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Title: Python Tool for Writing MCNP Unstructured Mesh Input Files

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Python Tool for Writing MCNP Unstructured Mesh Input Files

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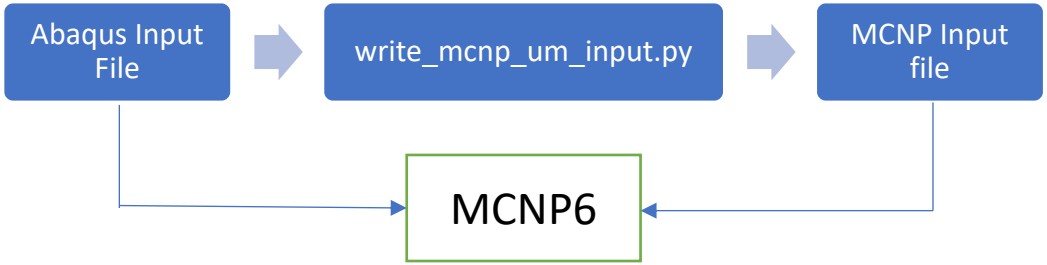
MCNP Unstructured Mesh (UM) Calculation

- An MCNP UM calculation requires two input file types:
  - MCNP input file
  - Abaqus input file(s)
- An Abaqus input file must have the correct Abaqus syntax rules and meet additional MCNP requirements.
- write_mcnp_um_input.py was developed to create an MCNP UM input file.




```
"""
import numpy as np
import os

from abaqus_input import read_abaqus
from abaqus_input import compute_global_model_extents
from abaqus_input import extract_mesh_data

from abq_part_elsets import  compute_part_elset_data
from abq_part_elsets import  compute_part_elset_material_data

from abq_part_data_checking import check_material_elset_numbers

#-----------------------------------------------------------------------
def write_mcnp_um_input(filein, fileout=None, eeout=None, meshinfo=None,
                        cellcards=None, surfacecards=None, datacards=None,
                        bgmaterial=0, lenconv=1.0, radiusext=1.0, denunit='g/cc',
                        writemeshinfo=False, writecomments=False):
```

Abaqus Input File

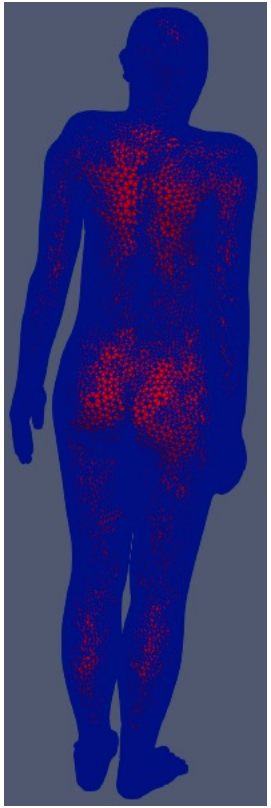
simple part model

```
*Part, name=Part-1000000
*Node
+--733 lines: 1,  1.4585610000, 1.1138850000, 33.1544720000--------
*Element, type=C3D4
+--2177 lines: 1,  1,  2,  3,  4-----------------------------------
*Nset, nset=Set-material_100, generate
1,   733,   1
*Elset, elset=Set-material_100, generate
1,   2177,   1
*Nset, nset=Set-statistic_100, generate
1,   733,   1
*Elset, elset=Set-statistic_100, generate
1,   2177,   1
*End Part
**
*Part, name=Part-2000000
*Node
+--728 lines: 1,  -2.9332100000, 3.7297810000, 31.2348880000-------
*Element, type=C3D4
+--2219 lines: 1,  1,  2,  3,  4-----------------------------------
*Nset, nset=Set-material_200, generate
1,   728,   1
*Elset, elset=Set-material_200, generate
1,   2219,   1
*Nset, nset=Set-statistic_200, generate
1,   728,   1
*Elset, elset=Set-statistic_200, generate
1,   2219,   1
*End Part
```

