitrary) ISOTXS nuclide labels to standard (ORIGEN) nuclide identifiers (IDs). This requires knowledge of the labels contained on the binary ISOTXS library and the nuclides to which they correspond. In many cases, this is as simple as mapping "U235_H" on the ISOTXS library to ORIGEN's "U235," but because the ISOTXS label is truly arbitrary, there can be labels such as "P9" or "LP," and an automatic conversion cannot be ensured to be correct (or detected when it fails).

- Elements such as "FE" and "NA" are not split into constituent nuclides because cross sections only exist for the element in the ISOTXS library and ORIGEN cannot currently update its nuclide-based reaction rates based on elemental reaction rates.

- A single, static system power value (total watts produced by the system) is allowed.

- Feedback of updated depletion isotopics to macroscopic transport cross sections is only performed for the nuclides that have been defined in the initial material. This is because the cross section-to-material mapping is performed when the input is read and data structures are distributed to all processes for the parallel computation. This is the only time such a send is allowed, and all data that are not needed are deleted.

Isotopics are currently not available on the HDF5 output file produced by PROTEUS.

2.1 DEPLETION INPUT

The PROTEUS input processor was modified to read depletion input similarly to the kinetics input, where the main input is read on "unic.inp" (see example in Figure 7), and additional input for the kinetics problem is read from "kinetics.inp." In the case of depletion, the additional input is called "depletion.inp" (an example is shown in Figure 8). A currently inconvenient feature of the input is the requirement for the user to define the mapping of cross-section nuclide names to actual names with multiple "NUCLIDE_ALIAS" commands. An example of a material assignment file is shown in Figure 9. Table 1 shows the complete set of input controls allowed in the "depletion.inp" file, with a table style consistent with other input definitions in the PROTEUS-SN user manual [3].

```
SN_TYPE                  LEG-TCHEBY
Theta_Resolution         2
Phi_Resolution           2
SEGMENT_ANGLE            2

DEBUG_PRINT_LEVEL         0
DEBUG_PRINT_SETUP         0
DEBUG_PRINT_FORMATION     0
DEBUG_PRINT_OUTER         0

THERMAL_POWER             1.0e2 !Watts

Scattering_Order          0
Tolerance_eigenvalue      1.0e-3
Tolerance_Fission         1.0e-3
Tolerance_Flux            1.0e-3

Iterations_Fission        400
Iterations_MaxUpScatter   5
Iterations_MinUpScatter   1
Iterations_scattering     20
Iterations_SA_CG          100
Iterations_PETSc          1000

SOURCEFILE_MESH           bench.ascii
SOURCEFILE_XS             bench_3g.anlxs
SOURCEFILE_MATERIAL       initial.assignment
```

Figure 7. Example of PROTEUS-SN main input (file "unic.inp").

```
INITIAL_MATERIAL_FILE    initial.assignment
DEPLETION_SOLVER ORIGEN_CRAM ! or ORIGEN_MATREX

TRANSITION_DEFINITION "/scale/scale_dev_data/origen_library/pwr.rev02.orglib"
REACTION_RESOURCE "/scale/scale_dev_data/origen.rev01.jeff252g"
YIELD_RESOURCE "/scale/scale_dev_data/origen_data/origen.rev05.yields.data"

! depletion time(s) ndiv    output files
TIME_STEP    8.64e4    1    step01.h5   step01.out    !1 day
TIME_STEP    8.64e5    1    step02.h5   step02.out    !10 days
TIME_STEP    8.64e6    3    step03.h5   step03.out    !100 days

!mapping of names of cross sections to names of nuclides for depletion
!              ISOTXS   actual
NUCLIDE_ALIAS      P9    pu239
NUCLIDE_ALIAS    O-16      o16
NUCLIDE_ALIAS    B-10      b10
NUCLIDE_ALIAS   U8__H     u238

EXPORT_ISOTOPICS isotopics.out
```

