Non-Linear Shape Optimization Using Local Subspace Projections – Supplementary Material

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1 Introduction

In this document, we present the details of the FEM framework used in our paper.

2 The Stiffness Matrix

In our representation, a 3d model is formed by two triangle meshes with boundary (inner and outer), that have identical topologies. Two corresponding triangles are connected to form a triangular prism. An additional node is introduced at the center of each edge of the prism in order to create "15-node wedge" elements. Each element has a local $(\xi, \eta, \zeta) = (\xi_1, \xi_2, \xi_3) = \boldsymbol{\xi}$ coordinate frame and a local node numbering, see Fig. 1.

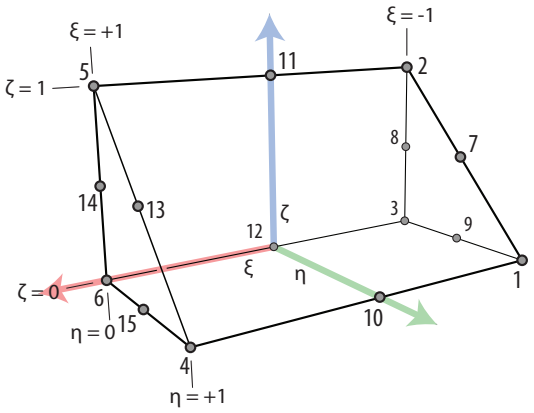

Figure 1: *15-node wedge element.*

Each node $i \in \{1, \ldots, 15 = n\}$ has a shape function $N_i : \Omega \to \mathbb{R}$, where Ω is the element interior. It holds that $N_i(\mathbf{p}_i) = 1$ and $N_i(\mathbf{p}_j) = 0$ for $i \neq j$, where $\mathbf{p}_k$ is the position of node k in the local coordinate frame. The shape functions form a partition of unity on Ω. Any quantity q_i that is defined at the nodal positions can be interpolated at a point $\mathbf{p} \in \Omega$ as $\sum q_i N_i(\mathbf{p})$.

Let $(\tilde{x}_i, \tilde{y}_i, \tilde{z}_i) = \tilde{\mathbf{x}}$ be the global coordinates of node i. Let

$$\tilde{X} = \begin{pmatrix} \tilde{x}_1 & \cdots & \tilde{x}_n \\ \tilde{y}_1 & \cdots & \tilde{y}_n \\ \tilde{z}_1 & \cdots & \tilde{z}_n \end{pmatrix}$$

be the 3-by-n matrix of global coordinates. The global coordinates are interpolated on Ω as $\tilde{X}\mathbf{N}$, where $N = (N_1, N_2, \ldots, N_n)^T$. Let $G(\mathbf{p})$ be the n-by-3-matrix-valued gradient of the shape functions N_i at $\mathbf{p}$ w.r.t. to the local coordinates s.t. $G_{ij}(\mathbf{p}) = \frac{\partial N_i}{\partial \xi_j}$. Then the Jacobi matrix of the transformation between global and local coordinates can be written as $J = \tilde{X}G = \frac{\partial \tilde{\mathbf{x}}}{\partial \boldsymbol{\xi}}$. The definition of the stiffness matrix requires the quantity $\frac{\partial \mathbf{N}}{\partial \tilde{\mathbf{x}}} = \overline{B} = GJ^{-1} \in \mathbb{R}^{n \times 3}$. Knowing the entries of $\overline{B}$, let

