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Athena-I CUBIT Journal Files

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1 Introduction

The Monte Carlo N-Particle (MCNP)¹ transport code version 6 (also known as MCNP6) has the capability for tracking particles on unstructured mesh (UM) geometry models embedded into constructive solid geometry (CSG) cells [1]. This feature has been developed for performing calculations of complex geometry models because manually creating CSG models is a time-consuming and error-prone process as the complexities of geometries increase.

The UM capability was originally designed to work with UM models created with the Abaqus software [2] and ASCII input files that it generates. The MCNP code version 6.0 and later can process UM models formatted as Abaqus input files. Starting with version 6.3, MCNP can also process HDF5 mesh input files. External codes must be used to generate Abaqus input files for MCNP UM calculations. CUBIT, the Sandia National Laboratory automated mesh generation toolkit, can generate a UM model formatted as an Abaqus input file [3]. However, the Abaqus input files exported from CUBIT cannot be used for MCNP simulations because it lacks the proper syntax. A Python script was developed to convert an Abaqus file created by CUBIT to an Abaqus file format that MCNP can process [4].

Creating UM models for complex geometries is not an easy task. The process of creating UM models in CUBIT for MCNP simulations is detailed in [4]. CUBIT provides several user interface options including a graphical user interface (GUI) and a command line interface. A GUI provides an easy way to use CUBIT without learning the CUBIT command syntax. When using CUBIT with either interface option, command lines are written into an ASCII file known as a journal file; this journal file can be edited and archived so that it can be played back in CUBIT to automatically generate a UM model.


This report describes the CUBIT journal files of the UM models developed for Athena-I. The Athena platform, an energy-tuning assembly, was developed to spectrally shape the National Ignition Facility (NIF) deuterium-tritium fusion neutron source to a thermonuclear (fusion) plus prompt fission neutron spectrum with capability to act as a short-pulse neutron source. MCNP6 was used for the Athena experiment design analysis [5]. An MCNP CSG input file of the Athena-I model is publicly available at <https://data.mendeley.com/datasets/bnvh2btjp3/1>. Based on this CSG input file, an Athena-I geometry model is created in CUBIT. This solid geometry is then meshed using two UM types: tetrahedral and hexahedral.

2 Athena Geometry Creation

Based on the MCNP CSG model, two primary methods in CUBIT are used to create Athena-I parts. Using a GUI, the Athena-I parts are built by using (i) geometry primitives (frustum and cylinder) to create shapes that are then modified and combined to create 3D volumes, or (ii) bottom-up geometry creation where vertices, curves, surfaces, and bodies are created to form 3D volumes. When executing CUBIT in a GUI mode, geometry creation commands are written into a journal file that is later edited to add comments and remove unnecessary commands.

Many parts of the Athena-I CUBIT model are built using the geometry primitives of frustum and cylinder commands. However, some parts are created using the bottom-up geometry creation in which vertices are drawn and connected by surfaces that are then lofted into a volume. This is a technique used when the Athena-I CSG file that the model is based on has a geometry defined by vertices, typically when MCNP macrobodies are used to define cells.

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A final version of the CUBIT journal file for creating the Athena-I model is attached . The solid Athena-I model created by this journal file is shown in Figure 1 and used to create the UM tetrahedral and hexahedral models described in Section 3 and 4, respectively.

