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Title: Introduction to MCNP6's Unstructured Mesh Capability (U)

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Intended for: The 18th Topical Meeting of the Radiation Protection & Shielding Division of ANS, Knoxville, TN

Los Alamos NATIONAL LABORATORY EST. 1943

LA-UR-14-25120

Introduction to MCNP6's Unstructured Mesh Capability

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For

RPSD 2014
Knoxville, TN

Hybrid Geometry

Abstract

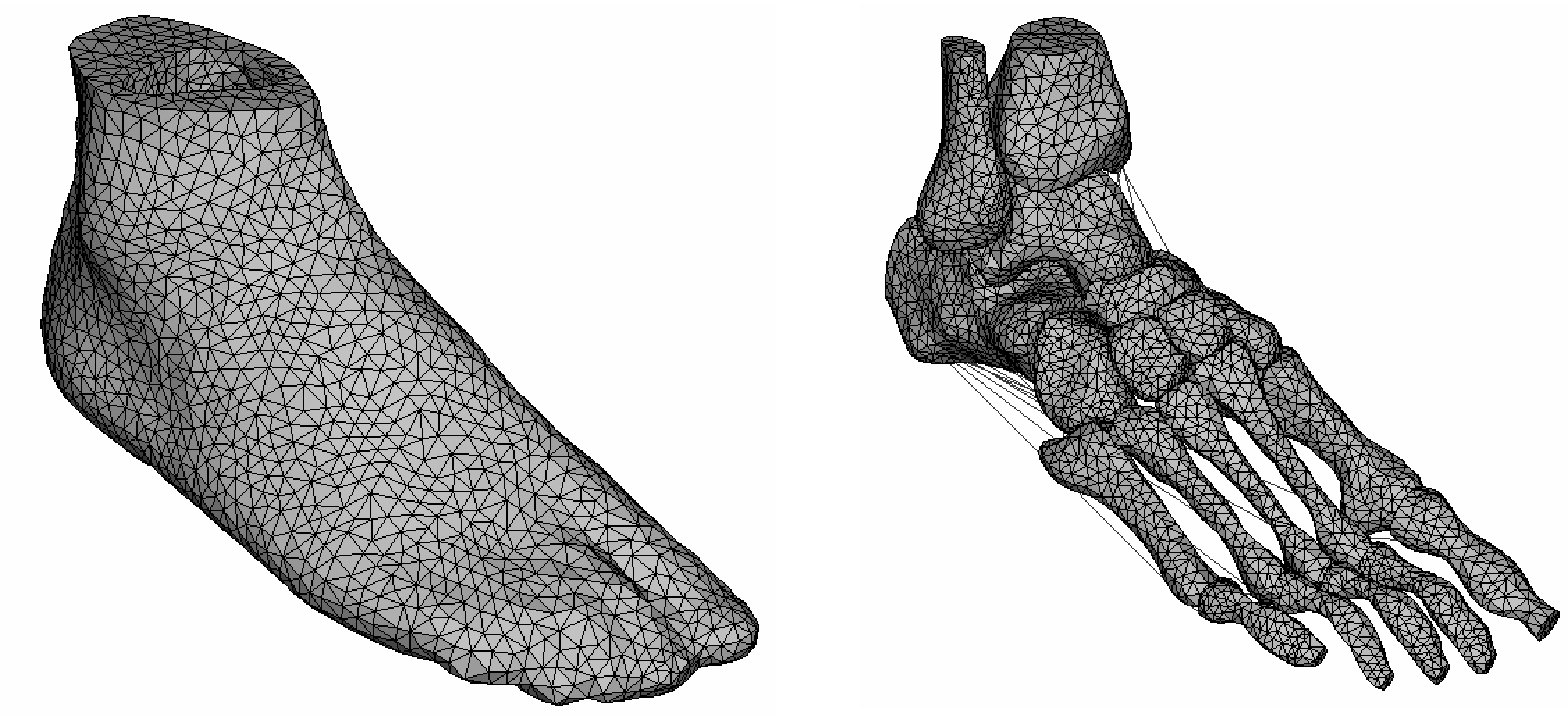
The presentation is intended to introduce MCNP users to the unstructured mesh capability by discussing basic concepts. A broad overview is presented along with relevant input and output features. Some performance results from two simple benchmark problems are presented.

Hybrid Geometry

What is the MCNP Unstructured Mesh (UM) Capability?

It is part of the new hybrid geometry capability that lets MCNP users embed "other" geometry representations of their geometry (e.g., unstructured and structured mesh) in the "legacy" constructive solid geometry (CSG) so that all representations of the geometry work together seamlessly.

How does an unstructured mesh affect modeling?

