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Title: MCNP6.3 Unstructured Mesh Performances

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MCNP6.3 Unstructured Mesh Performances

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LA-UR__

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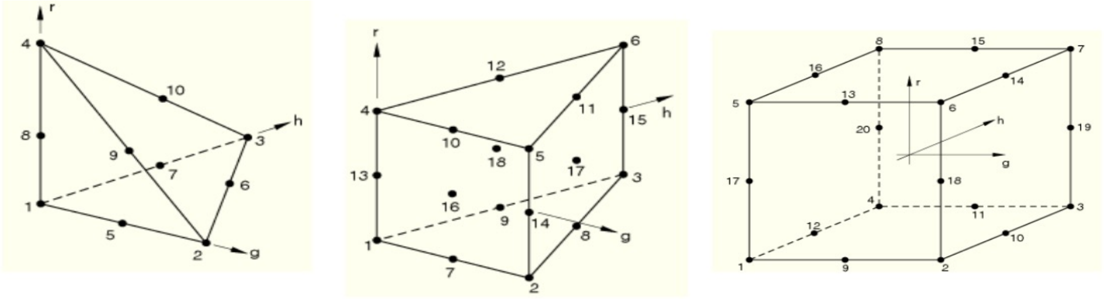
Unstructured Mesh (UM) Models

- **MCNP UM calculations require UM models created by other codes (not developed by the MCNP team). Element types must be selected when generating UM models.**
- The number of nodes and nodal locations define an element type.
  - Linear tetrahedron: 4 faces, 4 nodes at the vertices
  - Linear pentahedron: 5 faces, 6 nodes at the vertices
  - Linear hexahedron: 6 faces, 8 nodes at the vertices
  - Quadratic tetrahedron: 4 faces, 10 nodes at the vertices & on the edges midway between the vertices
  - Quadratic pentahedron: 5 faces, 15 nodes at the vertices & on the edges midway between the vertices
  - Quadratic hexahedron: 6 faces, 20 nodes at the vertices & on the edges midway between the vertices



Improvement in MCNP6.3 Unstructured Mesh Feature

- Element types used in UM models are problem-dependent. Linear hex and linear tet UM models are widely used.

- For comparable mesh qualities, linear tet models are typically larger than linear hex models.

- Code changes were made in MCNP6.3 to speed up calculations of linear hex and linear tet UM models.

- MCNP HDF5 UM input & output models (MCNP6.3 feature) can be visualized by ParaView.

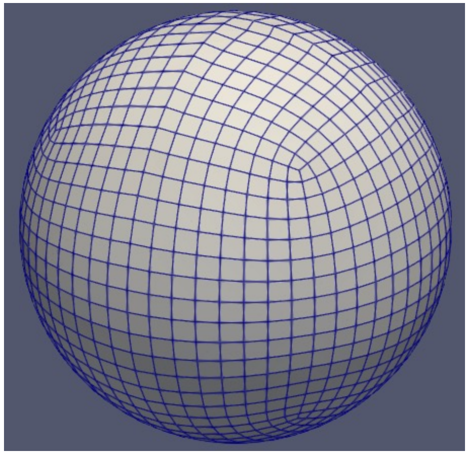
Godiva Sphere: ICSBEP Name = HEU-MeT-FAST-001

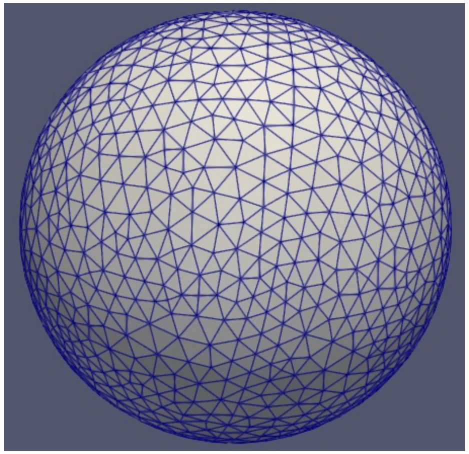
- Solid Model: HEU sphere with 8.7407 cm radius
- UM models were generated by Abaqus.

