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Title: l3d2vtk: An MCNPTools Utility to Enable LNK3DNT File Visualization & Post-processing

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`l3d2vtk`: An MCNPTools Utility to Enable LNK3DNT File Visualization & Post-processing

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Outline

Introduction & Motivation

MCNPTools Summary
- Software Overview
- Pre-existing Utilities
- New Utility: `l3d2vtk`
- Building, Testing, Installing, and Using

Example Interactive 3-D Visualization Workflow
- Problem Description
- Cards to Produce LNK3DNT File
- Visualization Techniques

Summary & Future Work

Introduction & Motivation

Objective: Provide a utility (among other utilities) that improves MCNP analysis post-processing and visualization capabilities.

- Much recent work to improve MCNP post-processing and visualization
  - Goals: Portable, open, easily interrogated by a user, no dependencies
    - Mesh tally-to-VTK conversion
    - EEOUT-to-VTK conversion (Kulesza and McClanahan, 2019)
  - Enables interactive, 3-D, visualization environments (e.g., ParaView)
- Why do this?
  - Provide physical insight into behaviors and trends
  - Error mitigation (easier to “see” errors than “read” them)
  - Improved communication with collaborators
- Why now?
  - Analyses are getting ever-more complicated
  - More flexible build, test, and deployment capabilities

MCNPTools Overview

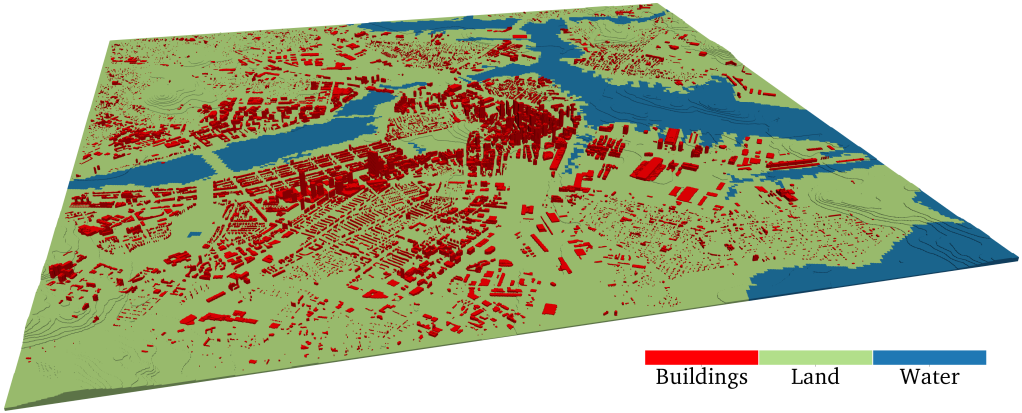
- Born out the continual need to process MCNP outputs
- Provides object-oriented access to MCNP output files
  1. `mctal` files
  2. `meshtal` (column-formatted Type B) files
  3. `ptrac` files
  4. LNK3DNT files
- Written in C++ and bound to Python (and Perl) via SWIG
  - Its true power: easily create custom post-processing applications
- Also includes utilities for common tasks
- First distributed via RSICC as version 3.8.0 with MCNP 6.2
  - Currently at version 5.1.0
  - Currently pursuing open-source release
- Discussed in MCNP Introduction and Intermediate Classes

Pre-existing MCNPTools Utilities

`l3dinfo`	Prints information about a LNK3DNT mesh file such as the geometry type, size of the mesh, and number of materials,
`l3dcoarsen`	Coarsens a LNK3DNT mesh to reduce the overall number of mesh voxels and re-smears material mixing fractions,
`l3dscale`	Scales a LNK3DNT mesh (e.g., to convert from centimeters to inches),
`mctal2rad`	Converts a text-based synthetic radiograph tally to a TIFF image,
`mergemctals`	Merges statistically independent tally files by computing aggregate mean and relative uncertainty values,
`mergemeshtals`	Merges statistically independent type B mesh tally files by computing aggregate mean and relative uncertainty values, and
`meshtal2vtk`	Converts a mesh tally file to one or more ASCII XML-based StructuredMesh VTK (`.vts`) files.

