LA-UR-24-23469

Approved for public release; distribution is unlimited.

Title: MCNP6(R) New Features and Improvements for Reactor Physics Applications

Author(s): Rising, Michael Evan
Armstrong, Jerawan Chudoung
Maldonado, Alexis
Vaquer, Pablo Andres
Weaver, Colin Andrew

Intended for: International Conference on Physics of Reactors (PHYSOR 2024), 2024-04-21/2024-04-24 (San Francisco, California, United States)

Issued: 2024-07-23 (rev.1)

Los Alamos NATIONAL LABORATORY

Los Alamos
NATIONAL LABORATORY

MCNP6® New Features and Improvements for Reactor Physics Applications

[1]Michael E. Rising, [1]Jerawan Armstrong, [2]Alexis Maldonado, [1]Pablo Vaquer, and [1]Colin Weaver

[1]XCP-3 and [2]NEN-5, LANL

International Conference on Physics of Reactors 2024 (PHYSOR 2024)

Sunday, April 21, 2024

LA-UR-24-23469

Acknowledgements

This work is supported by the Department of Energy through Los Alamos National Laboratory (LANL) operated by Triad National Security, LLC, for the National Nuclear Security Administration (NNSA) under Contract No. 89233218CNA000001.

This work is supported by the LANL MCNP Site Support Project, the LANL LDRD Program, and the DOE Nuclear Criticality Safety Program.

Thanks to the PHYSOR 2024 Topical meeting organizers for including us here.

Thanks to those who provided content to this workshop, including Jennifer Alwin, Simon Bolding, Forrest Brown, Jeffrey Bull, Alexander Clark, Micky Dzur, Colin Josey, Joel Kulesza, Scott Mosher, Josh Spencer, Kristin Stolte, and Sriram Swaminarayan.

Thanks to Jerawan Armstrong and Joel Kulesza for reviewing the content of this workshop.

MCNP® Trademark

MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Triad National Security, LLC, manager and operator of Los Alamos National Laboratory. Any third party use of such registered marks should be properly attributed to Triad National Security, LLC, including the use of the ® designation as appropriate.

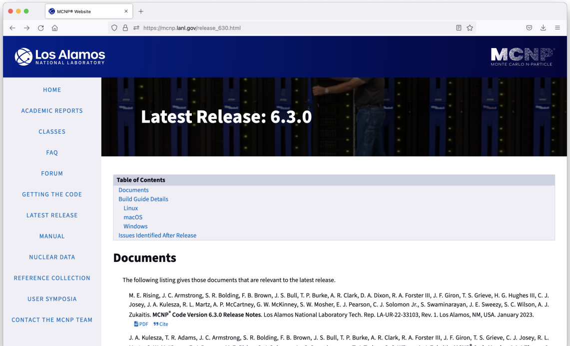
- Please note that trademarks are adjectives and should not be pluralized or used as a noun or a verb in any context for any reason.
- Any questions regarding licensing, proper use, and/or proper attribution of Triad National Security, LLC marks should be directed to trademarks@lanl.gov.

Outline

MCNP6.3 Overview

MCNP6.3 Release

- For the most up-to-date details on the latest release, see the Latest Release (https://mcnp.lanl.gov/release_630.html) tab on the MCNP website.



- The primary MCNP6.3 Release Notes [1], Theory & User Manual [2], Build Guide [3], and Verification and Validation Testing [4] documents can be found on the website and in the software distribution.

New Features

- **Fission-matrix-based convergence testing and acceleration**
- ***Multigroup cross section tallies for reactor analysis***
- Doppler broadening resonance correction
- Stochastic $S(\alpha, \beta)$ temperature mixing
- Mixed-material treatment for structured meshes
- ***New FMESH tally backend options***
- *Parallel PTRAC support*
- CMake build system
- ***HDF5-formatted output files and XDMF support***

Covered or partially discussed in this workshop

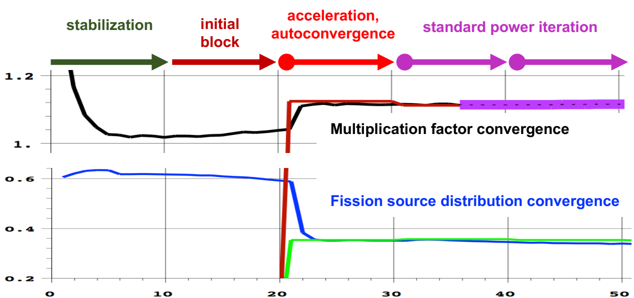
Improvements

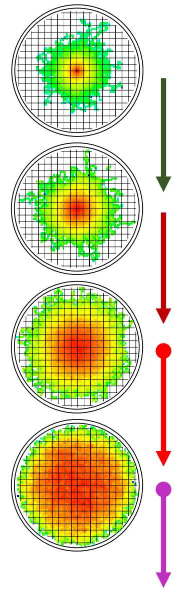
- ***New Qt-based plotter preview available as technology preview***
- All of the MCNP code meets Fortran 2008 and C++ 17 standard requirements
- Preliminary support for upcoming ENDF/B-VIII.1 data changes
  - For new $S(\alpha, \beta)$ format options
  - For photonuclear physics
- *Upgrade to use open-source version of CGMF 1.1.1*
- ***Improved unstructured mesh input file processing***
- ***Added unstructured mesh quality metrics and reporting***
- Decrease of delayed-gamma-line memory usage
- *Various deprecated features with plans for future removal*

Covered or partially discussed in this workshop

Fission-matrix-based Convergence Testing and Acceleration

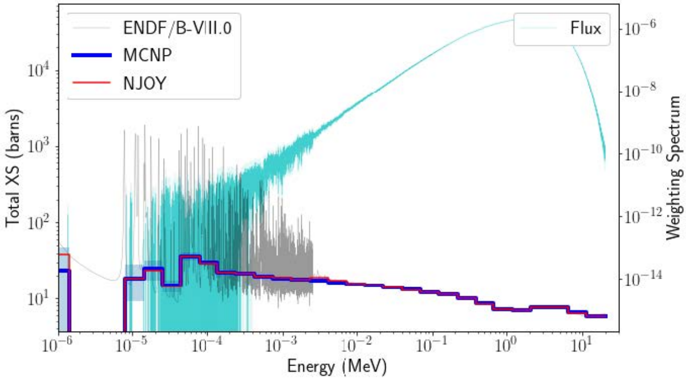
- Automated acceleration of the convergence of the fission source distribution
  - Eliminates user intervention and trial-and-error testing
  - Saves computational cost
- More robust statistical convergence and population testing
  - Ensuring the simulation has converged





Features for Advanced Reactor Analysis

- Unstructured mesh developments for high-fidelity reactor simulations
  - MCNP material properties based on element sets
  - Developed MCNP and ABAQUS based Reactor Multiphysics (MARM) framework for high temperature reactor analysis [5]
- Multigroup cross section tallies computed for coupling to deterministic, time-dependent reactor feedback codes [6]

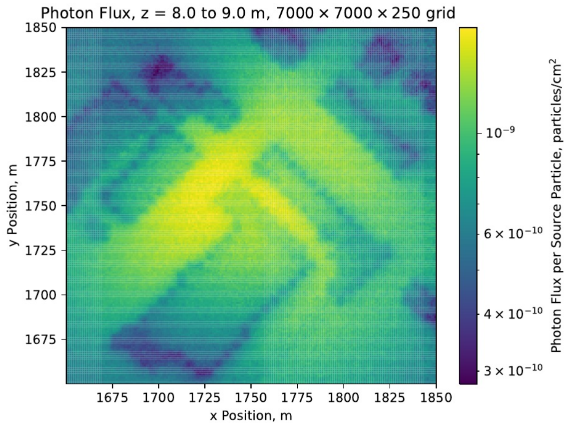


Los Alamos NATIONAL LABORATORY

Mesh Tally Backend Improvements Enabling Extreme-scale, High-fidelity Simulations [7]

- History and batch statistics
- Advanced MPI parallelism options
- Better performance on current problems
- Scaling to extreme scale for higher resolution future problems
  - E.g., full core reactor depletion

12.2 billion tally region problem run with new FMESH capability



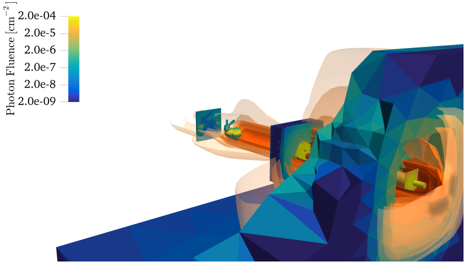
Introduction of the New File Formats (1)

- Introduced a flexible, Hierarchical Data Format (HDF5) to replace legacy binary and ASCII files
  - Permits natural organization
  - Parallel input/output can provide substantial performance
  - Parallel data transfer and distribution provides extensive mesh tally scalability
  - Intrinsic data-compression capability can provide 10–100× file size savings
  - Accessible via C, C++, Fortran, Python, Matlab, etc.
- The restart file (runtpe) now an HDF5 file in MCNP6.3.
- The ptrac file and unstructured mesh model / elemental edit files all now have an HDF5 option in MCNP6.3.

Introduction of the New File Formats (2)

- XDMF visualization through openly available software (e.g., ParaView, VisIt)
  - XML-formatted ASCII XDMF file can be easily interrogated via standard text editor
  - Permits many geometric representations: structured, unstructured, polyhedral, etc.
  - Low-overhead roadmap into the aforementioned HDF5 data file(s)
- HDF5+XDMF: directly accessible data files providing immediate visualization

Mesh Tally Results Visualized via ParaView



Simple Godiva Example (1)

Include last line if running with MCNP6.3, otherwise exclude.

Listing 1: godiva.mcnp.inp

```
 Godiva  Solid Bare HEU sphere  HEU-MET-FAST-001
1     100     4.7984e-02     -10      imp:n=1
2     0                       10      imp:n=0

10    so      8.7407

kcode  5000  1.0  50   250
ksrc   0 0 0
c
m100   92234.00c   4.9184e-04
       92235.00c   4.4994e-02
       92238.00c   2.4984e-03
c
fmesh4:n    geom=xyz  origin=-10 -10 -10
            imesh=10  iints=200
            jmesh=10  jints=200
            kmesh=10  kints=200
            out=xdmf              $ New out option in MCNP6.3
```

Los Alamos NATIONAL LABORATORY

Simple Godiva Example (2)

MCNP6.2

- Execution command:

```
mcnp6 i=godiva.inp n=godiva.  tasks 8
```

- Directory listing:

```
/
 |- godiva.inp
 |- godiva.o
 |- godiva.r
 |- godiva.s
 |- godiva.msht
```

- ~ 78 M Histories / hr

MCNP6.3

- Execution command:

```
mcnp6 i=godiva.inp n=godiva.  tasks 8
```

- Directory listing:

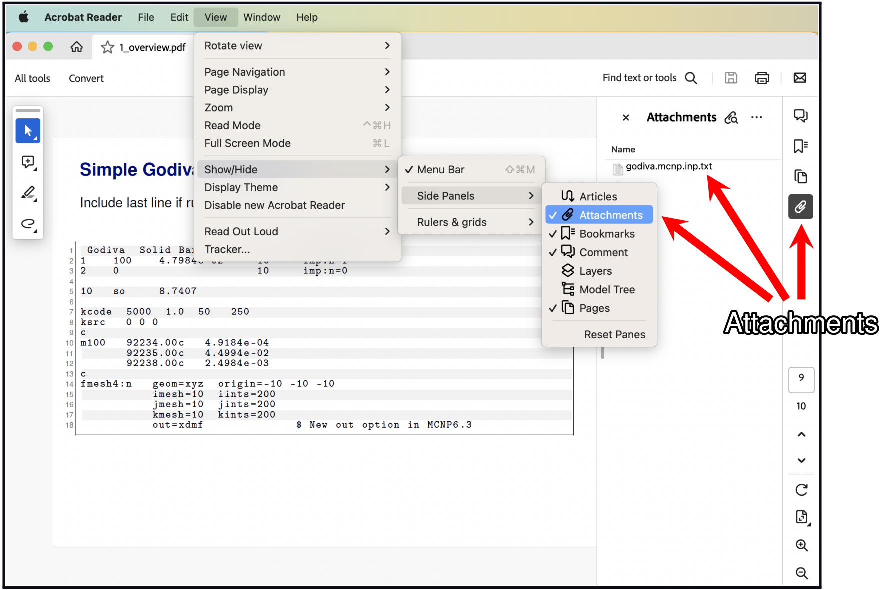
```
/
 |- godiva.inp
 |- godiva.o
 |- godiva.r.h5
 |- godiva.s
 |- godiva.msht.xdmf
```

  - `.h5` file extension for new HDF5 files
  - `.xdmf` file extension for new XDMF files
- ~ 710 M Histories / hr

Los Alamos NATIONAL LABORATORY

Extracting Inputs and Scripts from Workshop PDF

- Recommend downloading attachments and removing `.txt` file extension



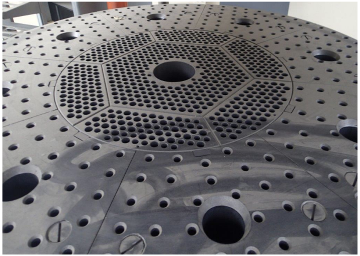
Deimos Project

LANL R&D Project

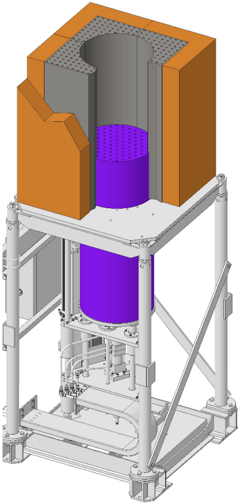
- Deimos is an ongoing LANL Laboratory Directed Research & Development (LDRD) project
- Motivation
  - Nuclear power reactor design, measurement, and validation for deep space missions
  - Small reactors need high assay low enriched uranium (HALEU) and/or particulate fuel
- Goals
  - Critical experiment design and measurement at Nuclear Criticality Exeriments Research Center (NCERC)
    - Schedule to be executed in 2024
  - Materials research for optimal coatings and moderator materials
  - Modeling and simulation work
    - Development of new MCNP features (e.g. Delta tracking capability)
    - Multi-physics calculations of Deimos

Deimos Experiment

- Compact Nuclear Power Source (CNPS) hexagonal graphite matrix and HALEU fuel from a critical experiment in the 1980s
- The HALEU TRISO fuel used in CNPS is used in the Deimos experiment
- Due to the Comet assembly weight restriction at NCERC, a beryllium reflector is used in parts where some of the original graphite was located in CNPS design



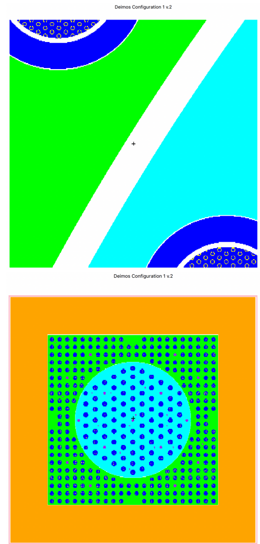
CNPS Graphite

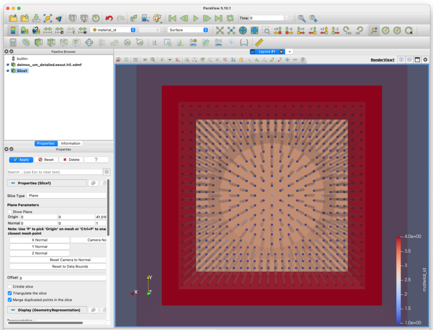


MCNP Deimos Models

- CSG TRISO Particulate Model
  - Most accurate / most computationally expensive
- CSG Homogenized Model (not shown)
  - Can be accurate / least computationally expensive
- Unstructured Mesh Models
  - Accuracy depends on how well model preserves volume/mass and shape

MCNP CSG TRISO Plotter Visualization





ParaView UM Visualization

Multi-physics Coupling

Coupling MCNP6.3 to Griffin

- MCNP6.3 calculates
  - Multigroup cross sections for Deimos reactor
  - Adjoint-weighted kinetics parameters
- Griffin, part of the NEAMS tools, calculates
  - Reactor dynamics, transient analysis
  - Heat conduction simulation
  - Includes deterministic (SN) transport
- For more discussion on multiphysics analysis techniques related to Deimos, see “Transient Modeling and Simulation for Deimos, an Advanced Reactor Experiment” in the Tuesday, 3:30-5:15 PM Experimental Reactor Physics technical session here at PHYSOR 2024.

MCNP
MONTE CARLO N-PARTICLE

NEAMS

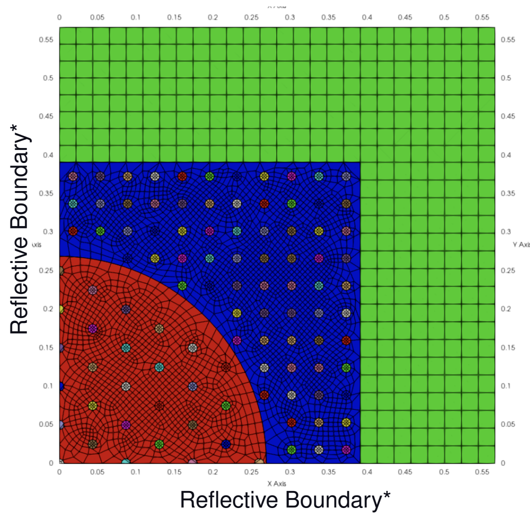
Griffin

Deimos Model Used in Workshop Exercises

- Using a quarter core (wth proper reflecting boundary conditions) unstructured mesh model of a simplified Deimos reactor model
  - Includes both the Abaqus and MCNP input files
  - Abaqus mesh model generated using CUBIT

- Both Abaqus and MCNP inputs electronically attached to this PDF
  - `deimos_um_simple.abaq.inp`
  - `deimos_um_simple.mcnp.inp`

Representative Deimos Quarter-core UM Model (different from workshop model)



Aside: MCNP UM Input File Construction

- Before venturing into a variety of new MCNP6.3 features
  - Open `LA-UR-24-23422_mcnp_um_input_files.pdf` document
  - "Constructing Input Files for MCNP Unstructured Mesh Simulations"

```
MCNP6_PHYSOR_2024_Workshop/
  MCNP6_PHYSOR_2024_Workshop.pdf
  outputs/
  supplemental/
    LA-UR-24-23422/
      LA-UR-24-23422_mcnp_um_input_files.pdf
      simple_deimos/
      simple_thermal/
```

- Additional exercises and scripts provided with this supplemental workshop material that allow for easier MCNP UM input file pre-processing and setup

Unstructured Mesh and HDF5

Unstructured Mesh Overview

Overview of Unstructured Mesh in MCNP6.3

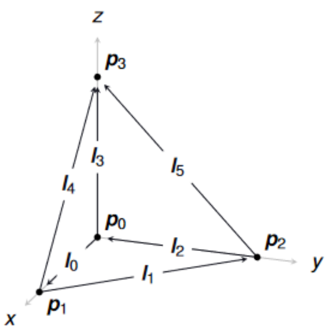
- Significant refactoring and modernization work done to clean-up existing and unused code paths
- Added mesh element quality assessment to the MCNP6.3 code
- Additional regression, verification, and validation testing with additional comment, warning, and fatal error messages
- New HDF5 input format option and HDF5+XDMF elemental edit output format option
  - The Abaqus input format can be used to produce the new HDF5 input format with the MCNP input (`mcnp6 i ...`) processing option
  - The elemental edit HDF5+XDMF output builds on top of the input HDF5 format such that it can be used as input for an initial calculation or for a restart calculation
- Reduced mesh input processing times and memory consumption
- Deprecated legacy UM Fortran utilities in favor of new Python-based scripts

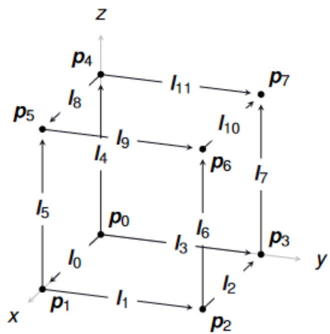
Mesh Elemental Quality Assessment

- Recent review of MCNP UM quality assessment and reporting work [8]
- Detailed discussion on calculating element quality [9, 10]
- Mesh-element quality is a thoroughly studied topic, e.g., [9, 11–13]
  - Also: International Meshing Roundtable [https://imr.sandia.gov]
  - Origins in mesh generation: calculate metrics and remesh toward optima
- The MCNP um_pre_op utility [14] has an "element checker"
  - Evaluates elemental Jacobian matrix determinant: go/no-go criterion
  - Must be run/inspected manually by a user; not implicitly in workflow
  - Invoked as, e.g., `um_pre_op -ec -o inp1034.ec.out um1034.abaq`
  - Looking for final line: "Total number of failed elements: 0"
- MCNP6.3 advances in mesh quality assessment
  - Quality metrics implemented for MCNP UM element types
    - Reproduced um_pre_op capability
    - Most-commonly used elements emphasized
    - Default enabled, opt-out available via embed card `elementchk` toggle

Approach to UM Quality Assessment (1)

- Start by focusing on linear tetrahedra and hexahedra
  - Most commonly used elements by MCNP UM practitioners
  - Most thoroughly studied elements by mesh-quality community
  - Identify metrics that can be characterized versus recommended ranges
  - All metrics exist on continua (i.e., no discrete and/or Boolean metrics)
  - Recommended ranges usually support FEA mesh-quality needs
  - This may lead to overly conservative recommended min/max values
  - Most consolidated source identified: Verdict library





Approach to UM Quality Assessment (2)

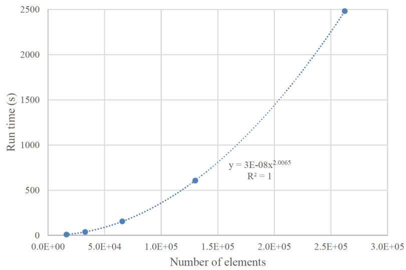
- Provide enough information to know if more information is needed
  - Provide information implicitly; don't require more workflow tasks
  - Ability to opt out in case mesh is "known to be good"
  - Elemental quality metric distribution information (a balancing act)
  - Number of elements inside / outside recommended ranges
  - Ample warning that more attention may be needed
  - Conservatism, until better guidance is available, is good
  - Education on how to learn more about mesh quality
- Warnings and Output Tables
  - Functional approach: warnings (below) and output tables
    - Warnings in standard output prompt user to inspect output tables
    - Output tables inform whether additional, external, study is necessary
  - (Conservative) warnings sent to standard output and output file...

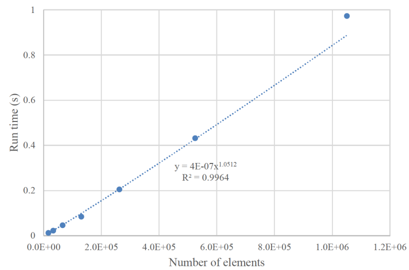
```
warning.  at least one element Maximum Edge Ratio outside recommended range.
warning.  at least one element Oddy outside recommended range.
warning.  at least one element Scaled Jacobian outside recommended range.
warning.  at least one element Shear outside recommended range.
warning.  at least one element Skew outside recommended range.
warning.  at least one element Stretch outside recommended range.
warning.  at least one element Taper outside recommended range.
```

Reduction in UM Initialization Computational Time

- For efficient particle tracking, the UM input processing includes a step to store neighbor-to-neighbor element information
- In MCNP6.2 this step is $O(N^2)$ and in MCNP6.3 this step is $O(N)$
- For large UM models, this is a significant improvement
  - For example, a city-sized UM model with 700k+ linear hexahedral element model had a 20x speedup in input processing time

UM Input Processing Times for MCNP6.2 (left) vs. MCNP6.3 (right)





Los Alamos NATIONAL LABORATORY

Reduction in UM Memory Consumption

- In MCNP6.2, UM models with many parts that have a large variance in the number of elements can lead to excessive amounts of unnecessary memory allocated
- This can be especially important when running MPI parallel calculations with a large number of ranks
- The example below is using a UM model of the ORNL PCA Problem

UM Memory Usage for MCNP6.2 (Devel) vs. MCNP6.3 (Mem)

Branch	Case	Mesh Init Time	Memory reported by top	RSS reported by top	Actual Savings	Expected Savings
Devel	1x1	49s	3.3 GB	2.8 GB	**1.7 GB**	**1.4 GB**
Mem	1x1	49s	1.6 GB	1.2 GB		
Devel	1x36	22s	6.0 GB	3.1 GB	**1.3 GB**	**1.4GB**
Mem	1x36	22s	4.7 GB	1.9 GB		
Devel	144x1	130s	416 GB	332 GB	**192 GB**	**201 GB**
Mem	144x1	37s	224 GB	144 GB		
Devel	72x1	70s	199 GB	161 GB	**94 GB**	**101 GB**
Mem	72x1	31s	105 GB	70 GB		
Devel	72x2	70s	193 GB	162 GB	**119 GB**	**101 GB**
Mem	72x2	28s	74. GB	27 GB		

MCNP Unstructured Mesh Geometry

- The MCNP unstructured mesh (UM) feature was implemented to allow MCNP to read in an Abaqus mesh file, generated by Abaqus, a multiphysics and finite element analysis code.
- The use of a mesh in MCNP allows a multiphysics code such as Abaqus to be used in tandem to perform neutronics analysis with MCNP and other analyses such as heat transfer with a separate code.
- Mesh quality is important
  - Mass/volume may not be preserved
  - Especially important for criticality calculations
- It is possible to generate a mesh, which reflects the geometry adequately for most purposes, and yet does not properly preserve mass and/or volume to the degree necessary for correct validation efforts using criticality safety benchmarks and shielding benchmarks.

Criticality Calculations using UM Geometry

Recent ICSBEP benchmarks modeled in MCNP6 UM [15].

HEU-MET-FAST-001: Godiva- bare, fast, spherical assembly of 94% 235U metal.

HEU-MET-FAST-007-037: HEU metal slabs moderated with polyethylene and reflected with polyethylene.

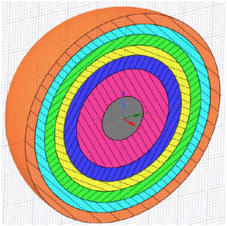
IEU-MET-FAST-007: Big Ten, a large, mixed-uranium cylindrical core with 10% average 235U enrichment, surrounded by a thick 238U reflector.

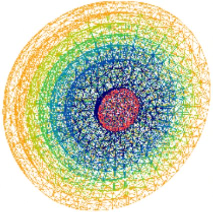
PU-MET-FAST-022: A bare, fast, spherical assembly of delta-phase plutonium metal, 98% 239Pu.

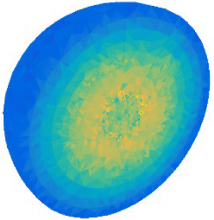
PU-SOL-THERM-001-001: A water-reflected 11.5-inch diameter sphere of plutonium nitrate solution.

