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MCNP® Visualization Approaches: An Overview

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Outline

Introduction & Motivation

Objective: broad overview of non-traditional MCNP visualization approaches

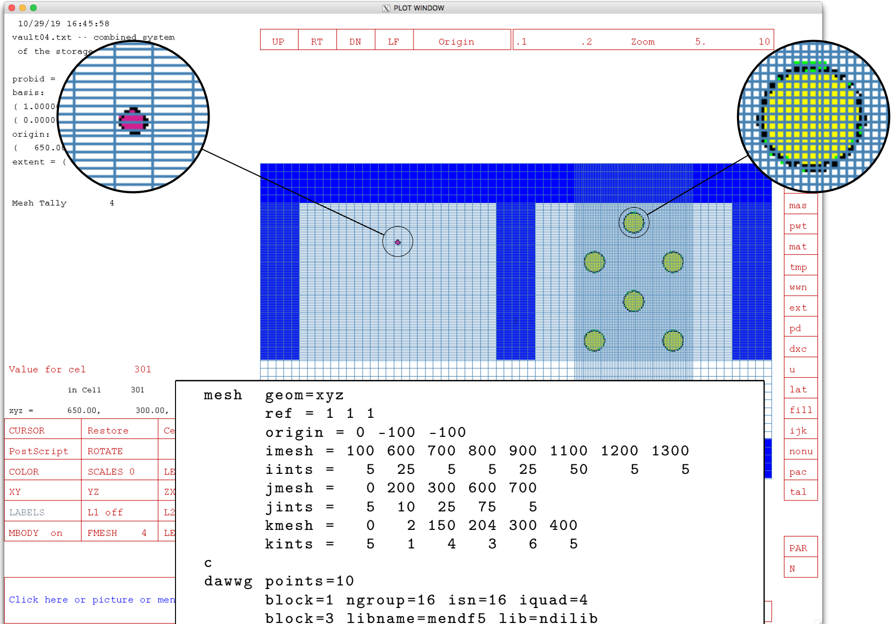
- The MCNP [1] plotter originated in the late 1970s
  - – Dated, and potentially unintuitive, interface (table vs. button)
  - – Limited interactivity—no click-and-drag capabilities
  - – Relies on X11 (unconventional setup for Windows users)
  - + 2-D slice plotter is precise (faithful zoomed geometry)
  - + Headless (`notek`) and batch-processing capability: speed & efficiency
  - + Cross-platform execution; multiple output capabilities (`file`, `printpts`)

↔

```
mcplot> help term
> Syntax: term n m
  Device type.
     ...
   n=1 specifies Tektronix 4010 using CGS.
   n=2 specifies Tektronix 4014 using CGS.
   n=3 specifies Tektronix 4014E using CGS. (DEFAULT)
   n=4115 specifies Tektronix using GKS and UNICOS.(DEFAULT)
   n=1 specifies Tektronix using the AIX PHIGS GKS library
     (DEFAULT) Check with your vendor for the proper
     terminal type if you are using a GKS library.
  The baud rate of the terminal is specified by m.
    (DEFAULT=9600)
```

https://en.wikipedia.org/wiki/Tektronix_4010.

LNK3DNT from MCNP CSG (`mcnp6 m i= vault04.txt`)




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

Geometry: `vault04.txt` from MCNP Criticality Class.

Converting LNK3DNT to VTK/XDMF+HDF5 [5–8]

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

```
> l3d2xdmf -V linkout
Processing file: linkout
  Found 3-D Cartesian (x,y,z) geometry.
  Reading materials... Done.
  Number of x mesh: 125
  Number of y mesh: 120
  Number of z mesh: 24
  Total number of mesh: 360000
  Writing XDMF file... Done.
  Processing mesh and writing HDF5 file...
    Finished 125 of 125 mesh layer iterations... Done.
```