mrcp-af.inp 1,11109836

```
*Instance, name=Part-80020000-1, part=Part-80020000
*End Instance
**
*Instance, name=Part-81000000-1, part=Part-81000000
*End Instance
**
*Instance, name=Part-82000000-1, part=Part-82000000
*End Instance
**
*Instance, name=Part-82010000-1, part=Part-82010000
*End Instance
**
*Instance, name=Part-82020000-1, part=Part-82020000
*End Instance
**
*Instance, name=Part-83000000-1, part=Part-83000000
*End Instance
**
*Instance, name=Part-84000000-1, part=Part-84000000
*End Instance
**
*Instance, name=Part-84010000-1, part=Part-84010000
*End Instance
**
*Instance, name=Part-84020000-1, part=Part-84020000
*End Instance
**
*Instance, name=Part-85000000-1, part=Part-85000000
*End Instance
```

mrcp-af.inp 11109429,11109836



Element sets and instances are used to define the MCNP pseudo-cells.

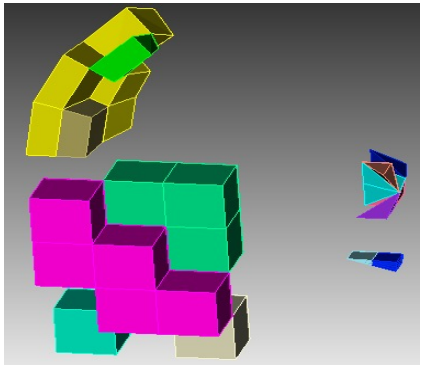
An Abaqus input file is from ICRP, 2020. Adult mesh-type reference computational phantoms. ICRP Publication 145. Ann. ICRP 49(3).

Abaqus Input File

complex part model

```
*Part, name=BLOCK-B
*Node
+-- 51 lines: 1,          -5.,          0.,          10.-------
*Element, type=C3D8R
+-- 12 lines: 13,    1,  19,  61,  24,  42,  77,  95,  73--------
*Elset, elset=SET_STATISTIC_004
 13, 15, 20, 21, 24
*Elset, elset=SET_STATISTIC_001
 37, 38, 39, 41, 44, 47, 48
*Elset, elset=SET_MATERIAL_001
 13, 15, 20, 21, 24, 37, 38, 39, 41, 44, 47, 48
** Section: Section-1-SET_MATERIAL_001
*Solid Section, elset=SET_MATERIAL_001, material=ALUMINUM_001
,
*End Part
**
*Part, name=HEMI-A
*Node
+-- 33 lines: 9,          -15.,          0.,          0.-------
*Element, type=C3D8R
+--  8 lines: 147, 302, 193, 192, 294, 218,  67,  66, 221-------
*Elset, elset=SET_STATISTIC_012
 147, 149
*Elset, elset=SET_STATISTIC_023
 150, 171
*Elset, elset=SET_STATISTIC_034
 151, 162
*Elset, elset=SET_STATISTIC_011
 160, 161
*Elset, elset=SET_MATERIAL_001
 147, 149
*Elset, elset=SET_MATERIAL_1008
 150, 151, 160, 161, 162, 171
** Section: Section-2-SET_MATERIAL_001
*Solid Section, elset=SET_MATERIAL_001, material=ALUMINUM_001
** Section: Section-3-SET_MATERIAL_1008
*Solid Section, elset=SET_MATERIAL_1008, material=WATER_1008
,
*End Part
```

```
*Assembly, name=Assembly
**
*Instance, name=HEMI-A-1, part=HEMI-A
*End Instance
**
*Instance, name=BLOCK-B-1, part=BLOCK-B
          0.,           0.,          -25.
*End Instance
**
*Instance, name=TET_ONLY-1, part=TET_ONLY
+--  2 lines: 10.,          15.,          -15.----
*End Instance
**
*Instance, name=HEX_WEDGE1-1, part=HEX_WEDGE1
+--  2 lines: 0.,           0.,          -22.-----
*End Instance
**
*End Assembly
```



```
C 1: HEMI-A-1, HEMI-A, statistic-11
1     1008    -1.000000       0  u=1  $ WATER_1008
C
C 2: HEMI-A-1, HEMI-A, statistic-12
2        1    -2.700000       0  u=1  $ ALUMINUM_001
C
C 3: HEMI-A-1, HEMI-A, statistic-23
3     1008    -1.000000       0  u=1  $ WATER_1008
C
C 4: HEMI-A-1, HEMI-A, statistic-34
4     1008    -1.000000       0  u=1  $ WATER_1008
C
C 5: BLOCK-B-1, BLOCK-B, statistic-1
5        1    -2.700000       0  u=1  $ ALUMINUM_001
C
C 6: BLOCK-B-1, BLOCK-B, statistic-4
6        1    -2.700000       0  u=1  $ ALUMINUM_001
C
C 7: TET_ONLY-1, TET_ONLY, statistic-1
7        1    -2.700000       0  u=1  $ ALUMINUM_001
C
C 8: HEX_WEDGE1-1, HEX_WEDGE1, statistic-2
8        1    -2.700000       0  u=1  $ ALUMINUM_001
C
9        0                    0  u=1  $ background
C
C LEGACY CELLS
10       0                 -999  fill=1 $ fill cell
11       0                  999
```

```
embed1 meshgeo=abaqus
       mgeoin=block_hemi_v5_simplified.inp
       meeout=block_hemi_v5_simplified.eeout
       length=1.000000E+00
       background=9
       matcell=1 1  $ WATER_1008
               2 2  $ ALUMINUM_001
               3 3  $ WATER_1008
               4 4  $ WATER_1008
               5 5  $ ALUMINUM_001
               6 6  $ ALUMINUM_001
               7 7  $ ALUMINUM_001
               8 8  $ ALUMINUM_001
```