Goals:

1. Determine engineering best practices for mesh parameters
2. Compare CSG, UM and experiment results

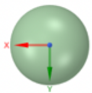




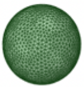


HEU-MET-FAST-001 Godiva

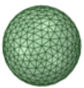
- UM meshing strategy: Element size control and mass correction



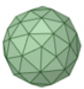
True Sphere (Radius = 8.741 cm)
Volume = 2797.4 cm^3 | Area=960.1 cm^2
SA/Vol = 0.343



Meshed Sphere (Max Edge Length = 1 cm)
Volume = 2785.6 cm^3 | Area = 957.6 cm^2
SA/Vol = 0.344



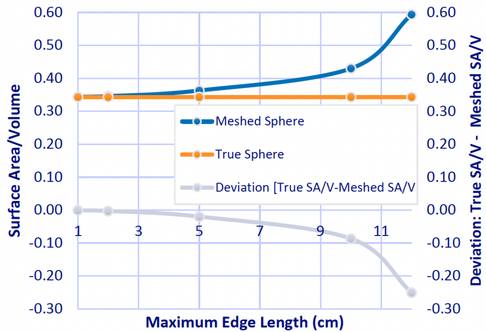
Meshed Sphere (Max Edge Length = 2 cm)
Volume = 2746.6 cm^3 | Area = 950.3 cm^2
SA/Vol = 0.346

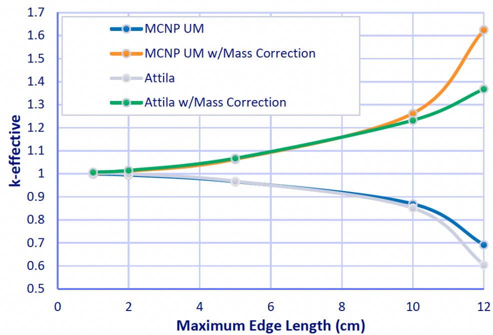


Meshed Sphere (Max Edge Length = 5 cm)
Volume=2480.9 cm^3 | Area=899.2 cm^2
SA/Vol = 0.363

Meshed Sphere (Max Edge Length = 10 cm)
Volume = 1748.3 cm^3 | Area = 752.2 cm^2
SA/Vol = 0.430

Meshed Sphere (Max Edge Length ≥ 12 cm)
Volume = 890.5 cm^3 | Area = 529.2 cm^2
SA/Vol = 0.594

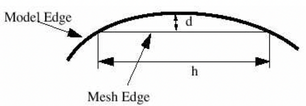


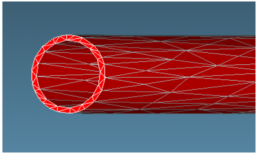


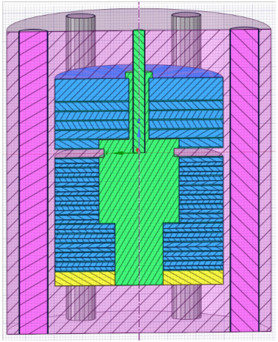
Los Alamos
NATIONAL LABORATORY

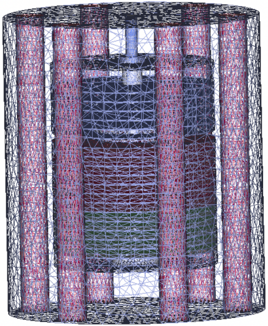
HEU-MET-FAST-007 Big Ten

- UM meshing strategy: Curvature Refinement
  - Allows the mesh to be automatically refined to match the curvature of the entities in the geometric model.
  - Mesh size is selected such that the distance of the model edge curve from the mesh edge (d) over the mesh edge length (h), d/h < 0.5
  - Useful values for d/h are typically in the range of 0.01 to 0.4 (smaller value=more refinement)



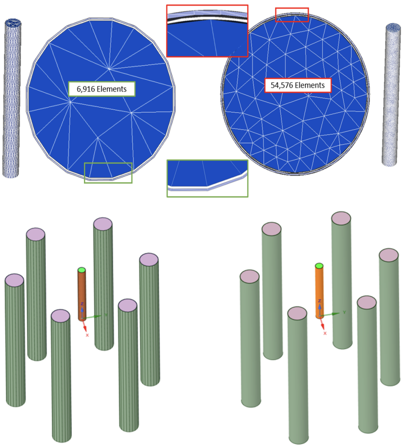


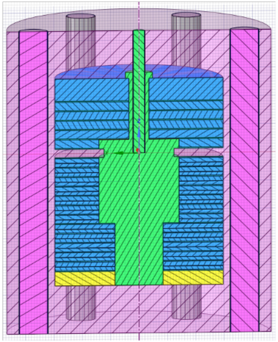


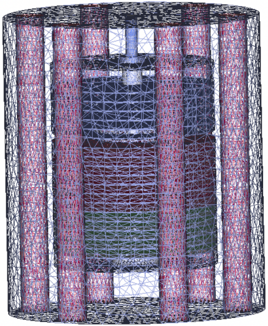


HEU-MET-FAST-007 Big Ten

- UM meshing strategy: Pre-faceting
  - 20-sided polygon vs. true cylinder
  - Radial tolerances strictly preserved
  - Mesh size substantially reduced







Critical Benchmark Validation Results

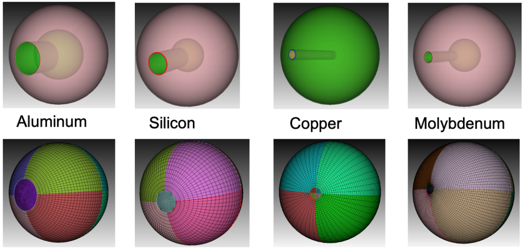
- Critical benchmarks with various materials and geometry have been studied for use with MCNP6 UM
- k-effective results that are within $\approx$ ½% experimental values when due care is applied to mesh quality, in preserving both the mass and shape.
- Mesh within mass and/or volume tolerances 1-2%
  - Volume within 2%, SA/V within 1%

Benchmark	Calc/Exp k-effective CSG	Calc/Exp k-effective UM
HEU-MET-FAST-001	1.0000	0.9984
HEU-MET-FAST-007-037	1.0030	1.0029
IEU-MET-FAST-007	0.9999	0.9995
PU-MET-FAST-022	0.9983	0.9960
PU-SOL-THERM-001-001	1.0058	1.0030

UM Verification and Validation Summary

- In the past couple of years, a dedicated UM verification and validation effort has been ongoing
- Focused on CSG vs. UM comparisons to ultimately understand the mesh quality requirements to obtain comparable results to a proper CSG benchmark model
- Both criticality safety benchmarks and shielding benchmarks have been studied
- UM testing will continue and ultimately become part of our standard V&V efforts in the future

Oktavian Shielding Benchmarks from SINBAD [16]



Aside: HDF5

Motivation

- MCNP output exists in many forms with various uses
  - Output file (`outp`)
    - Human-readable collection of relevant results
  - Data files (EEOUT, `mctal`, `meshtal`, `runtpe`, `ptrac`, etc.)
    - Uniquely formatted to support post-processing (plots, tables, etc.)
- Several of the data files can be written as binary
  - Fast, efficient storage
  - Non-standard formats; hard to parse (needs custom applications)
- MCNP data files are migrating toward HDF5 to eliminate this downside
  - Mesh tally (`fmesh`), `ptrac`, `runtape`, and UM output are implemented
  - Other files undergoing development and implementation

Introduction to HDF5

- HDF: Hierarchical Data Format
- Developed by The HDF Group – Non-profit organization
  - Spun off from Nat'l Center for Supercomp. Appl. at Univ. of Illinois
  - Central authority to ensure quality and prevent fragmentation
- BSD-like license, freely available, portable, numerous APIs
  - Official APIs: C, C++, Fortran, Java
  - Unofficial APIs: Julia, Matlab, Mathematica, Perl, Python, R
- Developed with speed and scalability in mind
- Binary format, which requires a program or API to read the data
- Three major objects: groups, datasets, and attributes

Groups	Containers for datasets or other groups (like a file system)
Datasets	Homogeneous n-dimensional arrays - Can contain complex objects, e.g., images
Attributes	Can be added to either groups or datasets

History of HDF5

- 1987: work to develop all-encompassing hierarchical object-oriented file
- 1990 and 1992: NSF grants provided crucial funding
  - NSF wanted to harmonize netCDF and HDF formats
  - Drove improved V&V basis
  - NASA selected HDF as its standard data and information system
- 1996: major redesign: went to current group & dataset approach
- More information in videos at: https://www.hdfgroup.org/about-us/

- HDF4 is older but actively supported
- HDF5 is current (and actively supported)
  - Attempts to address some HDF4 limitations

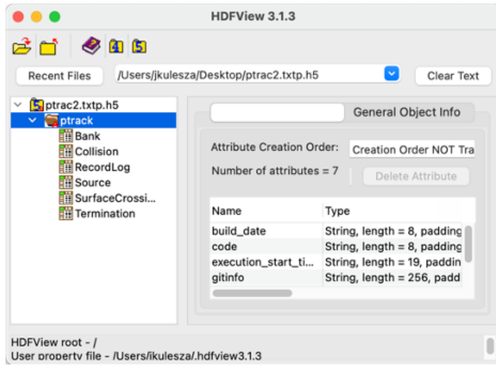
HDF5 is Binary, but Easily Interrogated

- Each group (e.g., `/ptrack/`) is like a filesystem directory
- Each dataset (e.g., `Bank`) is just an array of data that can be processed

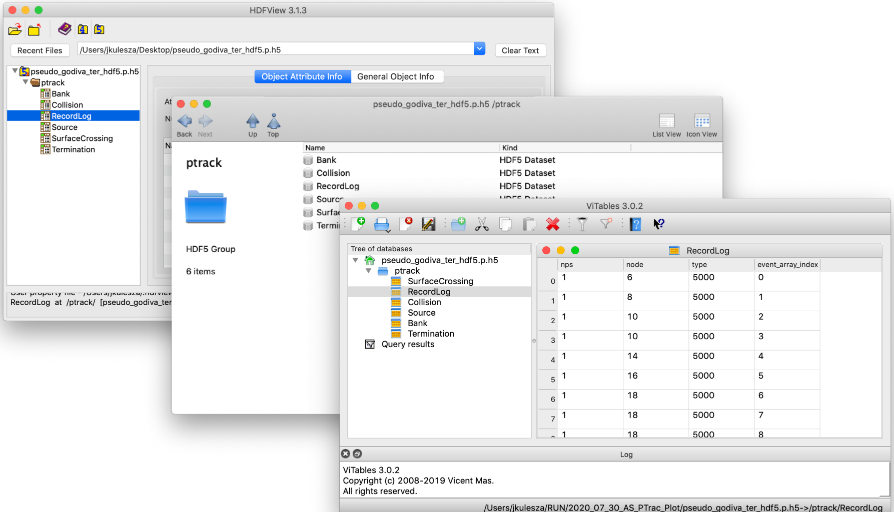
`h5ls` and `h5dump` for terminal usage

```
h5ls -r ptrac2.txtp.h5
/                            Group
/ptrack                      Group
/ptrack/Bank                 Dataset {0/Inf}
/ptrack/Collision            Dataset {12920729/Inf}
/ptrack/RecordLog            Dataset {12923729/Inf}
/ptrack/Source               Dataset {3000/Inf}
/ptrack/SurfaceCrossing      Dataset {0/Inf}
/ptrack/Termination          Dataset {0/Inf}
```

`HDFView` for graphical exploration



GUI Options: HDFView, HDF Compass, and ViTables



Los Alamos NATIONAL LABORATORY

Demo UM to HDF5 and Visualization in Paraview

Convert Abaqus Mesh File to HDF5

Step 1: Open MCNP Input File: `deimos_um_simple.mcnp.inp`

Step 2: Ensure `EMBED` card includes `hdf5file` keyword specifying the name of the HDF5-formatted model and elemental edit file:

Listing 2: UM Embed Card Input/Output File Information

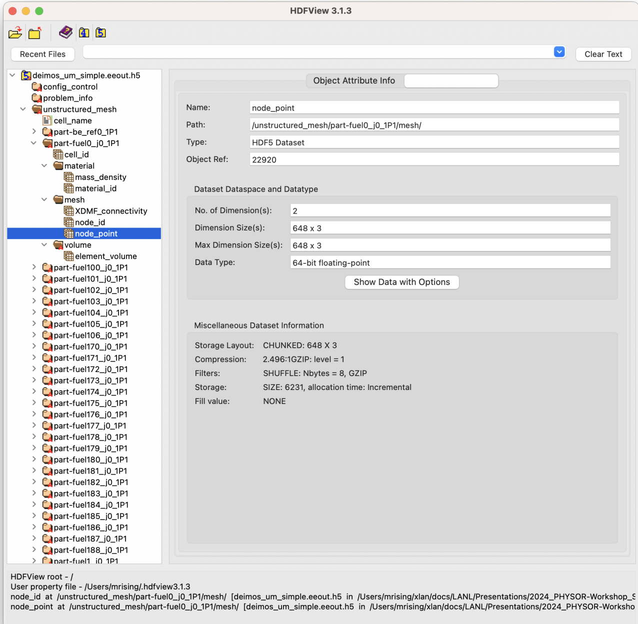
```
embed1 meshgeo=abaqus
       mgeoin=deimos_um_simple.abaq.inp
       hdf5file=deimos_um_simple.um.h5
```

Step 3: Run MCNP in input-processing only mode:

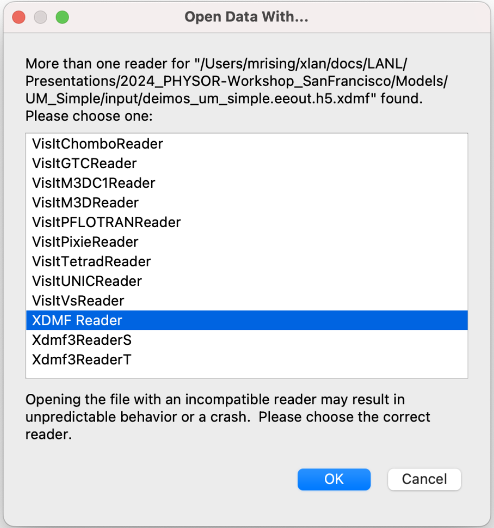
```
> mcnp6 i i=deimos_um_simple.mcnp.inp
```

A new HDF5 (.h5 extension) and XDMF (.h5.xdmf extension) file should now be in the current working directory.

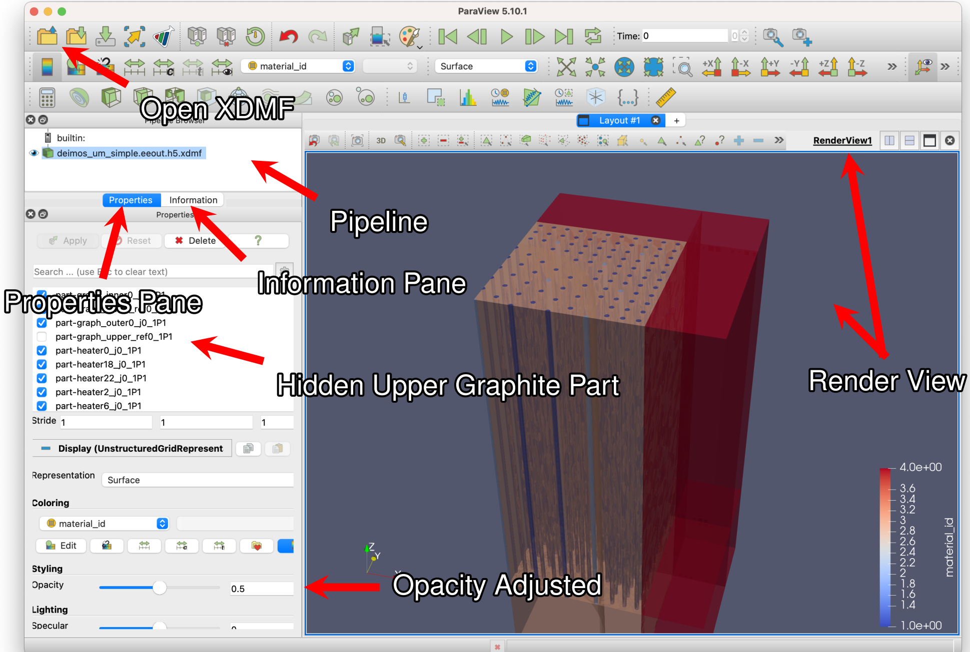
Mesh Information in HDF5 Format



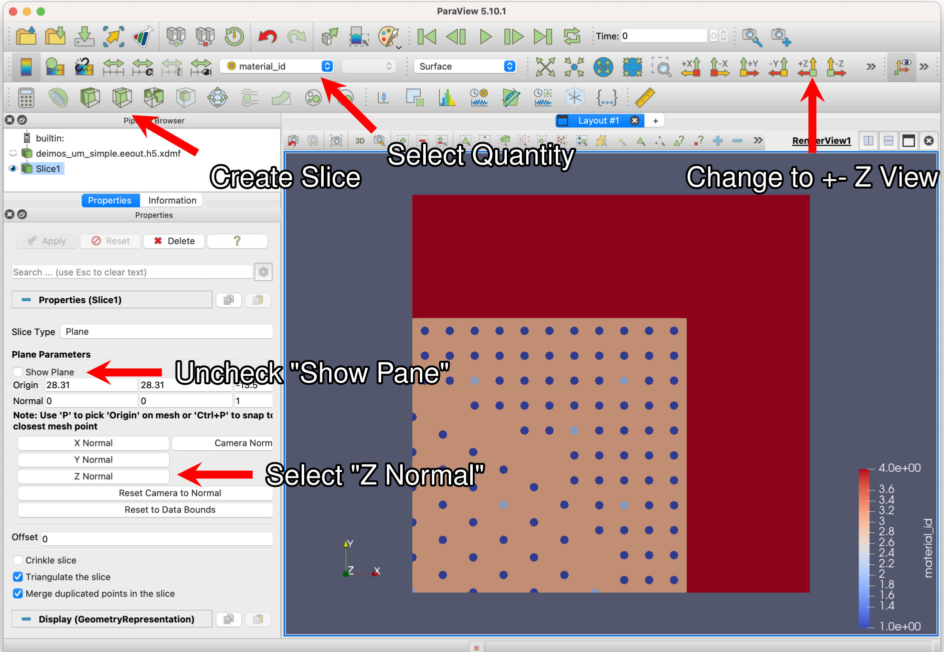
Open XDMF File in ParaView



View Mesh Model in ParaView



Add Slice Through Mesh Model in ParaView



Monte Carlo Simulation and Elemental Edits

Step 1: Open MCNP Input File: `deimos_um_simple.mcnp.inp`

Step 2: Ensure `EMBEE` card is included corresponding to `EMBED` card:

Listing 3: UM Embed Elemental Edit Card

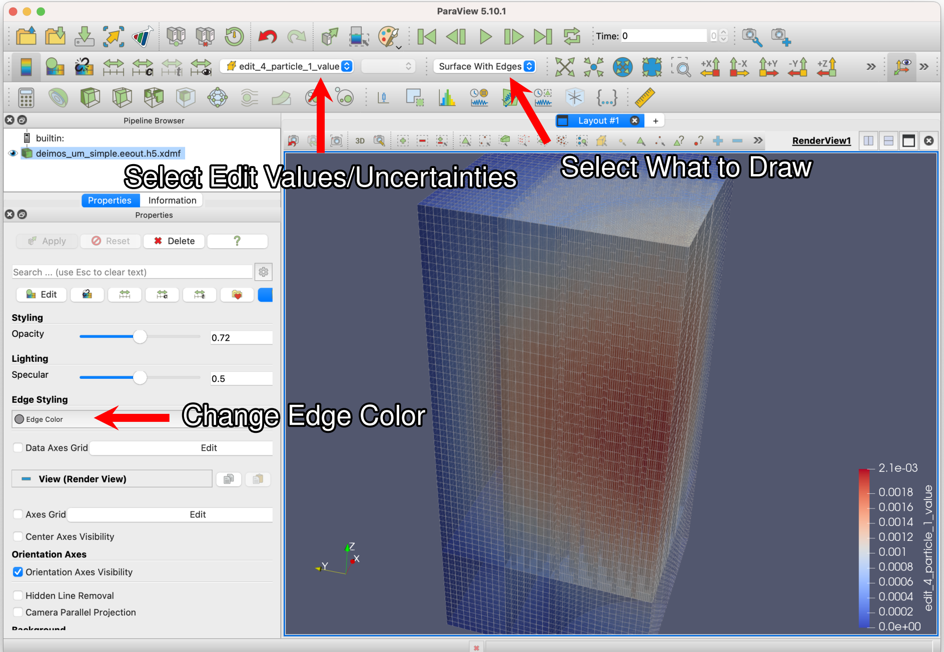
```
embee4:n embed=1 errors=yes
```

Step 3: Run MCNP in default input and cross section processing and Monte Carlo mode:

```
> mcnp6 i=deimos_um_simple.mcnp.inp tasks 8
```

The HDF5 (.h5 extension) and XDMF (.h5.xdmf extension) files now include the elemental edits.

View Elemental Edits in ParaView



Fission Matrix for Criticality Calculations

Fission Matrix Overview

Overview of the Integral Transport Equation for Multiplying System

- Consider Peierl's integral transport equation for a multiplying system:

$$S(\boldsymbol{p}) = \frac{1}{k}\int \mathcal{F}\big(\boldsymbol{p}', \boldsymbol{p}\big) S\big(\boldsymbol{p}'\big) \mathrm{d}p' \,,\ \boldsymbol{p} \equiv (\boldsymbol{r}, \boldsymbol{\Omega}, E)$$

- Where

$\boldsymbol{p}$ is the particle phase space
$\mathcal{F}(\boldsymbol{p}', \boldsymbol{p})$ is the transport operator – including leakage, collisions, scattering, and multiplication
k is the effective multiplication factor
$S(\boldsymbol{p})$ is the fission source

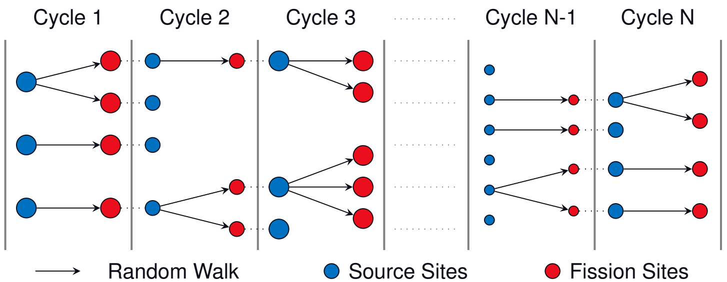
- Think of $\mathcal{F}(\boldsymbol{p}', \boldsymbol{p})$ as the operator that describes the transition of a neutron born from fission to the phase space of the next neutron born from an induced fission reaction

Power Iteration Method

- In MCNP, the power iteration technique is used to compute the final converged eigenvalue k and eigenfunction S of the system
  - Where the $k^{(i)}$ and $S^{(i)}$ are given for iteration index i

$$S^{(i+1)} = \frac{1}{k^{(i)}} \mathcal{F} S^{(i)}$$

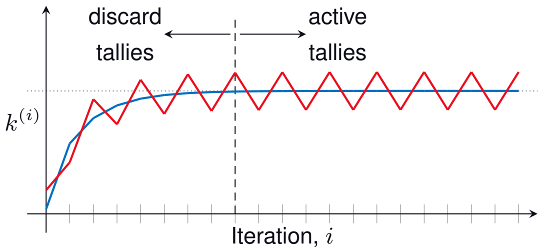
  - The next iteration $k^{(i+1)}$ and $S^{(i+1)}$ are computed during the Monte Carlo random walk ($\mathcal{F}$ operator)
  - Renormalization of the fission source (indicated by resized source sites) at beginning of each cycle



Monte Carlo Criticality Calculations Concerns

For the fundamental eigenvalue, k:

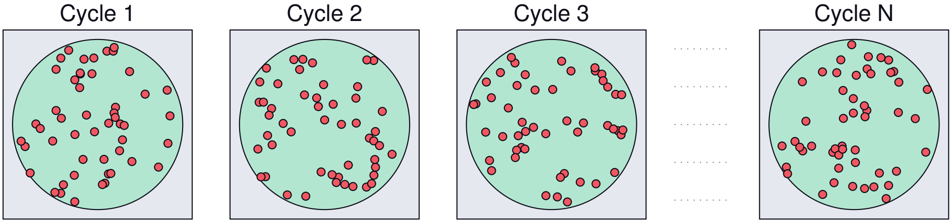
- Convergence
  - Assessing trends in k as a function of iteration, i, is straightforward
  - Use standard statistical testing to confirm converged eigenvalue
- Renormalization bias
  - Bias in k is non-conservative
  - Proportional to $^1/_N$ (N neutrons/cycle)
- Undersampling
  - Typically impacts eigenfunction S more than the eigenvalue k



Monte Carlo Criticality Calculations Concerns

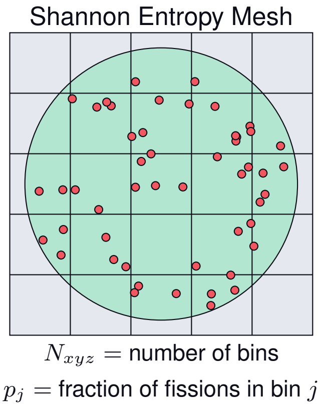
For the fundamental eigenvector, S:

- Convergence
  - Local fission source S takes longer to converge than integral k
  - Bias in source shape related to initial source guess
- Renormalization bias
  - Bias in S appears as a tilt
  - Like k, reduction in bias with more N neutrons/cycle
- Undersampling
  - Not enough N neutrons/cycle to cover the physical phase space
  - Clustering of neutrons may occur



Shannon Entropy of the Fission Source

- A uniformly spaced cartesian mesh is used to compute the Shannon Entropy
- Note that in MCNP6.3, the reported Shannon Entropy values have been changed from the absolute Shannon Entropy to the relative Shannon Entropy



- In MCNP6.2 and before:

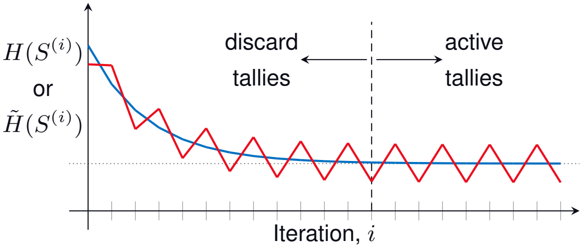
$$H(S) = -\sum_i^{N_{xyz}} p_j \ln(p_j)\,,$$

where $0 \le H(S) \le \ln(N_{xyz})$

- In MCNP6.3 and later:

$$\tilde{H}(S) = \frac{-\sum_i^{N_{xyz}} p_j \ln(p_j)}{\ln(N_{xyz})}\,,$$

where $0 \le \tilde{H}(S) \le 1$



Fission Matrix in Practice

- An alternative, or supplemental approach to computing the eigenvalue k and eigenfunction S of the system is to determine the $\mathcal{F}(\boldsymbol{p}', \boldsymbol{p})$ operator and compute its eigenvalues and eigenfunctions.

