PROTEUS-NODAL User Manual

Revision 0

Nuclear Science and Engineering Division

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Revision 0

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ABSTRACT

The PROTEUS-NODAL code is being developed as a three-dimensional (3D) neutron transport code based on homogenized geometry models of nuclear reactors. The code at present includes two solution options: diffusion theory and a nodal simplified P_3 (SP₃). The diffusion solution option is based upon the DIF3D-VARIANT P_N transport methodology where the transport options have not been implemented due to the desire to create a S_N based solution methodology. The diffusion solver works for Cartesian, hexagonal, and triangular-z geometries, while the SP₃ solution option is currently available for hexagonal-z geometry only. Both diffusion and SP₃ capabilities provide comparable solutions to DIF3D-VARIANT when using similar approximations. This document provides brief descriptions of inputs and outputs of the code.

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1. Introduction

The PROTEUS-NODAL code is being developed as a three-dimensional (3D) neutron transport code based on homogenized geometry models of nuclear reactors. The code presently includes two solution options: diffusion and a nodal simplified P_3 (SP₃). The diffusion solution is based upon the DIF3D-VARIANT P_N transport methodology [1,2] of which diffusion theory has only been implemented. The diffusion solver works for Cartesian, hexagonal, and triangular-z geometries while the SP₃ solution option is currently available for hexagonal-z geometry only. Both diffusion and SP₃ capabilities provide comparable solutions to DIF3D-VARIANT when using comparable approximations. This document provides users with a guide for using PROTEUS-NODAL including the basics of carrying out simulations using the code. *Note that the current version of the code is not parallel or threaded although significant research has been carried out on the subject as part of the NEAMS project.*

1.1 Input File Summary

Four input files are required to perform PROTEUS calculations (two other files are relevant only for certain simulations).

- a. Driver input file (*.inp)
- b. Multigroup cross section file (*.ISOTXS, *.anlxs)
- c. Mesh file (*.grid)
- d. Material assignment file (*.assignment)
- e. (Kinetics only) kinetics input file (*.inp)

The driver input file is a keyword-based free format text file that contains the simulation parameters such as angular cubature, parallelization, convergence criteria, and iteration limits.

The multigroup cross section file is a formatted file containing the multigroup cross sections for all the isotopes or materials of interest. Multigroup cross sections can be provided in either ANLXS, ISOTXS, or NODALXS formatted files.

The geometry details are given in a GRID formatted file which provides geometrical dimensions, region names, and boundary conditions and is part of the mesh generation toolkit [3]. In this manner, the results from the NODAL software can be visualized with the VTK file format which is also part of the toolkit. To define compositions and assign them to the geometrical regions we utilize the material assignment format that is already part of the PROTEUS framework.

The kinetics methodology is built on top of the existing steady state structure and is only relevant when running kinetics simulations. The kinetics input defines the timesteps to be simulated and requires material assignment files for each timestep along with delay cross section data and, if appropriate, a fixed source. The changes in materials or fixed source strength are assumed to drive the kinetics solution.

1.2 *Output File Summary*

Execution of the PROTEUS-NODAL software yields a text output file, a integral summary file NODAL_SUMMARY.out and visualization output of NODAL_SUMMARY.vtk. The text output file contains an echo of the inputs, eigenvalue iteration history, and timing summaries. The NODAL_SUMMARY.out file includes a region-to-composition map and block-integrated quantities such as power densities, neutron group fluxes, etc. The NODAL_SUMMARY.vtk can be used to plot composition, geometry, flux and power solutions using VisIt [4] or any visualization tools file which can read a VTK formatted data file.

2. Acquiring and Installing the Code

This chapter briefly describes how to obtain and install PROTEUS-NODAL. It lists the external library dependencies and also recommended compilers. For more specific (and up-to-date) compilation information including configuration options of the various packages, one should consult the installation documentation included with the distribution.

2.1 Acquiring the Code

The PROTEUS-NODAL source code is export-controlled and currently obtained through Argonne National Laboratory. Contact nera-software@anl.gov for distribution information. The distribution package includes source code, build instructions, benchmark examples and documentation.

2.2 External Library Dependencies

PROTEUS-NODAL achieves distributed memory parallelization using the Message Passing Interface (MPI) protocol and uses the MPI2 standard typically through the MPICH2 [5] library implementation. PROTEUS-NODAL also has essential dependencies on two external packages, the mesh partitioning package METIS [6] which comes from its dependency upon the mesh toolkit. Additionally, PROTEUS-NODAL optionally interfaces with data format library HDF5 [7] although it presently will not generate an hdf5 based output file. For help installing any of the packages for use with PROTEUS-NODAL, refer to the documentation included with the distribution, or contact nera-software@anl.gov.

PROTEUS-NODAL uses the METIS package to determine the mesh partitioning scheme for spatial domain decomposition. To download METIS, visit the webpage <http://glaros.dtc.umn.edu/gkhome/fsroot/sw/metis/OLD>. PROTEUS-NODAL is currently configured to use METIS 4.0 or METIS 5.0. To use METIS 4.0, no action is necessary. To use METIS 5.0, the pre-processing variable `PROTEUS_Use_METIS_VERSION_5` must be defined in `PROTEUS_Preprocess.h`.

2.3 Compiling the Code

Detailed compilation instructions are provided with the distribution, including suggested configuration options for many of the external dependencies. Once the external library dependencies have been downloaded and built, PROTEUS-NODAL is compiled using the provided makefile in the `/source` directory of the distribution. The makefile includes a second file, *Makefile.arch*, also located in the same directory.

2.3.1 Customization of *Makefile.arch*

Makefile.arch is a text file in the `/source` directory which contains typical compiler options and flags. We recommend you modify *Makefile.arch* to add an architecture-specific compilation section for your machine.

It is recommended to add a section to *Makefile.arch* for your machine similar to above where the machine name should be recovered earlier in the script using the “uname” or “dnsdomainname” UNIX functions. In the file, the locations of MPICH compiler, METIS, and HDF5 should be assigned. Note that the F90 compiler must be specified individually as it is used to compile one of the kinetics routines.

2.3.2 Customization of *PROTEUS_Preprocess.h*

The header file *PROTEUS_Preprocess.h* [8] controls various data assignments via pre-processor directives. Most of the contents of this file should remain unchanged for routine use. However, the top few definitions can be commented or uncommented to enable debug printing, and to enable compilation with optional dependencies.

2.3.3 Building the Targets

Once you have customized *Makefile.arch* and *PROTEUS_Preprocess.h*, invoke the “make all” command from Linux command prompt inside the /source directory. This command creates all of the targets (executables) in Table 1. Alternatively, type “make <target>” at the command line to create only a specific target.

