In Pursuit of An Alternative Formulation for Quadratically Complete PEM Elements

Herein we discuss an alternative formulation for quadratically complete PEM elements.

The Original Approach

Consider a representative 1D PEM element Ω subdivided into a number of segments γ_b and verticies v_a. Let us further suppose that at least three of the verticies are classified as nodes N_A, whose shape function values φ_N are known. We seek a linear transformation $\mathbf{M} : u_N \mapsto u|_{\gamma_b}$ such that the mapping $\mathbf{M}$ yields a piece-wise representation of $u|_{\gamma_b}$ on the set of segments which is both relatively "smooth" and "continuous." More precisely, we require that any $u|_{\gamma_b}$ obtained through $\mathbf{M}$ be the unique minimizer of a prescribed functional $\mathcal{F}$:

$$\mathcal{F} := \beta_0 \sum_{a \in \bar{\mathcal{B}}} \frac{h_a}{2} [\![u]\!]^2 \Big|_{v_a} + \beta_1 \sum_{a \in \mathcal{B}} \frac{h_a^3}{2} [\![n \nabla u]\!]^2 \Big|_{v_a} \tag{1}$$

which represents a weighted measure of compatibility and smoothness in the piece-wise representation of u over the element's segment partition. We will choose to represent each $u|_{\gamma_b}$ using a monomial basis, i.e.

$$u|_{\gamma_b}(x) = \sum_{\alpha \leq k} a_{\gamma_b}^{(\alpha)} x^\alpha = \mathbf{m} \cdot \mathbf{a}_{\gamma_b} \tag{2}$$

where $\mathbf{m}$ is a vector of monomials and $\mathbf{a}_{\gamma_b}$ is a vector of the corresponding (unknown) monomial coefficients for a given segment γ_b. Now, denote $\mathbf{a}$ as the vector of all segment monomial coefficients, and denote $\mathbf{u}$ as the vector of all nodal values. We may then formulate our minimum problem as

$$\min_{\mathbf{a}} \mathcal{F}(\mathbf{a}, \mathbf{u}), \tag{3}$$

and the unique minimizer of $\mathcal{F}$ will satisfy

$$\frac{\partial \mathcal{F}}{\partial \mathbf{a}} = \mathbf{0}. \tag{4}$$

Let us momentarily consider an individual vertex v_a which separates two segments, γ_{a1} and γ_{a2}. Note that

$$h_a[\![u]\!]^2\Big|_{v_a} = (\mathbf{a}_{\gamma_{a1}} - \mathbf{a}_{\gamma_{a2}}) \cdot [h_a \mathbf{m}_{v_a} \otimes \mathbf{m}_{v_a}] (\mathbf{a}_{\gamma_{a1}} - \mathbf{a}_{\gamma_{a2}}), \tag{5}$$

and

$$h_a^3[\![n\nabla u]\!]^2\Big|_{v_a} = (\mathbf{a}_{\gamma_{a1}} - \mathbf{a}_{\gamma_{a2}}) \cdot \left[h_a^3 \frac{\partial \mathbf{m}_{v_a}}{\partial n} \otimes \frac{\partial \mathbf{m}_{v_a}}{\partial n}\right] (\mathbf{a}_{\gamma_{a1}} - \mathbf{a}_{\gamma_{a2}}), \tag{6}$$

where we prescribe $h_a = (|\gamma_{a1}| + |\gamma_{a2}|)$ to obtain a proportional scaling of the two integral contributions to $\mathcal{F}$. If we define moment matrices $\mathbf{J}_{0a}$ and $\mathbf{J}_{1a}$ as

$$\mathbf{J}_{0a} \equiv h_a \mathbf{m}_{v_a} \otimes \mathbf{m}_{v_a} \tag{7}$$

$$\mathbf{J}_{1a} \equiv h_a^3 \frac{\partial \mathbf{m}_{v_a}}{\partial n} \otimes \frac{\partial \mathbf{m}_{v_a}}{\partial n} \tag{8}$$

then we may express the local contribution from vertex v_a to $\mathcal{F}$ as

$$\mathcal{F}_a = \frac{1}{2} \left\{ \begin{array}{c} \mathbf{a}_{\gamma_{a1}} \\ \mathbf{a}_{\gamma_{a2}} \end{array} \right\} \cdot \left(\beta_0 \left[\begin{array}{cc} \mathbf{J}_{0a} & -\mathbf{J}_{0a} \\ -\mathbf{J}_{0a} & \mathbf{J}_{0a} \end{array} \right] + \beta_1 \left[\begin{array}{cc} \mathbf{J}_{1a} & -\mathbf{J}_{1a} \\ -\mathbf{J}_{1a} & \mathbf{J}_{1a} \end{array} \right] \right) \left\{ \begin{array}{c} \mathbf{a}_{\gamma_{a1}} \\ \mathbf{a}_{\gamma_{a2}} \end{array} \right\}, \tag{9}$$

or more concisely:

$$\mathcal{F}_a = \frac{1}{2} \mathbf{a}_{\gamma_{a_{1,2}}} \cdot \mathbf{J}_a \mathbf{a}_{\gamma_{a_{1,2}}}. \tag{10}$$

The matrix $\mathbf{J}_a$ expressed in the above equation constitutes a local contribution from vertex v_a to the Jacobian of $\partial\mathcal{F}/\partial\mathbf{a}$ (i.e. to $\mathbf{J} = \partial^2\mathcal{F}/\partial\mathbf{a}\,\partial\mathbf{a}$, which will ultimately be inverted when we solve for the unknown monomial coefficients in each segment).

