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Verifying LNK3DNT Feature in MCNP6

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Outline

- MCNP LNK3DNT Feature
  - LNK3DNT file description
  - Embed a LNK3DNT file to MCNP6
- Using MCNPTools to create LNK3DNT files
  - One material elements
  - Mixed material elements
- Testing MCNP6 LNK3DNT Feature
  - Create MCNP input files for constructive solid geometry (CSG) and LNK3DNT problems.
  - Run CSG and LNK3DNT problems to compare the calculation results

MCNP6 LNK3DNT Feature

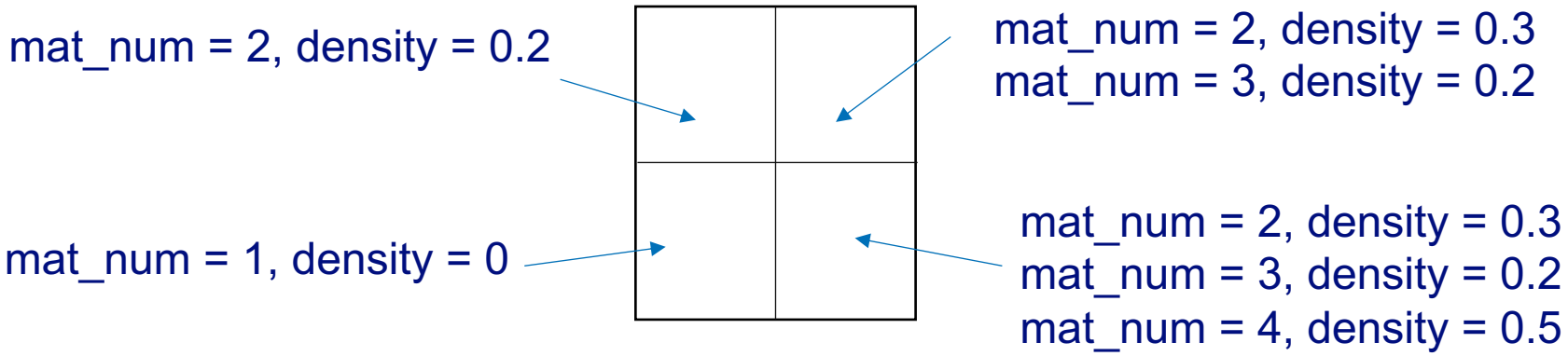
LN3DNT Structured Mesh and Material Model

- LNK3DNT is a binary file for LANL's PARTISN (PARallel, Time-dependent SN) code [1].

- A LNK3DNT file contains structured mesh geometries (1D, 2D, or 3D) and material numbers and densities of all elements in a mesh model.
  - Density type in a LNK3DNT file can be mass (g/cm^3) or atom (#/barn-cm) but cannot be both. **Density type information is not in a LNK3DNT file**.

- Each element in a LNK3DNT model may contain no materials (void), one material, or more than one materials (mixed materials).
  - A material in PARTISN is defined by a number, ZAIDS, and weight or atom fractions. A material definition is in Block-IV of a PARTISN input file. **ZAIDs and fractions are not in a LNK3DNT file**.

