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Brief Descriptions of PROTEUS-MOCEX Input Files

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Table of Contents

1. Introduction

PROTEUS-MOCEX [1] is the one of the 3D transport solver option available in PROTEUS code package. MOCEX can provide a faithful 3D transport solution for 3D heterogeneous configuration that can be represented using the extruded geometry model. This document describes the required input files for a PROTEUS-MOCEX calculation, which helps a user to perform a neurotics simulation with proper computational options. In order to perform a MOCEX calculation, a user needs to prepare the following four input files:

- *Driver input file*
- *Cross section file (*.ISOTXS, *.anlxs)*
- *Material assignment file (*.assignment)*
- *Mesh file (*. ascii)*

MOCEX adopts the cross section and material file formats of PROTEUS-SN. The detailed description of these input files can be found in the PROTUES-SN manual [2]. This document provides only the brief descriptions for first three input files and the PROTEUS-MOCEX manual will be prepared with a complete set of detailed descriptions and samples in the near future.

2. Input File Descriptions

2.1 Driver Input File

Upon execution, MOCEX searches for the driver input file, "mocex.inp" by default, in the current working directory. This input file is a plain text (ASCII) file that drives the MOCEX 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 "mocex_7g_L5T5.inp", the command line option "–input mocex_7g_L5T5.inp" should be added at the command line as below. The output file name can be added with "-output" as well.

$ {MOCEX executable -input mocex_7g_L5T5.inp -output mocex_7g_L5T5.out

2.1.1. Required Input Keywords

The following table shows the essential driver level input required in every MOCEX calculation. The keywords and values are not case sensitive. Default values are listed when applicable.

Table 1. Required Keywords for Driver Input File

Keyword	Input Data	Default Value	Description
SN_TYPE	*See SN manual*	-	Specifies the type of SN cubature to use.
THETA_RESOLUTION	[Integer > 0[]	-	Specifies the polar angle resolution of the SN cubature.
PHI_RESOLUTION	[Integer > 0]	-	Only applicable for product cubatures such as Leg-Tcheby. Specifies the azimuthal angle (x,y) resolution of the SN cubature.
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.

2.1.2. Optional Input Keywords

Other optional driver-level input options are listed in Table 2. They can be classified into the following groups: parallelization options, 2D ray-tracing options, iterative solver options, cross section options, boundary condition options, and CMFD options. Brief explanations of each option as well as the default values are provided.

Table 2. Auxiliary Keywords for Driver Input File

Keyword	Input Data	Default Value	Description
Parallelization Options			
SEGMENT_ANGLE	[Integer ≥ 0]	0	The number of segments to attempt in the angular directions. 0 = Code decides max parallelization 1=Serial 2 and up = # Processors (segments) in angle

Keyword	Input Data	Default Value	Description
SEGMENT_PLANE	[Integer ≥ 0]	0	The number of segments to attempt in the axial planes. 0 = Code decides max parallelization 1=Serial 2 and up = # Processors (segments) in axial planes
2D Ray-Tracing Options			
TRAJECTORY_AREA	[Real Value]	1.0D0	The maximum trajectory area to use.
BACK_PROJECTION	DOMAIN LOCAL VOLUME FULL	DOMAIN	Back-projection technique to employ.
EQUAL_AREA_SPACING	YES NO	NO	Use equal area cubature on the domain boundary is used for defining trajectories.
Iterative Solver Options			
EIGENVALUE_GUESS	[Real Value]	1.0	Guess for the initial eigenvalue.
ITERATIONS_FISSION	[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.
BASIC_BWO	YES NO	NO	Applies a basic bandwidth optimization to mesh (reorder mesh for minimum bandwidth with ICC preconditioner).
USE_WGS_KRYLOV	YES NO	NO	Specify whether WGS Krylov scheme is used in the eigenvalue calculation (recommended). (NO) MGS Krylov scheme is used
(For MGS Krylov) USE_MGS_FGMRES *(For WGS Krylov)* USE_WGS_FGMRES	YES NO	YES	USE the FGMRES algorithm in MGS/WGS Krylov Solver.

