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Title: MCNP6 Unstrucutred Mesh Capability(U)

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MCNP6 Unstructured Mesh Capability

Roger L. Martz

First New Mexico Workshop on Monte Carlo for Particle Therapy Treatment Planning

May 2011

MCNP6 Unstructured Mesh Capability

Abstract

This presentation presents an overview of MCNP6's unstructured mesh capability in contrast to the legacy constructive solid geometry capability with an emphasis on how it applies to medical physics and some other select applications. Some results are presented to demonstrate its validity and computational performance.

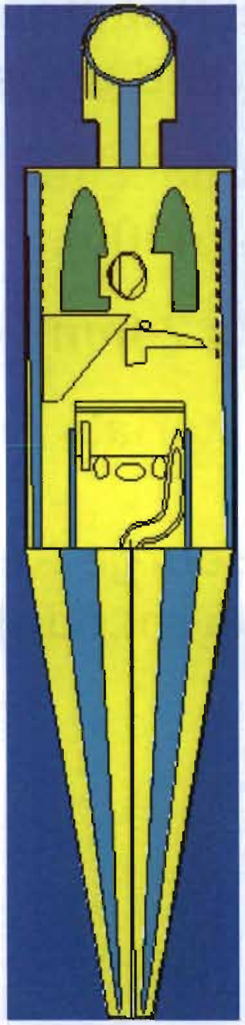
Talk Highlights

- More accurate representation of difficult geometry models
- Difficult models are easier to build
- Better visualization – geometry& results
- Faster Calculations

Something Old, Something New

CSG – Constructive Solid Geometry

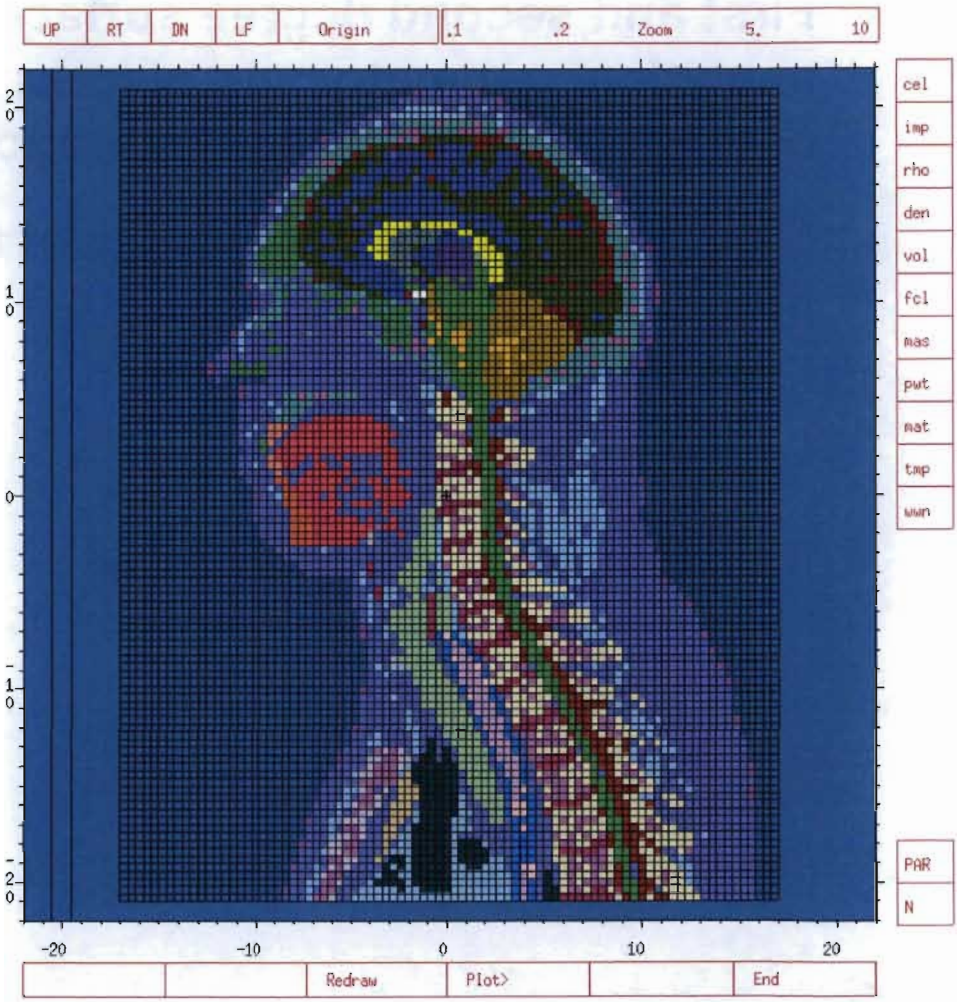
- **First and second degree surfaces of analytical geometry and elliptical tori combined with Boolean operations**
- **Can create analytical models of the human body**
  - MIRD human male
  - 40+ discrete cells
  - 3 Materials
    (D. Krstic and D. Nikezic, U. of Kragujevac, Serbia)



Lattice Geometry

- **Voxel Phantom of VIP-Man head and upper torso**
- **147 x 86 x 105 voxels (1,327,4100)**
- **2 x 2 x 2 mm**
- **41 materials / organs**

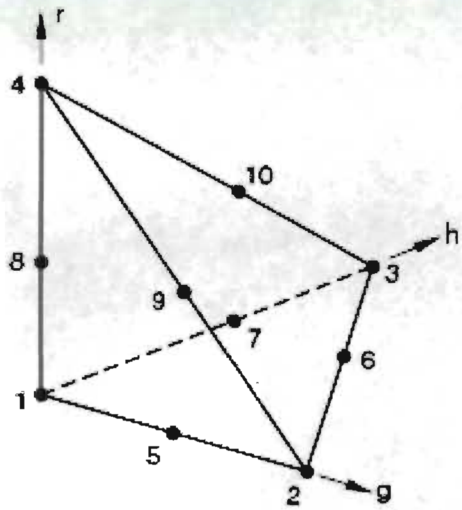
(By George Xu, RPI, xug2@rpi.edu)

