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Essential Boundary Conditions with Straight C^1 Finite Elements in Curved Domains

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Abstract

The implementation of essential boundary conditions in C^1 finite element analysis requires proper treatment of both the boundary conditions on second-order differentials of the solution and the curvature of the domain boundary. A method for the imposition of essential boundary conditions using straight elements (where the elements are not deformed to approximate a curved domain) is described. It is shown that pre-multiplication of the matrix equation by the local rotation matrix at each boundary node is not the optimal transformation. The uniquely optimal transformation is found, which does not take the form of a similarity transformation due to the non-orthogonality of the transformation to curved coordinates.

Key words: Numerical Methods
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1. Introduction

Finite elements having the C^1 property, for which the second-order derivatives of the discretized field are well-defined everywhere (including at element boundaries), admit the imposition of boundary conditions on the second-order derivatives. Even for the application of pure Dirichlet conditions, both the first and second derivatives in the direction tangential to the boundary should be specified at each node in order to constrain the value of the solution on the boundary between nodes. The application of essential boundary conditions in the coordinates local to the boundary (as opposed to global coordinates) requires taking the curvature of the boundary into account. This difficulty does

not exist with C^0 elements, for which boundary conditions need only account for the normal (or tangential) directions at each boundary node.

One method of handling curved boundaries is to deform the elements in order to approximately align the element edge with the boundary. [1, 2] (We use the term "edge" to denote the extent of the element, and "boundary" to denote the boundary of the non-discretized domain.) We focus here instead on using non-conforming elements which avoids nonlinear transformations of basis functions and integration quadrature sampling points and, in our opinion, simplifies the implementation.

The standard method for imposing essential boundary conditions in a coordinate system local to the boundary is to perform local rotations of the stiffness matrix at each node on the boundary. (See, for example, the overview in reference [3].) Thus the matrix equation

$$\mathsf{K}\mathbf{u} = \mathbf{b} \tag{1}$$

is transformed to

$$\mathsf{T}\mathsf{K}\mathbf{u} = \mathsf{T}\mathbf{b} \tag{2}$$

where T transforms to the appropriate boundary-oriented coordinates at each node. Ideally the transformation is such that the rows of equation (2) are either fully constrained or fully unconstrained by the boundary conditions, so that the constrained rows may then be replaced with the appropriate boundary conditions without reducing the solution space orthogonal to these constraints. What is meant here by a row being fully constrained by a boundary condition is discussed below.

2. Obtaining the optimal transformation

For concreteness we consider two-dimensional, triangular, reduced quintic finite elements [4], also known as the Bell triangle [5, 6] and the TUBA 3 element [7]. For these elements, the basis functions ν are orthogonal in the sense that

$$\mathcal{L}_i(\nu_j^w)|_v = \delta_{ij}\delta_{vw}. \tag{3}$$

where

$$\mathcal{L} = \begin{pmatrix} 1 & \partial_x & \partial_y & \partial_x^2 & \partial_x\partial_y & \partial_y^2 \end{pmatrix}. \tag{4}$$

The indices i and j range from 1 to 6; v and w range over all nodes. Here $|_v$ means "evaluated at node v," and δ is the Kronecker delta. In other words, for a given operation $\mathcal{L}_i$ there is exactly one basis function which evaluates to unity at node v; all others evaluate to zero. Thus $u|_v = U_i^v \nu_i^v$ with $U_i^v = \mathcal{L}_i(u)|_v$. One generally does not wants to impose boundary conditions in the global coordinate system ($\mathcal{L}_i(u)|_v = b$), but rather in the coordinate system local to the boundary ($\mathcal{L}'_i(u) = b$). Here

$$\mathcal{L}' = \begin{pmatrix} 1 & \partial_x & \partial_y & \partial_n^2 & \partial_t\partial_n & \partial_t^2 \end{pmatrix}, \tag{5}$$