File Sizes

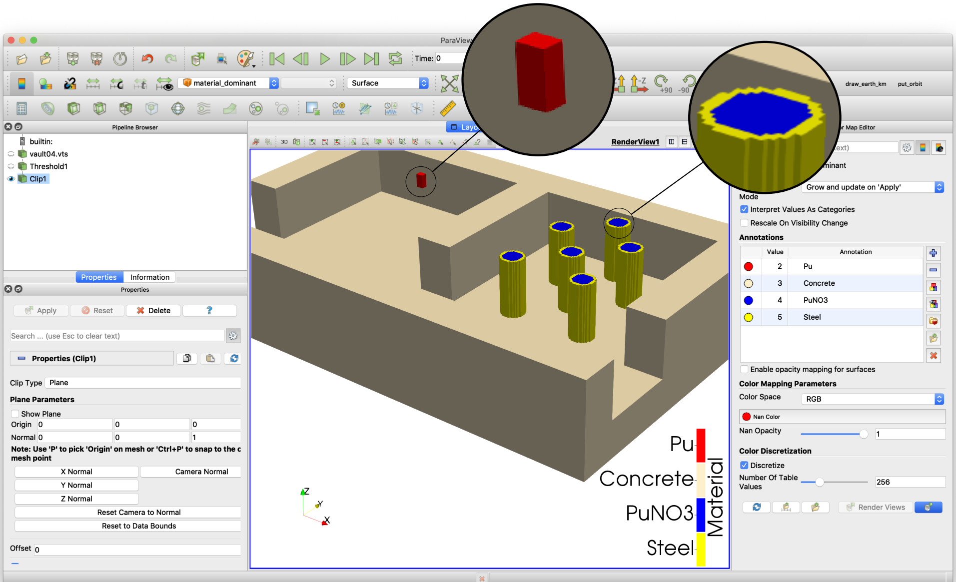
`linkout`: 8.3M

`lnk3dnt.vts`: 27M

`l3dfile.xdmf.h5`: 688k

Top: `l3d2vtk` (MCNPTools [2] v5.1.0+) [3].
Bottom: `l3d2xdmf` (LANL Only) [4].

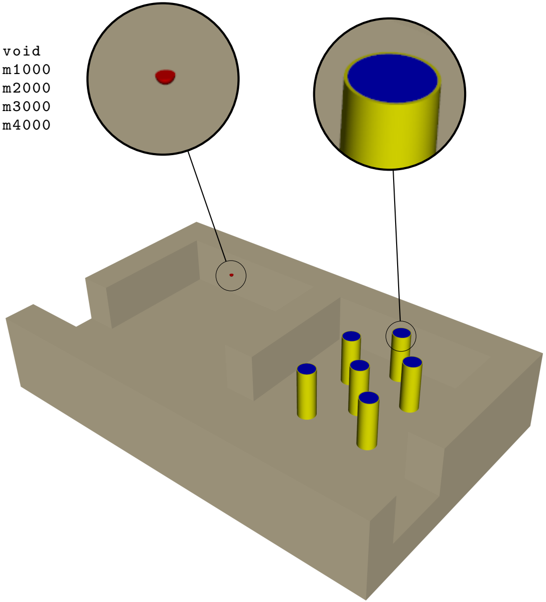
Interactively Viewing LNK3DNT Files [3]



Interface: ParaView [9], which is widely available at LANL for use on on desktop computers and/or through client-server connections to LANL HPC systems.

Compare with: Ray-traced CSG via Radiant [10]

```
colors {
  material     0     0    0    0  255   ! 0 void
  material    -1   255    0    0  255   ! 1 m1000
  material    -2   255  240  200  255   ! 2 m2000
  material    -3     0    0  255  255   ! 3 m3000
  material    -4   255  255    0  255   ! 4 m4000
}

visibility {
  materials_off  0
}

lights {
  light 0.0 0.0 -1.0  1.0
}

clipping {
  plane 0  0 0 150  0.0 0.0 1.0 false
}

image3d {
  background     255 255 255 255
  camera_pos     2048 -1250 1522
  view_angle     30.0
  view_focus     650 300 0
  view_pan       0 0
  view_up        -.34 0.43 0.83
  view_zoom       1.0
}
```

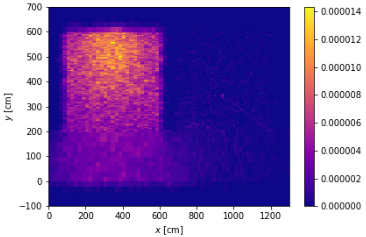


Generated with `radiant -t 4 -r 2560x2048 -a 4 radiant.inp runtpe`.