New Utility: `l3d2vtk` (MCNPTools 5.1.0)

- Converts spherical, cylindrical, and Cartesian LNK3DNT files to ASCII XML-based StructuredMesh VTK (`.vts`) files
- C++ application subject to serial processing



Building, Testing, and Installing `l3d2vtk`

- MCNPTools is provided with pre-compiled binary executables
  - Python wheel (`.whl`) files are also provided
- MCNPTools and its utilities are configured with CMake
- Linux & macOS build, test, and installation steps:
  1. `mkdir build && cd build`
  2. `cmake -DCMAKE_BUILD_TYPE=Release ..`
  3. `make`
  4. `ctest`
  5. `make install`
- Windows build, test, and installation via CMake GUI
- It is expected that all `ctest` tests pass, if not: seek help

Using `l3d2vtk`

```
> l3d2vtk --help
USAGE: l3d2vtk [--version] [--verbose] <LNK3DNT> [OUTPUT]

l3d2vtk converts a LNK3DNT file into an XML-formatted
StructuredGrid (.vts) VTK file.

OPTIONS:

--version, -v : Print version and exit

--verbose, -V : Produce standard output giving status
                (Default: False)

LNK3DNT       : LNK3DNT file name to convert

OUTPUT        : Converted LNK3DNT output name
                (Default: lnk3dnt.vts)
```

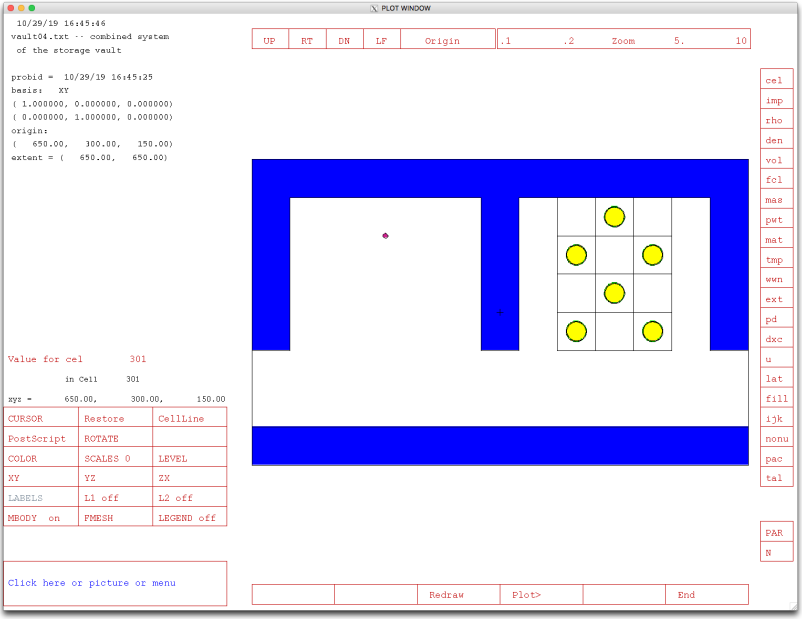
```
> l3d2vtk -V godiva_1mm_eighth.lnk
Processing file: godiva_1mm_eighth.lnk
  Found 3-D Cartesian (x,y,z) geometry.
  Reading materials...
  Constructing VTS file...
  Writing VTS file...
  Done.
```

Example Problem Description

- Fissile Material Storage Vault
  - A room has an incomplete array of $PuNO_3$-containing cylindrical tanks
  - A room has a small Pu sphere 1.5 m from the floor
  - Relatively few neutrons will travel from one room to another
    - Loosely coupled system
  - Adapted from an MCNP Criticality Class Case Study
    - Mesh tally added consistent with LNK3DNT mesh

