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MCNP Unstructured Mesh Elemental Quality Assessment

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Los Alamos National Laboratory

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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 & Motivation
- Element Checking with `um_pre_op`

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

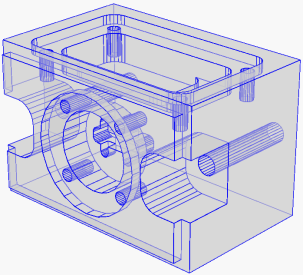
Other Mesh Quality Assessment Tools/Techniques
- Abaqus
- CUBIT
- ParaView, Interactive & Batch

Open Research Topics

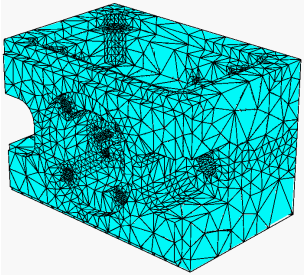
Introduction

This talk: review recent MCNP UM quality assessment & reporting work.
Slightly deeper into the details than Summer 2021 ANS UM quality presentation [2].
Not this talk: exhaustive discussion on calculating element quality [1, 3].

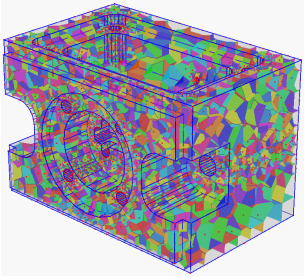
- Mesh-element quality is a thoroughly studied topic, e.g., [1, 4–6]
  - Also: International Meshing Roundtable [`https://imr.sandia.gov`]
- Origins in mesh generation: calculate metrics and remesh toward optima



1. Solid Geometry



2. Surface Mesh



3. Volume Mesh

Images from TetGen Website.

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 [8])

- The MCNP `um_pre_op` utility [9] 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 (see next slide):
  - 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

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

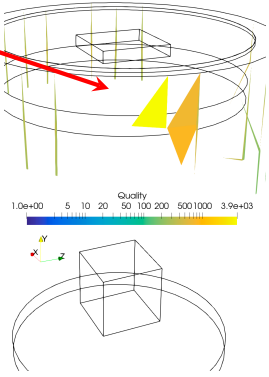
[1] Attila4MC [7] mesh generation engine.

Element Checking with `um_pre_op`

- Invoked as, e.g., `um_pre_op -ec -o inp1034.ec.out um1034.abaq`
- Looking for final line: "`Total number of failed elements:  0`"
- What about other metrics (e.g., those in Verdict [1])?

AspectDelta
AspectFrobenius
AspectGamma
AspectRatio
CollapseRatio
Condition
Distortion
EdgeRatio
Jacobian $\longrightarrow$ $\det\left(\begin{bmatrix} \sum_i \frac{\partial N_i}{\partial r} x_i & \sum_i \frac{\partial N_i}{\partial r} y_i & \sum_i \frac{\partial N_i}{\partial r} z_i \\ \sum_i \frac{\partial N_i}{\partial s} x_i & \sum_i \frac{\partial N_i}{\partial s} y_i & \sum_i \frac{\partial N_i}{\partial s} z_i \\ \sum_i \frac{\partial N_i}{\partial t} x_i & \sum_i \frac{\partial N_i}{\partial t} y_i & \sum_i \frac{\partial N_i}{\partial t} z_i \end{bmatrix}\right)$
MinimumAngle
RadiusRatio
RelativeSizeSquared
ScaledJacobian
Shape
ShapeandSize
Volume

High Aspect Ratio Elements

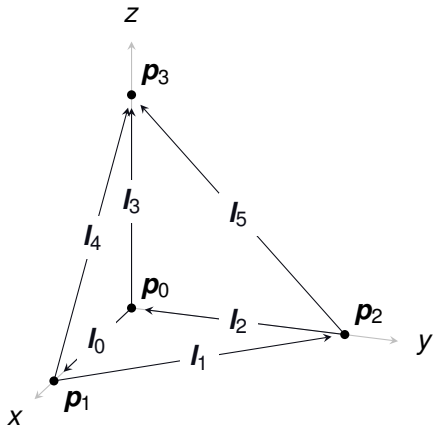


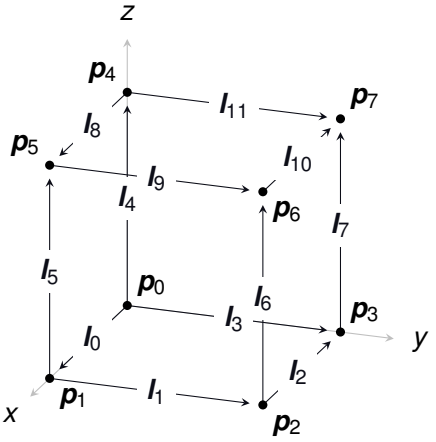
Measurement of element distortion relative to reference element in natural space (r, s, t); N_i: shape functions

