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Title: Athena-I Modeling with MCNP6.3

Author(s): Gladden, Bradley Jo
Armstrong, Jerawan Chudoung
Kelley, Karen Corzine

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Athena-I Modeling with MCNP6.3

Bradley Gladden

Mentors: Jerawan Armstrong, Karen Kelley

2023 MCNP User Symposium
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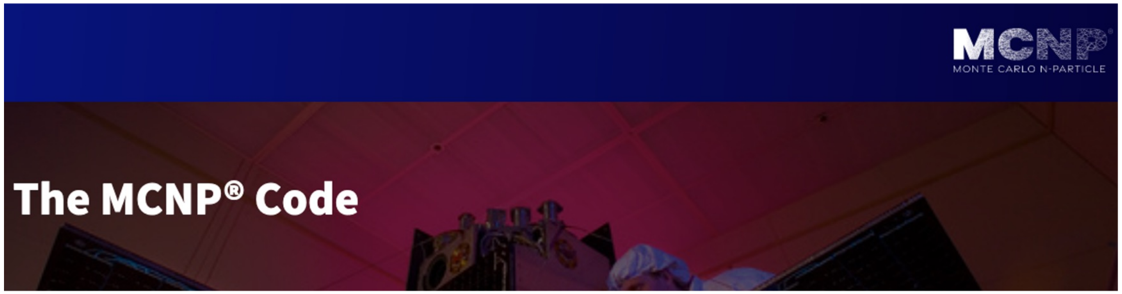
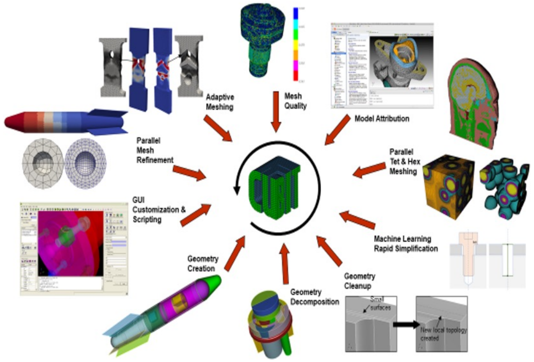
Outline

- Athena-I Overview
- Athena-I Unstructured Mesh (UM) Creation in CUBIT
- Athena-I Constructive Solid Geometry (CSG) and UM Modeling in MCNP6.3



https://mcnp.lanl.gov



https://cubit.sandia.gov

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Athena-I Overview

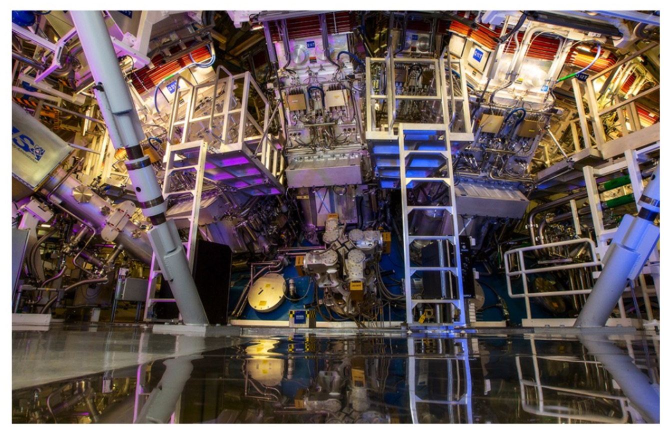
What is Athena-I?

- An experiment was designed by the Air Force Institute of Technology (AFIT) and conducted at the National Ignition Facility (NIF).
  - Designed to study the response of electronic devices to a neutron environment
  - Used prompt pulse from NIF high-density D-T neutron source
  - Used the energy tuning assembly called Athena-I to shape a D-T neutron source

- The Athena-I assembly contains foils and TLDs used to measure flux and dose from neutrons and photons.

https://www.afit.edu

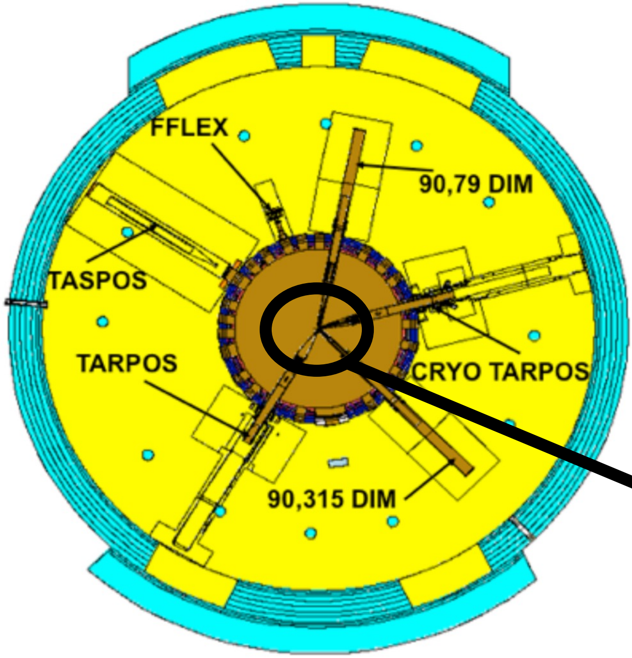
What Is the National Ignition Facility?