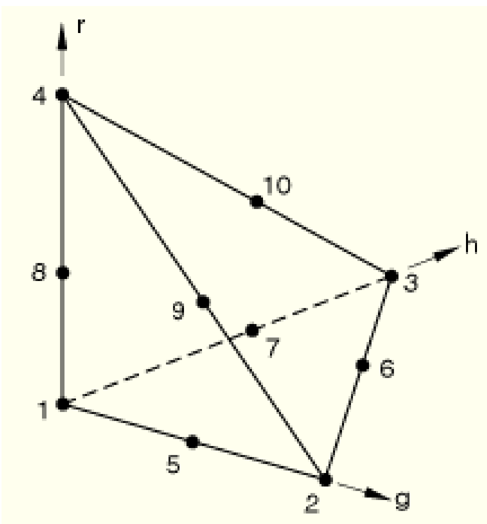


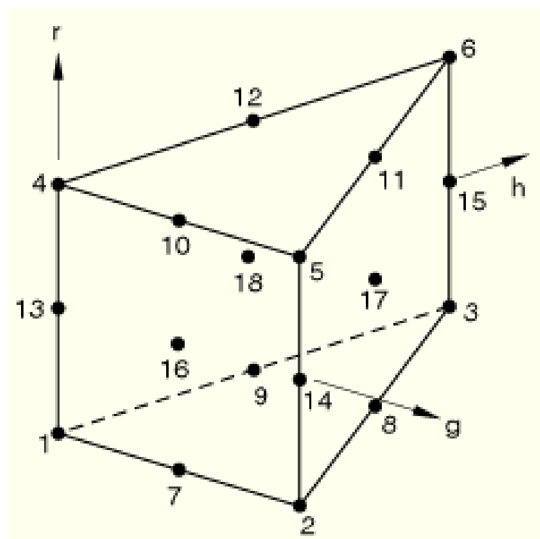
Jason Tak-Man Cheung and Ming Zhang, "Finite Element Modeling of the Human Foot and Footwear," 2006 ABAQUS Users' Conference.

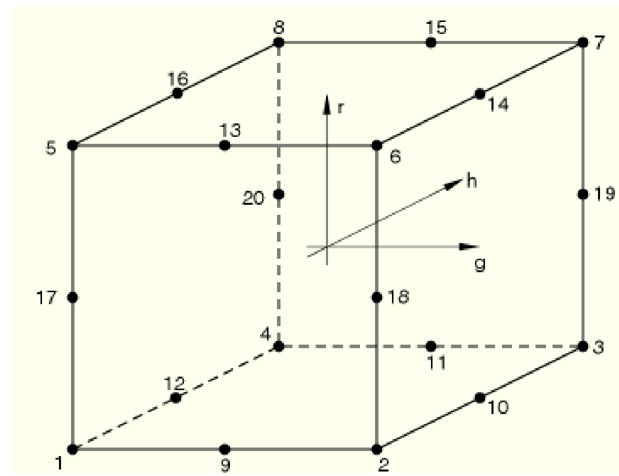
Objects and Definitions: elements or finite elements

The smallest building blocks

- **Unstructured polyhedrons with 4-, 5-, and 6-sides or faces generated by a meshing program. Surfaces may be bilinear or quadratic depending on the number of nodes.**







1st order – vertex nodes only; 2nd order – vertex + edge nodes

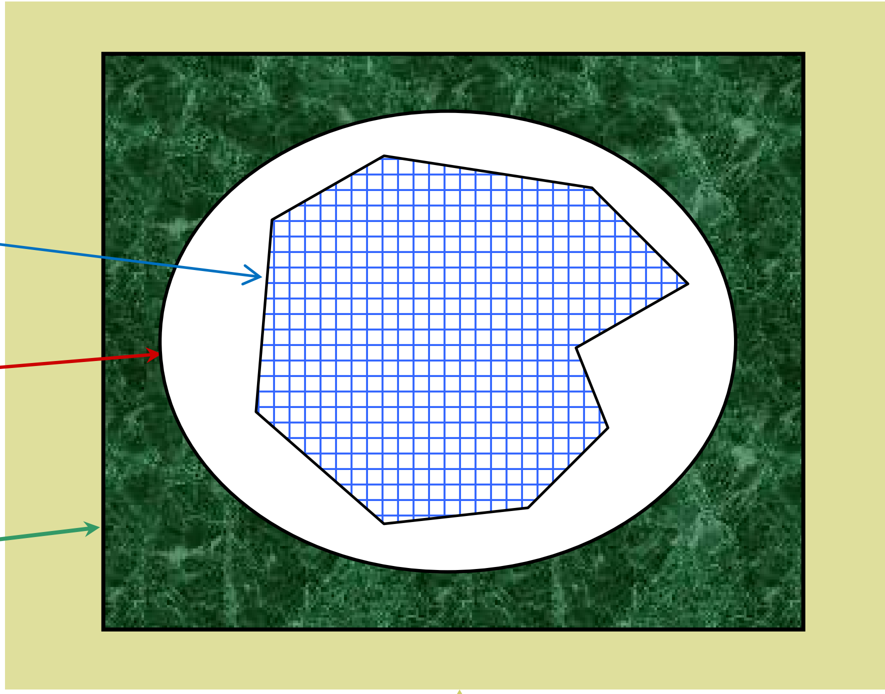
A Simple Hybrid Arrangement

Mesh universe with elliptical background cell and mesh

Unstructured or structured mesh (imp=1)