Geometry Type	# elements	# nodes	Volumes (cc)	Mass (g)	um/solid (mass)
Solid	N/A	N/A	2.79722E+03	5.24202E+04	
Linear Hex	7168	7989	2.78540E+03	5.21987E+04	0.995775
Linear Tet	35453	6584	2.78434E+03	5.21789E+04	0.995397
Quad Hex	7168	31081	2.79721E+03	5.24201E+04	0.999998
Quad Tet	35453	49940	2.79722E+03	5.24201E+04	0.999998

Same volumes & masses of UM models calculated by MCNP6.2 & MCNP 6.3

linear hex





linear tet

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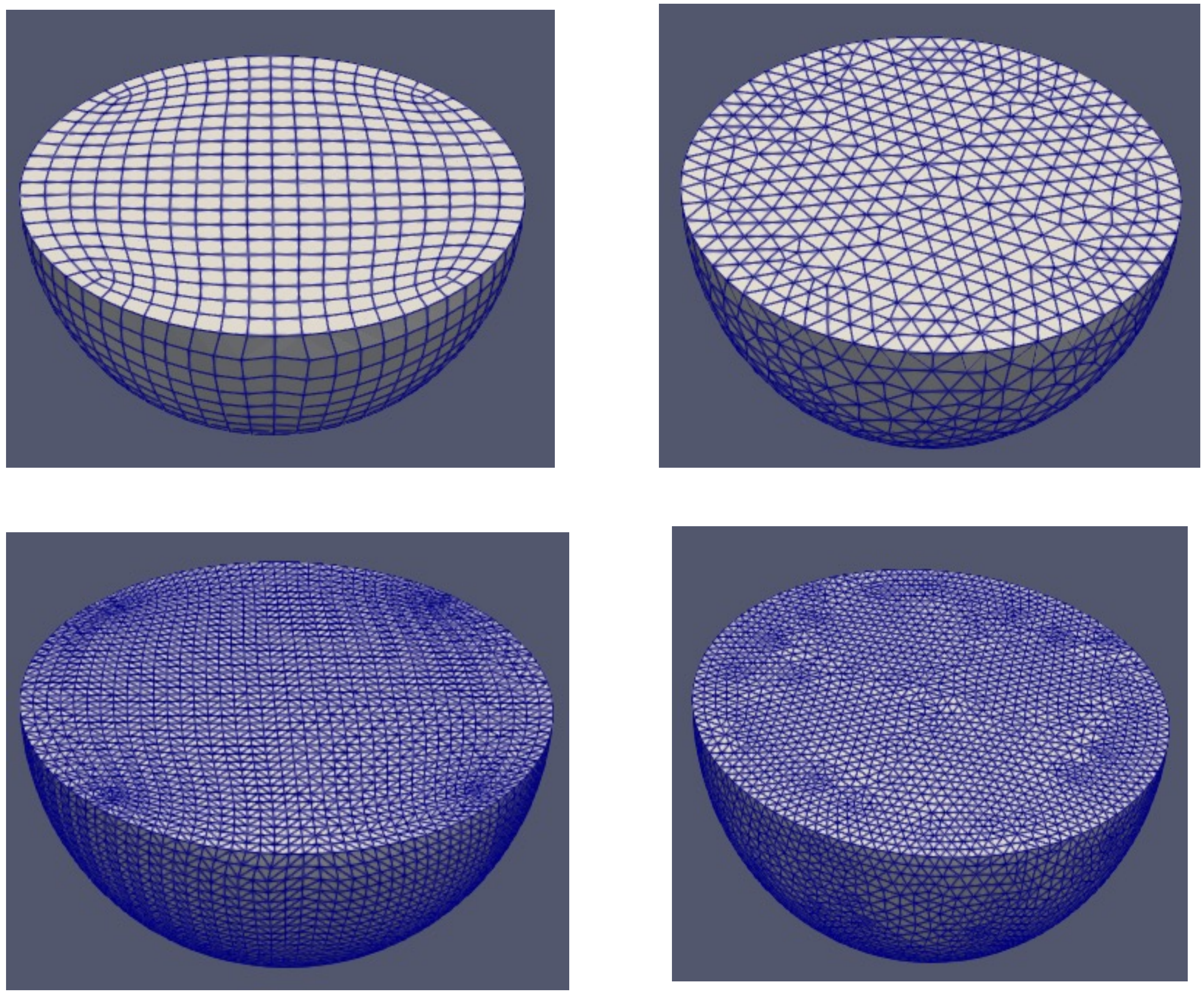
Godiva: UM Models Visualized by ParaView