THE WORLD'S LARGEST AND HIGHEST-ENERGY LASER

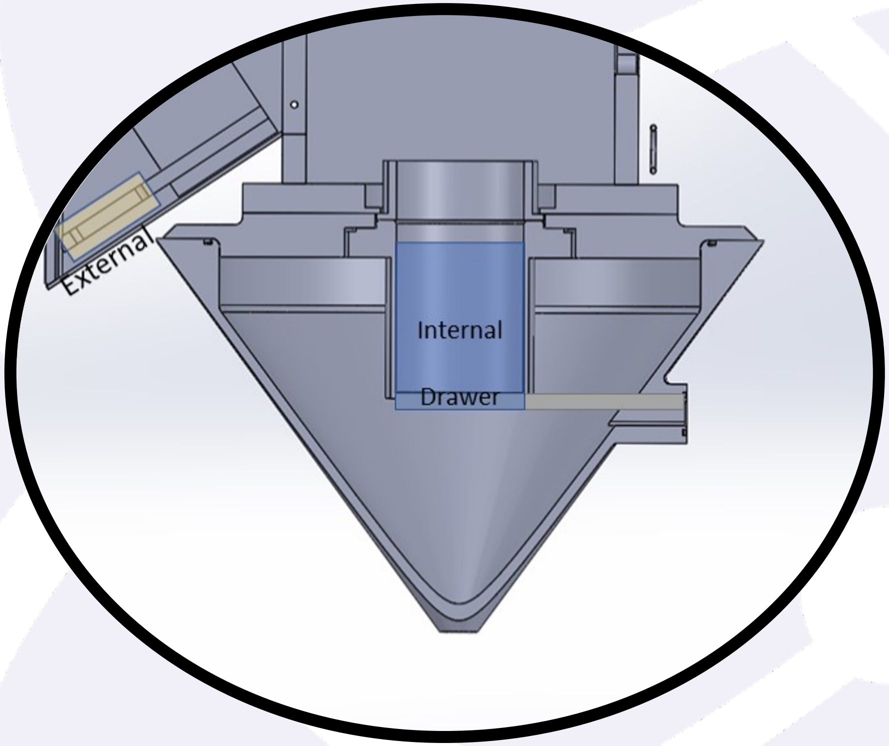
https://lasers.llnl.gov

Athena-I Experiment



NIF lasers produce D-T fusion neutrons

Figure 1. NIF Target Bay Area from Fusion Neutronics Meeting Simulation of Radiation Environment at NIF Presentation by Hesham Khater [1]



Athena-I energy tuning assembly measures effect on microelectronics

Figure 2. Athena Platform with Internal Drawer and External Arm from Athena: A Unique Radiation Environment Platform at the National Ignition Facility by Nick Quartemont et al [2]

Previous Athena-I Modeling

- MCNP6.2 was used for Athena-I modeling and analysis.
  - Created CSG model
  - Used two variance reduction methods:
    - Forced collisions
    - Weight windows, ADVANTG was used to generate weight window parameters
  - MODE n p e
  - Computational results and experimental data were comparable for neutrons
  - MCNP CSG input file was released to public [3]