write_mcnp_um_input

```
def write_mcnp_um_input(filein,
                        fileout=None,
                        eeout=None,
                        meshinfo=None,
                        cellcards=None,
                        surfacecards=None,
                        datacards=None,
                        bgmaterial=0,
                        lenconv=1.0,
                        radiusext=1.0,
                        denunit='g/cc',
                        writemeshinfo=False,
                        writecomments=False):
```

- A new algorithm is used to build an MCNP UM model: faster than um_pre_op, flexible to use, writing detailed mesh cell information.
- Extensive error checking on an Abaqus input file format.
- 40 Abaqus input files were used to test the Python code.

```
usage: write_mcnp_um_input.py [-h] -i <file.inp> [-o <file.mcnp>]
                              [-e <file.eeout>] [-mi <filename.info>]
                              [-cc <cellcards.txt>] [-sc <surfacecards.txt>]
                              [-dc <datacards.txt>] [-b <material_number>]
                              [-l <len_conversion>] [-re <radius_extension>]
                              [-du <density_unit>] [-wc] [-wm]

** Write MCNP Unstructured Mesh Input file **

optional arguments:
  -h, --help            show this help message and exit
  -i <file.inp>, --input <file.inp>
                        Abaqus input for constructing MCNP input file
  -o <file.mcnp>, --output <file.mcnp>
                        output file name
  -e <file.eeout>, --eeout <file.eeout>
                        eeout file name in EMBED card
  -mi <filename.info>, --meshinfo <filename.info>
                        a mesh information file name
  -cc <cellcards.txt>, --cellcards <cellcards.txt>
                        MCNP cell cards file to include
  -sc <surfacecards.txt>, --surfacecards <surfacecards.txt>
                        MCNP surface cards file to include
  -dc <datacards.txt>, --datacards <datacards.txt>
                        MCNP data cards file to include
  -b <material_number>, --back <material_number>
                        background material for MCNP input file
  -l <len_conversion>, --length <len_conversion>
                        a multiplication conversion factor to centimeters
  -re <radius_extension>, --radext <radius_extension>
                        a radius extension of a sphere surface for a fill cell
                        (in centimeters)
  -du <density_unit>, --densityunit <density_unit>
                        density unit option: g/cm^3 [default] or atoms/barn-cm
  -wc, --writecomments  write pseudo-cell comments in MCNP input file
  -wm, --writemeshinfo  write mesh information into mesh information file
```