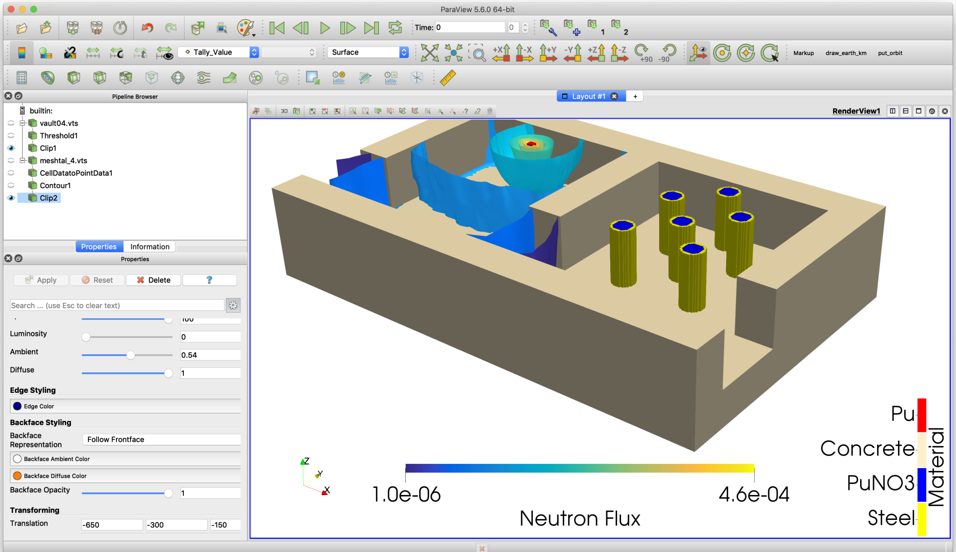
Mesh Tallies (fmesh)

- Several paths to a file that can be visualized interactively in 3-D space
  - MCNP6.2 and before: VTK via `meshtal2vtk` (MCNPTools v5.1.0)
  - MCNP6.3 New Option: `out=xdmf` (XDMF+HDF5)
- XDMF+HDF5 output in `runtpe.h5:/results/mesh_tally`
  - XDMF file must be kept with the runtape file
  - HDF5 results are useful independent of XDMF

```python
import h5py
import matplotlib.pyplot as plt
import numpy as np

f = h5py.File("vault04.txtr.h5", "r")
grid_x = f["/results/mesh_tally/mesh_tally_4/grid_x"]
grid_y = f["/results/mesh_tally/mesh_tally_4/grid_y"]
X, Y = np.meshgrid(grid_x, grid_y)
values = f["/results/mesh_tally/mesh_tally_4/mean"]
Z = values[0, 0, 5, :, :]
plt.pcolormesh(X, Y, Z, cmap="plasma")
plt.colorbar()

plt.xlabel("$x$ [cm]")
plt.ylabel("$y$ [cm]")
plt.tight_layout()

plt.savefig("vault04.png")
f.close()
```



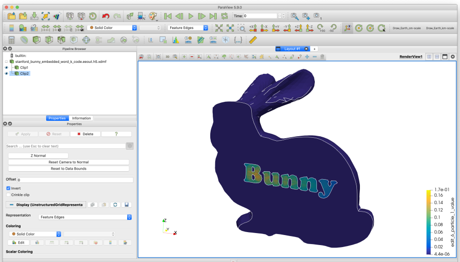
3-D, Interactive, Mesh Tallies + Geometry [3]



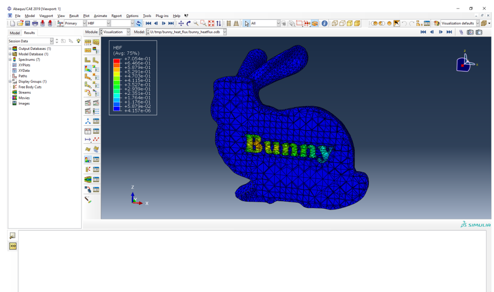
Mesh Tally Surfaces: Cell-to-point Data and Contour Filters.