Keyword	Input Data	Default Value	Description
(For MGS Krylov) ITERATIONS_MGS_KRYLOV *(For WGS Krylov)* ITERATIONS_WGS_KRYLOV	[Integer > 0]	1000	The maximum number of iterations in MGS/WGS Krylov solver.
(For MGS Krylov) BACKVECTORS_MGS_KRYLOV *(For WGS Krylov)* BACKVECTORS_WGS_KRYLOV	[Integer > 0]	30	The number of back vectors to employ in MGS/WGS Krylov solver.
(For MGS Krylov) TOLERANCE_MGS *(For WGS Krylov)* TOLERANCE_WGS	[Real Value]	0.1	Relative error target in MGS/WGS Krylov solver.
ITERATIONS_MGS_GS	[Integer > 0>]	1	The number of upscattering iterations in WGS Krylov solver (WGS Krylov solver only). 1= No upscattering iteration
Cross Section Options			
USE_CSAPI, USE_XSAPI	NO SUBGROUP (or SG) RESONANCETABLE (or RT)	NO	Indicates whether the subgroup or resonance table cross section library is to be used to generate cross sections. The cross section libraries are expected for heterogeneous geometry problems.
XSAPI_TOLERANCE_FSS	[Real Value]	1.0E-4	Targeted relative error on the fixed source problems for cross section generations.
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.
SCATTERING_ORDER	[Integer ≥ 0]	0	Legendre expansion order of the scattering kernel.
CHECK_XS_BALANCE	YES NO	NO	Check the cross section balance and correct total cross section if imbalance of cross section is detected.
Boundary Condition Options			

Keyword	Input Data	Default Value	Description
BC_ALIAS	*(For radial surface)* [Side set ID] [BCTYPE] *(For axial surface)* TOP <BCTYPE> Bottom <BCTYPE>	-	Assigns boundary condition at runtime to side set ID, top and bottom. Valid BCTYPE names are VOID or REFLECTIVE.

2.1.3. CMFD Input Keywords

MOCEX includes the coarse mesh finite difference (CMFD) acceleration capability [3] which can effectively accelerate an eigenvalue calculation. Table 2 presents the input keywords associated with the use of the CMFD acceleration. Note that the prerequisite for facilitating the CMFD acceleration is the coarse mesh structure. Thus, the MOCEX run with the CMFD acceleration requires the user-generated coarse mesh file that should be consistent with the fine meshes. It can be generated using the mesh tools such as CUBIT [4] and the PROTEUS mesh toolkit [5]. MOCEX is able to import the user-generated coarse mesh structure using the same format of the fine mesh file.

Table 3. CMFD Keywords for Driver Input File

Keyword	Input Data	Default Value	Description
Required Input Options			
USE_CMFD	*YES* *NO*	NO	Specify whether the CMFD acceleration is to be used in the eigenvalue calculations.
SOURCEFILE_COARSEMESH	*[Max 128 Characters]*	-	Specifies the UNIX file path to a CMFD mesh file.
CMFD Outer Iteration Options			
CMFD_ITERATION_FISSION	[Integer > 0]	100	The maximum number of outer iterations in each CMFD eigenvalue calculation.
CMFD_REDUCTION_EIGENVALUE	[Real Value]	0.1	Target error reduction of eigenvalue in CMFD calculation (partial convergence criterion).
CMFD_REDUCTION_FISSION	[Real Value]	0.1	Target error reduction of fission in CMFD calculation (partial convergence criterion).
CMFD_REDUCTION_FLUX	[Real Value]	0.1	Target error reduction of flux in CMFD calculation (partial convergence).

Keyword	Input Data	Default Value	Description
CMFD_TOLERANCE_EIGENVALUE	[Real Value]	1.0E-10	Relative target error of eigenvalue in CMFD calculation (Absolute convergence criterion).
CMFD_TOLERANCE_FISSION	[Real Value]	1.0E-10	Relative target error of fission in CMFD calculation (Absolute convergence criterion).
CMFD_TOLERANCE_FLUX	[Real Value]	1.0E-10	Relative target error of flux in CMFD calculation (Absolute convergence criterion).
CMFD_UNDERRELAXATION	[Real Value]	0.5	The under-relaxation parameter in CMFD prolongation process. 1.0 = No under-relaxation.
CMFD Krylov Solver (Inner Iteration) Options			
CMFD_BACKVECTORS_WGS_K	[Integer > 0]	30	The number of back vectors to employ in Krylov solver for WGS CMFD calculation.
CMFD_WGS_K_ITER	[Integer > 0]	100	The maximum number of inner Krylov iterations in each WGS CMFD calculation.
CMFD_TOLERANCE_WGS	[Real Value]	0.1	Relative error target in Krylov solver for WGS CMFD calculation.
Void (Low Density) Region Treatment Options			
CMFD_VOID_EXIST	YES NO	NO	Specify whether voided regions exist in CMFD meshes
CMFD_VOID_CRITERION	[Real Value]	1.0E-3	Tolerance of total macroscopic cross section for identifying voided regions.

