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Title: MCNP6: Unstructured Mesh -- Current Capabilities

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Intended for: Poster

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Unstructured Mesh – Current Capabilities

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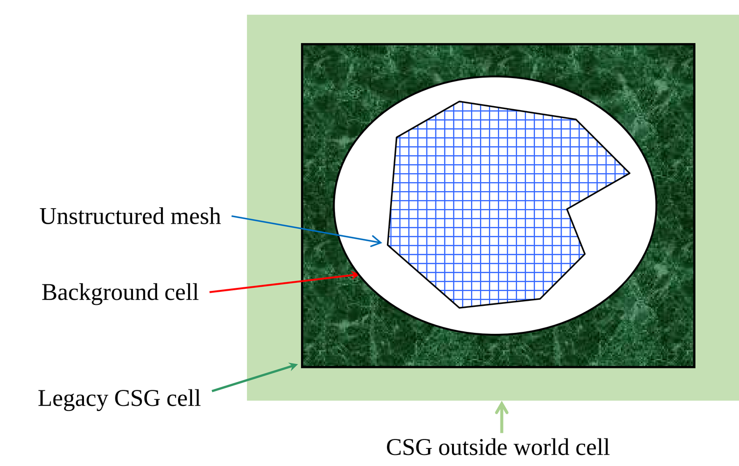
May 2015

LA-UR-15-22871

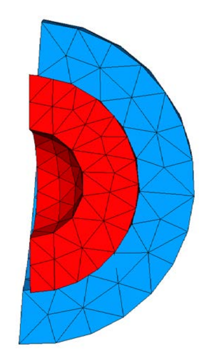
Unstructured Mesh Capability

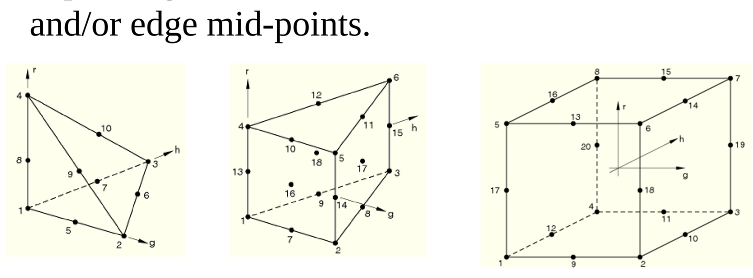
- An unstructured mesh (UM) representation of the geometry is embedded in a traditional (CSG) MCNP mesh universe giving rise to a hybrid geometry arrangement.
- Any degree of complexity in either geometry type is permitted.



Some of the Initial Requirements

- Track through overlaps & gaps in a non-contiguous mesh.
- Accumulate results on the mesh and output to a special file (eeout) for post-processing
- Support unstructured polyhedrons with 4-, 5-, and 6-sides (all in one model). Surfaces may be bilinear or quadratic depending on the number of nodes. Nodes are vertices and/or edge mid-points.





This is the only Monte Carlo radiation transport code on the entire planet that has this capability.

How are the models created?

A computer aided engineering (CAE) tool such as Abaqus/CAE or CUBIT can be used to create a 3-D solid model of the entity of interest.

or

A computer aided design (CAD) tool such as SolidWorks or SpaceClaim can create the 3-D solid model for import into the Attila4MC GUI for MCNP problem setup.

Recent Feature Additions

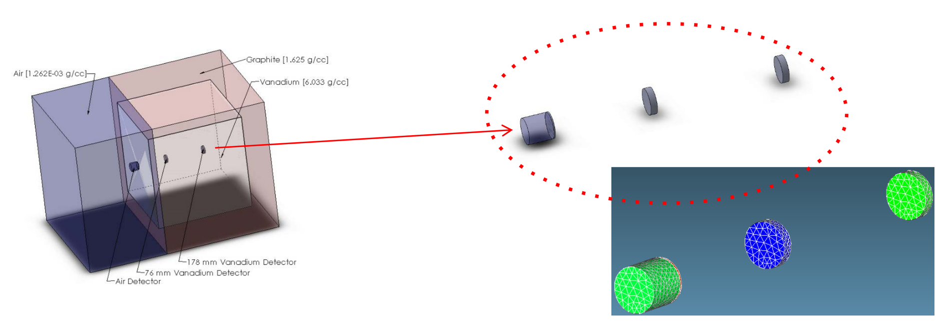
- Weight windows
- Supports multiple mesh geometries from different file reads
- Improved tracking for electrons and heavy charged particles
  All particle types now use the same top-level, UM tracking routine
- Allow non-uniform sampling of UM volume sources
- Select overlap treatment by part
- DXTRAN and point detector support
- Checking of twisted & deformed elements with the um_pre_op utility

Recent Important Bug Fixes, etc.