- In practice this can be done by
  - Discretizing the $\mathcal{F}(\boldsymbol{p}', \boldsymbol{p})$ operator such that the matrix $\bar{\mathcal{F}}$ includes elements which describe the next-generation fission neutrons produced in region I for each fission neutron born in region J

$$\mathcal{F}_{I,J} = \mathcal{F}(\boldsymbol{r}_J, \boldsymbol{\Omega}_J, E_J \rightarrow \boldsymbol{r}_I, \boldsymbol{\Omega}_I, E_I)$$

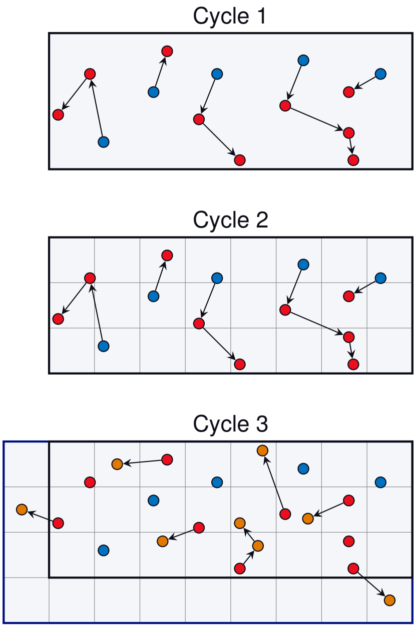
  - Computing the $\bar{\mathcal{F}}$ matrix elements using Monte Carlo
  - Computing the eigenvalues/eigenvectors with standard numerical solvers

- In MCNP, the fission matrix is discretized in the position $\boldsymbol{r}$ phase space, integrating over all angle $\boldsymbol{\Omega}$ and energy E transitions, such that

$$\mathcal{F}_{I,J} = \mathcal{F}(\boldsymbol{r}_J \rightarrow \boldsymbol{r}_I)$$

Fission Matrix Spatial Meshing

- The same uniformly spaced cartesian mesh is used for the fission matrix as that used for the Shannon entropy
- The first cycle of the criticality calculation will start without a pre-defined mesh
- The code uses a physics-based approach to automatically size the mesh
  - In the first cycle the RMS distance from birth to next fission location, L_{fiss}, is used for the physical mesh spacing along the x, y, and z axes
- In later cycles, if fission locations occur outside the mesh boundary the mesh is automatically extended preserving mesh spacing

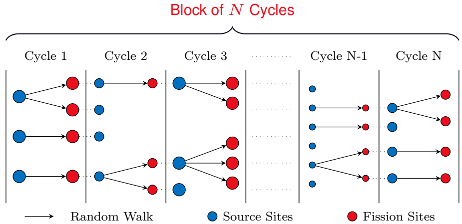


Reference Solution via the Fission Matrix

- Fission matrix and Shannon entropy
  - Sparse matrix storage: required for N_{xyz}^2-sized fission matrix to capture $\mathcal{F}_{I,J} = \mathcal{F}(\boldsymbol{r}_J \rightarrow \boldsymbol{r}_I)$ phase space transitions
  - Shannon entropy on same spatial (N_{xyz}-sized) mesh
- Power iteration and the fission matrix
  - Power iteration (PI) used for final eigenvalue k_{PI} and eigenvector S_{PI}
  - Fission matrix provides **reference solution** for global fission distribution
    - Compute fission matrix (FM) eigenvalue k_{FM} and eigenvector S_{FM}
    - Compare to k_{PI} and S_{PI}
    - Compute and compare Shannon entropy, $H(S_{FM})$ and $H(S_{PI})$
- Reference solution can be used for improved power iteration convergence testing, assessment, and acceleration

k and S Fission Source Metrics

- End-of-cycle vs. end-of-block metrics
  - Information from individual cycle
  - Combined information from multiple cycles



End-of-cycle metrics from the power iteration solution

- Track length k_{PI}, collision k_{PI}, and absorption k_{PI} estimators
- Shannon entropy $H(S_{PI})$, and its' marginal source distribution in x, y, and z, given as $H_x(S_{PI})$, $H_y(S_{PI})$, and $H_z(S_{PI})$, respectively

End-of-block metrics from the power iteration solution

- Slope of the (above) end-of-cycle metrics across all cycles in block
- Cumulative source distribution $\sum S_{PI}$, and average Shannon entropy, $\langle H(S_{PI}) \rangle$, across all cycles in block

End-of-block metrics from the fission matrix

- k_{FM}, S_{FM}, and $H(S_{FM})$

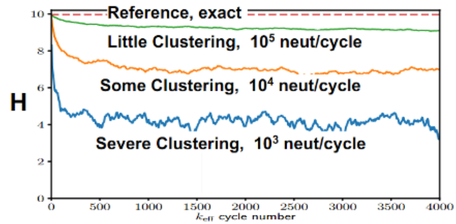
Statistical Testing for Convergence

- Slope tests
  - The power iteration end-of-cycle metrics should not trend in any direction once convergence has been achieved
  - Compute least-squares slope and uncertainty within block; if the slope is sufficiently small for all metrics, slope tests pass

- Shannon entropy test
  - Passes if $\langle H(S_{PI}) \rangle$ within 1% of $H(S_{FM})$
  - Sensitive to both convergence and population size

- Source $\sum S_{PI}$ and S_{FM} distribution tests
  - Kolmogorov-Smirnov test at 95% level
  - Chi-square 2-point test at 95% level
  - Relative entropy (Kullback-Liebler discrepancy) test at 95% level
    - Sensitive to both convergence and population size

Statistical Testing for Population Size



- Source renormalization leads to:
  - Bias in source shape
    - Too low in high-importance regions
    - Too high in low-importance regions
  - Undersampling/clustering
- Population size tests:
  - Shannon entropy test
    - Passes if $\langle H(S_{PI}) \rangle$ within 1% of $H(S_{FM})$
  - Fission source distribution test
    - Compare $\sum S_{PI}$ and S_{FM}
    - Relative entropy (Kullback-Liebler discrepancy) test at 95% level
- If these two tests pass, there is strong evidence that
  - Source convergence has been achieved
  - Population size is large enough such that source renormalization bias is negligible

Source Convergence Acceleration

- At end of each cycle
  - S_{FM} reference eigenvector is available from end of previous block of cycles
  - S_{PI} power iteration neutron source distribution at end of current cycle
- During inactive cycles, can optionally use S_{FM}/S_{PI} for importance sampling of fission source for each mesh region
  - Pushes neutron distribution toward S_{FM} reference eigenvector
  - Can reduce inactive cycles needed by a factor of 2–20
- In MCNP during the inactive cycles,
  - Iterate until Shannon entropy and fission matrix meshes are stable
  - Begin first block of cycles to compute reference source distribution from fission matrix
  - Once convergence has been reached the source importance sampling is disabled during active cycles

Primary Fission Matrix Options

- For the fission matrix convergence testing and acceleration methods, the `KOPTS` card includes some added capabilities

FMAT=yes/no
: Turns on the calculation of the fission matrix and uses this information to compute reference fission distribution metrics (e.g., Shannon entropy) to determine when the actual fission distribution reaches convergence.

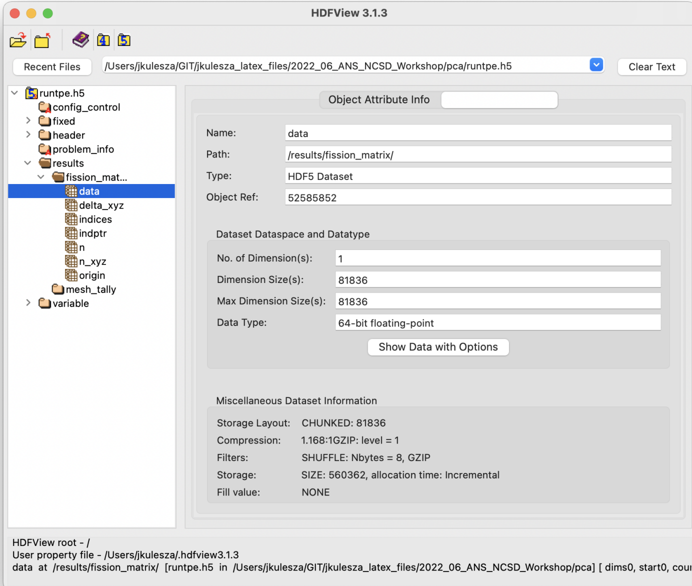
FMATCONVRG=yes/no
: Uses the reference fission-matrix fission distribution to automatically determine how many power iteration cycles must be discarded before active cycles begin. **In this case, the user-specified number of inactive cycles is ignored.**

FMATACCEL=yes/no
: Uses importance sampling based on the reference fission-matrix distribution to accelerate the convergence of the actual fission distribution. **This can reduce the number of inactive cycles needed in a simulation while the acceleration is applied prior to the active cycles.**

Fission Matrix Interrogation

Los Alamos
NATIONAL LABORATORY

Fission Matrix Interrogation in the HDF5 Runtape



`runtpe.h5/results/fission_matrix`

1-D data? Compressed-sparse storage!

An Aside on Compressed Sparse-row Storage

$$A = \begin{pmatrix} 7.5 & 2.9 & 2.8 & 2.7 & 0 & 0 \\ 6.8 & 5.7 & 3.8 & 0 & 0 & 0 \\ 2.4 & 6.2 & 3.2 & 0 & 0 & 0 \\ 9.7 & 0 & 0 & 2.3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.8 & 5.0 \\ 0 & 0 & 0 & 0 & 6.6 & 8.1 \end{pmatrix}$$

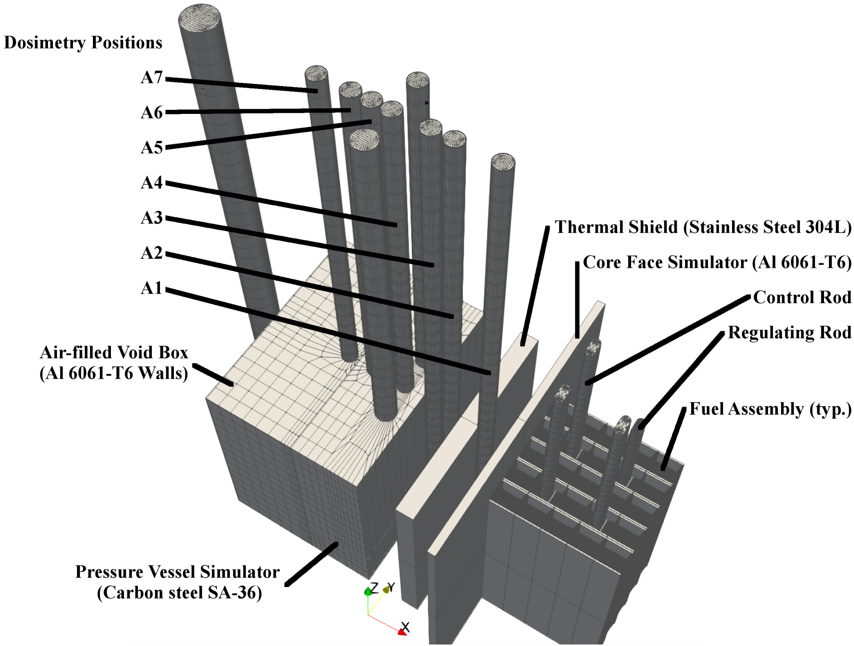
`rowptr:` $(\ 0\ \ 4\ \ 7\ \ 10\ \ 12\ \ 14\ \ 16\ )$

`colind:` $(\ 0\ \ 1\ \ 2\ \ 3\ \ 0\ \ 1\ \ 2\ \ 0\ \ 1\ \ 2\ \ 0\ \ 3\ \ 4\ \ 5\ \ 4\ \ 5\ )$

`val:` $(\ 7.5\ \ 2.9\ \ 2.8\ \ 2.7\ \ 6.8\ \ 5.7\ \ 3.8\ \ 2.4\ \ 6.2\ \ 3.2\ \ 9.7\ \ 2.3\ \ 5.8\ \ 5.0\ \ 6.6\ \ 8.1\ )$

Image from:
Elafrou et al., “A lightweight optimization selection method for Sparse Matrix-Vector Multiplication”, https://arxiv.org/abs/1511.02494.

Fission Matrix Interrogation Example [17–19]



Input file available at https://doi.org/10.2172/1601379

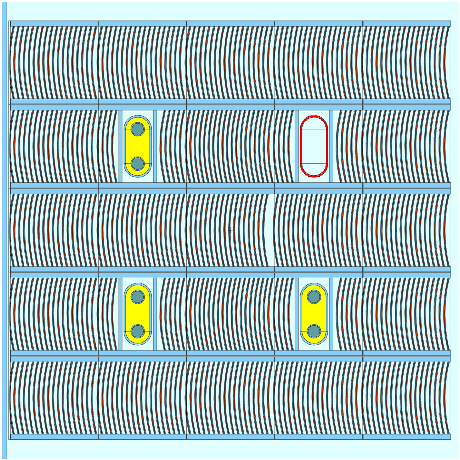
Fission Matrix Input Example

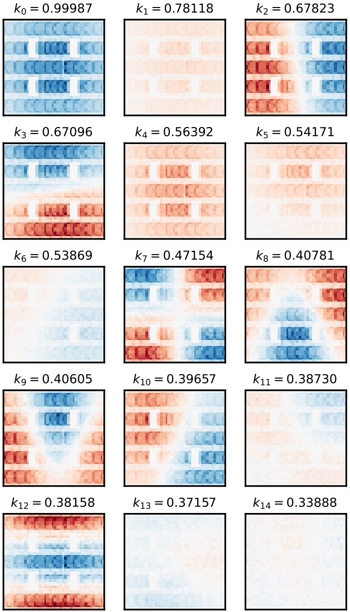
- Direct control can create a “preferred” fission-matrix mesh
- ORNL PCA example:

```
kcode 250000 1.000 50 250
kopts fmat=yes
hsrc    40 -20.41     20.25
        40 -19.275    19.275
        75 -36.35375 36.35375
```

- Beware of file size: the HDF5 runtapes can exceed several gigabytes

Fission Matrix Visualization Example





Los Alamos NATIONAL LABORATORY

See Kulesza and Josey, “Fission Matrix Processing Using the MCNP6.3 HDF5 Restart File”, https://doi.org/10.2172/1867160 for more information.

Demo Fission Matrix Calculation and Visualization

Modifications to MCNP Input File

Step 1: Open MCNP Input File: `deimos_um_simple.mcnp.inp`

Step 2: Insert fission matrix options:

Listing 4: Fission Matrix Options

```
kopts    fmat=yes
         fmatconvrg=yes
         fmataccel=yes
```

Step 3: Run MCNP (with threads if possible):

```
> mcnp6 i=deimos_um_simple.mcnp.inp tasks 8
```

Note: On a 2023 Apple M2 Max Macbook Pro, this simulation takes about 15 minutes

Fission Matrix Diagnostic Information

Listing 5: Shannon Entropy and Fission Matrix Mesh Information

```
comment.
comment. -----------------------------------------------------------------------
comment. The MESH (adaptive, axis-aligned, cartesian) to be used for computing
comment. Shannon entropy, fission-matrix tallies (if used), and source
comment. convergence checking is initially defined by:
comment.     max mesh spacing for automesh =  2.8216E+01
comment.
comment.     total mesh cells = 45
comment.
comment.     Xbins=    3   Xmin= 3.4730E-03   Xmax= 3.7887E+01   dx= 1.2628E+01
comment.     Ybins=    3   Ymin= 3.0571E-04   Ymax= 3.7877E+01   dy= 1.2625E+01
comment.     Zbins=    5   Zmin=-4.7496E+01   Zmax= 4.7487E+01   dz= 1.8997E+01
comment.
comment. the mesh will be automatically extended if necessary,
comment. preserving the original mesh cells and spacing.
comment. -----------------------------------------------------------------------
comment.
```

Fission Matrix Diagnostic Information

Listing 6: Fission Matrix Information

```
comment.
comment. ----------------------------------------------------------------------
comment.  FISSION MATRIX WILL BE COMPUTED to estimate dominance ratio,
comment.      based on fission sites only - not flights or collisions
comment.
comment.  The mesh for the fission matrix is the same as the entropy mesh,
comment.      using  45  mesh bins for tallying fission neutrons
comment.
comment.      Fission matrix mesh will be extended if
comment.         any fission sites are found outside this mesh.
comment.
comment.      Fission matrix tallies will be reset after cycle   1
comment.      Fission matrix eigenfunction will be found every  10 cycles.
comment.
comment.      Fission matrix dimensions:  45 x 45
comment.
comment.      Compressed-row-storage is used for the fission matrix.
comment.         max number of nonzero entries:  2025
comment.
```

Fission Matrix Diagnostic Information

Listing 7: Fission Matrix Convergence and Acceleration Information

```
comment.
comment.  FMATCONVRG option is being used.
comment.     Statistical tests on the neutron & fiss-matrix distributions
comment.     will be used to determine convergence & begin active cycles.
comment.     The 3rd entry on the KCODE card may be ignored.
comment.
comment.     Targets for statistical tests:
comment.       h_slope:   < 0.95 conf level,  or  < 0.0001
comment.       k_slope:   < 0.95 conf level,  or  < 0.0001
comment.       distribs:  < 0.95 conf level,  h_diff:  < 0.01
comment.
comment.
comment.  FMATACCEL option is being used.
comment.    Fission matrix will be used to ACCELERATE source convergence
comment.    of the neutron distribution during inactive cycles.
comment.    Importance-factor-limits:   min= 0.20,  max= 5.00
comment.
comment.
comment.  Keff of the fission matrix solution can be plotted using "kcode 4".
comment.  Hsrc of the fission matrix solution can be plotted using "kcode 5".
comment. ----------------------------------------------------------------------
comment.
```

Fission Matrix and Power Iteration Results

- Both fission matrix and power iteration k results provided
- Always use the power iteration k for production calculations

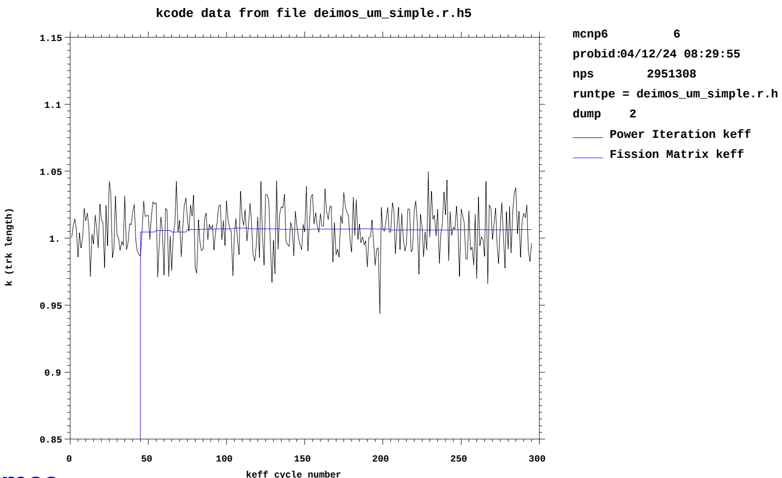
Listing 8: Fission Matrix and Power Iteration Results

```
. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
 Approximate results using the fission-matrix:
         fission matrix based on last  294  cycles
         fission matrix size =  175 x 175
         fission matrix based on fission sites only, not flights or collisions.
         fission matrix accuracy depends on mesh size.

         k-effective     = 1.00639
         dominance ratio = 0.59961
. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .


final k(col/abs/trk len) = 1.006662     std dev = 0.000665
```

Fission Matrix and Power Iteration Results

- Plot k-effective as a function of iteration:

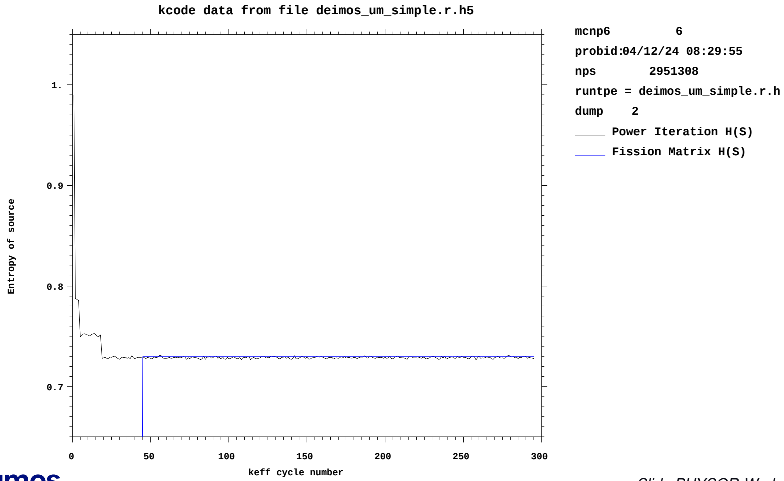
```
> mcnp6 r=deimos_um_simple.mcnp.r.h5 z
mcplot> kcode 3 label "Power Iteration keff" coplot
mcplot> kcode 4 label "Fission Matrix keff"
```



Fission Matrix and Power Iteration Results

- Plot $H(S)$ as a function of iteration:

```
> mcnp6 r=deimos_um_simple.mcnp.r.h5 z
mcplot> kcode 6 label "Power Iteration H(S)" coplot
mcplot> kcode 5 label "Fission Matrix H(S)"
```



Extract Fission Matrix, Calculate and Sort Eigenvalues & Eigenvectors, and Plot

- The fission matrix is accessible through the runtape
- Python script is available to extract, calculate, and plot eigenvalue and eigenvectors:

Listing 9: Header of fission_matrix_process.py

```
#!/usr/bin/env python3

import h5py
import matplotlib.pyplot as plt
import numpy as np
import scipy.sparse as sparse
import scipy.sparse.linalg as sla
from matplotlib.cm import get_cmap

SUPPORTED_RUNTAPE = [1, 0, 0]
```

Los Alamos NATIONAL LABORATORY

Complete script is electronically attached to this PDF, a modification of the same script from Kulesza and Josey, “Fission Matrix Processing Using the MCNP6.3 HDF5 Restart File”, https://doi.org/10.2172/1867160.

Extract Mesh Data

Listing 10: Matrix Extraction in fission_matrix_process.py

```python
def extract_fmat(runtape):
    """Returns the last saved fission matrix as a scipy.sparse.csr_matrix"""
    with h5py.File(runtape, "r") as handle:
        # Check runtape version
        version_file = handle["config_control"].attrs["version_file"]
        if any(SUPPORTED_RUNTAPE != version_file):
            print("Possibly incompatible runtape detected.")

        fmat = handle["results/fission_matrix"]

        n_dim = fmat["n"][()]
        indices = fmat["indices"][:]
        indptr = fmat["indptr"][:]
        data = fmat["data"][:]

        n_xyz = fmat["n_xyz"][:]
        delta_xyz = fmat["delta_xyz"][:]
        origin = fmat["origin"][:]

    return ( sparse.csr_matrix((data, indices, indptr), shape=(n_dim, n_dim)),
        n_xyz, delta_xyz, origin )
```

Calculate and Sort Eigenvalues & Eigenvectors

Listing 11: Eigenvalue/Eigenvector Calculation in fission_matrix_process.py

```python
def plot_eigs(mat, n_xyz, n_tot=6, n_col=2):
    """Retrieve eigenvalues/vectors, sort, reshape to 3-d object, and plot."""
    eigenvalues, eigenvectors = sla.eigs(mat, k=n_tot)

    # Clean up and sort the eigenvectors.
    sorted_eigvals = []
    sorted_eigvecs = []
    for i in np.argsort(-np.abs(eigenvalues)):
        val = eigenvalues[i]
        val = np.real(val) if np.real(val) == val else val
        sorted_eigvals.append(val)
        vec = np.real(eigenvectors[:, i].reshape(n_xyz[::-1]).transpose())
        if len(sorted_eigvals) == 1:
            vec = np.abs(vec)
        sorted_eigvecs.append(vec)
```


SciPy sparse linear algebra eigenvalue calculation:
https://docs.scipy.org/doc/scipy/reference/generated/scipy.sparse.linalg.eigs.html

Plot Eigenvalues & Eigenvectors

Listing 12: Eigenvalue/Eigenvector Plotting in fission_matrix_process.py

```
# Create example plot grid.
cmap = get_cmap("RdBu")
fig, ax = plt.subplots(int(n_tot / n_col), n_col, figsize=(3, 3 * 1.75))
aspect_ratio_z = delta_xyz[1] / delta_xyz[0]
for i in range(int(n_tot / n_col)):
    for j in range(n_col):
        k = i * (n_col) + j
        data = sorted_eigvecs[k]
        cbar_scaling = max(np.max(data), -np.max(-data))
        ax[i, j].matshow(
            data[:, :, int(n_xyz[2] / 2)].transpose(),
            cmap=cmap, origin="lower", aspect=aspect_ratio_z,
            vmin=-cbar_scaling, vmax=cbar_scaling,
        )
        ax[i, j].set_xticks([]); ax[i, j].set_yticks([])
        ax[i, j].set_title(
            f"$k_{{{k}}}={sorted_eigvals[k]:.5f}$",
            y=1.0, pad=3, fontsize=6,
        )
plt.savefig("eigenvalues.pdf", bbox_inches="tight")
```

Extracting Example Fission Matrix and Eigenmodes

Step 1: Open the Python script: `fission_matrix_process.py`

Step 2: Update plot and runtape file names at end of script:

Listing 13: Hardcoded Script File Names

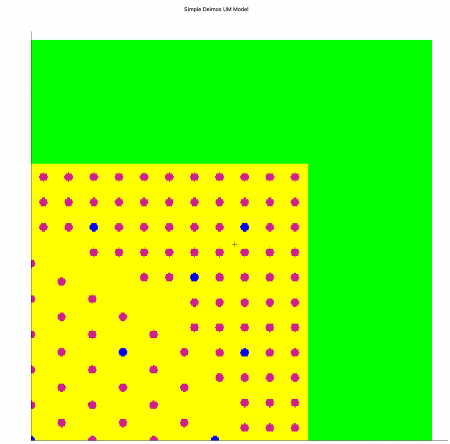
```
    plt.savefig("eigenvalues.pdf", bbox_inches="tight")

mat, n_xyz, delta_xyz, origin = extract_fmat("deimos_um_simple.r.h5")
plot_eigs(mat, n_xyz, 15, 3)
```

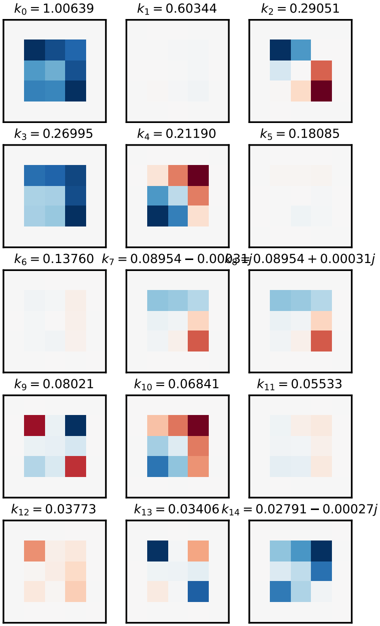
Step 3: Run Python script:

```
> python3 fission_matrix_process.py
```

Fission Matrix Visualization Example

- Default 3x3x5 fission matrix mesh

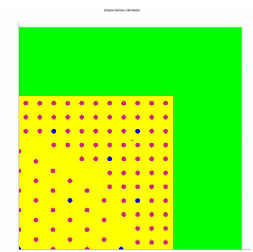


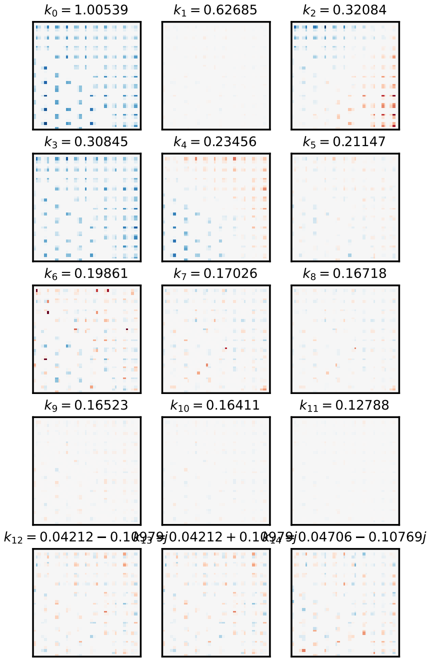


Fission Matrix Visualization Example

- For a more refined fission matrix solution, make Shannon entropy / fission matrix mesh finer using the `HSRC` card:

```
kopts   fmat=yes
        fmatconvrg=yes
        fmataccel=yes
hsrc     40       0   40
         40       0   40
         100    -50   50
kcode    10000   1.0   100    350
```





New Tally Features

FMESH Upgrades and HDF5+XDMF

Introduction

Since MCNP6.2, `FMESH` has undergone a substantial revision in capabilities.