UM Test Case 1034

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

- **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

```
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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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
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Radius Ratio	1.000E+00	3.000E+00	1.214E+00	1.114E-01	1.037E+00	1.610E+00	0	200	0.000
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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
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First-order Hexahedron Quality Metrics

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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
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Shear	3.000E-01	1.000E+00	5.455E-01	8.741E-02	3.366E-01	7.199E-01	0	800	0.000
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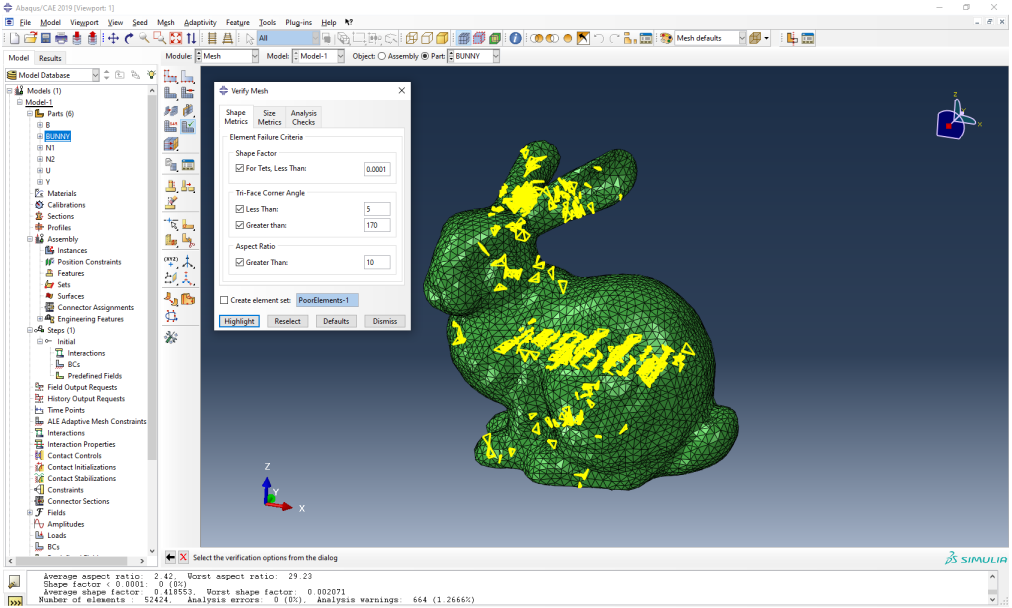
Taper	0.000E+00	5.000E-01	4.132E-01	4.785E-02	3.096E-01	5.552E-01	76	800	9.500

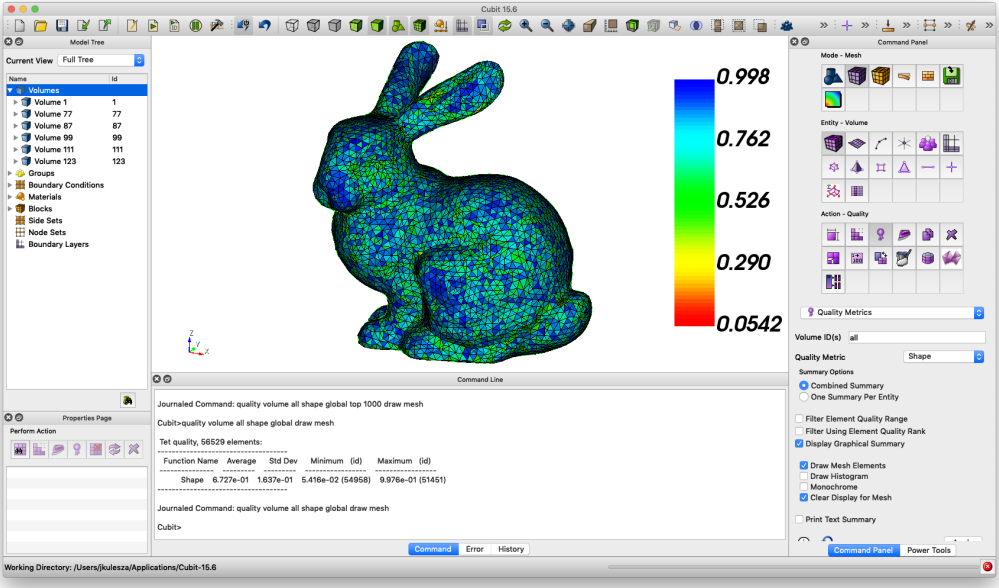
Outlier frequency

Mesh Assessment Tools: Abaqus [11]

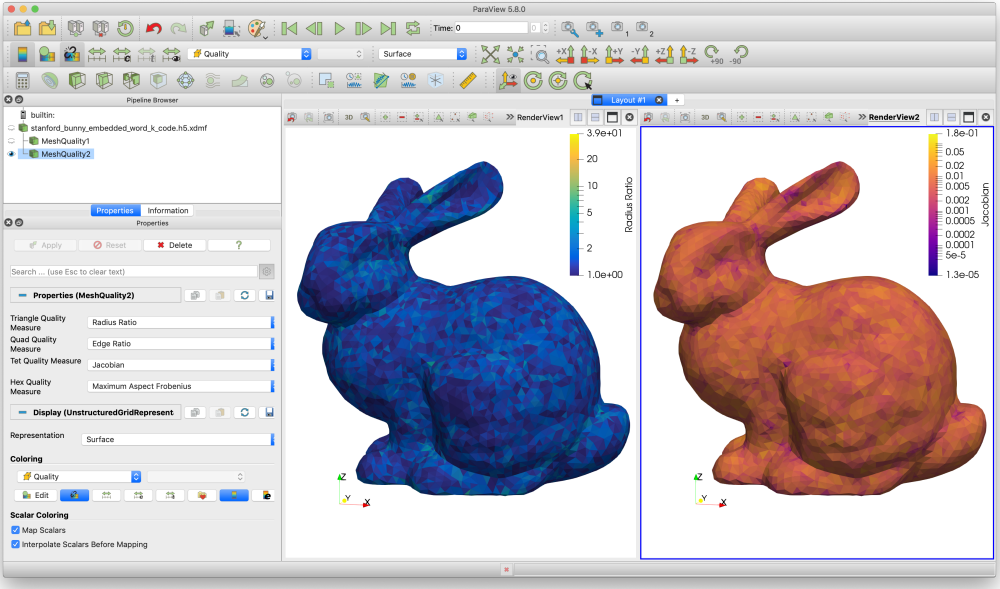


Geometry adapted from [10].

Mesh Assessment Tools: CUBIT [12]



Mesh Assessment Tools: ParaView (Interactive) [13]



See this ParaView issue for Overlaps.

Mesh Assessment Tools: ParaView (Batch)