$$B = \begin{pmatrix} \frac{\partial N_1}{\partial \tilde{x}} & 0 & 0 & \cdots & \frac{\partial N_n}{\partial \tilde{x}} & 0 & 0 \\ 0 & \frac{\partial N_1}{\partial \tilde{y}} & 0 & \cdots & 0 & \frac{\partial N_n}{\partial \tilde{y}} & 0 \\ 0 & 0 & \frac{\partial N_1}{\partial \tilde{z}} & \cdots & 0 & 0 & \frac{\partial N_n}{\partial \tilde{z}} \\ \frac{\partial N_1}{\partial \tilde{y}} & \frac{\partial N_1}{\partial \tilde{x}} & 0 & \cdots & \frac{\partial N_n}{\partial \tilde{y}} & \frac{\partial N_n}{\partial \tilde{x}} & 0 \\ 0 & \frac{\partial N_1}{\partial \tilde{z}} & \frac{\partial N_1}{\partial \tilde{y}} & \cdots & 0 & \frac{\partial N_n}{\partial \tilde{z}} & \frac{\partial N_n}{\partial \tilde{y}} \\ \frac{\partial N_1}{\partial \tilde{z}} & 0 & \frac{\partial N_1}{\partial \tilde{x}} & \cdots & \frac{\partial N_n}{\partial \tilde{z}} & 0 & \frac{\partial N_n}{\partial \tilde{x}} \end{pmatrix} \in \mathbb{R}^{6 \times 3n} \tag{1}$$

Let C be the 6-by-6 matrix representation of the stiffness tensor

$$C = \frac{E}{(1+\nu)(1-2\nu)} \cdot \begin{pmatrix} 1-\nu & \nu & \nu & & & \\ \nu & 1-\nu & \nu & & & \\ \nu & \nu & 1-\nu & & & \\ & & & \frac{1}{2}-\nu & & \\ & & & & \frac{1}{2}-\nu & \\ & & & & & \frac{1}{2}-\nu \end{pmatrix},$$

where E is Young's modulus in ν is Poisson's ratio, constant across all elements.

Then the stiffness matrix of one element is defined as

$$\mathbf{K}^e = \sum_{g=1}^{n_G} w_g \det(J(\mathbf{p}_g)) B(\mathbf{p}_g)^T C B(\mathbf{p}_g) \in \mathbb{R}^{3n \times 3n}.$$

The quantities $w_g, \mathbf{p}_g, g \in \{1, \ldots, n_G\}$ are the weights and nodes of a Gauss quadrature scheme, which remains constant. $\mathbf{p}_g$ are given in local coordinates. The global stiffness matrix of the assembly of elements is computed by pasting the entries of each $\mathbf{K}^e$ into the appropriate rows and columns determined by a global node numbering. If an entry in the global stiffness matrix has contributions from more than one element stiffness matrix, these contributions are accumulated.

3 Gradient of the Stiffness Matrix

Let the global node coordinates $\tilde{\mathbf{x}}$ be a function of shape parameters $\tilde{\mathbf{x}} = \tilde{\mathbf{x}}(\alpha_1, \ldots, \alpha_p)$. The goal is to compute $\frac{\partial \mathbf{K}^e}{\partial \alpha_i}$.

The gradient of the global coordinates w.r.t. the shape parameters $\frac{\partial \tilde{X}}{\partial \alpha_i} \in \mathbb{R}^{3 \times n}$ can be inferred from the parametrization of the shape. Then $\frac{\partial J}{\partial \alpha_i} = \frac{\partial \tilde{X}}{\partial \alpha_i} G$, because G only depends on the local coordinates of the Gauss quadrature points and thus not on the global coordinates.

The derivative of J^{-1} is given by $\frac{\partial J^{-1}}{\partial \alpha_i} = -J^{-1} \frac{\partial \tilde{X}}{\partial \alpha_i} G J^{-1}$. The derivative of $\overline{B}$ is given by $\frac{\partial \overline{B}}{\partial \alpha_i} = -G J^{-1} \frac{\partial \tilde{X}}{\partial \alpha_i} G J^{-1}$. From this the entries in $\frac{\partial B}{\partial \alpha_i}$ can be found by reordering like in Eq. 1.

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The derivative of $\det(J)$ is given by $\frac{\partial \det(J)}{\partial \alpha_i} = \mathrm{tr}\left(\mathrm{adj}(J)\frac{\partial \tilde{X}}{\partial \alpha_i}G\right)$, where "tr" denotes the trace and "adj" denotes the adjugate. Finally,

$$\frac{\partial \mathbf{K}^e}{\partial \alpha_i} = \sum_{g=1}^{n_G} w_g \left[\mathrm{tr}\left(\mathrm{adj}(J)\frac{\partial \tilde{X}}{\partial \alpha_i}G\right) B^T C B + \det(J)\left\{\left(\frac{\partial B}{\partial \alpha_i}\right)^T C B + \left[\left(\frac{\partial B}{\partial \alpha_i}\right)^T C B\right]^T\right\}\right], \quad (2)$$

where the arguments $\mathbf{p}_g$ have been left out for clarity.