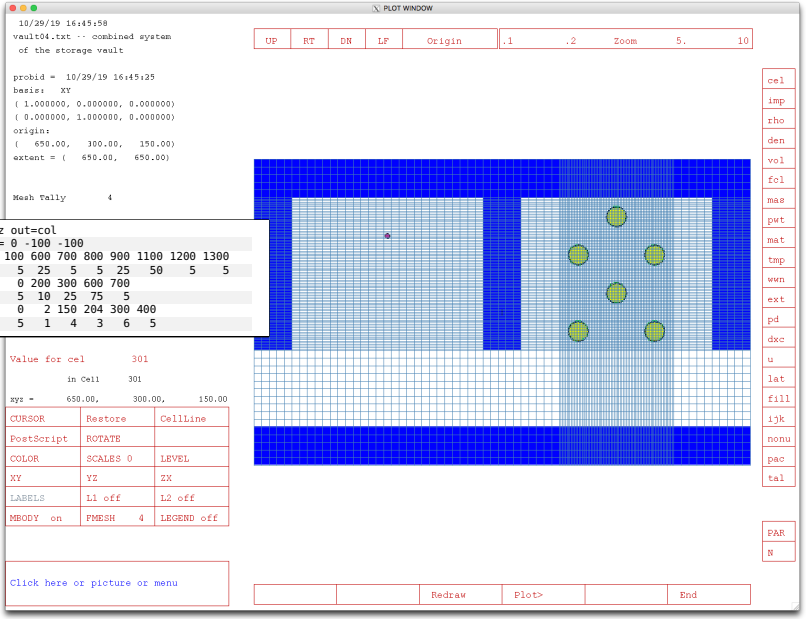
- Used as an example here because it
  - Is uncomplicated but of a size scale that is “interesting”
  - Demonstrates representing curvature on a Cartesian mesh

Plan View of Geometry

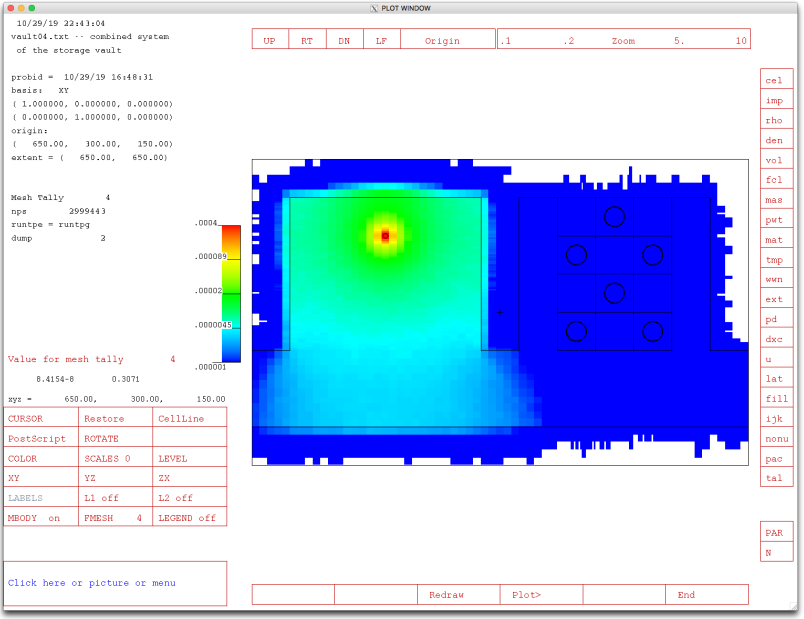


Geometry with Superimposed Mesh Tally Grid

```
1  fmesh4:n geom=xyz out=col
2           origin = 0 -100 -100
3           imesh = 100 600 700 800 900 1100 1200 1300
4           iints =   5  25   5   5  25   50    5    5
5           jmesh =   0 200 300 600 700
6           jints =   5  10  25  75   5
7           kmesh =   0   2 150 204 300 400
8           kints =   5   1   4   3   6   5
```