Figure 8. Example of PROTEUS-SN depletion input (file "depletion.inp").

```
! Material Definitions for C1P, C1, C2, AB, RB, RE, RD, RC
MATERIAL_DEF  C1P  PU239  0.0008    U238  0.0064   NA    0.0104    FE    0.0181    O-16   0.0149   !  0.050900
MATERIAL_DEF  C1   PU239  0.0008    U238  0.0064   NA    0.0104    FE    0.0181    O-16   0.0149   !  0.050900
MATERIAL_DEF  C2      P9  0.0008    U238  0.0054   NA    0.0110    FE    0.0181    O-16   0.0138   !  0.049800
MATERIAL_DEF  AB   U8__H  0.0080    NA    0.0088   FE    0.0244    O-16  0.0160                     !  0.057200
MATERIAL_DEF  RB   U8__H  0.0145    NA    0.0066   FE    0.0173    O-16  0.0290                     !  0.067400

! Assignment of materials to regions (regions names are defined by mesh)
REGION_ALIAS R_BLAN   RB
REGION_ALIAS R_CORE1  C1
REGION_ALIAS R_CORE2  C2

! Assignment of material properties to regions (MATERIAL_DEF interpreted as atom fractions)
REGION_PROPERTY R_BLAN    ATOM_DENSITY  0.067400
REGION_PROPERTY R_CORE1   ATOM_DENSITY  0.050900
REGION_PROPERTY R_CORE2   ATOM_DENSITY  0.049800
```

Figure 9. Example of PROTEUS-SN assignment input (file "initial.assignment").

Table 1. Auxiliary input controls for "depletion.inp"

Keyword	Input data	Default value	Function
INITIAL_MATERIAL_FILE	<Filename> <128 Character Name>	NO	Loads the initial material assignment file.
DEPLETION_SOLVER	ORIGEN_CRAM or ORIGEN_MATREX	NO	Whether to use Chebyshev Rational Approximation Method (CRAM) or legacy Matrix Exponential Method (MATREX).
TRANSITION_DEFINITION	<Filename> <128 Character Name>	depletion.td	Definition of the nuclides and transition to be included in the depletion problem. Basically, the sparsity pattern referred to in Eq. (4).
REACTION_RESOURCE	<Filename> <128 Character Name>	depletion.rr	A multigroup cross-section database for auxiliary reaction transition calculations. Basically, the data set referred to in Eq. (5).
YIELD_RESOURCE	<Filename> <128 Character Name>	depletion.yr	An energy-dependent fission yield file. Basically, the data set referred to in Eq. (6) and Eq. (7).
TIME_STEP	<Value> <Value> <Filename.out> <Filename.h5>	NO	Create a time step. First <Value> is length of the time step (seconds), second the number of substeps, and then (optionally) the name of an HDF5 dump file (.h5 extension) or region-wise edit file (.out extension).
NUCLIDE_ALIAS	<ISOTXS> <actual>	NO	Define a mapping from a nuclide name in the cross-section library to an actual nuclide, using the form "<e><a><m>," where <e> is the element symbol, <a> is the mass number, and <m> is the (optional) metastable indicator (e.g., "u235" or "am242m").
EXPORT_ISOTOPICS	<128 Character Name>	isotopics.out	

2.2 TEST PROBLEM

The test problem is a simplified model of a sodium-cooled fast reactor (SFR) core, taken from the SHARP/PROTEUS repository ("modules/unic/src/verification/SN2ND_Kinetics/bench07") and modified to include depletion. The test uses a three-group ANLXS[1] cross-section library with microscopic cross sections for U-238, Pu-239, Pu-240, Pu-241, O-16, and B-10 nuclides and group boundaries of 10 MeV, 800 keV, 80 keV, and 0.4 eV. Thus only updated number densities for these isotopes feed back into the transport code, although there are isotopic results from ORIGEN available for the full set of ~1200 isotopes. Notably missing from the library are fission products, so the eigenvalue will be considerably higher in this test than it should be. The geometry and mesh of the northeast quadrant are shown in Figure 10 (i.e., the *x*-axis and *y*-axis are lines of symmetry.