LN3DNT and MCNP Material Numbers



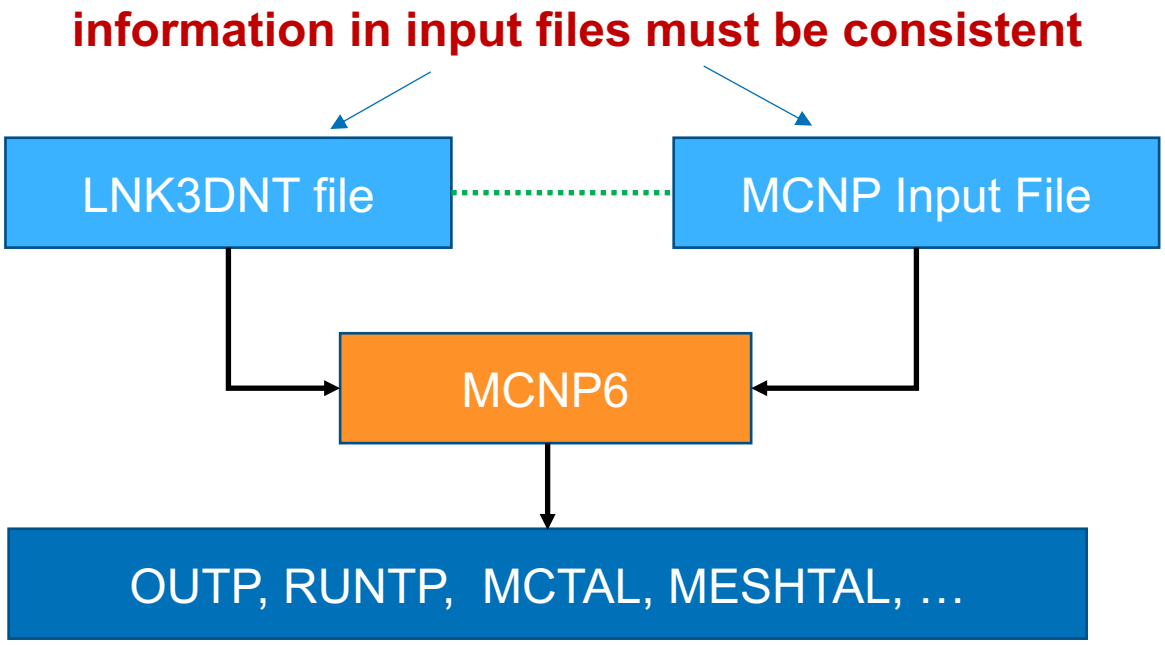
A simple description of a LNK3DNT model

- 1 is used for void in a LNK3DNT file, while 0 is used for void in MCNP.
- When a LNK3DNT file is processed by MCNP, material numbers are processed:

  Material Number in MCNP = Material Number in LNK3DNT - 1

MCNP6 LNK3DNT Calculations

- A LNK3DNT file can be imported into MCNP6 so that particles are tracked through a structured mesh geometry model (i.e., a set of elements formed a model).
- An EMBED card in an MCNP input file is used to map materials in a LNK3DNT file to pseudo cells in an MCNP input file.



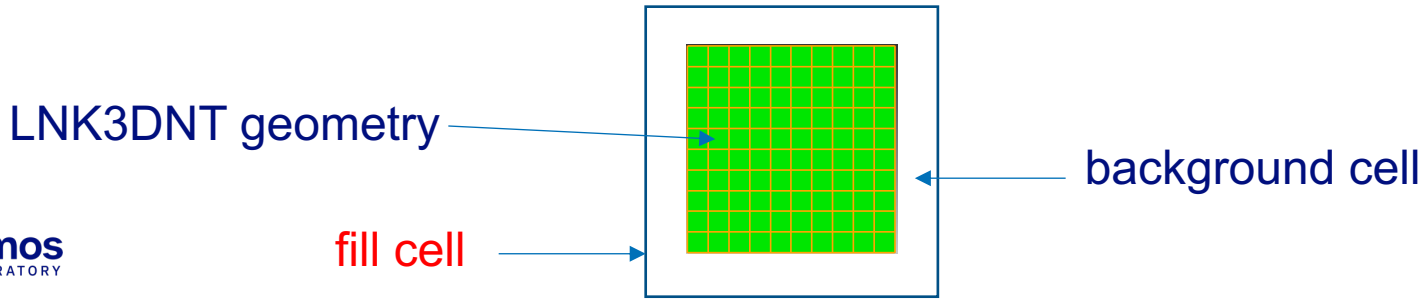
Interface LNK3DNT and MCNP Input Files

- Materials in a LNK3DNT file are mapped to pseudo cells in an MCNP input file. All material numbers in a LNK3DNT file must be mapped to pseudo cells in an MCNP input file [2].

- A pseudo cell is an MCNP cell defined with a null surface. Normal MCNP cell parameters may be assigned to a pseudo cell.

- Because a geometry in a LNK3DNT file is finite in extent, a background cell is required to serves as the background medium that the LNK3DNT model is placed. A background cell is also defined with a null surface.

- Background and pseudo cells must be grouped into a universe placed into a fill cell. A LNK3DNT geometry associated with pseudo cells must not be cropped by a fill cell. A fill cell is a traditional constructive solid geometry (CSG) cell that is defined by using surfaces.



