Analysis of several objective functions for optimization of hexahedral meshes

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Optimization of hexahedral meshes

The quality of the mesh has high repercussion on the numerical behaviour of FEM.

All elements should be valid.

What is a valid element?
2D element validity

Quadrilateral element

Reference element

\[ \begin{align*}
\xi_1 &= (-1, -1) \\
\xi_2 &= (1, -1) \\
\xi_3 &= (1, 1) \\
\xi_4 &= (-1, 1)
\end{align*} \]

\([-1, 1]^2\]

Physical element

\[ \mathbf{x}(\xi) \]

\[ \begin{align*}
\mathbf{x}(\xi) &= (x(\xi, \eta), y(\xi, \eta)) = \sum_{i=1}^{4} x_i N_i(\xi) \\
N_i(\xi) &= \frac{1}{4} (1 + \xi \xi_i)(1 + \eta \eta_i)
\end{align*} \]

Bilinear transformation

For FEM, one to one transformation is required

Positive Jacobian in the whole element

\[ J(\xi) = \det \left( \frac{\partial \mathbf{x}}{\partial \xi} \right) \]

\[ J(\xi) > 0, \ \xi \in [-1, 1]^2 \]
3D element validity

Hexahedral element

\[\begin{align*}
\xi_1 &= (-1, -1, -1) \\
\xi_2 &= (1, -1, -1) \\
\xi_3 &= (1, 1, -1) \\
\xi_4 &= (-1, 1, -1) \\
\xi_5 &= (-1, -1, 1) \\
\xi_6 &= (1, -1, 1) \\
\xi_7 &= (1, 1, 1) \\
\xi_8 &= (-1, 1, 1)
\end{align*}\]

valid element

\[J(\xi) = \det \left( \frac{\partial x}{\partial \xi} \right)\]

\[J(\xi) > 0, \quad \xi \in [-1, 1]^3\]
What conditions do ensure positive Jacobian?
Jacobian positivity of quadrilaterals

Subdivide the element in four triangles

\( J(\xi) > 0, \quad \xi \in [-1, 1]^2 \)

\[ J(\xi) = \det\left( \frac{\partial x}{\partial \xi} \right) \]
Jacobian positivity of quadrilaterals

Subdivide the element in four triangles

Ideal triangle

Physical triangle

\[ t_1 \text{ Jacobian matrix } \]

\[ A_1 = (x_2 - x_1, x_4 - x_1) \]
Jacobian positivity of quadrilaterals

Subdivide the element in four triangles

Ideal triangle

Physical triangle

$t_2$ Jacobian matrix

$$A_2 = (x_3 - x_2, x_1 - x_2)$$
Jacobian positivity of quadrilaterals

Subdivide the element in four triangles

Ideal triangle

Physical triangle

$A_3 = (x_4 - x_3, x_2 - x_3)$
Jacobian positivity of quadrilaterals

Subdivide the element in four triangles

Ideal triangle

Physical triangle

$t_4$ Jacobian matrix

$$A_4 = (x_1 - x_4, x_3 - x_4)$$
Jacobian positivity of quadrilaterals

Positive area of the triangles entail positive Jacobian of the bilinear transformation at vertices

$\det(A_i) > 0 \iff J(\xi_i) > 0$

$\quad i = 1, \ldots, 4$

Necessary condition
Positive Jacobian at vertices is **necessary and sufficient** condition for positive Jacobian in the whole element.

**Sufficient condition**

\[
\det(A_i) > 0 \iff J(\xi_i) > 0 \iff J(\xi) > 0 \\
\xi \in [-1, 1]^3
\]
And for a hexahedron?
Jacobian positivity of hexahedra

Subdivide the element in eight tetrahedra

\[ \tau_i = (x_1^i, x_2^i, x_3^i, x_4^i) \]
\[ i = 1, \ldots, 8 \]

Tetrahedron Jacobian matrix

\[ A_i = (x_2^i - x_1^i, x_3^i - x_1^i, x_4^i - x_1^i) \]
Jacobian positivity of hexahedra

Positive volume of each tetrahedra entail positive Jacobian of the trilinear transformation at vertices

\[
\det(A_i) > 0 \iff J(\xi_i) > 0 \implies J(\xi) > 0 \\
\xi \in [-1, 1]^3
\]

Necessary condition
Jacobian positivity of hexahedra

Does it ensure positive Jacobian in the whole element?

\[
\det(A_i) > 0 \iff J(\xi_i) > 0 \implies J(\xi) > 0
\]
\[
\xi \in [-1,1]^3
\]

Sufficient condition?

