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Title: MCNP6 Hybrid Geometry Development (U)

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MCNP6 Hybrid Geometry Development

Overview

ABSTRACT

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This presentation provides an overview of the new hybrid geometry capability in MCNP6. The modeling paradigm along with some implementation and user requirements are discussed. The new MCNP input cards are presented. Simple examples are shown to illustrate some of the relevant ABAQUS® features. Initial verification work is presented. Code design and implementation is briefly discussed. Recent accomplishments and near term goals are mentioned.

The BIG Picture Objectives of This Work

- **Support the KEA project in W-13 (immediate need)**
  - radiation effects / hostile environment
- **Serve as the foundation to replace the Eolus Grid Library (EGL)**
  - This new library is the **R**evised **E**olus **G**rid **L**ibrary (**REGL**)
- **Implement relevant features that will attract new "markets" for MCNP**
  - multi-physics users
  - CAE (computer aided engineering) users

Outline Of Objectives

- **Overview of the capability**
- **A quick view of the new MCNP Input Cards**
- **Concrete cylinder example / sample results from ABAQUS**
- **Some initial verification work**
- **Overview of code design & implementation**
- **Recent accomplishments**
- **Near term goals**

Capability Overview

Hybrid Geometry

Objectives of these next slides:

- **Provide the user with a basic understanding of**
  - the modeling paradigm used in this hybrid approach
  - some implementation & user requirements

Embedded mesh

- **Mesh geometry co-exists with MCNP cell-based geometry.**
  - read from separate input file
- **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 in place to support results on multiple instances or work with multiple mesh files simultaneously.

- **CAE tools like ABAQUS have their own set of terminology that is quite different from that used by MCNP.**

Some Geometry Requirements

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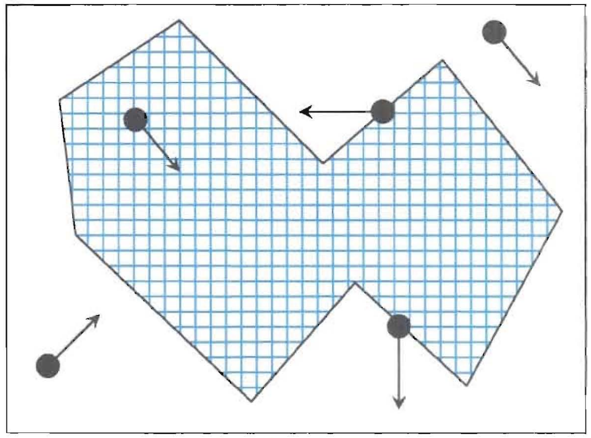
Irregular mesh body

Tracking considerations:

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



mesh universe / fill cell

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New Capability For MCNP6

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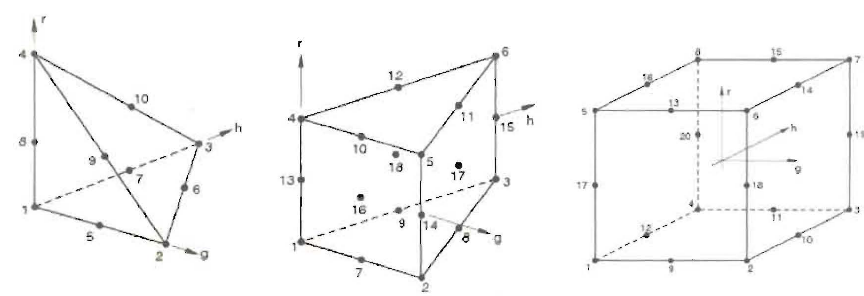
Current Implementation

Unstructured mesh with 4-, 5-, and 6-sided elements generated by the ABAQUS® finite element program. Surfaces may be bilinear.



Currently, no mid-point nodes permitted.

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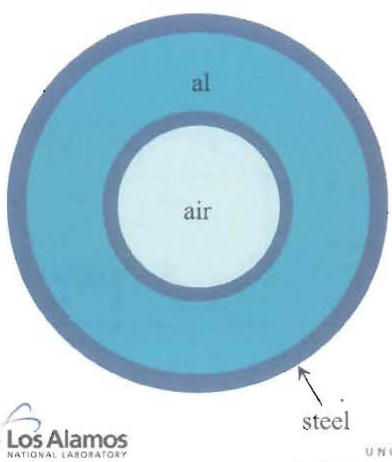
New Capability For MCNP6

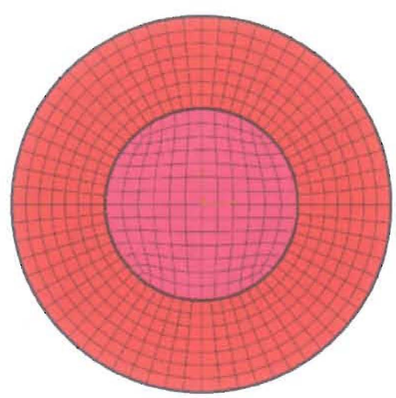
Parts contain element types:

- only tetrahedrons
- only prisms
- only hexahedrons
- prisms & hexahedrons

Example Geometry

Osaka Aluminum Sphere Benchmark Problem





Background: Constructing A Mesh Geometry

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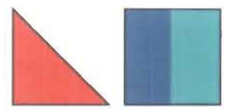
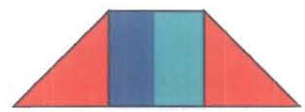
Created with ABAQUS

