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Title:	Recent Work on MCNP Unstructured Mesh Element Quality Assessment and Reporting
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Los Alamos
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Recent Work on MCNP Unstructured Mesh Element Quality Assessment and Reporting

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LA-UR-21-25293

Acknowledgements

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Clinton Stimpson (Sandia National Laboratories) provided several helpful clarifications on the Verdict library documentation [1].

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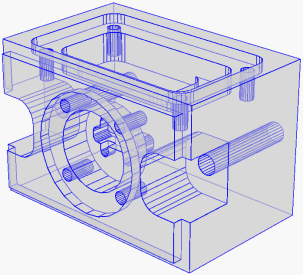
Outline

Introduction

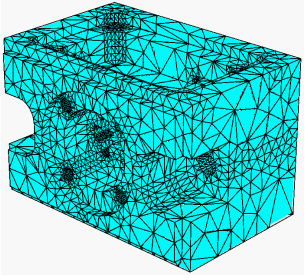
This talk: introduce recent MCNP UM quality assessment & reporting work.

Not this talk: equations to calculate element quality [1, 2].

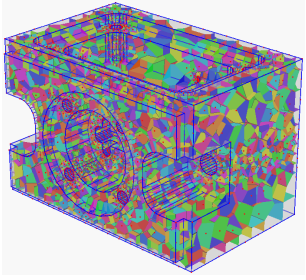
- Mesh-element quality is a thoroughly studied topic, e.g., [1, 3–5]
  - Also: International Meshing Roundtable [`https://imr.sandia.gov`]
- Origins in mesh generation: calculate metrics and remesh toward optima



1. Solid Geometry



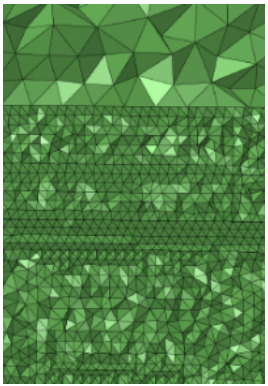
2. Surface Mesh



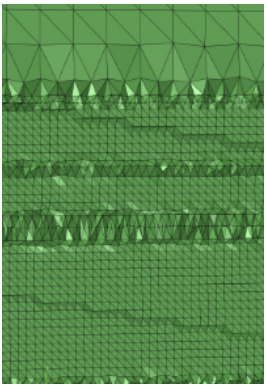
3. Volume Mesh

Motivation

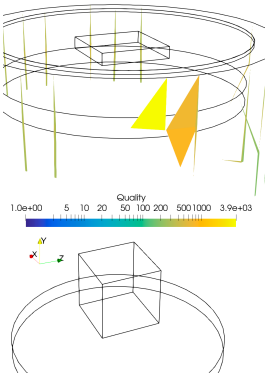
- Apparent increasing frequency of problematic MCNP UM calculations
- Appeared to result from questionable mesh
  - Threshold test for obscenity: “You know it when you see it.”
- Observed with multiple mesh generators (Simmetrix[1], TetGen [6])



Abaqus Mesh[2]



Attila4MC Mesh[2]



UM Test Case 1034

[1] Attila4MC mesh generation engine.
[2] Images from Tucker McClanahan (LANL Radiation Transport Applications Group).

Motivation, cont.

- The MCNP `um_pre_op` utility [7] has an “element checker”
  - Evaluates elemental Jacobian matrix determinant: go/no-go criterion
  - Must be run/inspected manually by a user; not implicitly in workflow

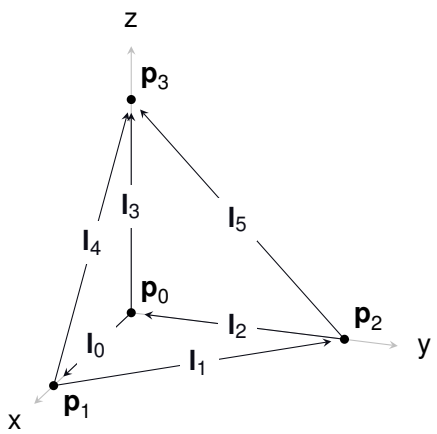
- Challenges with the element checker in practice:
  - Users would not exercise this capability
  - Lacks location information: hard to find/fix these elements in isolation
  - Go/no-go criterion is helpful, but it may not address tracking robustness