Background cell (csg filling cell; imp=1)

Legacy CSG cell (imp=1)



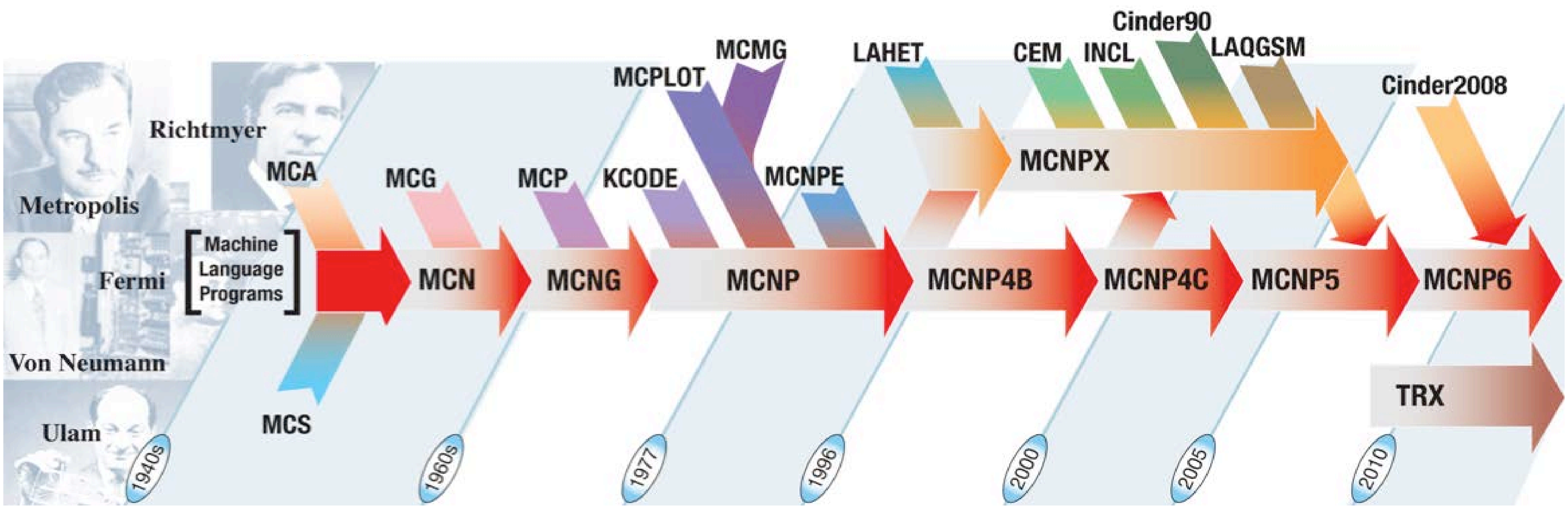
CSG outside world cell (imp=0)

Why use UM?

1) **Easier to create complex 3-D models with a state-of-the-art CAD/CAE tool.**
2) **Better geometry and results visualization.**
3) **Easier multi-physics integration with other mesh-based physics codes.**
4) **Better calculational performance for certain problems.**
5) **It's cool!**

A Brief History

- **MCNP has existed as MCNP since the mid-1970's.**
  - Initial geometry capability was Constructive Solid Geometry (CSG)
  - Macrobody capability was added (1980's) where the macrobody surfaces were translated into CSG surfaces.



A Brief History

- **Unstructured mesh (UM) development started in 2006**
  - Requested by LANL engineering community who standardized on Abaqus.
  - Any "code" that can write an Abaqus formatted input file with the appropriately named element sets can generate a viable mesh geometry for MCNP's use.
- **UM has been in MCNP6 since the 1st beta release.**
  - Each subsequent release has added more UM features and fixed any associated bugs.