Table 1. List of PROTEUS-NODAL Makefile Targets (Executables)

Target	Application
nodal.x	Steady state version of PROTEUS-NODAL-PN
nodal_sp3.x	Steady state version of PROTEUS-NODAL-SP3

2.3.4 Recommended Compilers and Architectures

PROTEUS-NODAL has been regularly compiled with the following Intel compiler version 13.1 or older on Intel hardware. Compilation with GNU compilers should be relatively straightforward using the flags “-ffree-line-length-0 -ffixed-line-length-0” on the FFLAGS line in *Makefile.arch*. However, the code is not routinely tested with the GNU compilers so minor changes may be required for successful compilation and execution.

3. A Brief Description of Methodologies

3.1 NODAL-PN

The NODAL methodology is a rewrite of the DIF3D-VARIANT methodology. In this methodology, we take the multigroup transport equation

$$\begin{aligned}\hat{\Omega} \cdot \vec{\nabla} \psi_g(\vec{r}, \hat{\Omega}) + \Sigma_{t,g}(\vec{r}) \psi_g(\vec{r}, \hat{\Omega}) &= W_g(\vec{r}, \hat{\Omega}) + S_g(\vec{r}, \hat{\Omega}) \\ W_g(\vec{r}, \hat{\Omega}) &= \int \Sigma_{s,g \rightarrow g}(\vec{r}, \hat{\Omega} \cdot \hat{\Omega}') \psi_g(\vec{r}, \hat{\Omega}') d\hat{\Omega}',\end{aligned}\quad (3-1)$$

where $g = 1, \dots, G$ and, using an P_1 angular approximation theory, recast it into the commonly known diffusion equation written in a functional form

$$\begin{aligned}\int dV \left[\vec{\nabla} \lambda(\vec{r}) D_g(\vec{r}) \vec{\nabla} \phi_g(\vec{r}) + \lambda(\vec{r}) \Sigma_{t,g}(\vec{r}) \phi_g(\vec{r}) \right] \\ = \int dV \left[\lambda(\vec{r}) \Sigma_{s,g \rightarrow g}(\vec{r}) \phi_g(\vec{r}) + \lambda(\vec{r}) S_g(\vec{r}) \right] - \sum_{\gamma} \int d\Gamma_{\gamma} \sum_K \hat{n}_{\gamma,K} V_K K_{\gamma} \Lambda_{\gamma}(\vec{r}) \chi_{g,\gamma}(\vec{r}),\end{aligned}\quad (3-2)$$

where the notation is mostly standard except for the boundary condition term appearing on the right hand side of this equation. In this case, these are necessary to define the interface current (odd parity flux) contributions to the flux solution within each spatial mesh. By spatially discretizing this system, we can collapse the system into the matrix relationship

$$\sum_{K,L} D_g P_{K,L} \phi_g + \Sigma_{t,g} F \phi_g = \Sigma_{s,g \rightarrow g} F \phi_g + F S_g - \sum_{\gamma} M_{\gamma} \chi_{g,\gamma}. \quad (3-3)$$

We can collect the matrices to write the compact form

$$A_g \phi_g = F S_g - \sum_{\gamma} M_{\gamma} \chi_{g,\gamma}, \quad (3-4)$$

which we can solve for the scalar flux

$$\phi_g = A_g^{-1} F S_g - \sum_{\gamma} A_g^{-1} M_{\gamma} \chi_{g,\gamma}. \quad (3-5)$$

To put this into a response matrix form, we impose continuity on the even- and odd-parity fluxes between spatial meshes and write

$$\varphi_{g,\gamma} = F_{\gamma}^{-1} M_{\gamma}^T \phi_g = F_{\gamma}^{-1} M_{\gamma}^T A_g^{-1} F S_g - F_{\gamma}^{-1} M_{\gamma}^T \sum_{\gamma'} A_g^{-1} M_{\gamma'} \chi_{g,\gamma'}. \quad (3-6)$$

Because we need to solve the global system of nodes simultaneously, we assume partial currents of the form

$$J_g^{\pm} = \frac{1}{4} \varphi_g \pm \frac{1}{2} \chi_g, \quad (3-7)$$

which leads to the response matrix relationships of

$$j_g^+ = R_g j_g^- + B_g S_g . \quad (3-8)$$

In PROTEUS-NODAL, the above system is setup assuming homogeneous cross sections within each spatial mesh although those cross sections can have a polynomial functionalization within the node. With this approach, orthogonal spatial basis functions internal and on the surfaces of the node are ideal when it comes to defining the spatial matrices. In DIF3D-VARIANT, the matrix-vector operations are manually unrolled for each surface and the red-black iteration is applied hierarchically in the axial and radial directions. In PROTEUS-NODAL, the red-black iteration is applied in 3D and we allow the compiler to determine the optimal matrix-vector operation. While we can show that the DIF3D-VARIANT approach is ideal in some reactor problems, using the full 3D sweeping in the partitioned matrix acceleration, matrix of PROTEUS-NODAL is always more efficient because of the better memory access pattern for the acceleration system and elimination of numerous intermediate vectors.

The DIF3D-VARIANT code actually chose the two level red-black scheme because of the memory constraints in the 1980s. With modern computers, we can handle a full red-black sweep over the entire domain for a given energy group as the total number of surface currents ($3 \cdot x \cdot y \cdot z < 25,000$ for most cases) and surface moments (3 for DIF3D-Nodal and 6 for DIF3D-VARIANT in diffusion $< 150,000$) leads to a small vector memory space (< 1.1 MB) which is within the typical cache size of most modern processors. More of an issue is the response matrix storage, which for 10,000 unique nodes leads to 12 MB of memory. Given both of these are still under the 32 MB level 3 cache, and unlikely to be less than the typical 2 MB of level 2 cache even with the two level iterative scheme, we can improve the convergence by removing the extra iteration needed in the two level scheme. It is important to note that in most fast reactor problems this alone should eliminate 25% to 50% of the computational effort.

It is important to note that this approach was tried before in DIF3D-VARIANT with a negative outcome. In the two level scheme of DIF3D-VARIANT, the response matrix storage was not split to explicitly handle the separated axial and radial components (i.e. the ideal approach). Instead, the memory access pattern had to be setup to access the response matrix components using offsets when computing the axial current based source for each radial plane, solving each radial system, and updating the outgoing axial currents. Regardless, upon inspection, the two-level approach was found to constitute fewer response matrix related flops per iteration. Thus the conclusion was that the performance of the full red-black sweep was not as good as the two level approach but this did not consider the restrictions placed on the cache sizes which were much smaller at the time of the tests (2-4 MB instead of today's 32 MB). While we implemented the full 3D sweep, we did not have time to contrast it against DIF3D-VARIANT. If in the future we find that two-level scheme is vastly superior to the 3D one, then we can switch to using the two-level scheme again.