2.2 Material Assignment Files (*.assignment)

The main role of material assignment file is to provide a mapping of material to 3D blocks defined in the mesh file. In MOCEX, the 3D heterogeneous domain is *internally* constructed by combining the 2D unstructured mesh file and the geometry extrusion information. Thus, the material

assignment file contains the additional geometry extrusion information. Upon execution of MOCEX, the material assignment file (*.assignment) file performs four functions:

- *Define materials or mixtures based on the isotopes in the cross section files*
- *Create 3D blocks by axially extruding 2D blocks in the mesh file*
- *Assign the materials to 3D blocks in the mesh*
- *Assign properties (e.g. density) to 3D blocks in the mesh*

The material assignment file uses simple keyword-based inputs in free format. It must be created by hand by the user, although scripting procedures can often be developed to speed the process. A python script is available to help a user create an assignment file in a more user-friendly manner. A comment starts with either "!" or "#".

2.2.1. Defining Materials

For defining materials, the relevant input keywords and formats of PROTEUS-SN are adopted. The detailed description can be found in the PROTEUS-SN manual [2].

2.2.2. Creation of 3D Blocks via Axial Extrusions

The specification of 3D block structures via the axial extrusion is a unique feature of material assignment file for MOCEX. The assignment file creates the 3D blocks with the following three steps:

- Step 1: Define a group of 2D blocks (referring to assembly) that will be collectively extruded in *Step 2* (*Input keyword: EXTRUDE*).
- Step 2: Extrude each assembly defined in *Step 1* with axial segmentations, which results in the 3D blocks along the axial direction (*Input keyword: ASSEMBLY*).
- Step 3: Define axial mesh structures that are consistent with the axial segmentations specified in *Step 2* (*Input keyword: ZGRID*).

The resulting 3D blocks become basic entities for material and property assignments in the subsequent processing steps. Figure 1 demonstrates the construction of 3D blocks from the 2D blocks with axial segmentations. Note that the driver input file should be updated with the axial boundary conditions as below.

```
BC_ALIAS    top             reflective  ! or void
BC_ALIAS    bottom          reflective  ! or void
```

Step 1				
Keyword	Name of 2D Block	Name of Assembly	-	-
EXTRUDE	MESHREGION_0011	ASSEMBLY_001		
EXTRUDE	MESHREGION_0012	ASSEMBLY_001		
EXTRUDE	MESHREGION_0013	ASSEMBLY_001		
EXTRUDE	MESHREGION_0020	ASSEMLBY_002		
Step 2				
Keyword	Name of Assembly	Name of 3D Block	Lower Axial Bound, cm	Upper Axial Bound, cm
ASSEMBLY	ASSEMBLY_001	BLOCK_001_01	0.00	20.00
ASSEMBLY	ASSEMBLY_001	BLOCK_001_02	20.00	40.00
ASSEMBLY	ASSEMBLY_002	BLOCK_002_01	0.00	20.00
ASSEMBLY	ASSEMBLY_002	BlOCK_002_02	20.00	40.00
Step 3				
Keyword	Lower Position, cm	Upper Position, cm	Number of Sub-divisions	-
ZGRID	0.00	20.00	4	
ZGRID	20.00	40.00	4	

Figure 1. Creation of 3D Blocks in Assignment File

2.2.3. Assigning Materials to 3D Blocks

For each 3D block, the material can be assigned using the REGION_ALIAS keyword shown in Figure 2.

Keyword	Name of 3D Block	Name of Material	-
REGION_ALIAS	BLOCK_001_01	FUEL	
REGION_ALIAS	BLOCK_001_02	FUEL	
REGION_ALIAS	BLOCK_002_01	COOLANT	
REGION_ALIAS	BLOCK_002_02	COOLANT	

Figure 2. Assigning Materials to 3D Blocks in Assignment File

2.2.4. Assigning Properties to 3D Blocks

The input keywords and formats for assigning properties to 3D blocks is the same as those for PROTEUS-SN. The detailed description can be found in the PROTEUS-SN manual [2].