See an example
Jacobian positivity of hexahedra

\begin{align*}
\mathbf{x}_1 &= (-1, -1, -1) \\
\mathbf{x}_2 &= (1, -1, -1) \\
\mathbf{x}_3 &= (1, 1, -1) \\
\mathbf{x}_4 &= (-1, 1, -1) \\
\mathbf{x}_5 &= (-1, 1, 6) \\
\mathbf{x}_6 &= (-1, -1, 6) \\
\mathbf{x}_7 &= (1, -1, 1) \\
\mathbf{x}_8 &= (1, 1, 1)
\end{align*}

rotate top cover -90° and elevate +5 edge \(x_5-x_6\)

8 tets are valid

\[\det(A_i) > 0 \iff J(\xi_i) > 0\]

\[i = 1, \ldots, 8\]
Jacobian positivity of hexahedra

Negative Jacobian!

\[ \begin{align*}
\mathbf{x}_1 &= (-1, -1, -1) \\
\mathbf{x}_2 &= (1, -1, -1) \\
\mathbf{x}_3 &= (1, 1, -1) \\
\mathbf{x}_4 &= (-1, 1, -1) \\
\mathbf{x}_5 &= (-1, 1, 6) \\
\mathbf{x}_6 &= (-1, -1, 6) \\
\mathbf{x}_7 &= (1, -1, 1) \\
\mathbf{x}_8 &= (1, 1, 1)
\end{align*} \]

\[ \text{det}(A_i) > 0 \iff J(\xi_i) > 0 \iff J(\xi) > 0 \]

Not sufficient condition
Local optimization
Local optimization

Goal: to obtain a valid mesh and improve the quality of the elements

Initial mesh → Optimization process → Optimized mesh
Local optimization

Iterative process
Each node is moved to a new position
Minimize an objective function

\[ x = \min K(x) \]
Objective function for quadrilaterals

\[ \sigma = \det(S) \]
\[ \|S\| \text{ is the Frobenius norm of } S \]

Shape quality measure of a triangle (mean ratio)

\[ q(S) = \frac{2\sigma}{\|S\|^2} = \frac{1}{\eta} \]

Regularized shape distortion measure

\[ \eta^*(S) = \frac{\|S\|^2}{2h(\sigma)} \]

Distortion of a quadrilateral

\[ \eta^*(x) = \left[ \frac{1}{4} \sum_{i=1}^{4} (\eta^*(S_i))^p \right]^{1/p} \]
Objective function for quadrilaterals

Objective Function

\[ K^*(x) = \frac{1}{N} \sum_{i=1}^{N} \left( \eta_i^*(x) \right)^p \]

\[ \sigma = \det(S) \]
\[ \|S\| \] is the Frobenius norm of S

Shape quality measure of a triangle (mean ratio)

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\[ \eta^*(x) = \left[ \frac{1}{4} \sum_{i=1}^{4} \left( \eta^*(S_i) \right)^p \right]^{1/p} \]
Objective function for hexahedra

\[ K^*(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} (\eta_i^*(\mathbf{x}))^p \]

Objective Function

Distortion of a hexahedron

\[ \eta^*(\mathbf{x}) = \left[ \frac{1}{8} \sum_{i=1}^{8} (\eta^*(S_i))^p \right]^{1/p} \]

Regularized shape distortion measure of a tetrahedron

\[ \eta^*(S) = \frac{\|S\|^2}{3h(\sigma)^{2/3}} \]
Hexahedral mesh optimization

- Optimization can be carried out by decomposing each element into simplices (triangles or tetrahedra).

- Objective function is based on the shape distortion measure of a simplex.

- For quadrilaterals, optimization guarantee the validity of the elements (Validity of 4 triangles is a necessary and sufficient condition for validity of the quadrilateral).

