Training on GEOUNED tool

J.P. Catalán, P. Sauvan and TECF3IR group

Energy Engineering Department.

Nuclear Engineering Area

Universidad Nacional de Educación a Distancia (UNED), Madrid, Spain

Introduction

GEOUNED code description

GEOUNED is a new conversion tool to convert CAD (B-rep) ↔ MC (CSG).

- Based on **FreeCAD** as interface for **Open CASCADE** CAD engine. Both tools are open source and actively supported.
- GEOUNED is open source located in GitHub.
- Programmed in Python 3. Used as script launched in a system console:
  - Automatization of repetitive/complex tasks (comments, density factors)
  - Extension of capabilities ⇒ high adaptability to specific problems
- Automatic void generation ⇒ essential for complex models
  - Complex enclosure shapes for void generation based on CAD solids => structured hierarchical voids producing cleaner inputs

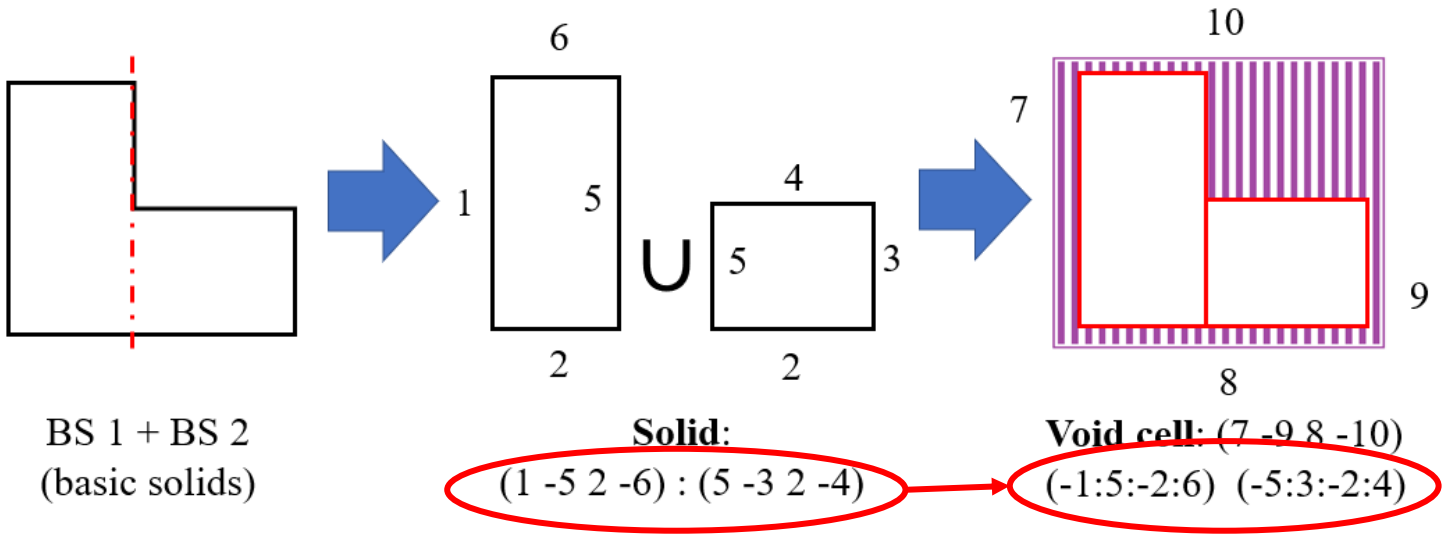
FreeCAD
Open Source parametric 3D CAD modeler

OPEN CASCADE

python™

GEOUNED basic performance

- The solids are decomposed in basic solids by splitting. GEOUNED splits for all the standard surfaces used in MCNP.
- The basic solids are suitable to be converted to CSG (Boolean operation of subspaces defined by surfaces).
- The void is generated automatically by intersecting void regions with the solids and using the complement of solids definition.



Installation and Execution

Windows and Linux

Python version

FreeCAD:

https://freecad.org current version for windows is 0.21.2.

GEOUNED:

Directly from GitHub repository: https://github.com/GEOUNED-code/GEOUNED

Or via pip

pip install git+https://github.com/GEOUNED-code/GEOUNED.git

Or using git (**currently recommended**)

git clone -b dev https://github.com/GEOUNED-code/GEOUNED.git

Python version in windows

FreeCAD has compilated libraries for a specific python version

Current version for FreeCAD 0.21.2 is 3.8.17. Versions ≥ 3.9 will not work

In windows FreeCAD comes with a compatible python executable located at*.

~FreeCAD 0.XX/bin>

With its own pip and wheel located at

~FreeCAD 0.XX/bin/Scripts>

*By default FreeCAD is located at C:\Program Files\

How to use it

GEOUNED is a python package and can be called from a python script

1. To find GEOUNED package and FreeCAD from the calling script: via pip, PYTHONPATH environment variable or path variable of sys module:

```
import sys
GEO_path='~/GEOUNED'
FreeCAD_path='~/FreeCAD' # not required for FreeCAD python
sys.path.append(GEO_path)
sys.path.append(FreeCAD_path) # not required for FreeCAD python
```

