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Title: Developing Python Codes for Processing MCNP Elemental Edit Outputs

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Developing Python Codes for Processing MCNP Elemental Edit Outputs

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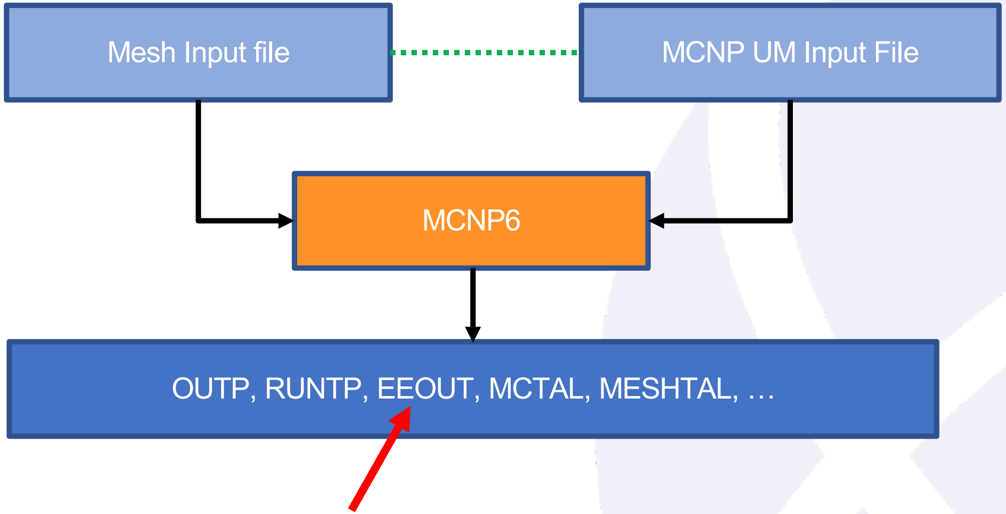
LA-UR-

Outline

1. MCNP unstructured mesh (UM) output files
2. Generating heat flux file for MCNP/Abaqus coupling calculations
3. Pseudo tallies
4. Add/Merge operation
5. Conclusion

MCNP Unstructured Mesh (UM): HDF5 EEOUT Files

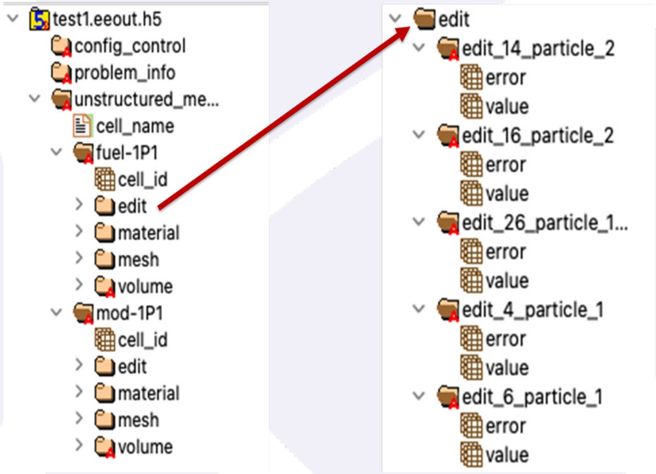


EEOUT (Elemental Edit OUTput) File Format:

- Flat File (ASCII or binary; MCNP 6.0 - 6.3 versions)
- HDF5 (binary; MCNP 6.3 version)

HDF5 Files

- Binary File format allows for writing and storing large complex data collections efficiently.
- HDF5 file is portable among different computing platforms.
- HDF5 file is easy to view, edit, and analyze using publicly available software tools or Python scripts.
  - HDF5/XDMF EEOUT files outputted by MCNP6.3 can be visualized with ParaView.
  - H5PY Python library can be used to extract data from HDF5 files.