Continuing, in DIF3D-VARIANT, there was a heavy focus placed on minimizing the vector storage of surface currents which arose due to the DIF3D-Nodal origination (where rotation of

current moments was not an issue). In PROTEUS-NODAL, the same convention was followed but because of the desire to use a Krylov solver (GMRES or FGMRES), an additional layer of expansion/contraction was necessary as the surface currents are multiply defined in some geometry setups (e.g. periodic and symmetry domains). In the previous work, the expansion/contraction approach resulted in a complex if branch operation in the main iterative (repeating) segment of the NODAL solver. In the updated PROTEUS-NODAL, both the DIF3D-VARIANT and the previous approaches were discarded as storing the full vector resulted in the minimal if branching during the iterative solver phase. While this does increase the memory usage slightly, it maximizes the potential success for threading as it allows the current vector components of each node to be independent memory targets.

Because of the rather minor success of energy parallelism and usage of GMRES/FGMRES, all aspects of the Krylov solver were removed as was the parallelism in energy concept. At the moment, the new version is thus completely serial although we are targeting OpenMP threading to allow it to better utilize the cores on a given node.

3.2 NODAL-SP3

The SP₃ equation, which is an approximated version of the P₃ equation, is known to be able to capture the major transport effects in both fast and thermal reactors. [9] With affordable additional computation cost, SP₃ can render significantly improved accuracy over the conventional diffusion equation. Moreover, it can be readily expanded for the full spatial kinetics by adopting the well-established methods for the diffusion equation. In order to support steady-state and transient analyses for routine design practices, the SP₃ nodal option was added to the PROTEUS-NODAL solver. Currently the SP₃ nodal option can provide the steady-state and transient solutions of the SP₃ equation for 3D hexagonal geometries.

In the SP₃ nodal capability, the SP₃ equation is efficiently solved by combining the 2D triangle based polynomial expansion nodal (TPEN) method and 1D nodal expansion method (NEM) for radial and axial directions, respectively. [10,11] The convergences of eigenvalue and fission source are accelerated by employing the diffusion CMFD method.

The 3D steady-state SP₃ equation with the transport approximation is given as:

$$\begin{bmatrix} -D_i & -2D_i \\ 0 & -D_i^2 \end{bmatrix} \begin{bmatrix} \nabla^2 \phi_i^0(\vec{r}) \\ \nabla^2 \phi_i^2(\vec{r}) \end{bmatrix} + \begin{bmatrix} \Sigma_{rg,i} & 0 \\ -\frac{2}{3}\Sigma_{rg,i} & \frac{5}{3}\Sigma_{t,i} \end{bmatrix} \begin{bmatrix} \phi_i^0(\vec{r}) \\ \phi_i^2(\vec{r}) \end{bmatrix} = \begin{bmatrix} q_i^0(\vec{r}) \\ q_i^2(\vec{r}) \end{bmatrix}, \quad (3-9)$$

where ϕ_i^k denotes the k -th flux moment on the i -th mesh, and the group index is omitted for brevity. The diffusion constant for the 2nd flux moment, D_i^2 , is defined as:

$$D_i^2 = \frac{3}{7\Sigma_{t,i}}. \quad (3-10)$$

By introducing a new solution variable $\hat{\phi}_i = \phi_i^0 + 2\phi_i^2$, Eq. (2-19) can be further simplified as:

$$\begin{bmatrix} -D_i & 0 \\ 0 & -D_i^2 \end{bmatrix} \begin{bmatrix} \nabla^2 \hat{\phi}_i(\vec{r}) \\ \nabla^2 \phi_i^2(\vec{r}) \end{bmatrix} + \begin{bmatrix} \Sigma_{rg,i} & -2\Sigma_{rg,i} \\ -\frac{2}{3}\Sigma_{rg,i} & \frac{4}{3}\Sigma_{rg,i} + \frac{5}{3}\Sigma_{t,i} \end{bmatrix} \begin{bmatrix} \hat{\phi}_i(\vec{r}) \\ \phi_i^2(\vec{r}) \end{bmatrix} = \begin{bmatrix} q_i^0(\vec{r}) \\ q_i^2(\vec{r}) \end{bmatrix}. \quad (3-11)$$

The currents for the 0th and 2nd flux moments can be determined using the following relations:

$$J_i^0(\vec{r}) = -D_i \nabla^2 \hat{\phi}_i(\vec{r}) = -D_i (\nabla^2 \phi_i^0(\vec{r}) + \nabla^2 \phi_i^2(\vec{r})), \quad (3-12)$$

$$J_i^2(\vec{r}) = -D_i^2 \nabla^2 \phi_i^2(\vec{r}). \quad (3-13)$$

For a set of homogenized hexagonal assemblies configured in a triangle lattice, the NODAL-SP₃ solver solves the two SP₃ equations for the radial and axial directions, which are coupled through the transverse leakages. To resolve the implicit couplings through the transverse leakage, the alternating nodal calculations for the radial and axial directions are performed. In this manner, the transverse leakage used for a one direction calculation is obtained from the solution of the other direction. Once the solution for one direction is obtained in the alternative solution process, the transverse leakage is updated and fed up to the subsequent calculation for the other direction. In the current implementation of the SP₃ nodal solver, the solution of the radial equation is determined by employing the 2D TPEN method and the 1D NEM is applied to the axial equation.

In the 2D SP₃ TPEN method, the solutions for individual hexagonal meshes are determined using the response matrix technique. The response matrix of each hexagon can be derived by solving the local problem for the hexagon using the local boundary conditions for surface currents and vertex fluxes. In this local problem, a hexagon node is divided into 6 triangular sub-nodes as shown in Figure 1 and an intra-nodal flux distribution is represented with a cubic polynomial. The intra-nodal flux distributions of six sub-meshes are simultaneously determined using the surface average incoming currents and vertex fluxes of hexagonal mesh along with additional constraints. Note that a single polynomial is used to represent the intra-nodal solution in the DIF3D-VARIANT method. In the TPEN method, the additional interfacial conditions on the internal surfaces are involved, which can adversely affect the solution accuracy. However, the TPEN approach is advantageous in that the flux variation within the homogenized node can be represented in a relatively concise form.

Figure 1. Discretization of Hexagonal Node in the TPEN Method

In each triangular node, the local coordinates x , u and p , which are perpendicular to triangle surfaces, are introduced as shown in Figure 1. Then, the intra-nodal fluxes for the 0th and 2nd flux moments are represented with the cubic polynomials having nine expansion coefficients to be determined:

$$\phi^m = c_o^m + a_x^m x + a_y^m y + b_x^m x^2 + b_u^m u^2 + b_p^m p^2 + c_x^m x^3 + c_u^m u^3 + c_p^m p^3. \quad (3-14)$$

Yielding the response matrix, the 9 expansion coefficients in Eq. (3-14) can be alternatively expressed in terms of the following 9 quantities defined on each triangular node: the average, x-moment and y-moment fluxes, surface average fluxes for three surfaces and vertex fluxes on three vertices. Consequently, a single hexagon has 54 unknowns in total for each flux moment. By noting that the vertex fluxes of hexagon are given and the continuity conditions are imposed on the triangle vertices and the internal surfaces, as shown in Figure 2, the number of unknowns to be determined is reduced to the following 31 quantities: average, x-moment and y-moment fluxes for the 6 triangular meshes, surface average fluxes for the 6 hexagon surfaces, surface average fluxes for the 6 internal surfaces and vertex fluxes on the hexagon center.