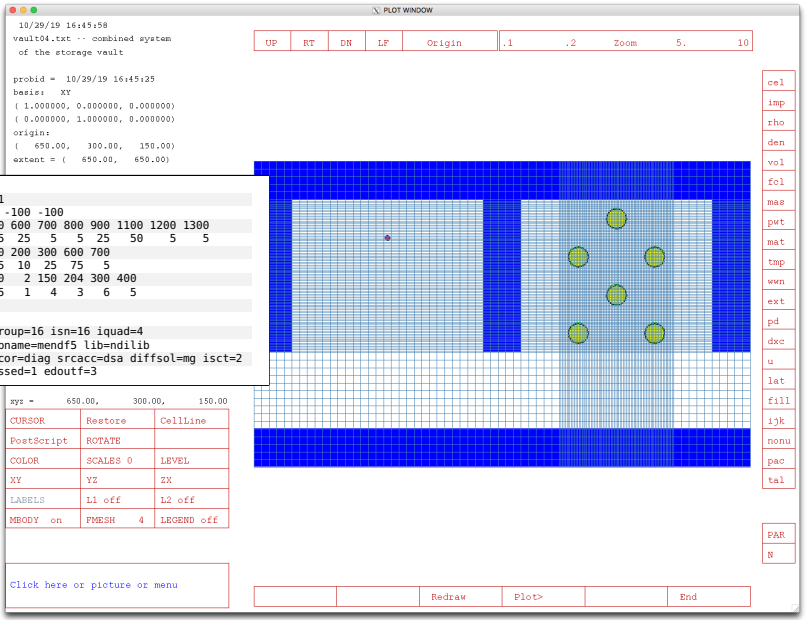


Geometry with Mesh Tally Results

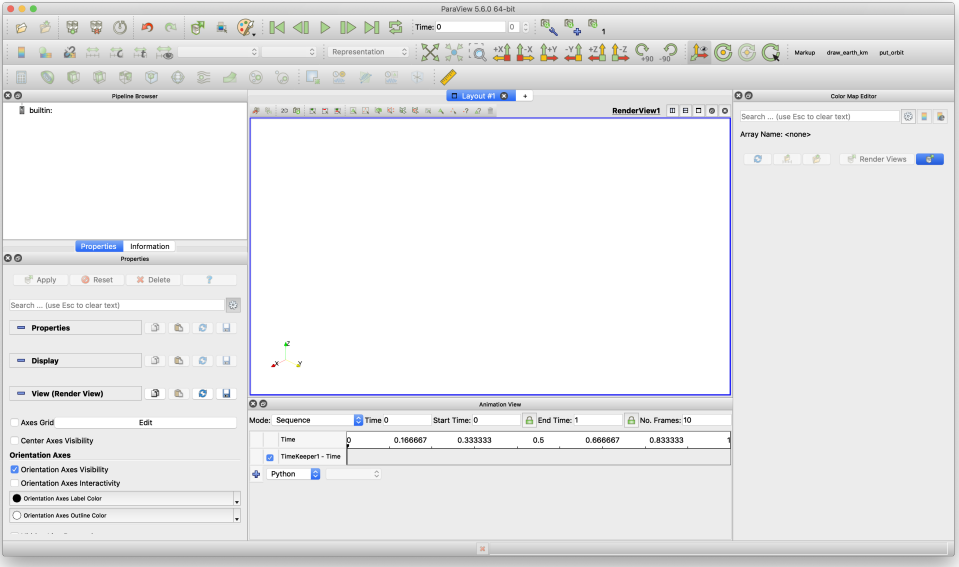


Cards to Produce LNK3DNT File (Run as `mcnp6 m i=...`)

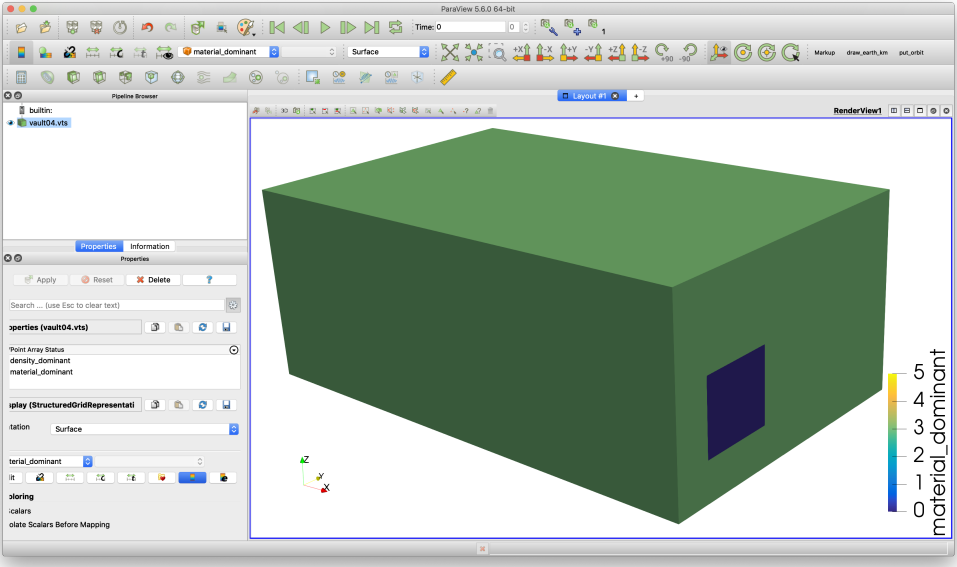
```
1  mesh   geom=xyz
2         ref = 1 1 1
3         origin = 0 -100 -100
4         imesh = 100 600 700 800 900 1100 1200 1300
5         iints =   5  25   5   5  25   50     5     5
6         jmesh =   0 200 300 600 700
7         jints =   5  10  25  75   5
8         kmesh =   0   2 150 204 300 400
9         kints =   5   1   4   3   6   5
10 c
11 dawwg points=10
12        block=1 ngroup=16 isn=16 iquad=4
13        block=3 libname=mendf5 lib=ndilib
14        block=5 trcor=diag srcacc=dsa diffsol=mg isct=2
15        block=6 massed=1 edoutf=3
```