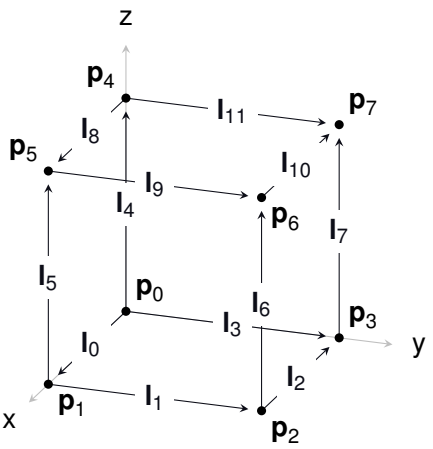
- Supplemental remarks on MCNP UM tracking and tracking robustness
  - MCNP UM tracking is element to element through a pseudocell
  - Computational equality term (10^{-10} cm: width of a hydrogen atom)
  - Tracking through a forest of slivers can be challenging

Bottom line: Can we help a user know when they may encounter trouble?

Approach to UM Quality Assessment

- Start by focusing on linear tetrahedra and hexahedra
  - Most commonly used elements by MCNP UM practitioners
  - Most thoroughly studied elements by mesh-quality community





Approach to UM Quality Assessment, cont.

- Identify metrics that can be characterized versus recommended ranges
  - All metrics exist on continua (i.e., no discrete and/or Boolean metrics)
  - Recommended ranges usually support FEA mesh-quality needs
    - This may lead to overly conservative recommended min/max values
  - Most consolidated source identified: Verdict library [1]

- **Provide enough information to know if more information is needed**
  - Provide information implicitly; don't require more workflow tasks
    - Ability to opt out in case mesh is "known to be good"
  - Elemental quality metric distribution information (a balancing act)
  - Number of elements inside / outside recommended ranges
  - Ample warning that more attention may be needed
    - Conservatism, until better guidance is available, is good
  - Education on how to learn more about mesh quality

Warnings & Output Tables

- Functional approach taken: warnings (below) and output tables (next)
  - Warnings in standard output prompt user to inspect output tables
  - Output tables inform whether additional, external, study is necessary

- (Conservative) warnings sent to standard output and output file...
  - if even one element exists outside a given metric's recommended range
  - if a negative Jacobian matrix determinant is found
    - This indicates a negative-volume element, usually from twist
  - ~~if elements are observed that no metrics are assessed for~~

```
warning.  at least one element Aspect Frobenius outside recommended range.
warning.  at least one element Min. Dihedral Ang. outside recommended range.
warning.  at least one element Scaled Jacobian outside recommended range.
```

Output Table Example

First-order Tetrahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Aspect Frobenius	1.000E+00	1.300E+00	1.163E+00	6.751E-02	1.028E+00	1.345E+00	6	200	3.000
Aspect Gamma	1.000E+00	3.000E+00	1.255E+00	1.097E-01	1.043E+00	1.560E+00	0	200	0.000
Aspect Ratio	1.000E+00	3.000E+00	1.409E+00	1.555E-01	1.101E+00	1.875E+00	0	200	0.000
Condition	1.000E+00	3.000E+00	1.167E+00	7.441E-02	1.030E+00	1.385E+00	0	200	0.000
Edge Ratio	1.000E+00	3.000E+00	1.544E+00	1.141E-01	1.249E+00	1.739E+00	0	200	0.000
Jacobian	1.000E-30	1.000E+30	3.499E-01	9.755E-02	1.906E-01	5.719E-01	0	200	0.000
Min. Dihedral Ang.	4.000E+01	7.053E+01	5.242E+01	6.730E+00	3.914E+01	7.227E+01	4	200	2.000
Radius Ratio	1.000E+00	3.000E+00	1.214E+00	1.114E-01	1.037E+00	1.610E+00	0	200	0.000
Scaled Jacobian	5.000E-01	7.071E-01	6.319E-01	8.458E-02	4.760E-01	8.573E-01	56	200	28.000
Shape	3.000E-01	1.000E+00	8.630E-01	4.960E-02	7.434E-01	9.724E-01	0	200	0.000

