

# OECD/NEA WPEC SG45

The way forward ...



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Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

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Paris (France) – Santa Fe, NM (USA)

- Input files for MCNP
- Input files for other codes?
- What can you do, you ask?

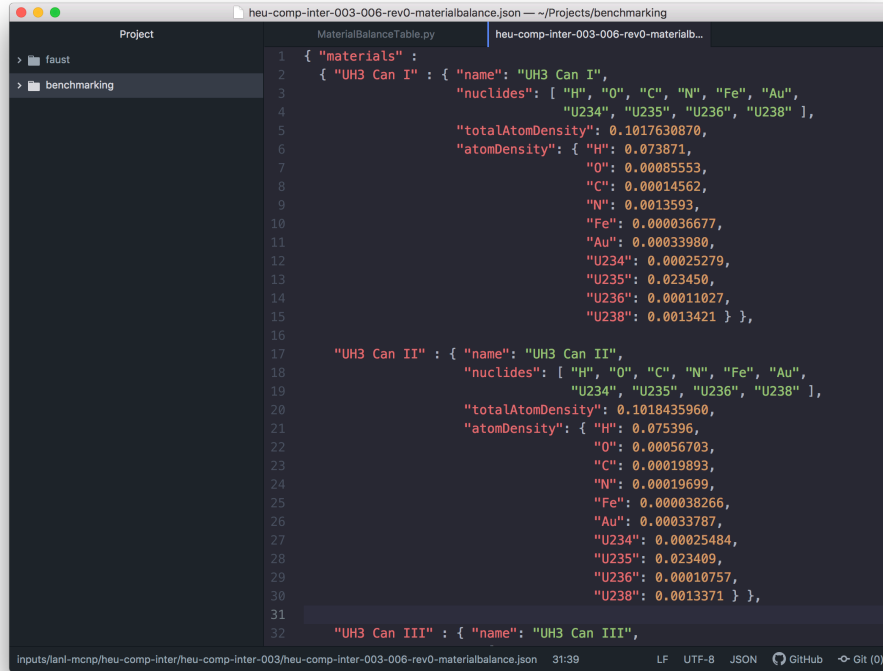


# Input files for MCNP

**The following general roadmap is proposed to produce a first set**

1. Make the repository for MCNP input files
2. Add a first set of cases from the LANL Whisper suite already under LANL QA
  - For example : ~100 Pu and/or HEU cases
  - Using the proper naming convention, archiving current LANL QA review documentation
  - Produce the material balance tables from the ICSBEP benchmark specifications
3. Verify the set against the material balance tables, review and correct discrepancies
4. Transform the set to be in line with the VaNDaL input requirements
  - Clean the files and add header information and standardised title
  - Replace material specifications using the verified material balance tables
  - Replace kcode card with the accepted VaNDaL default
5. Verify the generated input files using the appropriate policies against the originals
  - LANL Nuclear Criticality Safety division policies will be used
6. Verify and update the volume information in the material balance tables

# Input files for MCNP











```
1 { "materials" :  
2   { "UH3 Can I" : { "name": "UH3 Can I",  
3                     "nuclides": [ "H", "O", "C", "N", "Fe", "Au",  
4                                   "U234", "U235", "U236", "U238" ],  
5                     "totalAtomDensity": 0.1017630870,  
6                     "atomDensity": { "H": 0.073871,  
7                                       "O": 0.00085553,  
8                                       "C": 0.00014562,  
9                                       "N": 0.0013593,  
10                                      "Fe": 0.000036677,  
11                                      "Au": 0.00033980,  
12                                      "U234": 0.00025279,  
13                                      "U235": 0.023450,  
14                                      "U236": 0.00011027,  
15                                      "U238": 0.0013421 } },  
16  
17   "UH3 Can II" : { "name": "UH3 Can II",  
18                   "nuclides": [ "H", "O", "C", "N", "Fe", "Au",  
19                                   "U234", "U235", "U236", "U238" ],  
20                   "totalAtomDensity": 0.1018435960,  
21                   "atomDensity": { "H": 0.075396,  
22                                     "O": 0.00056703,  
23                                     "C": 0.00019893,  
24                                     "N": 0.00019699,  
25                                     "Fe": 0.000038266,  
26                                     "Au": 0.00033787,  
27                                     "U234": 0.00025484,  
28                                     "U235": 0.023409,  
29                                     "U236": 0.00010757,  
30                                     "U238": 0.0013371 } },  
31  
32   "UH3 Can III" : { "name": "UH3 Can III",
```



Benchmarked > inputs > lanl-mcnp > Details

master lanl-mcnp / pu-sol-therm / pu-sol-therm-006 History Q Find file Web IDE Clone

 Updated material comments in input files, added material balance tables  
Kristina Diane Yancey Spencer authored 8 hours ago 52556815

Name	Last commit	Last update
..		
 Review_Documentation	Updated material comments in input files, added mate...	8 hours ago
 pu-sol-therm-006-001-rev1-materialbal...	Updated material comments in input files, added mate...	8 hours ago
 pu-sol-therm-006-001-rev1.i	Updated material comments in input files, added mate...	8 hours ago
 pu-sol-therm-006-002-rev1-materialbal...	Updated material comments in input files, added mate...	8 hours ago
 pu-sol-therm-006-002-rev1.i	Updated material comments in input files, added mate...	8 hours ago
 pu-sol-therm-006-003-rev1-materialbal...	Updated material comments in input files, added mate...	8 hours ago
 pu-sol-therm-006-003-rev1.i	Updated material comments in input files, added mate...	8 hours ago

LANL is working on a proof of concept for automated verification with material balance tables and automated input file generation using policies

# Input files for MCNP

## **After this proof of concept, the long road:**

1. Meanwhile at LANL : process the Whisper files not yet under QA
  - Formal review and validation of the modeling, and add them to the stack
2. Rinse and repeat : add sets until all Whisper cases under QA are exhausted
  - Complete PU-MET-FAST and HEU-MET-FAST cases
  - Complete all other PU and HEU systems
  - Complete IEU and LEU systems
  - Complete U233 systems

## **After that : process the Steven Van der Marck suite and IAEA suite**

- Starting with the inputs that were NOT taken from ICSBEP appendices
- Eliminate the cases already in the VaNDaL MCNP suite

# Input files for other codes?

## Move on to other codes once some VaNDaL MCNP inputs are ready

1. Make the repository for < insert code name here > input files
2. Identify the input files for cases that are available in the VaNDaL MCNP repository
3. Verify the common set versus the VaNDaL MCNP repository
  - Verify the materials in the input file using the archived material balance table
  - Verify the geometry volumes in the input file using the archived material balance table
  - Verify the calculation results with VaNDaL MCNP results (applying the same policies)
4. Resolve all issues that were identified

# What can you do, you ask?



## We need the mass balance tables for verification purposes

- All tables you can contribute will be a time saver since it adds automated partial verification
- These will be used for input file verification for ANY calculation code

## Identify policies for the input generation

## Identify the source of isotopic abundances (and atomic masses)

## Review the documents we have produced or are producing

It's a lot of work but ...