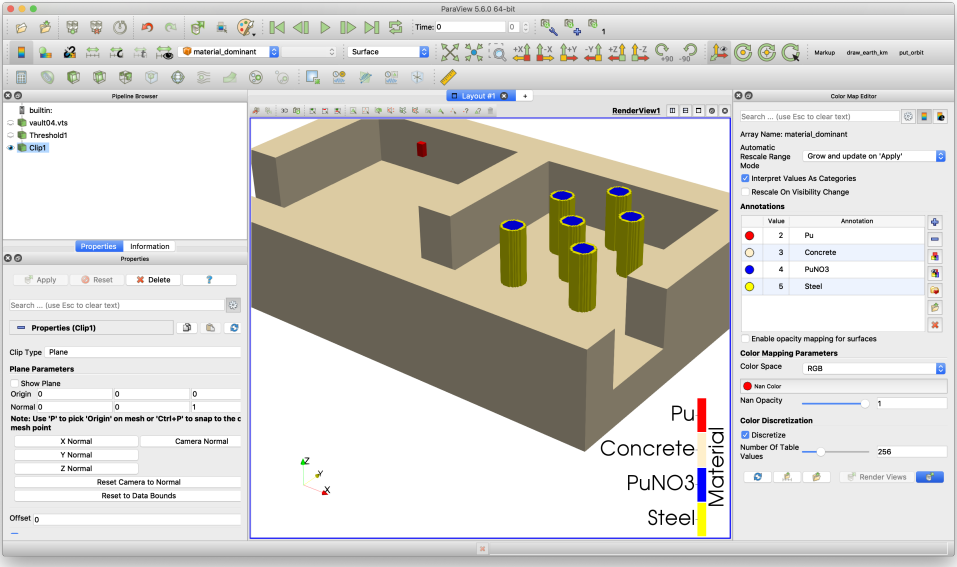
ParaView Interface Overview



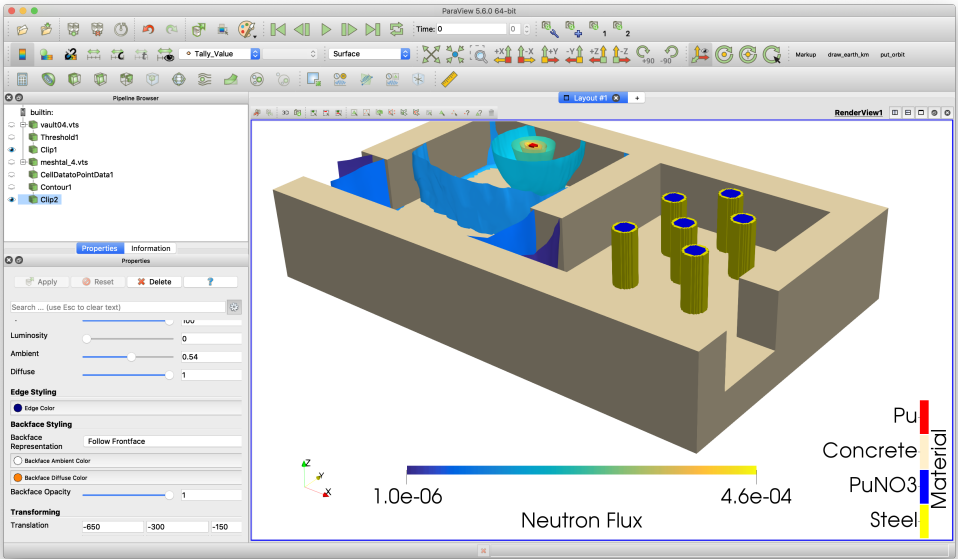
Load Geometry



Clip / Style Geometry & Legend



Insert Mesh Tally, Reformat as Isocontours, and Rescale



Summary & Future Work

Summary

- Provided update on latest MCNPTools capabilities and plans
- Presented new LNK3DNT-to-VTK (`l3d2vtk`) conversion utility
  - Also demonstrated mesh tally-to-VTK (`meshtal2vtk`) conversion utility
- Showed how to combine mesh tally results and voxelized geometry
  - ParaView used herein
  - Any application that supports VTK is permitted