EMBED Card of MCNP6.0-MCNP6.3

- An EMBED card in an MCNP input file is used to interface mesh and material information in a LNK3DNT file with cell and material information in an MCNP input file. An EMBED card is defined in the data block.

```
EMBED10  meshgeo=lnk3dnt
         mgeoin=meshmat
         background=13
         matcell=0 10
                 1 11
                 3 12
```

cell 13 (background cell and cell 10, 11, 12 (pseudo cells) must be in a universe 10 defined in the cell block.

meshgeo is for assigning a mesh geometry format.

mgeoin is for assigning a LNK3DNT filename. A file name must be lowercase.

background is for assigning a background cell.

matcell is for matching LNK3DNT material numbers with MCNP pseudo-cell numbers. **The 1st entries are material numbers in a LNK3DNT file minus 1,** and the 2nd entries are pseudo-cell numbers in an MCNP input file.

Densities in a LNK3DNT file must be mass densities when using MCNP6.0-MCNP6.3

MCNP Cell and Material Cards

```
Test Problem
10  0          0   u=10 imp:n=1
11 100  1.0    0   u=10 imp:n=1
12 200  1.0    0   u=10 imp:n=1
13 0           0   u=10 imp:n=1
20 0          -2   fill=10 imp:n=1
30 0           2   imp:n=0

2 s 20 20 20 30

m200    6000.66c 0.000150
        7014.62c 0.784431
        8016.62c 0.210748
       18000.35c 0.004671
m100    92235.50c 4.4994E-02
        92238.50c 2.4984E-03
        92234.50c 4.9184E-04
embed10 meshgeo=lnk3dnt
        mgeoin=meshmat
        background=13
        matcell=0 10 1 11 3 12
C other data cards are omitted.
```

Cell 10, 11, 12, 13 are pseudo cells.
Cell 13 is a background cell.
Cell 20 is a fill cell.

Pseudo cell Information:
material number in cell 10 is 0 (void)
material number in cell 11 is 100.
material number in cell 12 is 200.

MATCELL Information:
LNK3DNT material number 0 is mapped to cell 10.
LNK3DNT material number 1 is mapped to cell 11.
LNK3DNT material number 3 is mapped to cell 12.

LNK3DNT material 0 is void.
LNK3DNT material 1 is M100.
LNK3DNT material 3 is M200.

LNK3DNT material numbers are defined in a LNK3DNT file and fixed. MCNP cell numbers and material numbers are arbitrary.

EMBED Card of MCNP6.3.1 and later

- The DENTYPE keyword is required for MCNP6.3.1 and later.
- DENTYPE = MASS if mass densities (g/cm^3) are in a LNK3DNT file.
- DENTYPE = ATOM if atom densities (#/barn-cm) are in a LNK3DNT file

```
EMBED10  meshgeo=lnk3dnt
         mgeoin=test1
         dentype=mass
         background=13
         matcell=0 10
                 1 11
                 3 12
```

Density unit in test1 must be in g/cm^3

```
EMBED10  meshgeo=lnk3dnt
         mgeoin=test2
         dentype=atom
         background=13
         matcell=0 10
                 1 11
                 3 12
```

Density unit in test2 must be in #/barn-cm

If a LNK3DNT file with atom densities is used with MCNP6.0-6.3, then the calculation results are wrong. A user must know the density type in a LNK3DNT file and then use the dentype keyword to specify the density type.

Mixed Material Treatment in MCNP6.3

- Some elements in a LNK3DNT may contain multiple materials.

- MCNP6.0-MCNP6.2 cannot handle LNK3DNT files that have mixed material elements. If these LNK3DNT files were used with MCNP6.0-MCNP6.2, then the calculations may be incorrect.

- A mixed material treatment for MCNP LNK3DNT calculations was implemented in MCNP6.3.

- There is no limit on the number of materials in each elements. However, MCNP may not be able to handle a large LNK3DNT file due to a memory limitation. Currently, density values read from a LNK3DNT file are stored in an array of 4 dimensions.