- For hexahedra, optimization does not guarantee the validity of the elements (Validity of 8 tetrahedra is a necessary but not sufficient condition for validity of a hexahedra).
What other conditions may be used?
A hexahedron can be subdivided into 58 tetrahedra

The tetrahedra can be grouped in four groups:

- \( \alpha \) with 8 tets
- \( \beta \) with 24 tets
- \( \gamma \) with 24 tets
- \( \kappa \) with 2 tets

Sets of tetrahedra
Objective functions for hexahedra

\[ K^*(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} (\eta^*_i(\mathbf{x}))^p \]

Distortion of a hexahedron

\[ \eta^*(\mathbf{x}) = \left[ \frac{1}{32} \sum_{i=1}^{32} (\eta^*(S_i))^p \right]^{1/p} \]

Regularized shape distortion measure of a tetrahedron

\[ \eta^*(S) = \frac{\|S\|^2}{3h(\sigma)^{2/3}} \]
### Objective functions for hexahedra

<table>
<thead>
<tr>
<th>Conditions</th>
<th>Diagram</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>α</strong></td>
<td><img src="image1.png" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>α</strong></td>
<td><img src="image2.png" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>α</strong></td>
<td><img src="image3.png" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>α</strong></td>
<td><img src="image4.png" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>α</strong></td>
<td><img src="image5.png" alt="Diagram" /></td>
</tr>
<tr>
<td><strong>α</strong></td>
<td><img src="image6.png" alt="Diagram" /></td>
</tr>
</tbody>
</table>

- **α** **Necessary** but not sufficient conditions
- **α** **Necessary** nor sufficient conditions
- **α** **Necessary** nor sufficient conditions
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- **α** **Necessary** nor sufficient conditions
- **α** **Necessary** but **sufficient** conditions

**Note:** The diagrams illustrate the various conditions for hexahedra, with different combinations of α, β, γ, and κ.
Objective functions for hexahedra

Not necessary but \textbf{sufficient} conditions

\begin{align*}
\alpha & \quad \beta & \quad \gamma & \quad \kappa
\end{align*}

Only 30\% of valid elements satisfy this

\[ J(\xi) > 0, \quad \xi \in [-1, 1]^3 \]
Objective functions for hexahedra

\[ \alpha \beta \gamma \kappa \]

Not necessary but **sufficient** conditions

**Very restrictive conditions!**

rotate top cover -90°

\[ J(\xi) > 0, \ \xi \in [-1, 1]^3 \]
\[ \sigma(\tau) = 0 \]

Only 30% of valid elements satisfy this

Becomes into a flat tetrahedron
Objective functions for hexahedra

66% of valid elements satisfy this

Less restrictive sufficient conditions


Based on sum of volumes
Comparative study

Experiment
Goal: compare the untangling capability of different objective functions

First step
Generate high distorted elements with random vertices

Valid element $\rightarrow$ always exists feasible region for all vertices
Goal: compare the untangling capability of different objective functions

**Second step**
Optimize the element by moving one vertex

\[
x = \min K(x)
\]

Using different K

Does it continue being a valid element?

Free node
Comparative study

Same experiment with local meshes

- Valid and high distorted local mesh
- Optimize central node
- Valid local mesh after optimizing?
Percentage of valid elements/local meshes after optimizing

<table>
<thead>
<tr>
<th>Individual Elements</th>
<th>Local Meshes</th>
</tr>
</thead>
<tbody>
<tr>
<td>(α)</td>
<td>94%</td>
</tr>
<tr>
<td>(α, β)</td>
<td>88%</td>
</tr>
<tr>
<td>(α, γ)</td>
<td>67%</td>
</tr>
<tr>
<td>(α, κ)</td>
<td>39%</td>
</tr>
<tr>
<td>(α, β, γ, κ)</td>
<td>44%</td>
</tr>
<tr>
<td>(α, β, γ, κ, κ+)</td>
<td>86%</td>
</tr>
</tbody>
</table>

Comparative study


Percentage of valid elements/local meshes after optimizing

- Individual elements
- Local meshes

- $(\alpha)$: 94%
- $(\alpha, \beta, \gamma, \kappa^+)$: 92%
- $(\alpha, \kappa)$: 86%
- $(\alpha, \beta)$: 84%
- $(\alpha, \beta, \gamma, \kappa)$: 88%
- $(\alpha, \gamma)$: 59%
- $(\alpha, \beta, \gamma, \kappa)$: 92%
- $(\alpha, \gamma)$: 70%
- $(\alpha, \beta)$: 67%
- $\beta$: 39%
How optimize without simplex decomposition?
Objective functions for hexahedra

Using the weighted Jacobian matrix of the trilinear transformation

\[ S(\xi) = \frac{\partial x}{\partial \xi} \]

Reference element

Physical element

- \( \xi_1 = (-1, -1, -1) \)
- \( \xi_2 = (1, -1, -1) \)
- \( \xi_3 = (1, 1, -1) \)
- \( \xi_4 = (-1, 1, -1) \)
- \( \xi_5 = (-1, -1, 1) \)
- \( \xi_6 = (1, -1, 1) \)
- \( \xi_7 = (1, 1, 1) \)
- \( \xi_8 = (-1, 1, 1) \)