HDF5 EEOUT tree viewed with HDFView

Three Ways to Produce EEOUT Files

- Add option on EMBED card (**file names must be in all lower case**)

```
embed1 meshgeo=abaqus
       mgeoin=test1.inp
       meeout=test1.eeout
       length= 1.00000E+00
       background=        3
       matcell=  1   1   2   2
```

Option 1: ASCII EEOUT
Produces:
test1.eeout

```
embed1 meshgeo=abaqus
       mgeoin=test1.inp
       hdf5file=test1.eeout.h5
       length= 1.00000E+00
       background=        3
       matcell=  1   1   2   2
```

Option 2: HDF5 EEOUT
Produces:
test1.eeout.h5
test1.eeout.h5.xdmf

```
embed1 meshgeo=abaqus
       mgeoin=test1.inp
       meeout=test1.eeout
       hdf5file=test1.eeout.h5
       length= 1.00000E+00
       background=        3
       matcell=  1   1   2   2
```

Option 3*: Both
Produces:
test1.eeout
test1.eeout.h5
test1.eeout.h5.xdmf

*Bad for large data sets

Generating Abaqus Heat Flux Input File

Extract energy deposition and elemental volumes from ASCII EEOUT file, compute heat flux for each element, and write an Abaqus heat flux input file.

Two Python codes:

- ASCII EEOUT Files: eeout_to_inp.py
- HDF5 EEOUT Files: h5eeout_to_inp.py

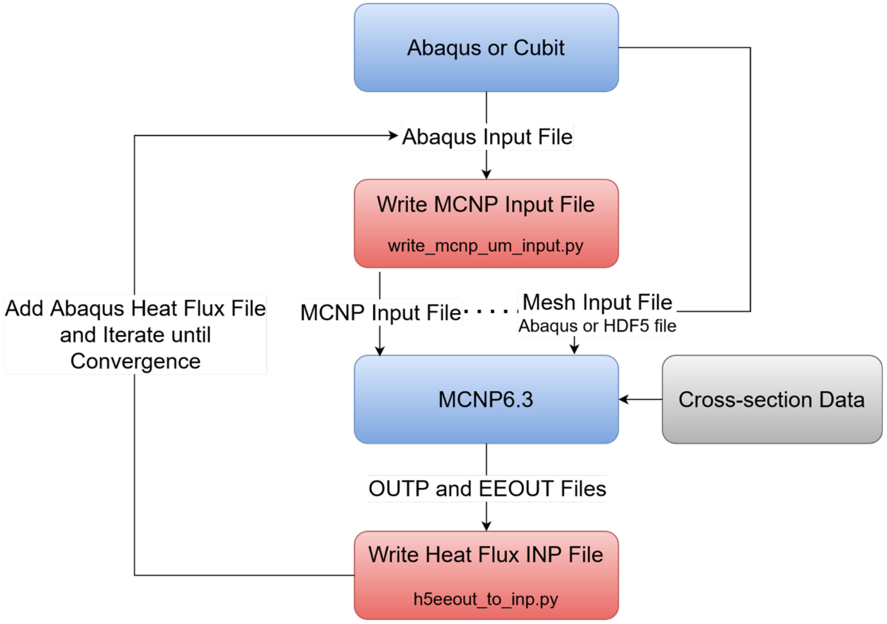
```
** STEP: Step-1
**
*Step, name=Step-1, nlgeom=NO
*Heat Transfer, steady state, deltmx=0.
1., 1., 1e-05, 1.,
*include, input=heatflux.inp
**
** BOUNDARY CONDITIONS
**
** Name: BC-1 Type: Temperature
*Boundary
Set-1, 11, 11, 1000.
**
```

Abaqus input file for heat transfer calculation

```
*amplitude, name=thermalAmplitude
0, 500.0
1, 500.0
1e+33, 500.0
*dflux, amplitude=thermalAmplitude
fuel-1.1, bf, 0.0008791459091281776
fuel-1.2, bf, 0.000858925988686834
fuel-1.3, bf, 0.0008337849284038419
fuel-1.4, bf, 0.0007818964855862113
fuel-1.5, bf, 0.0008136929202148363
fuel-1.6, bf, 0.0007244441603790287
fuel-1.7, bf, 0.0007469014558716738
fuel-1.8, bf, 0.0007183356470067473
fuel-1.9, bf, 0.0006557528548886173
fuel-1.10, bf, 0.000575632638423113
```

Abaqus heat flux input file

Generating Heat Flux file for MCNP/Abaqus Coupling Calculations



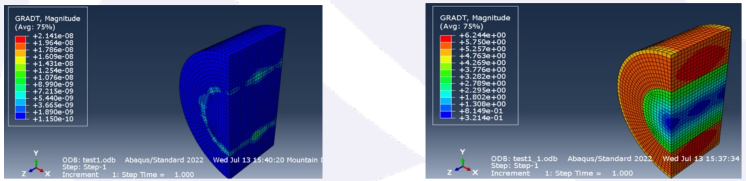
MCNP/Abaqus Coupling Calculations*

*This python code is just a small portion of a bigger project at LANL called MARM (MCNP Abaqus based Reactor Multiphysics) software package being developed for microreactor applications.