IDC(m,i,j,k)

IDC = densities
m = material number
i,j,k = structured grid numbers in i, j, k directions

Create LNK3DNT Files with MCNPTools

Create LNK3DNT Files

- An MCNP constructive solid geometry (CSG) model may be converted to a LNK3DNT file.
  - Use DAWWG and MESH cards and run MCNP with the m command line option.
  - Densities in a LNK3DNT file generated by MCNP are mass densities (g/cm^3).
  - No mixed material element in a LNK3DNT file.
  - The DAWWG and MESH cards may not work correctly for the MCNP input files that have complex CSG geometries.

- MCNPTools can be used to create LNK3DNT files [3].
  - Densities can be atom densities (#/barn-cm) or mass densities (g/cm^3).
  - Mixed material elements can be generated.

Only focus on using MCNPTools to create LNK3DNT files in this presentation.

Use MCNPTools to generate LNK3DNT File

```
import mcnptools
# make a LNK3DNT cylinder
l3d = mcnptools.Lnk3Dnt( mcnptools.Lnk3Dnt.RZT, # geometry
                                 3, # max number of materials
                                 2, # cells in i direction
                                 2, # cells in j direction
                                 4  # cells in k direction
                               )
# create mesh grids
l3d.SetIMesh( [ 0.00, 0.5, 1.0] )   # in cm
l3d.SetJMesh( [-1.0, 0.00, 1.0] )   # in cm
l3d.SetKMesh( [ 0.00, 0.25, 0.5, 0.75, 1.0] ) # in cm

# set materials for each element
# For LNK3DNT, "1" is a reserved material integer for void.
# MCNP will convert a mateiral number n in a LNK3DNT file to
# a material n-1 in MCNP.
for i in range(2):
     for j in range(2):
         for k in range(4):
             l3d.SetMaterials(     [2,3,4], i, j, k)
             l3d.SetDensities( [7.,2., 1.], i, j, k)

l3d.Save("test.l3d")
```

Methods:

- Set{I,J,K}Mesh()
  - defines the mesh grids along the i, j, k direction. The distances are in centimeters.
- SetMaterials()
  - defines the material ID in an element. A number of materials must be ≥ 1.
- SetDensities()
  - defines the density in an element. A density list is associated with a material ID list, and their lengths must be equal. Density values can be atom densities [#/barn-cm] or mass densities [g/cm^3]
- Save()
  - saves the generated LNK3DNT model into a file.

Convert Mass Density to Atom Density

```
"""avogad and aneut values are taken from MCNP"""
avogad  = 6.022043446928244e+23    # Avogadro's number
aneut   = 1.008664967              # Neutron mass in amu
avgdn   = 1e-24 * avogad / aneut

"""Atomic Weight Ratio (AWR) from xs_dir6.3 of U-isotope"""
awr = [233.02478975, 236.00581772,  232.03042798]   #[235, 238, 234]

"""Atom fraction"""
at_frac = [4.4994E-02, 2.4984E-03, 4.9184E-04]     #[235, 238, 234]

"""HEU mass density"""
den_HEU = 18.74 # g/cm^3

sf = sum(at_frac)
sw = 0.
for i in range(len(awr)):
    sw+= awr[i]*at_frac[i]

"""HEU atom density"""
rho_HEU = den_HEU * avgdn * sf/sw  # atoms/barn-cm
```

If mass fractions are given, then they can be converted to be atom fractions: atom_frac = mass_frac/awr

Compute Densities of Isotopes

```
"""
For given a density of a bulk material, compute densities of isotopes.
"""

"""Compute mass densities of isotopes"""
value   = den_HEU/sw
den_235 = at_frac[0]*awr[0] * value
den_238 = at_frac[1]*awr[1] * value
den_234 = at_frac[2]*awr[2] * value
print("\nmass density of U235, U238, U234, and total (g/cc)")
print(den_235, den_238, den_234, den_235 + den_238 + den_234)

"""Compute atom densities of isotopes"""
rho_235 = den_235 * avgdn / awr[0]
rho_238 = den_238 * avgdn / awr[1]
rho_234 = den_234 * avgdn / awr[2]
print("\natom density of U235, U238, U234, and total (at/b-cm)")
print(rho_235, rho_238, rho_234, rho_235 +rho_238 + rho_234)
```

Testing LNK3DNT Feature

Test Problems

- Three test problems taken from International Criticality Safety Benchmark Evaluation Project (ICSBEP) [4].
  - HEU-MET-FAST-001: Bare sphere of HEU.
  - HEU-MET-FAST-004: HEU sphere reflected by water.
  - PU-MET-FAST-001: Bare sphere of plutonium.