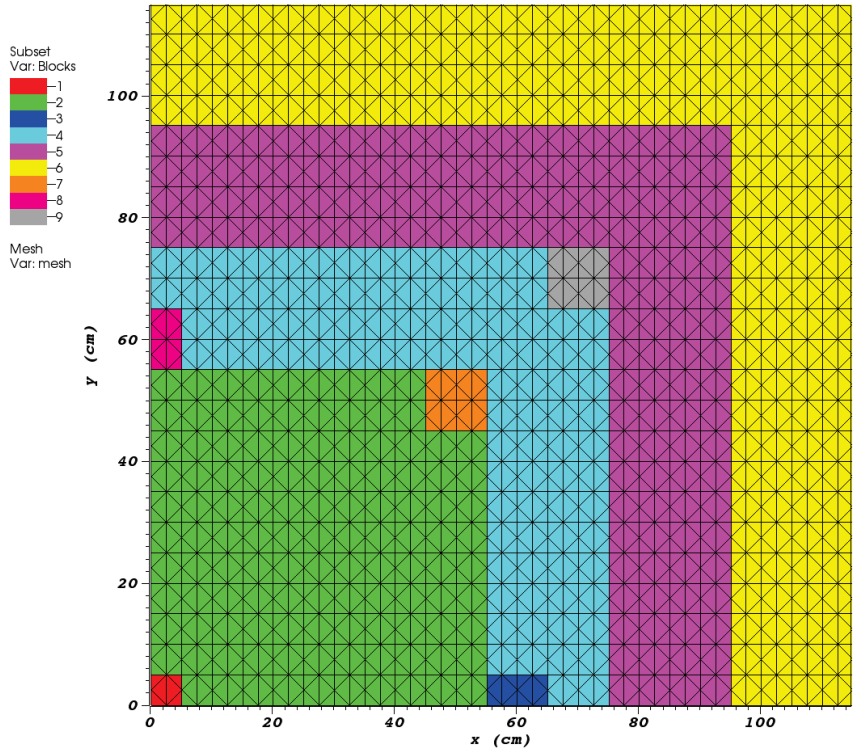


Figure 10. Simplified SFR test problem mesh and materials.

The nine materials in the problem are described in Table 2. The center rods and the rods on the *x*- and *y*-axes are inserted. The system is operated for 1157 days, in ten time steps of 115.7 days (1e7 seconds). The two fuel regions are homogenized with the coolant.

2.2.1 Results

The eigenvalue is shown in Figure 11, and scalar flux is shown in Figure 12 for each material. The power distribution as a function of time is shown in Figure 13. The absorption rate as a function of time is shown in Figure 14. The flux distributions are shown in Figure 15.

[1] The ANLXS library is a simple text format with the same information as the ISOTXS binary, converted to ISOTXS internally by PROTEUS-SN.

Table 2. Problem materials

Name	Description	Composition	Location	Color (see Figure 10)
R_REFL	Radial reflector	Na, Fe	Outermost	Yellow
R_BLAN	Radial blanket	U-238, O-16, Na, Fe	Next outermost	Magenta
R_CORE1	Inner fuel region	U-238, Pu-239, Na, Fe, O-16	Innermost	Green
R_CORE2	Outer fuel region	U-238, Pu-239, Na, Fe, O-16	Next innermost	Cyan
R_ROD1	Inserted control rod	Na, Fe, O-16, B-10, C	Origin	Red
R_ROD2	Inserted control rod	Na, Fe, O-16, B-10, C	*y*-axis	Pink
R_ROD3	Withdrawn control rod	Na	Along diagonal *y*=*x*, on edge of inner fuel region	Orange
R_ROD4	Withdrawn control rod	Na	Along diagonal *y*=*x*, on edge of outer fuel region	Grey
R_ROD5	Inserted control rod	Na, Fe, O-16, B-10, C	*x*-axis	Blue