Viewing UM Geometry & Results

- `um_post_op` could convert EEOUT to VTK [11]; recently unsuccessful
- Multiple post-processing capabilities exist, which include:
  - Attila4MC EEOUT-to-Tecplot [12, 13]
  - Python-based EEOUT-to-VTK [14]
  - Python-based EEOUT-to-Abaqus [15, 16]
- MCNP6.3: directly produce XDMF+HDF5 files from a UM calculation



EEOUT-to-VTK Converter



EEOUT-to-Abaqus Converter

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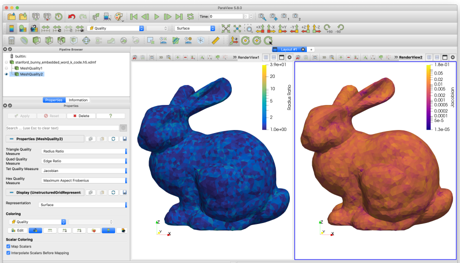
Geometry adapted from [17].

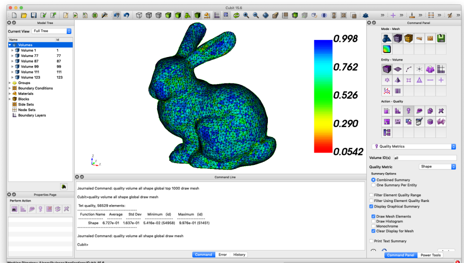
Assessing UM Elemental Quality

- MCNP6.3: Elemental quality assessment added to UM input processing
  - Default enabled with opt-out capability provided
  - The metrics assessed [18] are a subset of those in Verdict [19]
  - Goal: provide enough information to know when more is needed

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
...									
Jacobian	1.000E-30	1.000E+30	1.363E-02	1.583E-02	1.335E-05	1.758E-01	0	56529	0.000
Radius Ratio	1.000E+00	3.000E+00	1.892E+00	1.084E+00	1.003E+00	3.874E+01	4674	56529	8.268
...									



ParaView



Cubit [20]

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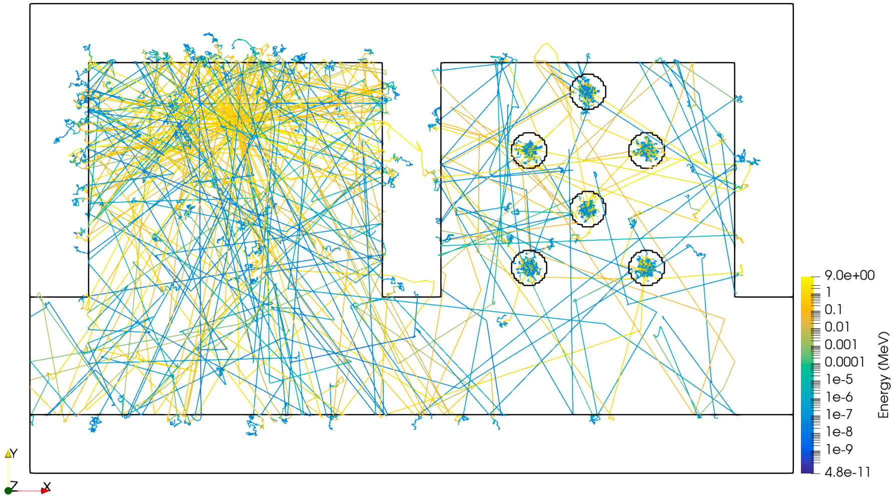
Both ParaView and Cubit provide the same elemental quality metrics as available in Verdict. Geometry adapted from [17].

`ptrac`: Processing & Viewing

- Legacy ASCII & Binary `ptrac` file parsing with MCNPTools
- MCNP6.3: Produce HDF5 ptrac files; works with multiprocessing
  - Can be directly parsed, or interpreted with MCNPTools v5.2.0+



Energy-shaded particle tracks from first 1000 histories.

Summary & Future Work

Summary

- Demonstrated several approaches to visualization beyond MCNP plotter
  - Looked at various MCNP data in isolation and combination
- Explored various interfaces: ParaView, matplotlib, Abaqus, Cubit
- Provided code snippets and supplemental references

Future Work

- Improved approach(es) for parsing `ptrac` data for visualization
- Real-time, interactive, CSG (active research topic)
  - In the meantime, incorporate faithful CSG with results
- Migration of other data to (XDMF+)HDF5 (`rssa`, `srctp`, etc.)