First-order Pentahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Jacobian	1.000E-30	1.000E+30	4.000E+00	9.428E-01	2.667E+00	5.333E+00	0	8	0.000

First-order Hexahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Diagonal	6.500E-01	1.000E+00	6.272E-01	1.245E-01	3.265E-01	9.421E-01	454	800	56.750
Jacobian	1.000E-30	1.000E+30	3.240E-03	9.033E-04	1.764E-03	5.296E-03	0	800	0.000
Maximum Edge Ratio	1.000E+00	1.300E+00	1.412E+00	2.042E-01	1.011E+00	1.914E+00	518	800	64.750
Oddy	0.000E+00	5.000E-01	7.909E+00	3.503E+00	2.269E+00	1.901E+01	800	800	100.000
Scaled Jacobian	5.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	228	800	28.500
Shear	3.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	0	800	0.000
Skew	0.000E+00	5.000E-01	3.981E-01	1.311E-01	3.355E-02	6.971E-01	172	800	21.500
Stretch	2.500E-01	1.000E+00	4.636E-01	6.928E-02	3.110E-01	6.480E-01	0	800	0.000
Taper	0.000E+00	5.000E-01	4.132E-01	4.785E-02	3.096E-01	5.552E-01	76	800	9.500

Metric name

Output Table Example

First-order Tetrahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Aspect Frobenius	1.000E+00	1.300E+00	1.163E+00	6.751E-02	1.028E+00	1.345E+00	6	200	3.000
Aspect Gamma	1.000E+00	3.000E+00	1.255E+00	1.097E-01	1.043E+00	1.560E+00	0	200	0.000
Aspect Ratio	1.000E+00	3.000E+00	1.409E+00	1.555E-01	1.101E+00	1.875E+00	0	200	0.000
Condition	1.000E+00	3.000E+00	1.167E+00	7.441E-02	1.030E+00	1.385E+00	0	200	0.000
Edge Ratio	1.000E+00	3.000E+00	1.544E+00	1.141E-01	1.249E+00	1.739E+00	0	200	0.000
Jacobian	1.000E-30	1.000E+30	3.499E-01	9.755E-02	1.906E-01	5.719E-01	0	200	0.000
Min. Dihedral Ang.	4.000E+01	7.053E+01	5.242E+01	6.730E+00	3.914E+01	7.227E+01	4	200	2.000
Radius Ratio	1.000E+00	3.000E+00	1.214E+00	1.114E-01	1.037E+00	1.610E+00	0	200	0.000
Scaled Jacobian	5.000E-01	7.071E-01	6.319E-01	8.458E-02	4.760E-01	8.573E-01	56	200	28.000
Shape	3.000E-01	1.000E+00	8.630E-01	4.960E-02	7.434E-01	9.724E-01	0	200	0.000

First-order Pentahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Jacobian	1.000E-30	1.000E+30	4.000E+00	9.428E-01	2.667E+00	5.333E+00	0	8	0.000