- The default `FMESH` configuration was heavily optimized.
- 3 new tally backends were added for various needs (mainly, larger tallies).
- MESHTAL is deprecated and replaced with an HDF5 + XDMF output format.
  (This format allows for much faster and easier postprocessing and analysis)

Tally Algorithms

It started as a side project - can we use MPI remote memory access to scale further than ever before?

Implemented 4 algorithms:

History	Basic history statistics without optimization.
Fast History	A tuned version of 6.2's `FMESH` algorithm, tracks changed indices to reduce memory bandwidth usage.
Batch	Threads share a tally array, so memory usage is reduced.
Batch RMA	The Batch algorithm, but using MPI-3 RMA to distribute tallies over all MPI ranks.

Infrastructure Changes

The MCNP code didn't support batch statistics in any way. A number of changes had to be made:

- `NPS` now has a batch size option.
- When any batch tallies are enabled, `KCODE` will resample the fission bank to a fixed size.

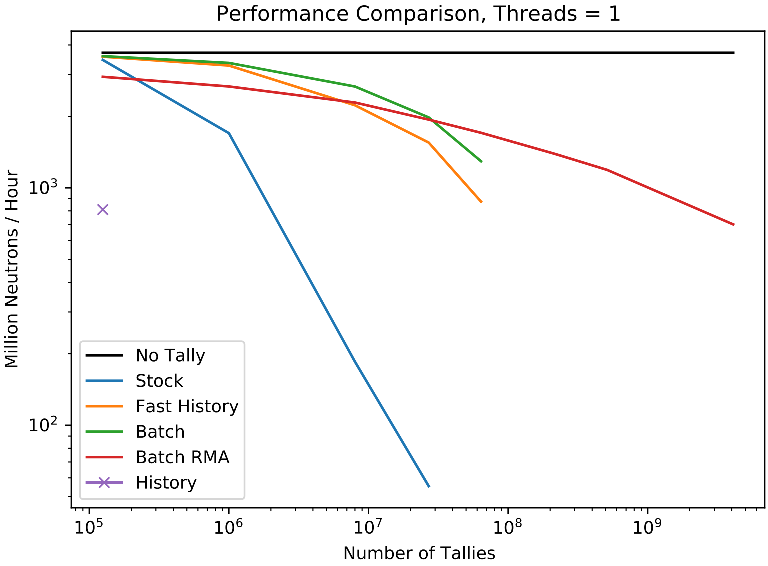
This means the RNG sequence will change if batch tallies are added!

Performance

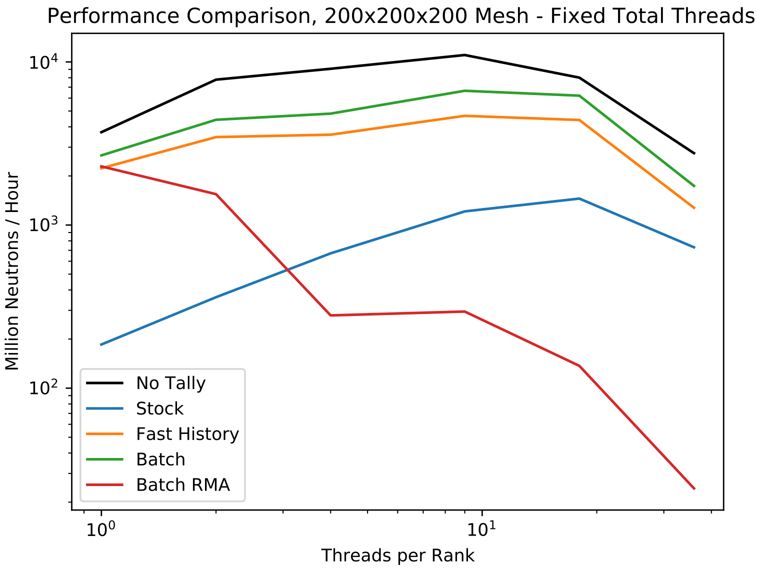
- Tested on a k-eigenvalue problem with a 10-cm, 10-g/cc ball of ^{235}U.
- Maximizes the effect of tally performance on the problem.
- Mesh was scaled from $50 \times 50 \times 50$ to $1600 \times 1600 \times 1600$
- Neutrons/hr and memory usage tallied
- Tested on 6 nodes of a cluster with 2 sockets, 18 cores each, 128 GB memory.
- Ran combinations of MPI, OpenMP.

Note: OpenMPI 3.1.6 + Omni-Path does not support `MPI_THREAD_MULTIPLE`, so threading performance is poor for Batch RMA.

Performance

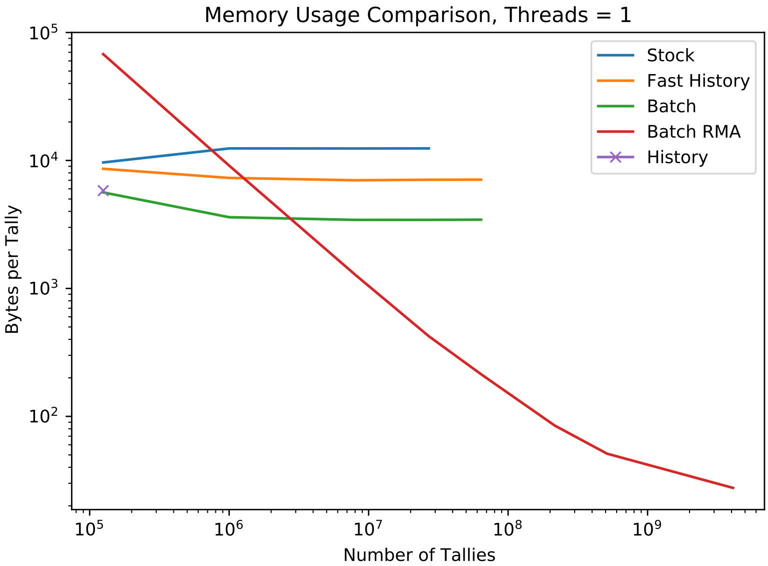


Performance



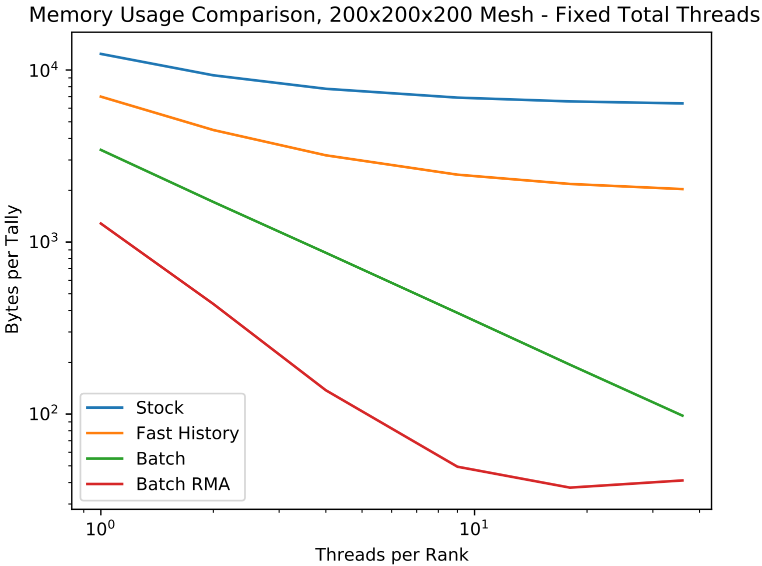
Los Alamos NATIONAL LABORATORY

Memory



Batch RMA has high overhead that dissipates for large problems.

Memory



Los Alamos NATIONAL LABORATORY

File Formats

Previous versions of the MCNP code used the MESHTAL format:

- ASCII output results in large file sizes.
- The binary to ASCII conversion was generally slow.
- It is tricky to bring into other tools (needs a processing script).

Version 6.3 uses HDF5 + XDMF:

- Binary file format for smaller sizes and faster IO.
- Trivial to load into ParaView, VisIt[1], Python, etc.
- (Optional) parallel HDF5 for even faster performance.

---

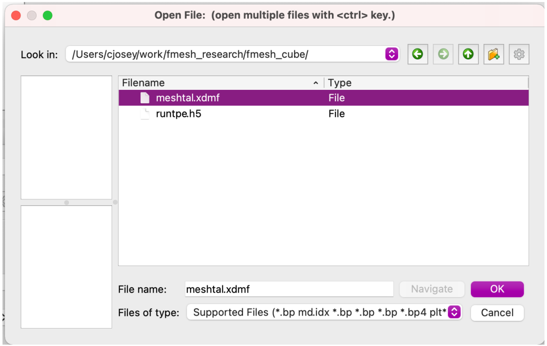
[1] Note that VisIt uses HDF5 1.8 at the time of this writing. MCNP outputs files that use the 1.10 format. Future versions of VisIt will use 1.10+. For now, `h5repack` can be used to convert to a 1.8 file.

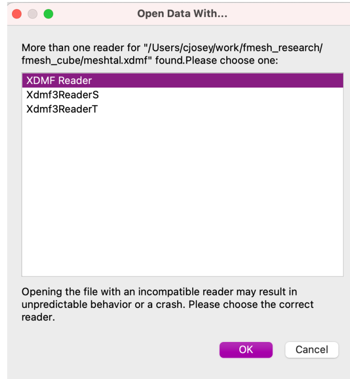
File IO Performance

216 million cell mesh, Lustre filesystem, 8 stripes, 1M stripe size, 8 MPI Ranks:

Method	Time (s)	File Size
MESHTAL	617.5	12 GB
HDF5 + XDMF	18.1	3.2 GB (in runtape)
Parallel HDF5 + XDMF	7.5	3.2 GB (in runtape)

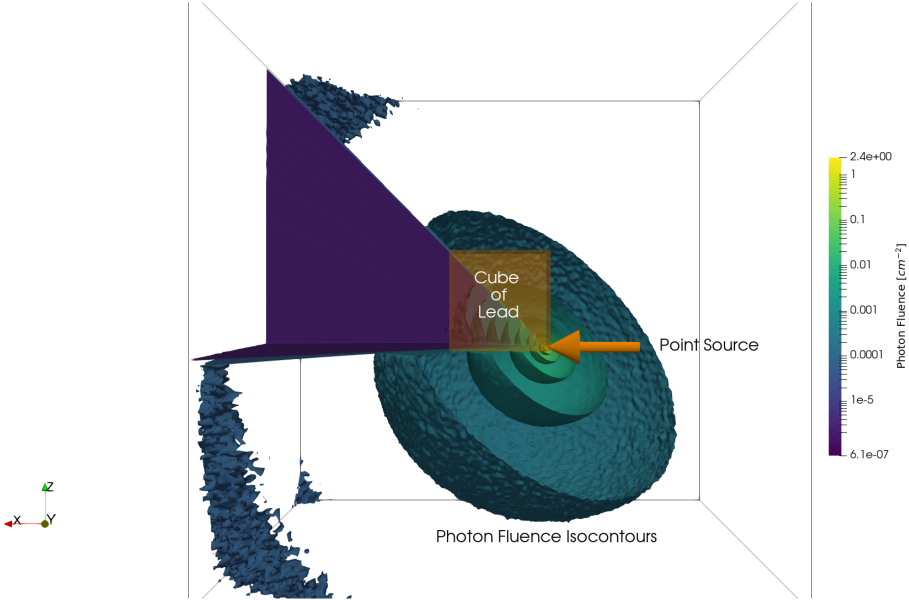
ParaView Example





Make sure to open with “XDMF Reader”, which is the reader for XDMF version 2 files.

ParaView Example - Point Source on Cube Corner



Python Example

Listing 14: Python 3.6+ Example for Reading FMESH

```python
import h5py
import numpy

def read_fmesh(filename, tally_id):
    with h5py.File(filename, 'r') as handle:
        group = handle[f"/results/mesh_tally/mesh_tally_{tally_id}"]

        data = {}
        # Transpose converts indices to x, y, z, e, t
        data["mean"] = numpy.transpose(group["mean"][()])
        data["relative_standard_error"] = \
            numpy.transpose(group["relative_standard_error"][()])
        data["grid_x"] = group["grid_x"][()]
        data["grid_y"] = group["grid_y"][()]
        data["grid_z"] = group["grid_z"][()]
        data["grid_energy"] = group["grid_energy"][()]
        data["grid_time"] = group["grid_time"][()]

        return data

data = read_fmesh("runtpe.h5", 4)
```

By slicing `group[‘‘mean’’]` instead of using `[()]`, one can load a portion into memory without loading all of it.

Summary

- New FMESH outperforms MCNP6.2's in most workloads.
- New modes allow for much lower memory usage for large problems.
- File formats are fast and easy to work with.

In the future, we expect to extend this capability to more parts of the MCNP code.

Special Tally Treatments for Multigroup Cross Sections

Motivation

- Historically, MCNP development has not been focused on nuclear reactor applications.
- Recent institutional investiments through the LANL Laboratory Directed Research & Development (LDRD) Program have focused on developing capabilities for nuclear reactor applications.
- **A new special tally treatment for multigroup cross section calculations is in the MCNP6.3 release**
- Work is continuing in this area, with a current focus on improved tracking algorithms (i.e., Delta tracking), improved energy deposition and burn-up/activation tallies, and new tooling to support efficient workflows for nuclear reactor applications
  - Note that several of these newly developed tools and/or improved capabilities will likely have an impact outside of nuclear reactor applications (e.g., radiation protection and shielding, criticality safety)

Background (1)

Multigroup cross sections are typically needed in deterministic transport and diffusion codes for reactor physics applications

- Accurate multigroup cross sections require the use of an appropriate weighting spectrum
- The weighting spectrum should be representative of the application that the multigroup cross sections are being used for

In simplified notation, the multigroup cross section can be computed as a ratio integrals,

$$\bar{\Sigma}_{x,g} = \frac{\langle \Sigma_x, \phi \rangle_g}{\langle \phi \rangle_g}, \text{ where}$$

$\bar{\Sigma}$ multigroup cross section

Σ continuous-energy cross section

ϕ weighting spectrum

x reaction channel

g incident-energy group

$\langle a, b \rangle$ the inner product of a and b integrated over all phase space

Background (2)

While the multigroup reaction cross sections are straightforward, the scattering angle/energy and fission energy terms are slightly more involved and limited (analog transport is used)

The multigroup Legendre moment, l, for the scattering matrix defining transitions from group g' to g is

$$\bar{\Sigma}_{sl,g'\to g} = \frac{\langle \Sigma_{sl}, \phi \rangle_{g'\to g}}{\langle \phi \rangle_{g'}}.$$

The multigroup fission neutron spectra is

$$\bar{\chi}_g = \frac{\sum_{g'=1}^{G} \left\langle \nu\Sigma_f, \phi \right\rangle_{g'\to g}}{\sum_{g=1}^{G} \sum_{g'=1}^{G} \left\langle \nu\Sigma_f, \phi \right\rangle_{g'\to g}},$$

which produces a normalized fission neutron energy spectrum. To separately obtain prompt and delayed fission neutron energy spectra, the integrals are binned by time.

Multigroup Cross Section Tally Options

Four new tally special treatment options (`FT` card) have been added to assist with reactor analyses:

- `SPM` Collision exit energy-angle scatter probability matrices
- `MGC` Flux weighted multigroup cross sections
- `FNS` Induced fission neutron spectra
- `LCS` Legendre coefficients for scatter reactions

These new multigroup tally capabilities have been thoroughly described and verified via code-to-code comparisons [6].

Flux-weighted Multigroup Cross Sections

`FTn MGC fg`

- `MGC` Flux weighted multigroup cross sections
- `fg` Flag for microscopic (barns) or macroscopic (1/cm) cross section calculation

Description of the Multiplier Bins for the `MGC FT` Option.

Bin #	Units	Values
1	$n/(cm^2 \cdot s)$	Flux (used as a divisor for the other bins)
2	sh/cm	Inverse velocity
3	barns	Total cross section
4	barns	Absorption cross section
5	barns	Fission cross section
6	barns	Total or prompt fission production cross section
7	barns	Delayed fission production cross section
8	barns	Fission heat production cross section
9	barns	Capture cross section (Absorption + Fission)
10	barns	Scatter cross section [Total − (Absorption + Fission)]

Flux-weighted Scattering Matrices and Fission Spectra

Multigroup scattering matrix options

`FTn SPM na` (cosine-binned scattering matrices)

- `SPM` Collision exit energy-angle scatter probability matrices
- `na` Integer number of equally-spaced cosine bins

`FTn LCS lo` (Legendre coefficient scattering matrices)

- `LCS` Legendre coefficients for scatter reactions
- `lo` Integer number of maximum Legendre scattering order

Multigroup fission energy spectra

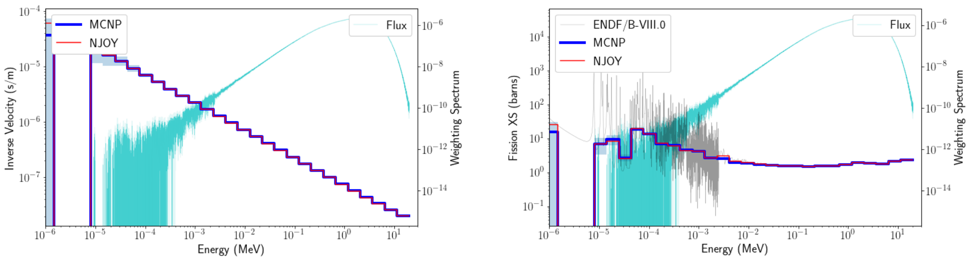
`FTn FNS nt`

- `FNS` Induced fission neutron spectra
- `nt` Integer number of delayed neutron time bins
  - If `nt` is not specified, then a `T` card needs to be used to specify time binning to separate various prompt and delayed neutrons emitted from fission.

Code-to-code Verification Efforts (1)

- Compared new multigroup special treatments to those produced using NJOY
  - Calculated a fine-group energy weighting spectrum with MCNP
  - Inserted the weighting spectrum into NJOY
  - Compared NJOY multigroup data to MCNP multigroup data
- Compared to other Monte Carlo codes that calculate multigroup cross sections

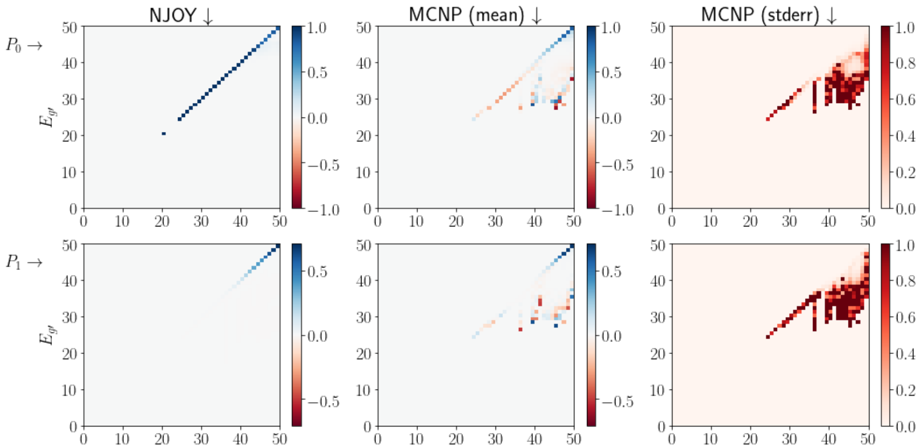
Multigroup Cross Section `MGC` Option Verification



Los Alamos NATIONAL LABORATORY

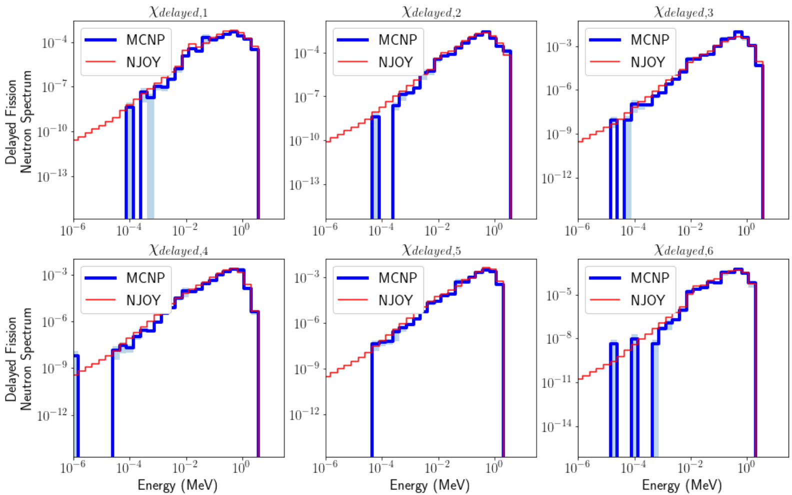
Code-to-code Verification Efforts (2)

Legendre Scattering Coefficient `LCS` Option Verification



Code-to-code Verification Efforts (3)

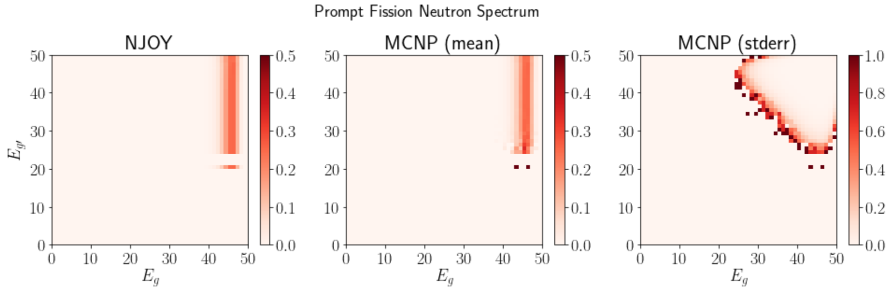
Delayed Fission Spectra `FNS` Option Verification



Summary

- The SPM and LCS options were compared to each other for internal consistency
- Besides any issues using NJOY with a fine-enough weighting spectrum and dealing with the statistical noise in the Monte Carlo tallies, everything looks good between NJOY and MCNP
- Some reactor pin-cell-like problems were used to compare to multigroup capabilities in other Monte Carlo codes

Prompt Fission Spectra FNS Option Verification



Demo FMESH and Multigroup Cross Section Calculations

Use Mesh Tally XDMF Output Option

Step 1: Open MCNP Input File: `deimos_um_simple.mcnp.inp`

Step 2: Ensure `FMESH` cards includes `out=xdmf` keyword-value option:

Listing 15: FMESH Card Tally Information

```
fmesh14:n   geom= xyz    out= xdmf
            origin= 0.0  0.0  -75.0
            imesh=   39  57        iints= 40  5
            jmesh=   39  57        jints= 40  5
            kmesh=  -47  47  87    kints= 10  100  10
            tally= fast_hist
C
fmesh24:n   geom= xyz    out= xdmf
            origin= 0.0  0.0  -75.0
            imesh=   39  57        iints= 40  5
            jmesh=   39  57        jints= 40  5
            kmesh=  -47  47  87    kints= 10  100  10
            tally= batch
```

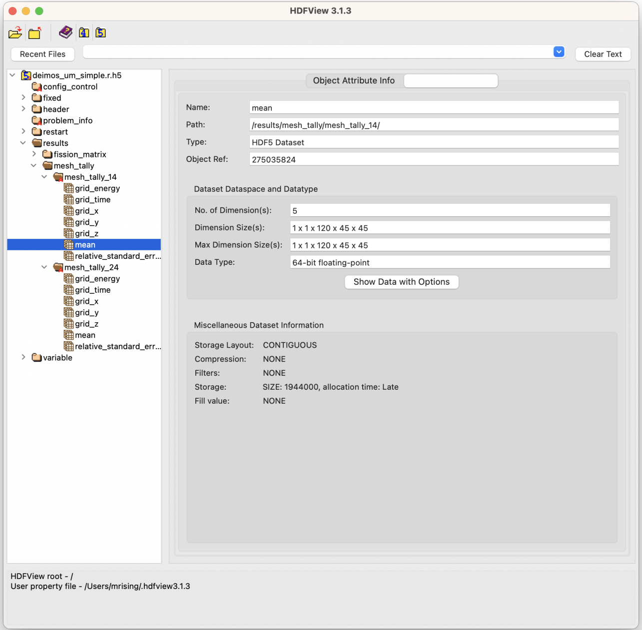
Step 3: Run MCNP (with threads if possible):

```
> mcnp6 i=deimos_um_simple.mcnp.inp tasks 8
```

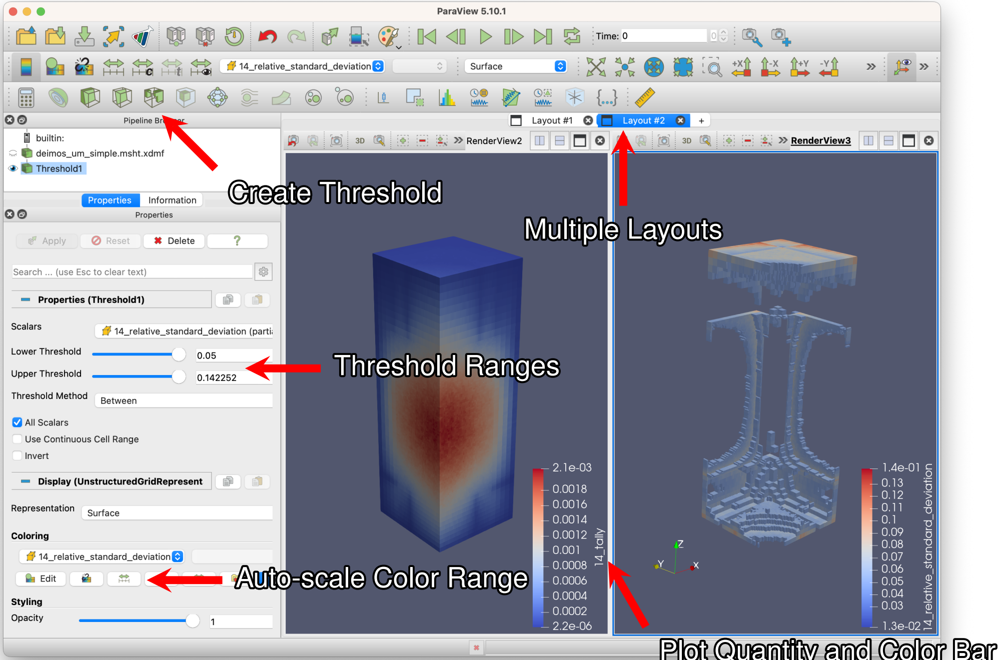
Los Alamos NATIONAL LABORATORY

Note: On a 2023 Apple M2 Max Macbook Pro,
this simulation takes about 15 minutes

Mesh Information in the HDF5 Runtape



View Mesh Tally Results in ParaView



Los Alamos
NATIONAL LABORATORY

Multigroup Tally Options in Input File

Step 1: Open MCNP Input File: `deimos_um_simple.mcnp.inp`

Step 2: Ensure `MGC`, `SPM`, `FNS`, and `LCS` special tally treatments and `PRDMP` card included in input file:

Listing 16: Multigroup Special Tally Treatment Input Information

```
C        TRISO Fuel   Inconel       Graphite             Beryllium
f34:n   (1 92i 94)   (95 5i 101)   (102 103 104 105)   (106)
ft34   mgc
e34    1e-11 99ilog 30.
C
f44:n   (1 92i 94)   (95 5i 101)   (102 103 104 105)   (106)
ft44   spm 20
e44    1e-11 99ilog 30.
C
f54:n   (1 92i 94)   (95 5i 101)   (102 103 104 105)   (106)
ft54   lcs 8
e54    1e-11 99ilog 30.
C
f64:n   (1 92i 94)   (95 5i 101)   (102 103 104 105)   (106)
ft64   fns 6
e64    1e-11 99ilog 30.
C
prdmp 2j 1
```

Step 3: Run MCNP (with threads if possible):

```
> mcnp6 i=deimos_um_simple.mcnp.inp tasks 8
```

Los Alamos NATIONAL LABORATORY

Note: On a 2023 Apple M2 Max Macbook Pro, this simulation takes about 15 minutes

Plot Cross Section Tallies with MCNP Plotter

- Can follow the sequence of MCNP plotter commands to visualize multigroup cross sections

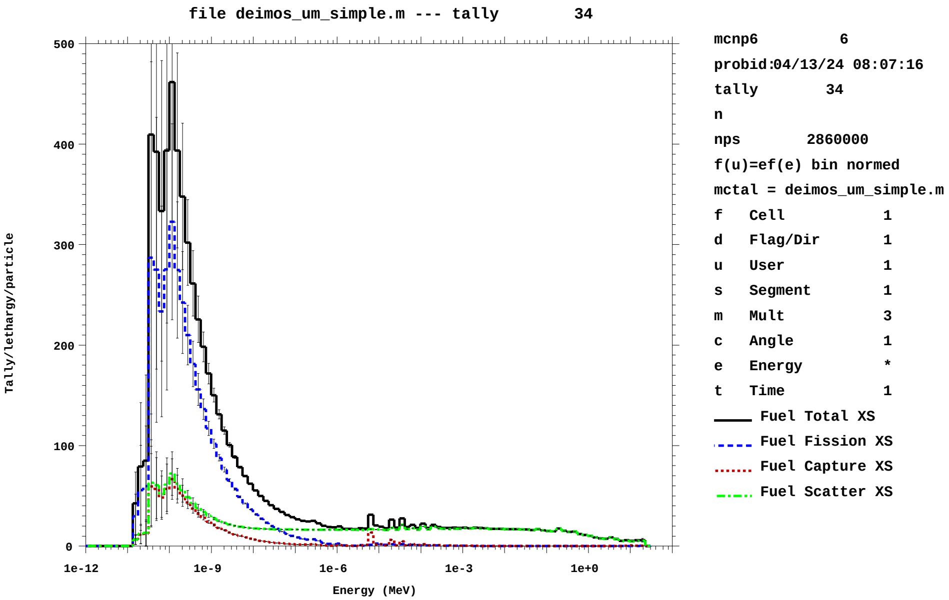
Listing 17: Complete MCPLOT COM File

```
rmctal deimos_um_simple.m
loglin lethargy
xlims 1e-12 1e2
thick 0.08
file fixed m 3 label "Fuel Total XS" coplot
fixed m 5 label "Fuel Fission XS" coplot
fixed m 4 label "Fuel Capture XS" coplot
fixed m 10 label "Fuel Scatter XS"
end
```

- Can also drive the MCNP plotter with this `COM` script:

```
> mcnp6 z com=mcplot_fuel.comin
```

Plot Cross Section Tallies with MCNP Plotter



Extracting Multigroup Tally with MCNPTools

Step 1: Ensure `mgxs.py` script and `deimos_um_simple.m` MCTAL file in working directory

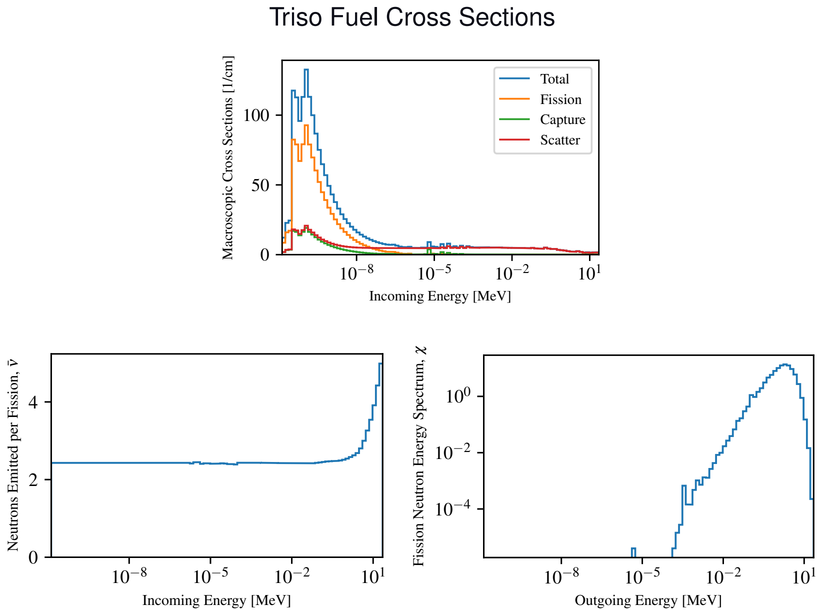
Listing 18: Header of Multigroup Tally Extraction Script

```
from mcnptools import Mctal, MctalTally
import numpy as np
import matplotlib.pyplot as plt
import pylab
```

Step 2: Run script:

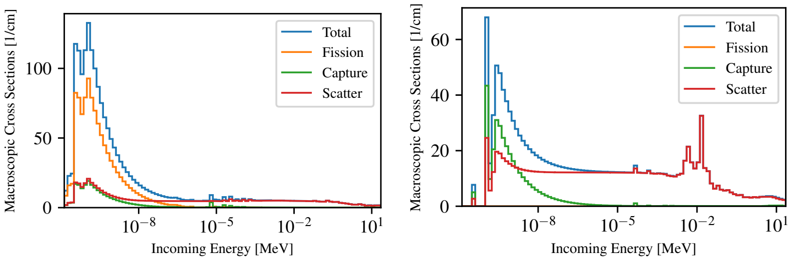
```
> python3 mgxs.py
```

Plot Cross Section Tallies with MCNP Plotter

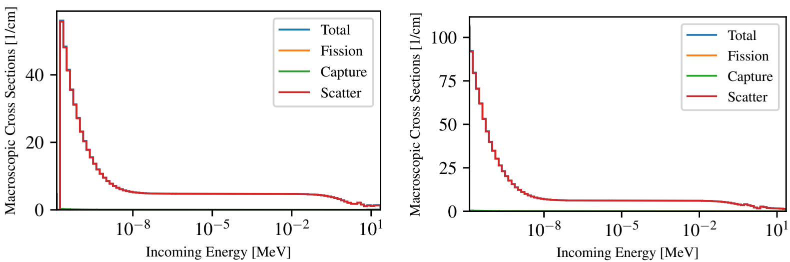


Plot Cross Section Tallies with MCNP Plotter

Triso Fuel (left) and Inconel (right) Cross Sections



Graphite (left) and Beryllium (right) Cross Sections



MCNP6.3 for Nuclear Criticality Safety

Los Alamos Scientific Laboratory, 30 December 1958 [20]

- On December 30, 1958 a nuclear criticality accident occurred in a processing facility at Los Alamos Scientific Laboratory.
  - Plutonium organic solution in an organic treatment tank;
  - single excursion;
  - one fatality, two significant exposures.

- Prior to the accident, the vessel contained two layers of aqueous and organic solutions.
  - A stirrer was started and abruptly forced solution up the tank wall, which caused a critical thickness to form in the central region.
  - The motion changed the system from subcritical to superprompt critical and an excursion occurred.
  - The system was driven permanently subcritical by the mixing of the layers.

Analysis Overview

- What effect does stirring have on a supercritical plutonium solution?
  - MCNP6.3 can be used to answer this question.
  - An input deck will be presented that utilizes universes, fills, and cones to model the vessel with the stirrer on and off.
  - The data card block will include standard cards to run a basic KCODE problem.
  - Additional data cards will be added to perform:
    - stochastic geometry calculations,
    - eigen-decomposition of the fission matrix,
    - visualization of the XDMF output of a FMESH, and
    - multigroup cross section generation.

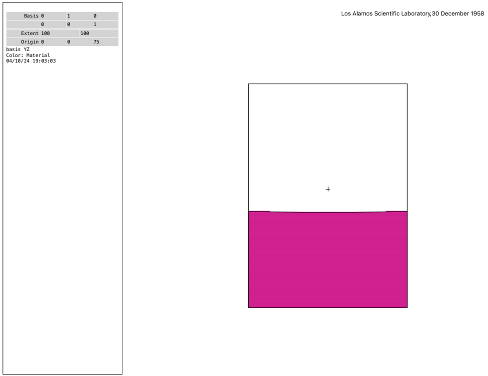
Basic Input Deck

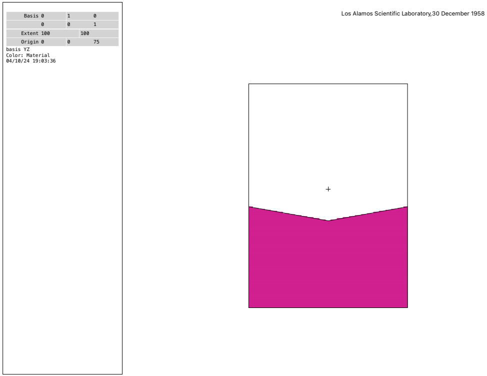
- A single-sheet cone is used to model the surface of the solution.
- The two infinite cells fill a finite right circular cylinder.
- A bounding sphere surrounds the system.

```
message: o=output.txt r=runtape.h5

Los Alamos Scientific Laboratory, 30 December 1958
10 1000 -0.98 +100              U=1    IMP:N=1
20 0          -100              U=1    IMP:N=1
30 0               -200         FILL=1 IMP:N=1
40 0               +200 -300           IMP:N=1
50 0                    +300           IMP:N=0

100 KZ 60 3300 +1                 <--- stirrer off
100 KZ 55 33   +1                 <--- stirrer on
200 RCC 0 0 0    0 0 141.5    50
300 SO 1000

MODE N
PRINT
PRDMP 2j 1
RAND GEN=2 SEED=3 STRIDE=1e6
M1000 1001 8 8016 4 94239 1
```

Qt-based Geometry Plotter

- The new Qt-based plotter can be accessed from the command line, mcnp6.qt inp= input.txt ip, and used to check the geometry.





Stochastic Geometry

- Stirring the solution creates a vortex but does not create extra mass.
  - The vertex of the cone must decrease to maintain the mass of the solution.
  - MCNP6.3 can be used to perform a stochastic volume calculation and determine the vertex coordinate through trial-and-error.

```
VOID
VOL 1.0
SDEF SUR=300 NRM=-1 DIR=D1 WGT=3141592.65359 <--- WGT=PI*(R=1000)**2
SI1 0 1
SP1 -21 1
SB1 -21 2
FC4 Solution Volume
F4:N ( 10 < 30 )
NPS 1E7
```

- The volume of the solution with the stirrer on and off is ~ 480,000 cm^3 when the vertex of the cone is 5 cm lower.

Los Alamos NATIONAL LABORATORY

Basic KCODE

- Add a basic KCODE block to the data cards
  - 10,000 particles/cycle, initial guess of 1.0, discard 50 cycles, 150 total cycles
  - Start initial fission sites at (0, 0, 50)

```
KCODE 10000 1.0 50 150
KSRC 0 0 50
```

- Stirrer off: final k(col/abs/trk len) = 1.006221 std dev = 0.001060
- Stirrer on: final k(col/abs/trk len) = 0.997261 std dev = 0.000951
- MCNP6.3's basic KCODE can answer the original question!
  - Stirring a supercritical plutonium solution can make the system subcritical.

Advanced KCODE

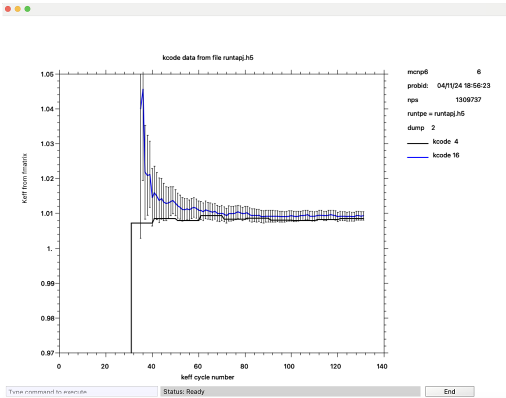
- Why does stirring the solution cause the system to be subcritical?
  - The system's fission matrix can be used to investigate this question.
  - A Shannon entropy grid is specified, the FMAT option is turned on, convergence and acceleration are enabled, and initial fission sites are sampled uniformly throughout the HSRC grid.

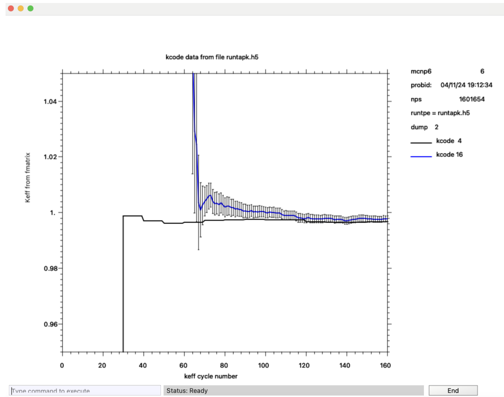
```
KCODE 10000 1.0 50 150
HSRC 25 -50 50    25 -50 50    25 0 150
KOPTS FMAT=YES FMATCONVRG=YES FMATACCEL=YES FMATSRC=YES
```

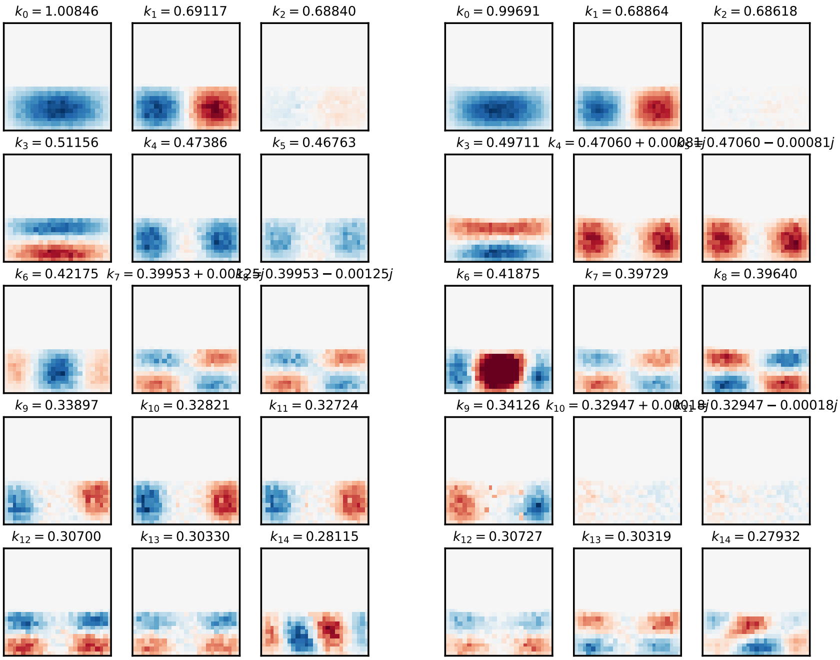
- Stirrer off:
  - Inactive cycles: 31
  - KCODE results: final k(col/abs/trk len) = 1.009300 std dev = 0.001234
  - FMAT results: k-effective = 1.00846 dominance ratio = 0.68271
- Stirrer on:
  - Inactive cycles: 60
  - KCODE results: final k(col/abs/trk len) = 0.997763 std dev = 0.001062
  - FMAT results: k-effective = 0.99691 dominance ratio = 0.69080

Fission Matrix Visualization

- The eigenvalues and eigenvectors of the fission matrix can be plotted and analyzed from the runtape.





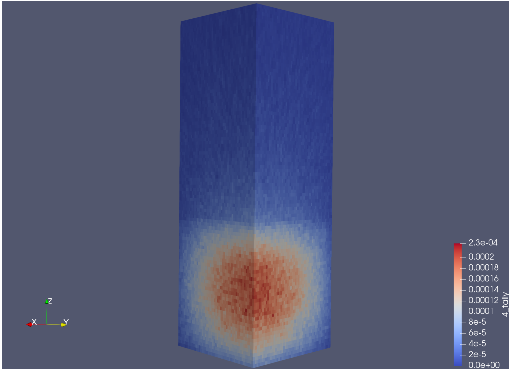

$k_0 = 1.00846$
$k_1 = 0.69117$
$k_2 = 0.68840$
$k_3 = 0.51156$
$k_4 = 0.47386$
$k_5 = 0.46763$
$k_6 = 0.42175$
$k_7 = 0.39953 + 0.00125j$
$k_8 = 0.39953 - 0.00125j$
$k_9 = 0.33897$
$k_{10} = 0.32821$
$k_{11} = 0.32724$
$k_{12} = 0.30700$
$k_{13} = 0.30330$
$k_{14} = 0.28115$
$k_0 = 0.99691$
$k_1 = 0.68864$
$k_2 = 0.68618$
$k_3 = 0.49711$
$k_4 = 0.47060 + 0.00081j$
$k_5 = 0.47060 - 0.00081j$
$k_6 = 0.41875$
$k_7 = 0.39729$
$k_8 = 0.39640$
$k_9 = 0.34126$
$k_{10} = 0.32947 + 0.00018j$
$k_{11} = 0.32947 - 0.00018j$
$k_{12} = 0.30727$
$k_{13} = 0.30319$
$k_{14} = 0.27932$

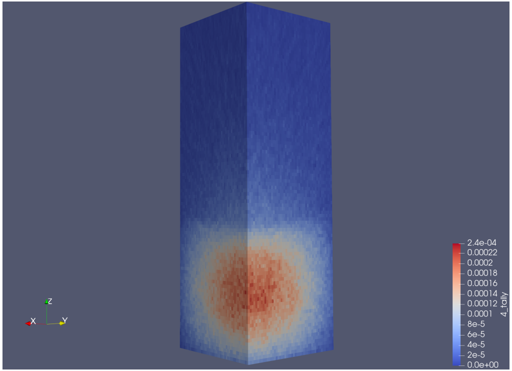
XDMF FMESH Visualization

- The FMESH tally's XDMF output can be used to generate a 3-dimensional plot of the flux.

```
FMESH4:N  GEOM=XYZ       ORIGIN=-50  -50  0
          IMESH=50       IINTS=100
          JMESH=50       JINTS=100
          KMESH=150      KINTS=100
          OUT=XDMF
```

- Plots can be generated with the ParaView software.
  - Getting it: https://www.paraview.org/download
  - Getting help with it: https://www.paraview.org/community-support
  - Issues: https://gitlab.kitware.com/paraview/paraview/-/issues


2.3e-04
0.0002
0.00018
0.00016
0.00014
0.00012
0.0001
8e-5
6e-5
4e-5
2e-5
0.0e+00
4_tally
Z
X
Y

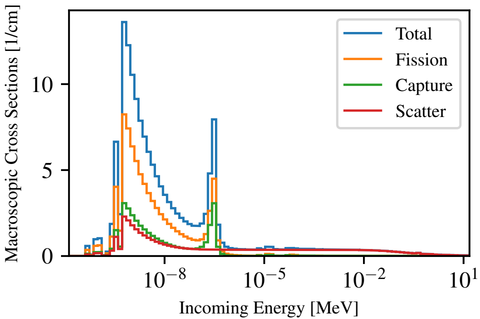

2.4e-04
0.00022
0.0002
0.00018
0.00016
0.00014
0.00012
0.0001
8e-5
6e-5
4e-5
2e-5
0.0e+00
4_tally
Z
X
Y

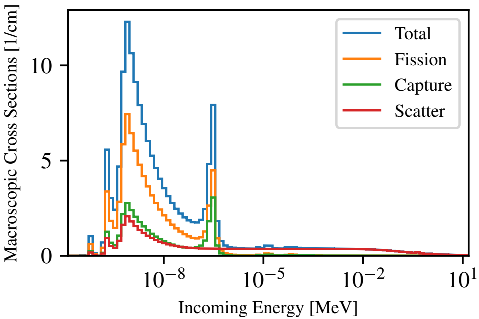
Multigroup XS Generation

- MCNP6.3 can be used to generate multigroup cross sections for use in deterministic transport software and multiphysics simulations.

```
VOL 4.75996E+05
F4:N ( 10 < 30 )
E4 1E-11 99ilog 20
FT4 MGC 1
```

- MCNPTools can be used to extract the multigroup cross section tallies from a MCTAL file.
  - Getting it: https://github.com/lanl/mcnptools


Macroscopic Cross Sections [1/cm]
0
5
10
10^{-8}
10^{-5}
10^{-2}
10^{1}
Incoming Energy [MeV]
Total
Fission
Capture
Scatter


Macroscopic Cross Sections [1/cm]
0
5
10
10^{-8}
10^{-5}
10^{-2}
10^{1}
Incoming Energy [MeV]
Total
Fission
Capture
Scatter

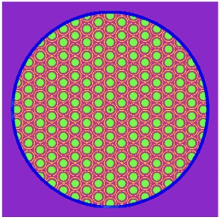
Final Thoughts

- MCNP6.3 is a powerful tool for analyzing nuclear systems.
- In KCODE problems, creating the geometry and defining materials are the most user intensive processes.
- It is easy to add data cards but using and interpreting them correctly can be challenging.
- Output files can now be analyzed and plotted easily.
- Multigroup cross sections should be generated for each configuration.
  - Using the “wrong” multigroup cross sections can introduce unnecessary nuclear data error into a calculation.
- Consider investigating some of MCNP6.3’s other tools and features such as mcnp_pstudy and KSEN.

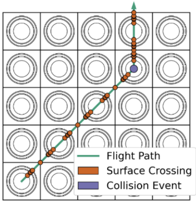
Future Work

Delta Tracking in MCNP6.4

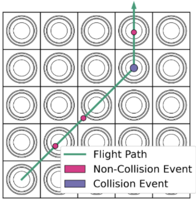
- Delta tracking (aka Woodcock tracking) is an alternative algorithm to the standard Monte Carlo surface-to-surface tracking algorithm
- Can be beneficial when collisions occur rarely with respect to the frequency that surfaces are crossed
- Implemented, tested, documented, and reviewed the Delta tracking capability – will be released in MCNP6.4
- Figures on right from Kristin Stolte ANS Summer 2023 presentation where discrete modeling of TRISO particles compared both tracking algorithms



Surface Tracking Algorithm

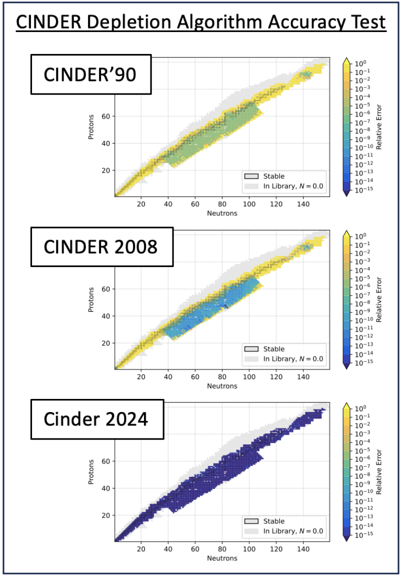


Delta Tracking Algorithm



Cinder Burn-up/Depletion in MCNP6.4

- The CINDER'90 code, used for material depletion and transmutation physics, was introduced into the MCNPX code in the early 2000's
  - Used inline for nuclear reactor depletion and activation/delayed particle emission physics
- Although it was planned, the CINDER 2008 code was never merged into MCNP6
- We are actively modernizing the code, with plans to release Cinder 2024 including improved numerical algorithms and better nuclear data



Credit: C. Josey CINDER Algorithm Improvements

Other Noteworthy Changes to Expect in MCNP6.4 (or earlier)

MONTE CARLO N-PARTICLE

- Generalized ZAID-specifier input processing (in MCNP6.3.1)
- New random number generator (see `RAND GEN=8` in MCNP6.3.1)
- Extended general sensitivity/uncertainty tally capabilities (`FSEN`)
- Completion of `FMESH` improvements to supplant `TMESH` capabilities
- Dynamically-linked source and tally capabilities
- More output data converted into HDF5-accessible formats
- And many more code enhancements, bug fixes, etc.
- For annual updates on MCNP6 code developments, consider attending our MCNP User Symposium (https://mcnp.lanl.gov/symposia.html)

Thanks!

Q&A

Backup Slides

References

[1] M. E. Rising, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, T. P. Burke, A. R. Clark, D. A. Dixon, R. A. Forster, III, J. F. Giron, T. S. Grieve, H. G. Hughes, III, C. J. Josey, J. A. Kulesza, R. L. Martz, A. P. McCartney, G. W. McKinney, S. W. Mosher, E. J. Pearson, C. J. Solomon, Jr., S. Swaminarayan, J. E. Sweezy, S. C. Wilson, and A. J. Zukaitis, "MCNP® Code Version 6.3.0 Release Notes," Tech. Rep. LA-UR-22-33103, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA, Jan. 2023.

[2] J. A. Kulesza, T. R. Adams, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, T. P. Burke, A. R. Clark, R. A. Forster, III, J. F. Giron, T. S. Grieve, C. J. Josey, R. L. Martz, G. W. McKinney, E. J. Pearson, M. E. Rising, C. J. Solomon, Jr., S. Swaminarayan, T. J. Trahan, S. C. Wilson, and A. J. Zukaitis, "MCNP® Code Version 6.3.0 Theory & User Manual," Tech. Rep. LA-UR-22-30006, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA, Sept. 2022.

References

[3] J. S. Bull, J. A. Kulesza, C. J. Josey, and M. E. Rising, "MCNP® Code Version 6.3.0 Build Guide," Tech. Rep. LA-UR-22-32851, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA, Dec. 2022.