2. Parameter definition through a config file.
3. Call the module for forward (CAD/MC) or reverse (MC/CAD) conversion.

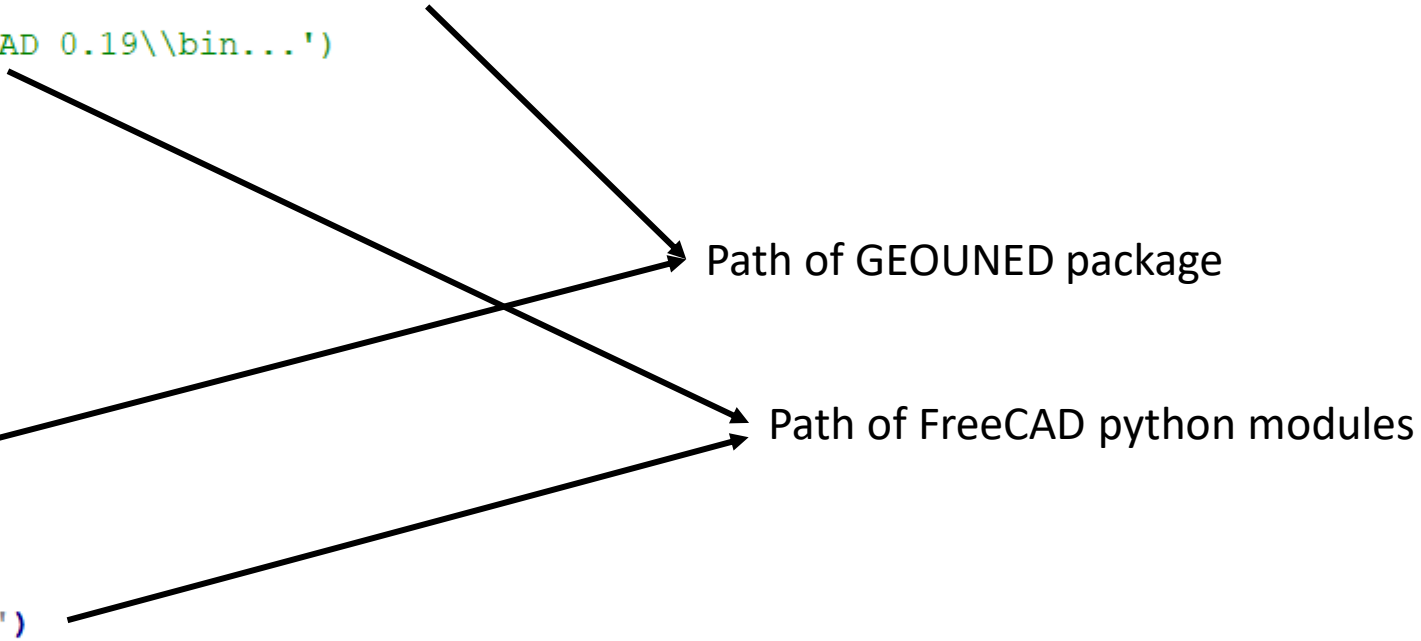
Example of script. Import modules

Windows

```
import sys
geo_path="C:\\Users\\Juan\\Documents\\GitHub\\GEOUNED\\GEOUNEDcode\\src"
sys.path.append(geo_path)
#sys.path.append('C:\\Program Files\\FreeCAD 0.19\\bin...')

import GEOUNED
from  GEOReverse.reverse import reverse
```

Linux

```
import sys

geo_path="/opt/geouned/v1.0/"

sys.path.append(geo_path)

# linux distribution
sys.path.append('/usr/lib64/freecad/lib64/')

import GEOUNED
from GEOReverse.reverse import reverse
```



Example of Script. Executing the modules

```python
runReverse = False
if len(sys.argv) < 2 :
    inifile = 'config.ini'

elif len(sys.argv) == 2 :
    if sys.argv[1] == '-r':
        runReverse = True
        inifile = 'configReverse.ini'
    else:
        inifile = sys.argv[1]

elif len(sys.argv) == 3:
    if   sys.argv[1] == '-r':
        runReverse = True
        inifile = sys.argv[2]
    elif sys.argv[2] == '-r':
        runReverse = True
        inifile = sys.argv[1]
    else:
        print('Bad option')
        exit()
else:
    print('Too many input arguments')
    exit()


if not runReverse :
    GEO = GEOUNED.GEOUNED(inifile)
    GEO.SetOptions()
    GEO.Start()

else:
    print(inifile)
    reverse(inifile)
```

Config files for forward and reverse conversion

For run the script

```
~>python geouned.py
```
← forward

```
~>python geouned.py -r
```
← reverse

Executing GEOUNED module

Executing reverse module

Example of the whole process

Let’s see an example: my configuration

Configuration

Parameter definition

Configuration File for CAD to MC conversion

In GEOUNED the configuration parameters are passed through a file that is read using parser capability of python.

The configuration file is divided in 5 sections:

1. Files
2. Parameters
3. Tolerances
4. MCNP numeric formats
5. Options

```
[Files]
title = my MCNP model
stepFile = myModel.stp
matFile = materials.txt
geometryName = myModel.i

[Parameters]
startCell = 10000
startSurf = 10000
```

Files

Set name of input and output files as well as the size of the region where the solid is defined

Parameter	Type: Default	Definition
stepFile	None	Name of the CAD file (in STEP format) to be converted.
matFile	None	Name of the file with the materials information.
geometryName	Step filename without ".stp" extension	Name of the output mcnp file
title	Step filename without ".stp" extension	Title of the model
outFormat	mcnp	Format for the output geometry. Available format are: mcnp, openMC_XML, openMC_PY, Serpent. Several output format can be written in the same geouned run.

Parameters I

Parameter	Type: Default	Definition
startCell	Integer: 1	Starting cell numbering label
startSurf	Integer: 1	Starting surface numbering label
UCARD	Integer: 0	Write universe card in the cell definition with the specified universe number (if value = 0 Universe card is not written)
volCARD	Boolean: True	Write the CAD calculated volume in the cell definition using the VOL card
volSDEF	Boolean: False	Write SDEF definition and tally of solid cell for stochastic volume checking.
dummyMat	Boolean: False	Write dummy material definition card in the MCNP output file for all material labels present in the model. Dummy material definition is “MX 1001 1”.
voidMat	Tuple (id,density,’text’): 0, not applied, ‘’	Assign a material defined by the user instead of void for cells without material definition and the cells generated in the automatic void generation. Example (100,1e-3,'Air assigned to Void')
sortEnclosure	Boolean: False	if enclosures are defined in the CAD models, the voids cells of the enclosure will be located in the output file in the same location where the enclosure solid is located in the CAD solid tree.
compSolids	Boolean: True	Join subsolids of STEP file as a single compound solid. Step files generated with SpaceClaim have not exactly the same level of solids as FreeCAD. It may a happened that solids defined has separated solids are read by FreeCAD as a single compound solid (and will produce only one MCNP cell). In this case compSolids should be set to False.
cellRange	List: []	Range of cell to be converted (only one range is allowed, e.g [100,220]). Default all solids are converted.
debug	Boolean:False	Write step files of original and decomposed solids, for each solid in the STEP file.