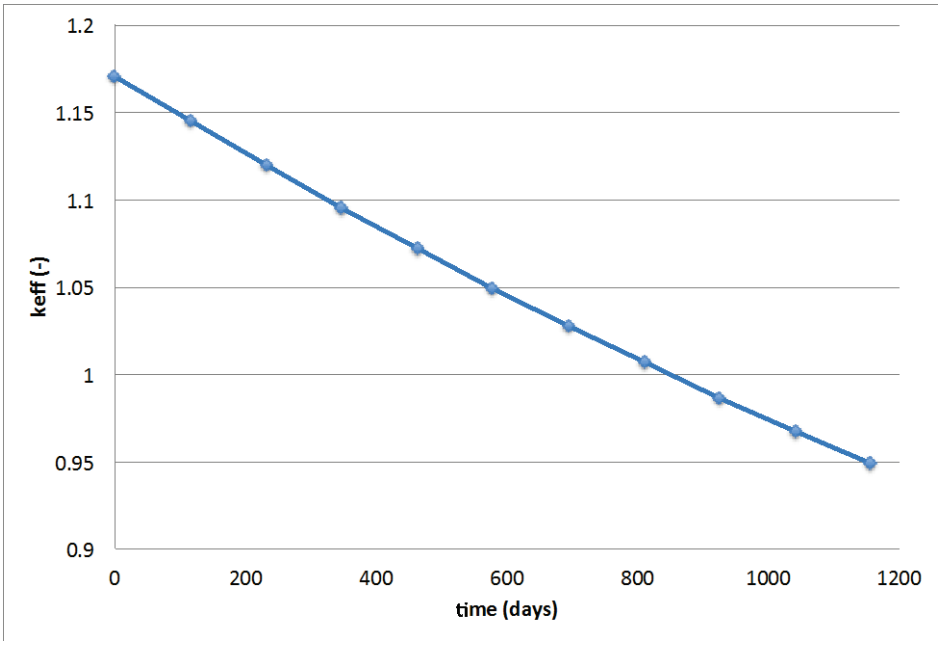


Figure 11. Eigenvalue for simple SFR problem.