Questions?

Contact Information

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Introduction & Motivation

LNK3DNT
- Generating from MCNP CSG, Converting to VTK/XDMF+HDF5, and Viewing
- Quick Comparison with Ray-traced CSG via Radiant

Mesh Tallies (`fmesh`)
- Converting to VTK, Producing as XDMF+HDF5, and Viewing

Unstructured Mesh
- Viewing UM Geometry & Results, Assessing Elemental Quality
- HDF5 Batch-processing Example

Particle Track (`ptrac`)
- New HDF5 Format; Example Processing & Viewing

Summary & Future Work

Backup Slides

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[14] J. A. Kulesza and T. C. McClanahan, “A Python Script to Convert MCNP Unstructured Mesh Elemental Edit Output Files to XML-based VTK Files,” Tech. Rep. LA-UR-19-20291, Rev. 2, Los Alamos National Laboratory, Los Alamos, NM, USA, Nov. 2019.

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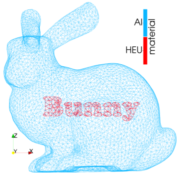
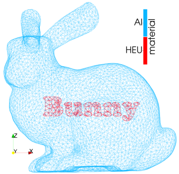
MCNP UM HDF5 Batch Use—Python (h5py)




```
#!/usr/bin/env python

import h5py
import numpy as np

f = h5py.File("stanford_bunny_embedded_word_k_code.h5", "r")

fluence = 0.0
volume = 0.0
for i in f["unstructured_mesh"]["instances"].items():
    e = i[1]["edits"]["edit_4_particle_1"]["values"]
    v = i[1]["volume"]
    fluence += np.inner(e, v)
    volume += np.sum(v)
print(f"Avg. Fluence: {fluence / volume:.3e}")
```

Avg. Fluence: $$\frac{\int \phi(\vec{x}) \mathrm{d}V}{\int \mathrm{d}V}$$

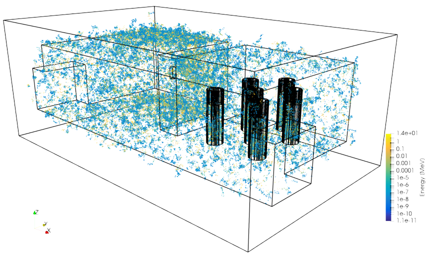
MCNP UM HDF5 Batch Use—ParaView (pvpython)

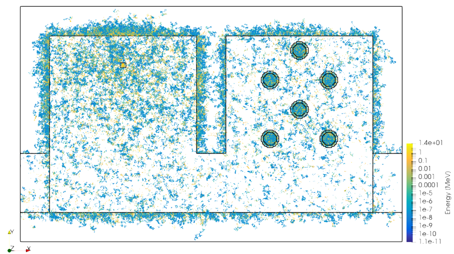



```
#!/Users/jkulesza/Applications/ParaView-5.8.0.app/Contents/bin/pvpython

import numpy as np
from paraview.simple import *
from paraview import servermanager as pvsm

# Setup ParaView.
paraview.simple._DisableFirstRenderCameraReset()
renderView1 = GetActiveViewOrCreate("RenderView")

# Load data.
bunny = XDMFReader(FileNames=["stanford_bunny_embedded_word_k_code.h5.xdmf"])

# Integrate and divide.
iv1 = IntegrateVariables(Input=bunny)
numer = np.array(pvsm.Fetch(iv1).GetCellData().GetArray("edit_4_particle_1_values"))[0]
denom = np.array(pvsm.Fetch(iv1).GetCellData().GetArray("Volume"))[0]
print("Avg. Fluence: {:.3e}".format(numer / denom))
```