In order to determine the above quantities uniquely, the following 25 constraints are imposed along with the incoming partial currents for the six hexagon surfaces:

- Neutron balance equation for each triangular meshes (6 constraints)
- x- and y-weighted residual equations for each triangle meshes (12 constraints)
- Surface current continuity for each internal surface (6 constraints)
- Source-free condition in the hexagon center (1 constraint)

The detailed derivation of response matrix and its solution technique can be found elsewhere [10,11].

In the 1D SP₃ NEM for the axial direction, the solution of each axial mesh is expanded using the 4th order orthogonal polynomials and its coefficients are determined through the conventional one-node nodal technique. In the current implementation of 1D NEM module of NODAL-SP3 solver, the following conditions/constraints are used to determine the intra-nodal flux shape for axial meshes:

- Node average flux
- Partial incoming currents at the top and bottom surfaces
- x- and y-weighted residual equations for the axial mesh

The axial nodal solver uses the node average flux and radial transverse leakage from the radial solution and it updates the axial currents on the top and bottom of hexagonal meshes. Hence, the axial nodal solver can be viewed as the embedded procedure on the radial solver to account for the axial streaming effect. The overall calculation procedure of NODAL-SP3 solver is illustrated in Figure 3.

Figure 2. Unknowns of Local Problem for Hexagon Node in the TPEN Method

Figure 3. Calculation Flow of PROTEUS-NODAL-SP3 Solver

4. Code Execution Syntax

PROTEUS-NODAL is executed via command line on Linux platforms. To perform a serial job with the steady state solver, type the following at the command prompt (assuming the executable is in the current directory or in the user's path):

```
$ nodal.x -input mydriver.inp -output mydriver.out
```

```
$ nodal_sp3.x -input mydriver.inp -output mydriver.out
```

The “-input” flag argument specifies that PROTEUS-NODAL should look for a specific driver input file in the location specified by the following argument. If the “-input” flag and argument is omitted, PROTEUS-NODAL looks for the driver input file in the current working directory with the default name “nodal.inp”. The output can be redirected from standard output to a file using the -output flag.

5. Input File Descriptions

This section describes the required input files for a PROTEUS-NODAL calculation:

- Driver input file
- Cross section file
- Mesh file
- Material assignment file

5.1 Driver Input File (*.inp)

Upon execution, PROTEUS looks for the driver input file, “nodal.inp”, in the current working directory. This input file is a plain text (ASCII) file that drives the PROTEUS calculation by specifying solver tolerances, the angular discretization, parallelization options, and other input options. Additionally, the UNIX file paths to the other input files (cross sections, mesh, and material assignment file) are specified. Input options are specified in the file by special keywords which can appear in any order.

To use a different file name for the driver input such as “nodal_5g_mesh1.inp”, you need to add the command line option “-input nodal_5g_mesh1.inp” at execution to alert PROTEUS of the driver input file name.

5.1.1 Required Input

Table 2 shows the essential driver level input required in every PROTEUS-NODAL calculation. The keywords and values are not case sensitive. Default values are listed when applicable.

Table 2. Required Keywords for Driver Input File

Keyword	Input Data	Default value	Description
SOURCEFILE_MESH	<Max 128 Characters>	-	Specifies the UNIX file path to a spatial geometry mesh file
SOURCEFILE_XS	<Max 128 Characters>	-	Specifies the Unix file path to a cross section data file
SOURCEFILE_MATERIAL	<Max 128 Characters>	-	Specifies the Unix file path to a material mapping file
THERMAL_POWER	<Real Value>	100.0	Specifies the thermal power (W unit) for properly normalizing the flux and power solutions

Keyword	Input Data	Default value	Description
			provided in output file

5.1.2 Optional Input

Other optional driver-level input options are listed in Table 3. They can be classified into the following groups: iterative solver options, cross section options, output file options and flowing fuel option.

Table 3. Input Cards in Driver Input File

Keyword	Input Data	Default value	Description
<i>Iterative Solver Options</i>			
EIGENVALUE_GUESS	<Real Value>	1.0	Guess for the initial eigenvalue.
MAX_FISSION_ITER	<Integer > 0>	100	Maximum number of outer (fission source) iterations.
TOLERANCE_EIGENVALUE	<Real Value>	1.0E-6	Targeted relative error on the eigenvalue.
TOLERANCE_FISSION	<Real Value>	5.0E-6	Targeted relative error on the fission source.
TOLERANCE_FLUX	<Real Value>	1.0E-7	Targeted relative error on the flux solution.
<i>Cross Section Options</i>			
USE_TRANSPORT_XS	YES NO	NO	Indicates that the transport corrected cross section is to be used as the “total” cross section. All anisotropic scattering data is ignored.
USE_DIF3D_CHI	YES NO	NO	Specify whether the composition-wise chi is to be used in the fission source update. Note DIF3D uses the composition-wise chi instead of isotopic-wise one.

Keyword	Input Data	Default value	Description
SOURCEFILE_DELAY	<Max 128 Characters>	-	Specifies the Unix file path to a DLAYXS file. NOTE: USE_FLOWINGFUEL should be turned on to make this input meaningful.
<i>Output File Options</i>			
EXPORT_SOLUTION_VTK	YES NO	NO	Export the output to a VTK file for visualization.
<i>Flowing Fuel Options</i>			
USE_FLOWINGFUEL	YES NO	NO	Activate the flowing fuel option
CHANNEL_INFO	1 st <Integer Value> 2 nd <Character Value> 3 rd <Real Value>	-	Define channel ID, name, and time spent outside the core (sec) 1 st : channel ID 2 nd : channel name 3 rd : time outside core (s) NOTE: USE_FLOWINGFUEL should be turned on to make this input work.

5.2 Cross Section File (*.ISOTXS, *.anlxs)

The cross section file consists of the multigroup cross sections for all isotopes and/or compositions in the problem. Multigroup cross sections must be provided in one of the following formats:

- ISOTXS (binary file)
- ANLXS (ASCII file)
- NODALXS (ASCII file)

The ISOTXS format is the preferred file format for cross section data used by PROTEUS-NODAL. The MC²-3 code [13] can be used to process multigroup cross sections in this format. Additionally, the DRAGON code [14] has a capability to generate an ISOTXS file. The Serpent [15] and OpenMC [16] Monte Carlo codes can be used to generate cross sections, for which their

cross section outputs should be converted to an ISOTXS format file using the GenISOTXS code [17]. Note that Serpent generates macroscopic cross sections only.

