OECD/NEA WPEC SG45

Policy driven input file generation applied to MCNP

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Introduction

Most organisations make choices to handle specific things when preparing input files for validation purposes

- Which elemental abundance data to use
- How to decompose specific elements
- Setting calculation precision

Consequences

- Differing calculation results between different organisations for the same case
  - Even when using the same code!
  - Illustrated by the intercomparison excercise
- Input files prepared by one organization are not necessarily correct for another

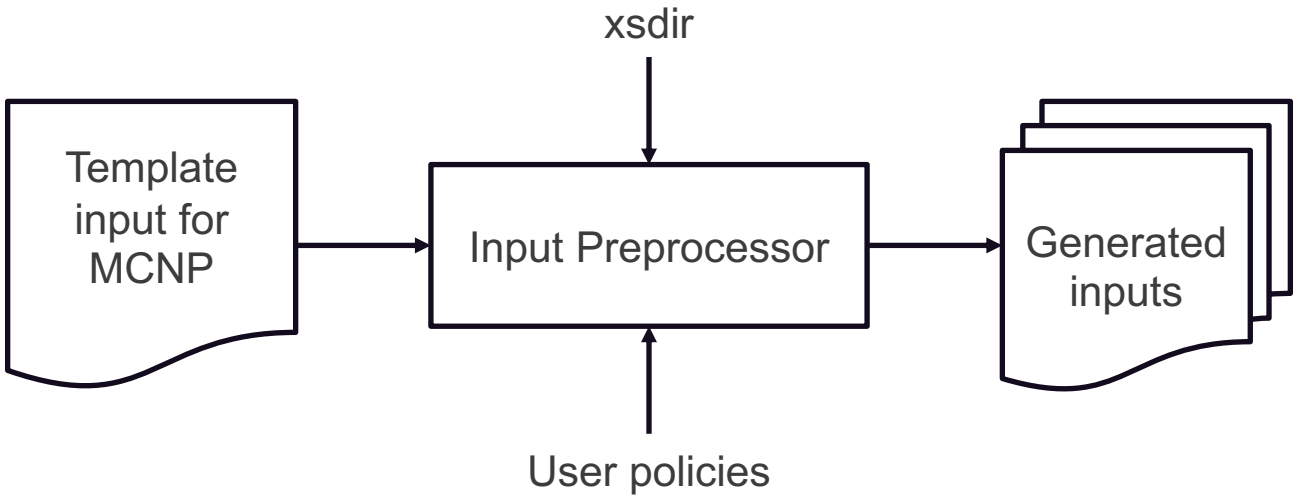
A solution : policy driven input generation

Maintain a single set of “template” input files for each code

- Follow the benchmark description as close as possible
- Devoid of specific library information or other organisational “choices”

Generate the input files at the request of the user

- Decompose elements based on nuclear data availability and user choices, etc.



Policy overview – elemental decompostion

An overview of identified policies available in the QA document

- See https://git.oecd-nea.org/science/wpec/sg45/documents

Abundance data policies

- There will be a default choice for the abundance data
- User defined abundance data can be provided as json files

Default treatment of isotopes with missing nuclear data files

- The missing isotopes in a natural element are corrected by renormalizing the abundances (i.e. the abundance of the missing isotope is distributed over all other isotopes)

```
{
  "abundances": {
    "H" : { "H1" : 1.0 },
    "He" : {"He3" : 1.34e-06, "He4": 0.99999866 },
    "Li" : { "Li6" : 0.0759, "Li7": 0.9241 },
    "C" : { "C12" : 0.9893, "C13": 0.0107 },
    "N": { "N14" : 0.99636, "N15": 0.00364 } }
}
```

Policy overview – elemental decompostion

Default decomposition can be overriden

- Through a user provided abundance file
- Applying special user policies

Decomposition policies will cover user overrides for select elements

- Decompose a user defined element as a single or its most abundant isotope
  - For example: H as H1, C as C12, N as N14, O as O16
- If a user defined isotope is missing, add its contribution to another user defined isotope (of the same element)
  - For example: add O18 to O17, add W180 to W182

A very special case (which should only happen for old libraries):

- Both the element and every isotope of the element have no nuclear data
- The missing element is removed and the atom density of the material is adjusted

Header information

Header information to trace these choices

- Keeping track of these choices is important
- Including them in the generated input files is the best way

```
c policy : userAbundanceFile
c abundances : /home/janedoe/abundances/abundances.lanl.ncs.json
c
c policy : userDecomposeSpecificElement
c element : O
c isotopes : O16
c
c policy : userDecomposeSpecificElement
c element : N
c isotopes : N14
c
c policy : userCalculationPrecision
c particles : 10000
c inactive cycles : 100
c active cycles : 500
```

Python coding

We've been working on an advanced MCNP input parser

```
# parse an existing input file
mcnp = McnpInput( 'pu-met-fast-001-000-rev4.mcnp' )

# retrieve and modify gallium in the materials
pu = mcnp.materials()[0]
ga = pu.composition[ '31000' ]
del pu.composition[ '31000' ]
pu.composition.update( { '31069' : 0.000826605216, '31071' : 0.000548594784 } )

# set kcode values
kcode = mcnp.criticalityCalculation()
kcode.nsrck = 10000
kcode.rkk = 1.
kcode.ikz = 100
kcode.kct = 600

# add kopts card
mcnp.data.append( McnpCriticalityCalculationOptions( kinetics = True ) )

# write the new file
newfile = mcnp.write()
```

Python coding

We have serialisation, deserialisation of json abundance files and decomposition of compositions using the underlying abundances

```
# create an abundance table
table = AbundanceTable( '/home/janedoe/abundances/abundances.lanl.ncs.json' )

# decompose gallium
composition = table.decompose( Element( 'Ga' ), 1.3752e-3 )

# transform to MCNP composition
mcnp_composition = { str( nuclide.z * 1000 + nuclide.a ) : comp
                     for nuclide, comp in composition.items() }
```

Example

Template MCNP file

```
pu-met-fast-001-000-rev4
1   1 4.029014e-2  -1   imp:n=1
2   0               1   imp:n=0

1   so  6.39157

mode n
totnu
kcode
ksrc 0. 0. 0.
c material 1: Plutonium
m1   94239 3.7047e-2
     94240 1.7512e-3
     94241 1.1674e-4
     31000 1.3752e-3
```

Generated MCNP file

```
pu-met-fast-001-000-rev4
c policy : defaultAbundanceFile
c policy : defaultCalculationPrecision
c policy : userCalculateEffectiveDelayedNeutronFraction
1   1 4.029014e-2  -1   imp:n=1
2   0               1   imp:n=0

1   so  6.39157

mode n
totnu
kcode 10000 1. 100 600
kopts kinetics=yes
ksrc 0. 0. 0.
c material 1: Plutonium
m1
     94239 0.037047
     94240 0.0017512
     31069 0.000826605216
     31071 0.000548594784
```