- Create 4 LNK3DNT models for each test problem.
  - One material for HEU-MET-FAST-001 & PU-MET-FAST-001 and two materials for HEU-MET-FAST-004; mass densities [**Homo-M**].
  - One material for HEU-MET-FAST-001 & PU-MET-FAST-001 and two materials for HEU-MET-FAST-004; atom densities [**Homo-A**].
  - Mixed materials where each material has only 1 nuclide; mass densities [**Mixmat-M**]
  - Mixed materials where each materials has only 1 nuclide; atom densities [**Mixmat-A**]

- Run KCODE calculations for CSG and LNK3DNT models using MCNP6 DEVEL branch.

MCNP LNK3DNT Input Files

```
Godiva  Solid Bare HEU sphere  HEU-MET-FAST-001 (homogeneous)
c ================================ cell block ======================
101         1          1        0   u=1           imp:n=1
104         0                   0   u=1           imp:n=1
105         0         -1000        fill=1        imp:n=1
106         0          1000                      imp:n=0

c ============================ surface block ======================
1000         so       10

c ============================ cell block ========================
m1        92234.00c   4.9184e-04     92235.00c   4.4994e-02
          92238.00c   2.4984e-03
embed01 meshgeo = lnk3dnt
        mgeoin = godiva_homo_m.l3d
        background =  104
        matcell = 1 101
        dentype=mass
```

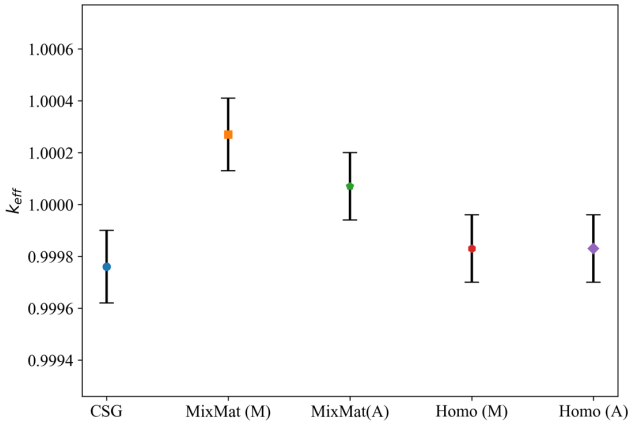
No mixed-material

```
Godiva  Solid Bare HEU sphere  HEU-MET-FAST-001 (mixed materials)
c ================================ cell block ======================
101         1        1    0    u=1           imp:n=1
102         2        1    0    u=1           imp:n=1
103         3        1    0    u=1           imp:n=1
104         0                  0    u=1           imp:n=1
105         0         -1000        fill=1        imp:n=1
106         0          1000                      imp:n=0

c ============================ surface block ======================
1000         so       10

c ============================ data block ========================
m1 92235.00c 1.0 $ U-235
m2 92238.00c 1.0 $ U-238
m3 92234.00c 1.0 $ U-234
embed01 meshgeo = lnk3dnt
        mgeoin = godiva_mixmat_m.l3d
        background =  104
        matcell = 1 101 2 102 3 103
        dentype=mass
```

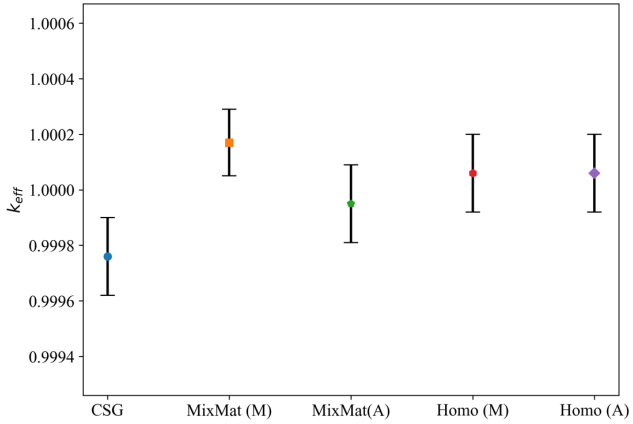
Mixed Materials

KCODE CALCULATIONS (HEU-MET-FAST-001)