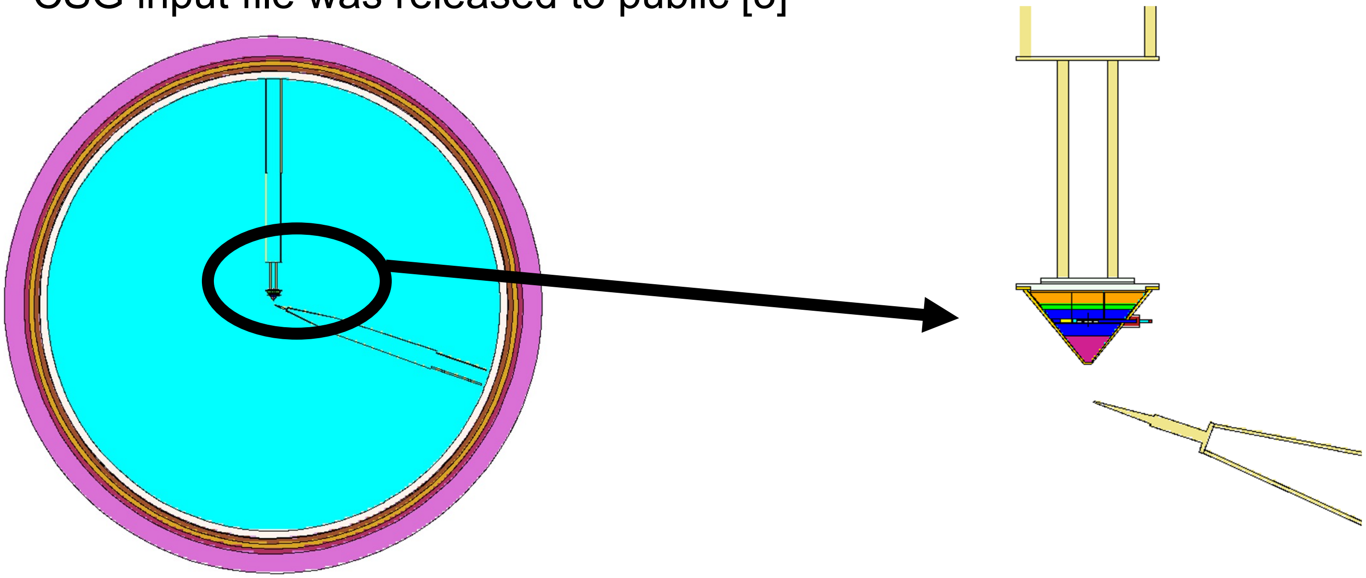


Figure 3. MCNP Plot of Athena-I Experimental Model

Athena-I Components

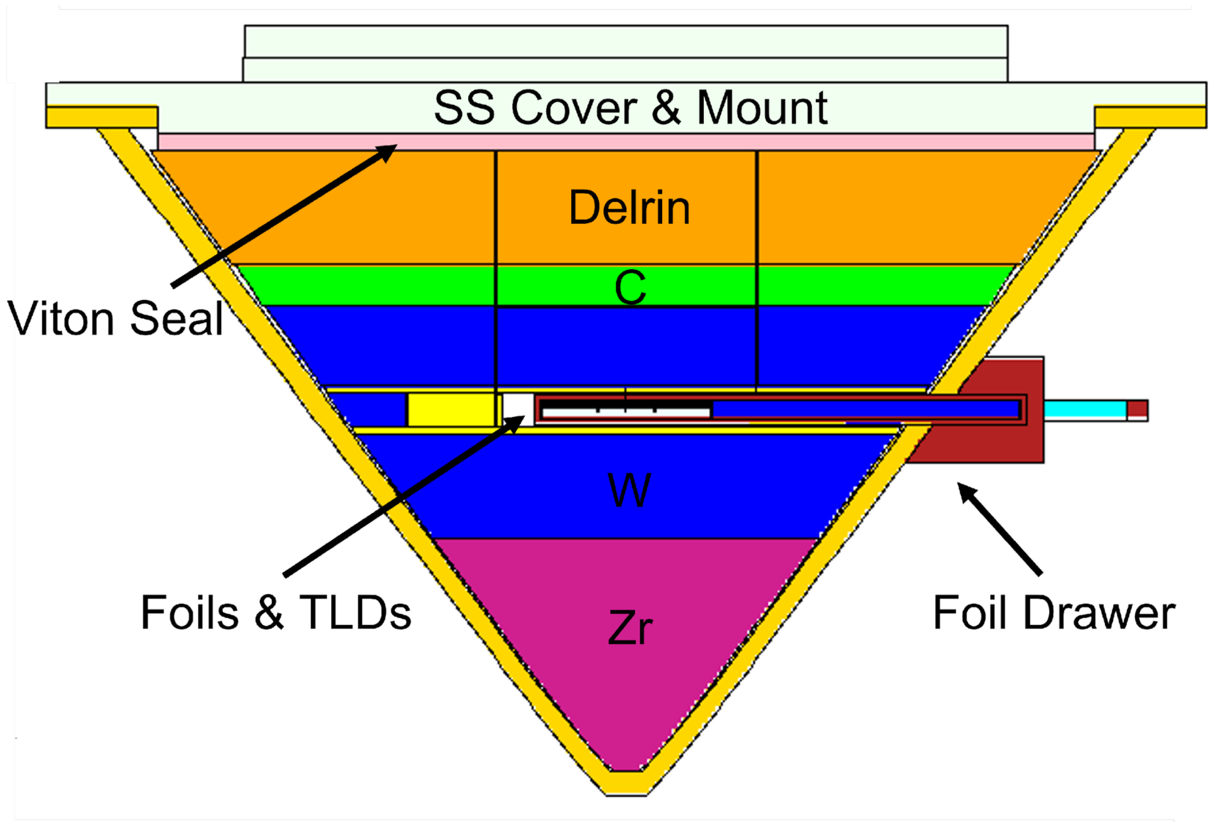


Figure 4. Athena-I Body

Athena-I Unstructured Mesh Models

CUBIT Geometry Creation

MCNP Input

Cells

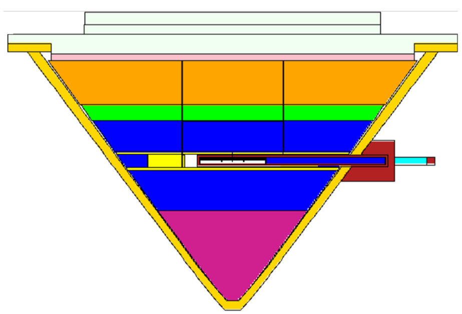
```
c Athena Body
10  22   -7.87      -10 11 60        imp:n,p=1 imp:e=0 $ Cone
```

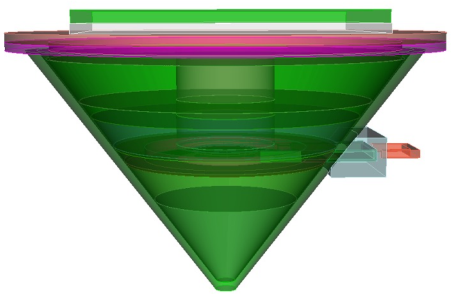
Surfaces

```
c Athena body surfaces
10 TRC  9.000 0 0 19.202 0 0 0.855 15.281      $ Outer body Athena
11 TRC  9.700 0 0 18.502 0 0 0.765 14.378      $ Inner body Athena
```

CUBIT Geometry

```
#----------------
# Outside Cone
#----------------

#Cell=Cone, Surface=Outer Body Athena
create frustum height 19.202 radius .855 top 15.281
rotate volume 1 about origin x direction z angle 90
rotate volume 1 about origin z direction z angle 90
move volume 1 x 18.601

#Cell=Cone, Surface=Inner Body Athena
create frustum height 18.502 radius .765 top 14.378
rotate volume 2 about origin x direction z angle 90
rotate volume 2 about origin z direction z angle 90
move volume 2 x 18.951

subtract volume 2 from volume 1
```





Cells

```
c TLD 100s
70  8   -1.29e-9   -80            imp:n,p,e=1  $ TLD 100
```

Surfaces

```
c TLDs
80 RPP 20.05 20.139 1.005 1.325 -0.16 0.16     $ TLD-100 #1
```

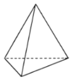
```
#Cell=TLD-100, Surface=TLD-100 #1
create vertex 20.139 1.005 -0.16
create vertex 20.05  1.005 -0.16
create vertex 20.139 1.005 0.16
create vertex 20.05 1.005 0.16
create vertex 20.139 1.325 -0.16
create vertex 20.05 1.325 -0.16
create vertex 20.139 1.325 0.16
create vertex 20.05 1.325 0.16
create surface vertex 713 711 707 709
create surface vertex 712 708 710 714
create volume loft surface 508 509

delete body 127 128
```

Figure 5. MCNP Geometry and Input

Figure 6. CUBIT Geometry and Journal File Inputs

CUBIT Mesh Generation

Tetrahedral



- Easy to mesh.
- Mesh qualities depend on geometries and meshing methods.