- **The final model is an "assembly" constructed with "instances" of "parts"**
- **Each "part" can consist of**
  - a single segment of one material
  - multiple segments of different materials
- **Each "part" can be meshed independently with different element types**
- **MCNP converts the assembly into a global mesh model for its use**



parts



assembly

Background: Constructing A Mesh Geometry

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Essential Implementation Tasks

- **How to map the material descriptions to the mesh?**
- **How to take advantage of MCNP's cell-base machinery?**

Background: Constructing A Mesh Geometry

Created with ABAQUS

- **Each part must contain element sets (elsets) of data for:**
  - materials
  - statistics
    - Collection of elements used for cell-based tallies & variance reduction
    - Can not encompass multiple materials
  - surfaces
    - Initial implementation required defining surfaces at the part and assembly level.
    - "Final" implementation will only need surfaces defined for each pseudo-cell.
    - Currently, both are needed.

Background: Constructing A Mesh Geometry

Creating ABAQUS Element Sets – elsets

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

where AAAA is one of the keywords:

material

statistic

surfset

cellsurf

_BBB is the set number following an underscore character

(see set number restrictions on the following slides)

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

Background: Constructing A Mesh Geometry

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Part Material Elsets

- Defined in ABAQUS under "sets".
- Multiple elsets are acceptable.
- Each element in a part must belong to one and only one material elset.
- All elements must belong to some material elset.
- The set number (_BBB) is the material number. This number must start at 1 and go to the max number present. E.g., if there are 5 materials, then the number must be 1 to 5, inclusive.

Background: Constructing A Mesh Geometry

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Part Statistic Elsets

- Defined in ABAQUS under "sets".
- Multiple elsets are acceptable.
- Each element in a part should belong to one and only one statistic elset.
- Any element not assigned to a statistic elset is assigned to a catch-all elset in that part.
- Each statistic elset must contain only one material.
- The set number (_BBB) is the statistic set number, must start at 001, and be unique throughout the part.

Background: Constructing A Mesh Geometry

Part Surface Set Elsets

- Defined in ABAQUS under "sets".
- Multiple elsets are acceptable.
- Each surface element in a part must belong to one and only one surface set elset.
- The set number (_BBB) is the surface set number and can be any number that is not already in use as a surface set number.
- Soon to be obsolete.

Background: Constructing A Mesh Geometry

Part Cellsurf Surfaces

- Defined in ABAQUS under "surfaces".
- All pseudo-cells in a part must have their surfaces defined in a "cellsurf" surface.
- Multiple surfaces are acceptable.
- Each surface element in a part must belong to one and only one cellsurf surface.
- The set number (_BBB) is the cell surface set number and can be any number that is not already in use as a cell surface set number for that part.

Background: Constructing A Mesh Geometry

Assembly Elsets

- All elements on the exterior surface of the assembly model must belong to an assembly surface set.
- The same rules apply to naming this surface set as for the part surface sets.
- No material or statistic elsets are specified at the assembly level; they are inherited from the parts.
- Soon to be obsolete.

Background: Constructing A Mesh Geometry

Future Part Elsets: Volume Source

- Optional, not required.
- Possible keywords: "source" or "volsource".
- Defined in ABAQUS under "sets".
- Multiple elsets will be acceptable.
- The set number (_BBB) is the volume source number. Numbering to be determined.

Background: Constructing A Mesh Geometry

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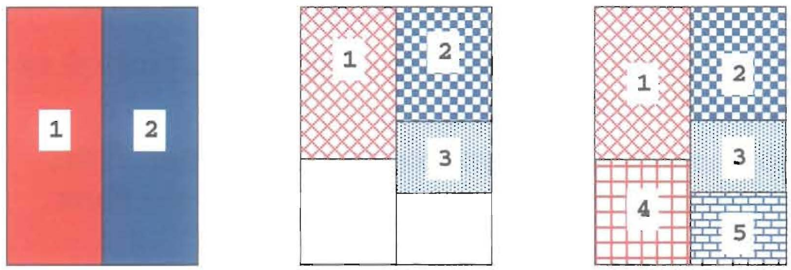
Pseudo-Cell Example



1 part with 2 materials

3 defined & 2 undefined statistical regions

5 pseudo-cells (always consecutively numbered from 1)

Background: Constructing A Mesh Geometry

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Pseudo-Cells

- **Each instance--material--statistic region is automatically mapped to a pseudo-cell.**
- **The numbering of the pseudo-cells starts at 1 and occur in the order in which ABAQUS instances the parts to construct the assembly and the order of the statistical regions within the part.**
- **There must be one MCNP cell for each mesh pseudo-cell.**
- **The MCNP cell must contain the correct material definition for the pseudo-cell. (users responsibility)**

Background: Constructing A Mesh Geometry

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Pseudo-Cell Table

- After the code processes the ABAQUS input file, a table appears in the output describing what it expects the pseudo-cells to be.
- The user should examine this table to ensure that the material assignments to the cells are correct.

Background: Constructing A Mesh Geometry

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Contact Pairs

- Contact pairs must be defined for all parts that "touch" or "appear to touch".

Modeling Considerations

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Contact Pair

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

This may be eliminated in the future, but is currently required.