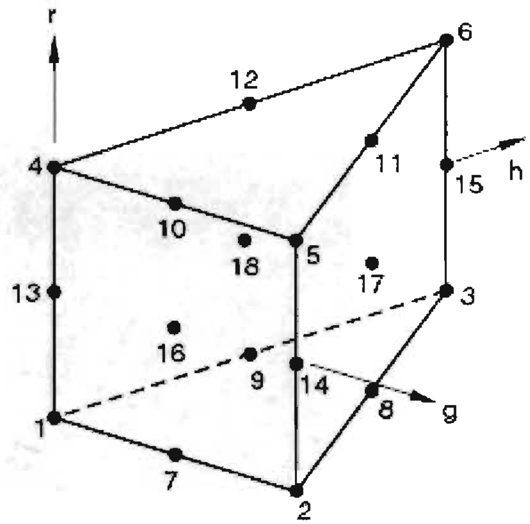


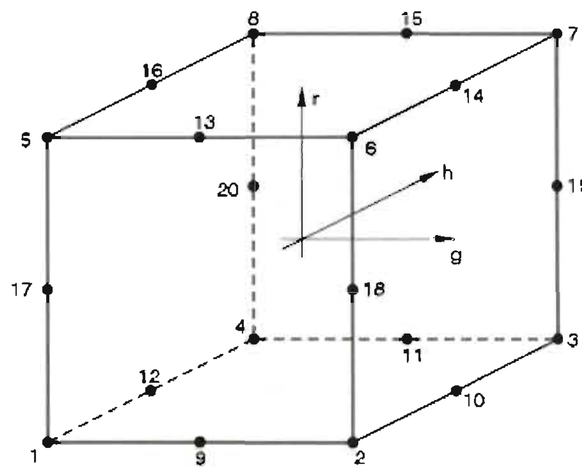
Unstructured Mesh: Finite Elements

The smallest building blocks

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

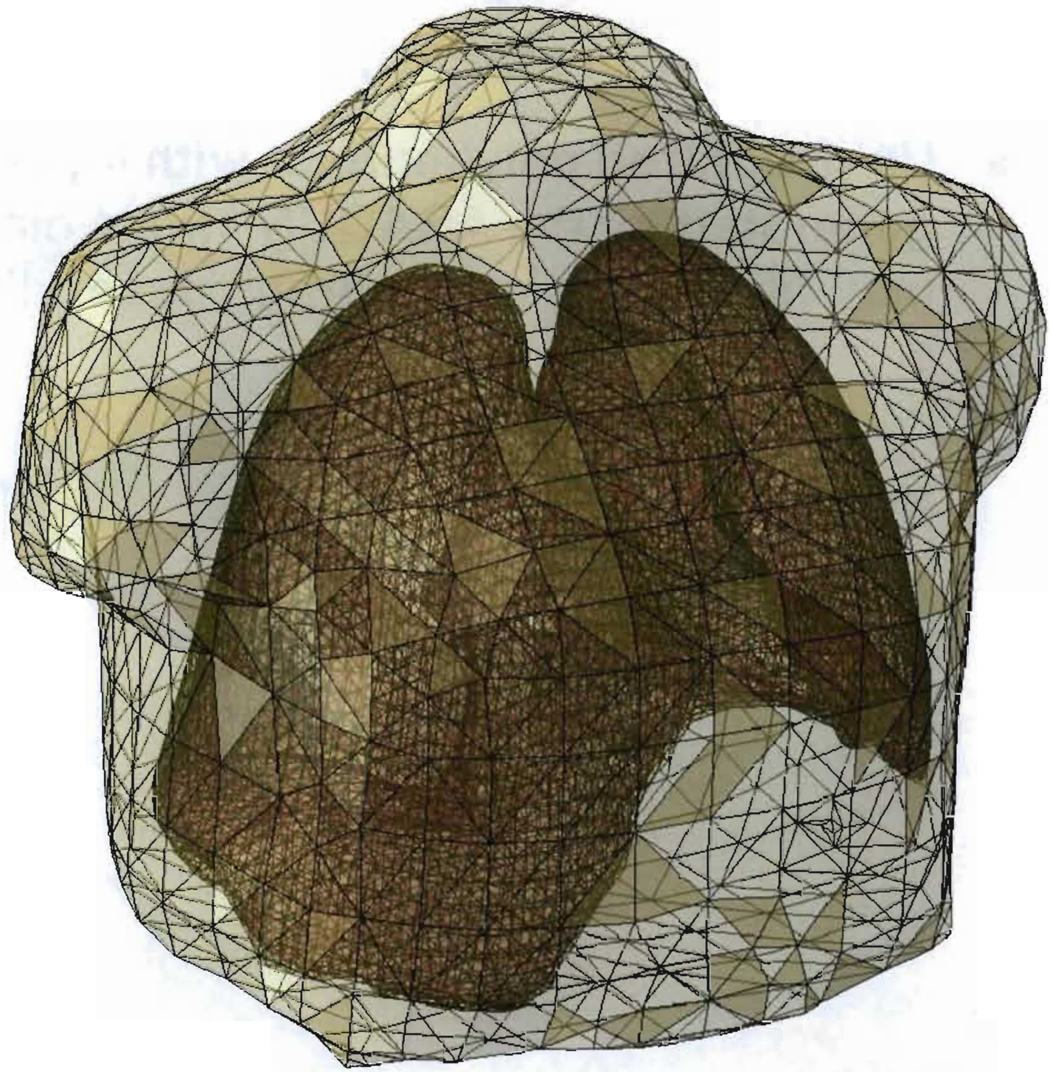






Unstructured Mesh Model: Chest & Lung

- More realistic
- 1st Order tetrahedra
- Courtesy George Xu, RPI, xug2@rpi.edu



CAD vs. CAE: A Simple View

CAD – Computer Aided Design

CAE – Computer Aided Engineering

- **Both utilized solid modeling engines.**
- **Some CAD tools may generate a mesh.**
- **CAE tools generate a mesh since they are integrated with finite element methods that generally support thermo-mechanical design, analysis, and simulation.**
  - CAE is CAD on steroids

Comments on Terminology

CAE tools have a well-established set of terminology that is different from MCNP terminology.

- NOTE: Some of the terminology may seem "different" from what MCNP users are accustomed. This arises due to the way the CAE / finite element users in the structural mechanics world have defined things. I have chosen to use their definitions where appropriate.

Object Definitions

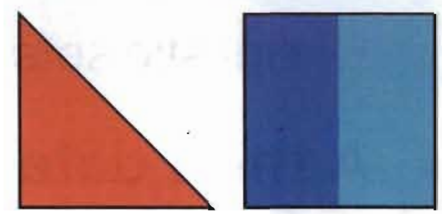
- **Mesh** - the collection of finite elements comprising the entire model.
- **Elsets** - a collection of elements or a sub-set of the mesh associated with a specific tag, label, or name.
- **Part** - the smallest geometric object created in the Abaqus CAE/tool.
- **Section** - a part segment or portion of a part
- **Instance** - a copy of a part used when constructing an assembly.
- **Assembly** - the largest geometric object created in the Abaqus CAE/tool.
- **Pseudo-cell** - an elset that has been mapped to an MCNP cell.
  - Meaning "cell - like"
  - I-Cell (inferred cell)

Constructing A Mesh Geometry

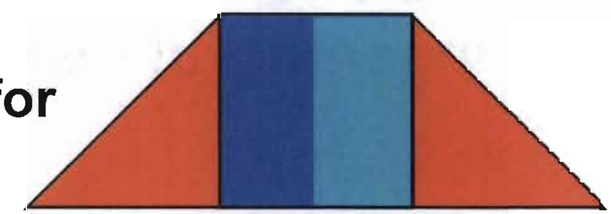
Constructing A Mesh Geometry: In The CAE Tool

Creating with ABAQUS

- **The final model is an "assembly" constructed with "instances" of "parts"**
- **Each "part" can consist of**
  - a single segment of one homogeneous material
  - multiple segments of different homogeneous materials
- **Each "part" can be meshed independently**
- **The mesh representation in MCNP is for the assembly**



parts



assembly

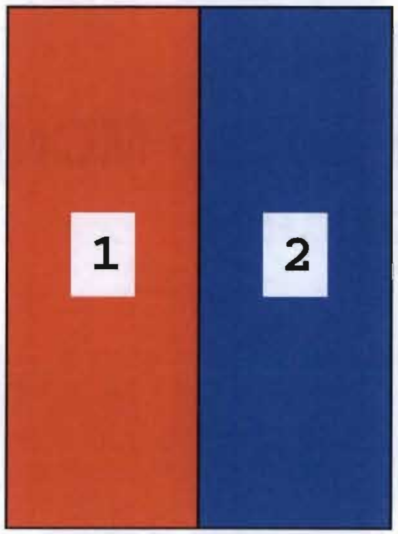
Constructing A Mesh Geometry: In The CAE Tool

- **Elements may be "tagged" with information by creating element sets (elsets).**
- **Each part must contain two data elsets:**
  - material sets
  - statistic sets
- **A third data elset will be optional in the near future:**
  - volume source sets
- **Materials should be numbered consecutively from 1 and meaningful material names should be defined.**

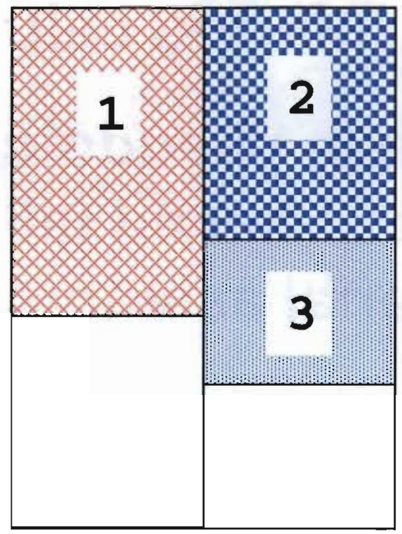
Constructing A Mesh Geometry: Pseudo-Cells

- Each homogeneous region in the mesh is referred to as a pseudo-cell or inferred cell.
- Want to map the mesh pseudo-cell to a legacy MCNP cell for things like cell-based tallies , variance reduction, and material assignment.

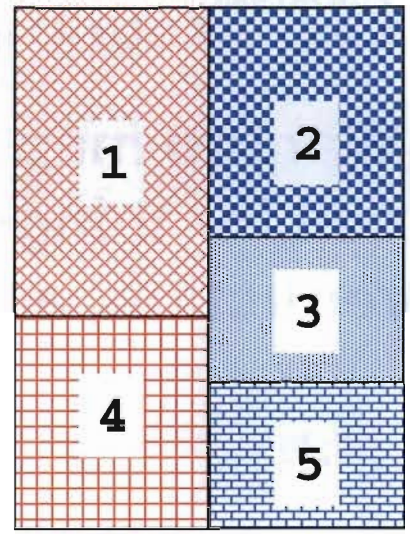
Constructing A Mesh Geometry: Pseudo-Cell Example



1 part with 2 materials



3 defined & 2 undefined statistical regions



5 pseudo-cells (always consecutively numbered internally from 1)

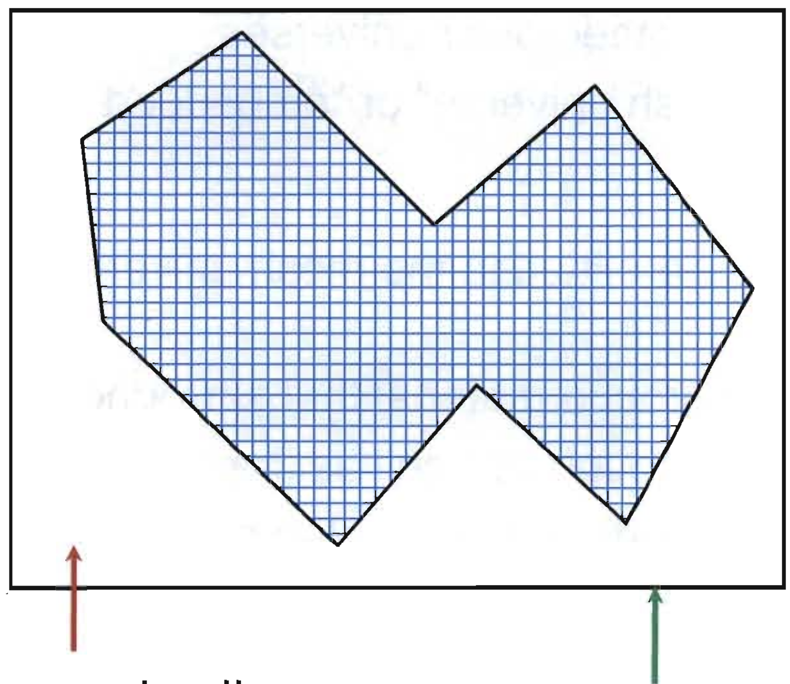
MCNP will tag untagged elements.

Constructing A Mesh Geometry: Putting It Together

- **An MCNP universe comprised of the mesh and a background cell.**
  - May not contain any other lower universes
  - Referred to as a “mesh universe” or “embedded universe”
- **Background Cell**
  - The only other cell permitted in the mesh universe with the embedded mesh geometry.
  - Serves as the background material that surrounds the mesh.
  - Particles can track through this cell as they enter and leave the mesh.
  - Serves as a “buffer” region between the mesh and the remaining CSG in the model.

