Generation of transport input file for PHITS format

(March 2024)

1. Introduction

As a trial of an extension work, PHITSFormat.py, is applied to generate PHITS geometry input files. PHITS[1] stands for the Particle and Heavy Ion Transport code System. This is a general-purpose Monte Carlo radiation transport code. Japan Atomic Energy Agency (JAEA) directly provides this code, following the Japanese export control rules. [For further information, please visit their web site. https://phits.jaea.go.jp]. PHITS geometry definition is very similar to the MCNP. Input formats of [MATERIAL], [SURFACE] and [CELL] sections are almost the same as those of MCNP, except for the definition of importance in [CELL]. Therefore, this PHITSFormat.py module is mainly based on MCNPFormat.py, being modified and added some codes for PHITS.

2. Overview

PHITSFormat.py outputs a ".inp" file.

geometryName	Generated PHITS Input File
test	test.inp

The generated PHITS input file can contain [CELL], [SURFACE], [MATERIAL] and [VOLUME] sections. The included sections depend on the config.ini setting.

Section	Description
[CELL]	Defined solid, void, and enclosure
[SURFACE]	Defined surface for a cell
[MATERIAL]	Applied dummy material for quick check
[VOLUME] off	Quoted CAD calculated volume for solid

In the geometry conversion, the available surfaces are listed below. Be careful not to use the other surface types in a prepared CAD file.

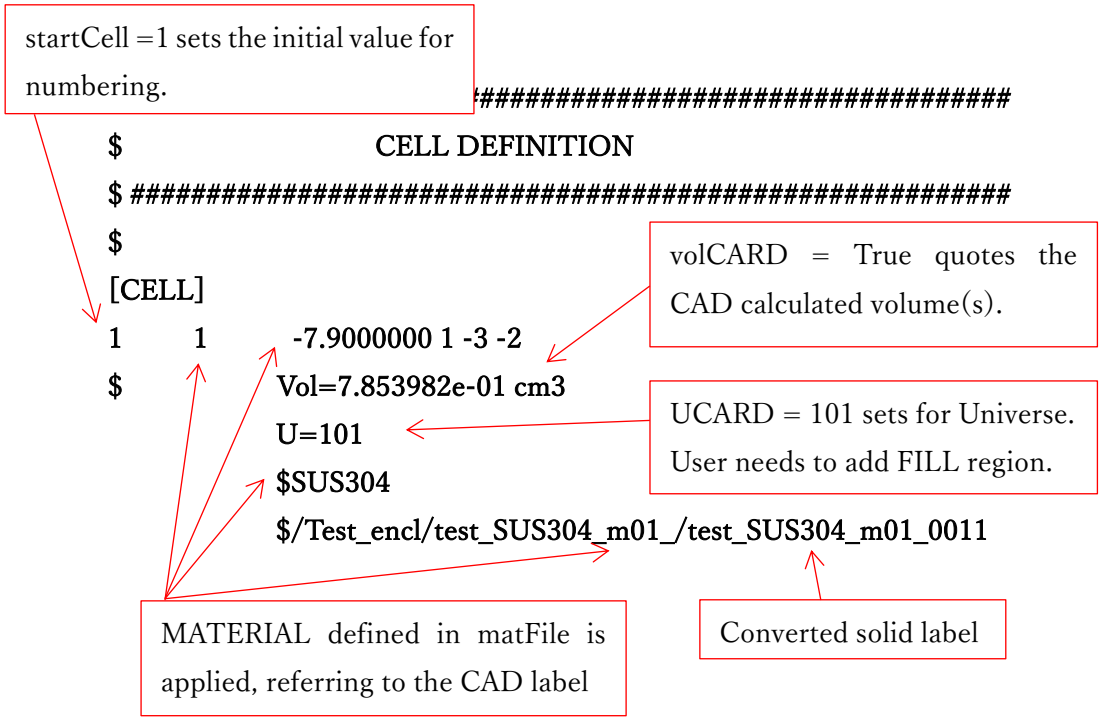
Surface	PHITS Surface Symbol
Plane	P, PX, PY, PZ
Cylinder	CX, CY, CZ, C/X, C/Y, C/Z, GQ
Cone	KX, KY, KZ, K/X, K/Y, K/Z, GQ
Sphere	S, SO
Torus	TX, TY, TZ

3. Overview of the Generated PHITS Input File

3.1. [CELL]