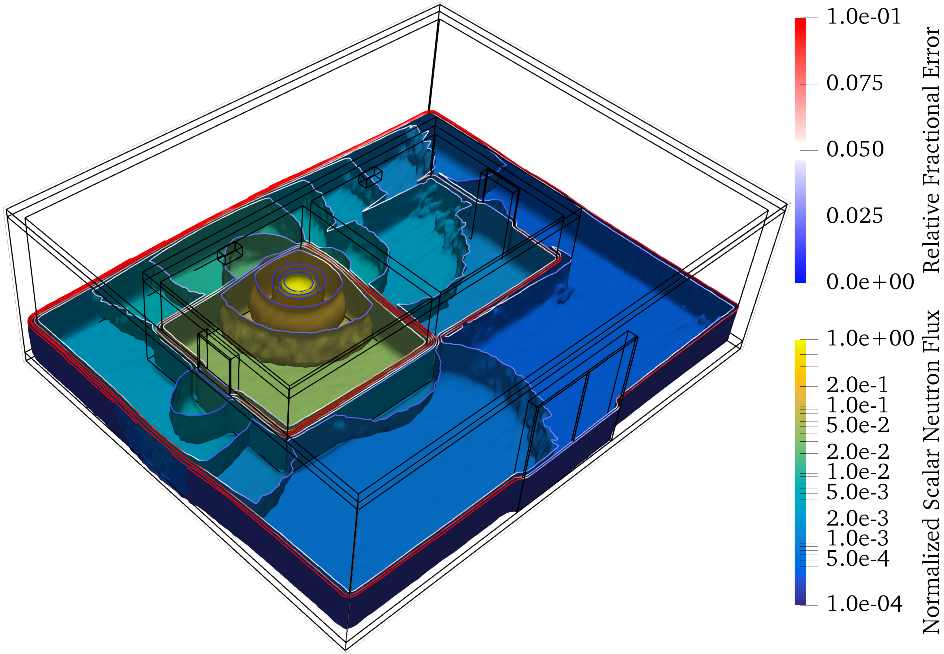
ptrac HDF5 Batch Use—Python (h5py)

```
#!/usr/bin/env python

import h5py
import numpy as np

f = h5py.File("ptrac.h5", "r")
x = f["ptrack/Collision"]["x"]
y = f["ptrack/Collision"]["y"]
z = f["ptrack/Collision"]["z"]
e = f["ptrack/Collision"]["energy"]
d = np.vstack((x, y, z, e))
np.savetxt("Collisions.csv", d.T, delimiter=",", header="x,y,z,e")
```