Parameters II

Parameter	Type: Default	Definition
cellSummaryFile	Boolean: False	Write an additional file with information on the CAD cell translated
cellCommentFile	Boolean: False	Write an additional file with comment associated to each CAD cell in the MCNP output file.
exportSolids	String: ‘’	Export CAD solid after reading. The execution is stopped after export, the translation is not carried out.
voidGen	Boolean: True	Generate voids of the geometry.
simplify	Sting: no	Simplify the cell definition considering relative surfaces position and using Boolean logics. Available options are: - no : no optimization - void : only void cells are simplified. Algorithm is faster but the simplification is not optimal. - voidfull : only void cells are simplified with the most optimal algorithm. The time of the conversion can be multiplied by 5 or more. - full : all the cells (solids and voids) are simplified.
minVoidSize	Float: 100	Minimum size of the edges of the void cell. Units are in mm.
maxSurf	Integer: 50	Maximum number of surfaces allowed in void cell definition. This number is the number of different surface label, if this label is used several times in the void definition, it will be counted only once.
maxBracket	Integer:30	Maximum number of brackets (solid complementary) allowed in void cell definition

Tolerances

Variable	Default	Definition
relativeTolerance	False	define the values as relative (True) or absolute in mm or rad.
relativePrecision	1e-6	relative precision in comparison between two numbers
generalDistance	1e-4	distance between objects
generalAngle	1e-4	angle between axis
planeDistance	1e-4	distance between parallel planes. Planes are assumed equal if distance between planes < 1e-4 mm
planeAngle	1e-4	angle between the normal of planes. Planes are parallel if angle < 1e-4
cylinderDistance	1e-4	distance between axis. Difference in radii size
cylinderAngle	1e-4	angle between axis
sphereDistance	1e-4	distance between centers. Difference in radii size
coneDistance	1e-4	distance between apex
coneAngle	1e-4	angle between semiangles/axis
torusDistance	1e-4	distance between Major/Minor radii/center
torusAngle	1e-4	angle between axis

MCNP numeric formats

variable	Default	Definition
P_abc	14.7e	A, B, C coefficients of MCNP general plane definition
P_d	14.7e	D coefficient of MCNP general plane definition
P_xyz	14.7e	Coefficients for PX/PY/PZ
S_r	14.7e	Radii SO/SX/SY/SZ/S
S_xyz	14.7e	X,Y,Z parameters in MCNP sphere definition
C_r	12f	Cylinder Radius
C_xyz	12f	X,Y,Z parameters in MCNP cylinder definition
K_xyz	13.6e	X,Y,Z parameters in MCNP cone definition
K_tan2	12f	Tangent in MCNP cone definition
T_r	14.7e	Torus Radius
T_xyz	14.7e	Torus X,Y,Z in MCNP definition
GQ_1to6	18.15f	1^{st} to 6^{th} parameters in GQ MCNP definition
GQ_7to9	18.15f	7^{th} to 9^{th} parameters in GQ MCNP definition
GQ_10	18.15f	10^{th} parameter in GQ MCNP definition

Options

Keyword	Default Value	Description
forceCylinder	False	Use cylinder (instead of cones) as ancillary surface where unclosed torus surfaces are involved in the solid definition.
newSplitPlane	True	New method to consider plane as cutting surface during the decomposition process. Former method split first planes perpendicular to X,Y,Z axis and then the other planes involved in the solid definition. New method group all parallel planes independently whether their normal are along X,Y,Z axes, and start the decomposition process cutting first with the group having the highest number of parallel planes.
enlargeBox	2	Enlarge box boundary when evaluating the constraint table during the simplification of the void cell definition. (unit is mm)
verbose	False	Print output warning during geouned run
nPlaneReverse	0	Threshold value to determine whether cut with parallel planes should be carried out first.
splitTolerance	0	Fuzzy tolerance value used in the FreeCAD function "BOPTools.SplitAPI.slice". This function is used during the solid decomposition process.
quadricPY	False	In openMC python script format, the cones or cylinders no aligned with the X,Y, or Z axis can be defined using the openmc.Cone or open.Cylinder methods but can also be defined with their quadric parameter. If "quadricPY" is True then all cones and cylinders will be defined in the openMC python script format under their quadric form

Configuration File for MC to CAD conversion

In GEOUNED the configuration parameters are passed through a file that is read using parser capability of python.

The configuration file is divided in 4 sections:

1. Settings
2. Levels
3. Cells
4. Materials
5. Options

Settings & Levels

Keyword	Default Value	Description
mcnpFile	None	Name of the MCNP input file
CADFile	None	Name of the file with the materials information.
outbox	None	Box size for conversion MC to CAD. All the cells should be inside this box

Keyword	Default Value	Description
UStart	0	**Universe to be converted to CAD. If UStart = 0 (default) the full model is translated. If UStart ≠ 0, only the universe UStart (and its nested universes) will be translated.**
levelMaX	**all**	**Level maximum of nested universe to be translated. If levelMax < highest nested universe level, cells inside the container cell whose level is levelMax will not be translated. This container cell will be the CAD solid written in the CAD file.**

Cells/Materials & Options

Keyword	Default Value	Description
rangeType	all (for cells) exclude (for materials)	**Define how to consider the range values. all : all the cells with any materials will be translated (range a no effect). include : include only cells/materials defined in range. exclude : exclude all cells/materials defined in range.**
range	**None (for cells) 0 (for materials)**	**List of cells or materials to be included/excluded during the conversion. The cells or material values can be entered as a single value or a range values. Single and range values entries are separated by colon. A range value is defined as is:ie where "is" is the starting value and "ie" the ending value of the range. Both "is" and "ie" values are considering in the range values. Range example: range = 1, 4, 6:10, 20, 45:100**