Constructing A Mesh Geometry: Mesh Universe

Mesh universe with rectangular background cell and mesh

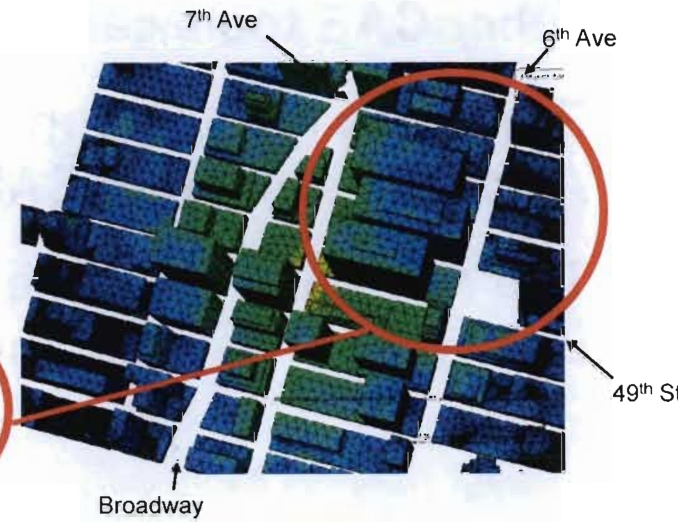


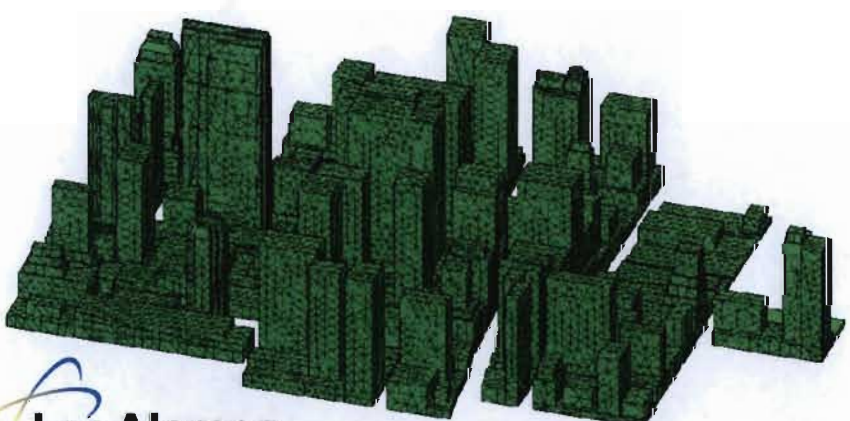
Constructing A Mesh Geometry: Alternatives

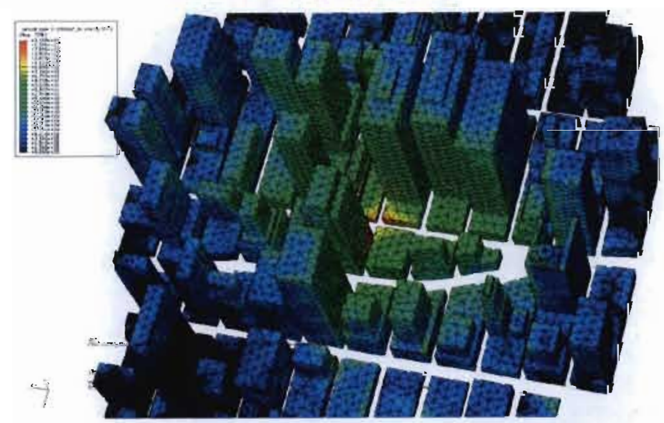
- **Other CAE tools can write an ABAQUS "inp" file.**
- **Programs exist to convert different data formats to a format that ABAQUS and other CAE tools can read. Examples follow.**
- **The ABAQUS "inp" file format is well defined. If the raw data exists, it is easy to convert it to the ABAQUS "inp" file format.**

Constructing A Mesh Geometry: Times Square Model

- Geometry based on 3D data sets (from LIDAR)
- This building-based model of Times Square, NY, includes explicit exterior walls and hollow interiors.







Constructing A Mesh Geometry: Asteroid Itokawa

Itokawa is an basalt asteroid measuring 535 x 294 x 209 meters.

Unstructured mesh geometry used for asteroid ablation and deflection studies.

Used Nagasaki neutron source (18-22 kT) to calculate energy deposition in MCNP.

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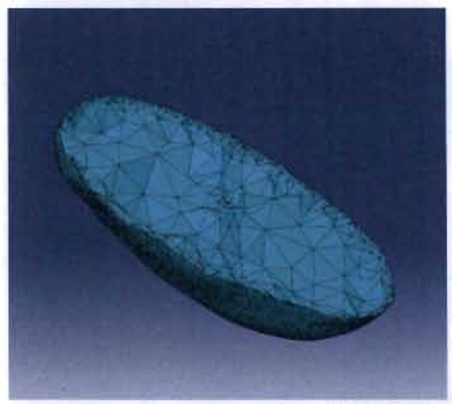
Abaqus mcnp

NASA steriolithographic data collected from Goldstone Radio Telescope.

Abaqus mcnp

Energy deposition on surface and interior (~12 m) of asteroid.



128,886 Tets

76 Meg for Mesh

Requirements & Restrictions

Requirements & Restrictions: Embedded Object

- **Mesh geometry co-exists with MCNP cell-based geometry.**
  - read from separate input file
  - MCNP input is often fairly small
- **Implemented as a universe.**
- **Ultimately, "many" instances of the same mesh or instances of "several" different mesh.**
  - Currently, one instance of one mesh has been tested.
  - Coding not currenlty in place to support results on multiple instances or work with multiple mesh files simultaneously. Planned for near future.

Requirements & Restrictions: Element Types

Parts contain certain combinations of element types:

- only tetrahedra
- only prisms (pentahedra)
- only hexahedra
- prisms & hexahedra

Requirements & Restrictions: Naming & Numbering

When Creating Element Sets – elsets

Required name format: ????AAAA????_BBB

where AAAA is one of the keywords:

material

statistic

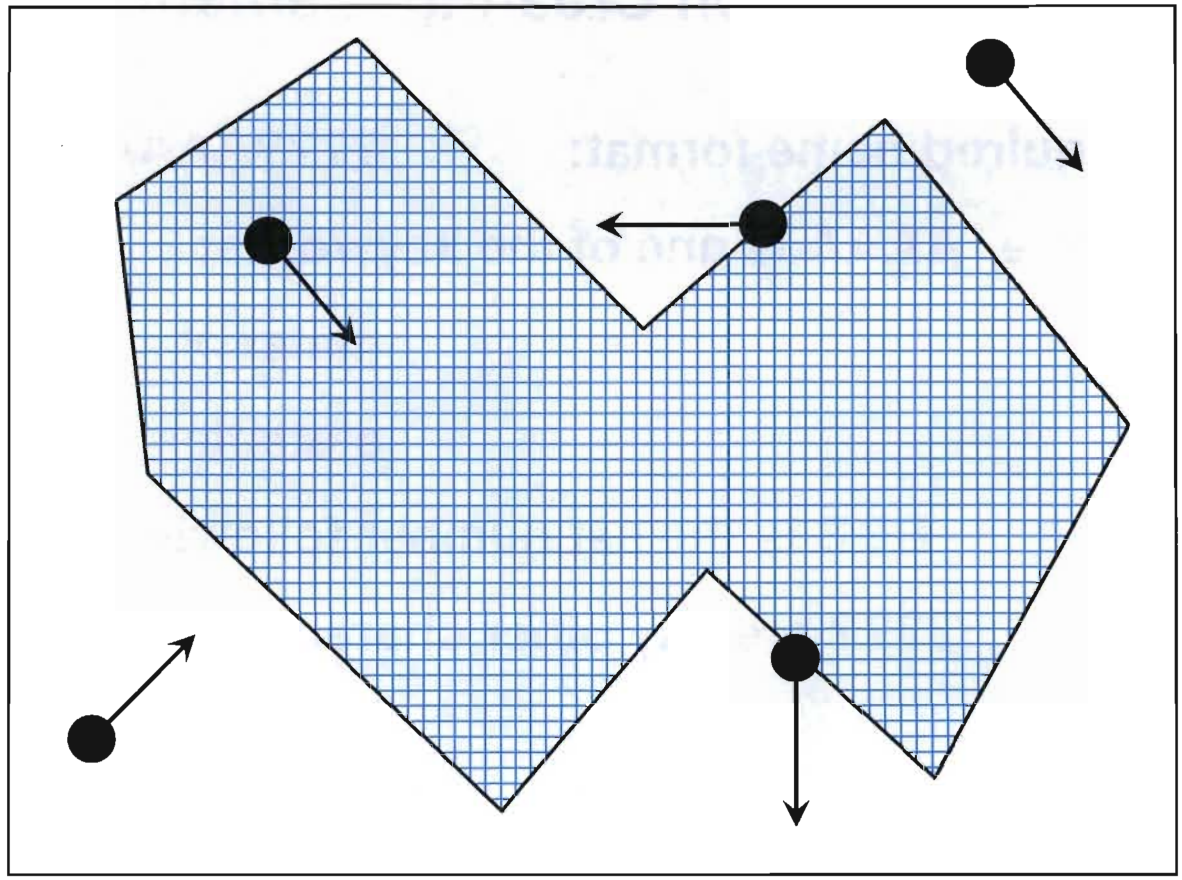
_BBB is the set number following an underscore character

???? are any other character or groups of characters

Requirements & Restrictions: Irregular Mesh Body

Tracking considerations:

1. Outside hitting
2. Outside missing
3. Inside
4. Leaving cleanly
5. Re-entrant



mesh universe / fill cell

Requirements & Restrictions: Assembling Parts

Two Basic Scenarios

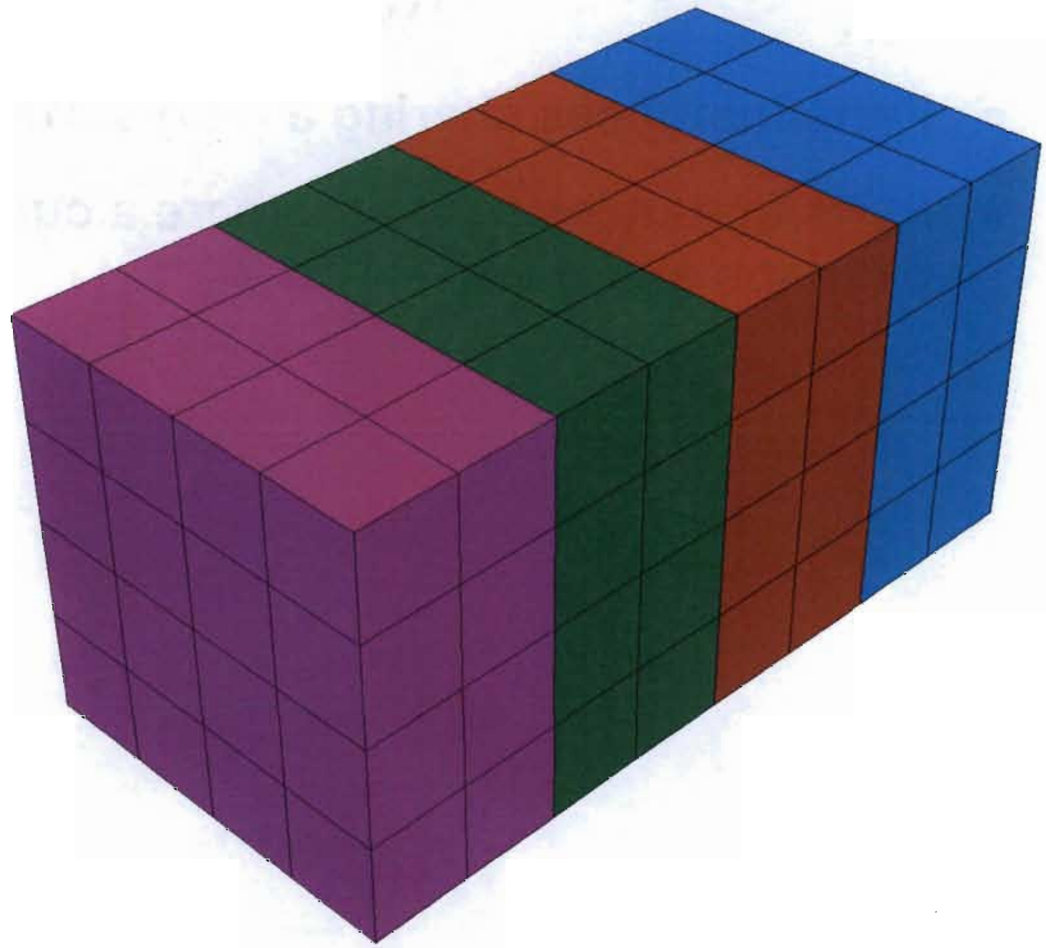
- Parts/Instances sharing a (flat) surface but not nodes.
- Parts/Instances trying to share a curved surface, resulting in overlaps and gaps.