- Not using simplifies problem set up.
- Using it reduces runtime for problems with many instances.

Modeling Considerations

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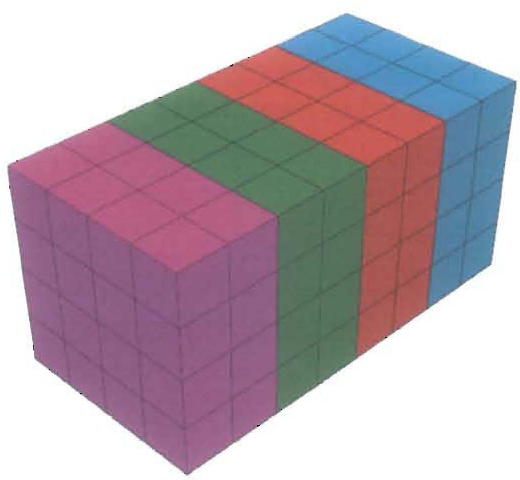
4 Parts

3 Contact Pair Surfaces

Redundant nodes on each contact pair surface



Modeling Considerations

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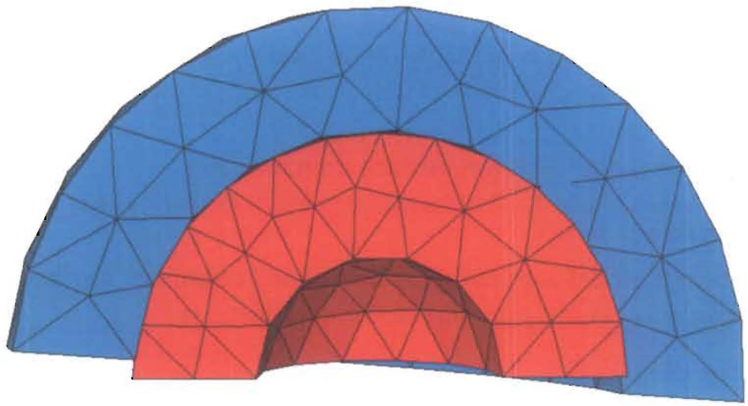
Two Parts On A Curved Surface



Modeling Considerations

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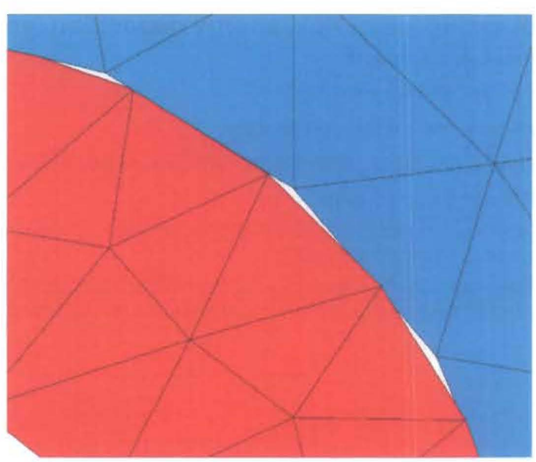
Gaps & Overlaps



Some Implementation Drivers

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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 pair surface
- **Multi-part model with overlaps and gaps / re-entrant surfaces**
  - most work required; may need to look at all elements

User has control over the model

More Implementation Drivers

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Additional Requirements

- **Path length estimates of flux, energy deposition, and/or fission energy 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 "fast" tracking is not efficient in producing results in the mesh, but is desirable for transport speed up where edits aren't needed.

Current Restrictions

- **Neutral particles only**
  - Charged particle tracking to be added later
- **Functionality with all variance reduction techniques has not been verified.**
  - Cutoffs, implicit capture, geometry splitting / roulette work
- **Using mcplot (2-D geometry plots) for mesh geometry does not work.**
- **Point detectors do not work.**
- **Surface tallies do not work inside the mesh.**
- **Non-lattice geometries only**

Input Cards

Embedded Mesh Universe

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- **Geometry mesh are embedded as the lowest level universe.**
- **Cell card requirements:**
  - At least one cell card with an embedded universe parameter "embu" along with the "u" parameter is needed to embed the mesh universe.
  - "embu" value must coordinate with the number on the "embed" data card.
  - One cell card with "embu" parameter 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 materials being numbered from 1 to the maximum number of materials.
  - All cell cards with the "embu" parameter must appear first.
  - Immediately following the "embu" parameter cards must be a cell card that serves as a "container" for the embedded mesh. This can be considered the background material in which the mesh resides. This must also have a "u" descriptor.

Embedded Mesh Universe

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- **Cell card requirements (cont.):**
  - After the container cell any number of cells should be OK in the embedded universe.
- **Example:**

```
c     *** Cell cards ***
c
     10      2  -7.8240  -8       embu=1  u=2
     11      1  -1.2230  -8       embu=1  u=2
     12      2  -7.8240  -8       embu=1  u=2
     13      3  -0.0012  -8       embu=1  u=2
     14      0           -8               u=2
     15      0            8  -9           u=2
     20      0          -10       fill=2
      6      0       10 -11
      7      0           11
```

Embedded Mesh Universe

Surface – To – Surface Tracking

- Change the "embu" parameter from postive to negative.
- Example:

```
c      *** Cell cards ***
c
       10    2  -7.8240  -8       embu=1    u=2
       11    1  -1.2230  -8       embu=-1   u=2
       12    2  -7.8240  -8       embu=1    u=2
       13    3  -0.0012  -8       embu=-1   u=2
       14    0           -8                 u=2
       15    0            8  -9             u=2
       20    0          -10       fill=2
        6    0       10 -11
        7    0           11
```

Positive embu value: element-to-element tracking in this cell.