linear

quadratic



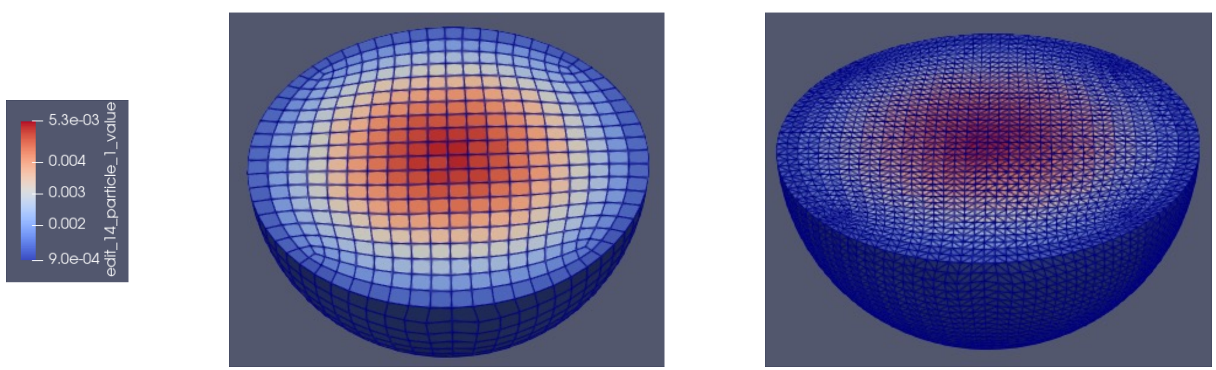
hex

tet

Godiva: MCNP6.2 & MCNP6.3 Results

- KCODE 10000 1 20 220; ENDF/B-VIII.0, Sequential run
- KEFF experiment value: 1.0023 (std dev = 0.0031)

	MCNP6.2		MCNP6.3	
	KEFF	Std Dev	KEFF	Std Dev
Linear Hex	0.99953	0.00044	0.999529	0.000439
Linear Tet	0.99886	0.00042	0.998858	0.000419
Quad Hex	0.99992	0.00041	0.999703	0.000420
Quad Tet	0.99987	0.00042	0.999869	0.000416



Neutron Fluence (n/cm^2)

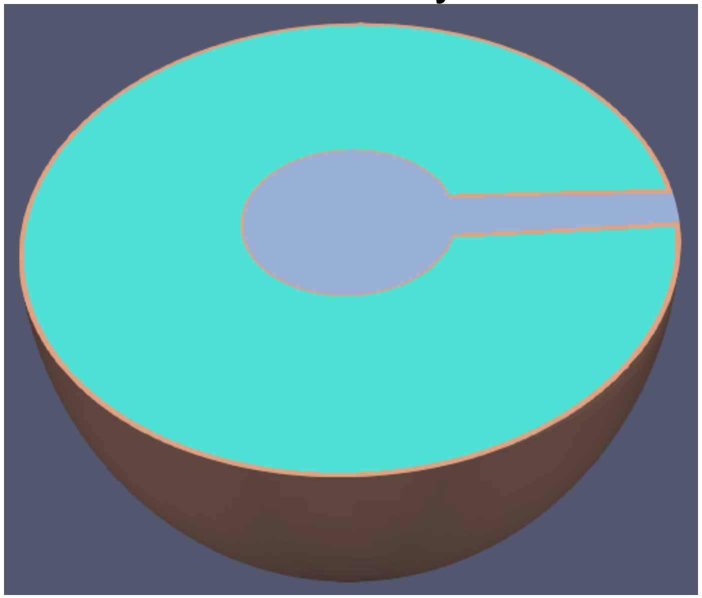
Godiva: MCNP6.2 & MCNP6.3 Computing Times

	6.2 Computing Time	6.3 Computing Time
Linear Hex	00:06:54	00:05:24
Linear Tet	00:08:20	00:06:12
Quadratic Hex	01:37:45	01:29:32
Quadratic Tet	01:07:59	01:02:41