Requirements & Restrictions: Flat Surfaces

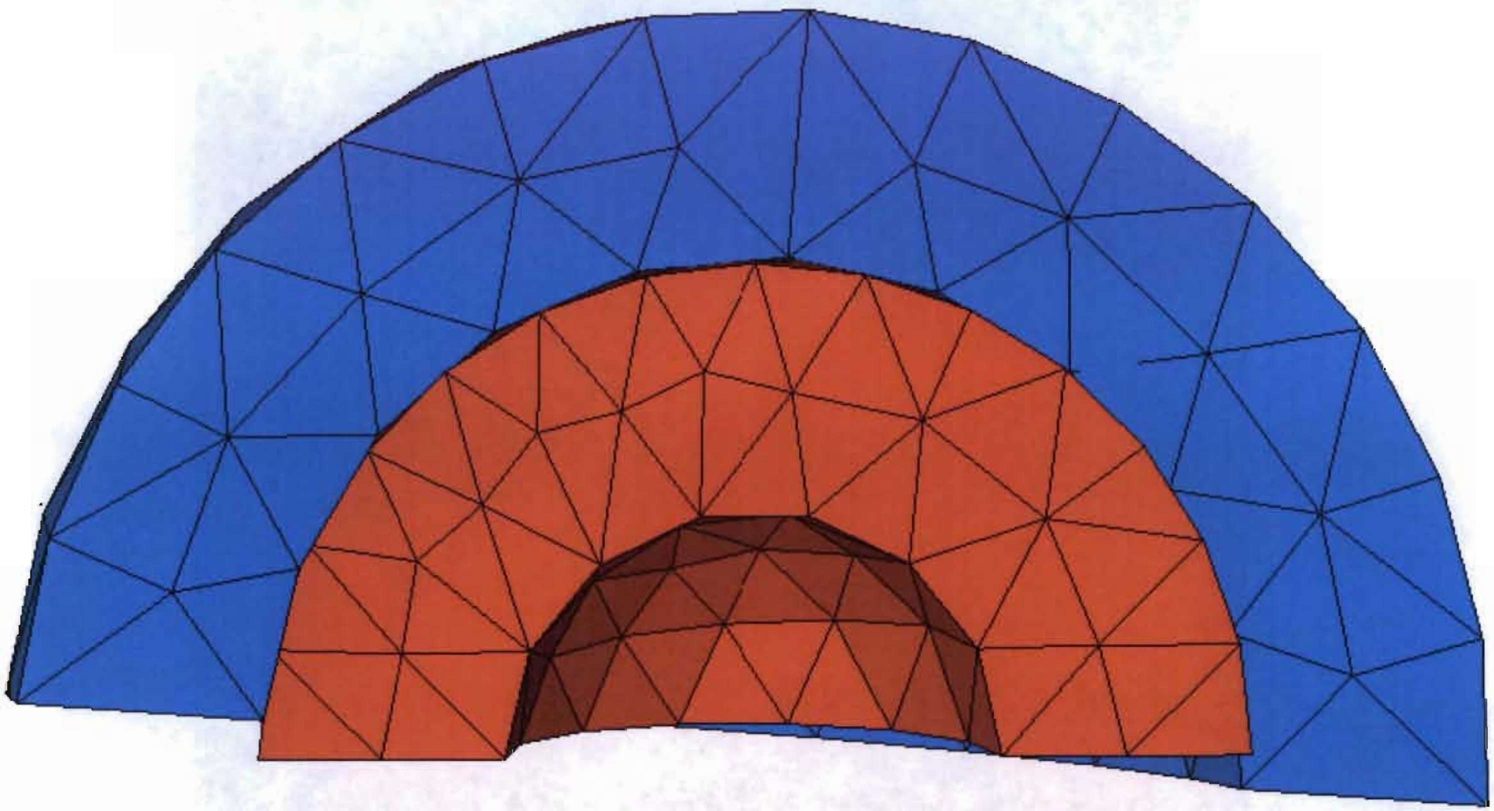
4 Parts

3 Contact Surfaces

Redundant nodes on each contact surface

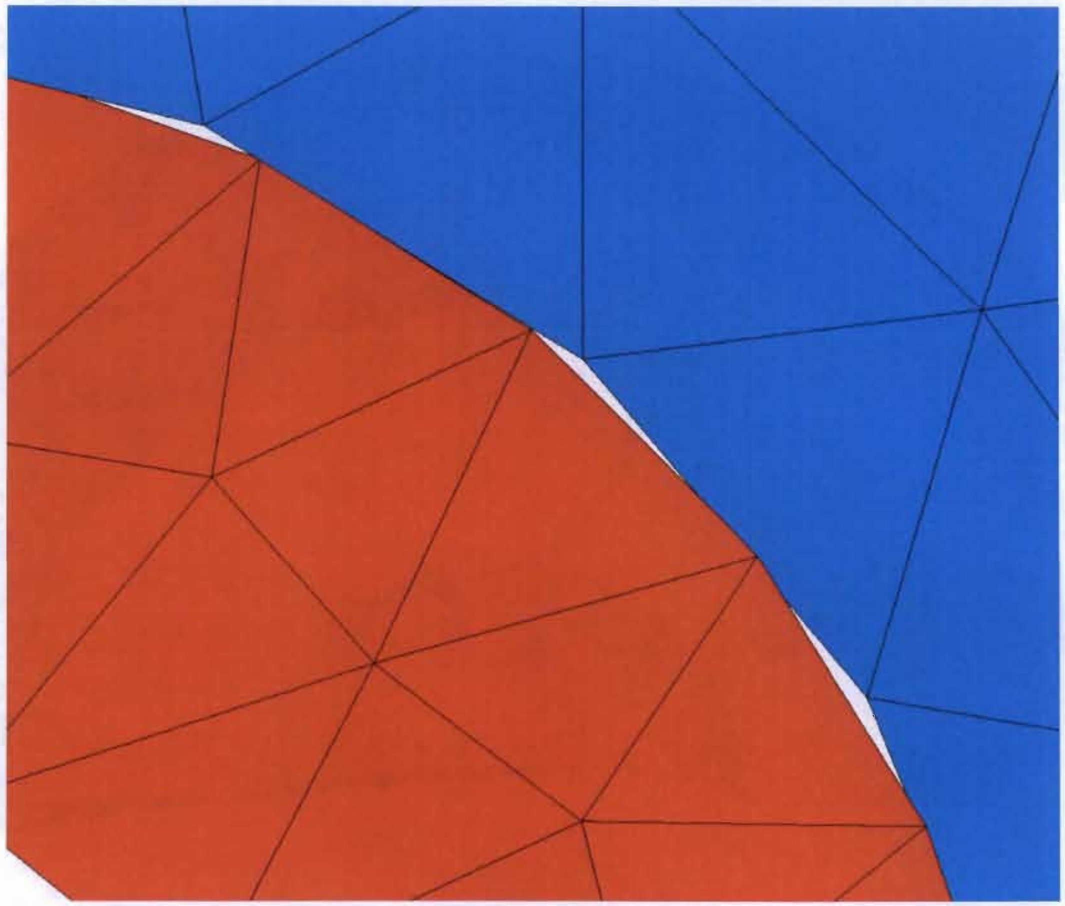


Two Parts On A Curved Surface



Requirements & Restrictions: Curved Surfaces

Gaps & Overlaps



Requirements & Restrictions: User Discretion

Modeling Considerations or "Style" Dictate Tracking Implementation

- **One part model with possibly many material sections**
  - quickest when tracking from element to element (use nearest neighbor search)
- **Multi-part model with flat-surface contact pairs**
  - more work required to find the next element on the other side of the contact surface
- **Multi-part model with overlaps and gaps / re-entrant surfaces**
  - most work required; may need to look at all surface elements

User has control over the model

Requirements & Restrictions: Results

- **Path length estimates of flux, energy deposition, and/or fission energy deposition by mesh element**
  - Referred to as "elemental edits"
  - NO statistical uncertainties on results
  - Results output (including mesh geometry) in a special file
  - Dictates tracking implementation
    - Path length estimation (like MCNP) produces result in each mesh element through which the particle tracks.
    - Surface-to-surface tracking is not efficient in producing results in the mesh, but is desirable for transport speed up where edits aren't needed.
- **Still need to connect to dose conversion cards**

Tracking On The Mesh

Unstructured Mesh Tracking

Ultimately, there will be at least two types of tracking implemented on the unstructured mesh:

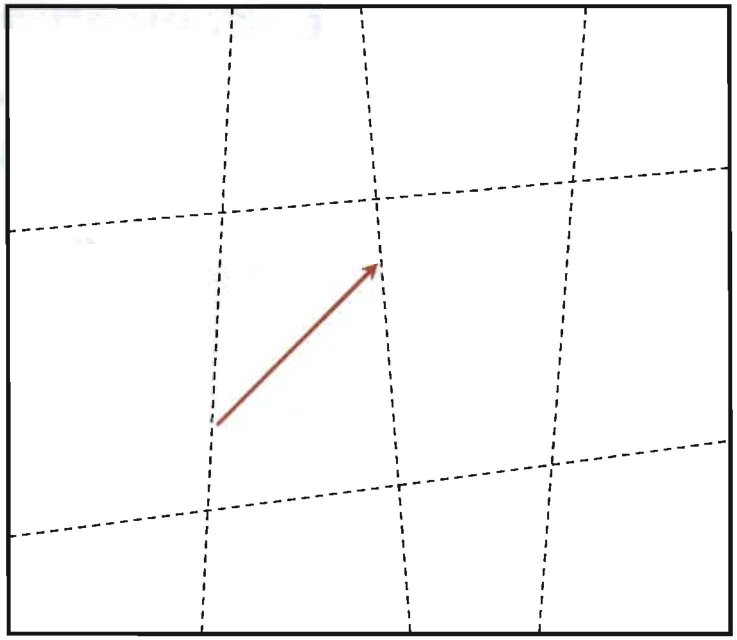
- Element-to-element
- Surface-to-surface

They primarily differ on the "granularity" of the geometry they use.