The ANLXS file format is a simple ASCII interpretation of the data provided in ISOTXS while the NODALXS file format was built to allow polynomial and tabulated data sets to be provided. Any ANLXS file format that is provided is converted into the appropriate ISOTXS file at runtime and both are converted to a NODALXS file for use in the NODAL solver.

The cross section file does not need to be located in the working directory. The UNIX file path to the cross section file must always be specified in the driver input file using the SOURCEFILE_XS keyword.

5.3 Geometry Specification

The geometry file is a GRID formatted file containing information on geometric dimensions, region names, and boundary conditions. The GRID file is part of the mesh generation toolkit [3] and thus the NODAL solutions can be visualized with the VTK option of the toolkit.

5.4 Material Assignment File (*.assignment)

The material assignment (*.assignment) file performs three main functions: (1) define materials or mixtures of the isotopes in the cross section file, (2) assign these materials to regions in the mesh, and (3) assign properties (e.g. density and temperature) to regions in the mesh. The material assignment file uses simple keyword-based inputs in a free format, as shown in Table 4. It is normally created by the user, although a Python script is available to speed up the process. Comments start with either “!” or “#”.

Table 4. Input Cards in Material Assignment File

Keyword	Input Data	Default value	Description
REGION_PROPERTY	1 st <Character Value> 2 nd <Character Value> 3 rd <Real / Integer Value>	-	Define region properties such as atom/mass density.
REGION_ALIAS	1 st <Character Value> 2 nd <Character Value>	-	Assign user-defined materials to regions.
MATERIAL_DEF	1 st <Character Value> 2 nd <Character Value> 3 rd <Real Value>	-	Create user-defined materials based on isotopes in the cross section file. Recursive definitions are allowed to create additional mixtures.

5.4.1 Defining Materials

The isotope names provided in the cross section files are all available for use in defining materials. Figure 4 demonstrates the definition of a material called FUEL from 8 isotopes appearing in the cross section file: “U234A”, “U235A”, etc... The keyword MATERIAL_DEF is used repeatedly to add compositions to the material FUEL with the given atom fractions. The sum of all atom fractions is renormalized to 1 inside PROTEUS-NODAL. In this way, the true atom densities can be given (in #/barn-cm) for easier recordkeeping or in the natural concentrations of the component molecule.

```
MATERIAL_DEF FUEL U234A    2.7572E-5
MATERIAL_DEF FUEL U235A    2.5533E-3
MATERIAL_DEF FUEL U236A    9.5684E-6
MATERIAL_DEF FUEL U238A    1.5316E-4
MATERIAL_DEF FUEL B10A     1.5539E-4
MATERIAL_DEF FUEL B11A     6.2547E-4
MATERIAL_DEF FUEL C12A     1.9521E-4
MATERIAL_DEF FUEL ALA      5.2751E-2
```

Figure 4. Material Definition in the Assignment File (Atom Fractions)

Figure 5 demonstrates the definition of a material called Water from 2 isotopes appearing in the cross section file, “H__1” and “O__16”. The negative fraction indicates that the value is given in terms of weight fraction rather than atom fraction.

```
MATERIAL_DEF Water H__1    -0.1121
MATERIAL_DEF Water O__16    -0.8879
```

Figure 5. Material Definition in the Assignment File (Weight Fractions)

Figure 6 demonstrates the definition of a material called Water from 2 isotopes appearing in the cross section file, “H1” and “O16”, as well as the definition of a material called Salt from isotopes “NA23” and “Chlor”. The fractions are assumed to be atom fractions since they are positive. The last MATERIAL_DEF line defines a mixture called Saline which is 0.9% Salt and 99.1% Water. This example demonstrates the recursive usage of the MATERIAL_DEF keyword. It is not permitted to mix weight fractions and atom fractions in the same definition of a material.


```
MATERIAL_DEF Water H1      2.0
MATERIAL_DEF Water O16     1.0

MATERIAL_DEF Salt  NA23     1.0
MATERIAL_DEF Salt  Chlor    1.0

MATERIAL_DEF Saline 0.009 Salt 0.991 Water
```

Figure 6. Recursive Material Definition in the Assignment File

5.4.2 Assigning Materials to Blocks

In the previous section, we defined a material called FUEL. We can assign this material (or any other composition appearing in the material assignment file or the cross section file) to a region in the mesh. The ASSEMBLY001 (block name was defined by the user during mesh creation) is supposed to be a fuel assembly. We can associate the material FUEL using the REGION_ALIAS keyword shown in Figure 7.

```
REGION_ALIAS      ASSEMBLY001      FUEL
```

Figure 7. Assigning a Material to a Block in the Assignment File

5.4.3 Assigning Block Properties

We have not yet accounted for the actual material density of the block, or any other properties. The previous step simply linked cross section data to a specific region. If macroscopic cross section data was provided, no further action is necessary since the number density is incorporated into the data. More typically, the cross section data file contains microscopic cross section data and the density must be assigned. Figure 8 demonstrates the assignment of total atom density to 5.6129E-02 atoms/barn-cm using the keywords REGION_PROPERTY and ATOM_DENSITY.

```
REGION_PROPERTY    ASSEMBLY001      ATOM_DENSITY    5.6129E-02
```

Figure 8. Assigning Total Atom Density to a Block in the Assignment File

Alternatively, the total mass density in g/cm³ can be assigned to a block as shown in Figure 9. When using the Density (g/cc) property, PROTEUS uses the mass specified in the ISOTXS file for each basic component to convert to number density.

```
REGION_PROPERTY    ASSEMBLY001      Density(g/cc)    8.595
```

Figure 9. Assigning Total Mass Density to a Block in the Assignment File

The keyword REGION_PROPERTY is therefore used to assign various properties to the mesh such as ATOM_DENSITY, Density(g/cc), TEMPERATURE(K), and MATERIAL_MODEL to each mesh region. This approach is similar to MCNP where the same material can be used for multiple regions but at different concentrations. For the standard PROTEUS-NODAL user, the only properties of interest are Density(g/cc) and ATOM_DENSITY.

An example of a complete assignment file for a fictitious problem is shown in Figure 10. This assignment file assigns materials to two blocks.

```
!MATERIAL_DEF      <Material Name> <Isotope Name> <Concentration>
!-----
MATERIAL_DEF      FUEL_ASSEMBLY    FUEL          0.7
MATERIAL_DEF      FUEL_ASSEMBLY    COOLANT        0.3
MATERIAL_DEF      REF_ASSEMBLY     REFLECTOR      1.0
!REGION_PROPERTY  <Region Name>   <Property>     <Initial Setting>
!-----
REGION_PROPERTY   ASSEMBLY001      Density(g/cc)  1.0
REGION_PROPERTY   ASSEMBLY002      Density(g/cc)  1.0
!REGION_ALIAS     <Region Name>    <Composition Name>
!-----
REGION_ALIAS      ASSEMBLY001      FUEL
REGION_ALIAS      ASSEMBLY002      REFLECTOR
```

Figure 10. Example PROTEUS-NODAL Assignment File

5.5 Flowing Fuel Modeling

PROTEUS-NODAL has a flowing fuel modeling capability which is essential feature for molten salt reactor analyses. In order to facilitate the flowing fuel module in PROTEUS-NODAL, a flow of molten salt or similar should be properly defined through the material assignment and driver input files along with a DLAYXS file which contains delayed neutron data. A process to setup the fuel flows can be categorized into flow path configuration and flow control.