Test #	ASCII EEOUT Avg Test Runtime (s)	HDF5 EEOUT Avg Test Runtime (s)	Percent Difference (%)	Performance Increase	Number of Elements
1	0.12	0.06	50.45	2.02	26,080
2	0.11	0.06	46.62	1.87	26,080
3	0.11	0.06	48.16	1.92	26,080
4	0.44	0.21	51.95	2.08	118,800
5	0.81	0.37	53.80	2.16	195,848

Performance results comparing the processing of Legacy ASCII EEOUT File to HDF5 files.

Neutron edit values of yttrium-hydride moderator with 19.75% enriched U-235 fuel, from left to right, edit type 4 (flux [particles/cm^2]), edit type 6 (energy deposition [MeV/g]).



Change in the Abaqus outputs when the heat flux file is added.

What is a Pseudo Tally

- Volume weighted tallies based on edit values
- Equivalent to MCNP tally avg. over a cell (i.e. F4, F6, and F7 tallies) but w/o
  - Statistical uncertainty
  - Tally fluctuation charts
- Pseudo tallies are over the pseudo cells
  - Pseudo cells are analogous to the cells in MCNP when using constructed solid geometry (CSG).
  - Pseudo cells define with the null surface (0) and contain UM models.

$$tally_i = \frac{\sum_{n=1}^{N} vol_n \cdot edit_n}{\sum_{n=1}^{N} vol_n}$$

$tally_i$	tally for pseudo-cell i form corresponding edit
vol_n	volume of element n
$edit_n$	edit result of element n
N	total number of elements in i

```
if embee_num == 0:
    for cname in cell_name:
        cell_mesh_data = mesh_data.get(cname)
        cell_edit_data = edit_data.get(cname)

        vol = np.array(cell_mesh_data[1])
        sum_vol = np.sum(vol)

        tally_dict = {}
        for key in cell_edit_data.keys():
            key_split_list = key.split('_')
            if key_split_list[1][-1] in ['4', '6', '7']:
                cur_edit_data = cell_edit_data.get(key)
                eitem = cur_edit_data[1]
                titem = cur_edit_data[2]
                value = np.array(cur_edit_data[3])
                tally = np.sum(vol*value)/sum_vol
                tally_dict[key] = [eitem, titem, sum_vol, tally]
            else:
                logging.eror("invalid embee number {key}")
                ret_code = 1
                return ret_code, cell_name, data
        data.append(tally_dict)
```

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Pseudo-tally results

- Input geometry
  - Same as the one used for generating the heat flux file
  - Cell 1:
    - Fuel: 19.75% enriched U-235
  - Cell 2:
    - Moderator: Yttrium-hydride

Cells	F4 tally [particles/cm^2]	F4 Error	Embee 4 Pseudo Tally [particles/cm^2]
1	7.36E-03	0.0003	7.36E-03
2	2.19E-03	0.0003	2.19E-03

Cells	F6 tally [MeV/g]	F6 Error	Embee 6 Pseudo Tally [MeV/g]
1	1.48E-03	0.0004	1.48E-03
2	3.53E-05	0.0004	3.53E-05

Pseudo tallies of neutron flux (4) and neutron energy deposition (6) versus MCNP standard tallies.

Cells	F4 tally [particles/cm^2]	F4 Error	Embee 4 Pseudo Tally [particles/cm^2]
1	1.59E-03	0.0006	1.59E-03
2	4.74E-04	0.0011	4.74E-04

Cells	F6 tally [MeV/g]	F6 Error	Embee 6 Pseudo Tally [MeV/g]
1	9.62E-05	0.0006	9.62E-05
2	1.55E-05	0.0012	1.55E-05

Pseudo tallies of photon flux (4) and photon energy deposition (6) versus MCNP standard tallies.

Add/Merge Operation

Consistency Check

Independent calculational runs of a problem using different seeds random seeds (and numbers of histories run).

Many HDF5 EEOUT from the runs. Check the mesh, material, and edit group structures to ensure that they are the same.

Add

Add the edit values from many independent runs together; results are **not weighted** by the number of histories from each run.

Merge

Add the edit values from the many independent runs; results are **weighted** by the number of histories from each run.