- Improved charged particle energy deposition
- Improved memory management
  Reduction by 20-50% of memory needed for calculations
- Improved background region tracking – now with an actual material assignment
- Resolved several tracking issues because of round off – includes handling large-sized mesh elements
- Fix so that F8 tallies work with UM
- UM coding is Fortran 2003 compliant

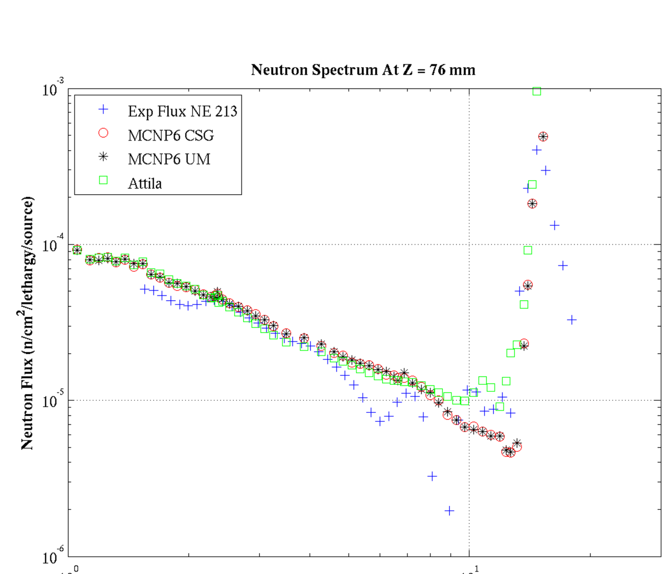
V&V with Vanadium Cube Benchmark

- Vanadium cube benchmark experiment from the Fusion Neutronics Source facility Japan Atomic Energy Research Institute.
- MCNP6 and Attila models developed from a single CAD model and used the same unstructured tet mesh.
- MCNP6 and Attila inputs prepared with the Attila4MC GUI.



- 47,640 tet (1st order) mesh elements
- Attila: S24 triangular Chebychev-Legendre quadrature, P4, Galerkin scattering treatment, FENDL-2.1 multigroup cross sections (175 neutron/42 gamma)
- MCNP6: 3E8 histories, ENDF/B-VII cross sections (for available isotopes)

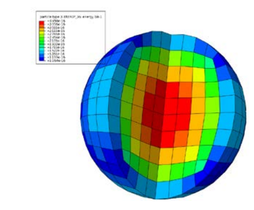
See: Proceedings of the ANS, 2013 National Meeting



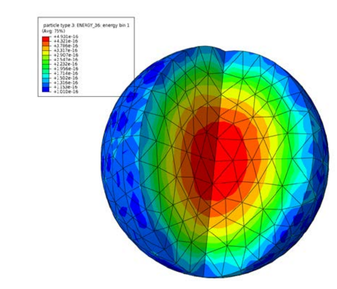
2nd Order Polyhedra Improve MCNP Mesh Calculations

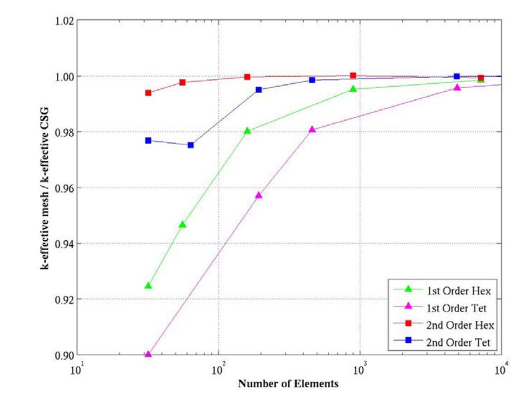
- Second order tetrahedral and hexahedral mesh elements more accurately reproduce the volume of curved objects.
- Fewer number of second order elements are required compared to first order.
- Fewer number of second order elements mean shorter calculation times by an order of magnitude to obtain the right answer with the same precision.