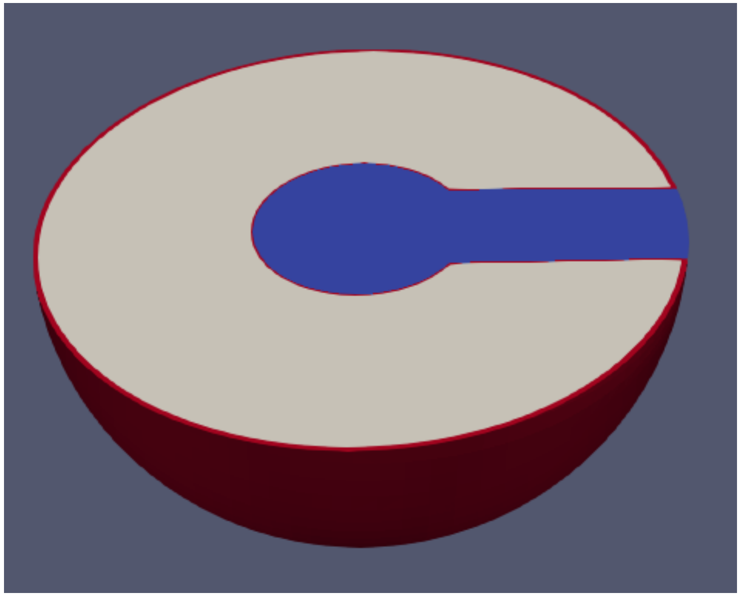
- For linear hex and tet, MCNP6.3 is faster than MCNP6.2.
- For quadratic hex and tet, MCNP6.2 and MCNP6.2 computing times are comparable. **No code changes were made in MCNP6.3 for quadratic element types.**
- For linear models, calculations of hex models are faster than calculations of tet models.
- Calculations of quadratic element models are significantly slower than calculations of linear element models. **Thus, quadratic element models are currently not used for large complex geometries.**

SINBAD Molybdenum and Silicon Oktavian Models

- Fixed source problems; 14 MeV D-T neutron source were in a center; F1Tally (sphere surface outside the Oktavians).
- UM Models (linear tet & linear hex) were generated by Cubit.
- MPI run (36 processes) on LANL HPC snow.
- Micky Dzur will present the MCNP6.3 verification of CSG and UM Oktavian models on Wednesday.



Mo

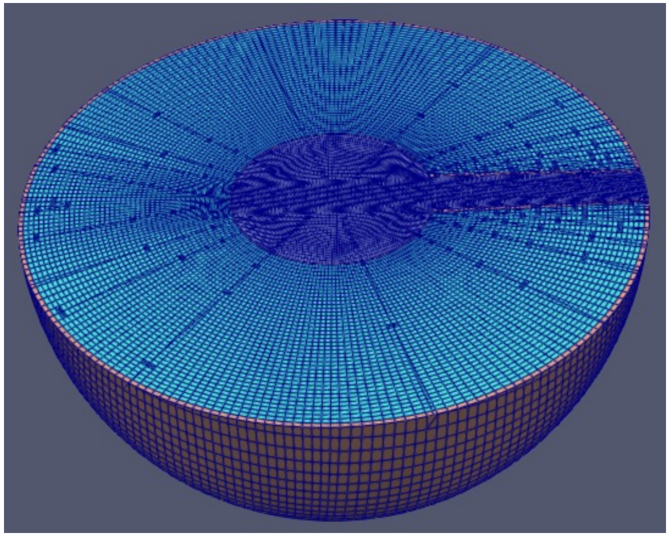


Si

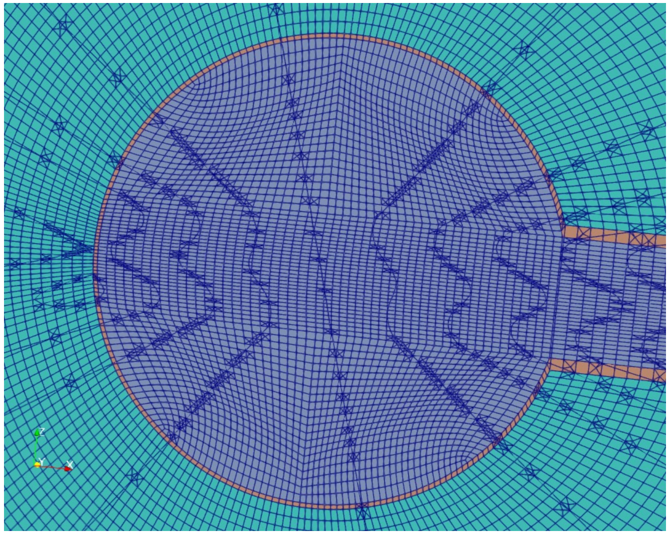
Mo Oktavian: Linear Hex Model

MCNP6.3 is significantly faster for not a *clean* UM model.