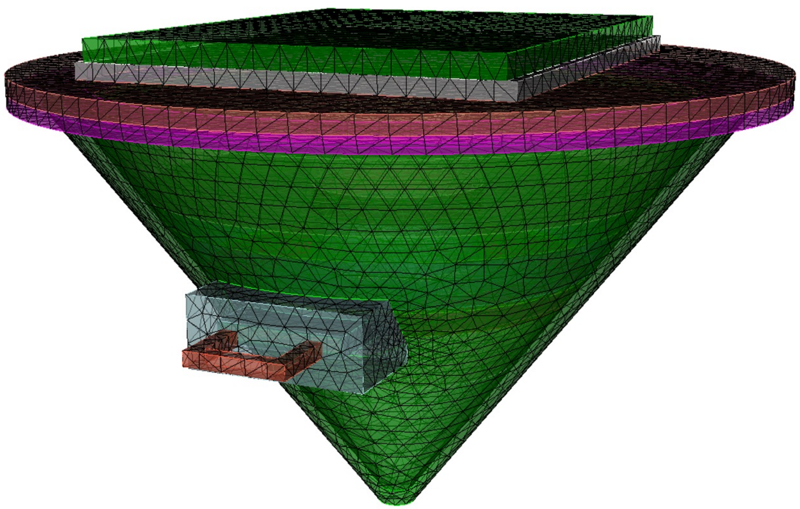
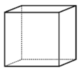


Figure 7. CUBIT Tetrahedral Mesh

Hexahedral



- Difficult to mesh.
- Mesh qualities depend on geometries and meshing methods.

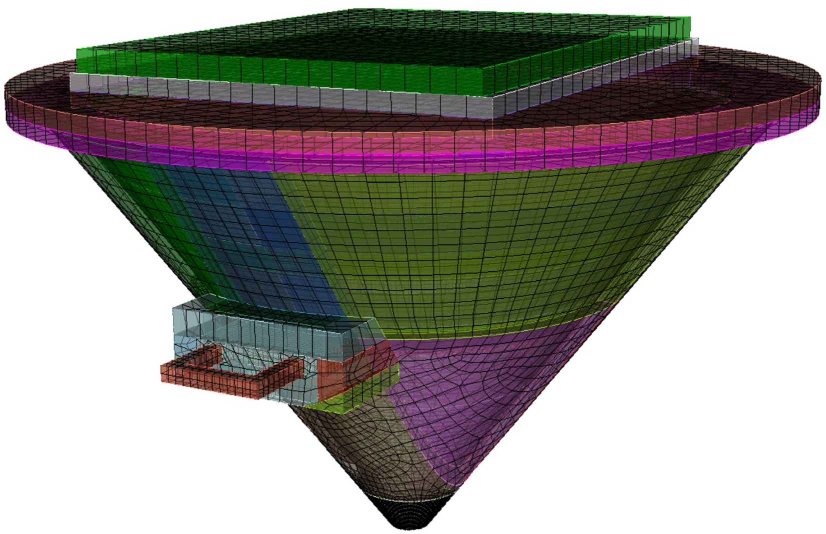


Figure 8. CUBIT Hexahedral Mesh

Mesh qualities: positive Jacobian & volumes of solid and meshed models are well-matched.

Tetrahedral Mesh

165,089 elements

- Meshable directly from geometry
- Contiguous mesh through entire geometry
- Mesh volume immediately within 3% of geometry volume, requires fewer elements than hexahedral
- Mesh immediately has positive Jacobian