Objects and Definitions

Paradigm Shift

- **Must recognize that this capability "marries" different "technologies".**
- **Each of these "technologies" was developed independently giving rise to terminology that one could consider unsettling because it is either new, different, conflicting, strange, weird, etc.**
  - Example: MCNP uses the concept of "cell" as the basic CSG building block. Abaqus uses the concept of "cell" when it refers to a 3-D region; a part may be a single cell or segmented into multiple cells.
- **One of the key concepts that was created to help the UM integrate with the MCNP world is the pseudo-cell; these are defined later. In a nutshell, this is a mechanism to let a <u>collection</u> of mesh elements have MCNP <u>cell-like</u> properties (e.g., IMP's) so that existing features are readily useable with the mesh.**

Objects and Definitions

- **The following slides will attempt to define some terminology as it relates to objects associated with the unstructured mesh capability.**
- **NOTE: Some of the terminology may seem “different” from what you are accustomed. This arises because of the way the CAE / finite element users in the structural mechanics world have defined things. Their definitions are used where appropriate.**

Objects and Definitions: mesh

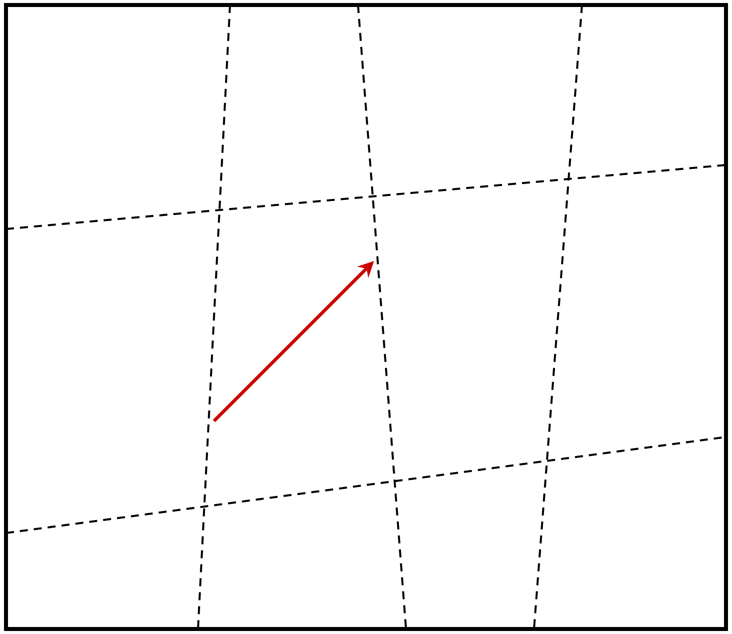
The collection of elements comprising the entire (meshed) model.

NOTE: There is a distinction between the solid model and the mesh model.

Think of the mesh as a representation of the solid model.

Element-to-Element Tracking

- **Tracking is from face-to-face of the element (barring a collision event or any other event that MCNP checks such as distance to dxtran surface).**
- **Path length results are collected for each element through which the particle travels.**
  - Therefore, collecting results such as flux (by element) adds very little overhead to the calculation.



12-element part

Objects and Definitions: edits

- **With element-to-element tracking on the unstructured mesh, results can be accumulated on each finite element through which particles pass.**
  - This is basically free.
- **Results on the unstructured mesh are referred to as "edits" or "elemental edits" to distinguish them from the tally results in the CSG.**
  - Results go to a special output file (eeout)
- **Edits are not intended to reproduce all of the tally functionality, such as**
  - Tally types F1, F2, F5
  - Statistical analysis, statistical checks, TFC's, empirical history score pdf, etc. (If these features are needed, use the appropriate statistical elset so that these things can be used with a collection of elements. See the discussion on statistical elsets below.)

Objects and Definitions: elsets

- **A collection of elements or a sub-set of the mesh associated with a specific tag, label, or name.**
  - Does not need to be contiguous.
  - Helps define the pseudo-cells.

Objects and Definitions: part

- **The smallest geometric object created in the CAD/CAE tool.**
  - Can contain a mesh representation
    - When created in Abaqus
  - Can be assigned attributes such as material #'s and density
  - Can be segmented into smaller pieces; these pieces are referred to as cells; if the part is not segmented then it is also a cell
    - When created in Abaqus

Objects and Definitions: instance

- **A copy of a part used when constructing an assembly**
- **1 part may be used many times**

Objects and Definitions: assembly

- **The largest geometric object created in the CAD/CAE tool**
  - Constructed from instances of parts
  - A composite object
  - The final mesh model from which MCNP creates its global mesh model
- **The Attila4MC mesher meshes the assembly**

Objects and Definitions: pseudo-cell

- An elset that has been mapped to an MCNP cell.
- This is a mechanism to let a collection of mesh elements have MCNP cell-like properties (e.g., IMP's) so that existing features are readily useable with the mesh.
- In essence, a group of elements (elset) has cell-like properties, but is not a traditional MCNP cell.

Pseudo: in scientific use, denoting close or deceptive resemblance to

Objects and Definitions: background cell

- A cell that serves as the background (or container or holding) cell for the mesh.
- An MCNP cell into which the mesh has been placed and basically is the csg cell that is “filled” into the universe.