Example Visualization: Criticality Accident Alarm System



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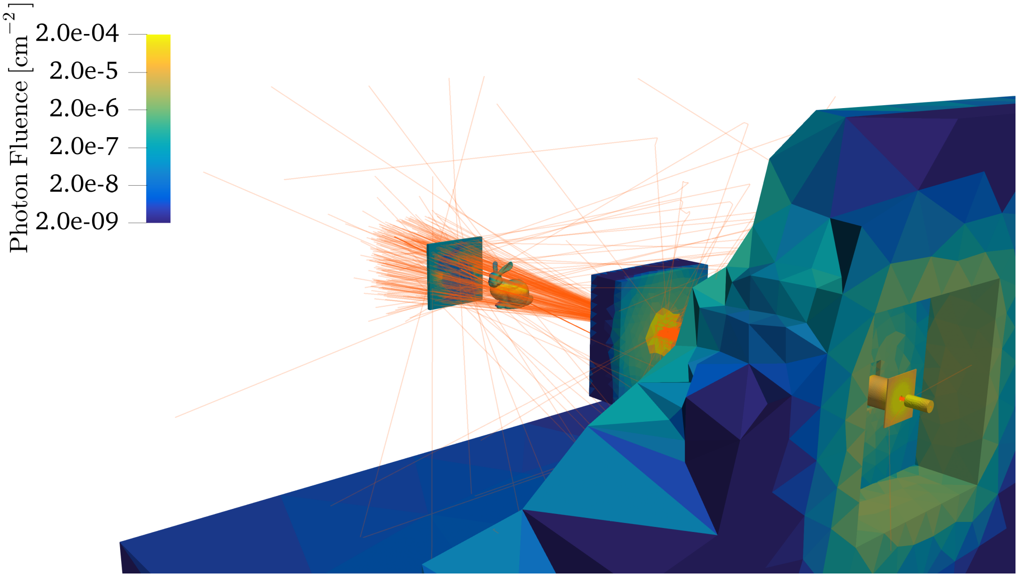
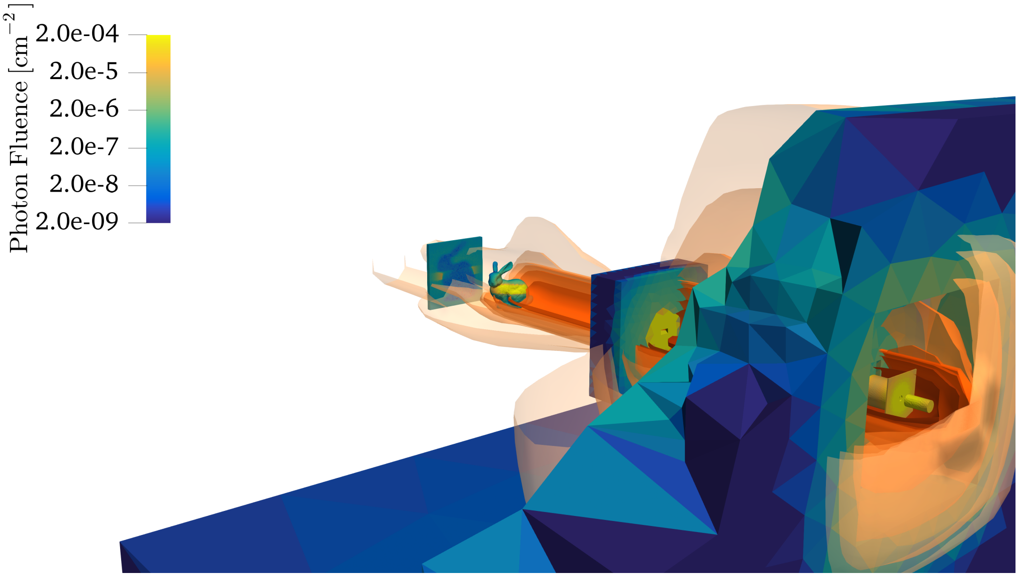
From [14, 22, 23].

Example Visualization: Notional Radiograph Facility



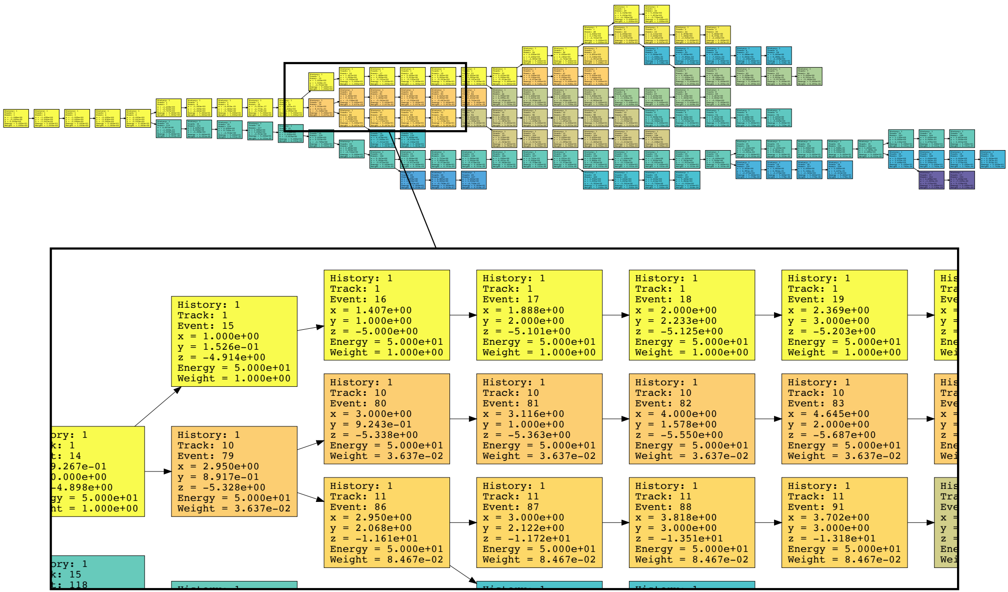
From [22].

Example Visualization: Notional Radiograph Facility, cont.



From [22].

Example Visualization: Particle Evolution via Graphviz [24]



From [22].