Negative embu value: surface-to-surface tracking in this cell.

Embedded Mesh Data Cards

Embedded Mesh Control Card

`EMBEDn  meshgeo=  mgeoin=  meeout=  meein= length=`

`n`	embedded mesh universe number (only one card currently permitted)
`meshgeo`	mesh geometry type Current permitted values: abaqus
`mgeoin`	mesh input file name
`meeout`	elemental edits output file name
`meein`	elemental edits input file name (valid only in continuation runs)
`length`	conversion factor to centimeters for all mesh dimensions in input and output

NOTE: all filenames must be lowercase

Elemental Edits Control Card

EMBEEn:<pl> embed= energy= time=

`n`	elemental edit number ending in 4, 6, or 7 follows tally convention current maximum of 4 cards
`<pl>`	particle designator from particle list current valid entrees: n or p
`embed`	embedded mesh universe number must correspond to a valid embed card #
`energy`	conversion factor from MeV/gm or jerks/gm for all energy related output
`time`	conversion factor from shakes for all time related output

Elemental Edit Energy Bins & Multipliers

EMBEBn B_1 B_2 ... B_k

`n` elemental edit number; 0 is not valid.

B_i monotonically increasing upper energy of the *i'th* bin.

EMBEMn M_1 M_2 ... M_k

`n` elemental edit number; 0 is not valid.

M_i monotonically increasing upper energy of the *i'th* bin.

Embedded Mesh Data Cards

Elemental Edit Time Bins & Multipliers

EMBTBn B_1 B_2 ... B_k

n — elemental edit number; 0 is not valid.

B_i — monotonically increasing upper time of the *i'th* bin. values in units of shakes (1 shake = 10^{-8} s)

EMBTMn M_1 M_2 ... M_k

n — elemental edit number; 0 is not valid.

M_i — monotonically increasing upper energy of the *i'th* bin.

Concrete Cylinder Example

Concrete Cylinder Geometry

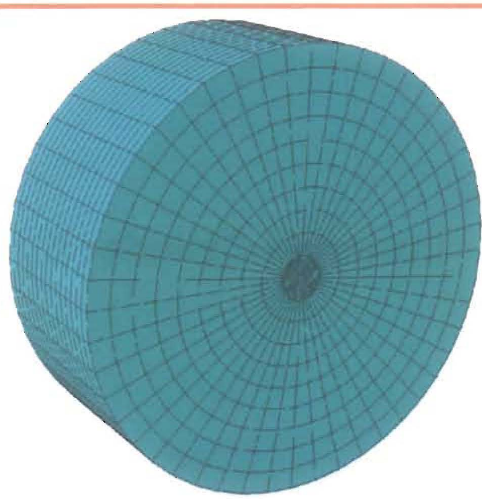
Objective: illustrate some of the mesh features and ABAQUS capabilities.

Concrete Cylinder Geometry

R = 100 cm

H = 80 cm

Source:
2 MeV neutrons;
mono-directional
along Z-Axis



Concrete Cylinder: 1 Part / 2 Mesh Zones

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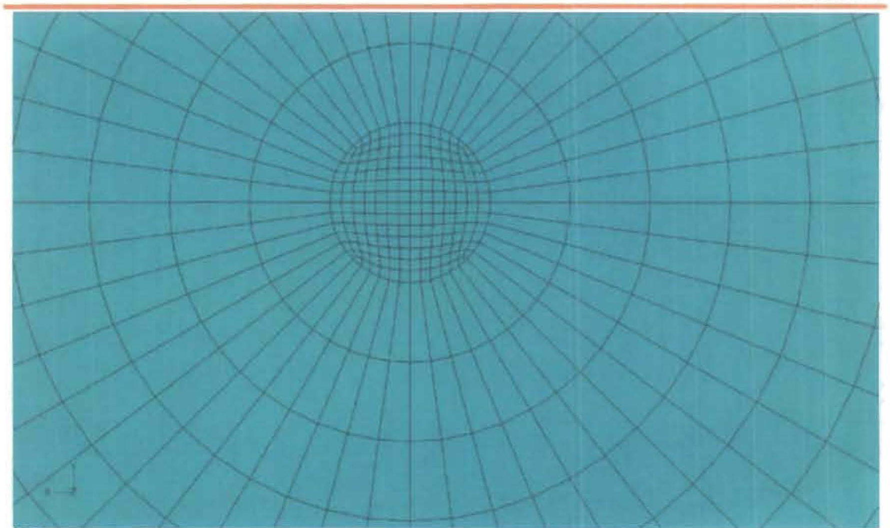