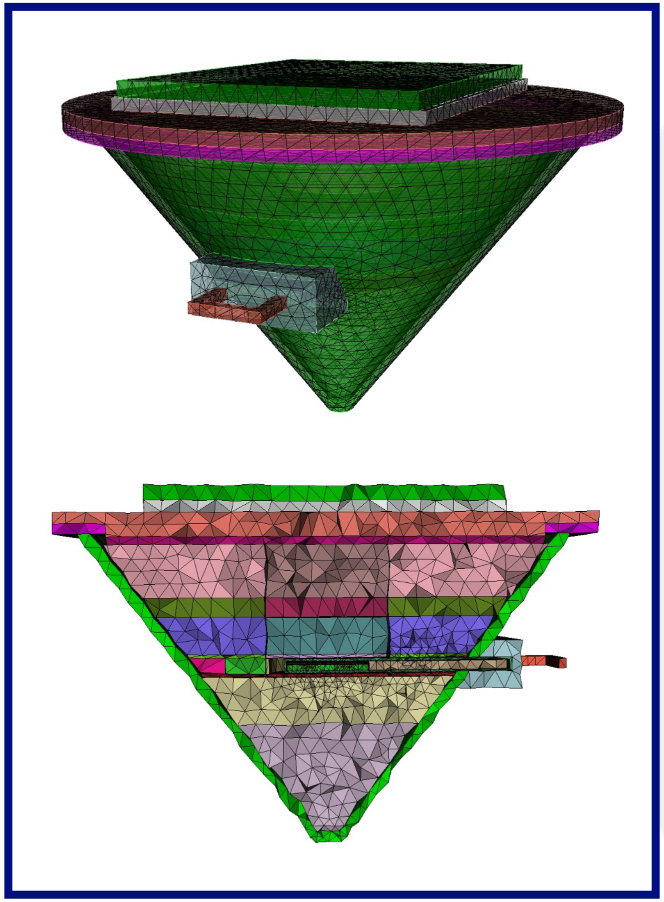


Figure 9. Isometric and Cross-Sectional View of Tet mesh model

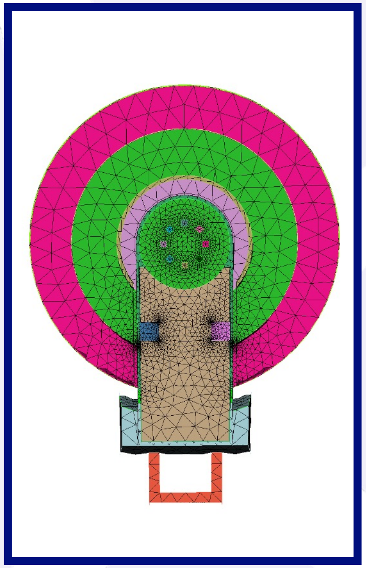


Figure 10. Top-Down View of Internal Drawer

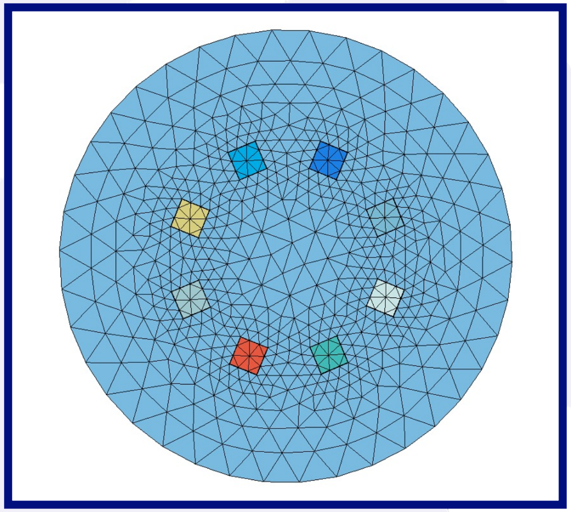


Figure 11 Zoomed View of TLDs Where Tally Calculations Occur (Foils are Below TLDs)

<u>Foils & TLDs</u>

Mesh automatically finer at flux and dose tally's locations

Hexahedral Mesh

1,107,965 elements

- Not meshable directly from geometry
- Contiguous mesh within each part
- Mesh volume within 3% of geometry volume after refinement, requires more elements than tetrahedral
- Mesh has positive Jacobian after much geometry preparation

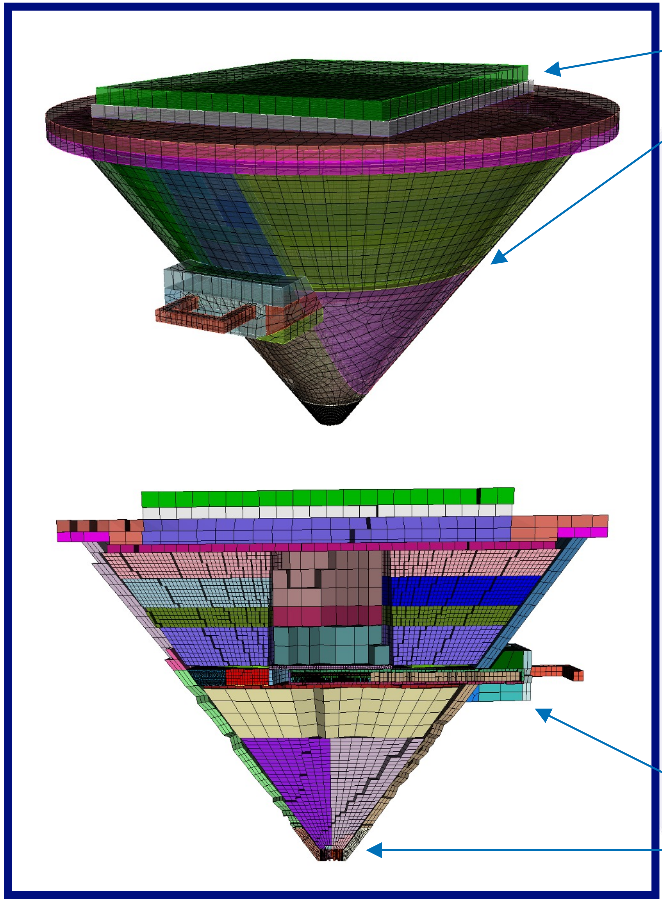


Figure 12. Isometric and Cross-Sectional View of Hex mesh model

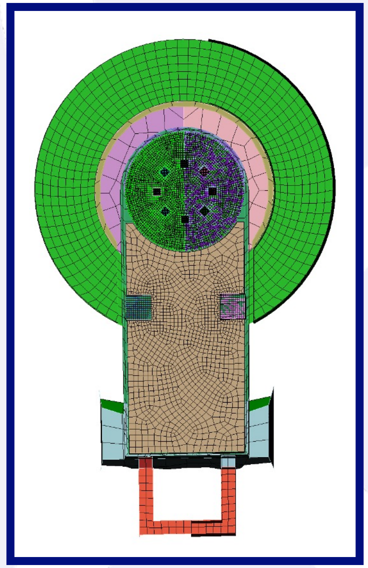


Figure 13. Top-Down View of Internal Drawer

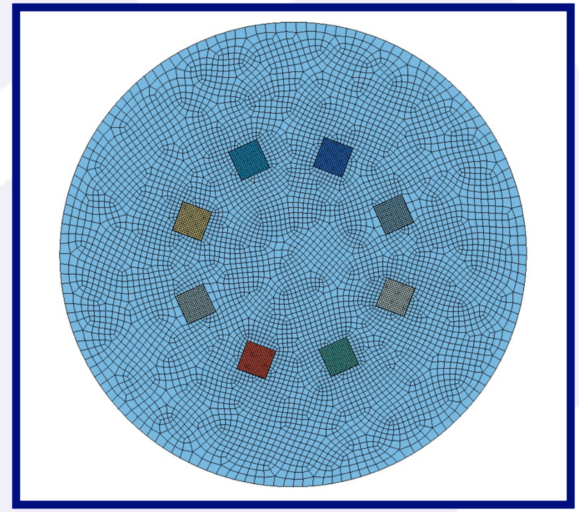


Figure 14. Zoomed View of TLDs Where Tally Calculations Occur (Foils are Below TLDs)