If the particular vertex in question had been a node, then

$$\mathcal{F}_a = \beta_0 \frac{h_a}{2} [\![u]\!]^2\Big|_{v_a} = \sum_i \left[\frac{1}{2} \mathbf{a}_{\gamma_{a_i}} \cdot \mathbf{J}_{0a} \mathbf{a}_{\gamma_{a_i}} - \mathbf{a}_{\gamma_{a_i}} \cdot \mathbf{B}_{0a} u_a + \frac{1}{2} u_a A_{0a} u_a \right] \tag{11}$$

where u_a denotes the nodal value at vertex v_a, $h_a = \sum_i |\gamma_{a_i}|$, and

$$A_{0a} \equiv \beta_0 h_a, \qquad \mathbf{B}_{0a} \equiv \beta_0 h_a \mathbf{m}_{v_a}. \tag{12}$$

If we sum the contributions from all verticies, then we are justified in writing $\mathcal{F}$ as a quadratic form:

$$\mathcal{F}(\mathbf{a}, \mathbf{u}) = \frac{1}{2} \mathbf{a} \cdot \mathbf{J}\mathbf{a} - \mathbf{a} \cdot \mathbf{B}\mathbf{u} + \frac{1}{2} \mathbf{u} \cdot \mathbf{A}\mathbf{u}. \tag{13}$$

The Proposed Alternative Approach

Let us propose the following representation for the element's shape functions defined on the set of all segments γ_b: suppose there exists some quadratic polynomial function $q(x) = \mathbf{m} \cdot \mathbf{a}_q$ such that $u|_{\gamma_b} = q + \hat{u}|_{\gamma_b}$, where the local segment functions $\hat{u}|_{\gamma_b} = \mathbf{m} \cdot \hat{\mathbf{a}}_{\gamma_b}$ are at most linear polynomials obtained from the solution of

$$\min_{\hat{\mathbf{a}}, \mathbf{a}_q} \mathcal{F}(\hat{\mathbf{a}}, \hat{\mathbf{u}}) \tag{14}$$

with

$$\hat{u}_a = u_a - \mathbf{m}_{v_a} \cdot \mathbf{a}_q, \tag{15}$$

or in matrix form

$$\hat{\mathbf{u}} = \mathbf{u} - \mathbf{Q}\mathbf{a}_q. \tag{16}$$

Thus, we must solve the augmented minimum problem

$$\min_{\hat{\mathbf{a}}, \mathbf{a}_q} \mathcal{F}(\hat{\mathbf{a}}, \mathbf{u} - \mathbf{Q}\mathbf{a}_q) \tag{17}$$

for both $\mathbf{a}_q$ (the element-wide quadratic coefficients), and $\hat{\mathbf{a}}$ (the "residual" segment coefficients) for a given setting of nodal values $\mathbf{u}$. Explicitly:

$$\mathcal{F}(\hat{\mathbf{a}}, \mathbf{u} - \mathbf{Q}\mathbf{a}_q) = \frac{1}{2}\hat{\mathbf{a}} \cdot \mathbf{J}\hat{\mathbf{a}} - \hat{\mathbf{a}} \cdot \mathbf{B}(\mathbf{u} - \mathbf{Q}\mathbf{a}_q) + \frac{1}{2}(\mathbf{u} - \mathbf{Q}\mathbf{a}_q) \cdot \mathbf{A}(\mathbf{u} - \mathbf{Q}\mathbf{a}_q), \tag{18}$$

and

$$\frac{\partial \mathcal{F}}{\partial \hat{\mathbf{a}}} = \mathbf{J}\hat{\mathbf{a}} - \mathbf{B}(\mathbf{u} - \mathbf{Q}\mathbf{a}_q) = \mathbf{0}, \tag{19}$$

$$\frac{\partial \mathcal{F}}{\partial \mathbf{a}_q} = \hat{\mathbf{a}} \cdot \mathbf{B}\mathbf{Q} - \mathbf{Q}^T\mathbf{A}(\mathbf{u} - \mathbf{Q}\mathbf{a}_q) = \mathbf{0}, \tag{20}$$

$$\begin{bmatrix} \mathbf{J} & \mathbf{B}\mathbf{Q} \\ \mathbf{Q}^T\mathbf{B}^T & \mathbf{Q}^T\mathbf{A}\mathbf{Q} \end{bmatrix} \begin{Bmatrix} \hat{\mathbf{a}} \\ \mathbf{a}_q \end{Bmatrix} = \begin{bmatrix} \mathbf{B} \\ \mathbf{Q}^T\mathbf{A} \end{bmatrix} \{ \mathbf{u} \}, \tag{21}$$

or more succinctly,

$$\mathbf{M}_a\mathbf{a} = \mathbf{M}_u\mathbf{u} \tag{22}$$

where $\mathbf{a}$ now denotes the vector of all unknown polynomial coefficients (both $\hat{\mathbf{a}}$ and $\mathbf{a}_q$).