- Model:
  - Number of elements = 702800
  - Number of nodes = 752503
- Computing Time (wall-clock):
  - MCNP6.2 = 02:56:42
  - MCNP6.3 = 00:43:30
- F41:p Figure of Merit:
  - MCNP6.2 = 13140
  - MCNP6.3 = 15928



Mat	Solid Vol (cc)	Meshed Vol (cc)	Mesh Vol/ Solid Vol
Mo	1.13804E+05	1.13719E+05	0.99925
Air	4.62006E+03	4.61679E+03	0.99930
Steel	6.36418E+03	6.35946E+03	0.99926



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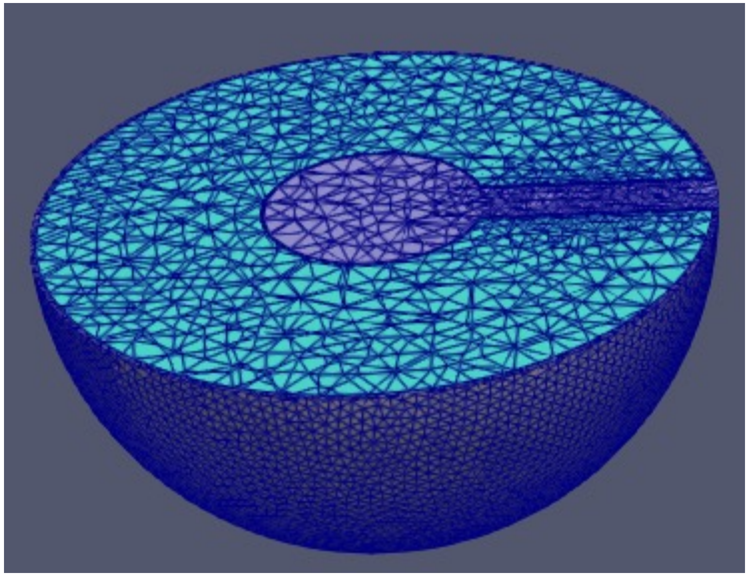
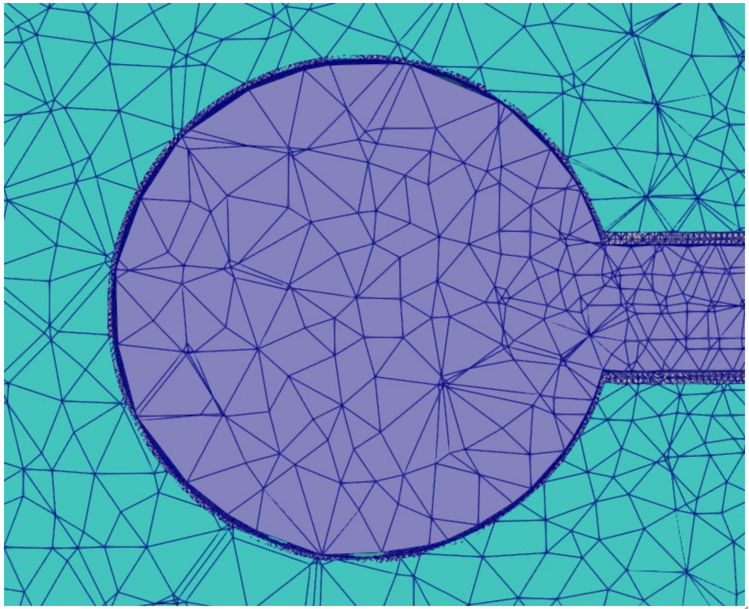
Not a clean UM model;
Overlap regions on steel shell

Mo Oktavian: Linear Tet Model

- Model:
  - Number of elements = 314135
  - Number of nodes = 93872
- Computing Time (wall-clock):
  - MCNP6.2 = 01:34:54
  - MCNP6.3 = 01:16:43
- F41:p Figure of Merit:
  - MCNP6.2 = 11165
  - MCNP6.3 = 12369