5.5.1 Flow Path Configuration

A flow of molten salt fuel is specified through REGION_PROPERTY keyword in assignment file. Using the CHANNEL_ID property name, the moving fuel regions are linked and PROTEUS-NODAL recognizes that the fuel flows through the blocks with the same channel ID from bottom to top direction. The two channel configurations shown in Figure 11 can be specified using the keywords given in Figure 12. In this example, the fuel in channel 1 will flow sequentially from A_01 to A_05 blocks and then return to the bottom of A_01 block.

Figure 11. Illustration of Flow Channel Configurations

Keyword	Block Name	Property Name	Value
REGION_PROPERTY	A_01	CHANNEL_ID	1
REGION_PROPERTY	A_02	CHANNEL_ID	1
REGION_PROPERTY	A_03	CHANNEL_ID	1
REGION_PROPERTY	A_04	CHANNEL_ID	1
REGION_PROPERTY	A_05	CHANNEL_ID	1
REGION_PROPERTY	B_01	CHANNEL_ID	2
REGION_PROPERTY	B_02	CHANNEL_ID	2
REGION_PROPERTY	B_03	CHANNEL_ID	2
REGION_PROPERTY	B_04	CHANNEL_ID	2
REGION_PROPERTY	B_05	CHANNEL_ID	2

Figure 12. Configuring Flow Paths in Assignment File

5.5.2 Fuel Flow Control

In PROTEUS-NODAL, the fuel flow can be controlled using two parameters: velocity of individual blocks having moving fuel and delayed time from outlet to inlet of each channel (outside of each channel). The velocities of individual blocks are assigned using VELOCITY property name which is available in REGION_PROPERTY keyword. An example of velocity specification is given in Figure 13. Note that velocities should be carefully defined with m/s unit such a way to preserve mass continuity of drifting precursors. The delayed time of each channel is specified using CHANNEL_INFO keyword in the driver input as illustrated in Figure 14. The first line in Figure 14 means the channel 1 named CH_001 has a delayed time of 5.0 sec.

Keyword	Block Name	Property Name	Value
REGION_PROPERTY	A_01	VELOCITY	2.751
REGION_PROPERTY	A_02	VELOCITY	1.179
REGION_PROPERTY	A_03	VELOCITY	0.323
REGION_PROPERTY	A_04	VELOCITY	1.179
REGION_PROPERTY	A_05	VELOCITY	2.751

Figure 13. Assigning Velocities to Blocks in Assignment File

CHANNEL_INFO	1	CH_001	5.0
CHANNEL_INFO	2	CH_002	5.0
CHANNEL_INFO	3	CH_003	5.0
CHANNEL_INFO	4	CH_004	5.0
CHANNEL_INFO	5	CH_005	50.0

Figure 14. Assigning Delayed Times in Driver Input

6. Output Files

Upon execution, as illustrated in Figure 15, PROTEUS-NODAL produces three basic types of outputs: (1) a main output text file, (2) a summary output file, and (3) a VTK file.

Figure 15. Schematic Illustration of Input and Output Files

6.1 Main Output File

The main text-based output is printed to a standard output or to a file if the “-output” option is used. The output contains confirmation that the input was imported successfully, parallel timing summaries, and eigenvalue iteration history results.

At the top of the file, the various input options are echoed and errors are produced if the input files were not successfully imported. This section is followed by the outer iteration history which reports the eigenvalue (and other quantities) as the calculation proceeds. At the end of the outer iteration history, the final eigenvalue is reported along with an error estimate. At the end of the output file, a timing history provides an overview of where time was spent in the calculation.

6.2 Summary Output File

The summary of full solution in the entire domain is exported to an organized ASCII file for detailed analysis. The summary output file, named NODAL_SOLUTION.out, contains the following data: (1) region configuration and associated material mapping, (2) region-wise integrals for flux, power and fission source, (3) mesh-wise distributions for flux and power, and additionally (4) mesh-wise distributions for precursor if the flowing fuel option is turned on. These data are edited out with the user-friendly table format. Note that the total power is normalized to the user-specified value of THERMAL_POWER given in the main driver input.

6.3 VTK File

PROTEUS-NODAL exports the full 3D solutions in the VTK file format with the EXPORT_SOLUTION_VTK option on in the main driver input. The resulting VTK file, named NODAL_SOLUTION.vtk, is readable by VisIt or any visualization software which accepts a VTK format. This option can be invoked to visually examine or demonstrate the full 3D NODAL solutions.

7. Example Problems

The test case selected as an example problem is a steady-state calculation for a 3D full core with flowing PuCl_3 molten salt fuel. The following input files are required to solve this problem:

- Main driver input file
- Geometry & mesh file
- Cross section file
- Material assignment file

Examining the driver input file in Figure 16, we see that the paths to the mesh, cross section data, and material assignment file are clearly defined by the SOURCEFILE_MESH, SOURCEFILE_XS, and SOURCEFILE_MATERIAL keywords. For this test case, SOURCEFILE_DELAY should be specified to calculate the delayed neutron contributions to the total neutron fluxes with respect to the speed of flowing fuel salt. In addition, the time for which the moving fuel spends from outlet to inlet of each channel is specified using CHANNEL_INFOR keyword. The mesh and full solution is exported to a VTK file named NODAL_SUMMARY.vtk if EXPORT_SOLUTION_VTK is set to YES.

```

THERMAL_POWER 100.0

MAX_FISSIION_ITER      100
EIGENVALUE_GUESS      1.0
TOLERANCE_EIGENVALUE  1.0e-5
TOLERANCE_FISSION     1.0e-4
TOLERANCE_FLUX        1.0e-4

SOURCEFILE_MATERIAL    MSR.CaseA.assignment
SOURCEFILE_GRID        MSR.grid

USE_TRANSPORT          YES
SOURCEFILE_XS          MoltenChloride_33g.ISOTXS
SOURCEFILE_DELAY       MoltenChloride_33g.DLAYXS

EXPORT_SOLUTION_VTK    YES

USE_FLOWINGFUEL YES
! <ID> <NAME> <DELAY TIME, sec>
CHANNEL_INFO 1 CHANNEL_0001 5.0
CHANNEL_INFO 2 CHANNEL_0002 5.0
CHANNEL_INFO 3 CHANNEL_0003 5.0
CHANNEL_INFO 4 CHANNEL_0004 5.0
CHANNEL_INFO 5 CHANNEL_0005 50.0

```

Figure 16. Driver Input File for Example Case

The cross section file is generated using MC²-3. The details of cross section generation are presented in Reference 13. In this test case, the isotopic cross sections for fuel, blanket, and shield regions are generated with homogeneous mixture.