An example of parameter setting in config.ini

Parameter	Example Setting
matFile =	materials.txt
voidGen =	True
voidMat =	(100, -1.21e-3, 'Air assigned to Void')
volCARD =	True
UCARD =	101
startCell =	1
cellRange =	(0,100)
sortEnclosure =	True
simplify =	No



When UCARD is set, the fill region is not defined. Therefore, the user needs to add its filling cell definition with FILL parameter. In addition, without such modification, PHIG-3D fails to visualize. As a recommendation, at first comment out the UCARD setting in config.ini and check whether geometry conversion is appropriate or not. Then set UCARD to output PHITS geometry file.

```
$ ###################################
$                    VOID CELLS
$ ###################################
$
8       100     -1.2100e-03 29 -30 31 -32 33 -34 (28:-27:26:-25:-24:23)
$               Vol=1.0 cm3
                U=101
                $'Air assigned to Void'
                $Automatic Generated Void Cell. Enclosure(-6.5, 6.5, -6.5, 6.5, -6.5,
6.5)
                $Enclosed cells : ()

9       100     -1.2100e-03 -35 (-29:30:-31:32:-33:34)
$               Vol=1.0 cm3
                U=101
                $Inner void
10      -1        35
$               Vol=1.0 cm3
                U=101
                $Outer void$

$ ###########################################################
$                       ENCLOSURE 1
$ ###########################################################
$
6       0         -28 27 -26 25 24 -23 (21:-20:-18:17:14:-13) (11:(-12:(15:(-16:(20:
                -19) (-21:22)) (-17:21:-20)) (18:21:-20:-16)) (-14:21:-20:-18:17))
                (13:21:-20:-18:17:-12)

                $Automatic Generated Void Cell. Enclosure(-5.5, 5.5, -5.5, 5.5, -5.5,
5.5)
                $Enclosed cells : (5)
```

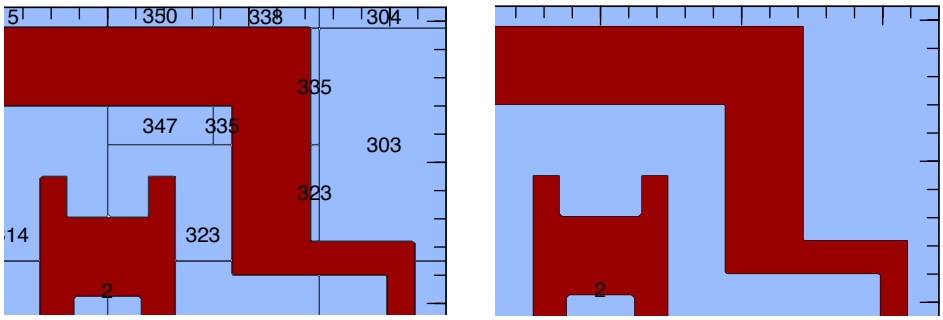
voidGen = True
When this is True, the void cells are generated to cover all solid cell regions.

Void volumes are not calculated.
Set at 1.0cm^3 tentatively.

voidMat = (100, -1.21e-3, 'Air assigned to Void')
is applied to all void cells except for enclosure cells

sortEnclosure = True
Only when the CAD file contains the enclosure information. The defined enclosure void cell definitions come appear.

When the “voidGen = True”, the void cells are automatically generated. However, for PHITS input file, there is a difference from the other output files like MCNP, OpenMC, and Serpent. Basically, the void cells are generated through the same method of GEOUNED. Using the generated outer-most void surface, originally named the “Graveyard” sphere surface for MCNP, as a boundary, the inner voids are merged into new one void.