First-order Hexahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Diagonal	6.500E-01	1.000E+00	6.272E-01	1.245E-01	3.265E-01	9.421E-01	454	800	56.750
Jacobian	1.000E-30	1.000E+30	3.240E-03	9.033E-04	1.764E-03	5.296E-03	0	800	0.000
Maximum Edge Ratio	1.000E+00	1.300E+00	1.412E+00	2.042E-01	1.011E+00	1.914E+00	518	800	64.750
Oddy	0.000E+00	5.000E-01	7.909E+00	3.503E+00	2.269E+00	1.901E+01	800	800	100.000
Scaled Jacobian	5.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	228	800	28.500
Shear	3.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	0	800	0.000
Skew	0.000E+00	5.000E-01	3.981E-01	1.311E-01	3.355E-02	6.971E-01	172	800	21.500
Stretch	2.500E-01	1.000E+00	4.636E-01	6.928E-02	3.110E-01	6.480E-01	0	800	0.000
Taper	0.000E+00	5.000E-01	4.132E-01	4.785E-02	3.096E-01	5.552E-01	76	800	9.500

Verdict-recommended range

Output Table Example

First-order Tetrahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Aspect Frobenius	1.000E+00	1.300E+00	1.163E+00	6.751E-02	1.028E+00	1.345E+00	6	200	3.000
Aspect Gamma	1.000E+00	3.000E+00	1.255E+00	1.097E-01	1.043E+00	1.560E+00	0	200	0.000
Aspect Ratio	1.000E+00	3.000E+00	1.409E+00	1.555E-01	1.101E+00	1.875E+00	0	200	0.000
Condition	1.000E+00	3.000E+00	1.167E+00	7.441E-02	1.030E+00	1.385E+00	0	200	0.000
Edge Ratio	1.000E+00	3.000E+00	1.544E+00	1.141E-01	1.249E+00	1.739E+00	0	200	0.000
Jacobian	1.000E-30	1.000E+30	3.499E-01	9.755E-02	1.906E-01	5.719E-01	0	200	0.000
Min. Dihedral Ang.	4.000E+01	7.053E+01	5.242E+01	6.730E+00	3.914E+01	7.227E+01	4	200	2.000
Radius Ratio	1.000E+00	3.000E+00	1.214E+00	1.114E-01	1.037E+00	1.610E+00	0	200	0.000
Scaled Jacobian	5.000E-01	7.071E-01	6.319E-01	8.458E-02	4.760E-01	8.573E-01	56	200	28.000
Shape	3.000E-01	1.000E+00	8.630E-01	4.960E-02	7.434E-01	9.724E-01	0	200	0.000

First-order Pentahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Jacobian	1.000E-30	1.000E+30	4.000E+00	9.428E-01	2.667E+00	5.333E+00	0	8	0.000

First-order Hexahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Diagonal	6.500E-01	1.000E+00	6.272E-01	1.245E-01	3.265E-01	9.421E-01	454	800	56.750
Jacobian	1.000E-30	1.000E+30	3.240E-03	9.033E-04	1.764E-03	5.296E-03	0	800	0.000
Maximum Edge Ratio	1.000E+00	1.300E+00	1.412E+00	2.042E-01	1.011E+00	1.914E+00	518	800	64.750
Oddy	0.000E+00	5.000E-01	7.909E+00	3.503E+00	2.269E+00	1.901E+01	800	800	100.000
Scaled Jacobian	5.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	228	800	28.500
Shear	3.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	0	800	0.000
Skew	0.000E+00	5.000E-01	3.981E-01	1.311E-01	3.355E-02	6.971E-01	172	800	21.500
Stretch	2.500E-01	1.000E+00	4.636E-01	6.928E-02	3.110E-01	6.480E-01	0	800	0.000
Taper	0.000E+00	5.000E-01	4.132E-01	4.785E-02	3.096E-01	5.552E-01	76	800	9.500

Observed distribution (mean, standard deviation, minimum, maximum)