Objects and Definitions: mesh universe

- **An MCNP universe comprised of the mesh and the background cell.**
  - May not contain any other lower universes

MCNP UM I/O

Embedded Mesh Universe

- **Geometry mesh is embedded as the lowest level universe.**
  - No universe can be placed within it.
- **Cell card requirements:**
  - One cell card for each mesh “pseudo-cell”.
    - Check the mcnp “outp” file for a table showing how the code expects the “pseudo-cells” to match with the mesh regions. Correct material names in this table are dependent upon the material rules cited above.
  - There must be a cell card that serves as a “background” for the embedded mesh. Think of this as the cell that substitutes or stands-in for the mesh. Another way of stating this is that this cell is the smallest cell into which the mesh can fit. (See next slide for examples.) This can be considered the background material in which the mesh resides and is essential for the unstructured mesh to work correctly. This cell must also have a “u” descriptor. See the “background” key word on the embed card.

Embedded Mesh Universe: Cell Cards

- **Cell card requirements:**
  - There can be no cells outside of the background cell in the embedded mesh universe; put CSG cells outside the universe in order to build the remainder of the hybrid geometry.
  - The background cell and pseudo-cell descriptions appear as normal MCNP cell descriptions except they must contain a null surface; enter a zero (0) for the null surface description.

- **Example:**

```
c    *** Cell cards ***
c
     10     2  -7.8240   0              u=2   $ pseudo-cell
     11     1  -1.2230   0              u=2   $ pseudo-cell
     12     2  -7.8240   0              u=2   $ pseudo-cell
     13     3  -0.0012   0              u=2   $ pseudo-cell
     14     0            0              u=2   $ background cell
     20     0          -10     fill=2         $ fill the mesh universe
      6     0       10 -11
      7     0           11
```

MCNP Output: Pseudo-Cell Cross Reference Table

Lists for each pseudo-cell that it knows about,

- **The corresponding MCNP cell number**
- **The instance number**
  - This is the same as the pseudo-cell number as long as there aren't any partitioned parts where partitions have different material or statistic elset numbers
- **The part number**
- **The material number**
- **The material name**

```
***********************************************************************************************
* Pseudo-Cell Cross Reference Table                                                           *
***********************************************************************************************
  Pseudo-Cell #    MCNP6 Cell #    Instance #    Part #    Material #    Material Name
  -------------    ------------    ----------    ------    ----------    -------------
              1              11             1         2             2    material-cube_02
              2              12             2         3            10    material-source_10
              3              13             3         1             1    material-cube__01
***********************************************************************************************
```

Embedded Mesh Data Cards: Geometry

Embedded Mesh Control Card

```
EMBEDn  meshgeo=  mgeoin=  meeout=  meein= length=
        background=  matcell=  filetype=  gmvfile=
        overlap=
```

`n`	embedded mesh universe number n, must match a valid universe # from cell cards
`meshgeo`	mesh geometry type Current permitted values: abaqus, lnk3dnt
`mgeoin`	mesh geometry input file name
`meeout`	elemental edits output file name
`meein`	elemental edits input file name (valid only in continuation runs)

NOTE: all filenames must be lowercase

Embedded Mesh Data Cards: Geometry

Embedded Mesh Control Card (cont.)

```
EMBEDn  meshgeo=  mgeoin=  meeout=  meein=   length=
        background=  matcell=  filetype=  gmvfile=
        overlap=
```

`length`	conversion factor to centimeters for all mesh dimensions in input and output
`background`	cell number of the background cell for the mesh
`matcell`	pairs of numbers: 1st number = mesh material number (actually, the mesh pseudo-cell) 2nd number = MCNP cell number (i.e., the pseudo-cell #)

Embedded Mesh Data Cards: Edits

Elemental Edits Control Card

`EMBEEn:<pl>   embed=   energy=   time=`

`n`	**elemental edit number ending in 4, 6, or 7; follows tally convention; indep. of tally #'s**
`<pl>`	**particle designator from particle list**
`embed`	**embedded mesh universe number; must correspond to a valid embed card #**
`energy`	**conversion factor from MeV/gm for all energy related output**
`time`	**conversion factor from shakes for all time related output**
`errors`	**statistical uncertainties: no (default); yes**

Embedded Mesh Data Cards: Edit Modifiers

- **`EMBEB` – energy bin break points**
- **`EMBEM` – energy bin multipliers**
- **`EMBTB` – time bin break points**
- **`EMBTM` – time bin multipliers**
- **`EMBEM` – energy bin multipliers**
- **`EMBDE` / `EMBDF` – dose energy flux conversion factors**

Embedded Mesh Data Cards: Volume Source

Volume Source Sampling

- **A source elset or elsets are defined via Attila4MC.**
- **An element is selected proportional to the total source volume. That is, proportional to its volume divided by the total mesh source volume.**
- **A position is selected by rejection uniformly in the element’s volume.**
- **No longer need to use cookie-cutter cells. Model the phase-space of the volume source exactly.**