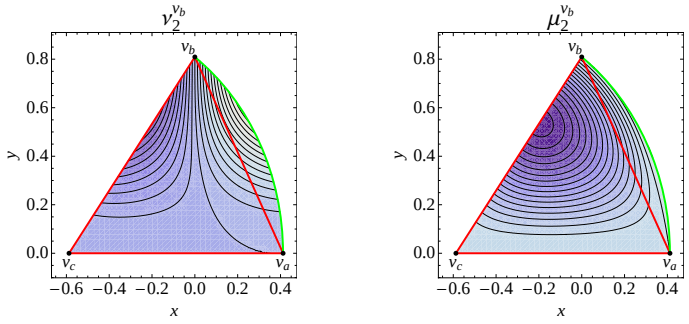

Figure 1: Contour plots of two functions are shown within a finite element having two vertices, v_a and v_b, lying on a curved boundary (green arc). *Left*: the basis function $\nu_2^{v_b}$, which is constructed such that $\partial_x(\nu_2^{v_b})|_{v_b} = 1$. *Right*: the trial function $\mu_2^{v_b}$, which is constructed such that $\partial_n(\mu_2^{v_b})|_{v_b} = 1$.

where n and t are coordinates normal and tangential to the boundary at the given node. Note that $\partial_t(\partial_n u)$ is generally not equal to $\partial_n(\partial_t u)$ when the boundary is curved; usually one wants to constrain the former rather than the latter.

For a node v_b lying on a boundary, it can easily be shown that $\mathcal{L}'(u)|_{v_b} = \mathsf{r}^{v_b}\mathcal{L}(u)|_{v_b}$, where

$$\mathsf{r}^{v_b} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & n_x & n_y & 0 & 0 & 0 \\ 0 & -n_y & n_x & 0 & 0 & 0 \\ 0 & 0 & 0 & n_x^2 & 2n_xn_y & n_y^2 \\ 0 & -\kappa n_y & \kappa n_x & -n_xn_y & n_x^2 - n_y^2 & n_xn_y \\ 0 & -\kappa n_x & -\kappa n_y & n_y^2 & -2n_xn_y & n_x^2 \end{pmatrix}. \tag{6}$$

The curvature $\kappa = \hat{n} \cdot d\hat{t}/d\ell$, where $\hat{n}$ is the outward normal unit vector to the boundary, $\hat{t}$ is the tangent unit vector, and $\hat{t}\, d\ell = d\mathbf{x}$ for a differential displacement $d\mathbf{x}$ along the boundary. For nodes v_i not lying on the boundary no transformation needs to be made, so we may set $\mathsf{r}^{v_i} = \mathsf{I}$, the identity matrix.

It is tempting at this point to assume that T in equation (2) should simply be $\mathsf{R} = \mathrm{diag}(\mathsf{r}^v)$, the block-diagonal matrix with block-elements r^v. This procedure, while stable, will not yield the optimal results. What one wants, in order that the residual be constrained as much as possible when imposing an essential boundary condition on $\mathcal{L}'_i(u)|_{v_b}$, is a new set of trial functions μ_i^v, such that

$$\mathcal{L}'_i(\mu_j^v)|_{v_b} = \delta_{ij}\delta_{v_b v}. \tag{7}$$

Let us stipulate that these new trial functions are a linear combination of the old basis functions,

$$\mu_i^v = \mathsf{s}_{ij}^v \cdot \nu_j^v, \tag{8}$$

so as to preserve the important property of the Ritz-Galerkin method that the residual is orthogonal to the basis functions (in the inner-product sense). By using equations (5) and (8) to eliminate $\mathcal{L}'$ and μ in equation (7), and then using equation (3), it is found that $\mathsf{s}^v = [(\mathsf{r}^v)^{-1}]^\top$:

$$\mathsf{s}^{v_b} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & n_x & n_y & \kappa n_y^2 & -\kappa n_x n_y & \kappa n_x^2 \\ 0 & -n_y & n_x & 2\kappa n_x n_y & -\kappa(n_x^2 - n_y^2) & -2\kappa n_x n_y \\ 0 & 0 & 0 & n_x^2 & n_x n_y & n_y^2 \\ 0 & 0 & 0 & -2n_x n_y & n_x^2 - n_y^2 & 2n_x n_y \\ 0 & 0 & 0 & n_y^2 & -n_x n_y & n_x^2 \end{pmatrix} \tag{9}$$

for boundary nodes v_b. Let $\mathsf{S} = \mathrm{diag}(\mathsf{s}^v)$. If equation (1) is the result of constructing the discretized system via the Ritz-Galerkin procedure with trial functions ν, then equation (2) is obtained by using μ as trial functions instead of ν, with $\mathsf{T} = \mathsf{S}$. It can be seen in figure 2 that taking $\mathsf{T} = \mathsf{S}$ results in significantly less error than $\mathsf{T} = \mathsf{R}$.