Output Table Example

First-order Tetrahedron Quality Metrics

Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
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Aspect Ratio	1.000E+00	3.000E+00	1.409E+00	1.555E-01	1.101E+00	1.875E+00	0	200	0.000
Condition	1.000E+00	3.000E+00	1.167E+00	7.441E-02	1.030E+00	1.385E+00	0	200	0.000
Edge Ratio	1.000E+00	3.000E+00	1.544E+00	1.141E-01	1.249E+00	1.739E+00	0	200	0.000
Jacobian	1.000E-30	1.000E+30	3.499E-01	9.755E-02	1.906E-01	5.719E-01	0	200	0.000
Min. Dihedral Ang.	4.000E+01	7.053E+01	5.242E+01	6.730E+00	3.914E+01	7.227E+01	4	200	2.000
Radius Ratio	1.000E+00	3.000E+00	1.214E+00	1.114E-01	1.037E+00	1.610E+00	0	200	0.000
Scaled Jacobian	5.000E-01	7.071E-01	6.319E-01	8.458E-02	4.760E-01	8.573E-01	56	200	28.000
Shape	3.000E-01	1.000E+00	8.630E-01	4.960E-02	7.434E-01	9.724E-01	0	200	0.000

First-order Pentahedron Quality Metrics

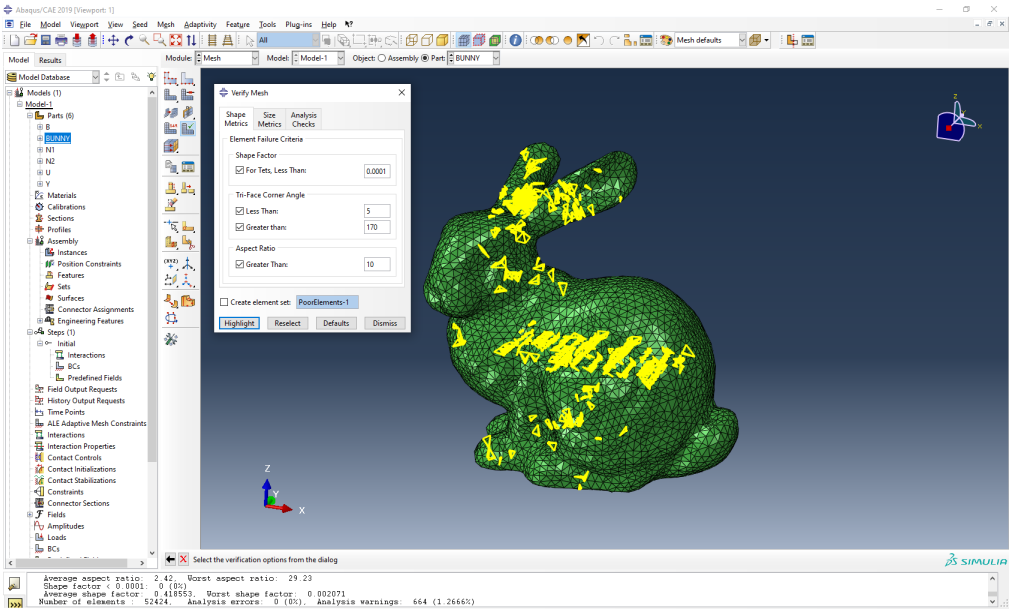
Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Jacobian	1.000E-30	1.000E+30	4.000E+00	9.428E-01	2.667E+00	5.333E+00	0	8	0.000