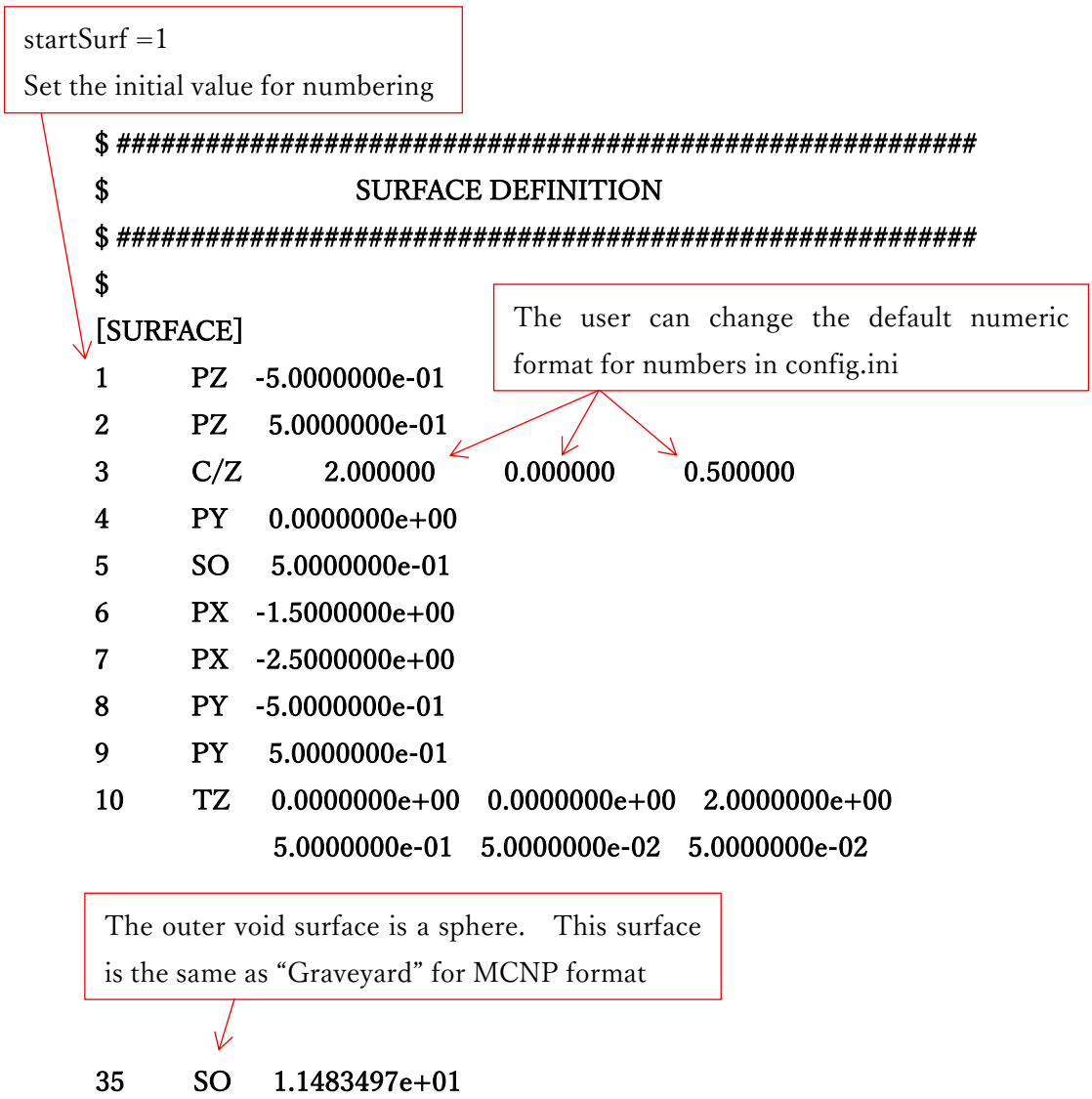
Left) An example of the auto-generated void cells. Right) Unified the generated void cells.

Please note for the PHITS geometry file that “voidGen = True” and any enclosure(s) or envelope(s) are NOT defined in the CAD file, the auto-generated void cells are unified as the inner void cell. The merged void cell(s) is/are eliminated and not written in the .inp file. In opposite, when a user sets enclosure(s) or envelope(s), the auto-generated void cells are NOT unified like the other geometry input format.

3.2. [SURFACE]

An example of parameter setting in config.ini

Parameter	Example Setting
startSurf =	1
P_xyz =	14.7f
S_r =	14.7e
S_xyz =	14.7e
C_r =	12f
C_xyz =	12f
T_r =	14.7e
T_xyz =	14.7e



The surface definitions are described in this section. The start surface number is changeable with “startSurf = (specific number)”. When the “voidGen = True”, the outer and inner void boundary surface is a sphere shape. If you output the MCNP format file at the same time, this surface is the same as the “Graveyard” surface. The available surface types are also the same as using MCNP geometry input file. The surface types are listed in 2. Overview section.