<u>Foils & TLDs</u>

Mesh must be refined to properly characterize flux and dose

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Athena-I CSG vs UM Models

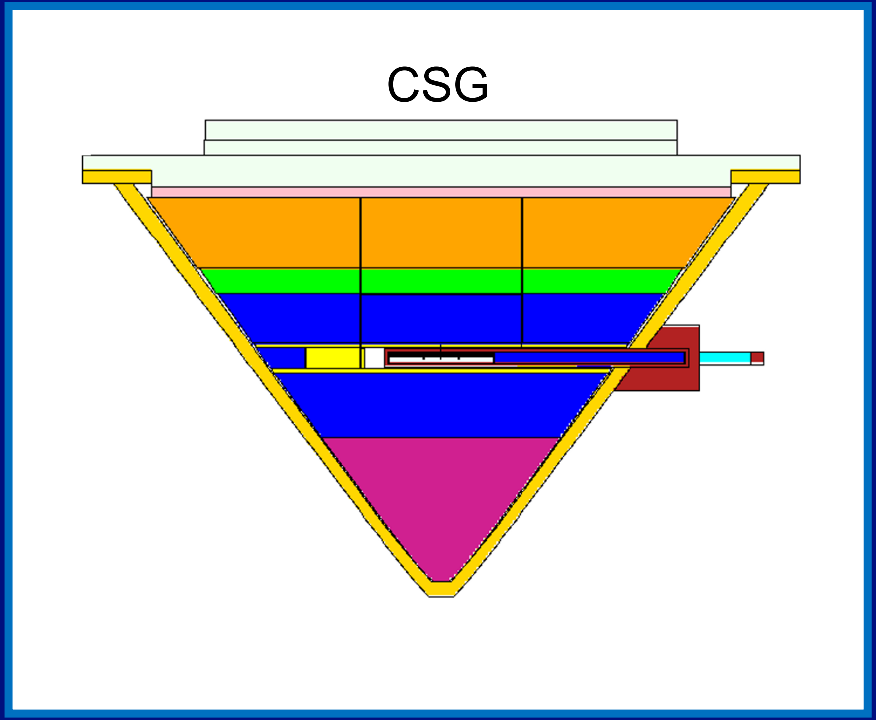
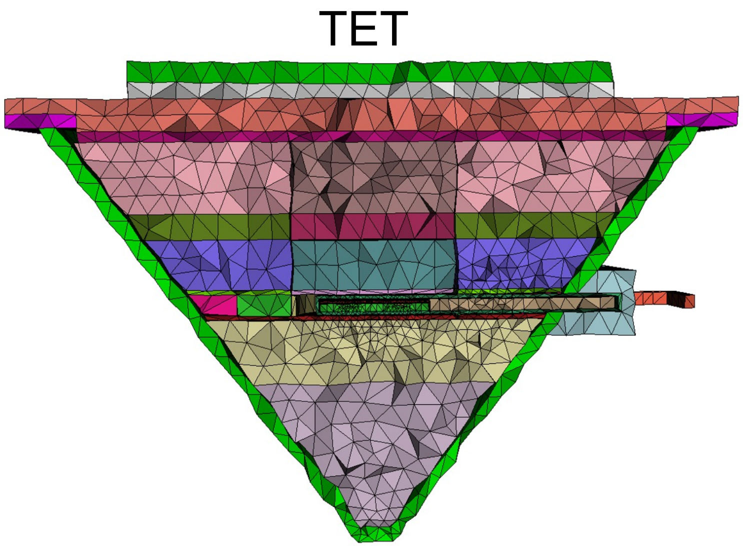
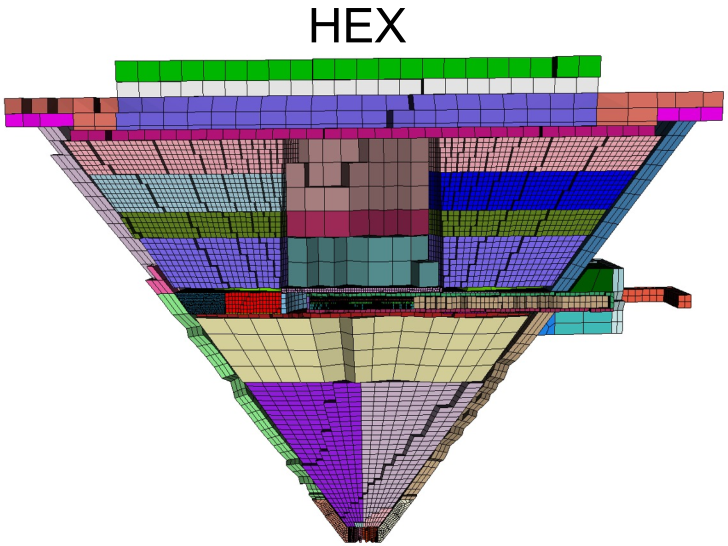


Figure 15.Athena-I CSG Model



(Contiguous Mesh Through Entire Geometry)

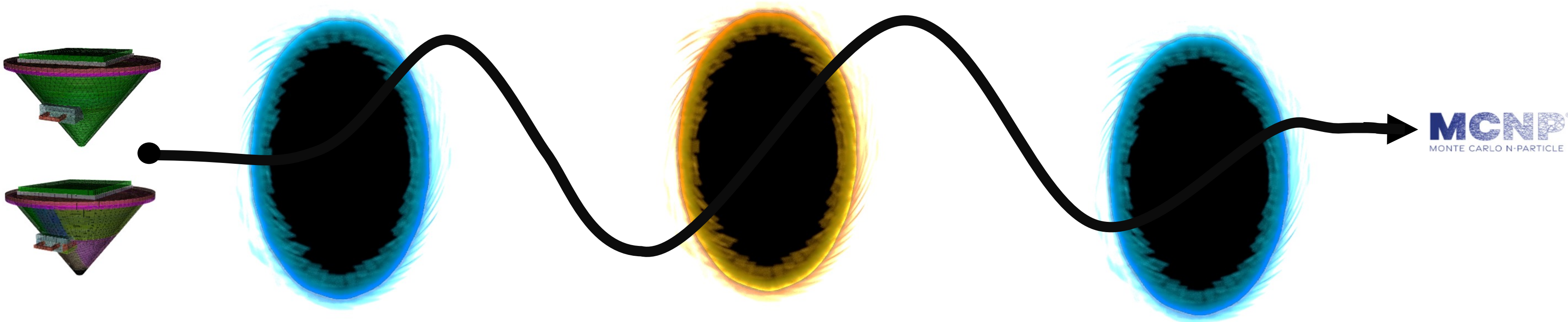
Figure 16. Cross-sectional View of Tet mesh in CUBIT