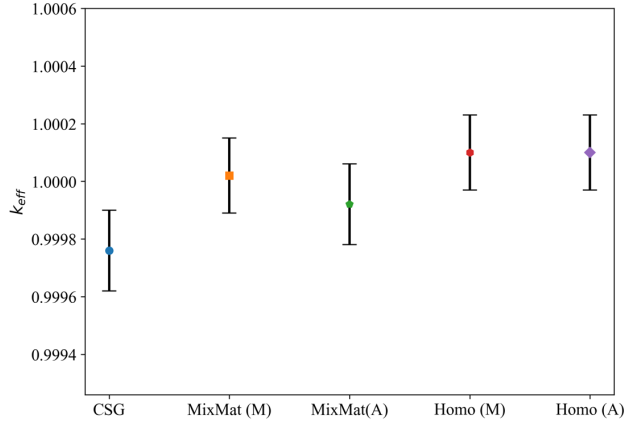
- Experimental Value: 1.00000 ± 100 pcm



10 elements



40 elements

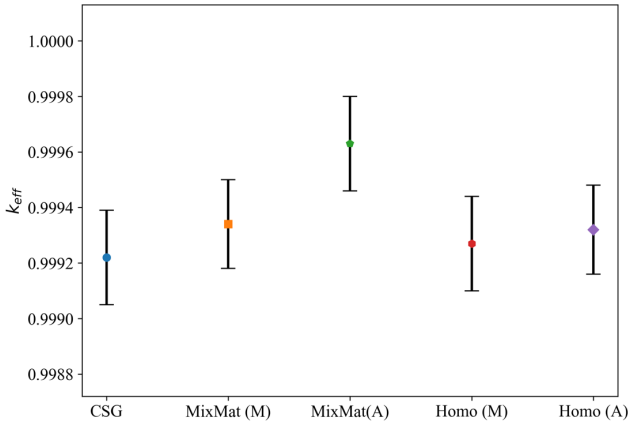


20 elements

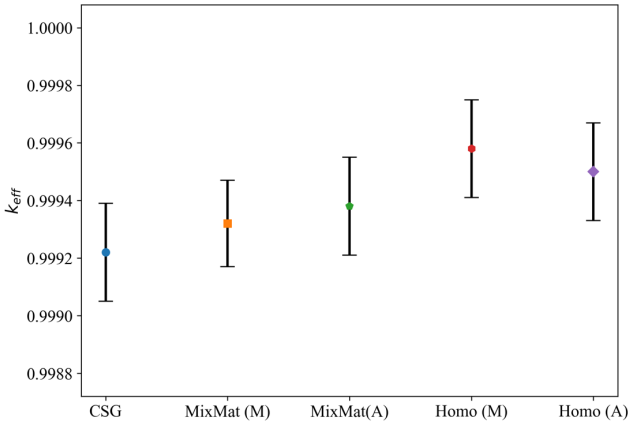
Homo = 1 material in each element

KCODE CALCULATIONS (HEU-MET-FAST-004)