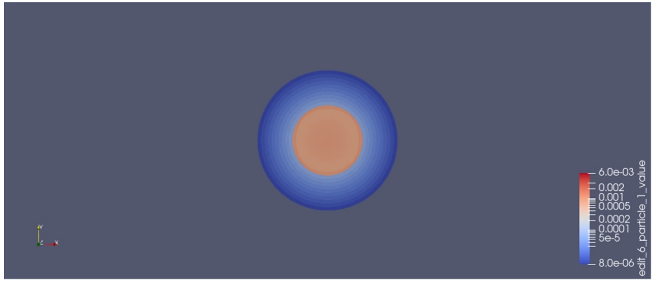
Add/Merge Results

Neutron Energy Deposition [MeV/g] Log Scale: 8E-06 to 6E-03

Test1.eeout.h5

Nps: 1E6

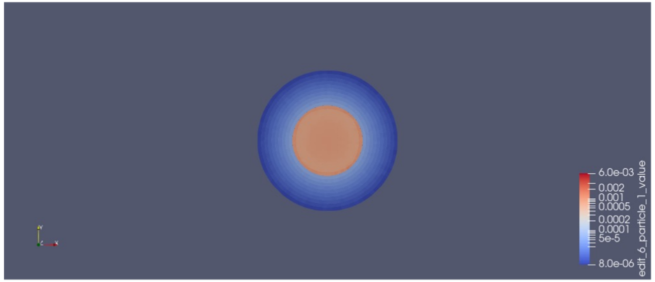
Rand seed =3456235679



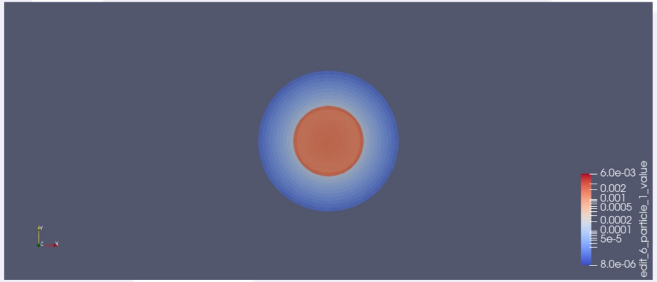
Test2.eeout.h5

Nps: 1E5

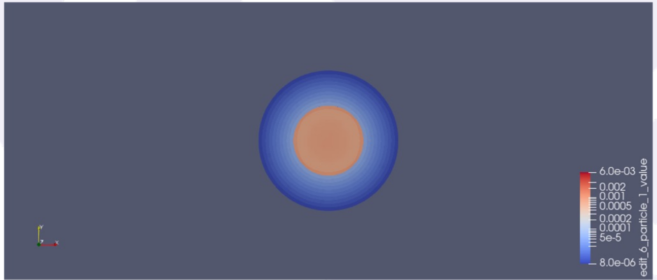
Rand seed=17854369



Add Results



Merge Results



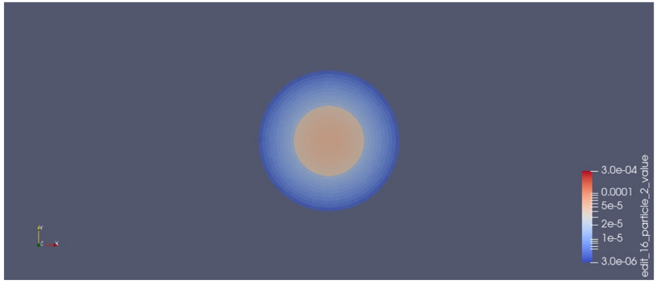
Add/Merge Results

Photon Energy Deposition [MeV/g] Log Scale: 3E-06 to 3E-04

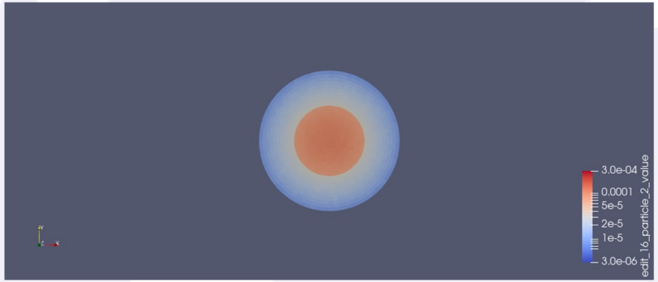
Test1.eeout.h5

Nps: 1E6

Rand seed =3456235679



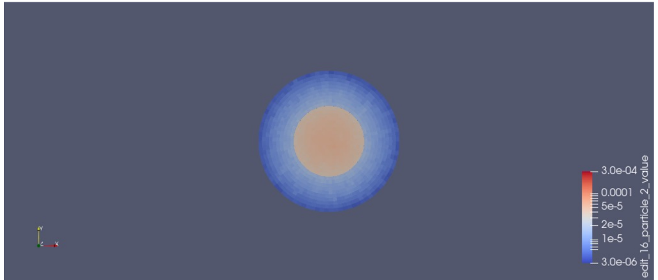
Add Results



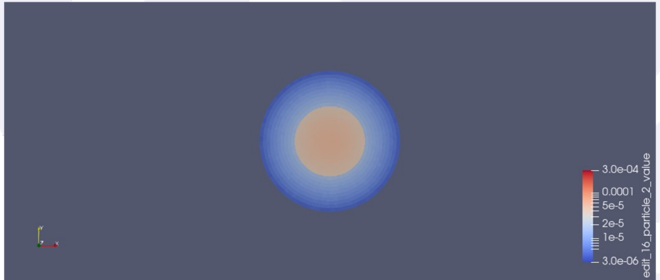
Test2.eeout.h5

Nps: 1E5

Rand seed=17854369



Merge Results



Conclusion

- We developed four python codes for processing HDF5 EEOUT files outputted by MCNP6.3. These Python codes use H5PY Python library. They will be released to public.
  - h5eeout_to_inp.py
  - pseudo_tally.py
  - add_eeout_h5.py
  - merge_eeout_h5.py

H5PY was imported

```python
def get_h5eeout_data(eeout_filename, edit_num=6):
    """
    Get data from an HDF5 EEOUT file.

    Parameters
    ----------
    eeout_filename : string
        An HDF5 EEOUT file.
    edit_num : integer, optional
        An EMBEE number. The default is 6.

    Returns
    -------
    ret_code : integer
        A return code.
    cell_name : list of string
        A list of cell names.
    mesh_data : dictionary
        Keys are cell_name and values are mesh data lists (density and volume).
    edit_data : dictionary
        Keys are cell_name and values are edit data lists.

    """
    ret_code = 0
    cell_name = []
    mesh_data = {}
    edit_data = {}

    if not os.path.isfile(eeout_filename):
        logging.error(f'{eeout_filename} file does not exist')
        ret_code = 1