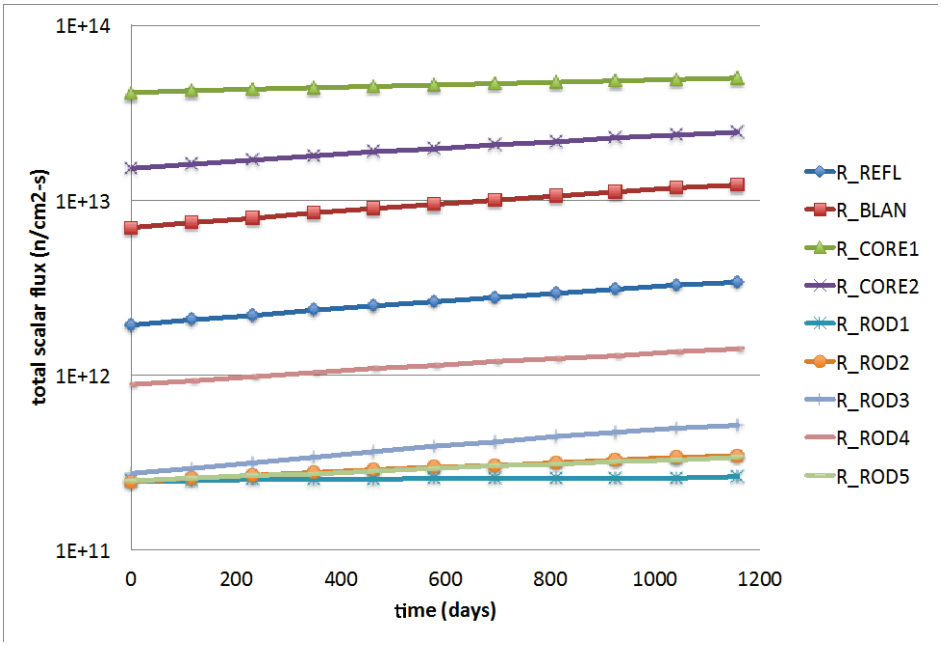
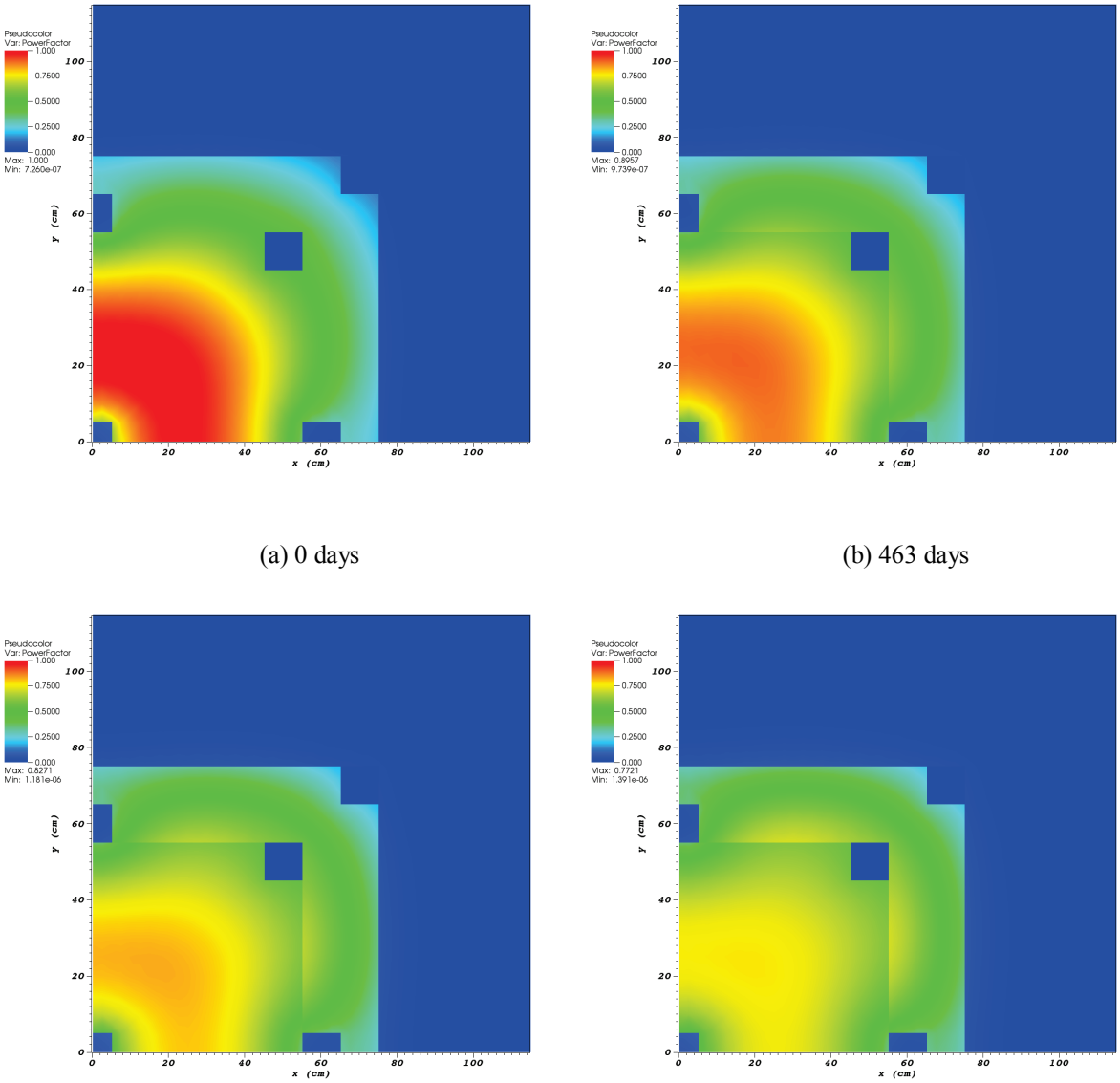


Figure 12. Total scalar flux in each material for simple SFR problem.