Keyword	Default Value	Description
splitTolerance	**0**	**Fuzzy tolerance value used in the FreeCAD function "BOPTools.SplitAPI.slice". This function is used during the solid decomposition process.**

ConfigReverse.ini example

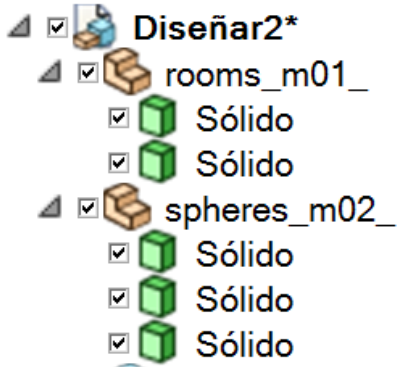
```
[Setting]
inputFile = my_CSG_model
CADFile = modelCAD

# CSG format allowed are mcnp or openMC_XML
inFormat = mcnp

# box dim in cm
# box entries xmin xmax ymin ymax zmin zmax
outBox = -500 500 -500 500 0 1000

[Levels]
UStart = 0
levelMax = all

# For cell and materials "rangeType" value may be all, include, exclude
# range example is : 2:20, 34, 38, 100:200
[Cells]
rangeType = all
#range = 1:13

[Materials]
rangeType = exclude
range = 0

[Options]
splitTolerance = 0.01
```

Materials definition

Material number, density and name are defined in a file

```
# Materials and density
# FORMAT: NUM DENS NAME
# 0 1.0 EXPLICITELY DEFINED VOID MATERIAL
9001 7.8     Eurofer
9004 9.5     LiPb
9006 0.7     Water
9013 7.93    SS316L
9010 8.2     Inconel718
9016 0.01    Helium
9017 11.34   Pipe Shield
9018 11.34   Tank Shield
9019 0.35    Tank insulator
9020 0.35    Cold trap insulator
9021 11.34   Cold trap shield
9022 11.34   Pump Shield
9023 0.67    Molecular Sieve
9024 2.7014  St909 alloy
```

Materials are assigned in the CAD tree at any level



Key text for material _mXX_dYY.YY_
XX number of material
YY.YY dilution/density correction factor (optional)

Model preparation

Good practices

Preparation of CAD neutronic model

The CAD neutronic model should be suitable for conversion:

1. The surface types are restricted to those supported by MC codes*.(mandatory)
   *Up to second order surfaces & tori with axis parallel to X, Y and Z axis

2. No interferences between solids. (desirable)

3. Reduction of unnecessary complexity. (desirable)

This part is the CAD side. Hereafter we will focus on SpaceClaim.

Preparation of CAD neutronic model

In some models arises some problems during the conversion that are in the part of the CAD tool.

1. Some solids in STEP format in SpaceClaim are not saved properly. This can be detected by opening the solid in FreeCAD.

Solution: Save the model in IGS format, open it in SpaceClaim and save again in STEP format.

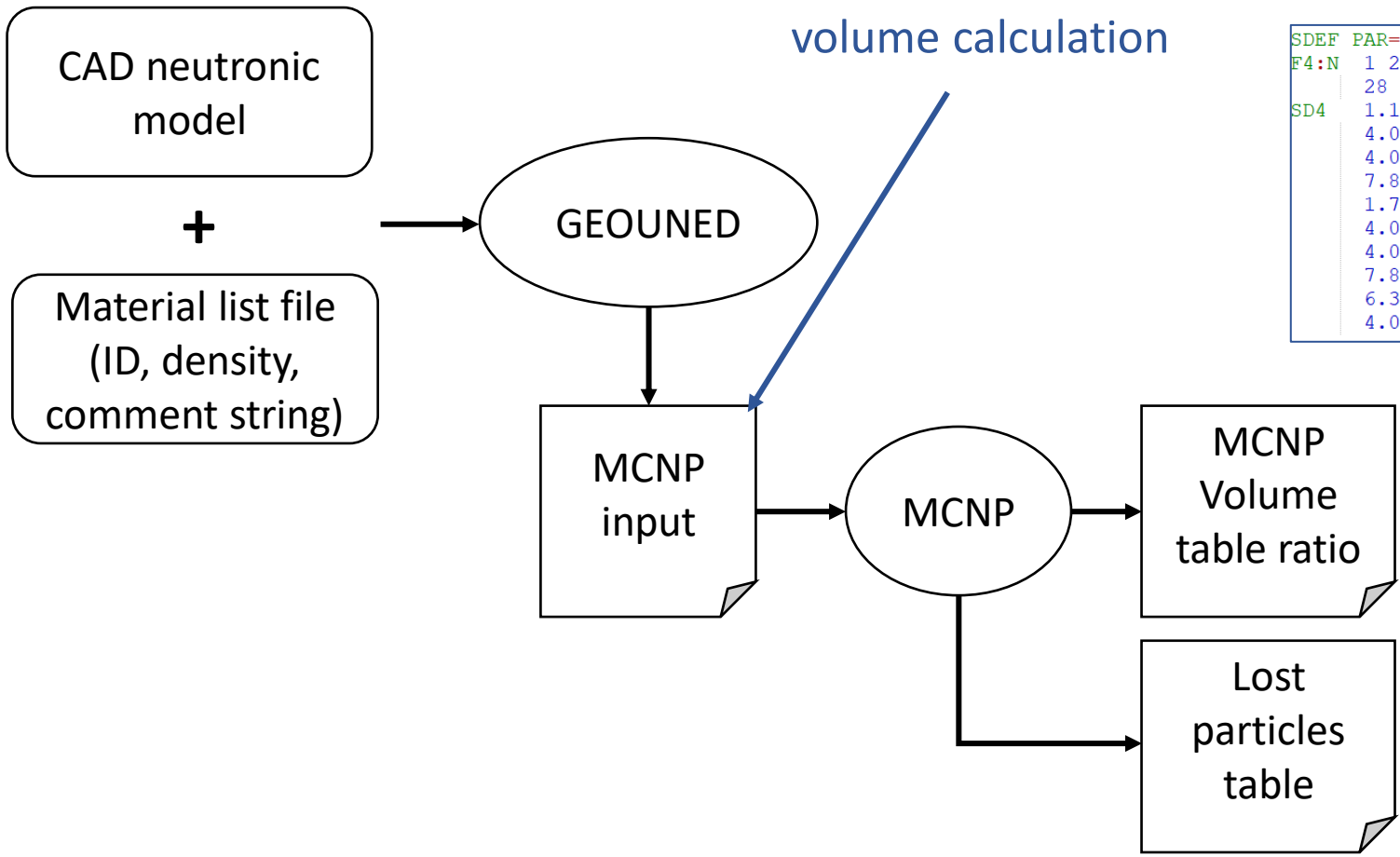
2. Solids with very small details and faces (with no sense from the point of view of the neutronic analysis)