(see the next two slides for details)

Element-to-Element Tracking

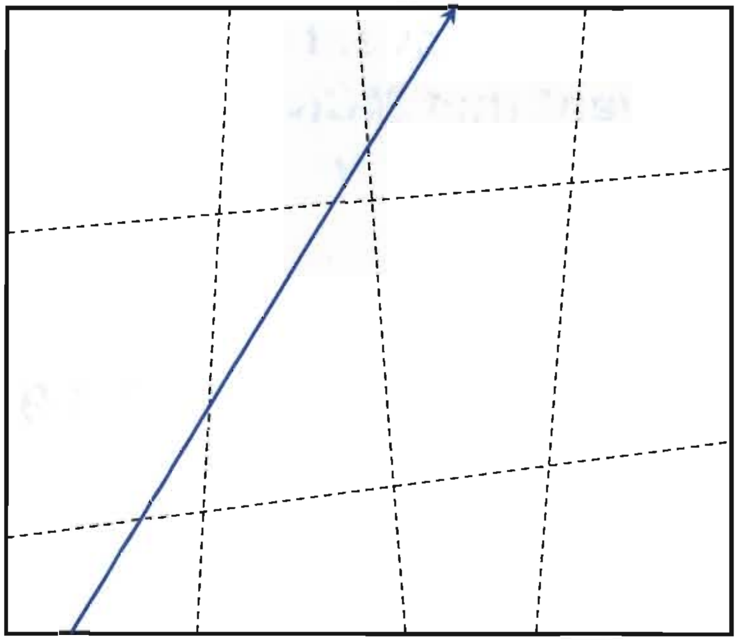
- Tracking is from face-to-face of the element (barring a collision event or any other event that MCNP checks such as distance to dxtran surface).
- Path length results are collected for each element that the particle travels through.



12-element part

Surface-to-Surface Tracking

- **Tracking is from surface-to-surface of the part (barring a collision event or any other event that MCNP checks such as distance to dxtran surface).**
- **No path length results are collected on the elements.**

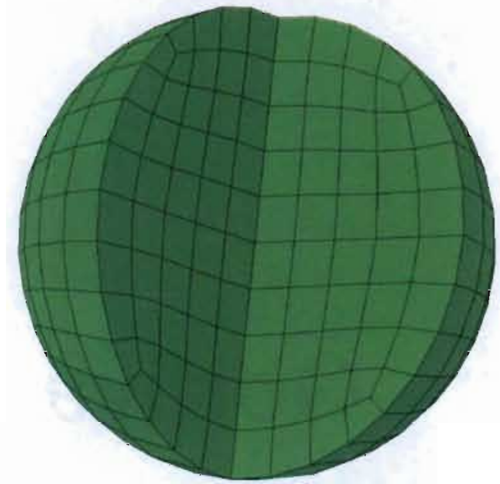


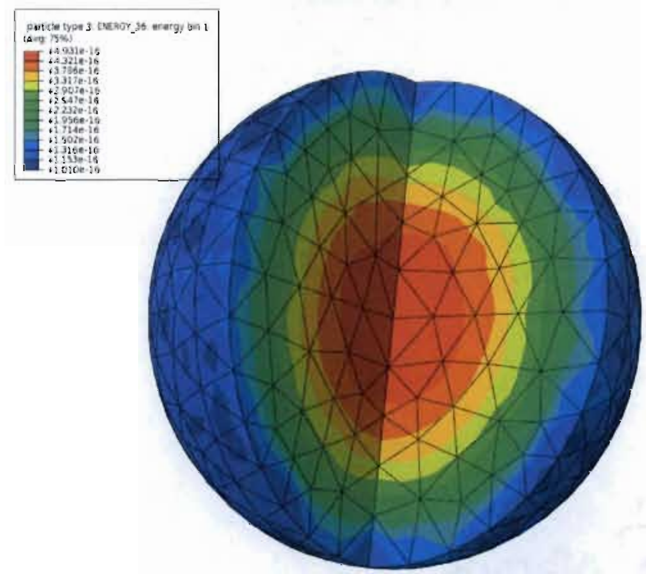
12-element part

Godiva Benchmark Example

Godiva: Highly Enriched Uranium Sphere

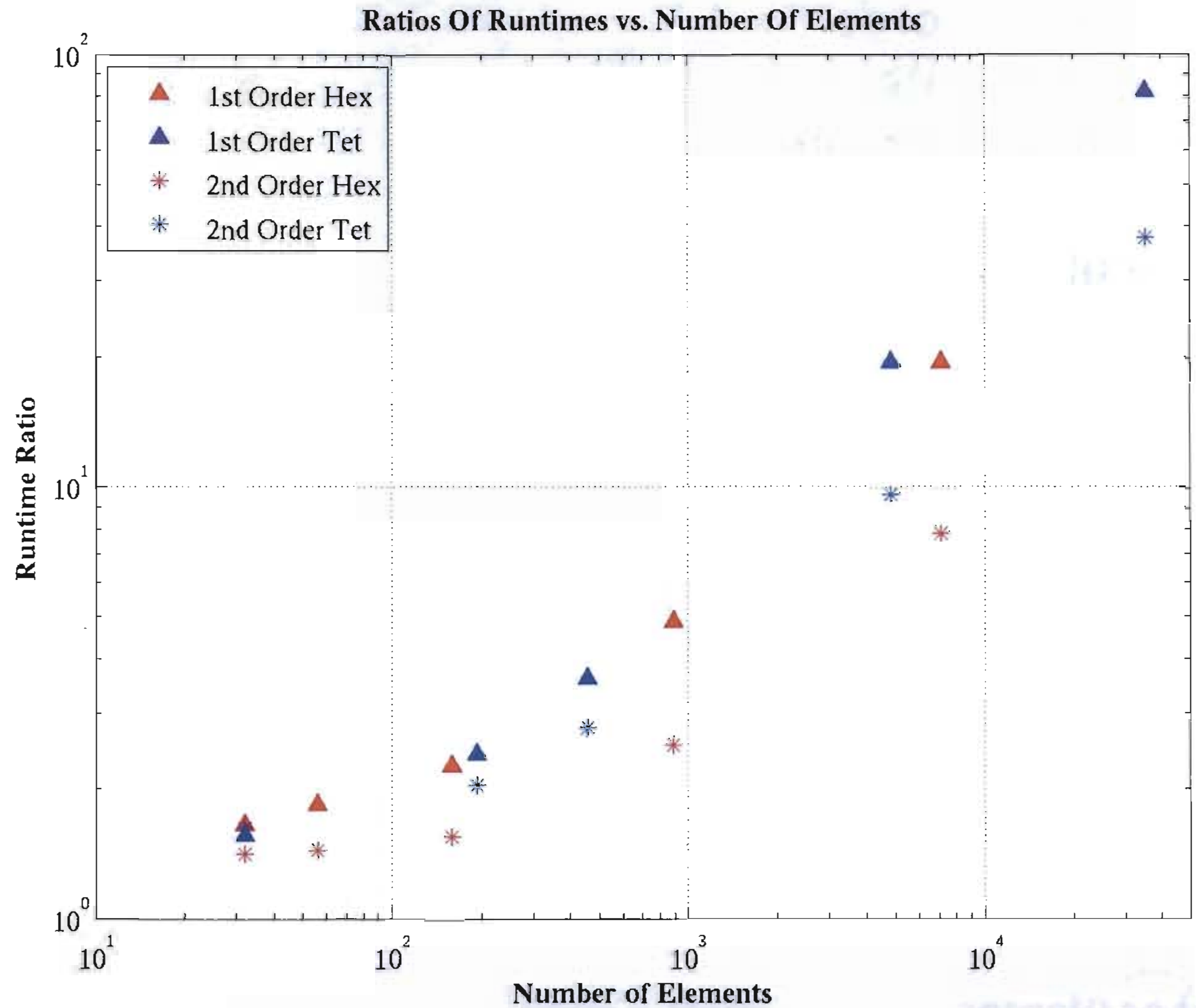
- Criticality benchmark
  - Well understood
  - Poses a challenge for mesh with its curved surface
- MCNP Calculations
  - ENDF/B-VII cross sections
  - Mode n, p
  - 300 histories / cycle
  - 100 inactive cycles
  - 900 active cycles
  - 64-bit Redhat 5
  - Intel Xeon X5450 @ 3.0 GHz