Mat	Solid Vol (cc)	Meshed Vol (cc)	Mesh Vol/ Solid Vol
Mo	1.13804E+05	1.13435E+05	0.99676
Air	4.62006E+03	4.44270E+03	0.96161
Steel	6.36418E+03	6.36336E+03	0.99987





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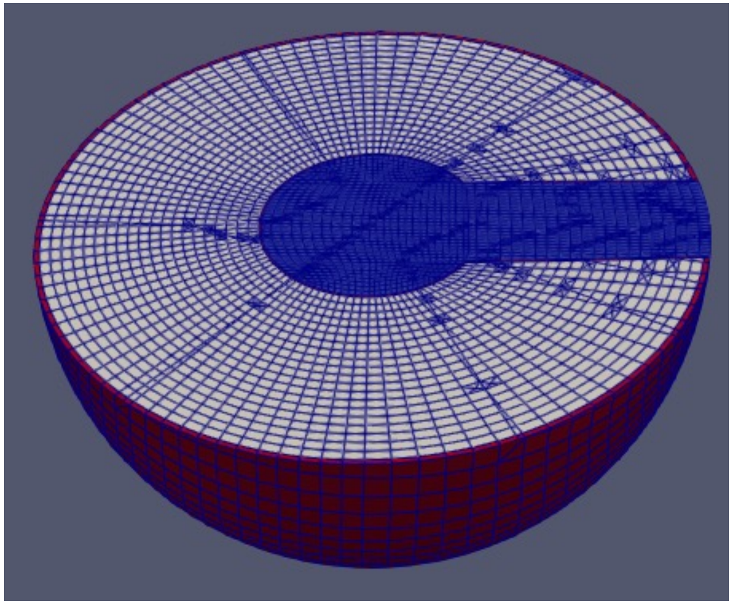
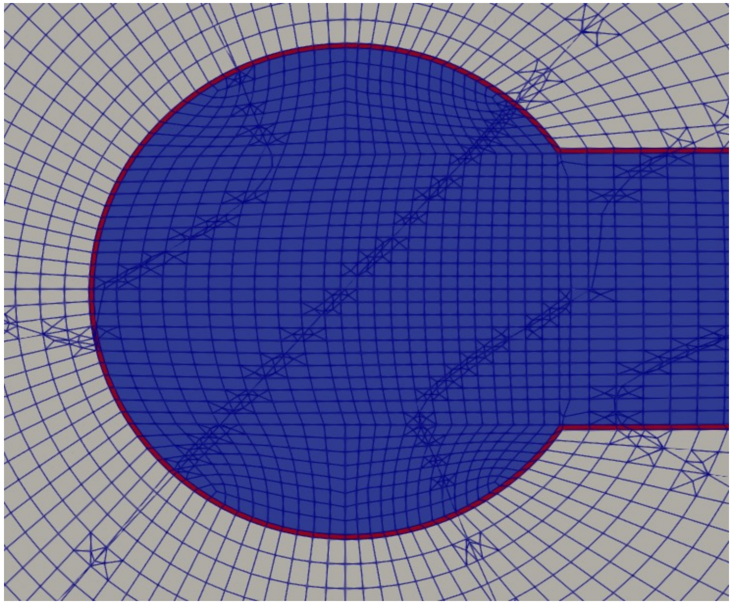
Si Oktavian: Linear Hex Model

- Model:
  - Number of elements = 111200
  - Number of nodes = 126712
- Computing Time (wall-clock):
  - MCNP6.2 = 00:46:21
  - MCNP6.3 = 00:35:42
- F41:p Figure of Merit:
  - MCNP6.2 = 38837
  - MCNP6.3 = 48163

Mat	Solid Vol (cc)	Meshed Vol (cc)	Mesh Vol/ Solid Vol
Si	1.06535E+05	1.06302E+05	0.99781
Air	6.22685E+03	6.21731E+03	0.99847
Steel	6.08503E+03	6.07160E+03	0.99779