Pointwise distortion

\[ \eta^*(\xi) = \frac{\|S(\xi)\|^2}{3h(\sigma(\xi))^{2/3}} \]

\( \xi \in [-1, 1]^3 \)

Global distortion

\[ \eta^*_\Omega = \frac{1}{V_\hat{\Omega}} \int_{\hat{\Omega}} \eta^*(\xi) \, d\hat{\Omega} \]
Objective functions for hexahedra

Using the weighted Jacobian matrix of the trilinear transformation

\[ S(\xi) = \left( \frac{\partial x}{\partial \xi} \right) \]

Reference element

\[ \xi_1 = (-1, -1, -1) \]
\[ \xi_2 = (1, -1, -1) \]
\[ \xi_3 = (1, 1, -1) \]
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\[ \xi_7 = (1, 1, 1) \]
\[ \xi_8 = (-1, 1, 1) \]

Physical element

Objective function

\[ K^*(x) = \frac{1}{M} \sum_{m=1}^{M} \eta^*_{\Omega m}(x) \]
Objective functions for hexahedra

Numerical quadrature of the distortion

\[ \int_{\hat{\Omega}} \eta^*(\xi) \, d\hat{\Omega} \approx \sum_{i,j,k=1}^{2} w_{ijk} \, \eta^*(\xi_{ijk}) \]
Objective functions for hexahedra

Numerical quadrature of the distortion

\[ \int_{\hat{\Omega}} \eta^*(\xi) \, d\hat{\Omega} \approx \sum_{i,j,k=1}^{2} w_{ijk} \eta^*(\xi_{ijk}) \]

adaptive distribution of quadrature points
Comparative study

Strategies for optimization of hexahedral meshes and their comparative study, Engineering With Computers,
DOI 10.1007/s00366-016-0454-1

Percentage of valid elements/local meshes after optimizing

- $x(\xi)$: 99%
- $(\alpha)$: 94%
- $(\alpha, \beta, \gamma, \kappa)$: 92%
- $(\alpha, \kappa)$: 86%
- $(\alpha, \kappa)$: 92%
- $(\alpha, \beta, \gamma, \kappa)$: 84%
- $(\alpha, \beta)$: 88%
- $(\alpha, \beta, \gamma, \kappa)$: 59%
- $(\alpha, \beta, \gamma, \kappa)$: 70%
- $(\alpha, \gamma)$: 67%
- $(\alpha, \gamma)$: 44%
- $(\alpha, \gamma)$: 39%

Individual elements
Local meshes
Conclusions

Good results and less computationally expensive than others

In real meshes:
Conclusions

Use in the last steps of optimization

In real meshes:
Thanks for your attention.

Any questions?
Less restrictive sufficient conditions

Objective functions for hexahedra

Validity of each alpha tetrahedron

Positive Jacobian at vertices
Objective functions for hexahedra

Group $\beta$ in groups of 2
Sum of volumes of each group $> 0$

Positive Jacobian at edges
Objective functions for hexahedra

Positive Jacobian at faces

Group gamma in groups of 4
Sum of volumes of each group > 0
Objective functions for hexahedra

Positive Jacobian in the inner

Sum of volumes of \( \kappa > 0 \)
Objective functions for hexahedra

Validity of each alpha tetrahedron

\[ \eta^*(S) = \frac{||S||^2}{3h(\sigma)^{2/3}} \]

Imposes validity and shape
Objective functions for hexahedra

Sum of volumes of each group $> 0$

- $\delta = 0.5$

- $h'(\sigma)^{-1} = 2 - \frac{\sigma}{h(\sigma)}$

  i.e. $\sigma = \sigma(\beta_1) + \sigma(\beta_2)$

Imposes only barriers
Objective functions for hexahedra


Objective function (simplified)

\[ k^* = \sum \eta^*(S_{\alpha_1}) + \sum \frac{1}{h'(\sigma_{\beta_1} + \sigma_{\beta_2})} + \sum \frac{1}{h'(\sigma_{\gamma_1} + \sigma_{\gamma_2} + \sigma_{\gamma_3} + \sigma_{\gamma_4})} + \frac{1}{h'(\sigma_{\kappa_1} + \sigma_{\kappa_2})} \]

\[ K^*(x) = \sum_{m=1}^{M} (k^*_m)^p(x) \]

M: number of hexahedra of the local mesh