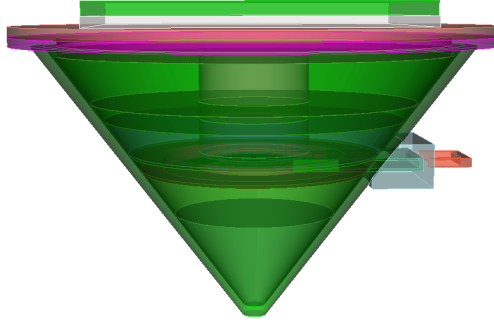

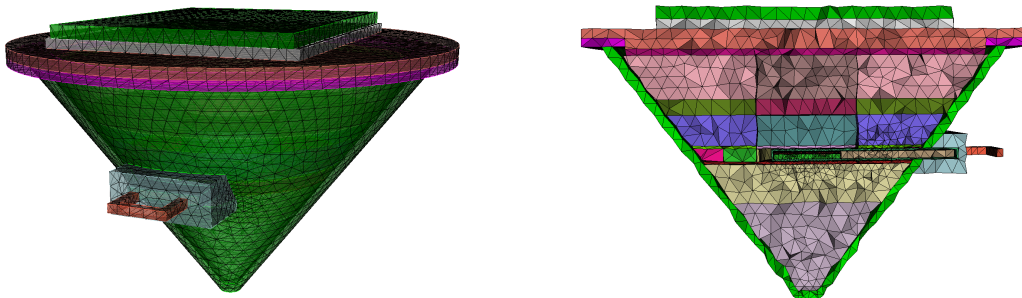


Figure 1. Athena-I Solid Geometry created in CUBIT

3 Athena Linear Tetrahedral Model

A linear tetrahedral element has 3 faces and 4 nodes at the vertices. To prepare the geometry for meshing, all volumes are imprinted and merged. Imprinting geometry is necessary to ensure that touching geometries will have identical mesh patterns. The merge command is then used to merge the touching geometries into one, typically by combining coincident surfaces. The entire model is meshed with tetrahedral elements to create a contiguous mesh between each volume. Although this is not required for the model, the tetrahedral shape easily conforms to complex geometry creating a cohesive mesh pattern. This tetrahedral model has 165,089 elements. The mesh can also be refined in volumes of interest, such as the foils and thermoluminescent detectors (TLDs), where the tallies are calculated in MCNP. The automatic sizing of the tetrahedral mesh in CUBIT for this model creates a fine enough mesh in these locations for the volume difference between the geometry and the mesh to remain within 3%, which is typically sufficient for the UM analysis in MCNP. A sample

CUBIT Python script used to check volumes is attached .




(a) Isometric view of Athena-I Tetrahedral Mesh (b) Cross-sectional view of Athena-I Tetrahedral Mesh

Figure 2. Athena-I Tetrahedral Mesh

Mesh generation is typically an iterative process. If a mesh quality is not good enough, a mesh may be deleted and a different technique should be used. Several mesh quality metrics are available in CUBIT, but currently it is unknown if these quality metrics are applicable to mesh models for MCNP UM simulations. The solid and meshed volumes should agree as much as possible ($\leq 3\%$). The Jacobian should be positive, as elemental volumes and Jacobian are used by the MCNP UM tracking methods. Thus we ensure that the Athena-I UM tetrahedral and hexahedral models pass the volume and Jacobian metrics. After a mesh has passed quality metrics, the next steps in CUBIT include (i) creating materials, (ii) creating blocks and assigning materials to the blocks, and (iii) exporting a UM model as an Abaqus input file. This Abaqus input is later processed by

the `cubit_to_mcnp.py` script [4] to convert to an Abaqus input file that MCNP can interpret. The Athena-I tetrahedral model is shown in Figure 2.

A CUBIT journal file of the Athena-I linear tetrahedral model is attached . Note that CUBIT version 16.10 and earlier generates a different Abaqus input file for each run when using the same CUBIT journal file, but this CUBIT issue was fixed in version 16.12.

4 Athena Linear Hexahedral Model

A linear hexahedral element has 6 faces and 8 nodes at the vertices. The hexahedral model is generated from the same 3D solid geometry as the tetrahedral model. However, when imprinting and merging all volumes, the drawer case is left unmerged due to the intricate shape affecting the mesh on neighbouring volumes. MCNP requires that the mesh is contiguous within each part, but the connectivity is not required between parts.

While hexahedral meshing can typically save computing time in MCNP due to the more robust tracking methods for hexahedral shapes, the process of developing and fitting a mesh is more extensive than for tetrahedral meshing. Parts that are not immediately meshable require geometrical alterations to mesh. For the Athena-I hexahedral mesh, several volumes with small surfaces including the drawer screws, viton seal, the cover bottom and adapter offset, and multiple inner components are altered to extend an acceptable connecting surface to include the small and unmeshable surfaces. Volumes with complex shapes such as the cover top, drawer case, and drawer handle mount are created by uniting multiple geometries together into one volume. These parts require a sweep surface modification to create surfaces that are acceptable to mesh together. Most of the Athena-I parts aside from the foils and TLDs require at least one webcut to break the intricate volumes into multiple simpler meshable ones. The foils and TLDs, where the tally measurements occur, are small enough and made of simple enough geometry to generally be meshable without modification. The mesh is set to be finer in these parts to achieve a mesh with good enough qualities.

The most complex part to prepare is the outside cone shown in Figure 3. The cone has complications in it, being hollow and containing a hole for the drawer insert. This is solved by webcutting the cone into several volumes, including cutting out the hole and creating smaller volumes at the tip of the part to accommodate the slope. This creates a part that is able to be meshed cohesively, with a finer mesh on the smaller pieces to ensure the mesh qualities are acceptable.