One may still want to transform $\mathbf{u}$ to boundary-oriented coordinates at the boundary nodes to facilitate the construction of the stiffness matrix, for example. Letting $\mathbf{u}' = \mathsf{R}\mathbf{u}$ (which is the correct transformation of $\mathbf{u}$) and $\mathsf{T} = \mathsf{S} = (\mathsf{R}^{-1})^\top$ (which is the correct transformation of K) yields

$$\mathsf{T}\mathsf{K}\mathsf{T}^\top \mathbf{u}' = \mathsf{T}\mathbf{b}. \tag{10}$$

Note that this is *not* equivalent to performing a similarity transformation of K since T is not an orthogonal matrix unless $\kappa = 0$. In the case of C^0 elements where the second derivatives are not constrained by boundary conditions, only the upper-left 3×3 sub-matrices of R and S are relevant, the transformation becomes a similarity transformation.

3. Surface terms

For C^1 elements the trial functions are twice differentiable, and therefore two integrations by parts may be performed when constructing the weak-form equations. Thus there are two types of surface terms which must be considered:

1. terms of the form
$$\oint_{\partial\Omega} d\ell\ \hat{n} \cdot \mathbf{F}\, \mu_i^v; \text{ and} \tag{11}$$
2. terms of the form
$$\oint_{\partial\Omega} d\ell\ \hat{n} \cdot \mathsf{G} \cdot \nabla \mu_i^v, \tag{12}$$

where $\mathbf{F}$ and G are arbitrary functions of space. All surface terms arising a single integration by parts will be of the first form. Those arising from terms which have been integrated by parts twice can in general be written as a combination of both types.

For any reduced quintic finite element having an edge on a straight boundary, only six trial functions are nonzero anywhere on that edge: $\mu_1^{v_a}$, $\mu_3^{v_a}$, $\mu_6^{v_a}$, $\mu_1^{v_b}$, $\mu_3^{v_b}$, and $\mu_6^{v_b}$ where v_a and v_b are the two vertices of the edge. The surface terms are therefore nonzero only in the weak-form equations formed using these trial functions. Essential Dirichlet boundary conditions are imposed by replacing precisely these equations with the boundary condition equation. Therefore, surface terms of the first type make no contribution when Dirichlet boundary conditions are imposed.

Terms of the second type may be re-written

$$\oint_{\partial\Omega} d\ell\ \hat{n} \cdot \left[\mathbf{G}_n \hat{n} + \mathbf{G}_t \hat{t}\right] \cdot \nabla \mu_i^v, \tag{13}$$

where $\hat{t}$ is the unit vector tangent to the domain boundary. Again, there are only six trial functions for which $\partial_t \mu_i^v$ is nonzero anywhere on the edge (the same six μ_i^v which are nonzero on the edge); therefore, the term involving $\mathbf{G}_t$ will vanish when Dirichlet boundary conditions are imposed. There are four trial functions for which $\partial_n \mu_i^v$ are nonzero on the edge: $\mu_2^{v_a}$, $\mu_5^{v_a}$, $\mu_2^{v_b}$, and $\mu_5^{v_b}$. The weak-form equations obtained with these trial functions are precisely the ones which are replaced when imposing Neumann boundary conditions.

To summarize, when the domain boundaries are straight, all surface terms vanish under the imposition of Cauchy conditions (both Dirichlet and Neumann conditions together). Of course, this is only appropriate when considering fourth-order differential equations; otherwise, two integrations by parts should never be performed. When considering second-order differential equations, for which only one integration by parts should be performed, all surface terms vanish under the imposition of Dirichlet conditions. This is not surprising, as the application of additional boundary conditions (as natural boundary conditions, for example) would be expected to over-determine the system.