```python
# 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 [3])

- 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
- Element Checking with `um_pre_op`

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

Adult male phantrom from [14].

Backup Slides

References

[1] C. J. Stimpson, C. D. Ernst, P. K. and. P. P. Pébay, and D. Thompson, "The Verdict Geometric Quality Library," Tech. Rep. SAND2007-1751, Sandia National Laboratories, Albuquerque, NM, USA, Mar. 2007.

[2] J. A. Kulesza, "Recent Work on MCNP Unstructured Mesh Element Quality Assessment and Reporting," in *Transactions of the Summer 2021 American Nuclear Society Meeting*, (Providence, RI, USA; June 14–16), 2021.

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References

[6] P. P. Pébay, D. Thompson, J. Shepherd, P. Knupp, C. Lisle, V. A. Magnotta, and N. M. Grosland, "New Applications of the Verdict Library for Standardized Mesh Verification Pre, Post, and End-to-End Processing," in *Proceedings of the 16th International Meshing Roundtable* (M. L. Brewer and D. Marcum, eds.), (Seattle, WA, USA; October 15–17), pp. 535–552, 2008.

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[8] H. Si, "TetGen, a Delaunay-Based Quality Tetrahedral Mesh Generator," *ACM Trans. on Mathematical Software*, vol. 41, pp. 11:1–11:36, Feb. 2015.

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[10] Stanford Computer Graphics Laboratory, "The Stanford 3D Scanning Repository," Aug. 2017.

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

References

[12] Sandia National Laboratories, “CUBIT Toolkit.”