The mesh input is generated for a 3D core in the GRID format, as shown in Figure 17. The input is directly read by PROTEUS-NODAL, which can also be verified by using the mesh generation toolkit. The detailed information on generating a GRID file is presented in Reference 3. The region names, such as FUEL_A_1, BLK____1, etc., specified in ASSEMBLY card are used in the material assignment file to link between region and material. Figure 18 is a snapshot of the VTK plot at the core center.

```

Element_Order 1
Element_Scheme PRISMS
GEOMETRY XYZ

RITZ_XY      3
RITZ_Z       3
RITZ_SOURCE  3
RITZ_SURFACE 1

! Define Grid
XGRID      0.000      45.000      2
XGRID      45.000      90.000      2
(cut)
XGRID      280.000     325.000      2
XGRID      325.000     370.000      2

YGRID      0.000      45.000      2
YGRID      45.000      90.000      2
(cut)
YGRID      280.000     325.000      2
YGRID      325.000     370.000      2

ZGRID      0.000      45.000      2
(cut)
ZGRID      435.000     480.000      2

! Define BCs
BOUNDARY_CONDITION -X VOID
BOUNDARY_CONDITION +X VOID
BOUNDARY_CONDITION -Y VOID
BOUNDARY_CONDITION +Y VOID
BOUNDARY_CONDITION -Z VOID
BOUNDARY_CONDITION +Z VOID

! Define Assemblies
!BLK      Assembly
ASSEMBLY  BLK      BLK____1      0.000      45.000
ASSEMBLY  BLK      BLK____2      45.000      90.000
(cut)

```



```

!Shield Assembly
ASSEMBLY SHD SHD 0.000 45.000
ASSEMBLY SHD SHD 45.000 90.000
(cut)

!A Type
ASSEMBLY CORE_A_1 FUEL_A_1 0.000 45.000
ASSEMBLY CORE_A_1 FUEL_A_2 45.000 90.000
(cut)
ASSEMBLY CORE_D_3 BLK___4 390.000 435.000
ASSEMBLY CORE_D_3 BLK___5 435.000 480.000

! Define ALIAS
ALIAS A1 CORE_A_1
ALIAS A2 CORE_A_2
(cut)
ALIAS D2 CORE_D_2
ALIAS D3 CORE_D_3

ALIAS S SHD
ALIAS B BLK

! Define GRID MAP
! 1 2 3 4 5 6 7 8 9 10 11 12
GRIDMAP 12 S S S S S S S S S S S S
GRIDMAP 11 S B B B B B B B B B B S
GRIDMAP 10 S B B A3 A3 A3 B3 B3 B3 B B S
GRIDMAP 9 S B A3 A3 A2 A2 B2 B2 B3 B3 B S
GRIDMAP 8 S B A3 A2 A1 A1 B1 B1 B2 B3 B S
GRIDMAP 7 S B A3 A2 A1 A1 B1 B1 B2 B3 B S
GRIDMAP 6 S B C3 C2 C1 C1 D1 D1 D2 D3 B S
GRIDMAP 5 S B C3 C2 C1 C1 D1 D1 D2 D3 B S
GRIDMAP 4 S B C3 C3 C2 C2 D2 D2 D3 D3 B S
GRIDMAP 3 S B B C3 C3 C3 D3 D3 D3 B B S
GRIDMAP 2 S B B B B B B B B B B S
GRIDMAP 1 S S S S S S S S S S S S

```

Figure 17. Mesh File for Example Case

Figure 18. Region Map from the Mesh File at the Core Center

Part of the assignment file is shown in Figure 19. The MATERIAL_DEF card is used to define compositions with isotopes, which can be recursively used as shown in the example. PUCL3 and SHD are first defined and then those are used to define FUEL_1 using the MATERIAL_DEF card. The REGION_PROPERTY card specified total atom number densities for the regions which are defined in the mesh file. The same card is used to determine CHANNEL_IDS which should be corresponding to the channel IDs defined in the main driver input. The velocities in m/s within channels are defined using VARIABLE_DEF, which are used in the REGION_PROPERTY card to assign velocities to channels.

```

MATERIAL_DEF      PUCL3      NA23I      6.3881E-03
MATERIAL_DEF      PUCL3      CL35I      2.3642E-04
(cut)
MATERIAL_DEF      SHD        B11_S      2.70469E-02
MATERIAL_DEF      SHD        C___S      7.51711E-03
(cut)
MATERIAL_DEF      REFL       MG25S      1.22652E-04
MATERIAL_DEF      REFL       MG26S      1.35039E-04

! Fuel Definition
MATERIAL_DEF      FUEL_1     PUCL3      1.86456217E-02
MATERIAL_DEF      FUEL_1     SHD        6.92523721E-02
(cut)
MATERIAL_DEF      BLK__5     BUCL3      1.87460867E-02
MATERIAL_DEF      BLK__5     SHD        6.92523721E-02

! Region-Material Map
REGION_ALIAS      FUEL_A_1    FUEL_1
REGION_ALIAS      FUEL_A_2    FUEL_2
(cut)
REGION_ALIAS      BLK__4      BLK__4
REGION_ALIAS      BLK__5      BLK__5
REGION_ALIAS      SHD         SHD

! Region Properties - Atom_Density
REGION_PROPERTY    FUEL A 1    ATOM DENSITY    8.78979938E-02

```

```

REGION_PROPERTY    FUEL_A_2    ATOM_DENSITY    6.72562088E-02
(cut)

REGION_PROPERTY    SHD            ATOM_DENSITY    1.38504744E-01

!Define Flow channel
REGION_PROPERTY    FUEL_A_1    CHANNEL_ID    1
REGION_PROPERTY    FUEL_A_2    CHANNEL_ID    1
(cut)
REGION_PROPERTY    BLK_____4    CHANNEL_ID    5
REGION_PROPERTY    BLK_____5    CHANNEL_ID    5

! Region Properties - Velocity (m/s)
VARIABLE_DEF    FUEL_V_1 =    2.751
VARIABLE_DEF    FUEL_V_2 =    1.179
(cut)
VARIABLE_DEF    BLK___V_4 =    0.0282
VARIABLE_DEF    BLK___V_5 =    0.0261

REGION_PROPERTY    FUEL_A_1    VELOCITY    FUEL_V_1
REGION_PROPERTY    FUEL_A_2    VELOCITY    FUEL_V_2
(cut)
REGION_PROPERTY    BLK_____4    VELOCITY    BLK___V_4
REGION_PROPERTY    BLK_____5    VELOCITY    BLK___V_5

```

Figure 19. Material Assignment File for Example Case.