Another Example

ITER Demonstration Calculation

ITER model (20 degree section used for detailed analysis of diagnostic ports) calculation with MCNP6 Version 1.0

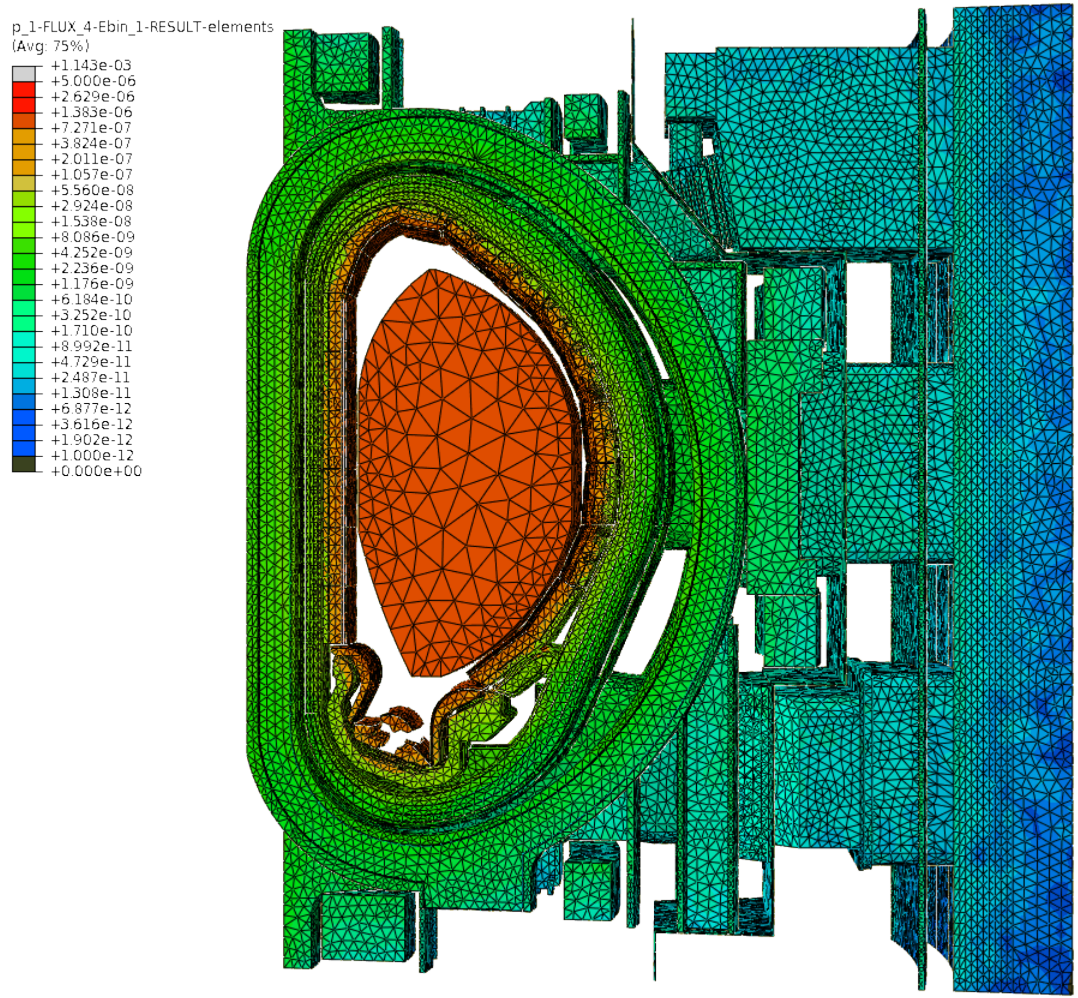
14.1 MeV mono-energetic neutron source using mesh volume source methodology.

Void region mesh removed to aid calculation performance and memory requirements (~4.5 GB/cpu).

2,073,968 1st order tets in 309 cells

Reflecting boundary conditions

100 million histories run with 55 slave nodes. ~7.5 minutes setup time using parallel input processing.
~ 6.25 hours wall clock time with Intel Xeon E5-2670 chips @ 2.6 GHz running 64-bit Chaos Linux.



Total neutron flux

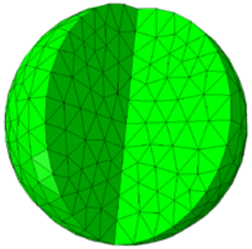
Performance

Performance

Direct Comparison

The following slides show a comparison between CSG and UM for the Godiva and Osaka benchmarks where

- **The models use only 1st order tets.**
- **Each tet in the UM is modeled exactly using combinations of arb surfaces in CSG.**
  - 1-to-1 comparison between a CSG cell and an UM element.