Total Energy Deposition: 3-D View With ¾ Geometry

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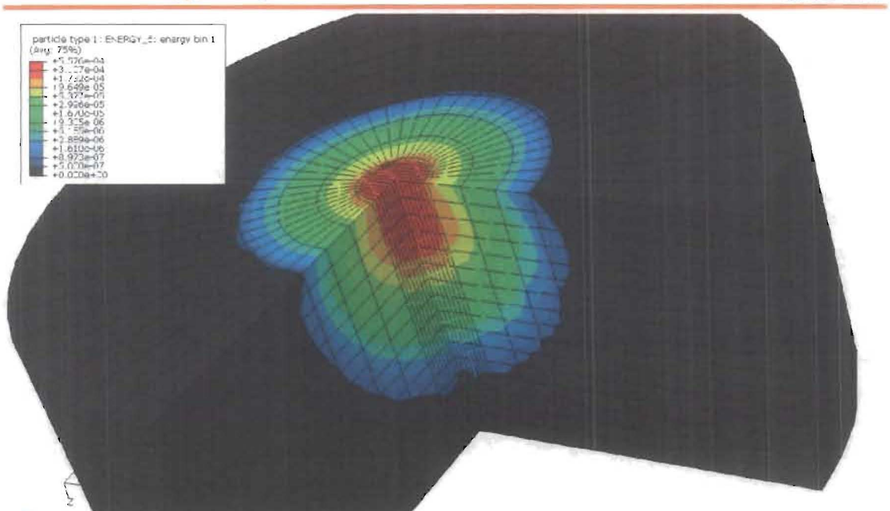

Total Energy Deposition: 3-D View With Half Geometry

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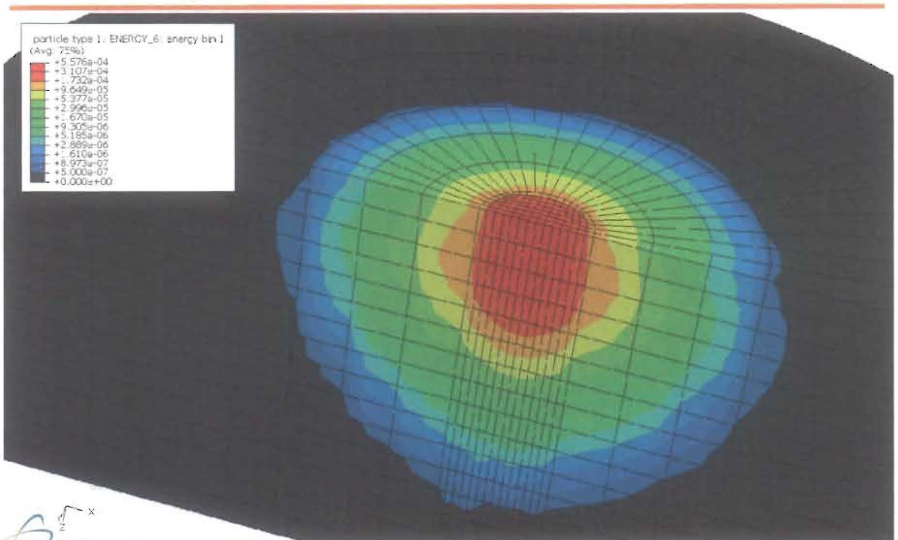

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Total Energy Deposition: 2-D View

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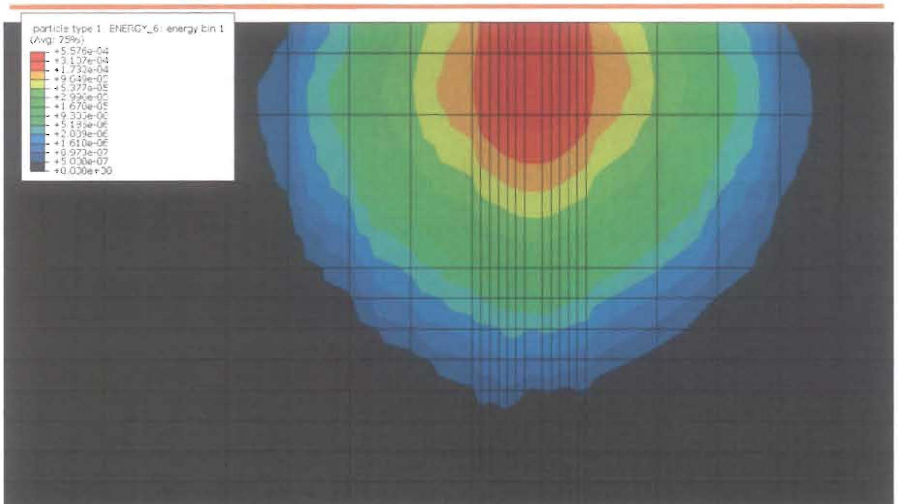

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Concrete Cylinder: total neutron flux & geometry

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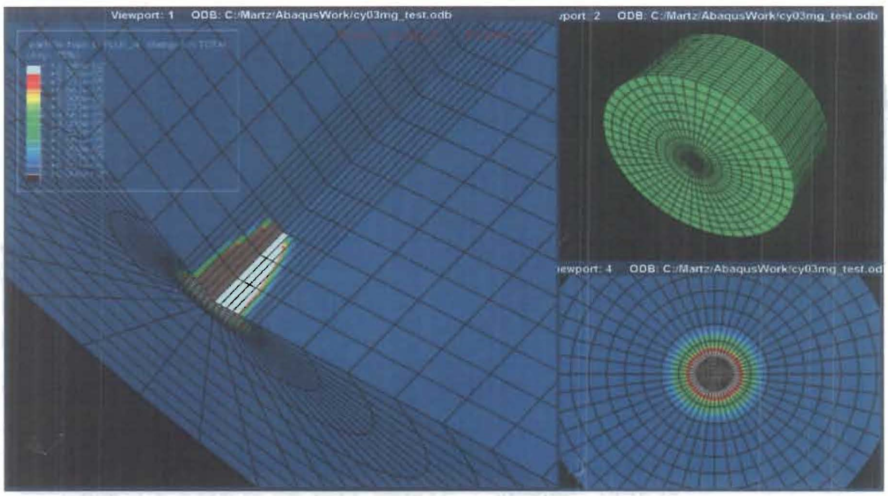