Once the four inputs (driver, cross section, mesh, and material assignment inputs) are prepared, the following command executes the code:

```
$ nodal.x -input user.inp -output user.out
```

```
$ nodal sp3.x -input user.inp -output user.out
```

We have assumed that the executable and input files all reside in the working directory. After execution, the following files are produced:

- user.out
- NODAL_SUMMARY.out
- NODAL_SUMMARY.vtk

The first file, `user.out`, is the main text-based output file containing the eigenvalue and timing, as shown in Figure 20. The second file, `NODAL_SUMMARY.out`, is the formatted output file containing the full solution. The last file, `NODAL_SUMMARY.vtk`, is a VTK format file containing power, group flux, and precursor data for plotting using the visualization software, as illustrated in Figure 21.

[illegible]

```

.....00.....0000.....000000000000.....000000000000.....00.....00.....0000000000.....
.....00.....000.....0000000000.....0000000000.....00.....00.....0000000000.....
.....
.....Argonne National Laboratory Neutronics Package.....
.....A steady-state solver of the multigroup nodal diffusion equation.....
.....Geometry inputs include Cartesian 1:3-D, hexagonal & triangular 2:3-D.....
.....
.....Primary code authors.....Current Institution.....Contact Email.....
.....-----
.....Yeon Sang Jung.....Argonne National Lab.....yjung@anl.gov.....
.....Michael A. Smith.....Argonne National Lab.....masmith@anl.gov.....
.....Chang Ho Lee.....Argonne National Lab.....clee@anl.gov.....
.....
[NODAL]...Successfully imported the NODAL input (all errors reported above).....
[NODAL]...Obtaining the response matrices.....
(cut)
[NODAL]...Ritz Source order.....3
[NODAL]...Ritz Surface order.....1
[NODAL]...Hexagonal pitch.....0.000000000E+00
[NODAL]...Number of X, Y, Z meshes ( 24, 24, 18).....
[NODAL]...Number of unique regions in the domain.....26
[NODAL]...Number of active nodes.....10368
[NODAL]...Number of unique surfaces.....32544
[NODAL]...Number of boundary surfaces.....2880
[NODAL]...Number of surfaces per node.....6
[NODAL]...Number of volume moments per node per group.....20
[NODAL]...Number of surface moments per surface per group.....3
[NODAL]...Number of volume moments per group.....207360
[NODAL]...Number of surface moments per group.....195264
[NODAL]...Finite element mesh projection number of elements.....41472
[NODAL]... Number of spatial dimensions.....3
[NODAL]...Global space-angle degrees of freedom.....13286592
[NODAL]...Source type information.....
[NODAL]... Is a fission source present.....Yes
[NODAL]... Is a fixed source present.....No
[NODAL]... Is upscattering present (thermal system).....No
[NODAL]... Number of groups with up-scattering.....0
[NODAL]... Is a fission source present.....
[NODAL]...Outer iteration control variables.....
[NODAL]... Maximum inverse power iterations.....100
[NODAL]... No acceleration will be used.....
[NODAL]... Targeted error on the eigenvalue.....1.000E-05
[NODAL]... Targeted error on the fission source.....1.000E-04
[NODAL]... Targeted error on the flux solution.....1.000E-04
[NODAL]...Flowing Fuel Modeling.....Yes
[NODAL]...Solving the preceding NODAL system of equations
=NODAL Fission Source Iteration | MG GS | Within-group Gauss-Siedel |
=NODAL Seconds|Itr|Eigenvalue | Error | Fis Err|Flux Err| Wielandt | Dom |Iter Error | Total| Grp Max Err|Grp Max Itr|Grp Min Itr|P-grid|
=NODAL 2.4|001|1.03637E+00| 3.5E-02|3.3E-01| 1.7E-01| F 1.000E+30| 0.000| 1 1.7E-01| 132| 0 0.0E+00| 1 4| 1 4| F |
=NODAL 2.4|002|9.92517E-01| 4.4E-02|2.0E-01| 3.6E-02| F 1.000E+30| 0.000| 2 3.6E-02| 132| 0 0.0E+00| 1 4| 1 4| F |
=NODAL 2.4|003|1.01557E+00| 2.3E-02|6.8E-02| 1.5E-02| F 1.000E+30| 0.000| 3 1.5E-02| 132| 0 0.0E+00| 1 4| 1 4| F |
(cut)
=NODAL 2.4|017|1.01328E+00| 3.4E-07|8.2E-05| 1.5E-05| F 1.000E+30| 0.000| 10 1.5E-05| 132| 0 0.0E+00| 1 4| 1 4| F |
[NODAL]...!!!SUCCESS!!! All convergence criteria satisfied at iteration .....17
[NODAL]...Final eigenvalue.....1.01327958
[NODAL]...Final error on the eigenvalue.....3.441E-07
[NODAL]...Final error on the fission source.....8.223E-05
[NODAL]...Final error on the multi-group flux solution.....1.459E-05
[NODAL]...Total number of fission source iterations.....17
[NODAL]...Total computational time required for real solve (seconds).....42.109641
[NODAL]...Successfully exported the NODAL solution to the VTK file.....
[NODAL].....
[NODAL]...Timing history information for total job.....
[NODAL]...Total cumulative program time.....45.08
[NODAL]...Wall clock time.....Date (02/21/2018)...Time (14:05:14).....
[NODAL]...Wall clock time.....Date (02/21/2018)...Time (14:06:03).....
[NODAL]...Total cumulative wall clock time.....49.00
[NODAL].....
[NODAL]...| Id |Event Name | Total | Time(seconds) |
[NODAL]...| | Measure | Avg/Call | Total |Percent|
[NODAL]...| 1|Reading and converting all Inputs except XS | 1| 0.7551| 0.7551| 1.67|
[NODAL]...| 2|Obtaining and Linking XS | 0| 0.0000| 0.0000| 0.00|
(cut)
[NODAL]...| 10|Solving the forward transport equation | 1| 42.1096| 42.1096| 93.41|
[NODAL]...| 11|Fission source iteration | 17| 2.4478| 41.6126| 92.31|
(cut)
[NODAL]...| 22|Within-group flux solution | 561| 0.0492| 27.6256| 61.28|
[NODAL]...| 23|Within-group current solution | 561| 0.0369| 20.6941| 45.90|
[NODAL]...| 24|Normalizing flux and power distributions | 2| 0.0763| 0.1527| 0.34|
[NODAL]...| 25|Native HDF5 export | 0| 0.0000| 0.0000| 0.00|
[NODAL].....

```

Figure 20. Main Output for the Test Case

Figure 21. Power Density (left), Fast Neutron Flux (middle), and Precursor Family 1 (right) for the Test Case Plotted in VisIt

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