First-order Hexahedron Quality Metrics

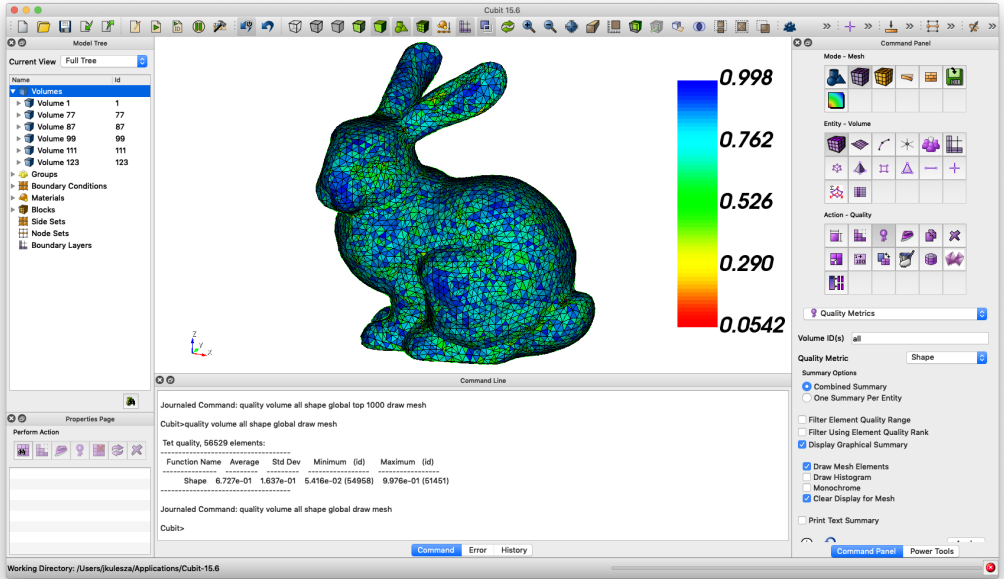
Metric	Rec. Min.	Rec. Max.	Mean	Std. Dev.	Calc. Min.	Calc. Max.	# Outside	# Checked	% Outside
Diagonal	6.500E-01	1.000E+00	6.272E-01	1.245E-01	3.265E-01	9.421E-01	454	800	56.750
Jacobian	1.000E-30	1.000E+30	3.240E-03	9.033E-04	1.764E-03	5.296E-03	0	800	0.000
Maximum Edge Ratio	1.000E+00	1.300E+00	1.412E+00	2.042E-01	1.011E+00	1.914E+00	518	800	64.750
Oddy	0.000E+00	5.000E-01	7.909E+00	3.503E+00	2.269E+00	1.901E+01	800	800	100.000
Scaled Jacobian	5.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	228	800	28.500
Shear	3.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	0	800	0.000
Skew	0.000E+00	5.000E-01	3.981E-01	1.311E-01	3.355E-02	6.971E-01	172	800	21.500
Stretch	2.500E-01	1.000E+00	4.636E-01	6.928E-02	3.110E-01	6.480E-01	0	800	0.000
Taper	0.000E+00	5.000E-01	4.132E-01	4.785E-02	3.096E-01	5.552E-01	76	800	9.500

Outlier frequency

Mesh Assessment Tools: Abaqus [9]

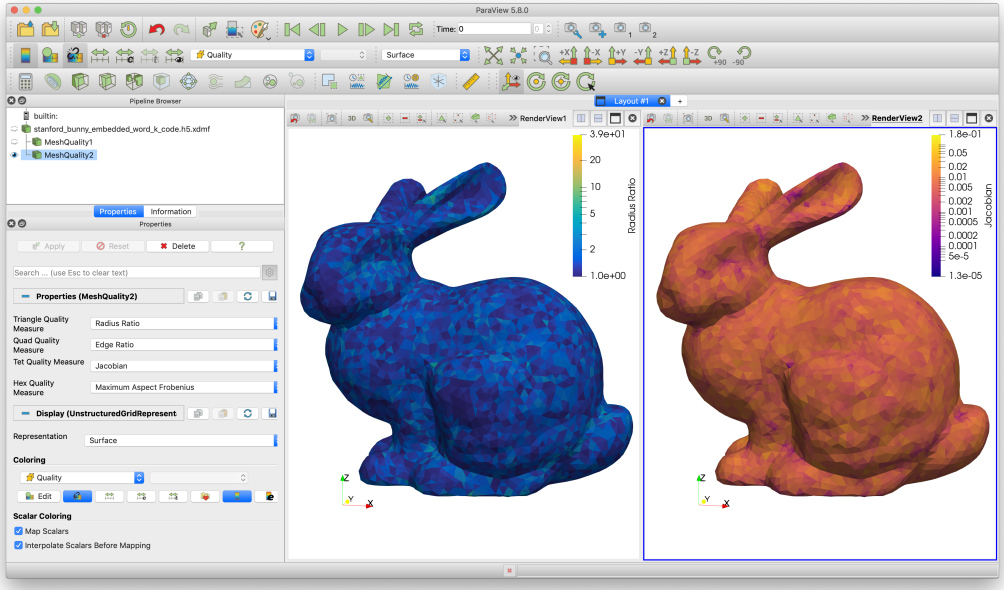


Mesh Assessment Tools: CUBIT [10]



Geometry adapted from [8].