3.3. [MATERIAL]

An example of parameter setting in config.ini

Parameter	Example Setting
matFile =	materials.txt
dummyMat =	True
voidMat =	(100, -1.21e-3, 'Air assigned to Void')

materials.txt

```
# Materials and density
# FORMAT: ID DENS NAME
01 7.9 SUS304
02 2.20 Concrete
```

dummyMat = True
When this is True, [MATERIAL] section is added in the input file.

```
$ ############################################################
$                        MATERIAL DEFINITION
$ ############################################################
$ All material labels present in this model are listed below
$ Need to change the dummy material definition(H2O1) to appropriate one(s)
$
[MATERIAL]
$ Change dummyMat M1 to SUS304, Density = 7.9g/cm3
 M1          H 2 O 1
$ Change dummyMat M2 to Concrete, Density = 2.2g/cm3
 M2          H 2 O 1
$ Change dummyMat M100 to 'Air assigned to Void', Density = 0.00121g/cm3
 M100        H 2 O 1
```

All material definitions are set dummy H2O1.

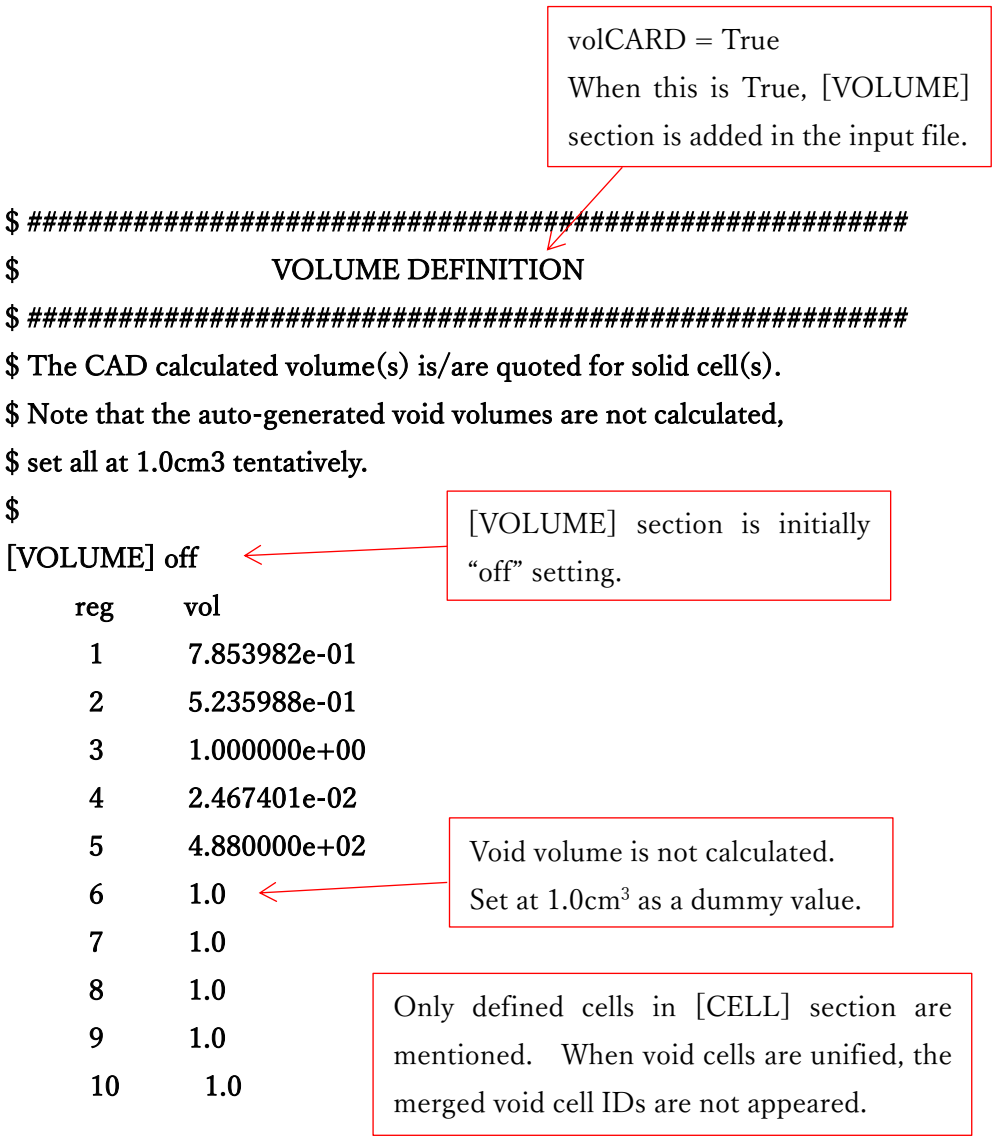
voidMat = (100, -1.21e-3, 'Air assigned to Void')
When the void material is applied, the material number is also written. The density is set at negative value.