3. Sample Inputs

3.1 Driver Input File

```
! Parallel processing
SEGMENT_ANGLE            1
SEGMENT_PLANE            1

! Angles
THETA_RESOLUTION         3
PHI_RESOLUTION           3
SN_TYPE                  LEG-TCHEBY

! Convergence criteria
ITERATIONS_FISSION       150
EIGENVALUE_GUESS         1.0
```

```
TOLERANCE_EIGENVALUE     1.0e-5
TOLERANCE_FISSION        1.0e-5
TOLERANCE_FLUX           1.0e-5

! Iterative solver option
USE_WGS_KRYLOV           YES
TOLERANCE_WGS            0.05d
BACKVECTORS_WGS_KRYLOV   10

! Mesh and material assignment input files
SOURCEFILE_MESH          ../00_Mesh/pin_1x1.ascii
SOURCEFILE_MATERIAL      ../00_Mesh/pin_1x1_3d.assignment

! Cross section input file
SOURCEFILE_XS            ../../../00_XSLIB/THERMAL_11G.ISOTXS
USE_TRANSPORT_XS         NO
SCATTERING_ORDER         1

! Boundary conditions
BC_ALIAS    top              reflective
BC_ALIAS    bottom           reflective
BC_ALIAS    SIDESET_00000001 reflective
BC_ALIAS    SIDESET_00000002 reflective
BC_ALIAS    SIDESET_00000003 reflective
BC_ALIAS    SIDESET_00000004 reflective
BC_ALIAS    SIDESET_00000005 reflective
BC_ALIAS    SIDESET_00000006 reflective
BC_ALIAS    SIDESET_00000007 reflective
BC_ALIAS    SIDESET_00000008 reflective
```

Figure 3. Sample Driver Input File

3.2 Assignment Input File

```
! ZGRID <Lower Position in cm> <Upper Position in cm> <subintervals to apply>

ZGRID         0.0        20.0    5
ZGRID        20.0        40.0    5

! EXTRUDE <Name of 2D mesh region> <Name of assembly>

EXTRUDE              FUEL  ASM2D001
EXTRUDE              CLAD  ASM2D002
EXTRUDE               MOD  ASM2D003

! ASSEMBLY <Assembly Name> <Region Name> <Lower Axial Bound> <Upper Axial Bound>

ASSEMBLY  ASM2D001 REG2D001_3D001        0.0       20.0
ASSEMBLY  ASM2D001 REG2D001_3D002       20.0       40.0

ASSEMBLY  ASM2D002 REG2D002_3D001        0.0       20.0
ASSEMBLY  ASM2D002 REG2D002_3D002       20.0       40.0

ASSEMBLY  ASM2D003 REG2D003_3D001        0.0       20.0
ASSEMBLY  ASM2D003 REG2D003_3D002       20.0       40.0

! REGION_PROPERTY <Name of mesh region> {<property> <initial setting>}

REGION_PROPERTY  REG2D001_3D001 ATOM_DENSITY  1.00000E+00
REGION_PROPERTY  REG2D001_3D002 ATOM_DENSITY  1.00000E+00

REGION_PROPERTY  REG2D002_3D001 ATOM_DENSITY  1.00000E+00
```

```
REGION_PROPERTY  REG2D002_3D002 ATOM_DENSITY  1.00000E+00

REGION_PROPERTY  REG2D003_3D001 ATOM_DENSITY  1.00000E+00
REGION_PROPERTY  REG2D003_3D002 ATOM_DENSITY  1.00000E+00

! REGION_ALIAS <Name of assembly region> <Name of Material>

REGION_ALIAS     REG3D001_3D001     MAT_FUEL
REGION_ALIAS     REG3D001_3D002     MAT_FUEL

REGION_ALIAS     REG3D002_3D001     MAT_CLAD
REGION_ALIAS     REG3D002_3D002     MAT_CLAD

REGION_ALIAS     REG3D003_3D001     MAT__MOD
REGION_ALIAS     REG3D003_3D002     MAT__MOD

! MATERIAL_DEF <Material name> {<isotope name> <concentration>}

MATERIAL_DEF          MAT_FUEL      XS_FUEL  1.00000E+00
MATERIAL_DEF          MAT_CLAD      XS_CLAD  1.00000E+00
MATERIAL_DEF          MAT__MOD      XS__MOD  1.00000E+00
```