Concrete Cylinder: total neutron flux movie

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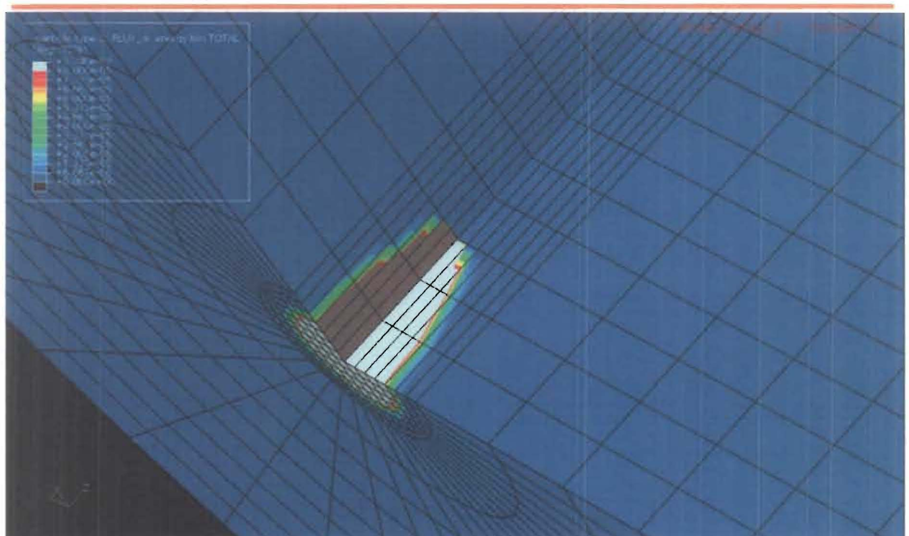
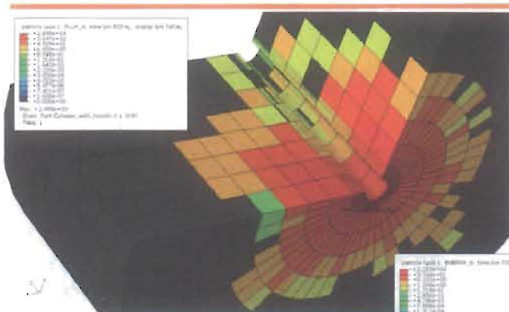
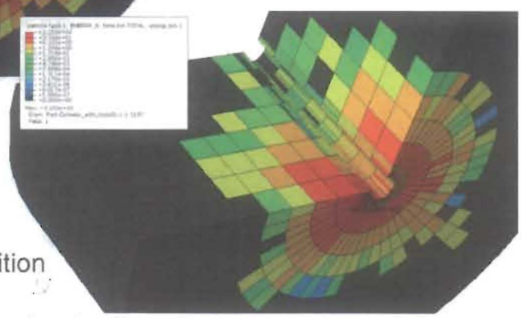


Concrete Cylinder With Penetration (5 cm radius)



Total neutron flux



Total neutron energy deposition

Initial Verification

Initial Verification

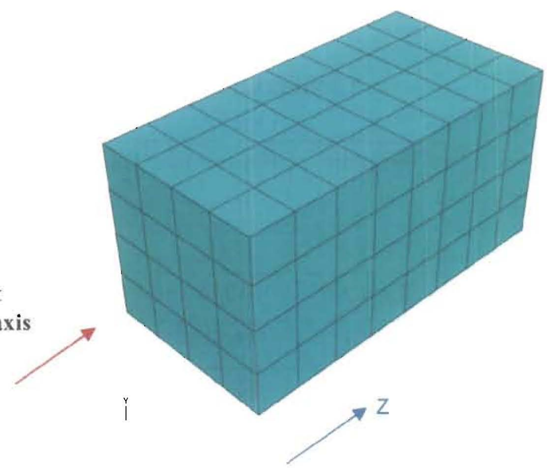
Objective: verify that the mesh tracking is functioning properly.

NOTE: The following calculations were conducted in 2008 and may not reflect current code performance.

Fixed Source Calculations

Concrete slab:
40 cm x 40 cm x 80 cm

2 MeV neutrons @ 4 point source locations clustered at the origin parallel to the Z-axis



Fixed Source Calculations

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Concrete Slab

- **Hex mesh cases:**
  - 10 x 10 x 10; 1 part / 1 instance
  - 5 x 5 x 5; 1 part / 1 instance
  - 2 x 2 x 2; 1 part / 1 instance
- **For each mesh case, create an equivalent MCNP cell model, where <u>each</u> hex mesh element is an MCNP cell.**

Effect Of Increasing Number Of Mesh

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Hex Mesh Results

1 eV – 2 MeV
1 million histories; AMD Opteron 2.2 GHz

Problem	Elements	Element Scaling	Runtime (min)	Runtime Scaling
10 x 10 x 10	128	1	5.96	1
5 x 5 x 5	1024	8	15.5	2.6
2 x 2 x 2	16000	125	131.0	22.0
1 x 1 x 1	128000	1000	1246.6	209.2

Tracking Agreement

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Concrete Slab: Hex Mesh

- Now, create an equivalent MCNP cell model, where each MCNP cell is an ABAQUS® "part".
- Observation: results from tracking on the unstructured mesh elements are identical to the results from tracking with the MCNP cells.