        return ret_code, cell_name, mesh_data, edit_data

    h = h5py.File(eeout_filename,'r')

    # check path
    um = 'unstructured_mesh'
    cn = 'cell_name'
    path = f'/{um}/{cn}'
    if path not in h:
        logging.error(f'{path} is not a path in {eeout_filename}')
        ret_code = 2
        return ret_code, cell_name, mesh_data, edit_data

    # get cell name dataset
    cell_label = list(h[path])
    path_name = []
    for c in cell_label:
        name = c.decode('utf-8').strip()
        path_name.append(f'/{um}/{name}')
        cell_name.append(name)
```

References

1. J. A. Kulesza, T. R. Adams, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, T. P. Burke, A. R. Clark, R. A. Forster III, J. F. Giron, A. S. Grieve, C. J. Josey, R. L. Martz, G. W. McKinney, E. J. Pearson, M. E. Rising, C. J. Solomon Jr., S. Swaminarayan, T. J. Trahan, S. C. Wilson, and A. J. Zukaitis, “MCNP Code Version 6.3.0 Theory & User Manual,” Los Alamos National Laboratory, Los Alamos, NM, USA, LA-UR-22-30006.
2. V. K. Mehta, J. C. Armstrong, D. V. Rao, and D. Kotlyar, "Capturing multiphysics effects in hydride moderated microreactors using MARM”, Annals of Nuclear Energy, Vol 172 (2022), https://doi.org/10.1016/j.anucene.2022.109067.

Abstract

The MCNP code can track particles on unstructured mesh (UM) geometry models and tally quantities of interests in finite elements. It writes these quantities of interests into a file known as an elemental edit output (EEOUT) file. MCNP6.3 can create two EEOUT file formats: ASCII and HDF5. The results in EEOUT files are typically processed for further analysis and/or multiphysics calculations, such as MCNP/Abaqus coupling calculations. An HDF5 EEOUT file format is a new feature in MCNP6.3, and this work focuses on developing Python codes for post-processing HDF5 EEOUT files.