For more information see: LA-UR-09-7320



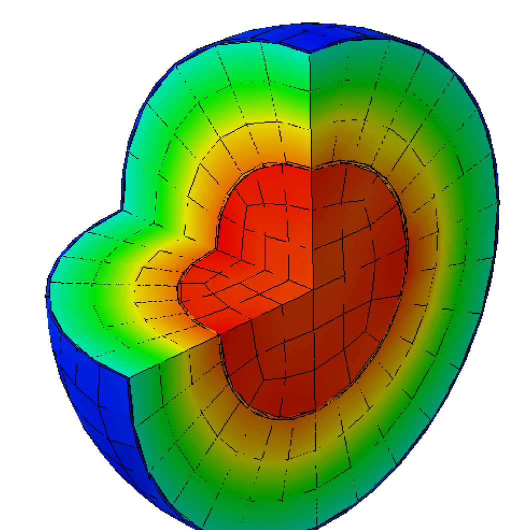
Godiva criticality benchmark sphere





Parallel Input

- UM problem setup requires nested-loops in several parts of the code. These loops can be time-intensive.
- Can speed this up by running mpi.
  - Want 1 mpi slave node for each instance. The minimum number of mpi processes to specify should be 1 + number of instances in the model.
  - Each instance or part will then have a dedicated processor for its input. At this time, multiple processors per instance or part are not implemented and there is no load balancing.
  - Still limited by the instance / part with the largest number of elements.
- The most efficient parallel input processing takes place when all parts have approximately the same number of elements and there is more mpi processes than instances.
  - < ~30,000 elements per part is a key number for efficient input processing.
  - When there are fewer processes than instances – divide and conquer.



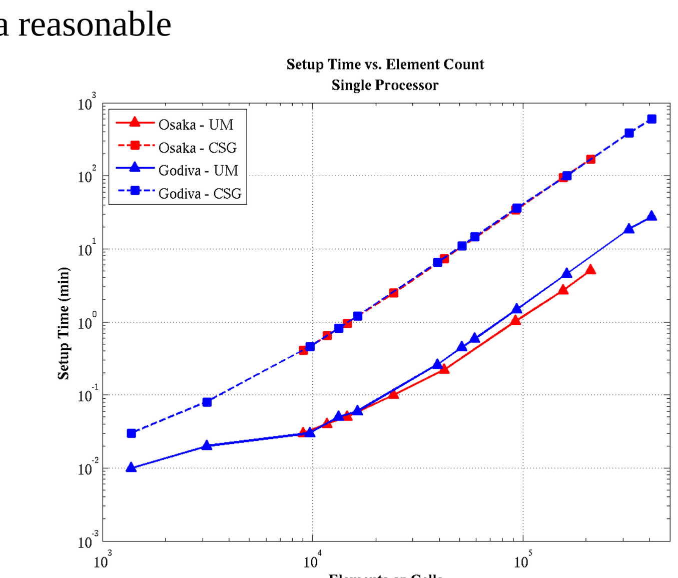
Osaka Benchmark Spheres

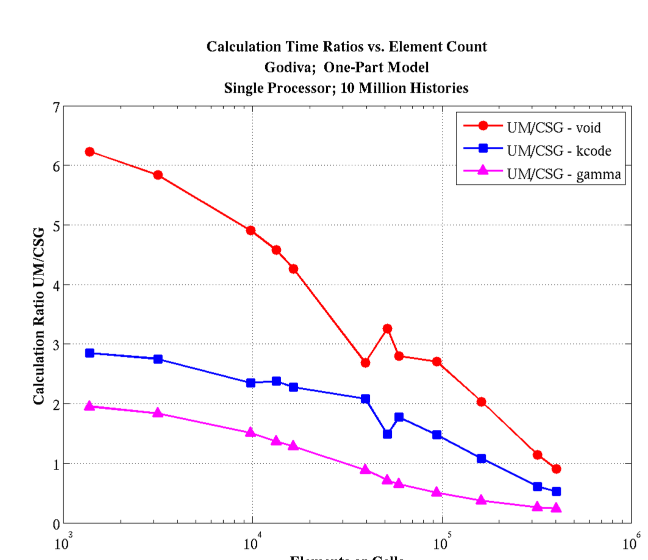
CSG and UM Performance Comparison

Figures below 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 in CSG using combinations of arb surfaces.
  - Thanks to Kevin Marshall, et al., of the Radiation Science's Group, AWE Plc. for providing the program to convert the Abaqus .inp file into an MCNP CSG input deck.
- 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.

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





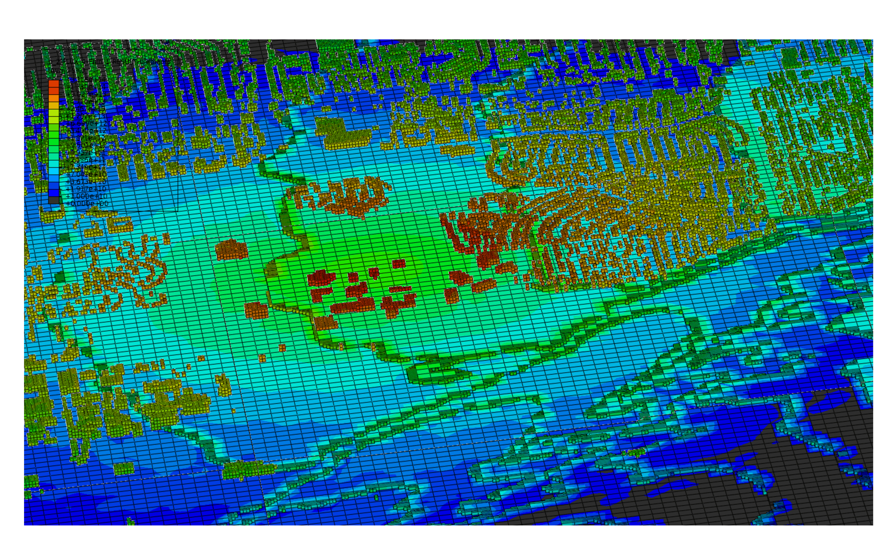
As the problem detail increases, UM calculation times are shorter compared to CSG.