Increase In Runtime

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Concrete Slab: Prism vs. Hex vs. Tet

10 cm faces; 1eV – 2 MeV
1 million histories; AMD Opteron 2.2 GHz

Problem	Mesh Runtime (min)	Cell Runtime (min)	Ratio
Hex	5.96	1.09	5.5
Prism	7.17	1.09	6.6
Tet	9.66	1.09	8.9

Effect Of Increasing Number Of Mesh Thru Types

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Hex vs. Prism vs. Tet: Another View

10 cm faces; 1eV – 2 MeV
1 million histories; AMD Opteron 2.2 GHz

Problem	Elements	Element Scaling	Runtime (min)	Runtime Scaling
Hex	128	1	5.96	1
Prism	256	2	7.17	1.2
Tet	640	5	9.66	1.6

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Increase In Runtime

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Concrete Slab: Influence of Contact Pairs

10 x 10 x 10 Hex elements; 1 eV – 2 MeV
1 million histories; AMD Opteron 2.2 GHz

Problem	Mesh Runtime (min)	Cell Runtime (min)	Ratio
No contact pair surfaces	5.96	1.09	5.5
3 contact pair surfaces	12.74	1.09	11.7

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Criticality Calculations

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Uranium Slab

10 x 10 x 10 Hex elements; 128 total
120 cycles; 20 discarded cycles; 2000 histories/cycle
AMD Opteron 2.2 GHz

Case	Eigenvalue	Uncertainty	Time (min)	Runtime Scaling
4 cells	1.67934	0.00147	0.19	1.0
4 parts	1.67934	0.00147	2.90	15.3
1cell	1.67411	0.00189	0.19	1.0
1 part	1.67411	0.00189	0.87	4.6
lattice	1.68257	0.00188	0.28	1.5

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Criticality Calculations

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Uranium Slab

Hex elements
120 cycles; 20 discarded cycles; 2000 histories/cycle
AMD Opteron 2.2 GHz

Problem	Elements	Element Scaling	Runtime (min)	Runtime Scaling
10 x 10 x 10	128	1	0.87	1
5 x 5 x 5	1024	8	2.12	2.4
2 x 2 x 2	16000	125	19.64	22.6

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Godiva Sphere

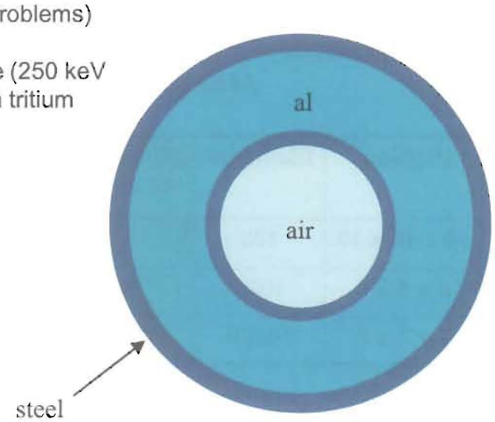
120 cycles; 20 discarded cycles; 5000 histories/cycle
AMD Opteron 2.2 GHz

Case	Hex Elements	Eigenvalue	Uncertainty	Volume (cm^3)	Time (min)
1	1536	0.99576	0.00086	2.74413E+3	4.96
2	5096	0.99771	0.00079	2.77201E+3	10.60
3	11664	0.99883	0.00089	2.77938E+3	21.98
4	35984	1.00011	0.00082	2.78615E+3	63.29
5	73984	0.99692	0.00088	2.78892E+3	119.14
REF	1 Cell	1.00209	0.00087	2.79751E+3	0.28

Osaka Aluminum Sphere

(From SINBAD Benchmark Problems)

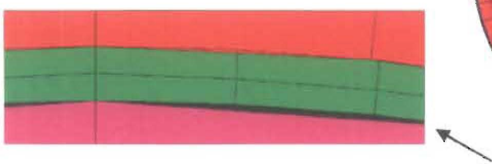
D-T neutron generator source (250 keV deuteron beam bombarding a tritium target) at center of air cavity

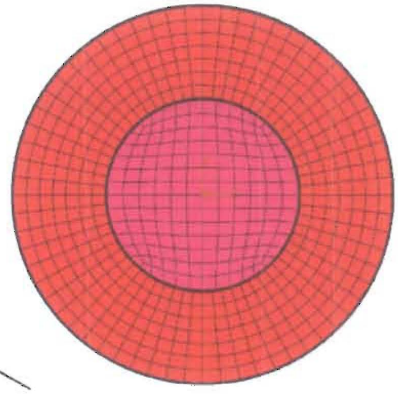


Fixed Source Benchmark

Osaka Aluminum Sphere

4 parts; 72104 hex elements





Gaps & Overlaps

Embedded Mesh Capability For MCNP6

Conclusions From This Work

- **The new mesh capability is working correctly in the sequential version.**
- **Tracking on the unstructured mesh is more expensive.**
  - modeling considerations or "style" has impact on runtime
- **Optimization of the mesh tracking routines is needed.**
- **More verification is required.**

Code Design & Implementation

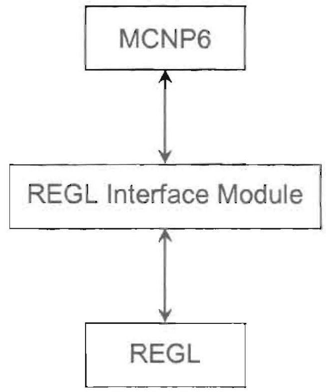
Code Design & Implementation

Objective: discuss some high-level code issues.