[4] C. J. Josey, A. R. Clark, J. A. Kulesza, E. J. Pearson, and M. E. Rising, "MCNP® Code Version 6.3.0 Verification & Validation Testing," Tech. Rep. LA-UR-22-32951, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA, Dec. 2022.

[5] V. K. Mehta, J. Armstrong, D. V. Rao, and D. Kotlyar, "Capturing Multiphysics Effects in Hydride Moderated Microreactors using MARM," *Annals of Nuclear Energy*, vol. 172, p. 109067, 2022.

[6] R. B. Wilkerson, G. McKinney, M. E. Rising, and J. A. Kulesza, "MCNP Reactor Multigroup Tally Options Verification," Tech. Rep. LA-UR-20-27819, Los Alamos National Laboratory, Oct. 2020.

[7] C. J. Josey and J. A. Kulesza, "Improved FMESH Capabilities in the MCNP 6.3 Code," Tech. Rep. LA-UR-21-26363, Los Alamos National Laboratory, July 2021.

References

[8] J. A. Kulesza, J. C. Armstrong, T. C. McClanahan, and S. Swaminarayan, “MCNP Unstructured Mesh Elemental Quality Assessment,” Tech. Rep. LA-UR-21-26362, Los Alamos National Laboratory, Los Alamos, NM, USA, July 2021. MCNP User Symposium Presentation.

[9] C. J. Stimpson, C. D. Ernst, P. K. and. P. P. Pébay, and D. Thompson, “The Verdict Geometric Quality Library,” Tech. Rep. SAND2007-1751, Sandia National Laboratories, Albuquerque, NM ,USA, Mar. 2007.

[10] J. A. Kulesza, “MCNP Code Version 6.3.0 Unstructured-mesh Quality Metrics & Assessment,” Tech. Rep. LA-UR-20-27150, Los Alamos National Laboratory, Los Alamos, NM, USA, Sept. 2020.

[11] P. M. Knupp, “Achieving Finite Element Mesh Quality Via Optimization of the Jacobian Matrix Norm and Associated Quantities. Part II—A Framework for Volume Mesh Optimization and the Condition Number of the Jacobian Matrix,” *International Journal for Numerical Methods in Engineering*, vol. 48, pp. 1165–1185, May 2000.

References

[12] P. M. Knupp, "Algebraic Mesh Quality Metrics for Unstructured Initial Meshes," *Finite Elements in Analysis and Design*, vol. 39, pp. 217–241, Jan. 2003.

[13] P. P. Pébay, D. Thompson, J. Shepherd, P. Knupp, C. Lisle, V. A. Magnotta, and N. M. Grosland, "New Applications of the Verdict Library for Standardized Mesh Verification Pre, Post, and End-to-End Processing," in *Proceedings of the 16th International Meshing Roundtable* (M. L. Brewer and D. Marcum, eds.), (Seattle, WA, USA; October 15–17), pp. 535–552, 2008.

[14] R. L. Martz, "The MCNP6 Book On Unstructured Mesh Geometry: User's Guide For MCNP 6.2," Tech. Rep. LA-UR-17-22442, Los Alamos National Laboratory, Los Alamos, NM, USA, Mar. 2017.

[15] J. L. Alwin and J. B. Spencer, "Utilizing Unstructured Mesh Geometry in Criticality Calculations and Criticality Accident Alarm System Analysis," Presentation LA-UR-21-25913, Los Alamos National Laboratory, Los Alamos, NM, USA, June 2021.

References

[16] M. R. Dzur, J. C. Armstrong, and C. A. D'Angelo, "CUBIT for MCNP Unstructured Mesh Analysis of Oktavian Benchmarks," Presentation LA-UR-22-30541, Los Alamos National Laboratory, Los Alamos, NM, USA, October 2022.

[17] I. Remec and F. B. K. Kam, "Pool Critical Assembly Pressure Vessel Facility Benchmark," Tech. Rep. NUREG/CR-6454, Oak Ridge National Laboratory, Oak Ridge, TN, USA, July 1997.

[18] J. A. Kulesza and R. L. Martz, "Evaluation of the Pool Critical Assembly Benchmark with Explicitly Modeled Geometry Using MCNP6," *Nuclear Technology*, vol. 197, pp. 284–295, Mar. 2017.

[19] J. A. Kulesza and R. L. Martz, "Evaluation of the Pool Critical Assembly Benchmark with Explicitly Modeled Geometry using MCNP6's Unstructured Mesh Capabilities," in *Proceedings of 16th International Symposium on Reactor Dosimetry (ISRD16)*, (Santa Fe, NM, USA; May 7–12), ASTM International, 2017. Accompanying presentation: LA-UR-17-23854.

References

[20] T. P. McLaughlin, S. P. Monahan, B. G. Ryazanov, N. L. Pruvost, V. V. Frolov, and V. I. Sviridov, *A Review of Criticality Accidents*. 2000.

[21] U. Ayachit, *The ParaView Guide*. Kitware, Inc., community ed., June 2018.

[22] 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.

[23] J. A. Kulesza, J. L. Alwin, J. D. Hutchinson, E. F. Shores, and R. C. Little, “l3d2vtk: An MCNPTools Utility to Enable LNK3DNT File Visualization & Post-processing,” in *Transactions of the Winter 2019 American Nuclear Society Meeting*, vol. 121, pp. 1233–1236, Nov. 2019.

References

[24] H. Childs, E. Brugger, B. Whitlock, J. Meredith, S. Ahern, D. Pugmire, K. Biagas, M. Miller, C. Harrison, G. H. Weber, H. Krishnan, T. Fogal, A. Sanderson, C. Garth, E. W. Bethel, D. Camp, O. Rübel, M. Durant, J. M. Favre, and P. Navrátil, "VisIt: An End-User Tool For Visualizing and Analyzing Very Large Data," in *High Performance Visualization–Enabling Extreme-Scale Scientific Insight*, pp. 357–372, Oct. 2012.

[25] J. A. Clarke and E. R. Mark, "Enhancements to the eXtensible Data Model and Format (XDMF)," in *HPCMP User's Group Conference 2007. High Performance Computing Modernization Program: A Bridge to Future Defense*, (Pittsburgh, PA, USA; June 18–21), pp. 322–327, 2007.

[26] "XDMF Model and Format." Website, Mar. 2019.

Qt-based Geometry and Tally Plotter

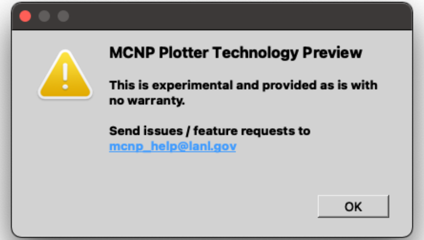
Outline

- Geometry Plotter
  - Introduction of new features
  - Brief look at each panel
  - Live demo
- Tally Plotter
  - New viewport
  - Live demo

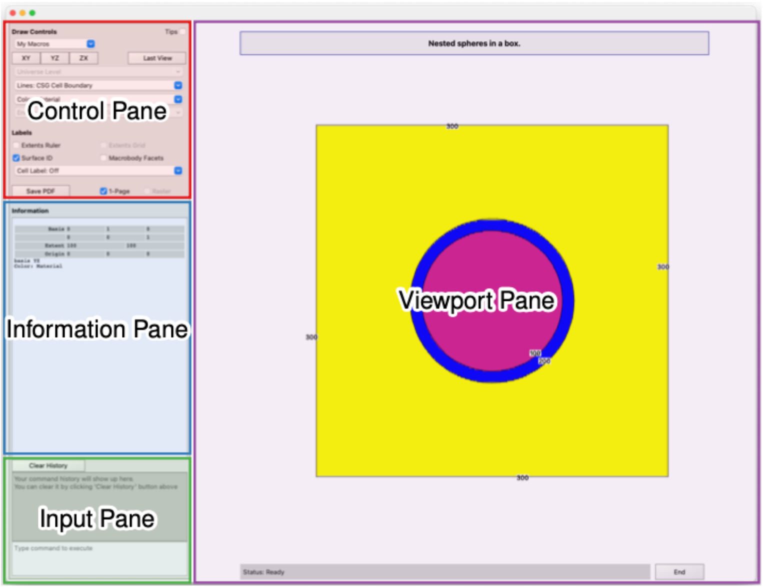
New Plotter Features

- Qt-based render window (no X-Server required)
- Modern buttons (geometry plotter)
- Command box supporting > 29 characters
- Mouse control to pan, zoom, and rotate slices
- New plotter view file formats (png, pdf)
- Macro support

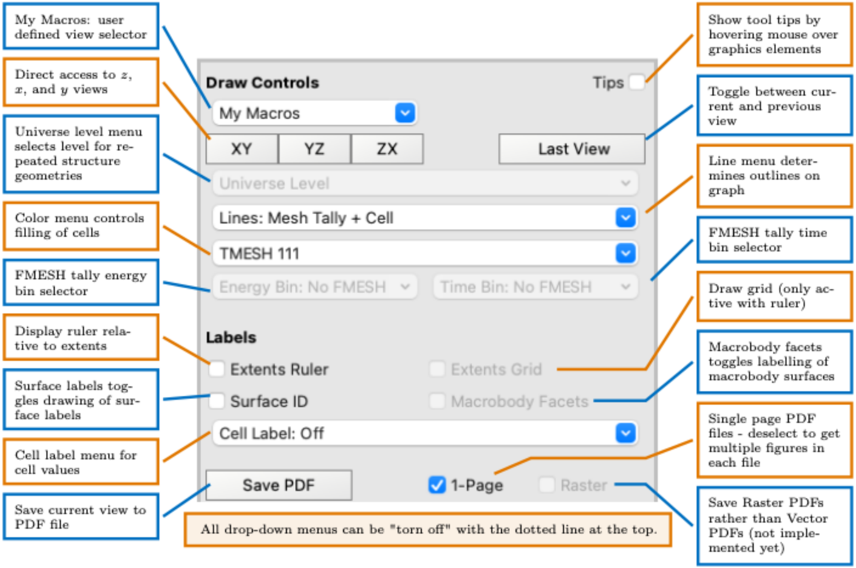
New plotter is shipping with MCNP6.3



Geometry Plotter First Look



Control Pane (1)

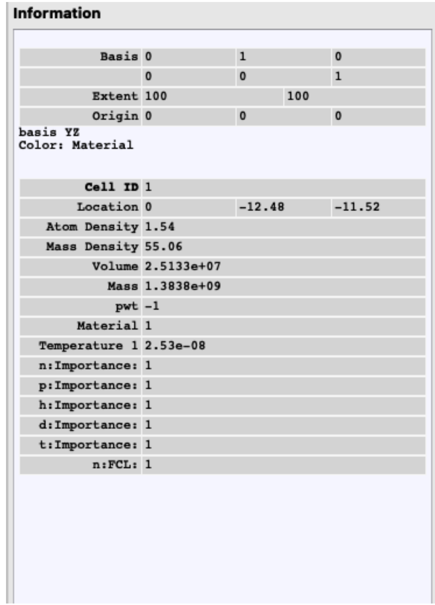


Control Pane (2)

- "My Macros" functionality
  - Similar to reading a COM file on the execution line
  - More later
- "Last View" expands on limitations of "Restore" button
  - Resets all parameter(s) to previous parameter(s) instead of a select few
- "Tips" button allows user to hover over a feature for quick help text
- "Save PDF" button
  - Available as a new command: `savepdf`
  - Raster PDF functionality to come

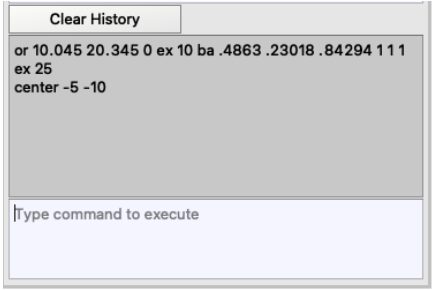
Information Pane

- Contains all information present in X-based plotter by default
  - Basis, Extent, Origin
- Click in a cell for more information on that cell.
  - Old plotter only showed what was selected in the right-hand control panel
  - Now shows all information relevant to problem
- Will also show information on an overlaid FMESH mesh
  - Runtape information, tally value/error of selected voxel, voxel indices



Input Pane

- The old “Click here or picture or menu” box only supported 29 characters of input
  - or 10.045 20.345 0 ex 10 ba .4863 .23018 .84294 1 1 1
- New input is “infinite” for all practical one-liners
  - Also supports command recall with up- and down-arrows
- Messy history can be cleared with “Clear History” button, but command recall with arrow keys still works
- Error messages are still presented in the command-prompt window



Viewport Pane

- Can now interact directly with keyboard and mouse:
  - Click and drag to pan
  - Shift-Click and drag to rotate
  - Ctrl-Click and drag to zoom in and out
  - Ctrl-[Arrow Key] to pan
    - Ctrl-Shift-[Arrow Key] to pan more
  - Ctrl-[+/-] to zoom at origin
    - Ctrl-Shift-[+/-] to zoom more
- Status bar now tells you when the plotter is working

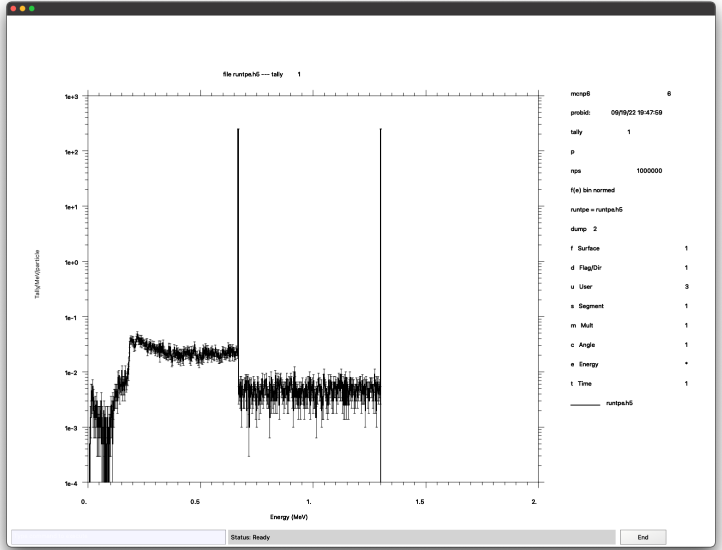
These features will be shown in the demo

Geometry Plotter Live Demo

- Show macro functionality with lost particle use-case
- Demo more complex geometry
  - Compare X-plotter speed
  - Show new `savepdf`, `savepng` commands

Tally Plotter Viewport

- Largely the same look as the old tally plotter, though modernized



Tally Plotter Live Demo

- Show classic tallies
  - Arrow key recall
- Show FMESH tally
  - Tie into geometry plotter

MCNP6.3 Visualization Approaches

How to Use These Slides

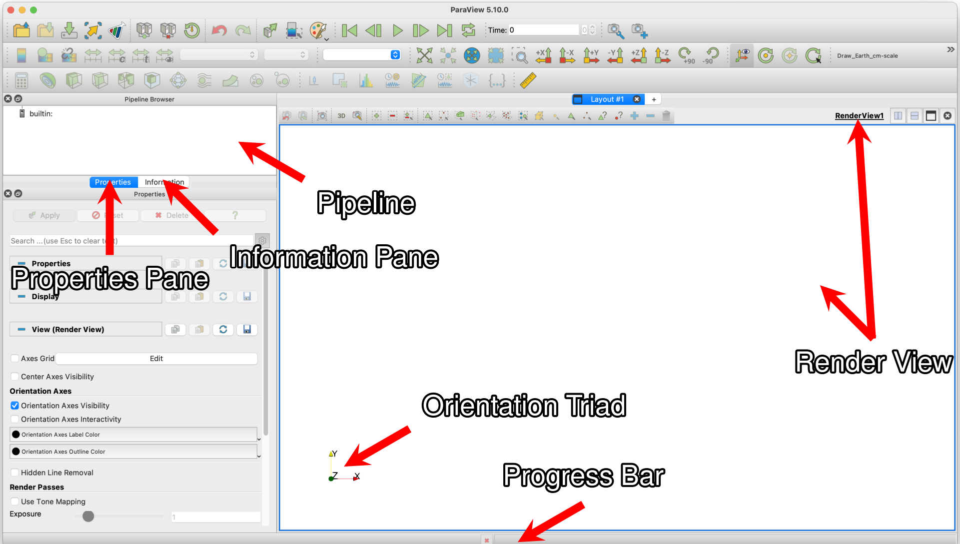
- Intended to be useful as a reference
  - Can be used independent of ParaView [21] being open
- GUI elements labeled to establish nomenclature
  - When "clicks" are necessary, steps are numbered to give click order
  - Additional information in lower-right "callout" boxes
- Recommended approach: focus on presentation and experiment after
  - Prevents "getting lost" while the presentation is underway
  - Experimentation is how skill and "muscle memory" is built

ParaView Introduction

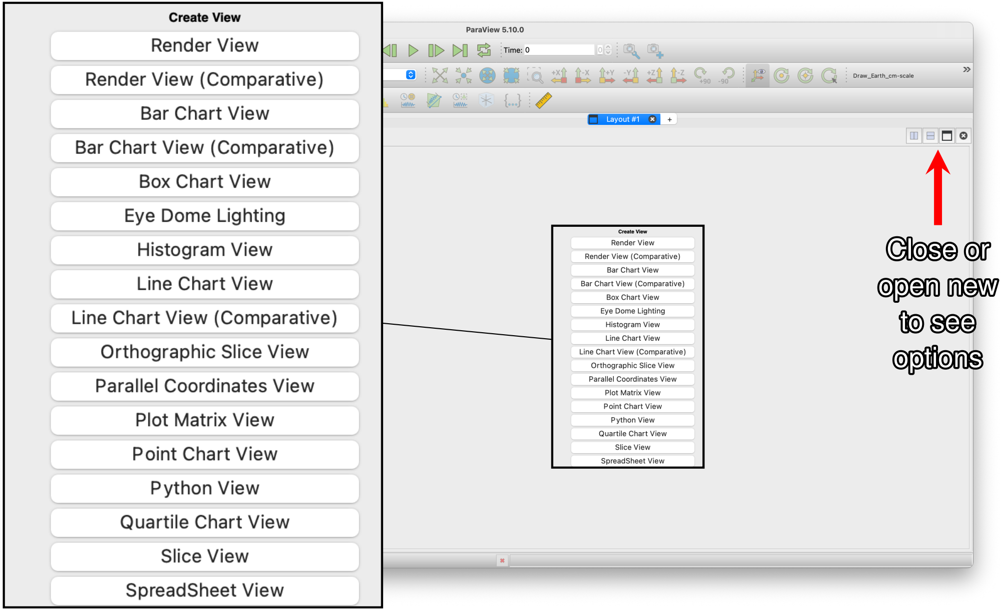
- Open-source & cross-platform software
- Maintained by Kitware Inc.
  - Kitware also maintains CMake, VTK, etc.
- Supported by, among others:
  - Advanced Simulation and Computing Program
  - Army Research Laboratory
  - Los Alamos National Laboratory
  - Sandia National Laboratories

- Getting it: `https://www.paraview.org/download`
- Getting help with it: `https://www.paraview.org/community-support`
- Issues: `https://gitlab.kitware.com/paraview/paraview/-/issues`

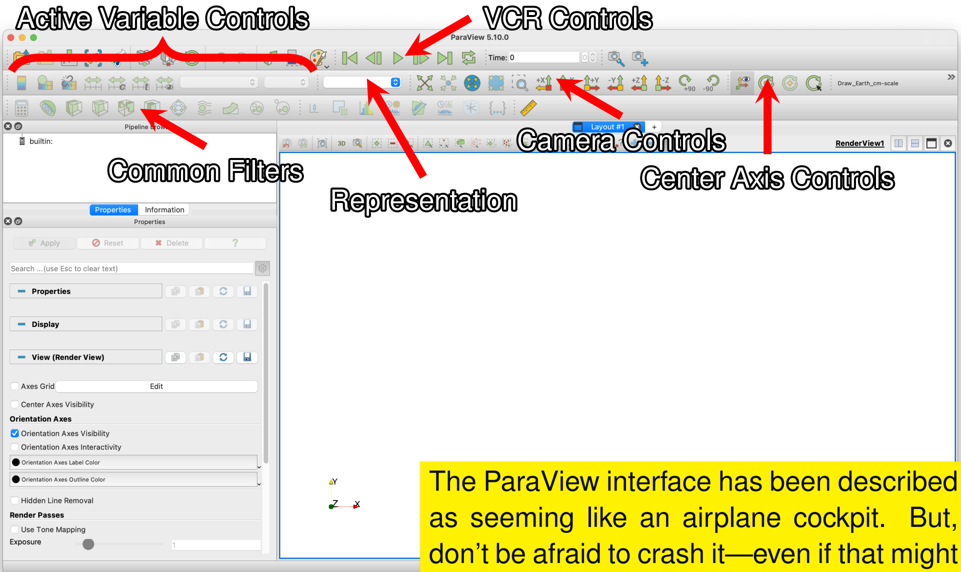
ParaView Interface Overview—Main Components



Views other than the Render View



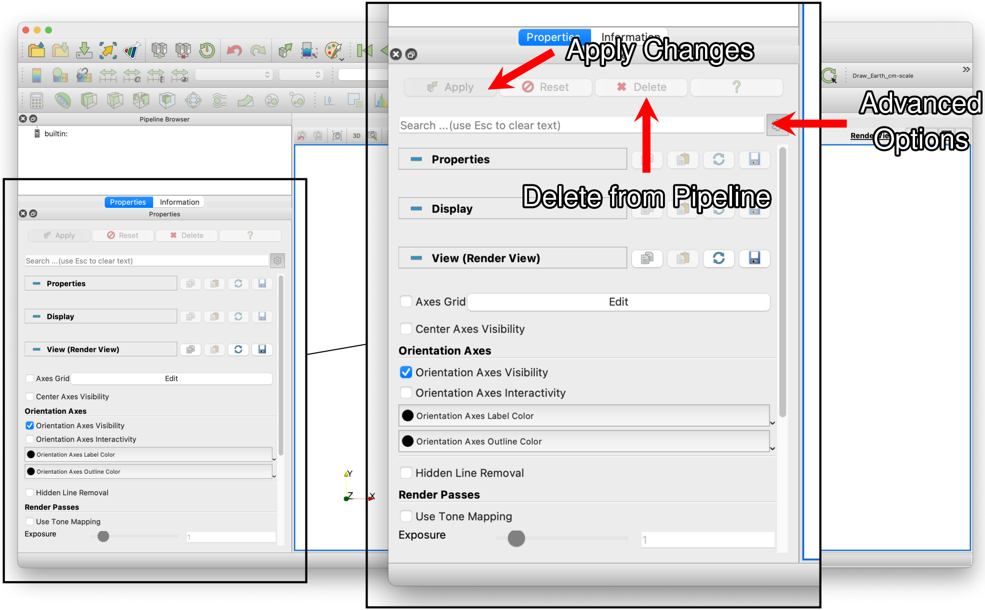
ParaView Interface Overview—Toolbars



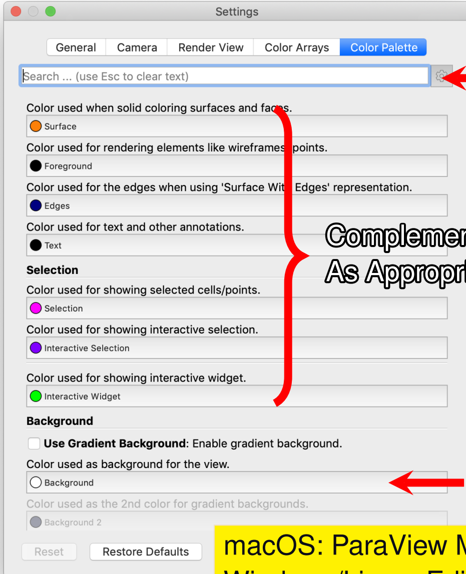
The ParaView interface has been described as seeming like an airplane cockpit. But, don't be afraid to crash it—even if that might (rarely) happen from time to time...

Los Alamos NATIONAL LABORATORY

ParaView Interface Overview—Properties Pane



Render View Colors (Settings, Color Palette Tab)



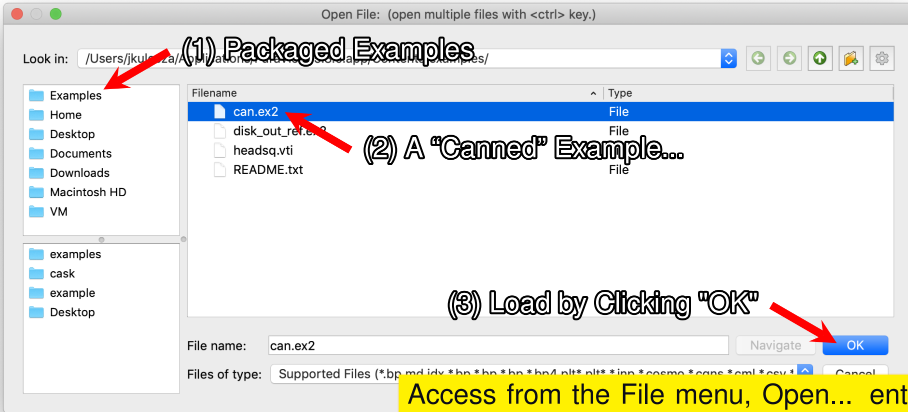
Advanced Options

Complement the Background, As Appropriate

Background Color

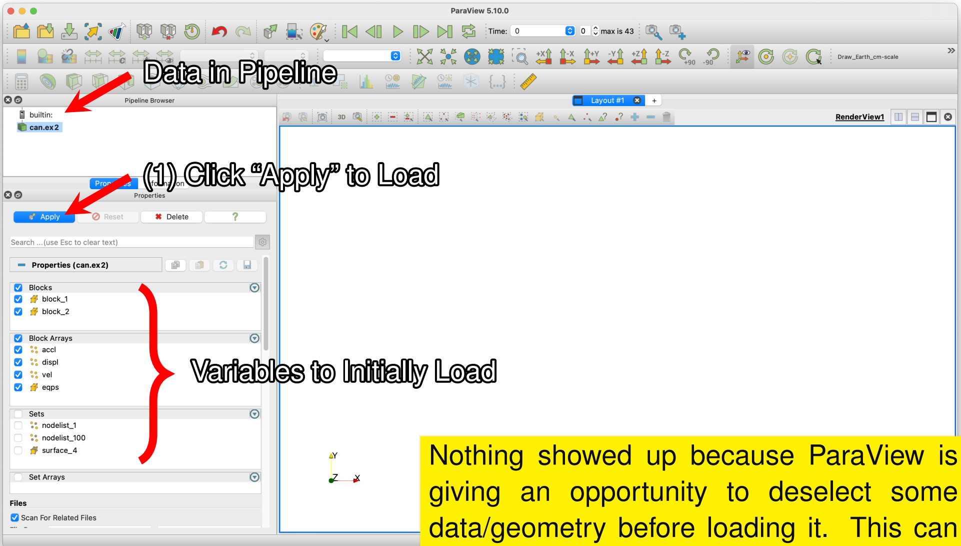
macOS: ParaView Menu→Preferences
Windows/Linux: Edit Menu→Settings

Loading (Example) Data to View



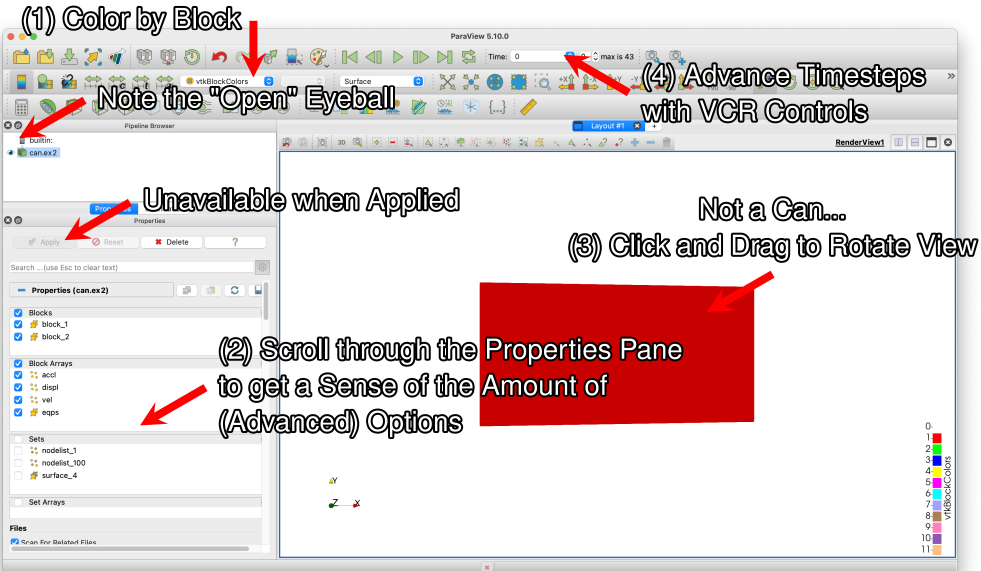
Access from the File menu, Open... entry. Some simple data files are provided with ParaView that can be used for familiarization and/or experimentation.