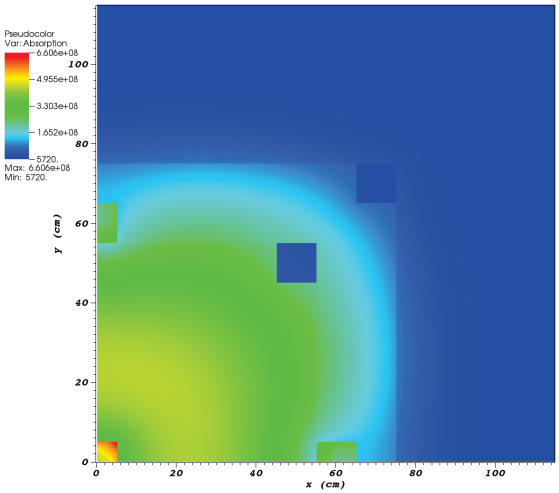
(a) 0 days

(b) 463 days

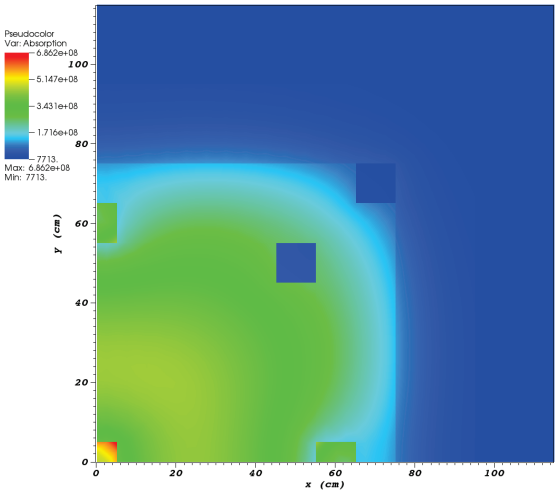
(c) 810 days

(d) 1157 days

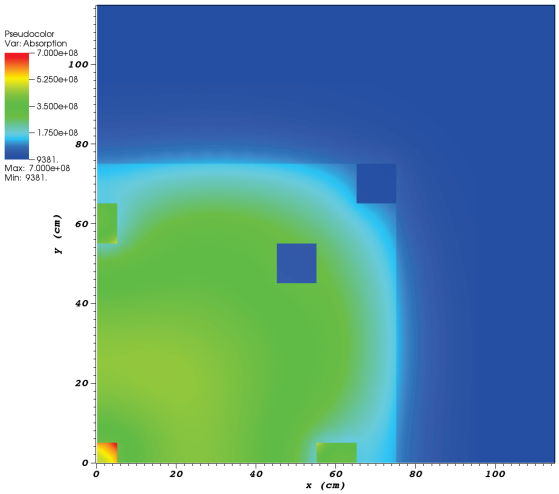
Figure 13. Power distribution in SFR core at various times.