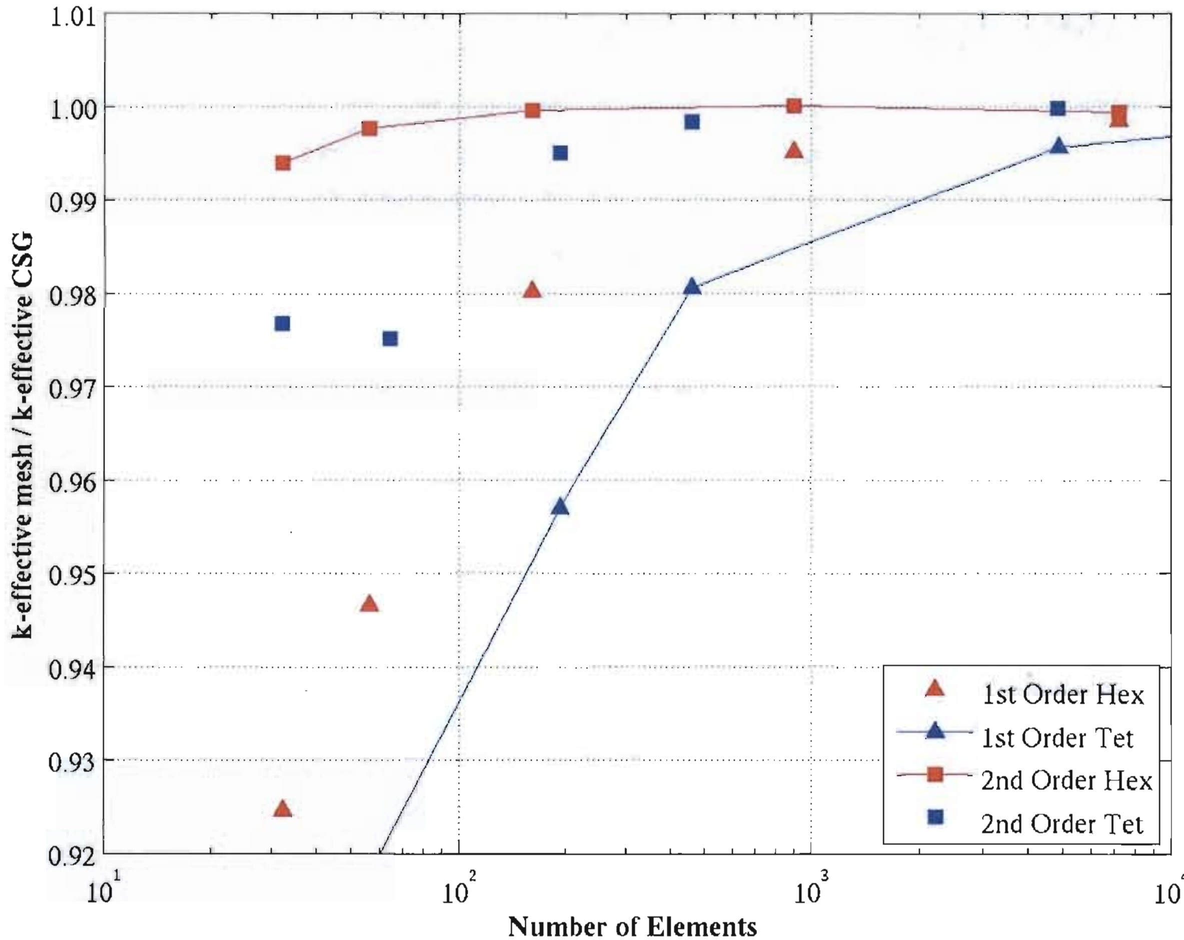
Godiva: Speed Up Improvements

Substantial gains!



Godiva: K-Effective Ratio vs. Number of Elements

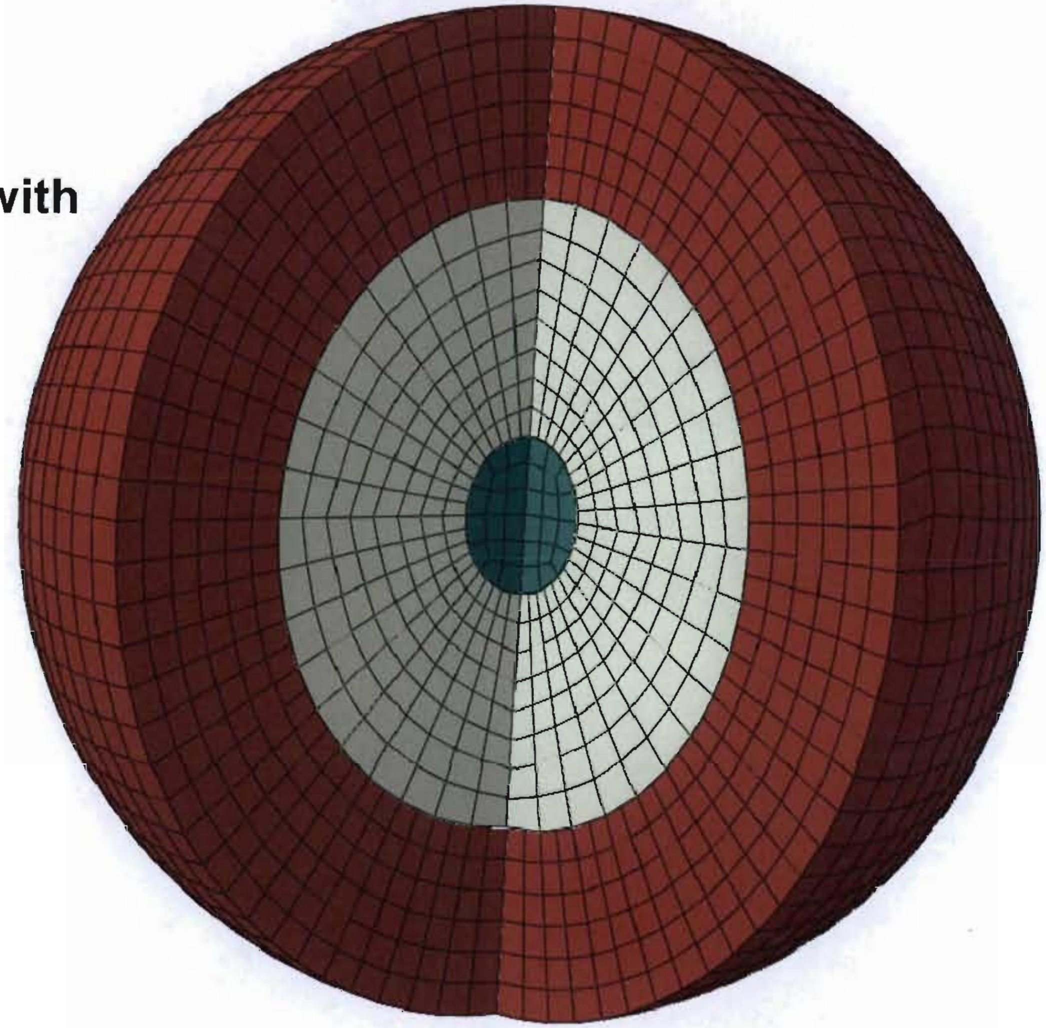
Fewer 2nd order elements are needed to obtain and accurate result



Osaka Benchmark Example

Osaka: Fusion Neutronics Shielding Benchmark

- **Fixed Source Calculation**
  - Well understood
  - Poses a challenge for mesh with its overlaps & gaps
- **MCNP Calculations**
  - ENDF/B-VII cross sections
  - Mode n
  - 64-bit Chaos Linux
  - AMD Opteron @ 2.3 GHz