- Void geometry is limiting case.
- Which "physics" in use affects performance.

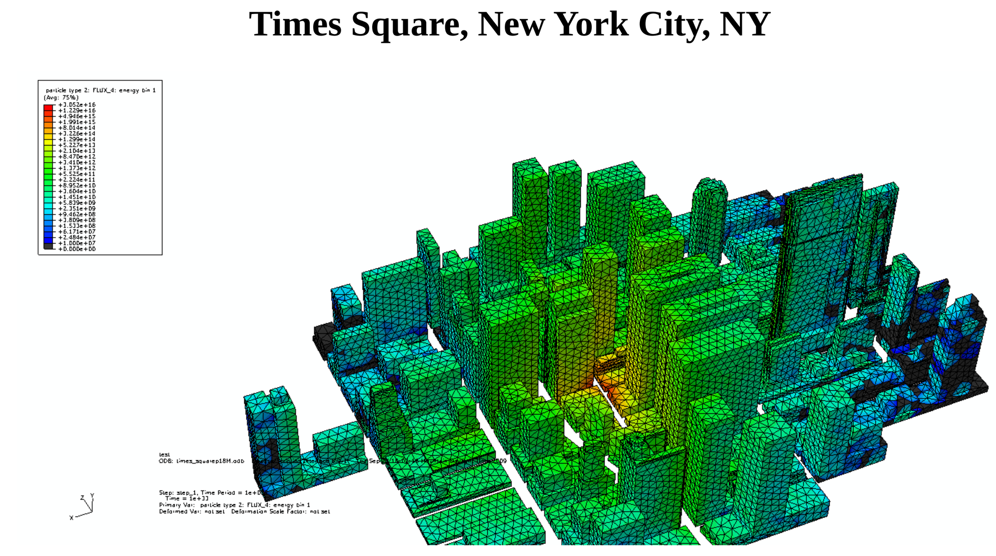
See: *Nuclear Technology*, Vol. 184, Nov. 2013.

Gamma flux from simulated "Fat Man-like" explosions

Kirtland, AFB, Albuquerque, NM

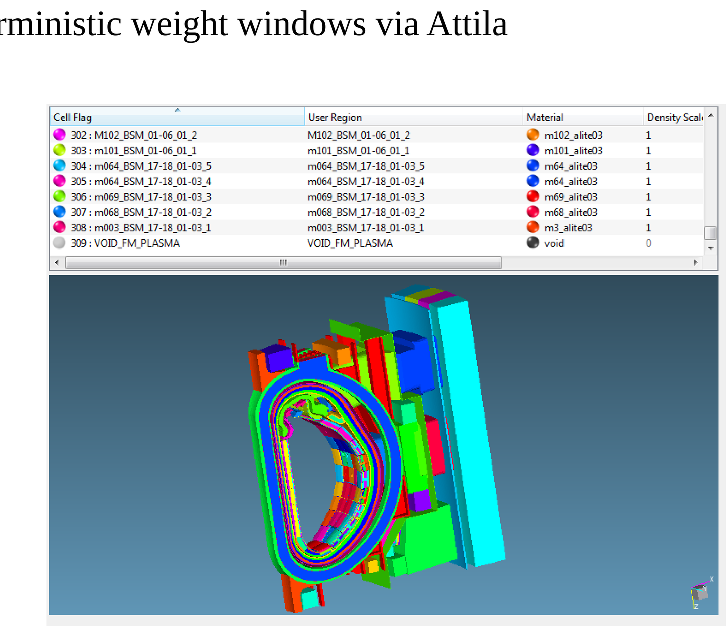


Times Square, New York City, NY



Varian Medical's Attila4MC Setup Tool for MCNP6

- Generate geometry with SpaceClaim or Solidworks. (alternative to Abaqus/CAE)
- Generate mesh with Simmetrix mesher in Attila4MC.
- Setup MCNP6 input via Attila4MC GUI.
- Generate deterministic weight windows via Attila



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.