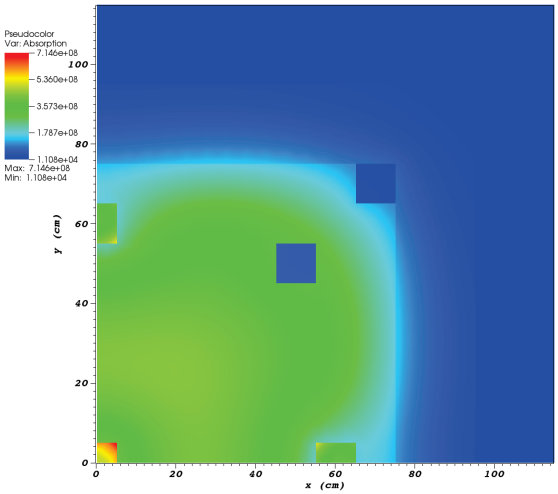
(a) 0 days



(b) 463 days

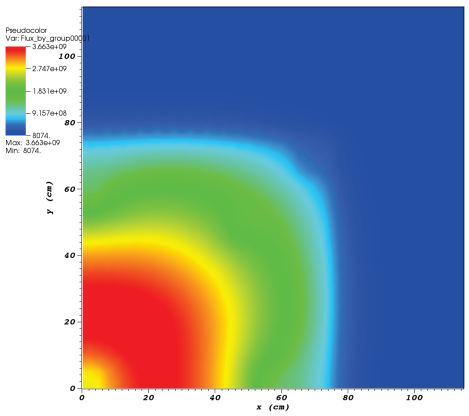


(c) 810 days

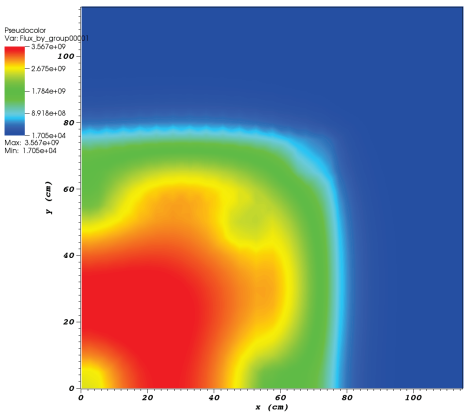


(d) 1157 days

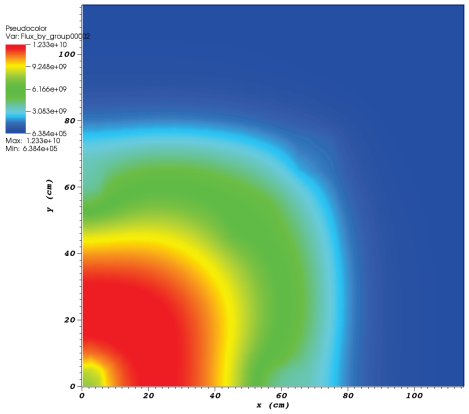
Figure 14. Absorption rate distribution in SFR core at various times.



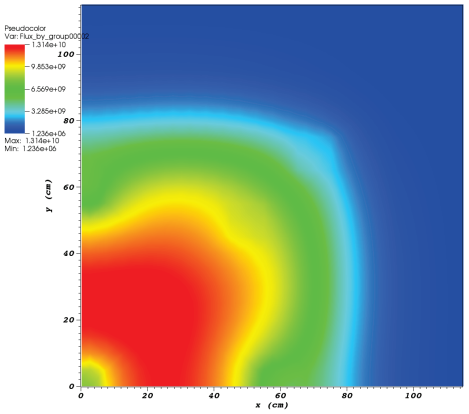
(a) fast flux at 0 days



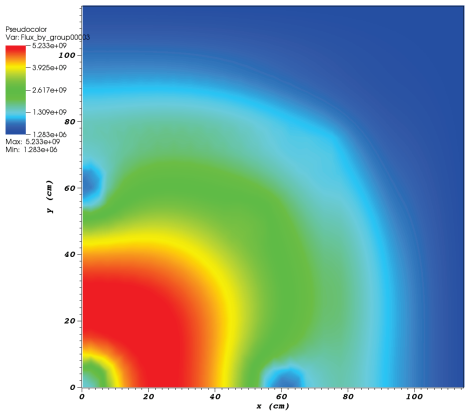
(b) fast flux at 1157 days



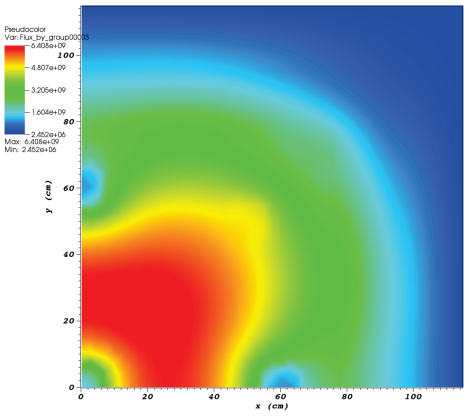
(c) intermediate flux at 0 days



(d) intermediate flux at 1157 days



(e) thermal flux at 0 days



(f) thermal flux at 1157 days

Figure 15. Fast flux, intermediate, and thermal distribution in SFR core at various times.