Solution: Running the SpaceClaim functions Split Edges, Extra Edges, Small Faces and Inexact Edges until all tests give you 0 problems.

3. Similar surfaces that produces lost particles.

Solution: GEOUNED can handle part of this kind of surfaces by modifying the tolerances and number formats. This also can be managed by using replace surface function of SpaceClaim to be sure that the surface are the same.

Automatic model verification



Automatic SDEF and Tally definition for statistical volume calculation

volSDEF = True

GEOUNED source and tally definition

```
SDEF PAR=N NRM=-1 SUR=119 WGT=3.8587656e+07
F4:N  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27
      28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48
SD4   1.1305650e+09 1.1305650e+09 7.5037500e+08 9.3375000e+07 4.0172000e+04
      4.0172000e+04 4.0172000e+04 4.0172000e+04 4.0172000e+04 4.0172000e+04
      4.0172000e+04 4.0172000e+04 8.0955088e+05 2.0400000e+04 7.8209324e+04
      7.8209324e+04 1.6336282e+05 3.3696000e+06 1.5459226e+05 1.7518889e+04
      1.7518889e+04 3.5507600e+04 5.5126400e+04 7.5080951e+03 7.5080951e+03
      4.0172000e+04 4.0172000e+04 4.0172000e+04 4.0172000e+04 4.0172000e+04
      4.0172000e+04 4.0172000e+04 4.0172000e+04 9.4808928e+05 7.8209324e+04
      7.8109292e+04 3.3696000e+06 1.7722898e+05 1.7518889e+04 1.7518889e+04
      6.3198480e+04 7.5080951e+03 7.5080951e+03 2.3680000e+04 1.8912388e+05
      4.0263600e+04 1.8000000e+06 4.9896000e+07
```

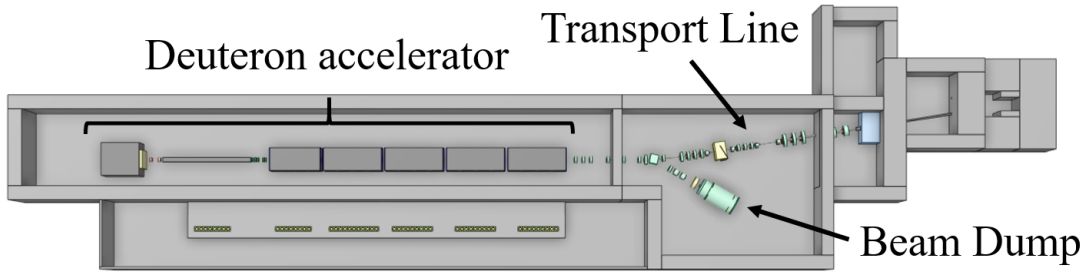
Tally normalized by CAD volume should be one if the solid is right

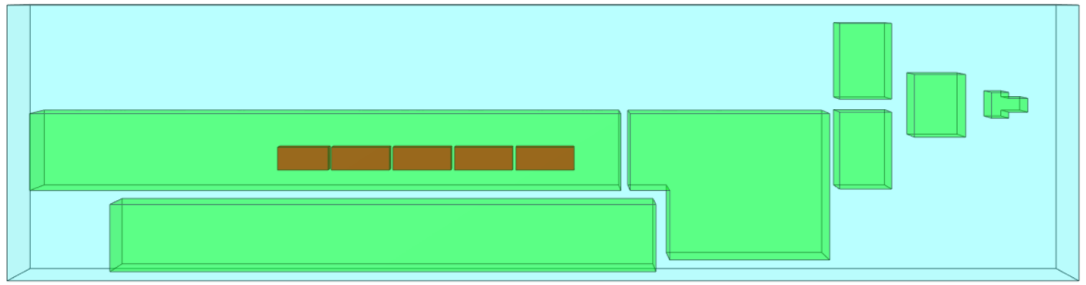
Void generation

Enclosures & envelopes

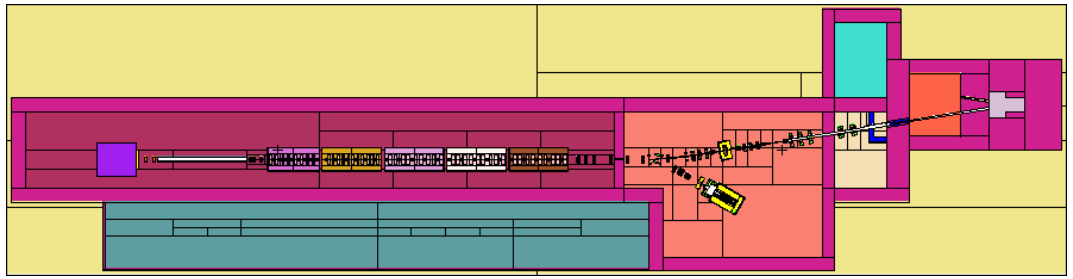
Enclosures and envelopes

IFMIF-DONES: complex void structure





Hierarchical nested enclosure structure



IFMIF-DONES MCNP model (pz = 0)

CAD solids can be used to void generation (enclosures) or exclusion regions (envelopes).