not in um_pre_op

Example Output Files

```
No description
C
C Abaqus Input File: mrcp-af.inp
C
C High-Level Mesh Information:
C   Number of Parts:     187
C   Number of Instances: 187
C   Number of Materials: 187
C
C Details of mesh information are in file: mrcp-af.info
C
C PSEUDO CELLS
C
C 1: Part-1000000-1, Part-1000000, statistic-100
1      100    -0.000000       0  u=1  $ Material_100
C
C 2: Part-2000000-1, Part-2000000, statistic-200
2      200    -0.000000       0  u=1  $ Material_200
C
C 3: Part-3000000-1, Part-3000000, statistic-300
3      300    -0.000000       0  u=1  $ Material_300
C
C 4: Part-3010000-1, Part-3010000, statistic-301
4      301    -0.000000       0  u=1  $ Material_301
C
C 5: Part-3020000-1, Part-3020000, statistic-302
5      302    -0.000000       0  u=1  $ Material_302
C
C 6: Part-3030000-1, Part-3030000, statistic-303
6      303    -0.000000       0  u=1  $ Material_303
C
C 7: Part-4000000-1, Part-4000000, statistic-400
7      400    -0.000000       0  u=1  $ Material_400
C
C 8: Part-4010000-1, Part-4010000, statistic-401
8      401    -0.000000       0  u=1  $ Material_401
C
C 9: Part-4020000-1, Part-4020000, statistic-402
9      402    -0.000000       0  u=1  $ Material_402
C
```

no density in a file

```
embed1 meshgeo=abaqus
       mgeoin=mrcp-af.inp
       meeout=mrcp-af.eeout
       length=1.000000E+00
       background=188
       matcell=1 1  $ Material_100
               2 2  $ Material_200
               3 3  $ Material_300
               4 4  $ Material_301
               5 5  $ Material_302
               6 6  $ Material_303
               7 7  $ Material_400
               8 8  $ Material_401
               9 9  $ Material_402
              10 10  $ Material_403
              11 11  $ Material_404
              12 12  $ Material_405
              13 13  $ Material_500
              14 14  $ Material_501
              15 15  $ Material_600
              16 16  $ Material_700
              17 17  $ Material_800
              18 18  $ Material_801
              19 19  $ Material_802
              20 20  $ Material_803
              21 21  $ Material_804
              22 22  $ Material_805
              23 23  $ Material_806
              24 24  $ Material_807
              25 25  $ Material_808
              26 26  $ Material_900
              27 27  $ Material_910
              28 28  $ Material_1000
              29 29  $ Material_1010
              30 30  $ Material_1100
              31 31  $ Material_1110
              32 32  $ Material_1200
              33 33  $ Material_1210
              34 34  $ Material_1300
              35 35  $ Material_1400
              36 36  $ Material_1500
              37 37  $ Material_1600
```

```
number of parts: 187
number of instances: 187
number of materials: 187

total  number of nodes: 2523963
total  number of elements: 8582677

total  number of linear tet elements: 8582677
```

```
*** part name: Part-1000000
*** number of nodes: 733
*** element_type: c3d4
    number of elements: 2177
*** elset keywords: material
    elset number: 100
    number of elements in this set: 2177
*** elset keywords: statistic
    elset number: 100
    number of elements in this set: 2177
```

```
*** part name: Part-2000000
*** number of nodes: 728
*** element_type: c3d4
    number of elements: 2219
*** elset keywords: material
    elset number: 200
    number of elements in this set: 2219
*** elset keywords: statistic
    elset number: 200
    number of elements in this set: 2219
```

```
*** part name: Part-3000000
*** number of nodes: 2528
*** element_type: c3d4
    number of elements: 8296
*** elset keywords: material
    elset number: 300
    number of elements in this set: 8296
*** elset keywords: statistic
    elset number: 300
    number of elements in this set: 8296
```