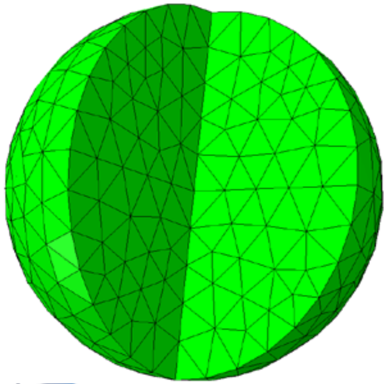


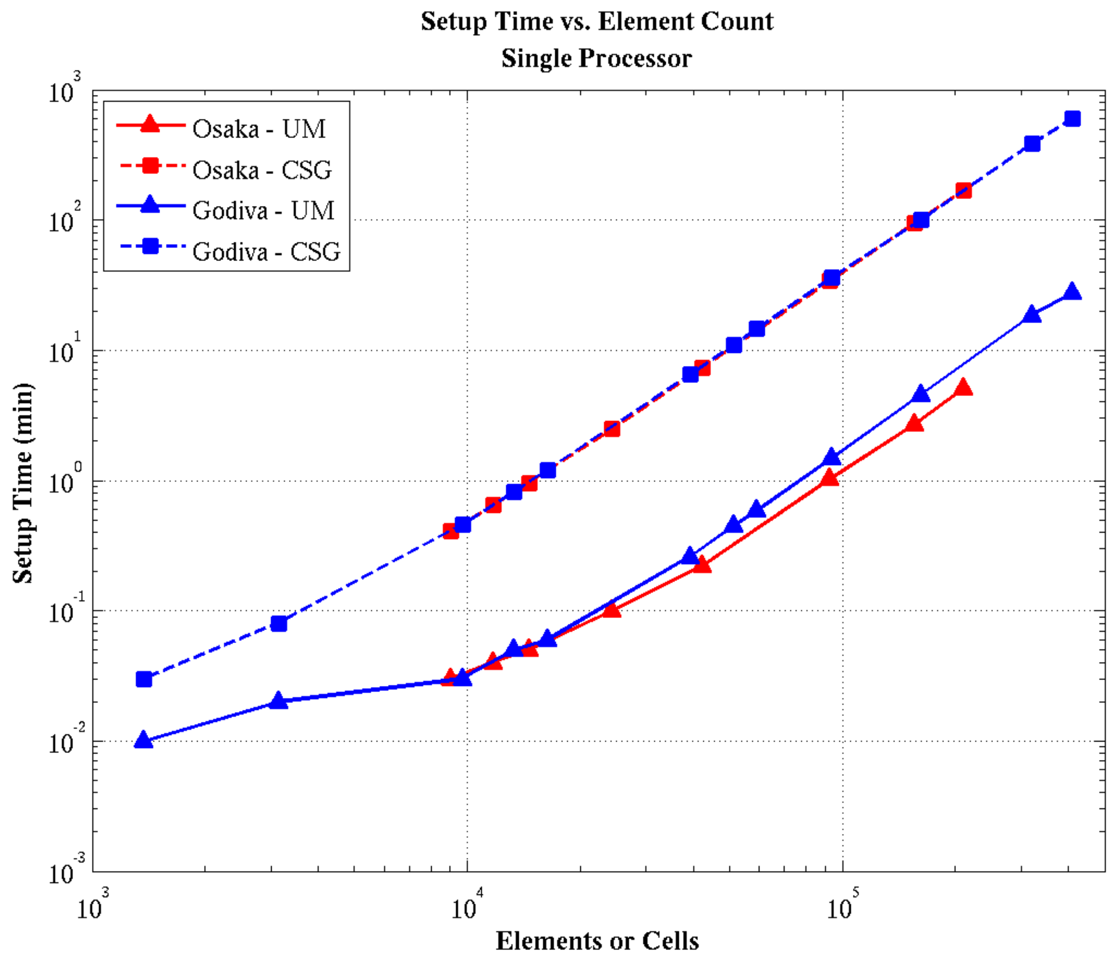
- **The total number of histories were chosen so that the most detailed models could be run in a reasonable amount of time with 1 processor.**
- **See: Roger L. Martz and Kevin M. Marshall, "A Notable Comparison of Computational Geometries in MCNP6 Calculations," Nuclear Technology, 184 (Nov 2013).**

MCNP6 Unstructured Mesh Performance Comparison

Problem setup time for large element/cell counts is ~40 times faster with unstructured mesh.

There is 1 CSG cell for each mesh element – producing an apples to apples comparison.