Moving Around / Controls



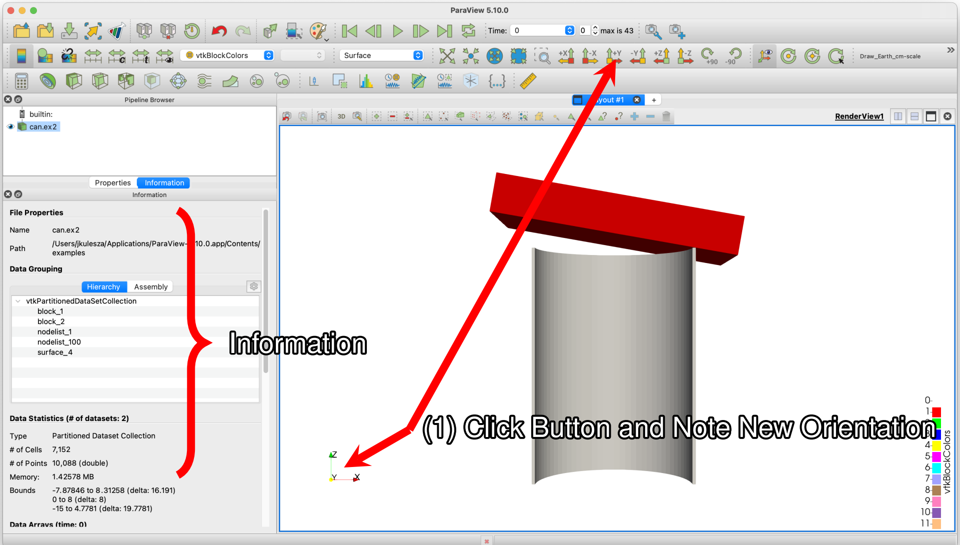
Nothing showed up because ParaView is giving an opportunity to deselect some data/geometry before loading it. This can save time/memory.

Moving Around / Controls (Properties Tab)

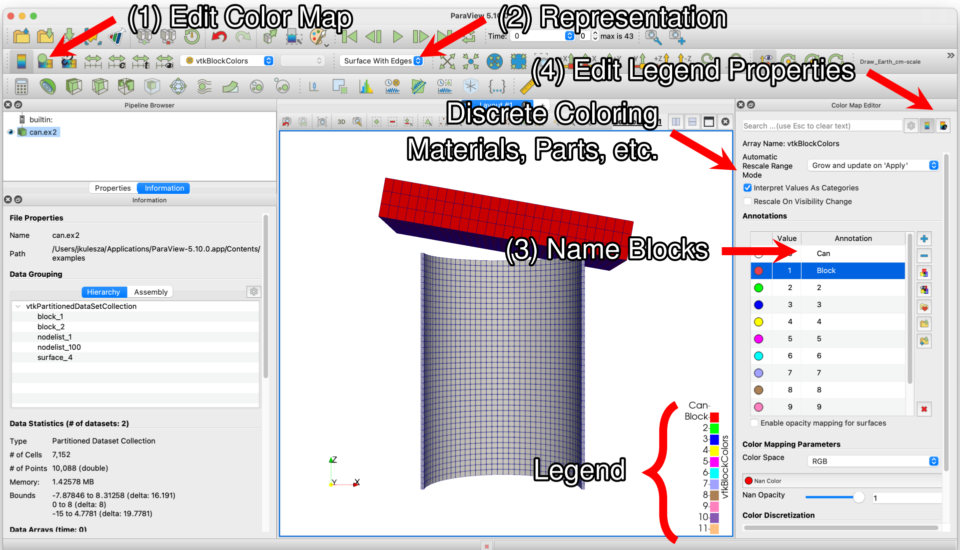


Los Alamos NATIONAL LABORATORY

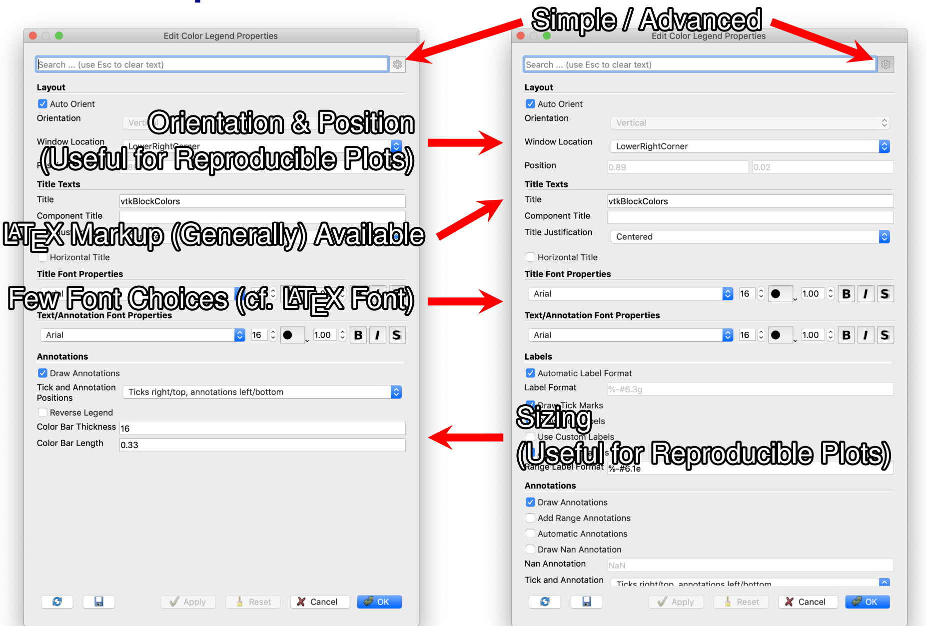
Moving Around / Controls (Information Tab)



Moving Around / Controls (Coloring & Legends)



Edit Color Map



Common MCNP Output Operations / Manipulations

Motivating Calculation Geometry & Results

- Focus: UM geometry and results
  - EEOUT file converted to an ASCII Unstructured VTK File (.vtu) [22]
  - HDF5+XDMF output files (not available in MCNP6.2 and earlier)
- Focus: FMESH-based mesh tallies
  - MESHTAL file converted to an ASCII Structured VTK File (.vts)
  - HDF5+XDMF output files (not available in MCNP6.2 and earlier)

- The needed HDF5+XDMF files are provided
  - Conversion processes shown next for completeness

- Other possibilities (not covered here)
  - Particle tracks
  - Point data (collisions, fissions, etc.)
  - Voxelized CSG representations [23]
  - Weight-window mesh files

MCNP UM File Format Conversion

- MCNP6.2 and earlier: use conversion script electronically attached to [22]
- MCNP6.3: direct `embed` XDMF+HDF5 output via `hdf5file=`*filename*
- Example conversion execution looks like:

```
> ./Convert_MCNP_eeout_to_VTK.py caas_hybrid.mcnp.eeout
Processing caas_hybrid.mcnp.eeout...
  Found 1 edit(s).
  Processing ENERGY_6 edit...
    Processing & Validating EDIT_6_RESULT_...
    Maximum          value: 1.19052e-02
    Minimum positive value: 3.21896e-14
    Minimum          value: 0.00000e+00
    Processing & Validating EDIT_6_ERROR_...
    Maximum          value: 1.00000e+00
    Minimum positive value: 8.86076e-04
    Minimum          value: 8.86076e-04
```

- Resulting file: `caas_hybrid.mcnp.eeout.vtu`

MCNP Mesh Tally File Format Conversion

- MCNP6.2 and earlier: use `meshtal2vtk` script with MCNPTools 5.2.1+
- MCNP6.3: direct `fmesh` XDMF+HDF5 output via `out=xdmf`
- Example `meshtal2vtk` execution looks like:

```
> meshtal2vtk meshtal
Processing mesh tally: 14 -> meshtal_14.vts
  Smallest non-zero tally value:  1.58150e-03
             Largest tally value:  3.57728e-02
```

- As before: the values are useful for setting log-scaled colorbar bounds

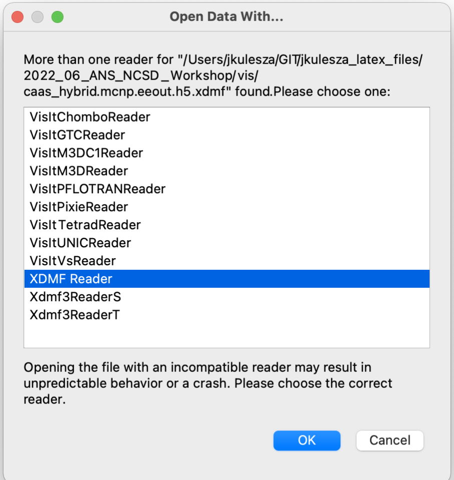
Introduction to XDMF [25, 26]

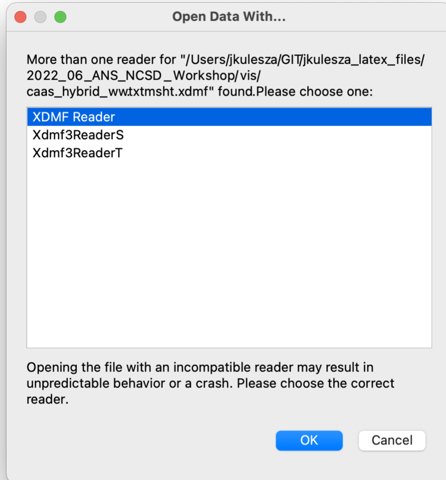
- ASCII, XML-formatted, file
  - Standard, albeit not actively developed, file format
  - Supports various structured and unstructured geometries
  - Can contain data and/or **contain pointers into HDF5 files**

- Cross-platform & open-source support (direct visualization of output)
  - ParaView [21]
  - VisIt [24]

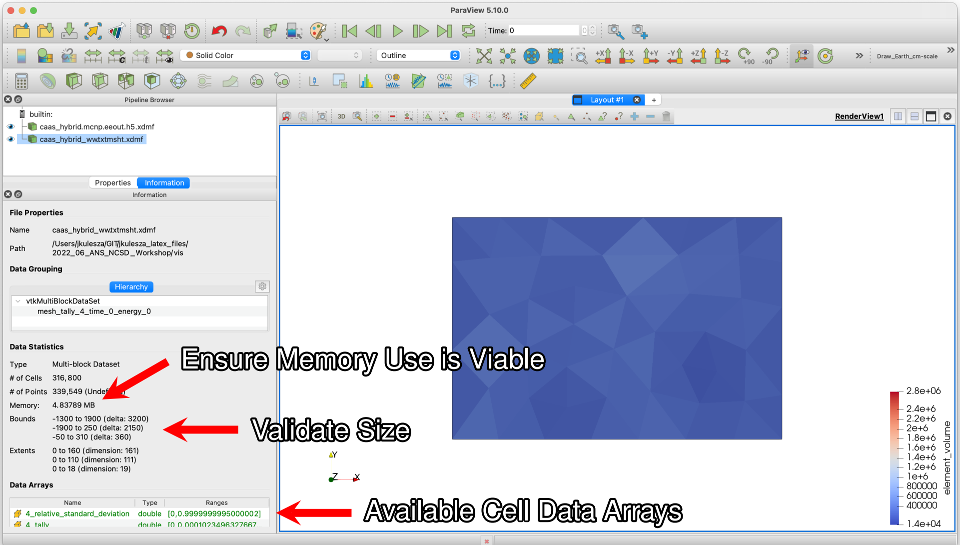
- No additional MCNP library dependencies
  - MCNP outputs are XDMF version 2

Loading XDMF Version 2 Files

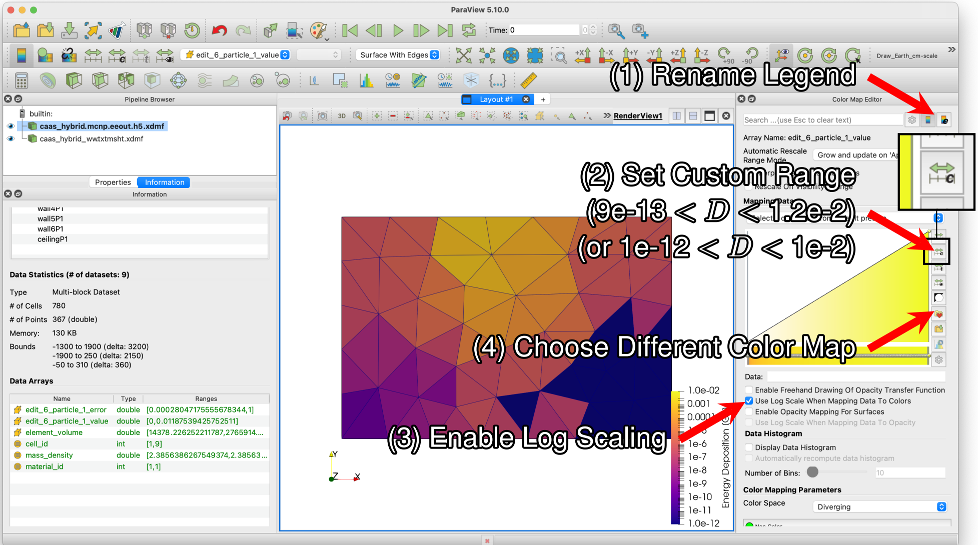




After Loading, Check the File “Information”

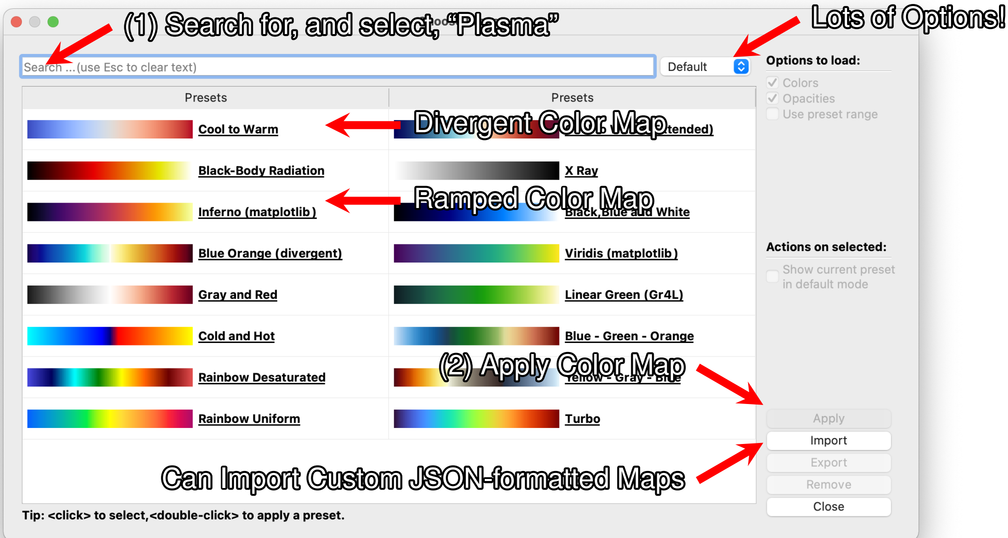


Logarithmically Scaled Coloring & Rename Legend

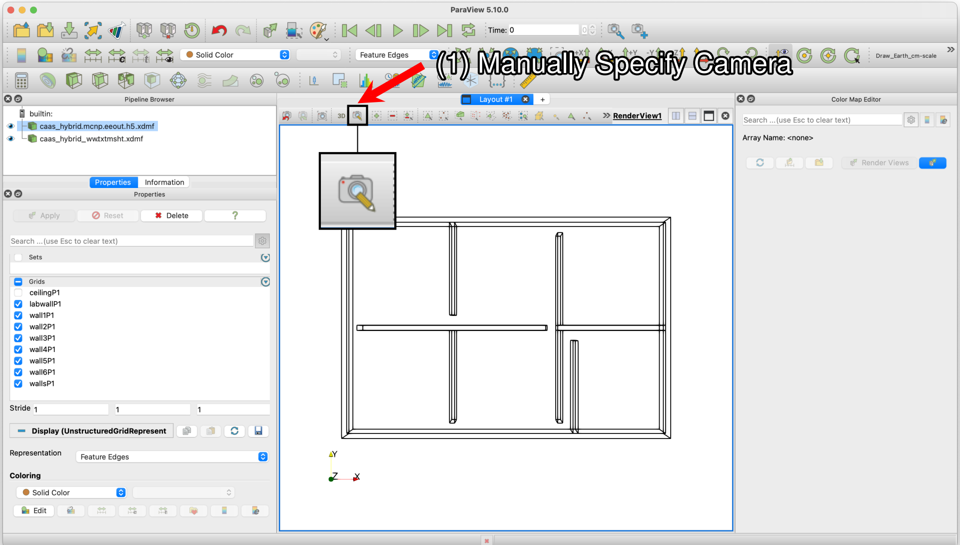


Select Edit 6 values to color by.
Units are calculated as gray from
MeV/g $\times 1.6022 \times 10^{-10}$ Gy · g/MeV $\times$ 2.9 fission^{-1} $\times$ 10^{15} fissions.

Color Map Selection

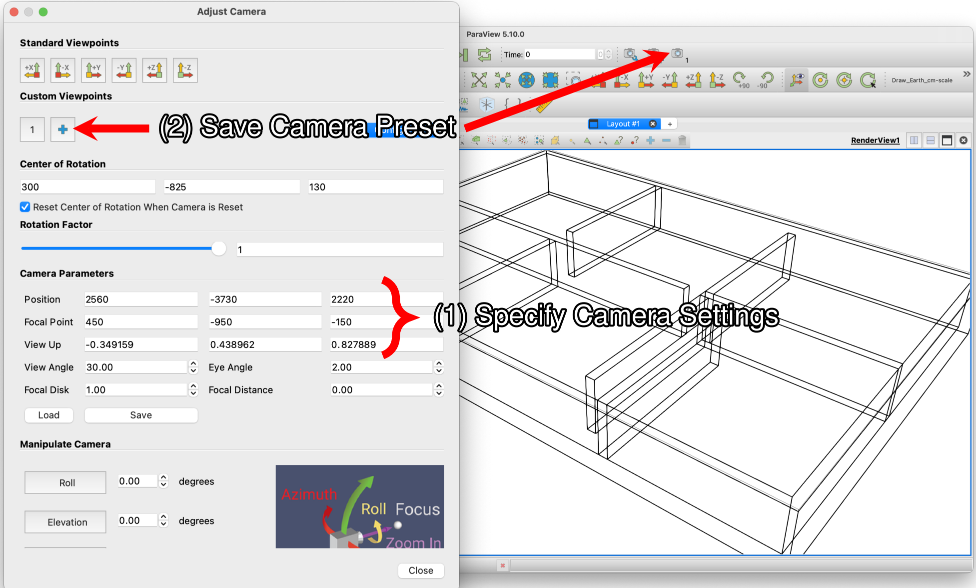


UM Feature-edges Only



Deselect ceiling grid, change UM representation to "Feature Edges", color as black, set line width to 3.

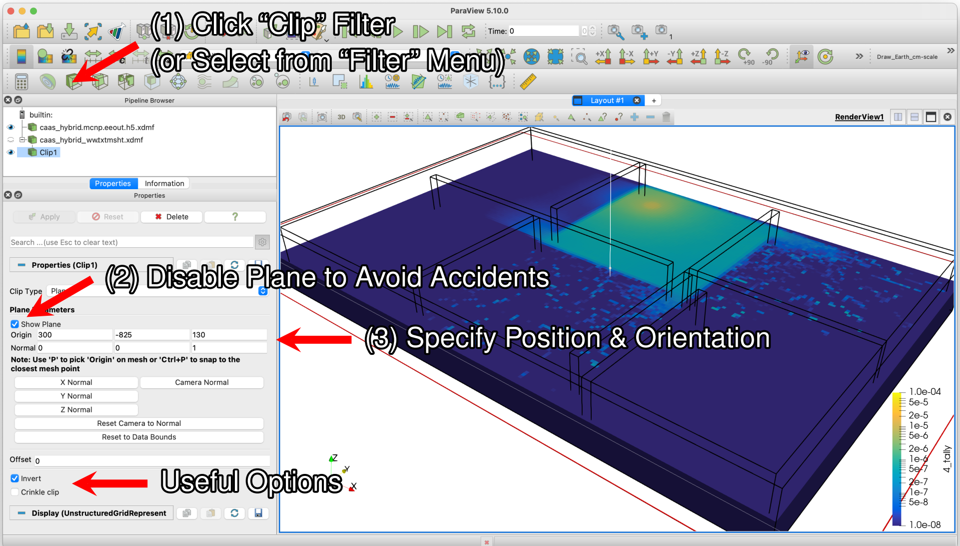
Specify Camera Settings



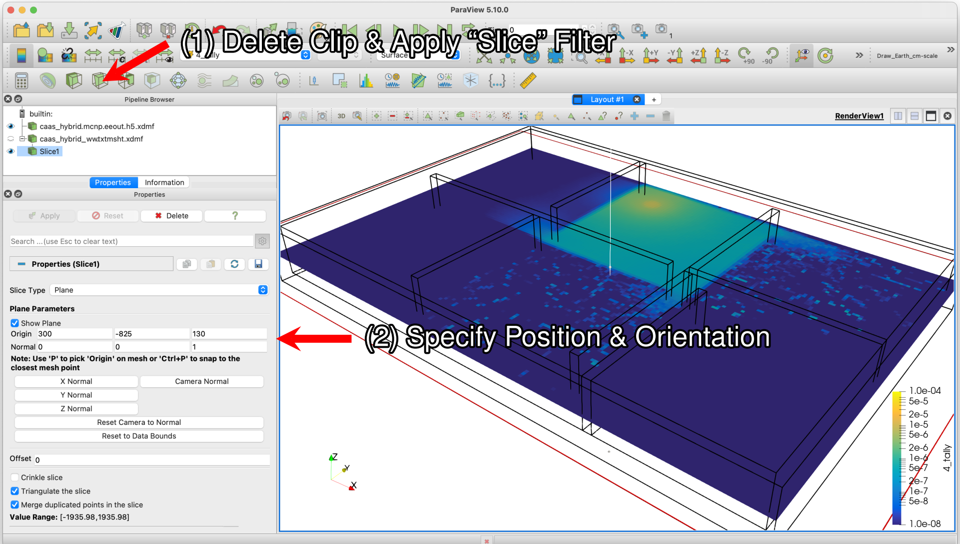
Operations of Interest

- Clips and slices
- Isocontours
  - Cell-to-point data conversion
  - Lighting considerations
  - Overlaying relative fractional uncertainties
  - Probing & manually annotating values
- Assessing mesh quality
  - Segregating and finding particular elements

Clip (Hide Half Space)

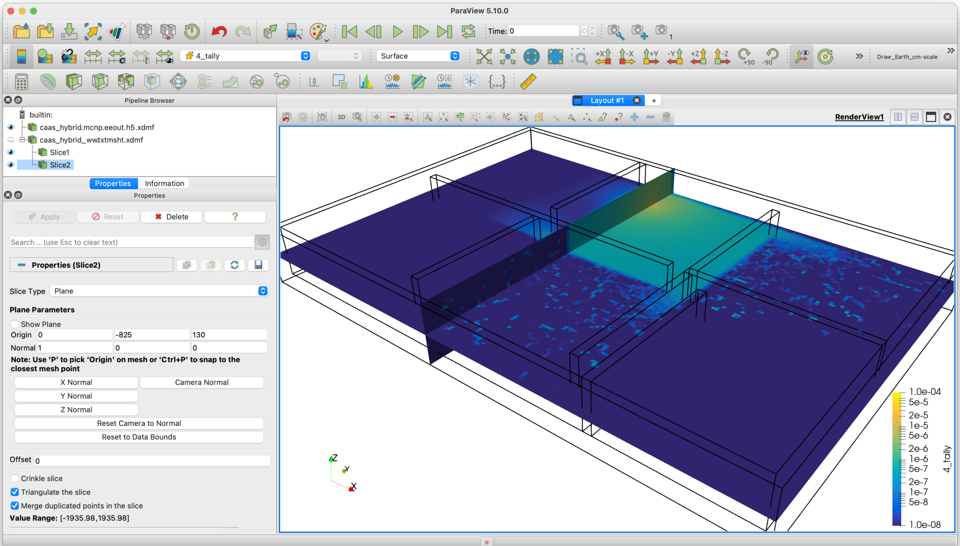


Slice



Los Alamos NATIONAL LABORATORY

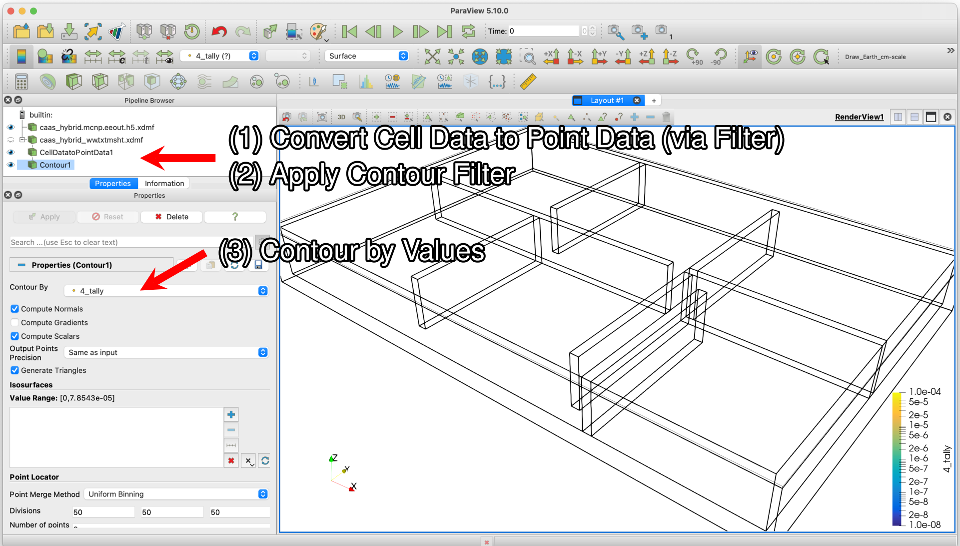
Another Slice ($x, y, z = 0, -825, 130 \perp x$)