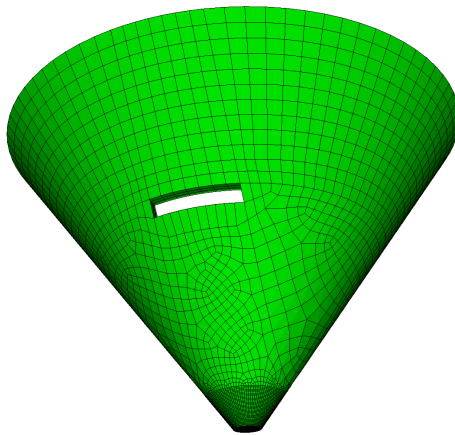



Figure 3. Outer cone of Athena-I Hexahedral Mesh

In all cases of geometry manipulations, the resulting volumes are imprinted and merged to maintain them as one connected part. Smaller volumes and those where the fluence is of particular interest (foils and TLDs) are meshed to a finer resolution. The hexahedral model has 1,107,965 elements, which is significantly larger than the tetrahedral model. This is likely due to the conical shape of the Athena-I geometry being a better fit for a tetrahedral shape in CUBIT since only one mesh shape is used at a time. Other methods and software may be used to create mixed element types (i.e., hexahedral and pentahedral shapes). The hexahedral mesh in this case is also finer, which is necessary to create a quality mesh and ensure the volume difference between the geometry and mesh are within 3%. As with the tetrahedral model, the attached CUBIT Python script is used to check these volumes.

A CUBIT journal file of Athena-I linear hexahedral model is attached . This journal file is commented with the part and cell names where each geometry is modified to prepare for meshing. After the mesh is generated, the next CUBIT commands are to create materials, create blocks that correspond with the Athena-I parts, and assign MCNP material numbers to the blocks. The UM model is exported from CUBIT as an Abaqus input file, which is later processed by the `cubit_to_mcnp.py` script to convert the file to one that MCNP can read [4]. The Athena-I hexahedral mesh is shown in Figure 4.

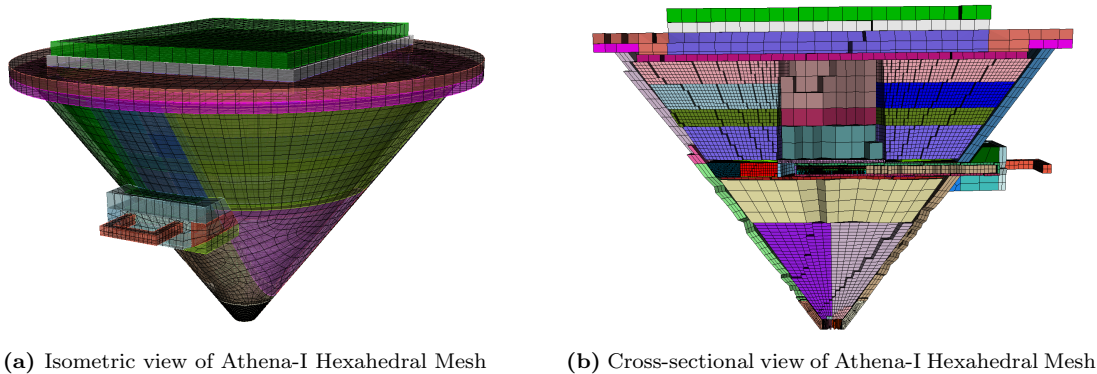


Figure 4. Athena-I Hexahedral Mesh

5 Conclusions and Future Work

CUBIT is used to create the Athena-I solid geometry and generate a tetrahedral and hexahedral mesh. The tetrahedral mesh model is easier to create than the hexahedral mesh model, as minimal geometry preparation is required for tetrahedral meshing, while hexahedral meshing requires more geometrical preparation in order to mesh. Meshing is an iterative process, including quality checks, to ensure MCNP can properly transport particles within the mesh universe. Only two mesh quality metrics (volumes and Jacobian) are considered when meshing the tetrahedral and hexahedral Athena-I model. After a suitable mesh is obtained, the process of creating an Abaqus model for MCNP UM simulations includes creating materials, grouping volumes into blocks to define each cell from the CSG MCNP input as a block as well as to assign a corresponding material number. This is necessary to create a UM MCNP input file that is directly comparable to the CSG input in MCNP. Finally, the tetrahedral and hexahedral models are exported as Abaqus files and converted to a readable Abaqus format for use in MCNP UM calculations. The CUBIT commands used to create these two models are placed in the ASCII files known as journal files which are attached in this report. In future work, the models can be recreated in CUBIT 16.12, which will allow the user to export CUBIT files directly to a readable Abaqus format in MCNP. Additionally, the meshing capabilities on the Athena-I model can be further explored by generating second-order tetrahedral and hexahedral meshes.

Acknowledgment

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References

- [1] Joel A. Kulesza et al. *MCNP[®] Code Version 6.3.0 Theory & User Manual*. Tech. rep. LA-UR-22-30006, Rev. 1. Los Alamos, NM, USA: Los Alamos National Laboratory, Sept. 2022. URL: <https://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-22-30006>.

- [2] Dassault Systemes. *Abaqus/CAE - finite element analysis software*. <https://www.3ds.com/products-services/simulia/products/abaqus/abaquscae/>.
- [3] Sandia National Laboratories. *CUBIT - geometry and mesh generation toolkit*. <https://cubit.sandia.gov>.
- [4] Jerawan C. 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. URL: <https://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-23-21715>.
- [5] 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). URL: <https://doi.org/10.1016/j.nima.2021.165777>.