Mesh Assessment Tools: ParaView (Interactive) [11]



Geometry adapted from [8].
See this ParaView issue for Overlaps.

Mesh Assessment Tools: ParaView (Batch)

```
# Load modules and process files; see full Python file attached to presentation...

# Iterate through mesh quality metrics and print statistics.
def print_metrics(metric_type, metrics, data):
    for q_metric in metrics:
        if metric_type == "Linear Tetrahedron": data.TetQualityMeasure = q_metric
        elif metric_type == "Linear Hexahedron": data.HexQualityMeasure = q_metric
        else: raise ValueError("Unknown mesh quality metric type.")
        q = np.array( paraview.servermanager.Fetch(data).GetCellData().GetArray("Quality"))
        print( f"{q_metric:<24s} {q.mean():10.3e} {np.std(q):10.3e} {np.min(q):10.3e} {np.max(q):10.3e}")
    return


# Define metrics to query.
q_metrics_lintet = [
    "Aspect Frobenius", "Aspect Gamma", "Aspect Ratio", "Condition", "Edge Ratio", "Jacobian",
    "Minimum Dihedral Angle", "Aspect Beta", "Scaled Jacobian", "Shape",
]
q_metrics_linhex = [
    "Diagonal", "Jacobian", "Maximum Edge Ratio", "Oddy", "Scaled Jacobian", "Shear",
    "Skew", "Stretch", "Taper",
]

# Execute query and print metrics.
print(f"{'Metric':<24s}  {'Mean':10s} {'Std. Dev.':10s} {'Minimum':10s} {'Maximum':10s}")
print_metrics("Linear Tetrahedron", q_metrics_lintet, meshQuality)
print_metrics("Linear Hexahedron", q_metrics_linhex, meshQuality)
```

Mesh Assessment Tools: ParaView (Batch) Output

Metric	Mean	Std. Dev.	Minimum	Maximum
Aspect Frobenius	1.163e+00	6.751e-02	1.028e+00	1.345e+00
Aspect Gamma	1.255e+00	1.097e-01	1.043e+00	1.560e+00
Aspect Ratio	1.409e+00	1.555e-01	1.101e+00	1.875e+00
Condition	1.167e+00	7.441e-02	1.030e+00	1.385e+00
Edge Ratio	1.544e+00	1.141e-01	1.249e+00	1.739e+00
Jacobian	3.499e-01	9.755e-02	1.906e-01	5.719e-01
Minimum Dihedral Angle	5.242e+01	6.730e+00	3.914e+01	7.227e+01
Aspect Beta	1.214e+00	1.114e-01	1.037e+00	1.610e+00
Scaled Jacobian	6.319e-01	8.458e-02	4.760e-01	8.573e-01
Shape	1.632e+00	1.461e-01	1.300e+00	2.079e+00
Diagonal	6.272e-01	1.245e-01	3.265e-01	9.421e-01
Jacobian	3.240e-03	9.033e-04	1.764e-03	5.296e-03
Maximum Edge Ratio	1.412e+00	2.042e-01	1.011e+00	1.914e+00
Oddy	7.909e+00	3.503e+00	2.269e+00	1.901e+01
Scaled Jacobian	5.455e-01	8.741e-02	3.366e-01	7.199e-01
Shear	5.455e-01	8.741e-02	3.366e-01	7.199e-01
Skew	3.981e-01	1.311e-01	3.355e-02	6.971e-01
Stretch	4.636e-01	6.928e-02	3.110e-01	6.480e-01
Taper	4.132e-01	4.785e-02	3.096e-01	5.552e-01

Data table synthesized from two separate executions for brevity.