(Contiguous Mesh in Each Part)

Figure 17. Cross-sectional View of Hex mesh in CUBIT

Generating Abaqus and MCNP Input Files



Export to Abaqus
Instance blocks in 3D

Convert Abaqus for MCNP
Python Tool:
cubit_to_mcnp.py [4]

Generate MCNP input
Python Tool:
write_mcnp_um_input.py [5]

CUBIT journal files of Athena-I were released to public [6].

Athena-I Modeling with MCNP6.3

Athena-I Calculations with MCNP6.3

- Create equivalent MCNP CSG and UM input files
  - UM models are hybrid, only Athena-I body are meshed
- Use ENDF/B 8.0 nuclear data
- MODE N P
- NPS = 1E8
- PRDMP 1E8 1e8 1 1
  - Generate MCTAL file
- Do not use force collisions
- Use WWG (weight window generator) to generate weight window parameters
  - Cell-based weight windows
  - Generate weight window parameters for CSG, Tet, and Hex models

- All runs are on snow (LANL's HPC machine) using 1 node with 36 tasks
- Weight windows improve efficiencies for neutrons, but not for photons
- CSG weight window parameters are not useful for Tet and Hex models
- CSG, Tet, and Hex results are comparable.

MCN6.3 Results of CSG Model

No Weight Window

Wall-clock Time = **00:50:19**

Tally	Fluence [#/cm^2]	Rel. Error	FOM
14	3.2116E-04	0.0024	106
194	3.3231E-04	0.0078	9.8
204	9.7235E-05	0.0179	1.9

WWG 14 10
WWP:N 4 j 3 -1 0

WWG 204 10
WWP:P 5 j 100 -1 0

- Cannot use WWG to generate "good" weight window parameters
- Photon tally results are not reliable, and weight windows are not useful for photons

Weight Window: neutron

Wall-clock Time = **00:04:58**

Tally	Fluence [#/cm^2]	Rel. Error	FOM
14	3.2440E-04	0.0071	117
194	3.3536E-04	0.0101	57
204	9.3761E-05	0.0222	12

Weight Window: neutron, photon

Wall-clock Time = **00:03:11**

Tally	Fluence [#/cm^2]	Rel. Error	FOM
14	3.1934E-04	0.0030	1080
194	3.2332E-04	0.0083	137
204	1.0048E-04	0.0283	12

Tallies
14: Neutron Fluence for Entire Foil Pack
194: TLD Neutron Fluence
204: TLD Photon Fluence

MCN6.3 Results of Tet Model

No Weight Window

Wall-clock Time = **01:02:18**

Tally	Fluence [#/cm²]	Rel. Error	FOM
14	3.2171E-04	0.0024	84
194	3.2873E-04	0.0079	7.6
204	9.7371E-05	0.0179	1.5

CSG Weight Window

Wall-clock Time = **01:46:47**

Tally	Fluence [#/cm²]	Rel. Error	FOM
14	3.1931E-04	0.0020	80
194	3.2101E-04	0.0058	9.4
204	1.0306E-04	0.0498	1.3

WWG 14 10
WWP:N 4 j 3 -1 0

- CSG weight window parameters are not effective for a Tet model
- Tet weight window parameters generated by WWG improve computational efficiency for neutrons.

Tet Weight Window: neutron

Wall-clock Time = **00:12:40**

Tally	Fluence [#/cm²]	Rel. Error	FOM
14	3.2227E-04	0.0034	164
194	3.2405E-04	0.0089	34
204	9.6798E-05	0.0222	5.4

Tallies
14: Neutron Fluence for Entire Foil Pack
194: TLD Neutron Fluence
204: TLD Photon Fluence

MCN6.3 Results of Hex Model

No Weight Window

Wall-clock Time = **01:01:28**

Tally	Fluence [#/cm²]	Rel. Error	FOM
14	3.1650E-04	0.0024	87
194	3.0320E-04	0.0079	7.7
204	8.9832E-05	0.0178	1.5

CSG Weight Window

Wall-clock Time = **01:32:29**

Tally	Fluence [#/cm²]	Rel. Error	FOM
14	3.1449E-04	0.0028	55
194	3.0260E-04	0.0070	8.7
204	8.2388E-05	0.0536	1.4

WWG 14 10
WWP:N 4 j 3 -1 0

- CSG weight window parameters are not effective for a Hex model
- Hex weight window parameters improve computational efficiency for neutrons

Hex Weight Window: neutron

Wall-clock Time = **00:12:26**

Tally	Fluence [#/cm²]	Rel. Error	FOM
14	3.1436E-04	0.0031	304
194	2.9828E-04	0.0088	37
204	8.8497E-05	0.0226	5.6

Tallies
14: Neutron Fluence for Entire Foil Pack
194: TLD Neutron Fluence
204: TLD Photon Fluence

Computing Times

Model	Number of Elements	Computing Time	
		no weight windows	weight windows
CSG	N/A	00:50:19	00:04:58
Tet	165,089	01:02:18	00:12:40
Hex	1,107,965	01:01:28	00:12:26

A tracking algorithm for hex models was improved in MCNP6.3. The hex model is significantly larger than the tet model, but the computing times are not significantly different.

