

# Progress on SG45 tools

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# Agenda

1. SG45 software tools
  1. Policy driven input file generation for MCNP
  2. Storing and manipulating calculation and experimental results
2. SG45 deliverables
3. Beyond SG45 ...



# SG45 software tools



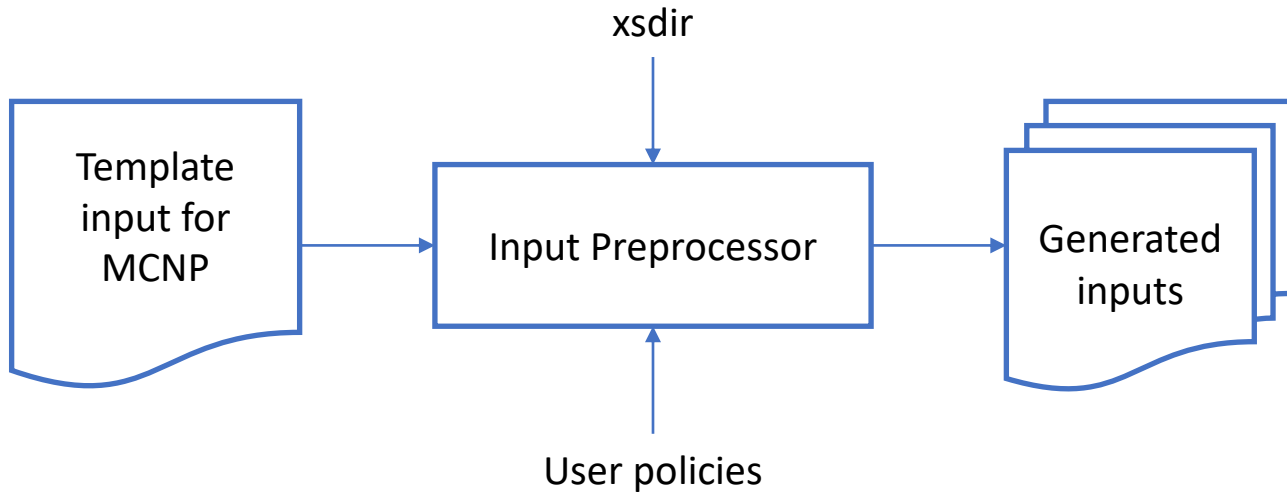
# Template input files for MCNP

- 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 exercise
  - Input files prepared by one organization are not necessarily correct for another



# Template input files for MCNP

- 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.



# Template input files for MCNP

## 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
```



# Template input file generation

- The LABS repository now has over 500 input files
  - Still the old MCNP input files using ENDF/B-VII.1 nuclear data files
  - The associated material balance tables will be used to generate the template files
- Additional verification of the input files using the input parser
  - Removing unused materials
  - Adding missing 'e' in numbers using scientific notation
  - Some “interesting” typos in card names: e.g. MCNP accepts `m2t` instead of `mt2`
- Code to compare the material balance tables to the MCNP input files
- The final template files will be produced once these verifications are complete
  - These files and the material balance tables will be released to SG45



# Policy driven input file generation

- Code to decompose elements based on abundance data is completed
  - Default and user provided abundance data in json files
  - Policies implemented as modification to that abundance data
- Code to analyse a user's xsdir file for available nuclear data is completed
- MCNP input parser handles all cards that we need
  - Additional customisation can be added on a case by case basis
- For the final tool, some assembly is still required
  - This tool will be released as open source in the future



# Tools for calculation results

```
[ { "type" : "effectiveMultiplicationFactor",
  "data" : { "values" : [ 1.0000 ],
            "uncertainties" : [ 0.0001 ] } },
{ "type" : "sensitivityProfile",
  "response" : "effectiveMultiplicationFactor",
  "parameter" : "crossSection",
  "particleId" : "neutron",
  "nuclide" : "U235",
  "reaction" : "fission",
  "material" : "total",
  "data" : { "values" : [ -1.7129e-17, 1.4106e-09 ],
            "uncertainties" : [ 0.0034, 0.0033 ],
            "structure" : [ { "name" : "energy-in",
                              "type" : "histogram",
                              "limits" : [ 1e-11, 10.0, 20.0 ],
                              "unit" : "MeV" } ],
            "units" : { "value" : "%/%", "uncertainty" : "relative" } } } ]
```



# Extensions for calculation results

- Added additional types for our purposes
  - Pulsed sphere time of flight spectra
  - Reaction rate ratios
- Advanced filtering on results
- Added capability of case-by-case comparison of results for sets of benchmarks
  - Can be used calculation-to-calculation and calculation-to-experiment comparison
  - Plotting and report generation will use these special types of results



# SG45 deliverables



# Beyond SG45 ...