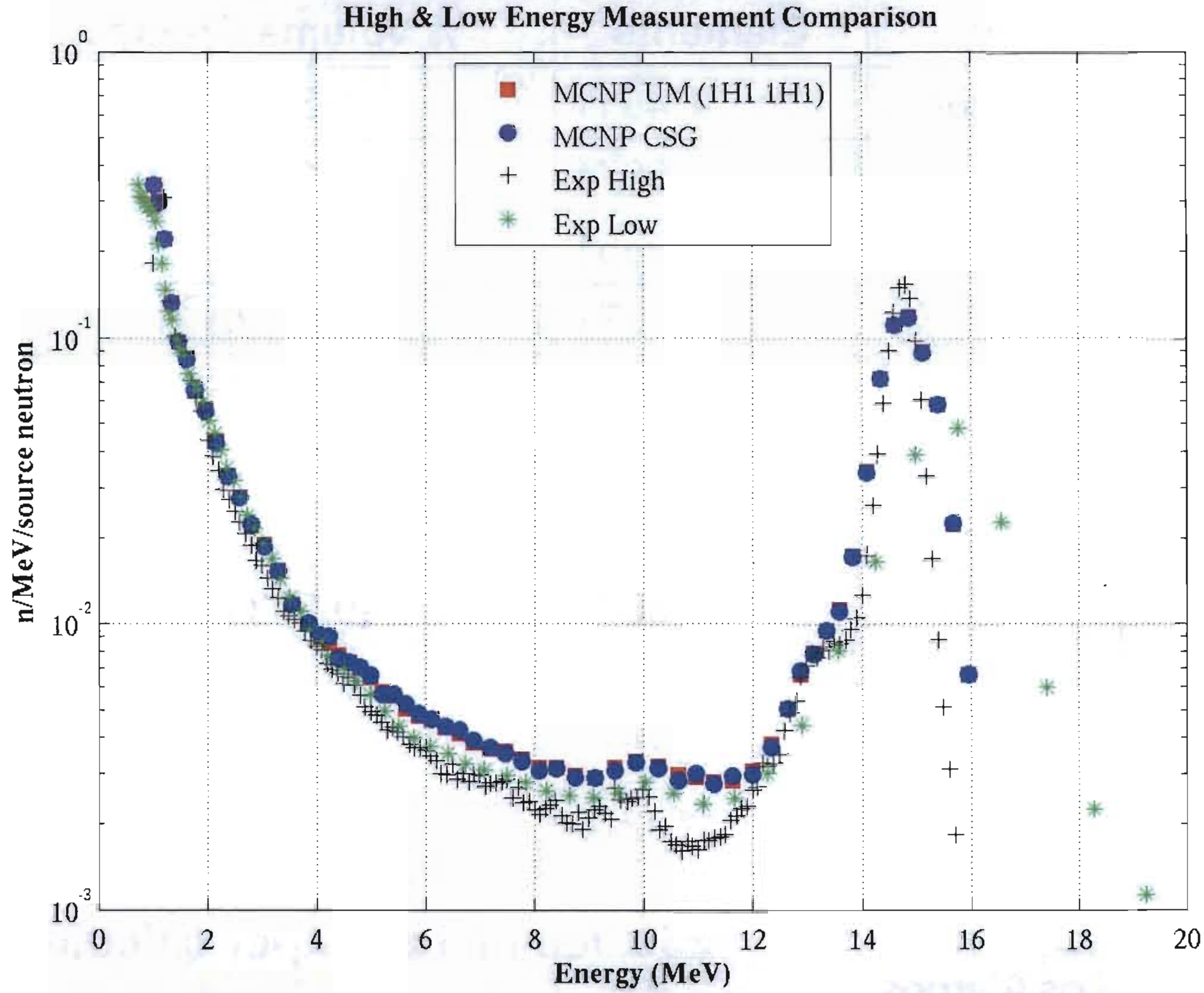


Osaka: Neutron Leakage Comparison w/ Experiment

5 million histories

Largest error on any energy bin: 4.5%

Typical error on energy bins: 1%



Osaka: Neutron Leakage Comparison -- Tetrahedra

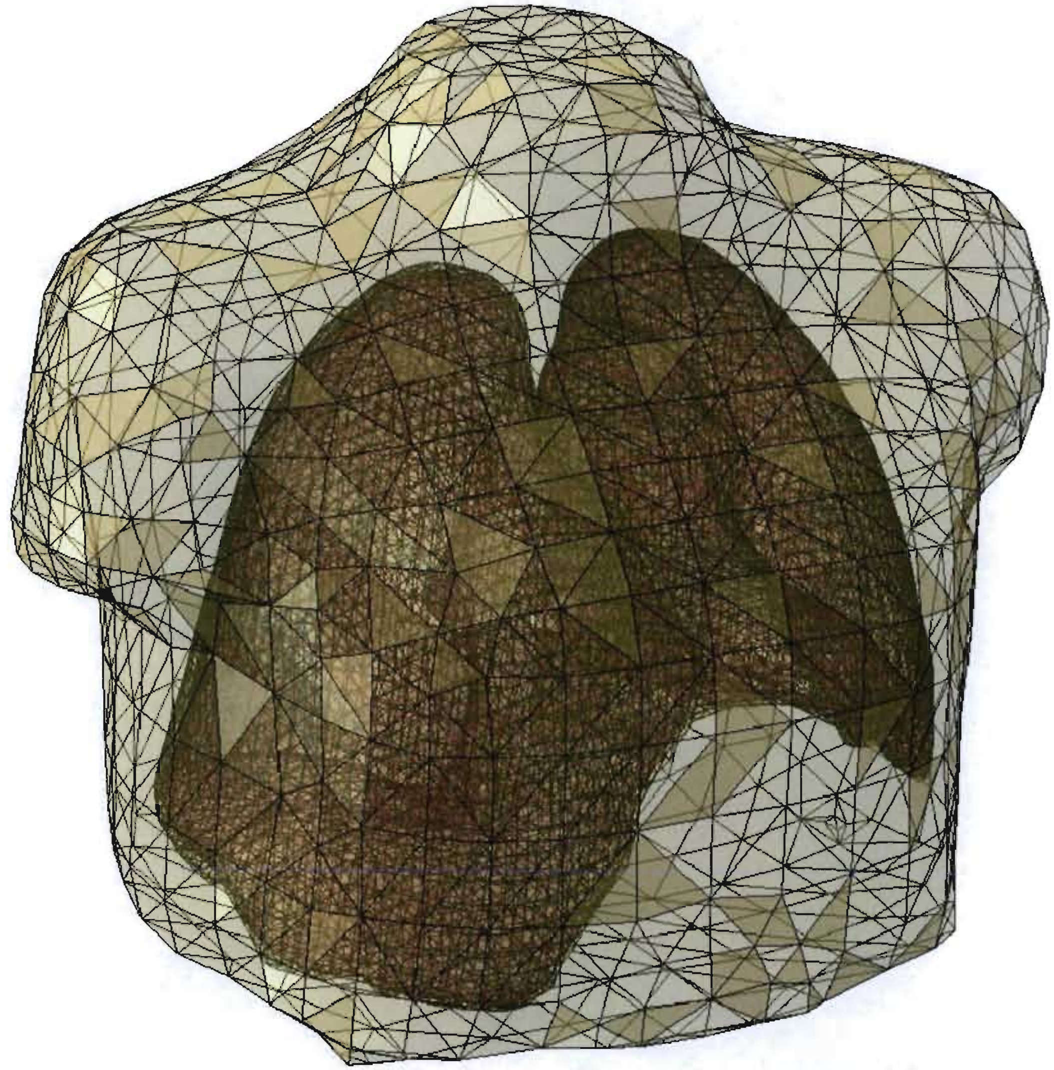
Type	Elements	% Volume Change	% Leakage Change
1^{st} Order	4011	-3.524	2.646
	6674	-1.818	4.294
	10651	-1.533	2.607
	17971	-1.122	2.629
	118256	-0.3305	0.8581
2^{nd} Order	4011	-0.01982	2.528
	6674	-0.003497	4.358
	10651	-0.002331	2.562
	17971	-0.001166	2.531
	118256	0.0	0.9009

250,000 histories per calculation

Unstructured Human Torso

Unstructured Human Torso: Energy Deposition Results

- ^{60}Co Source
- Mono-directional beam



Last Words

More Work To Do

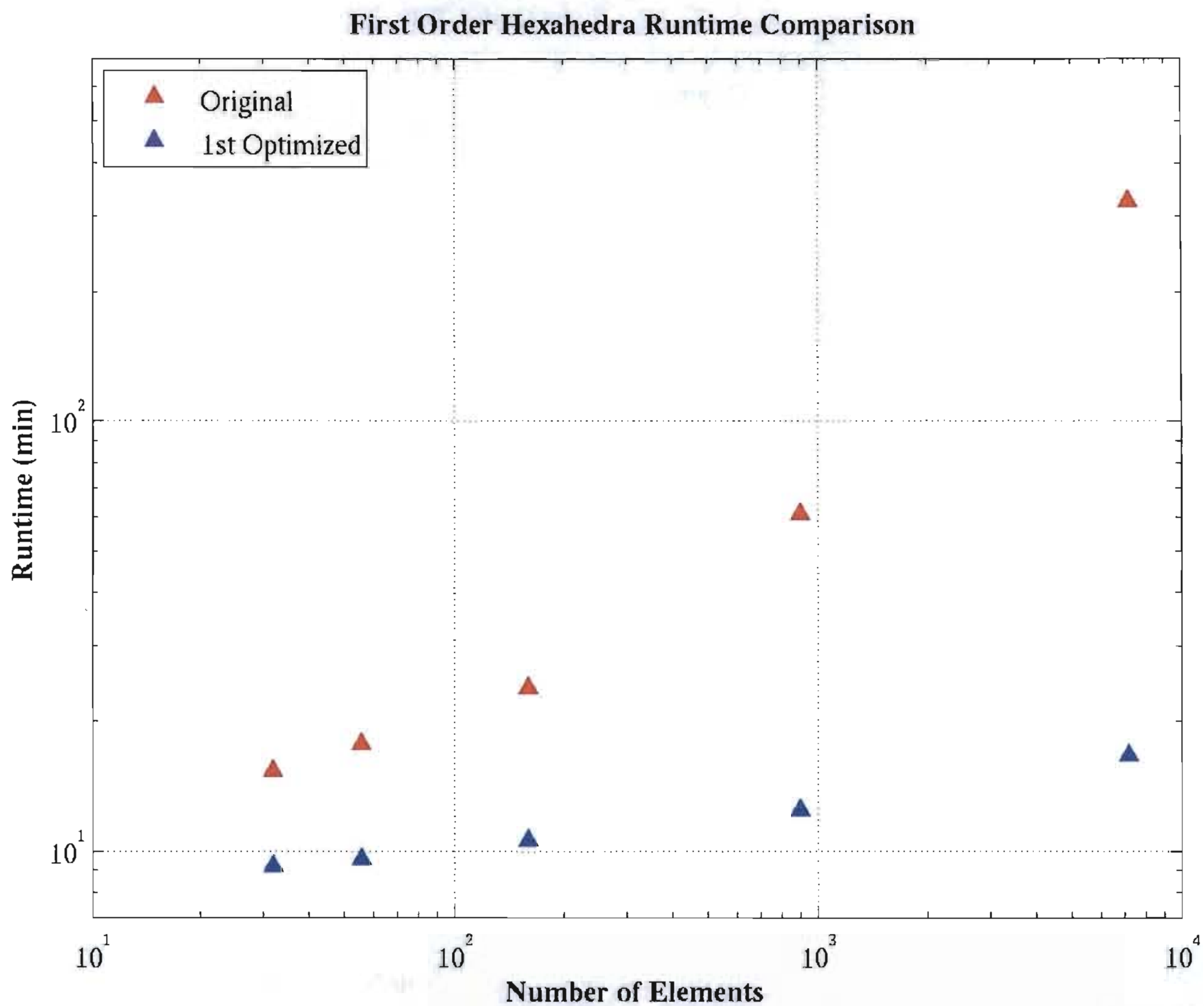
- Connecting to other features – progressing
- More V&V