Open Research Topics

- Linear 4- and 6-sided elements have been extensively studied
  - Begs the question: What metrics can be devised for...
    - quadratic elements that we currently permit?
    - general (arbitrary-order?) polyhedra?
  - What metrics are most relevant to Monte Carlo transport?

- Can we find formulae relating quality metrics to Monte Carlo tracking?
  - How will this depend on tracking methods vs. finite-precision math?
  - Could these weight mesh-generation algorithm optimization?
  - Before getting to this, we probably need general guidance...

- We (particle-transport practitioners) are a small part of this field...
  - **How can we maximize both our impact and benefit?**

Summary & Future Work

Summary

- Garbage in leads to garbage out
- Quality metrics implemented for MCNP UM element types
  - Reproduced `um_pre_op` capability
  - Most-commonly used elements emphasized
  - Default enabled, opt-out available via `embed` card `elementchk` toggle
- Pre- and post-MCNP-calculation mesh interrogation methods described

Future Work (beyond finalizing [2])

- Develop additional quality metrics for other MCNP UM element types
  - Collaboration opportunities (who is interested?)
- Identify reasonable MCNP-centric recommended min/max values
  - Heuristically determined first, analytically determined to follow

Questions?

Introduction & Motivation

MCNP Unstructured Mesh Quality Assessment
- Approach that Guided Implementation
- Warning & Output Table Examples

Other Mesh Quality Assessment Tools/Techniques
- Abaqus
- CUBIT
- ParaView, Interactive & Batch

Open Research Topics

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Backup Slides

References

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[9] Dassault Systèmes Simulia Corp., "Abaqus/CAE." Website.

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[11] U. Ayachit, *The ParaView Guide*. Kitware, Inc., community ed., June 2018.

Complete Script Listing (also Electronically Attached)

```
#!/Users/jkulesza/Applications/ParaView-5.9.0.app/Contents/bin/pvpython

import numpy as np
from paraview.simple import *
import sys

# Load data set, create render view, merge blocks, apply filter.
paraview.simple._DisableFirstRenderCameraReset()
xdmf = XDMFReader(FileNames=[sys.argv[1]])
renderView1 = GetActiveViewOrCreate("RenderView")
mergeBlocks = MergeBlocks(Input=xdmf)
meshQuality = MeshQuality(Input=mergeBlocks)

# Load modules and process files; see full Python file attached to presentation...

# Iterate through mesh quality metrics and print statistics.
def print_metrics(metric_type, metrics, data):
    for q_metric in metrics:
        if metric_type == "Linear Tetrahedron": data.TetQualityMeasure = q_metric
        elif metric_type == "Linear Hexahedron": data.HexQualityMeasure = q_metric
        else: raise ValueError("Unknown mesh quality metric type.")
        q = np.array( paraview.servermanager.Fetch(data).GetCellData().GetArray("Quality"))
        print( f"{q_metric:<24s} {q.mean():10.3e} {np.std(q):10.3e} {np.min(q):10.3e} {np.max(q):10.3e}")
    return


# Define metrics to query.
q_metrics_lintet = [
    "Aspect Frobenius", "Aspect Gamma", "Aspect Ratio", "Condition", "Edge Ratio", "Jacobian",
    "Minimum Dihedral Angle", "Aspect Beta", "Scaled Jacobian", "Shape",
]
q_metrics_linhex = [
    "Diagonal", "Jacobian", "Maximum Edge Ratio", "Oddy", "Scaled Jacobian", "Shear",
    "Skew", "Stretch", "Taper",
]

# Execute query and print metrics.
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print_metrics("Linear Tetrahedron", q_metrics_lintet, meshQuality)
print_metrics("Linear Hexahedron", q_metrics_linhex, meshQuality)
```