Nested structure of the enclosures (several levels) can be defined

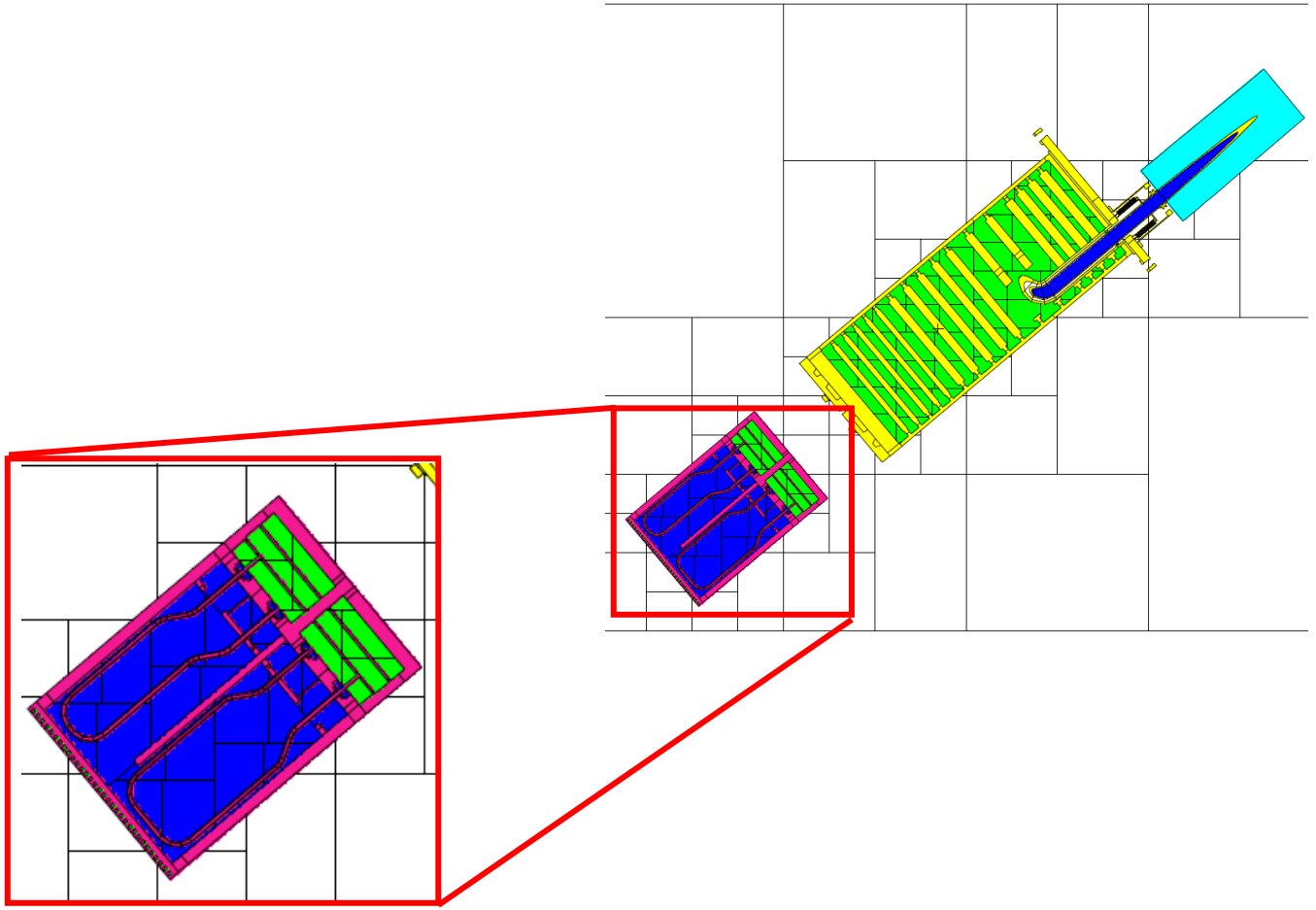
- 1st level: outermost enclosure
- 2nd level: room enclosures
- 3rd level: Superconducting Radio Frequency Modules

Structured hierarchical voids producing cleaner inputs

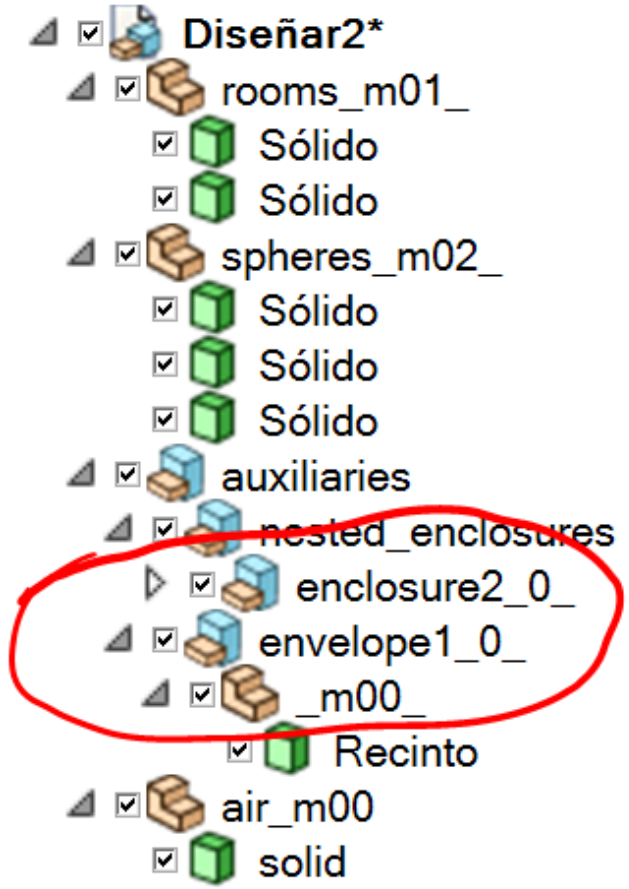
Easy material assignment

Other example of enclosure

Enclosures to define LiPb and water



Definition of enclosure and envelopes



Enclosures are defined in the CAD tree by the key word ‘enclosureX_Y_’