This includes only when “dummyMat = True” is in the config.ini setting. All material labels in the model are listed. Pay attention that the applied material is a dummy(H2O1). The users need to change the dummy definition to the appropriate one(s). To take a quick look at PHIG-3D, this dummy material is set as a default. In addition, the density of the voidMat is set at a NEGATIVE value in config.ini.

3.4. [VOLUME]

An example of parameter setting in config.ini

Parameter	Example Setting
volCARD =	True



This includes only when "volCARD = True" is in the config.ini setting. This section is initially an "off" setting. The CAD calculated volume(s) is/are quoted for solid cell(s). Note that the auto-generated void volumes are not calculated, set all at 1.0cm^3 tentatively. These volumes are also written in the [CELL] section. Use [VOLUME], when a user needs to set the solid volume(s) for calculation or when a user checks [T-VOLUME] result.

4. Examples (Tested with PHITS Version = 3.310)

An example of parameter setting in config.ini

Parameter	Example Setting
stepFile =	test.step
geometryName =	test
matFile =	materials.txt
outFormat =	phits
volCARD =	True
dummyMat =	True
#UCARD =	Comment out
startCell =	1
startSurf =	1
voidMat =	(100,-1.21e-3,'Air assigned to Void')

The conversion process is the same with the other formats.

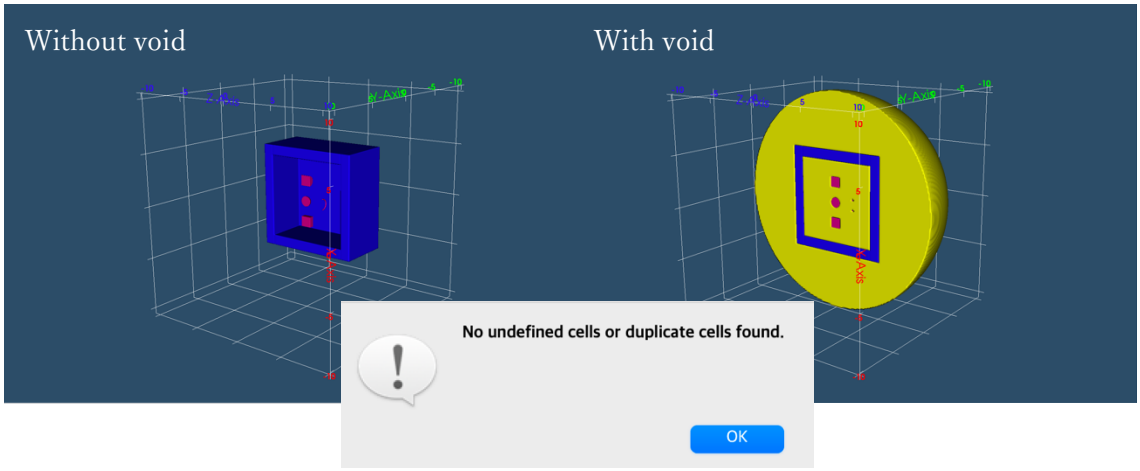
1. Set "outFormat = phits" in config.ini. GEOUNED can output multiple geometry formats at the same time. Below case generates 5 geometry formats.