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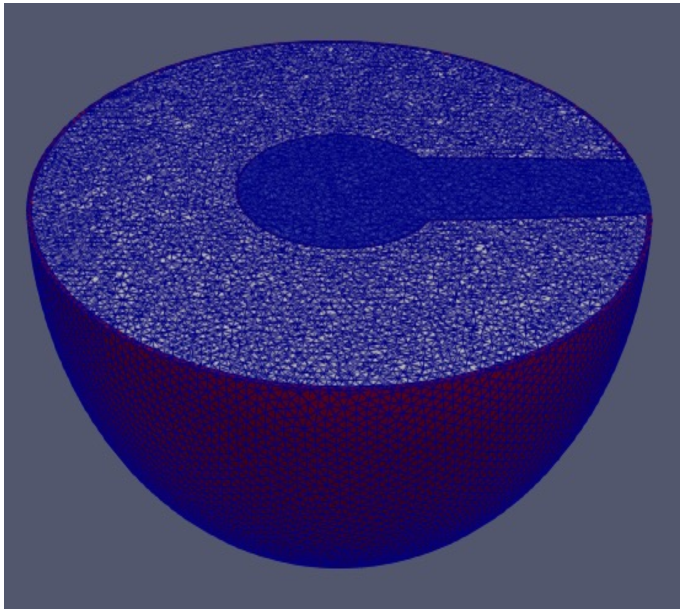
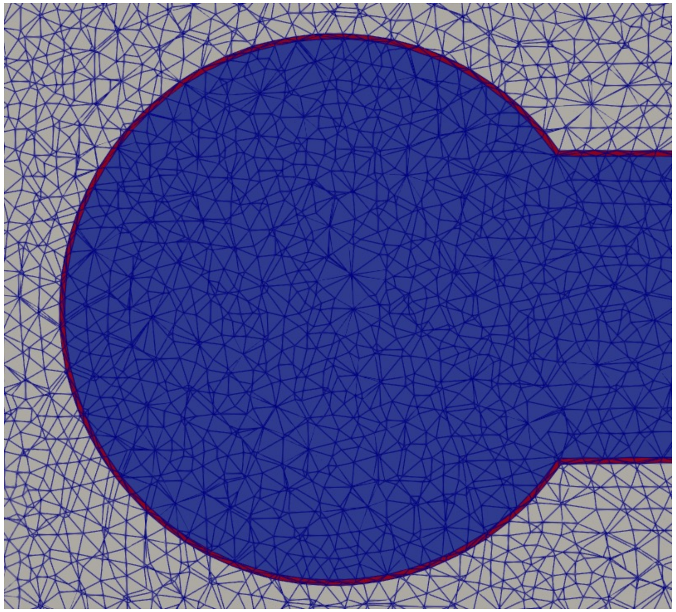
Si Oktavian: Linear Tet Model

- Model:
  - Number of elements = 1036892
  - Number of nodes = 198905
- Computing Time (wall-clock):
  - MCNP6.2 = 04:11:11
  - MCNP6.3 = 01:12:28
- F41:p Figure of Merit
  - MCNP6.2 = 20952
  - MCNP6.3 = 24924

Mat	Solid Vol (cc)	Meshed Vol (cc)	Mesh Vol/ Solid Vol
Si	1.06535E+05	1.06512E+05	0.99978
Air	6.22685E+03	6.20313E+03	0.99619
Steel	6.08503E+03	6.08461E+03	0.99999

MCNP6.3 is significantly faster for a large model.





Conclusion

- Code changes were made to MCNP6.3 to speed up calculations of linear tet and linear hex models.
- Running test problems showed that MCNP6.3 calculations were faster than MCNP6.2 calculations.
- For large models with comparable mesh qualities, calculations of linear hex models are significantly faster than calculations of linear tet models.
- Future work is to develop a new tracking method for linear hex models to improve the performance and memory usage.
  - Linear hex models are typically used for large complex models and MCNP/Abaqus calculations at LANL.
- A new feature for MCNP calculations using quadratic UM models is requested by LANL users. Godiva calculations showed that it is computationally expensive for quad hex and tet UM models.
  - Future work is to develop a new tracking method for quad hex UM models to speed up calculations and verify calculation results.

Abstract

The implementation of the unstructured mesh (UM) feature in MCNP6.3 has changed to improve performance and reduce memory usage compared to MCNP6.2. UM models of the Godiva reactor generated with Abaqus and UM models of the Oktavian benchmark experiments generated with Cubit were run with both MCNP6.2 and 6.3. In this presentation, the computing times and results of these simulations are compared.