Future Work

- Migrate MCNP output files to more-common HDF5-based formats
  - Runtape, `ptrac`, UM EEOUT, mesh tally
- Create interactive 3-D representation of CSG

Questions?

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Summary & Future Work

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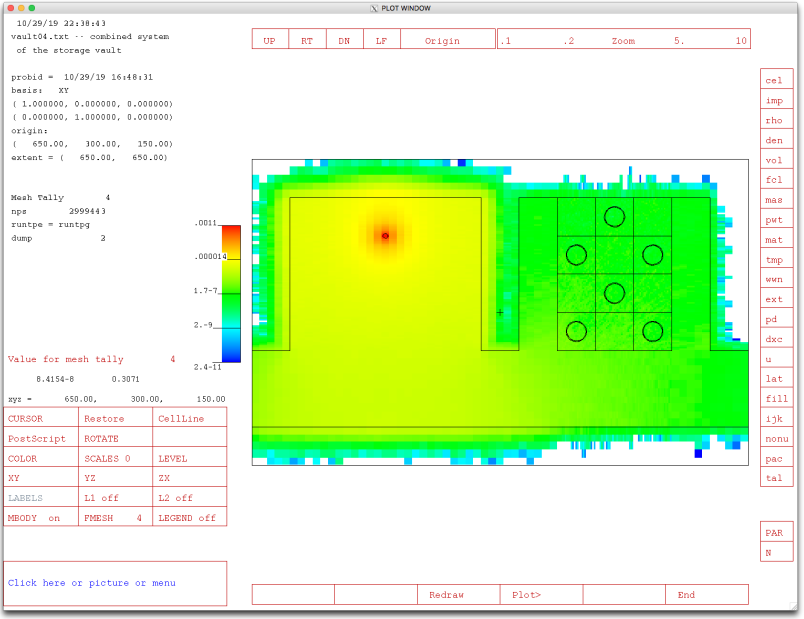
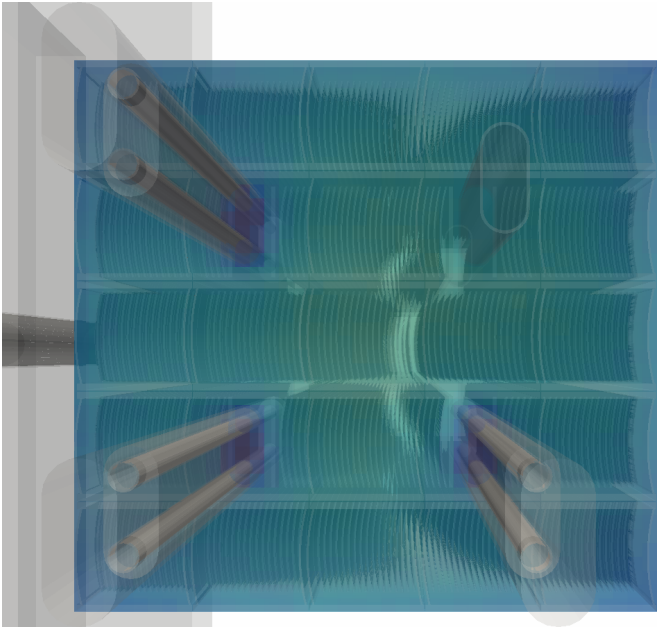
Backup Slides

References

J. A. Kulesza and T. C. McClanahan, “A Python Script to Convert MCNP Unstructured Mesh Elemental Edit Output Files to XML-based VTK Files,” Los Alamos National Laboratory, Los Alamos, NM, USA, Tech. Rep. LA-UR-19-20291, rev. 1, Sep. 2019. [Online]. Available: http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-19-20291

Geometry with Unscaled Mesh Tally Results



Unstructured Mesh Geometry & Overlaid Mesh Tally