2.2.2 Analysis

Qualitatively, results for the initial implementation of depletion inside PROTEUS-SN appear reasonable. The eigenvalue shown in Figure 11 decreases as Pu-239 is consumed more than it is generated by U-238. The lack of fission products in the test library leads to no initial sharp drop as fission products burn in and equilibrate. The total scalar flux in Figure 12 for each material shows they are all increasing with time. This is expected due to the fixed power, consumption of fissile material, and hardening of the spectrum. The power distribution in Figure 13 shows flattening with time, and the outer core region power ("R_CORE2") begins to show a discontinuity due to isotopic differences. The absorption rate as a function of time is shown in Figure 14 and shows the effect of the control rods where they are inserted at the origin and on the x-axis and y-axis. The other two rod locations are pure sodium and do not exhibit the absorption rate of the uranium/plutonium/sodium homogenized fuel mixture. The flux distributions shown in Figure 15 exhibit the spectrum hardening, with the fast and intermediate flux extending to the core periphery. The magnitudes are increasing as well to compensate for loss of fissile material.

3. CONCLUSION

This report has documented the implementation of an initial depletion capability in the PROTEUS-SN code via the ORIGEN API depletion package. The results for a simple SFR test problem look qualitatively reasonable. Future work will address three main avenues of improvement: PROTEUS cross-section library integration, transport/depletion coupling enhancement, and liquid fuel modeling enhancement.

ORIGEN tracks ~1200 nuclides explicitly, many of them short-lived fission products with no appreciable cross section. However, ~300 nuclides have evaluated cross sections, and it is important that they all be included in a general-purpose library for PROTEUS. Otherwise, the proper feedback on the neutron transport properties of the system (i.e., macroscopic cross sections) due to isotopes introduced solely from depletion is neglected. In some systems, such as fast reactors, using a small problem-specific library may be easy to justify. However, if PROTEUS-SN is to be a general nuclear system code, a general library must exist and must be included with the distribution. Another issue with the libraries currently in ISOTXS format is that nuclides have arbitrary labels (e.g., "U5H" or "FP"), which are used in case there are two variants of a nuclide that have undergone different self-shielding or flux-weighting processes. Currently, the user is required to input the mapping of the nuclides to an actual nuclide in ORIGEN. A solution is to have in addition to the arbitrary label, an optional standard nuclide identifier, such as the seven-digit IZZZAAA, where I is the isomeric state, ZZZ is three digits of atomic number, and AAA is three digits of atomic mass (e.g., U-235 is 0092235, Am-242*m* is 1095242, and elemental carbon is 0006000. If the standard nuclide identifier was found, it would enable ORIGEN to directly map a physical nuclide to each ISOTXS library nuclide, and the user would not be required to put this mapping in the input file.

Transport/depletion coupling should be enhanced in future work by implementing a predictor/corrector methodology, whereby much more accurate solutions in time can be obtained. Additionally, the ability to specify time-dependent power levels and to produce HDF5 outputs of the isotopic distributions must be implemented.

Separate depletion zones introduce nonphysical isotopic distributions in a fuel that is constantly mixing. Therefore, more development is needed before liquid fuel systems such as molten salt reactors can be modeled. Specifically, additional development is needed so that fuel zones designed to allow variations in density, temperature, and cross section do not create separate depletion zones. Liquid fuel also experiences intermittent decay and fission product removal while in the out-of-core part of the loop. If this is a desirable system to model with PROTEUS-SN, then an appropriate liquid fuel model must be developed.

4. REFERENCES

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