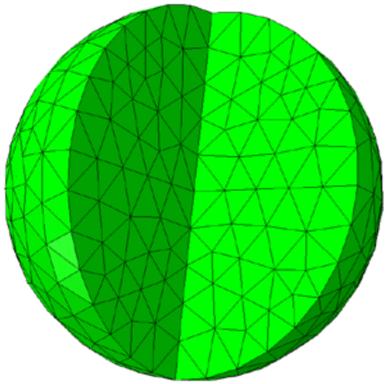


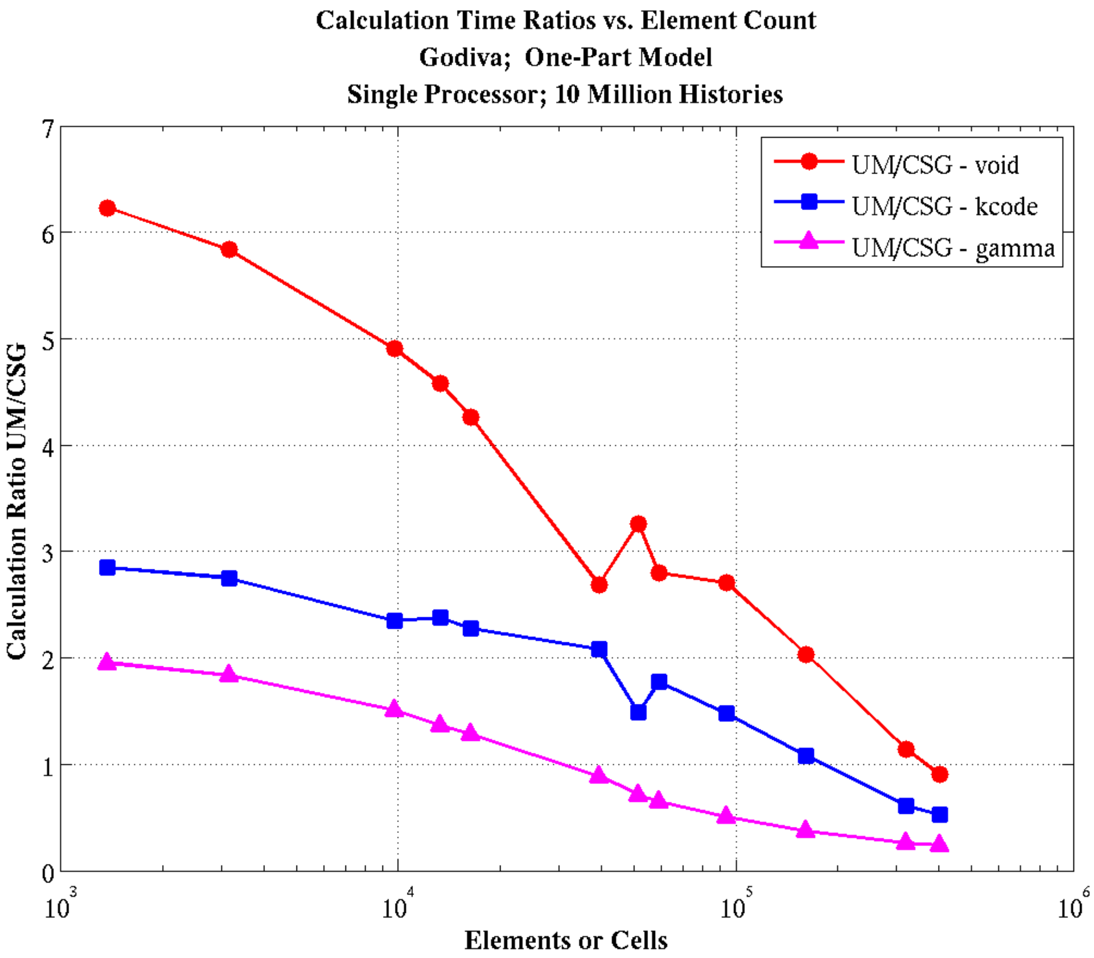


MCNP6 Unstructured Mesh Performance Comparison

As the problem detail increases, unstructured mesh calculation times are shorter.

There is 1 CSG cell for each mesh element – producing an apples to apples comparison.





Expert Advice, Opinion, & Perspective

Expert Advice, Opinion, & Perspective

Mesh & The Monte Carlo Method

The mesh in MCNP is used for 2 basic purposes:

1. **Define boundaries between parts (i.e., cells)**
   - More elements or 2nd order elements may be required to accurately represent the boundary and the associated volume and mass that it encloses.
2. **Collect edit results for visualization**
   - Mesh granularity should be increased in areas of large gradients for better representation during visualization.

Expert Advice, Opinion, & Perspective

Using somebody's already generated CAD file

- **May contain too many irrelevant features for the MCNP model**
  - Time may be required to "de-feature" the existing model
    - SpaceClaim tools make this an easier task
- **May contain unsupported element types such as 2-D surface elements**
  - Totally un-useable without a great deal of work
- **Fidelity of the model may not be good enough for MCNP**
  - Dimensions may not be very accurate
  - Parts may not touch other parts exactly where they should
  - Time will be required to fix