 # format of the converted geometry :
outFormat = mcnp, openMC_PY, openMC_XML, serpent, phits

2. Run GEOUNED

% python geouned.py

3. Send the output .inp file to PHIG-3D and check the geometry.



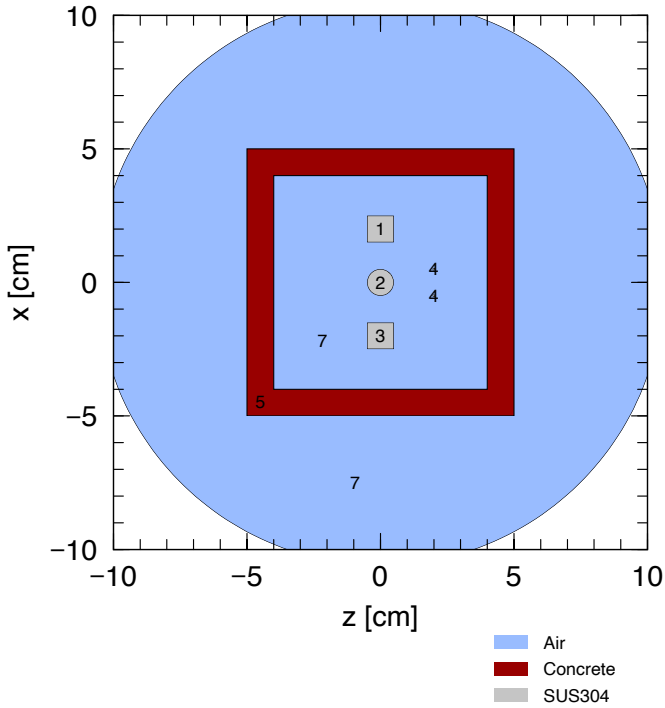
4. Prepare for PHITS calculation. Add "infl:{*filename*}" to insert the geometry input file and check the geometry with icntl=8.

```
[Parameters]
 icntl = 8
 maxcas = 10000
 maxbch = 1
 negs = 1

 infl: {test.inp}
```

add "infl:{*filename*}"

```
[Source]
 s-type = 9
   proj = electron
     e0 =   1.0
     x0 =   0.0
     y0 =   0.0
     z0 = -2.0
     r1 =   0.0
     r2 =   3.0
 factor =   1.0
    dir =   all
```

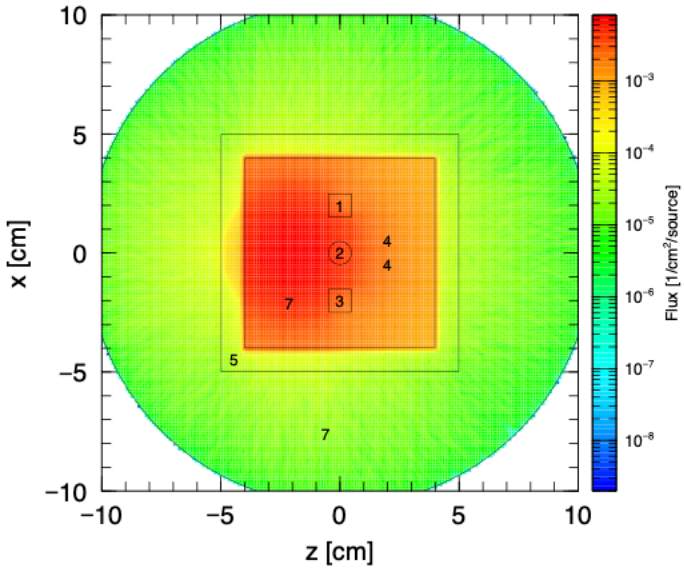



```
[Mat  Name  Color]
    mat    name        color
     1     SUS304      gray
     2     Concrete    darkred
    100    Air         pastelblue
```

```
[T-Track]
    mesh =   xyz
  x-type = 2
      nx = 200
    xmin = -10
    xmax = 10
   ...
```

Cell 1: Cylinder
Cell 2: Sphere
Cell 3: Square with planes
Cell 4: Torus
Cell 5: Square with planes
Cell 7: Sphere (Inner Void)
(Cell 6: Merged in Cell 7)

5. Start out PHITS calculation.



1MV electrons are emitted to the all directions from a 3.0cm sphere source at (x, y, z) = (0.0, 0.0, -2.0).

5. Related files

GEOUNED/scripts/config.ini
GEOUNED/src/GEOUNED/__init__.py
GEOUNED/src/GEOUNED/Write/Functions.py
GEOUNED/src/GEOUNED/Write/PHITSFormat.py
GEOUNED/src/GEOUNED/Write/WriteFiles.py

Reference:

[1] T. Sato, Y. Iwamoto, S. Hashimoto, T. Ogawa, T. Furuta, S. Abe, T. Kai, Y. Matsuya, N. Matsuda, Y. Hirata, T. Sekikawa, L. Yao, P.E. Tsai, H.N. Hunter, H. Iwase, Y. Sakaki, K. Sugihara, N. Shigyo, L. Sihver and K. Niita, Recent improvements of the Particle and Heavy Ion Transport code System - PHITS version 3.33, J. Nucl. Sci. Technol. 61, 127-135 (2024)