Figure 4. Sample Assignment Input File for a 3D Problem with Macroscopic Cross Sections

```
! ZGRID <Lower Position in cm> <Upper Position in cm> <subintervals to apply>

ZGRID         0.0        20.0    5
ZGRID        20.0        40.0    5

! EXTRUDE <Name of 2D mesh region> <Name of assembly>

EXTRUDE              FUEL  ASM2D001
EXTRUDE              CLAD  ASM2D002
EXTRUDE               MOD  ASM2D003

! ASSEMBLY <Assembly Name> <Region Name> <Lower Axial Bound> <Upper Axial Bound>

ASSEMBLY  ASM2D001 REG2D001_3D001        0.0       20.0
ASSEMBLY  ASM2D001 REG2D001_3D002       20.0       40.0

ASSEMBLY  ASM2D002 REG2D002_3D001        0.0       20.0
ASSEMBLY  ASM2D002 REG2D002_3D002       20.0       40.0

ASSEMBLY  ASM2D003 REG2D003_3D001        0.0       20.0
ASSEMBLY  ASM2D003 REG2D003_3D002       20.0       40.0

! REGION_PROPERTY <Name of mesh region> {<property> <initial setting>}

REGION_PROPERTY  REG2D001_3D001 ATOM_DENSITY  3.74648E-02
REGION_PROPERTY  REG2D001_3D002 ATOM_DENSITY  3.74648E-02

REGION_PROPERTY  REG2D002_3D001 ATOM_DENSITY  4.27669E-03
REGION_PROPERTY  REG2D002_3D002 ATOM_DENSITY  4.27669E-03

REGION_PROPERTY  REG2D003_3D001 ATOM_DENSITY  7.44336E-02
REGION_PROPERTY  REG2D003_3D002 ATOM_DENSITY  7.44336E-02

! REGION_ALIAS <Name of assembly region> <Name of Material

REGION_ALIAS     REG3D001_3D001     MAT_FUEL
```

```
REGION_ALIAS     REG3D001_3D002     MAT_FUEL

REGION_ALIAS     REG3D002_3D001     MAT_CLAD
REGION_ALIAS     REG3D002_3D002     MAT_CLAD

REGION_ALIAS     REG3D003_3D001     MAT__MOD
REGION_ALIAS     REG3D003_3D002     MAT__MOD

! MATERIAL_DEF <Material name> {<isotope name> <concentration>}

MATERIAL_DEF          MAT_FUEL         U235  2.48293E-04
MATERIAL_DEF          MAT_FUEL         U238  7.65991E-03
MATERIAL_DEF          MAT_FUEL          O16  2.95566E-02

MATERIAL_DEF          MAT_CLAD         ZR90  4.26303E-03
MATERIAL_DEF          MAT_CLAD         FE56  1.36597E-05

MATERIAL_DEF          MAT__MOD           H1  4.96224E-02
MATERIAL_DEF          MAT__MOD          O16  2.48112E-02
```

Figure 5. Sample Assignment Input File for a 3D Problem with Microscopic Cross Sections

For comparison between the assignment inputs for MOCEX and SN2ND, the sample assignment input for SN2ND is shown in Figure 6. Note that this is for a 2D problem, while the assignment input for MOCEX is for a 3D problem. As discussed in the previous section, the input keywords ZGRID, EXTRUDE, and ASSEMBLY are for use in MOCEX only. For a 3D problem with SN2ND, a 3D mesh file for it should be provided.

```
! REGION_PROPERTY <Name of mesh region> {<property> <initial setting>}

REGION_PROPERTY             FUEL ATOM_DENSITY  3.74648E-02
REGION_PROPERTY             CLAD ATOM_DENSITY  4.27669E-03
REGION_PROPERTY              MOD ATOM_DENSITY  7.44336E-02

! REGION_ALIAS <Name of assembly region> <Name of Material>

REGION_ALIAS                FUEL     MAT_FUEL
REGION_ALIAS                CLAD     MAT_CLAD
REGION_ALIAS                 MOD     MAT__MOD

! MATERIAL_DEF <Material name> {<isotope name> <concentration>}

MATERIAL_DEF            MAT_FUEL         U235  2.48293E-04
MATERIAL_DEF            MAT_FUEL         U238  7.65991E-03
MATERIAL_DEF            MAT_FUEL          O16  2.95566E-02

MATERIAL_DEF            MAT_CLAD         ZR90  4.26303E-03
MATERIAL_DEF            MAT_CLAD         FE56  1.36597E-05

MATERIAL_DEF            MAT__MOD           H1  4.96224E-02
MATERIAL_DEF            MAT__MOD          O16  2.48112E-02
```

Figure 6. Sample Assignment Input File for a 2D Problem with Microscopic Cross Sections for SN2ND (Equivalent to Figure 5)

References

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2. E. R. Shemon, M. A. Smith and C. H. Lee, "PROTEUS-SN Methodology Manual", ANL/NE-14/5, Argonne National Laboratory, June 30, 2014.
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