The preceding arguments fail in the case of curved boundaries because in that case there is generally no curve between v_a and v_b along which more than one of the trial functions associated with v_a or v_b vanishes. Therefore the surface terms must be retained, even with the imposition of Cauchy boundary conditions. Put differently, the basis $\{\nu\}$ cannot satisfy essential homogeneous Dirichlet or Neumann conditions along the entire curved boundary, only at the nodes. Curved C^1 elements that do satisfy essential homogeneous Dirichlet and Neumann conditions along an approximate boundary have been developed by Qing and Li [2]. Exact satisfaction of essential conditions along an approximate boundary is likely not a significant advantage over the method discussed here except for applications that are both particularly sensitive to boundary conditions and in which strictly homogeneous boundary conditions are being applied.

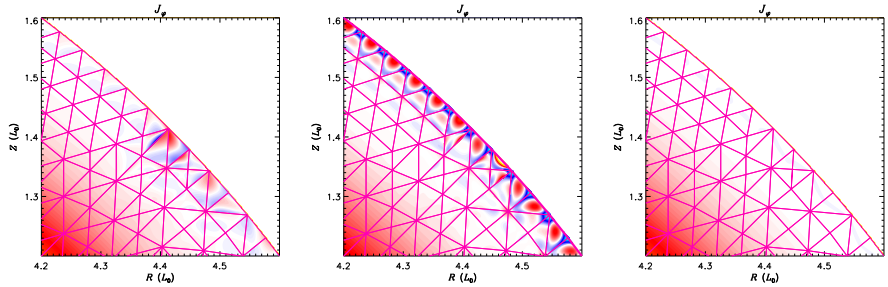

Figure 2: Illustrated here is the toroidal current density of the solution to the Grad-Shafranov equation in a circular domain, using three different methods of applying homogeneous Dirichlet conditions on ψ. *Left*: The boundary conditions are applied without applying any transformation to the matrix equation; *Center*: the transformation is applied assuming $\mathsf{T} = \mathsf{R}$; *Right*: the transformation is applied assuming $\mathsf{T} = \mathsf{S}$.

4. Numerical Examples

As examples, we present numerical solutions to the Grad-Shafranov equation,

$$-\nabla \cdot \left(\frac{\nabla \psi}{R^2} \right) = \frac{dp}{d\psi} + \frac{F}{R^2} \frac{dF}{d\psi}, \tag{14}$$

with various treatments of boundary conditions, in cylindrical coordinates (R, Z). This equation describes pressure balance in a magnetized plasma in toroidal geometry, where p is the thermal pressure, F/R is the toroidal component of the magnetic field, and $J_\varphi = -R\nabla \cdot (\nabla\psi/R^2)$ is the toroidal component of the electrical current density. The solution ψ is uniquely determined by the profiles p and F, together with boundary conditions on ψ. We obtain a solution with an iterative method described in detail in reference [8] using the M3D-C^1 code [9]. Although this second-order differential equation does not require integration by parts, we integrate by parts once for the purpose of illustration, to obtain

$$A_{ij}^{vw} = \int_\Omega d^2x \, \frac{1}{R^2} \nabla \nu_i \cdot \nabla \nu_j - \oint_{\partial\Omega} d\ell \, \frac{1}{R^2} \nu_i^v \, \hat{n} \cdot \nabla \nu_j \tag{15}$$

$$B_i^v = \int_\Omega d^2x \, \left(\nu_i^v \frac{dp}{d\psi} + \frac{F}{R^2} \frac{dF}{d\psi} \right). \tag{16}$$

Equation 14 is specific to toroidal geometry, so $d^2x = R\, dR\, dZ$ here.

First, we show that the method we have proposed (with $\mathsf{T} = \mathsf{S}$) yields better results than two other choices: $\mathsf{T} = \mathsf{I}$ (the identity matrix) and $\mathsf{T} = \mathsf{R}$. Here, a circular boundary having radius $R_C = 2$ and centered at $(3, 0)$ is used, so $\kappa = 1/R_C = 1/2$. Homogeneous essential Dirichlet conditions are imposed on ψ. Both p' and FF' are taken to approach zero smoothly at the boundaries, so the analytic solution will have J_φ also smoothly approaching zero. The numerical solutions of J_φ for the various cases are shown in figure 2.