MCNP Total Neutron Fluence Results

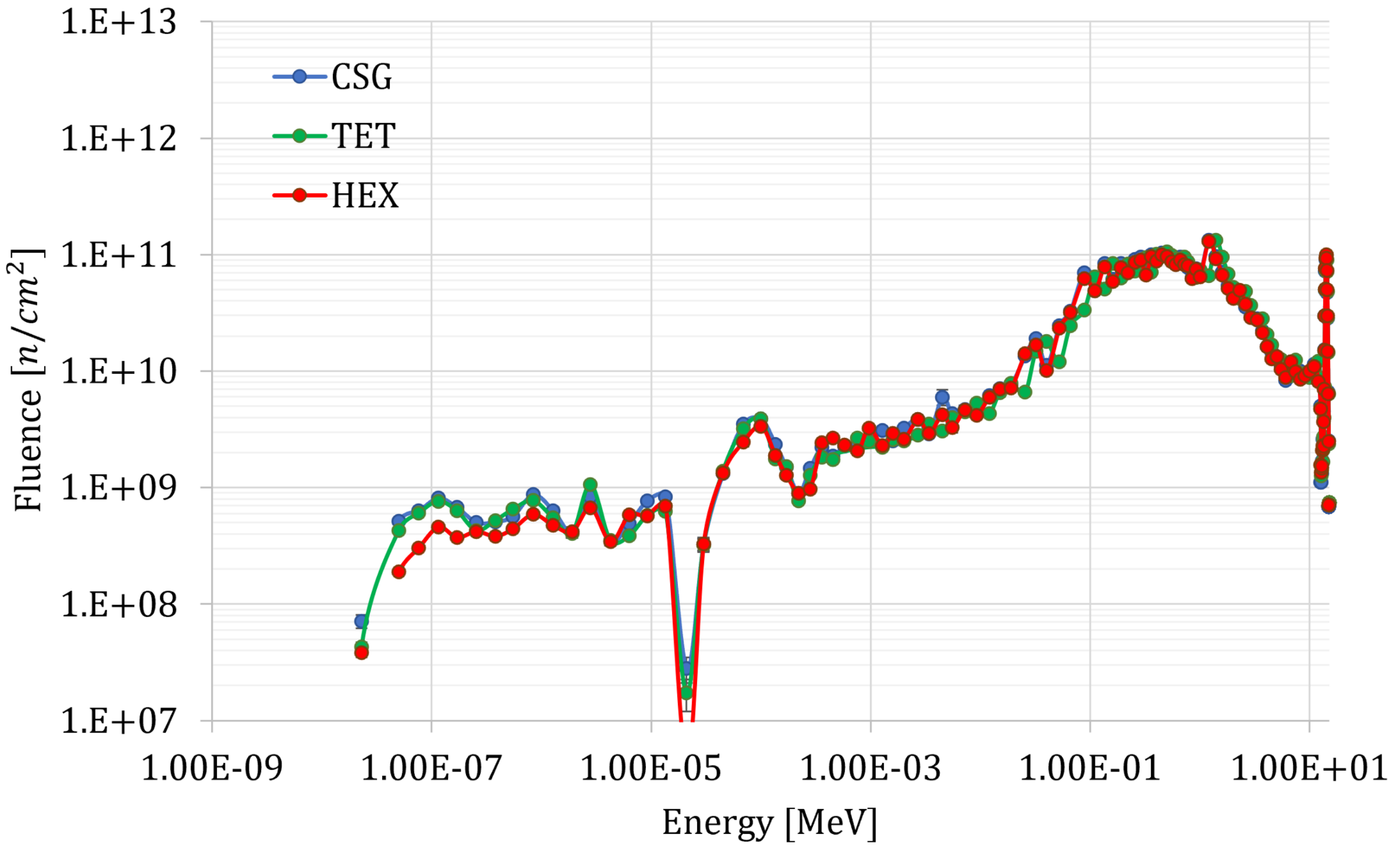


Figure 18. Total Neutron Fluence in Internal Drawer for CSG and UM Model Results from MCNP. Gamma fluence is not included because the experimental and calculation results were not reliable.

Conclusions and Future Work

- **Conclusions:**
  - Created Tet and Hex models of Athena-I in CUBIT
  - Made equivalent CSG and UM input files for MCNP6.3
  - Applied WWG to generate weight window parameters for CSG, Tet, and Hex calculations.
    - CSG weight window parameters are not effective for Tet and Hex models
    - For CSG, Tet, and Hex models, weight windows improve computational efficiencies for neutron tallies but not for photon tallies

- **Future work:**
  - Neutron, photon, and electron transport calculations (MODE N P E)
  - Investigate other variance reductions to improve efficiencies for photon tallies

Acknowledgement: We would like to thank Darren Holland (Air Force Institute of Technology) and Nick Quartemont (Air Force Nuclear Weapons Center) for providing information on the Athena-I CSG model.

Questions?

References

1. Heshham Khater. “Simulation of Radiation Environment at the NIT”, Lawrence Livermore National Laboratory, LLNL-PRES-840208 (2023)
2. Nicholas Quartemont et al. “ATHENA: A unique radiation environment platform at the National Ignition Facility”. In: Nuclear Instruments and Methods in Physics Research 131 (2021)
3. Nicholas Quartemont. “NIF ATHENA Experiment”, Mendeley Data, V1, doi: 10.17632/bnvh2btjp3.1 (2021)
4. Jerawan Armstrong. “Using CUBIT to Create Unstructured Mesh Models for MCNP Simulations”. Tech. rep. LA-UR-23-21715. Los Alamos, NM, USA: Los Alamos National Laboratory, Feb. 2023
5. Jerawan Armstrong and Karen Kelley. “Generating MCNP Input Files for Unstructured Mesh Geometries”. Tech. rep. LA-UR-23-28515. Los Alamos, NM USA: Los Alamos National Laboratory, Jul. 2023
6. Bradley Gladden et al. “Athena-I CUBIT Journal Files”, Tech. rep. LA-UR-23-28395. Los Alamos NM, USA: Los Alamos National Laboratory, Jul. 2023

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Neutron fluence results are consistent with previously made CSG model
Slightly lower values at around 0.1 MeV than experimental results