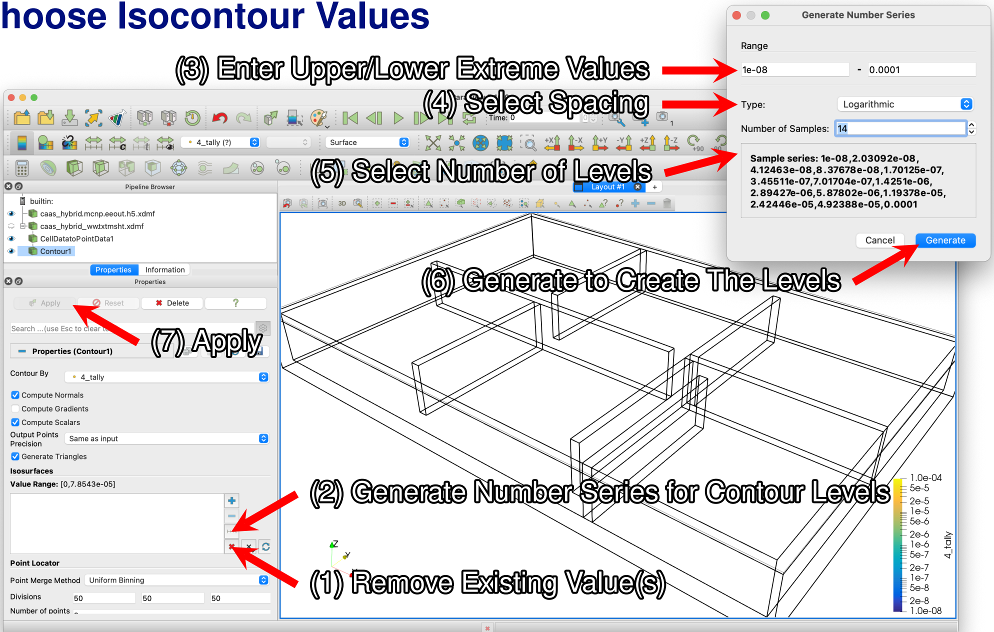
Los Alamos NATIONAL LABORATORY

Isocontours & Lighting Considerations

Apply Contour Filter and "Contour By" Value



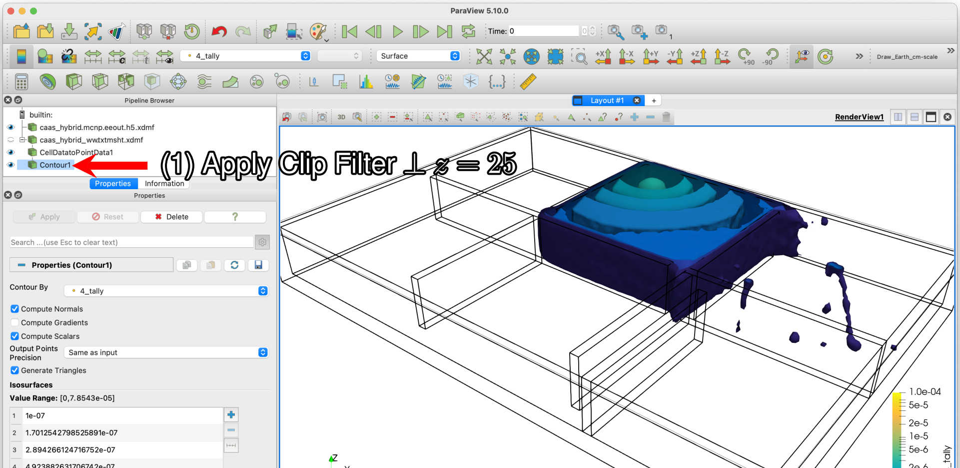
Choose Isocontour Values



Los Alamos NATIONAL LABORATORY

Also adjust coloring by value to be consistent with contour range.

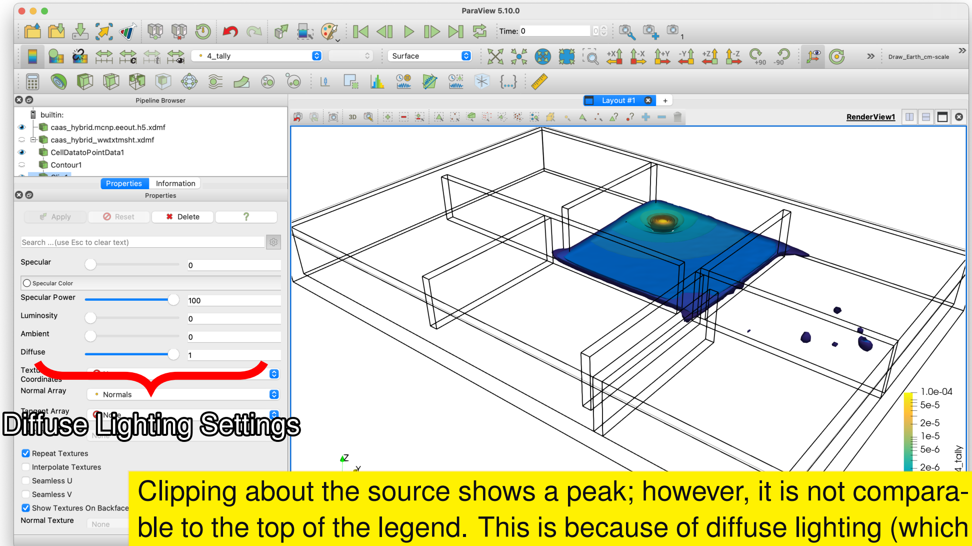
Observe Isocontour Results & Trends



Peak and emanations about source. Significant attenuation in walls

Can also overlay other results (particle tracks, etc.).

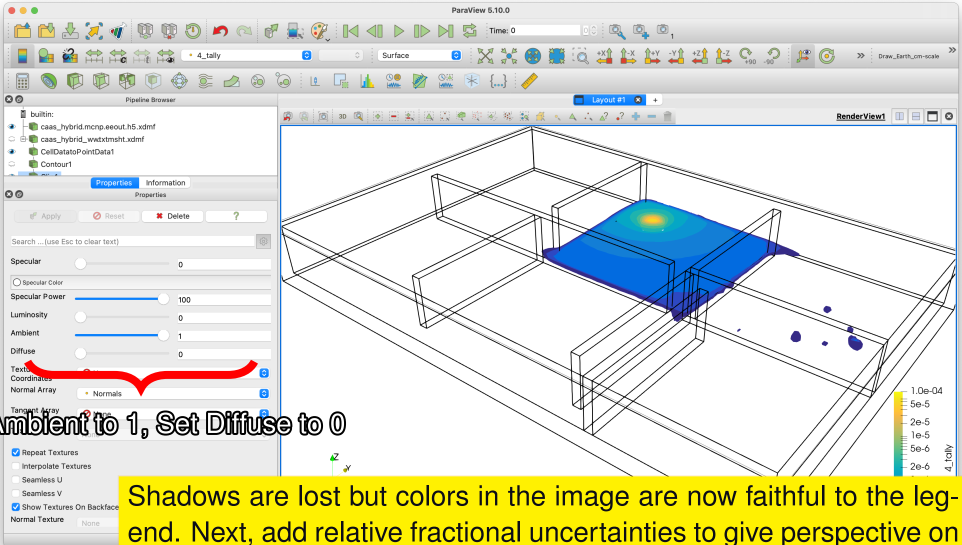
Clip Isocontour & Observe Shadows



Clipping about the source shows a peak; however, it is not comparable to the top of the legend. This is because of diffuse lighting (which gives shadows but "darkens" the colors).

Los Alamos
NATIONAL LABORATORY

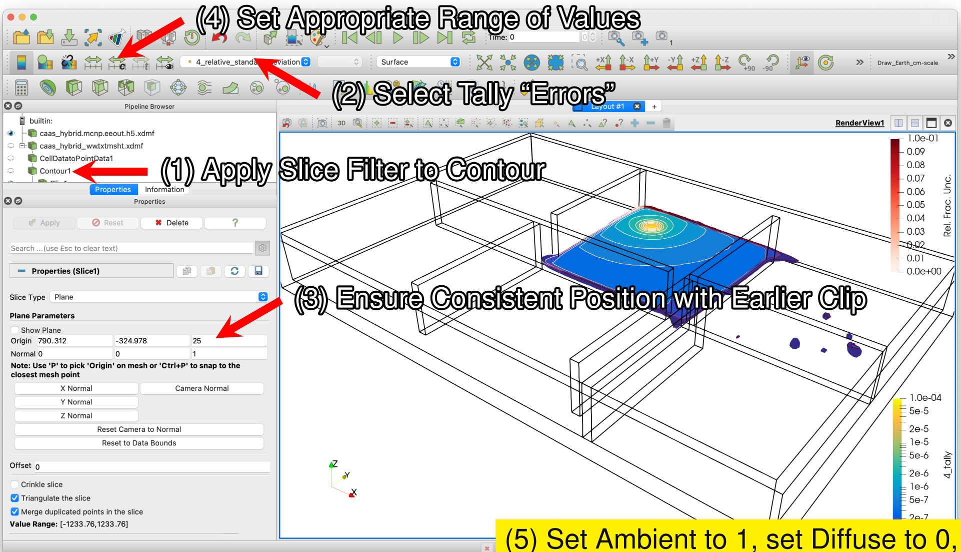
Adjust from Diffuse to Ambient Lighting



Set Ambient to 1, Set Diffuse to 0

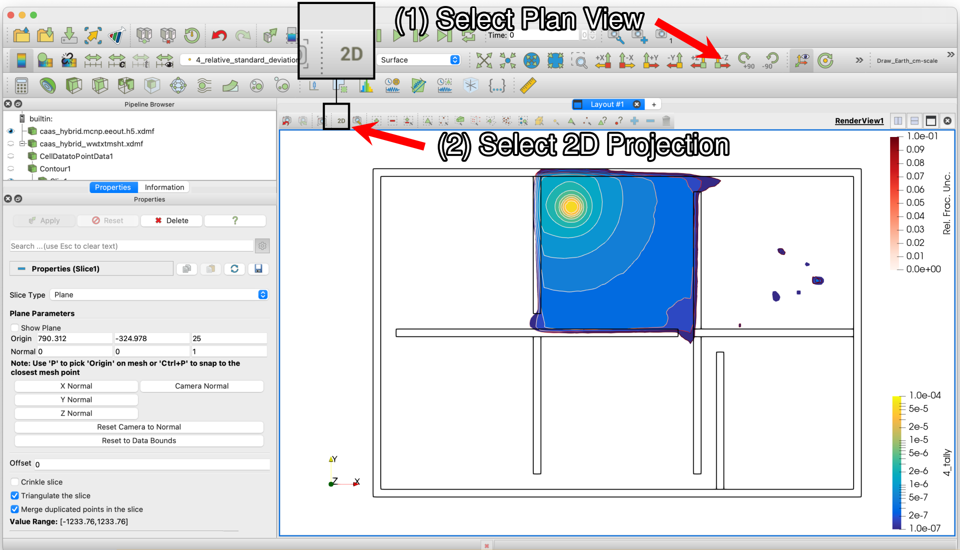
Shadows are lost but colors in the image are now faithful to the legend. Next, add relative fractional uncertainties to give perspective on results.

Add Relative Fractional Uncertainties



(5) Set Ambient to 1, set Diffuse to 0, set line width to 2.

2D Plan View



Gives a more “traditional” representation of geometry and results.

Assessing Mesh Quality

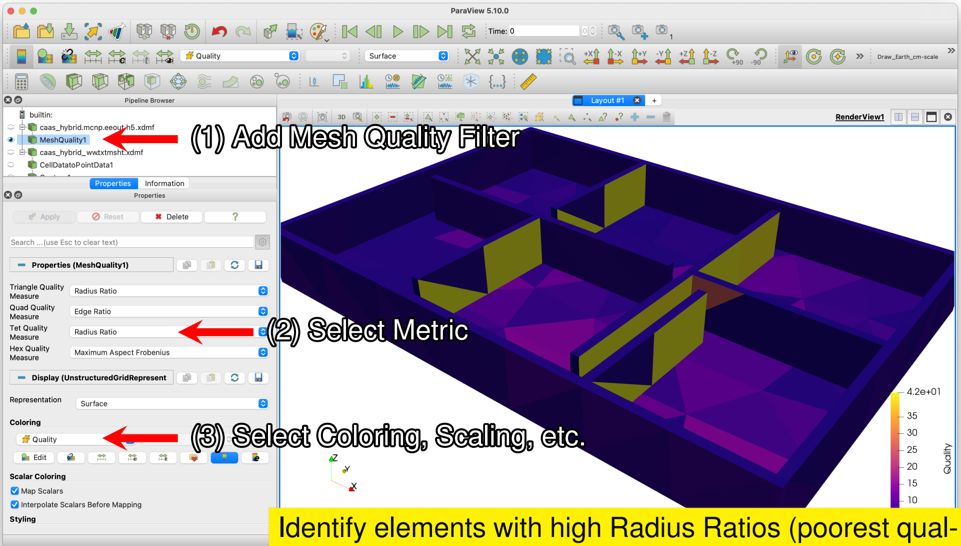
What is “Mesh Quality”

- Mesh element “quality” can be assessed by a variety of metrics
  - Deterministically calculated
  - Useful for mesh-generation algorithms
  - Useful for deterministic engineering calculations

- Body of knowledge mainly for linear tetrahedra and hexahedra
  - Verdict library [9] summarizes these metrics
  - ParaView incorporates Verdict

- Useful for Monte Carlo transport to identify undesirable elements
  - Negative-Jacobian elements have negative volume
    - Problematic for edits
  - “Paper-thin” elements can challenge particle tracking

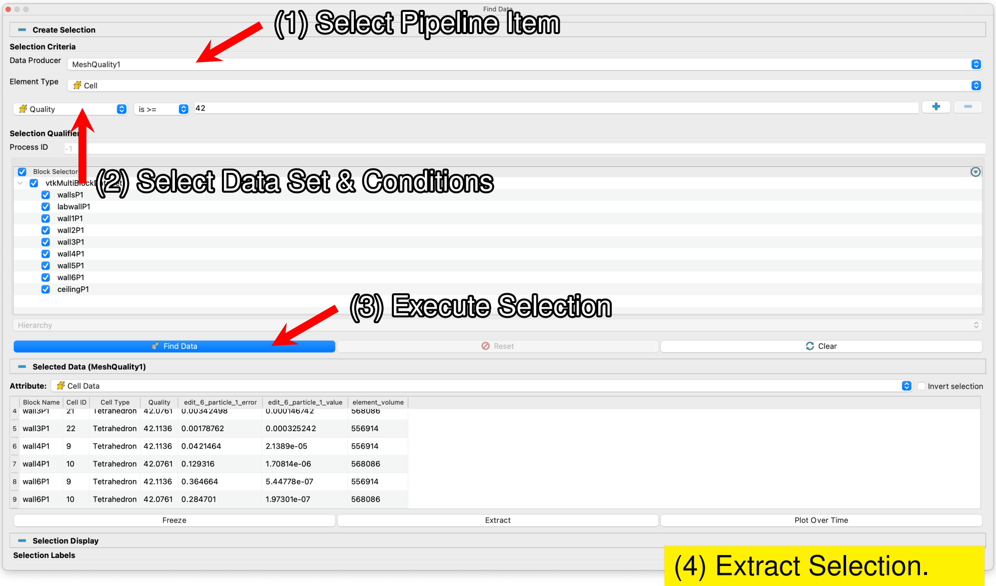
Mesh Quality Filter & Finding Elements



Identify elements with high Radius Ratios (poorest quality). To do this: (4) Edit menu: Find Data.

Hide all other pipeline components.

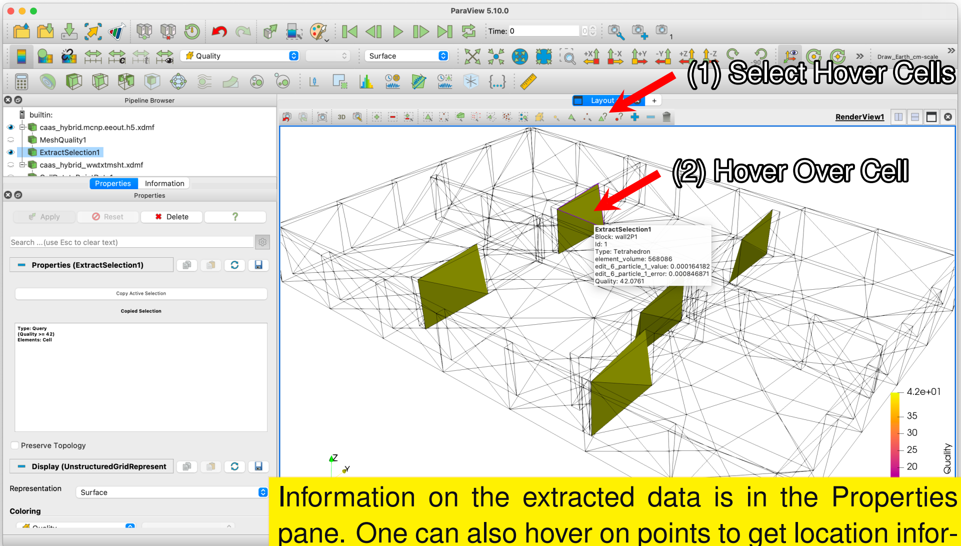
Find Data Dialog Use



Los Alamos NATIONAL LABORATORY

Note that this dialog may need to be scrolled vertically to expose all elements.

Viewing & Interrogating Specific Elements



Information on the extracted data is in the Properties pane. One can also hover on points to get location information.

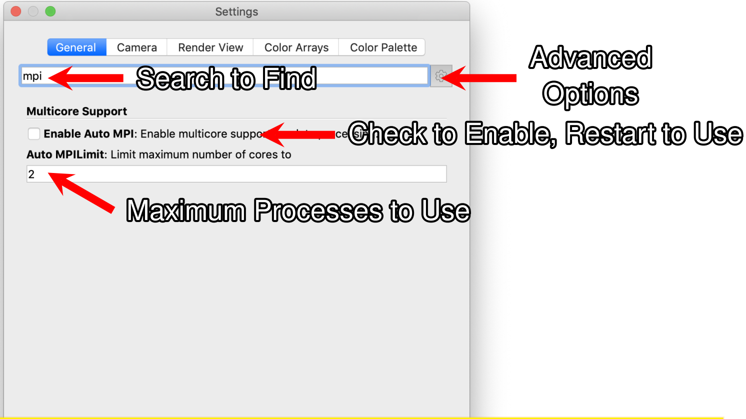
Los Alamos NATIONAL LABORATORY

Other (Advanced?) ParaView Topics

Brief Overview of Other Topics

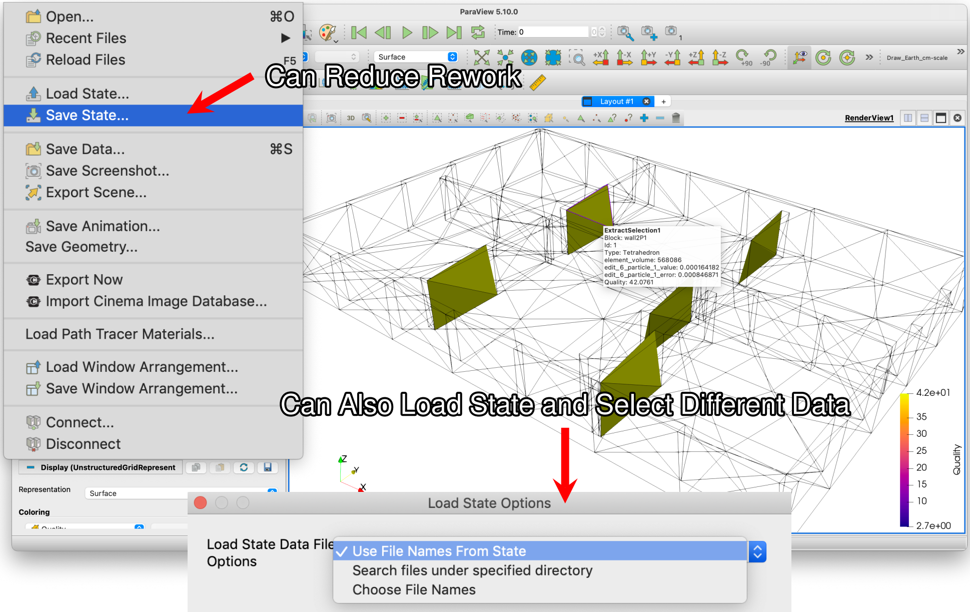
- MPI Parallelism
- Toggling Geometry via Blocks
- Saving ParaView State
- Camera Linking
- Recording Traces (Macros)
- Client-server Connections
- Animation

MPI Parallelism (Settings, General Tab)

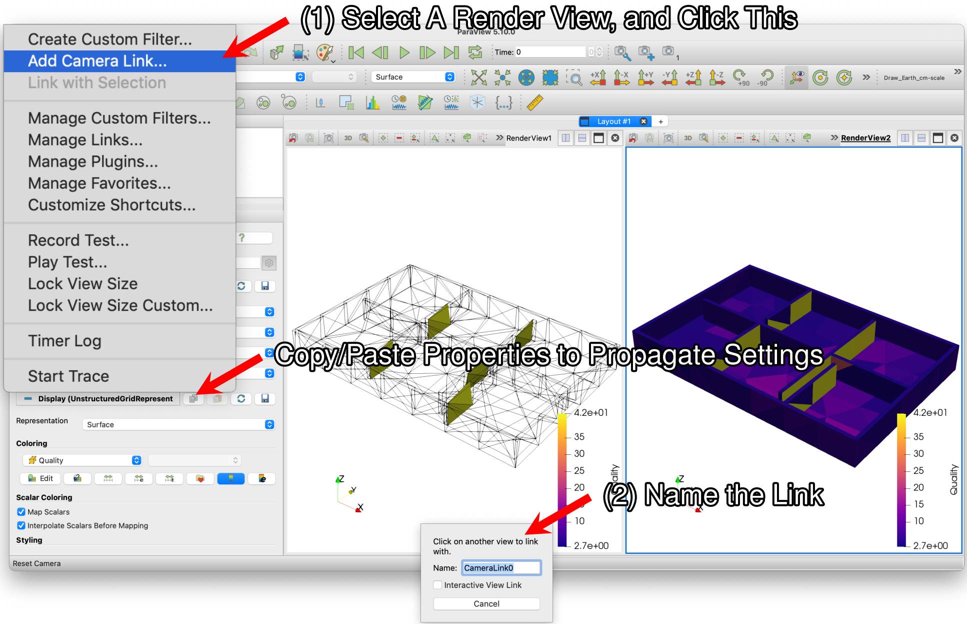


Requires MPI on your system (and running). Also, depending on your system firewall settings, you may see a number of MPI processes launch and be forced to dismiss allow/block requests. This means: start with a few processes to see how your system behaves.

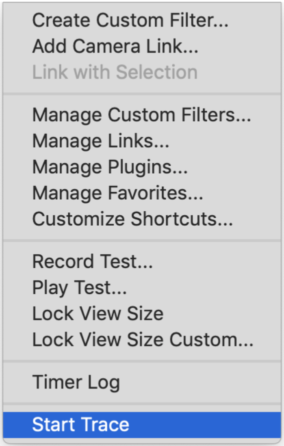
Saving ParaView State (File Menu)

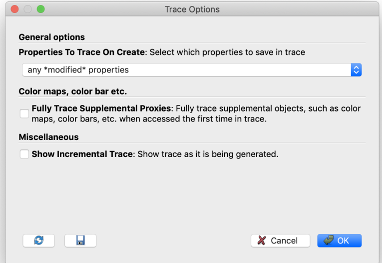


Camera Linking (Tools Menu)

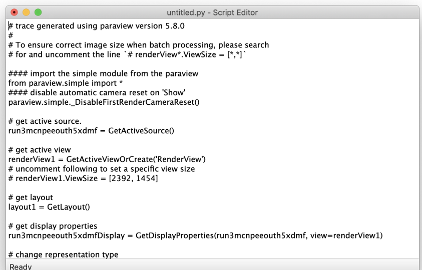


Recording Macros (Traces, Tools Menu)



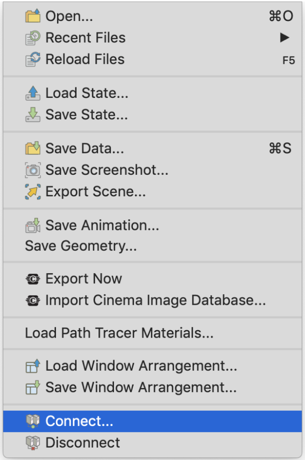


Stop Trace

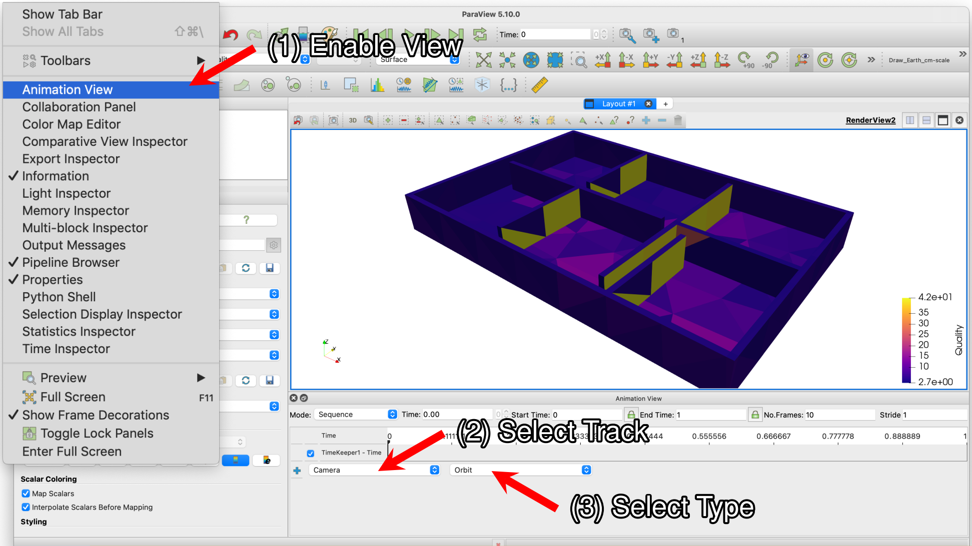


Client-server Connections

- Negates downloading data
- Provide parallel processing via MPI
- Institution-specific configuration
- LANL uses a PVSC configuration file
- `https://hpc.lanl.gov/paraview_usage`
- Remote memory monitoring
  - View: Memory Inspector



Animation



Python tracks can perform scripted actions every frame (every tick).