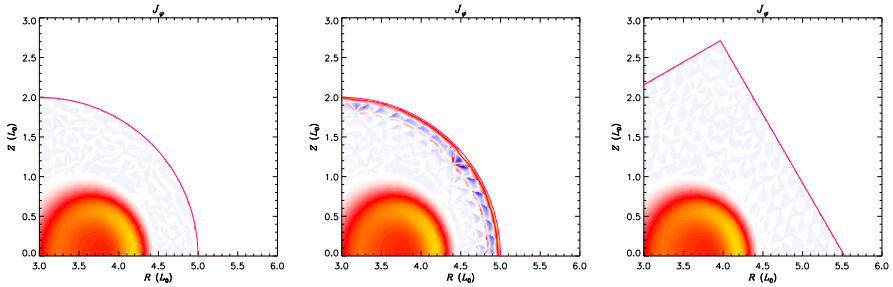

Figure 3: *Left*: The toroidal current density of the solution to the Grad-Shafranov equation in a circular domain; *Center*: the same case, but with the surface term omitted; *Right*: the same case, with the surface term omitted, in a (rotated) rectangular domain. In each case inhomogeneous Dirichlet conditions have been imposed on ψ. Given these conditions, omitting surface terms only results in errors for curved boundaries.

Forgoing the transformation leads to visible errors in the numerical solution near the boundary, but the choice $\mathsf{T} = \mathsf{R}$ leads to even greater errors, perhaps surprisingly. The third case presented in figure 2, and clearly the most accurate, is that in which the transformation $\mathsf{T} = \mathsf{S}$ is used.

Next, we show that the surface term in equation (15) may be neglected when Dirichlet conditions are applied to ψ if the boundaries are straight, but not if they are curved. For the curved configuration we again use a circular boundary of radius 2 centered at $(3, 0)$. For the straight configuration we use a square boundary that has been rotated by 30° to show that the orientation of the boundary is not relevant. The boundary conditions in this case are inhomogeneous in order to show that the homogeneity of the boundary conditions is not relevant either. Specifically, the boundary value of ψ is calculated to be consistent with an externally applied vertical field, as would be present in a tokamak. In figure 3 it is shown that significant errors in the numerical solution arise in the circular case when the surface term is neglected, but not in the straight case. This is consistent with the analysis of section 3.

5. Summary

The basis functions ν of the reduced quintic finite element are constructed to obey an orthogonality condition on their derivatives with respect to the global coordinate system (x, y). When applying essential boundary conditions, it is important to transform the matrix equations so that each row is either fully constrained or unconstrained by the boundary condition. We have shown that the appropriate transformation of the stiffness matrix is not R, the transformation matrix from global coordinates to boundary-oriented coordinates. Instead, it is preferable to use the transformation S, which transforms the *trial functions* ν to a new set μ so as to satisfy the orthogonality condition equation (7). These trial functions are optimal in the sense that the application of essential

boundary conditions constrains the non-orthogonal part of the residual to the maximum extent possible given boundary conditions of the form $\mathcal{L}_i'(u) = b$. In the case of C^0 elements for which only first-order derivatives may be constrained with boundary conditions, R and S obtain the same form, and therefore the two approaches yield the same result. Only in the C^0 case, or when $\kappa = 0$, does the appropriate transformation of the stiffness and the solution vector take the form of a similarity transform.

In the special case of straight boundaries, the surface terms arising from integrating the weak-form equations by parts will not contribute to the final set of equations when certain essential boundary conditions are applied. Specifically, surface terms arising from a single integration by parts will not contribute when Dirichlet boundary conditions are applied; and surface terms arising from two integrations by parts will not contribute when Cauchy conditions are applied (and depending on the form of the term, only one of these conditions may need to be applied). These boundary conditions need not be homogeneous. For curved boundaries, surface terms must always be retained (except for particular natural boundary conditions), as the method described here does not permit the satisfaction of essential homogeneous Dirichlet or Neumann boundary conditions along the curved boundary. However, these conditions will be satisfied within the accuracy of the finite element.

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