Preliminary Results

A simple MATLAB test script was created for the 1D PEM problem depicted in Figure 1. This test was constructed to verify the completeness of

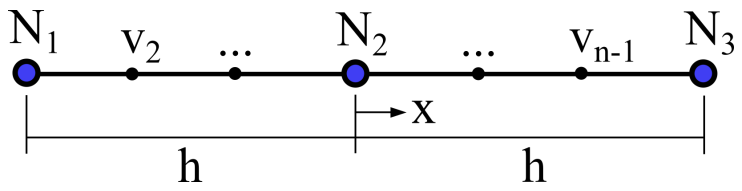

Figure 1: A representative 1D partitioned element, Ω.

the resulting shape functions, and to determine the rank sufficiency (or the condition number) of the system of equations expressed in (22).

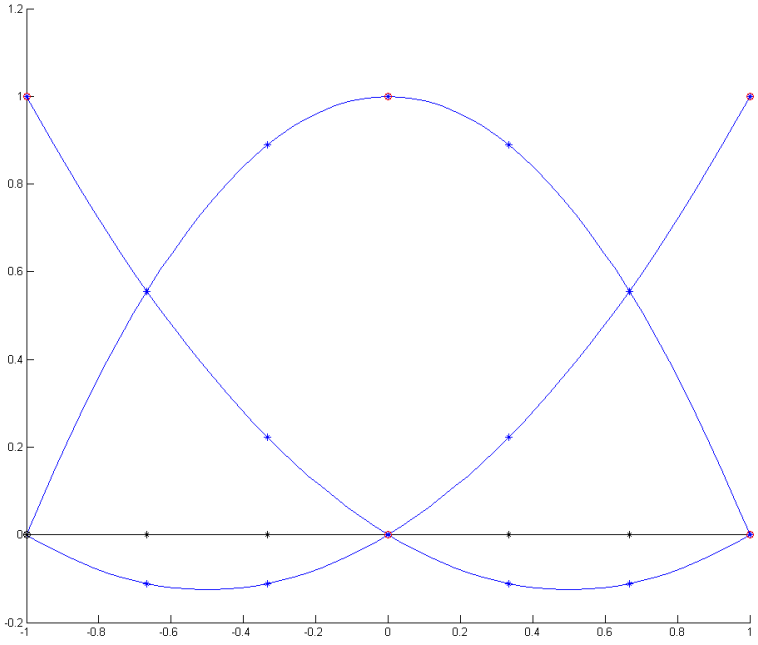

Figure 2: The resulting PEM quadratic nodal interpolants (consistent with the Lagrange interpolating polynomials).

Initial attempts pursued the case where $q(x)$ was allowed to be an arbitrary quadratic function (i.e. $q(x) = a_q^{(0)} + a_q^{(1)}x + a_q^{(2)}x^2$), and where each segment's local variations $\hat{u}|_{\gamma_b}$ were prescribed to be arbitrary linear functions (i.e. $\hat{u}|_{\gamma_b} = \hat{a}_{\gamma_b}^{(0)} + \hat{a}_{\gamma_b}^{(1)}x$), such that the resulting shape functions in a given segment assumed the form:

$$u|_{\gamma_b} = (a_q^{(0)} + \hat{a}_{\gamma_b}^{(0)}) + (a_q^{(1)} + \hat{a}_{\gamma_b}^{(1)})x + a_q^{(2)}x^2. \tag{23}$$

This, however, led $\mathbf{M}_a$ to be rank deficient, as the constant and linear coefficients could take on arbitrary non-zero values such that $a_q^{(0)} = -\hat{a}_{\gamma_b}^{(0)}$ or $a_q^{(1)} = -\hat{a}_{\gamma_b}^{(1)}$, even if the nodal values were identically zero. Consequently, it was observed that any enrichment $q(x)$ would need to consist of polynomials not already contained in the space of piece-wise linear polynomials represented by the segment coefficients.

Secondary attempts which restricted $q(x)$ to be a second-order monomial (i.e. $q(x) = a_q^{(2)}x^2$) succeeded in achieving rank-sufficiency, and produced shape functions which were quadratically complete (see Figure 2.)

An examination of the condition number for $\mathbf{M}_a$ via a parameter sensitivity analysis revealed that $\kappa(\mathbf{M}_a) \approx O(h^4)$ (consistent with the $O(h^{2k})$ approximation, derived previously), in affirmation of previous speculation that ill-conditioning in the PEM linear systems is largely a consequence of the choice of polynomial basis (namely, the monomial basis).