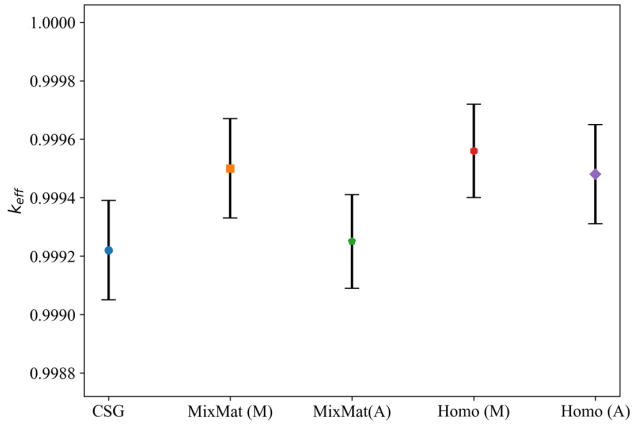
- Experimental Value: 0.99850 ± 110 pcm



15 elements



60 elements

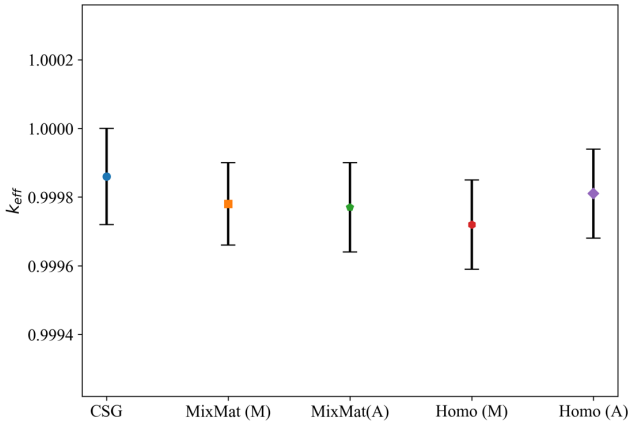


30 elements

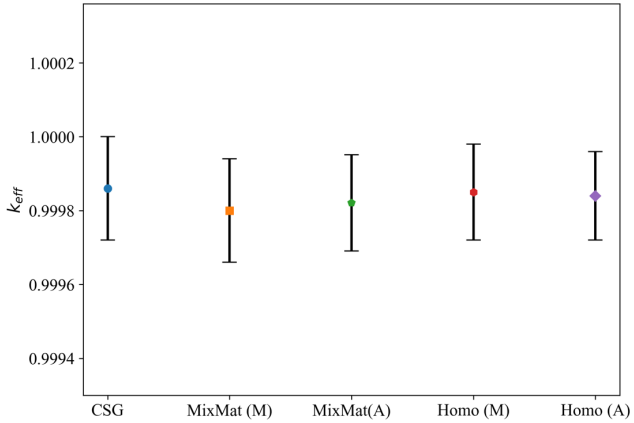
Homo = 1 material in each element

KCODE CALCULATIONS (PU-MET-FAST-001)

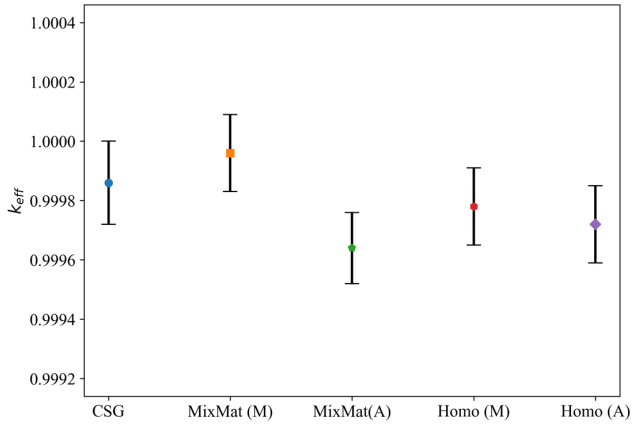
- Experimental Value: 1.00000 ± 200 pcm



10 elements



40 elements



20 elements

Homo = 1 material in each element

Conclusion and Future Work

- KCODE calculations with 1-D spherical mixed material LNK3DNT files can replicate experimental criticality results.
- Further work is required to test cylindrical and Cartesian mixed material LNK3DNT geometries with KCODE calculations.
- Need to investigate why the mixed material atom and mass density models produce varying k_{eff} .

Questions?

References

1. Ray E. Alcouffe, Randal S. Baker, Jon A. Dahl, Erin J. Davis Thomas G. Sallera, Scott A. Turner, Robert C. Ward, and Robert J. Zerr. Partisn: A time-dependent, parallel neutral particle transport code system. Technical Report LA-UR-08-07258, Los Alamos National Laboratory, Los Alamos, NM, USA, 14 September 2017.
2. Lawrence J. Cox. LNK3DNT Geometry Support: User Guidance for Creating and Embedding. Technical Report LA-UR-11-01654, Los Alamos National Laboratory, Los Alamos, NM, USA, March 2011.
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4. Nuclear Energy Agency. International Handbook of Evaluated Criticality Safety Benchmark Experiments. The Organization for Economic Cooperation and Development, Paris, FR, 2020.

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