X corresponds to the number of the enclosure
Y corresponds to the upper level of enclosures

Envelopes are defined in the CAD tree by the key word ‘envelopeX_Y_’

X corresponds to the number of the envelope
Y corresponds to the upper level of enclosures

Debug & log files

fuzzySurfaces file

Indicates which surfaces have been considered equal regarding the tolerance and which ones not.
So far, only distances of planes and cylinders are saved.

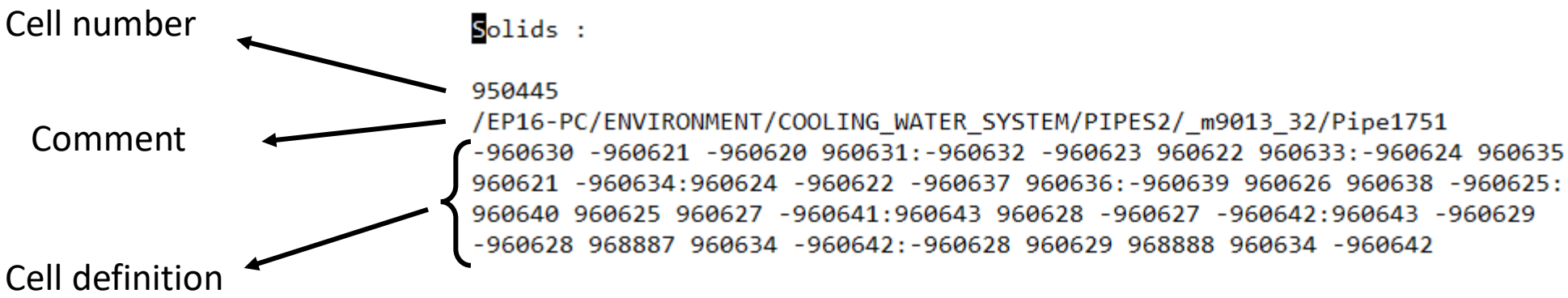
- planes: independent term Δd $(aX + bY + cZ + d = 0)$
- Cylinders: distance between axis and ΔR

The criteria to be in the file is that evaluated quantity is $\in (0.5 \times tolerance, 2 \times tolerance)$

```
Same surface : False
Plane distance / Tolerance : 0.003982017722591991 0.002
 40      P    6.4278761e-01 -7.6604444e-01  2.2415620e-13  1.7668000e+03
 0       P    6.4277701e-01 -7.6605334e-01  4.5401709e-06  1.7668004e+03

Same surface : True
Plane distance / Tolerance : 0.0013033170507696923 0.002
 25      P    6.4278761e-01 -7.6604444e-01  2.2415620e-13  1.7668000e+03
 0       P    6.4277701e-01 -7.6605334e-01  4.5401709e-06  1.7668001e+03
```

Suspicious solids

"Warning_Solids_definition.txt" file contains information about MC definition of suspicious solids

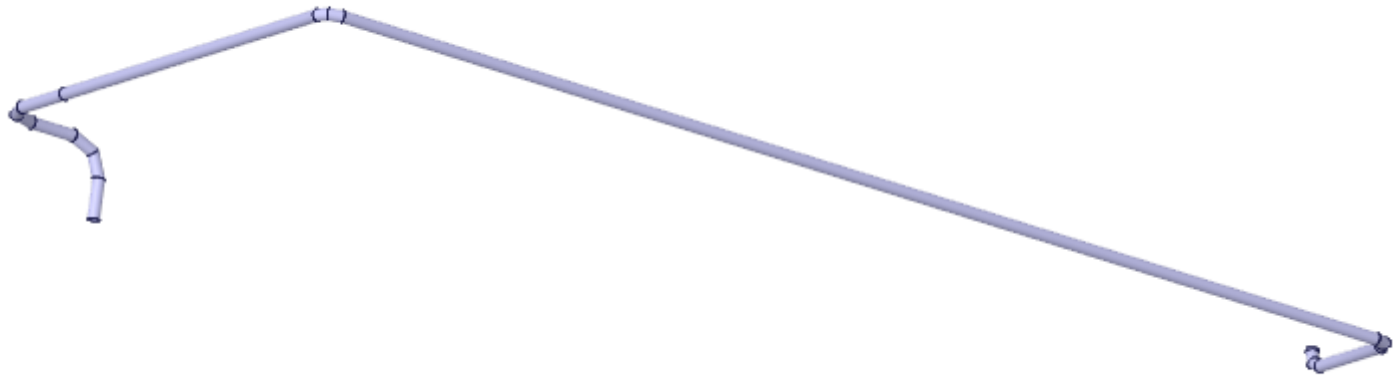


The suspicious solids are saved in "Suspicious_solids" folder that contains two STEP files for each solid the original and decomposed (split) version.