It took about 20 seconds to process this Abaqus input file on a laptop. ~8.5M elements

Other Uses of The Python Tool

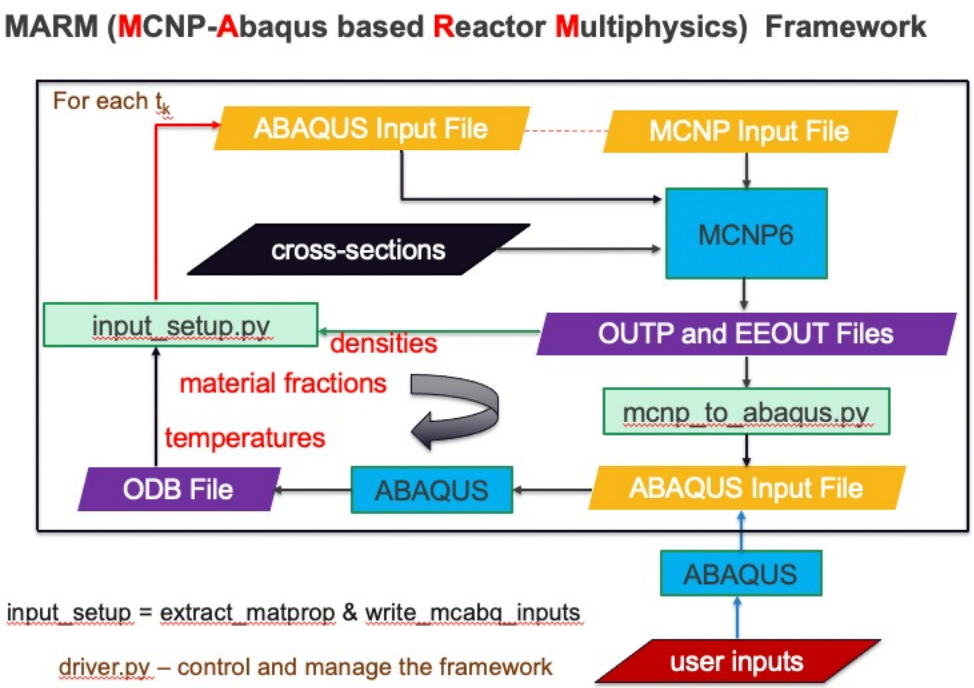
- A prototype for refactoring MCNP routines used to process an Abaqus input file.

  Python prototype

  ⬇

  Fortran production

- Integrate into MCNP-Abaqus Multiphysics Calculation Framework.



Conclusions

- Writing an MCNP input file for an unstructured mesh geometry can be a tedious, bookkeeping exercise.
- A new Python code was developed to process an Abaqus input file and write a corresponding MCNP input file to define the mesh geometry and material definition.
  - The Python code does extensive error checking on an Abaqus input format.
  - The Python code is significantly faster than and more options than um_pre_op.
  - The Python code provides detailed mesh geometry mapping between Abaqus and MCNP models.
- 40 Abaqus input files were used to verify this python code. MCNP input files generated by the Python code match those produced by um_pre_op.
- **write_mcnp_um_input.py should be used to write an MCNP input file instead of um_pre_op since um_pre_op is not updated in MCNP 6.3 version and write_mcnp_um_input.py is more flexible to use and provides detailed mesh information mapping.**