4 The Mass Matrix

The mass matrix of an element can be written as

$$\mathbf{M}^e = \sum_{g=1}^{n_G} w_g \det(J(\mathbf{p}_g))H(\mathbf{p}_g),$$

where H is a $3n$-by-$3n$ matrix that does not depend on the global coordinates. Therefore it can be precalculated once for every Gauss quadrature node $\mathbf{p}_g$ and then used for every element.

The gradient of the mass matrix is

$$\frac{\partial \mathbf{M}^e}{\partial \alpha_i} = \sum_{g=1}^{n_G} w_g \mathrm{tr}\left(\mathrm{adj}(J)\frac{\partial \tilde{X}}{\partial \alpha_i}G\right) H.$$

5 Equations of Motion

Let $\mathbf{K}$ be the global stiffness matrix and $\mathbf{M}$ the global mass matrix. The finite element equations of motion for vibrations are given by

$$\mathbf{K}\ddot{\mathbf{u}} + \mathbf{M}\mathbf{u} = 0.$$

By solving the generalized eigenvalue problem

$$\mathbf{K}\mathbf{v}_i = \lambda_i \mathbf{M}\mathbf{v}_i,$$

the solutions to the original equations of motion are given as harmonic oscillations with frequencies of $f_i = \frac{\sqrt{\lambda_i}}{2\pi}$.

The derivatives of λ_i are given by

$$\frac{\partial \lambda_i}{\partial \alpha_j} = \mathbf{v}_i^T\left(\frac{\partial \mathbf{K}}{\partial \alpha_j} - \lambda_i \frac{\partial \mathbf{M}}{\partial \alpha_j}\right)\mathbf{v}_i.$$

The derivatives of f_i are given by

$$\frac{\partial f_i}{\partial \alpha_j} = \frac{1}{4\pi\sqrt{\lambda_i}}\frac{\partial \lambda_i}{\partial \alpha_j}.$$

6 Derivatives of eigenvalues and eigenvectors

The following applies for non-repeated eigenvalues. Each eigenpair fulfills the equations

$$\mathbf{K}\mathbf{v}_i = \lambda_i \mathbf{M}\mathbf{v}_i, \quad \mathbf{v}_i^T \mathbf{M}\mathbf{v}_i = 1.$$

Assuming that all quantities depend on a shape parameter p_j, the first partials are given by

$$(\mathbf{K} - \lambda_i \mathbf{M})\frac{\partial \mathbf{v}_i}{\partial p_j} - \mathbf{M}\mathbf{v}_i \frac{\partial \lambda_i}{\partial p_j} = \left(\lambda_i \frac{\partial \mathbf{M}}{\partial p_j} - \frac{\partial \mathbf{K}}{\partial p_j}\right)\mathbf{v}_i,$$
$$2\mathbf{v}_i^T \mathbf{M}\frac{\partial \mathbf{v}_i}{\partial p_j} = -\mathbf{v}_i^T \frac{\partial \mathbf{M}}{\partial p_j}\mathbf{v}_i.$$

This can be expressed using block matrix notation as

$$\begin{pmatrix} \mathbf{K} - \lambda_i \mathbf{M} & -\mathbf{M}\mathbf{v}_i \\ 2\mathbf{v}_i^T \mathbf{M} & 0 \end{pmatrix}\begin{pmatrix} \frac{\partial \mathbf{v}_i}{\partial p_j} \\ \frac{\partial \lambda_i}{\partial p_j} \end{pmatrix} = \begin{pmatrix} \left(\lambda_i \frac{\partial \mathbf{M}}{\partial p_j} - \frac{\partial \mathbf{K}}{\partial p_j}\right)\mathbf{v}_i \\ -\mathbf{v}_i^T \frac{\partial \mathbf{M}}{\partial p_j}\mathbf{v}_i. \end{pmatrix}$$

This $(N+1)\times(N+1)$ system has a unique solution if λ_i is a non-repeated eigenvalue.