Treatment of problematic solids

Example of a solid with errors

Typical pipe after script to pass from tori to cylinders



Error in the decomposition. Strange surface type

Decomposing solid: 3/17
bad Surface type <SurfaceOfRevolution object>
bad Surface type <SurfaceOfRevolution object>
bad Surface type <SurfaceOfRevolution object>

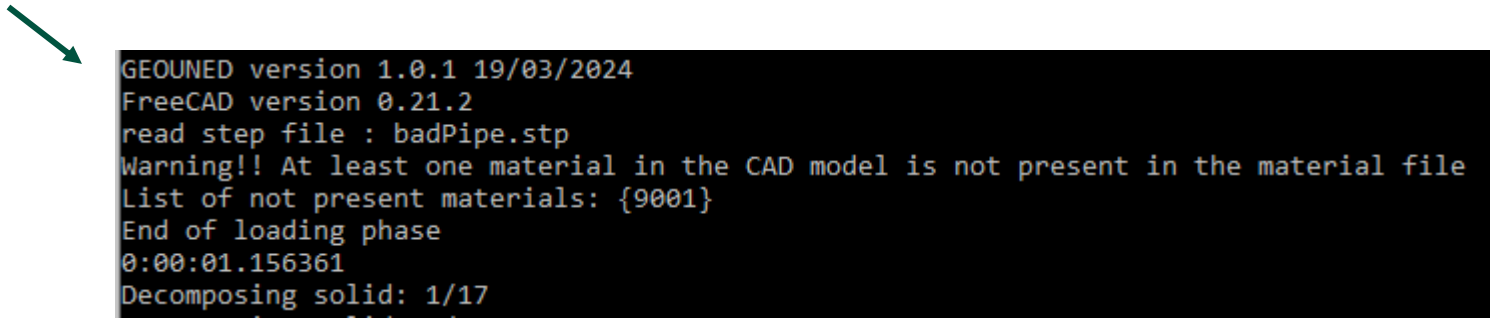
Let's see how to check this in FreeCAD!

Reporting errors

The errors found during a conversion case should be reported using Issues of github.

Ideally the steps to follow:

1. Try to isolate the error as much as possible (within our capabilities and knowledge).
2. Send always the message of error that is in the console: strange type of surface, unexpected exit, python exception…
3. Include in the github issue all the files used in the conversion as well as the GEOUNED version used (it is always at the beginning of the translation*).



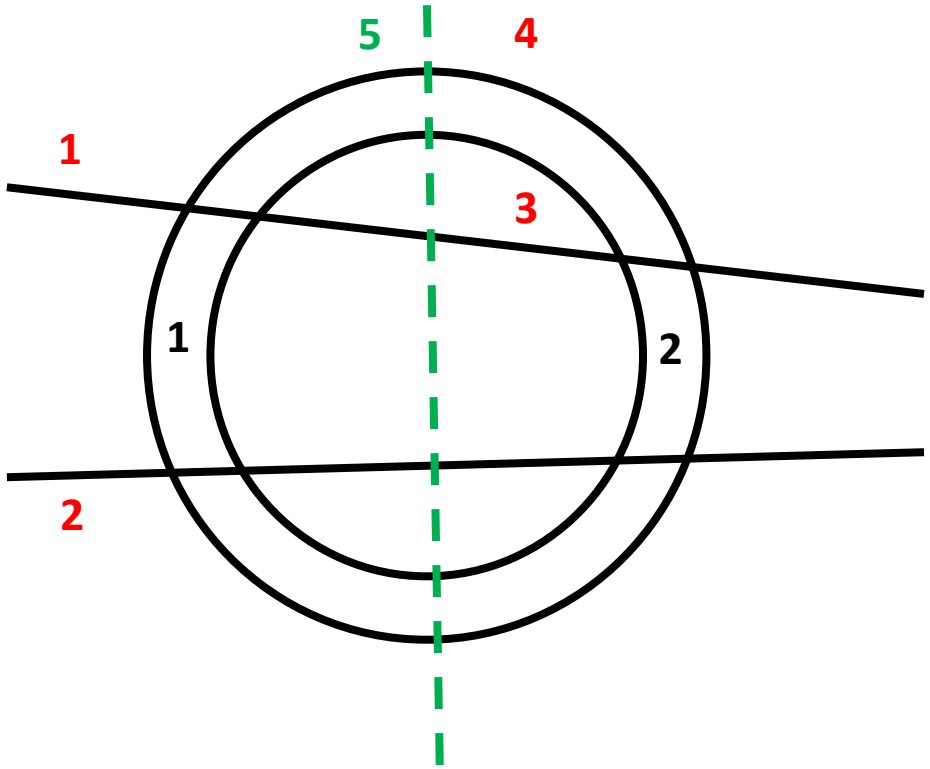
* Always the first option is to try the last version of dev branch (git pull) to check if your problem is already solved

Identified Issues

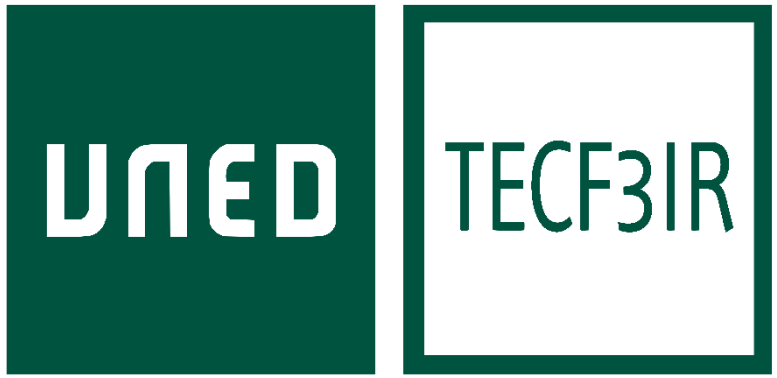
Identified Issues

The communicated issues have been solved so far.

1. Tori can be handled without simplification. Is simplification is activated additional planes are removed and the problem arise again.



If the solid is represented by region 1 and additional plane is required to separate from 2 region. Only the faces cannot do that.



FUSION FOR ENERGY

THE EUROPEAN JOINT UNDERTAKING FOR ITER AND THE DEVELOPMENT OF FUSION ENERGY

Thank you for your attention

GEOUNED code development has been partially supported by the Ministerio de Ciencia e Innovación (MICINN), Spain under Plan Estatal I+D+i - Retos de la Sociedad, project PID2019-109362RA-I00