Modular Design

The REGL

- not dependent on MCNP
- useable by any code that adheres to its interface
- the calling code provides / receives a minimum amount of information to / from the library



Division of Responsibilities

The REGL handles

- its own memory management
- reading / writing "mesh" files
- all mesh tracking functions / edits on mesh
- passes error codes, etc. back to calling code

MCNP handles

- user interface for input
- provides necessary data & parameters
  - e.g., distance to collision, output file unit number, editing cross sections
- receives tracking results
  - e.g., position, next cell number, error codes

Affected MCNP6 Routines / Files

LA-UR-09-00???

- **User interface / input**
  - chekit, newcrd, oldcrd, nextit, nxtit1, newcd1, mcnp_input, pass1, rdprob, imcn
- **Parallel**
  - msgcon, msgtsk
- **Memory**
  - fixcom, pblcom, setdas, expung
- **Source**
  - sourcb, sourck, crit1_mod, acegam, colidk
- **Transport / Tracking**
  - hstory, mcrun, startp
- **Other**
  - prinv, tpefil, bankit

- **Added**: regl_interface_mod (1824 lines of code)

Some Conventions

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- **MCNP variables**
  - declared in MCNP routines and adhere to MCNP convention
- **regl_interface_mod**
  - public variables declared here begin with `rgli_`
  - public subroutines & functions begin with `rgli_`

    `rgli` = Revised Grid Library Interface
- **REGL**
  - public subroutines & functions begin with `regl_`

    `regl` = Revised Eolus Grid Library
  - library variables should not be accessed directly

REGL Module Overview

LA-UR-09-00???

Lines of Code	Module	Function
3366	regl_read_abaqus_mod	ABAQUS input parser
2903	regl_isoparametric_mod	bi-linear / tri-linear intersection
1418	regl_track_mod	mesh tracking
1093	regl_load_mod	mesh setup / take down / I/O
931	regl_graphics_edit_mod	graphics & editing
793	regl_skdtree_mod	build / manipulate skd-tree
616	regl_hit_mesh_mod	handles entering the mesh
271	regl_global_mod	memory management
118	regl_find_mesh_mod	locating points in elements
630	regl_utilityl3_mod	high-level utilities
972	regl_utilityl2_mod	mid-level utilities
766	regl_utilityl1_mod	low-level utilities

13877 lines of code, including comments. ~10-20% of which can be deprecated and removed. Not current.

Handling The Mesh

LA-UR-09-00???

Spatial KD-Tree (SKD-Tree)

- **The kd-tree is well know as an effective data structure for storage & manipulation of point objects.**
  - considered unsuitable for non-zero sized objects
- **skd-tree is an extension, using a spatial discriminator, that supports efficient containment & intersection searches.**
  - eliminates duplication of objects that extend over multiple sub-spaces

Handling The Mesh

LA-UR-09-00???

Spatial KD-Tree (SKD-Tree)

- Assume mesh object contains `N` mesh elements.
- Associated with each element (i.e., tree node) is a safety box which is the smallest rectangular box (parallel to the 3 coordinate axes) which fully encloses all mesh elements in the sub-tree.
- Associate with each element is a "key" which is the element centroid.
- By alternately finding the median coordinate of the keys in the 3 coordinate directions, we keep bisecting the set of keys.
- This tree is a balanced binary tree with exactly `2N-1` nodes on $\log_2 N$ levels, allowing searching in logarithmic time.
- The tree is constructed in $O(N \log_2 N)$ time.
- The collection of nested overlapping boxes guarantees that queries are rigorous and free of "collisions".

Tracking On The Mesh

LA-UR-09-00???

Isoparametric Methods

- Intersection and containment routines (for each mesh type) using methods similar to those used by finite element codes such as ABAQUS.

Accomplishments

Accomplishments

Important Development Milestones To Date:

1. **Methods for "working with" unstructured mesh researched and programmed.**
   - Implemented with planar and bilinear surfaces for intersection & containment
   - skd-tree for searching mesh
   - Contact pairs, re-entrant particles, gaps / overlaps
2. **ABAQUS input parser**
3. **Mesh edit results file & visualization**
4. **Serial, omp, and mpi versions of the code are being tested.**
5. **Presented some preliminary results at the ANS RPSD08 meeting**

Near Term Goals

Near Term Goals

Next Several Months

1. Continue testing & "bug" fixing
2. Resolve integration issues
3. Present user interface to MCNP Change Control Board
4. Implement surface-to-surface fast tracking
5. Implement quadratic surfaces
6. Technical society presentations
7. Documentation
8. Interest others in using these tools or fund further development