Conclusion

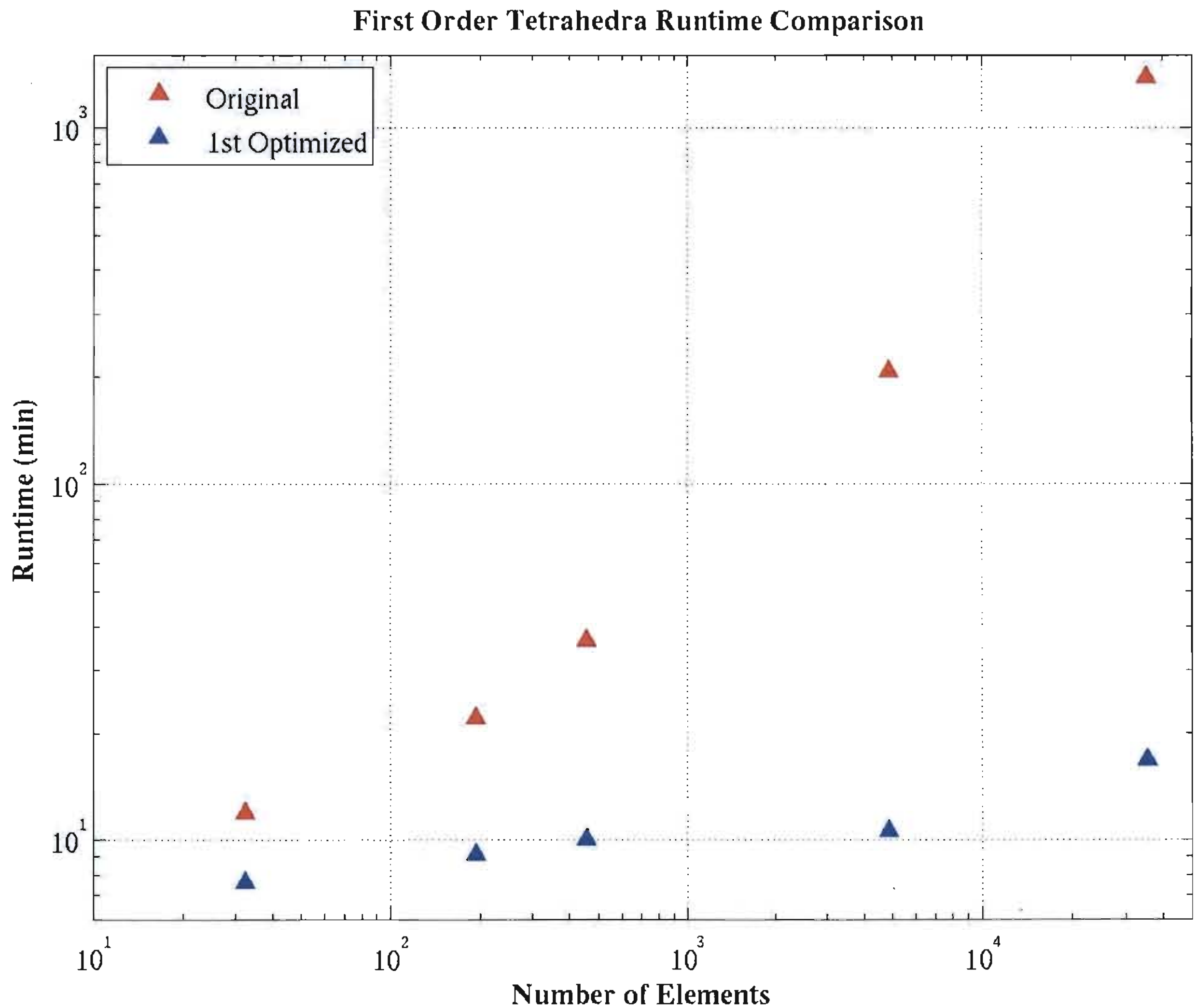
- Unstructured mesh capability shows great promise

Extra Slides

Godiva

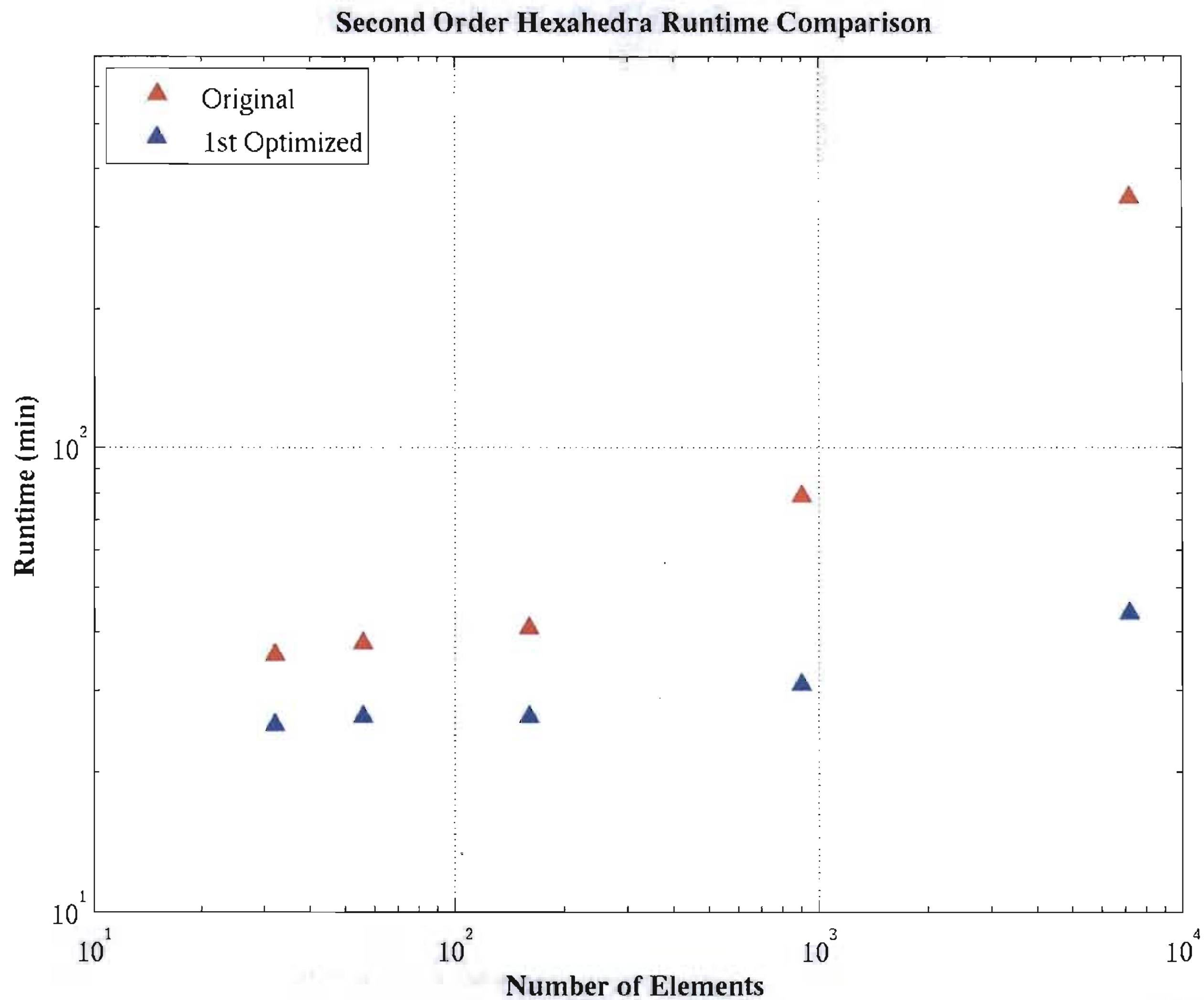

First Order Hexahedra Runtime Comparison
Original
1st Optimized
Runtime (min)
10^2
10^1
10^1
10^2
10^3
10^4
Number of Elements

Godiva



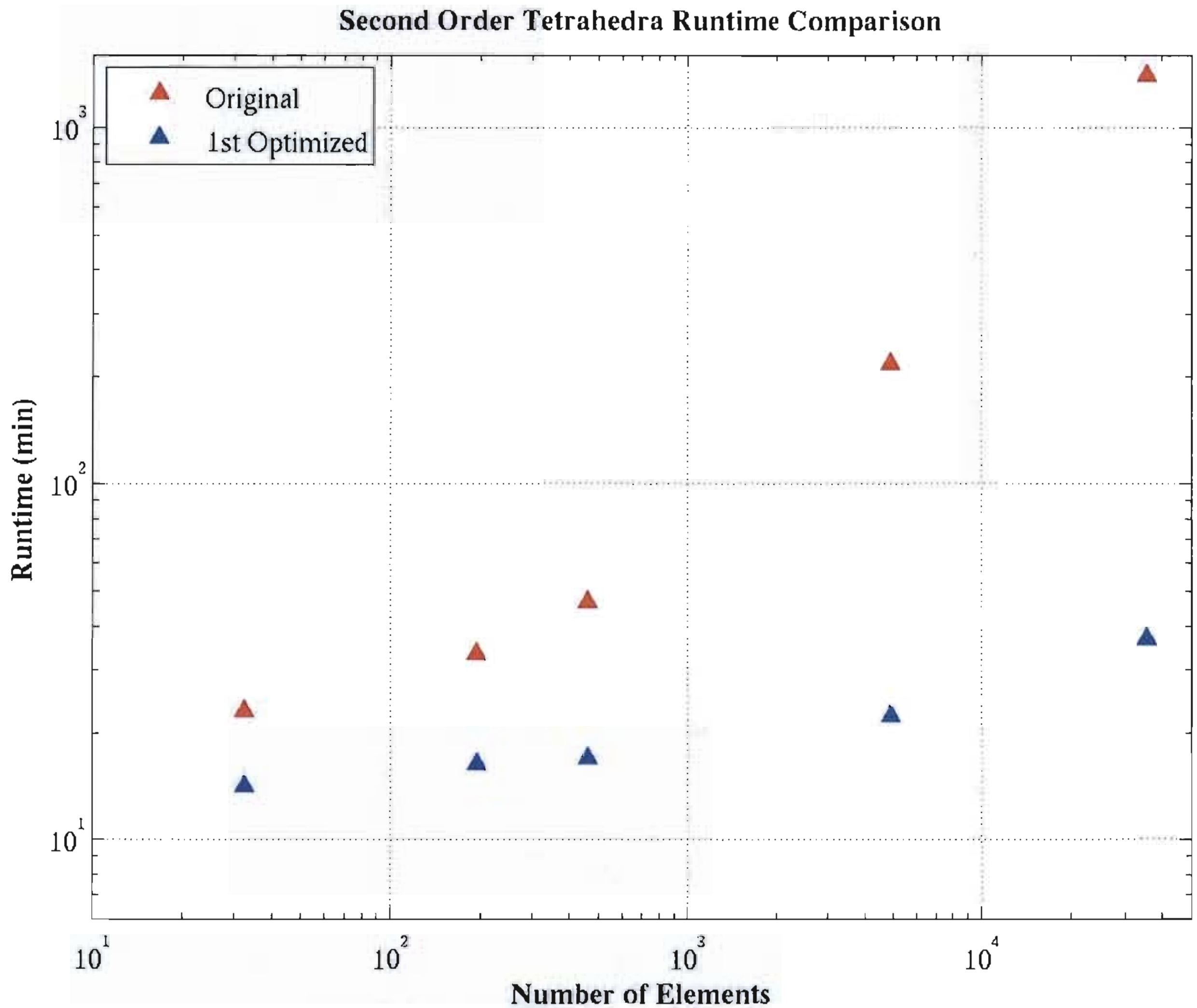
First Order Tetrahedra Runtime Comparison
Original
1st Optimized
Runtime (min)
10^3
10^2
10^1
10^1
10^2
10^3
10^4
Number of Elements

Godiva



Second Order Hexahedra Runtime Comparison
Original
1st Optimized
Runtime (min)
10^2
10^1
10^1
10^2
10^3
10^4
Number of Elements

Godiva


Second Order Tetrahedra Runtime Comparison
Original
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10^{2}
10^{1}
10^{1}
10^{2}
10^{3}
10^{4}
Number of Elements