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

[14] C. H. Kim, Y. S. Yeom, N. Petoussi-Henss, M. Zankl, W. E. Bolch, C. Lee, C. Choi, T. T. Nguyen, K. Eckerman, H. S. Kim, M. C. Han, R. Qiu, B. S. Chung, H. Han, and B. Shin, “Adult Mesh-type Reference Computational Phantoms,” Tech. Rep. ICRP Publication 145, International Commission on Radiological Protection (ICRP), Ottawa, Ontario, Canada, 2020.

Example Jacobian Matrix Determinants

Calculating the first-order tetrahedron Jacobian matrix determinant is simply

$$q = (\boldsymbol{l}_2 \times \boldsymbol{l}_0) \cdot \boldsymbol{l}_3. \tag{1}$$

Handling first-order hexahedra is more involved. First calculate

$$\begin{aligned}
\boldsymbol{x}_0 &= (\boldsymbol{p}_1 - \boldsymbol{p}_0) + (\boldsymbol{p}_2 - \boldsymbol{p}_3) + (\boldsymbol{p}_5 - \boldsymbol{p}_4) + (\boldsymbol{p}_6 - \boldsymbol{p}_7) \\
\boldsymbol{x}_1 &= (\boldsymbol{p}_3 - \boldsymbol{p}_0) + (\boldsymbol{p}_2 - \boldsymbol{p}_1) + (\boldsymbol{p}_7 - \boldsymbol{p}_4) + (\boldsymbol{p}_6 - \boldsymbol{p}_5) \\
\boldsymbol{x}_2 &= (\boldsymbol{p}_4 - \boldsymbol{p}_0) + (\boldsymbol{p}_5 - \boldsymbol{p}_1) + (\boldsymbol{p}_6 - \boldsymbol{p}_2) + (\boldsymbol{p}_7 - \boldsymbol{p}_3)
\end{aligned}$$

and then form the nine matrices

$$\begin{aligned}
A_0 &= \begin{bmatrix} \boldsymbol{l}_0 & \boldsymbol{l}_3 & \boldsymbol{l}_4 \end{bmatrix}, & A_1 &= \begin{bmatrix} \boldsymbol{l}_1 & -\boldsymbol{l}_0 & \boldsymbol{l}_5 \end{bmatrix}, & A_2 &= \begin{bmatrix} \boldsymbol{l}_2 & -\boldsymbol{l}_1 & \boldsymbol{l}_6 \end{bmatrix} \\
A_3 &= \begin{bmatrix} -\boldsymbol{l}_3 & -\boldsymbol{l}_2 & \boldsymbol{l}_7 \end{bmatrix}, & A_4 &= \begin{bmatrix} \boldsymbol{l}_{11} & \boldsymbol{l}_8 & -\boldsymbol{l}_4 \end{bmatrix}, & A_5 &= \begin{bmatrix} -\boldsymbol{l}_8 & \boldsymbol{l}_9 & -\boldsymbol{l}_5 \end{bmatrix} \\
A_6 &= \begin{bmatrix} -\boldsymbol{l}_9 & \boldsymbol{l}_{10} & -\boldsymbol{l}_6 \end{bmatrix}, & A_7 &= \begin{bmatrix} -\boldsymbol{l}_{10} & -\boldsymbol{l}_{11} & -\boldsymbol{l}_7 \end{bmatrix}, & A_8 &= \begin{bmatrix} \boldsymbol{x}_0 & \boldsymbol{x}_1 & \boldsymbol{x}_2 \end{bmatrix}
\end{aligned}.$$

Example Jacobian Matrix Determinants, cont.

Finally, using the column vectors $\boldsymbol{a}_0, \boldsymbol{a}_1, \boldsymbol{a}_2$ in matrix A, introduce the notation

$$\det(A) \equiv \boldsymbol{a}_0 \cdot (\boldsymbol{a}_1 \times \boldsymbol{a}_2),$$

so the first-order hexahedron Jacobian matrix determinant is

$$q = \min\left(\min_{i=0,\ldots,7}(\det(A_i)), \frac{\det(A_8)}{64}\right). \tag{2}$$

Complete Script Listing (also Electronically Attached)

```python
#!/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)

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```

Abstract

This talk describes the implementation and interpretation of MCNP unstructured mesh (UM) elemental quality metrics.

The talk begins with a review of the `um_pre_op` element-check capability that is available with the MCNP code, version 6.2. Then, a newly implemented collection of elemental quality metrics implemented during UM input processing in the upcoming release of the MCNP code, version 6.3, are described. These new metrics are automatically, but optionally, calculated to provide the analyst immediate feedback on the UM with no additional effort. The talk concludes with a review of several other approaches to interactively calculate and examine elemental quality metrics.