Implementing the finite element method

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January 22, 2009

1   Local and Global Assembly

The basic strategy which is employed in constructing the discrete equations which are solved is that we integrate the equations under consideration on each element in the mesh and then we add these terms into the global matrices and vectors at the rows and columns corresponding to the nodes of that element. The integration of the equations over each node is referred to as local assembly while the construction of the overall linear system from these contributions is referred to as global assembly.

2   The reference element

The key advantage of this approach of local and global assembly is that evaluate the shape functions on a single reference element and then transform this element to represent each actual element in the mesh. We therefore only store the shape functions and their derivatives once for each element space we deal with. If there are N basis functions per element then local assmbly consists of testing those N functions with N test functions to produce an $N \times N$ matrix.

3   Local Coordinates

The reference hypercube element is easily represented as the Cartesian product of intervals. Conventionally, the interval is $[-1, 1]$. For simplices (triangles and tetrahedra) life is more complicated. A solution is to use $n + 1$ coordinates to represent the n-dimensional simplex. For example in this system the vertices of the reference triangle are $(1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$.

An n-dimensional vector space can have only n independent vectors so clearly these coordinates cannot be independent. In fact the coordinates are related by the relation:

$$\left(\sum_{i=1}^{\dim} \xi_i \right) = 1 \tag{1}$$

Consider a triangle with vertices $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ in global coordinates. This local coordinate system has a number of interesting properties:

1. If (ξ_1, ξ_2, ξ_3) are the local coordinates of a point $\mathbf{p}$ then the global coordinates are given by $\xi_1 \mathbf{v}_1 + \xi_2 \mathbf{v}_2 + \xi_3 \mathbf{v}_3$.

2. The centroid (barycentre) of the triangle has local coordinates $(1/3, 1/3, 1/3)$

3. If $\mathbf{p}$ lies in the triangle then all its local coordinates are positive. Conversely, if $\mathbf{p}$ lies outside the triangle it has at least one negative local coordinate.

4. If $\mathbf{p}$ lies on the edge opposite vertex i then $\xi_i = 0$.

5. If A is the area of $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ then the area of the triangle $\{\mathbf{v}_i, \mathbf{v}_j, \mathbf{p}\}$ is equal to $\xi_k A$ where (i, j, k) is some permutation of $(1, 2, 3)$.

These properties apply with the obvious modifications in dimensions other than 2. Due to the last of these properties, this system of coordinates is frequently referred to as area (in two dimensions) or volume (in three dimensions) coordinates. The term "barycentric coordinates" is also used to describe this system.

3.1 The interval element

The observent reader will have noticed that local coordinates for simplex elements vary in the interval $[0, 1]$ while local coordinates for hypercube elements vary in the interval $[-1, 1]$. What, then, is the appropriate local coordinate for the one dimensional interval element - which can be seen either as a simplex or as a hypercube? The answer is somewhat arbitrary but in Fluidity the choice is made that interval elements are treated as simplices.

4 Shape functions in local coordinates

An advantage of the local coordinate systems is that the shape functions which are employed as the basis for finite element spaces can frequently be written as the product of one dimensional functions. So, for example, the P1 (linear) element on the reference triangle has basis functions:

$$n_1(\xi_1, \xi_2, \xi_3) = \xi_1 \tag{2}$$
$$n_2(\xi_1, \xi_2, \xi_3) = \xi_2 \tag{3}$$
$$n_3(\xi_1, \xi_2, \xi_3) = \xi_3 \tag{4}$$

For a slightly more complex example, the P2 (quadratic) element on the interval can be given by:

$$n_1(\xi_1, \xi_2) = \xi_1(2\xi_1 - 1) \tag{5}$$
$$n_2(\xi_1, \xi_2) = (2\xi_1)(2\xi_2) \tag{6}$$
$$n_3(\xi_1, \xi_2) = \xi_2(2\xi_2 - 1) \tag{7}$$

5 Change of coordinates

Having written the shape functions in local coordinates, we are now in a position to evaluate bilinear forms of these shape functions. If we take the simplest case of the mass matrix in one dimension we have:

$$\mathrm{M}(i, j) = \int_E n_i(\xi_1, \xi_2) n_j(\xi_1, \xi_2) \mathrm{d}x \tag{8}$$

To evaluate this integral it is necessary to change coordinates so that the coordinate in the integrand matches that over which we are integrating:

$$\mathrm{M}(i, j) = \int_0^1 n_i(\xi_1, 1 - \xi_1) n_j(\xi_1, 1 - \xi_1) \frac{\mathrm{d}x}{\mathrm{d}\xi_1} \mathrm{d}\xi_1 \tag{9}$$

Note also that we have used equation (1) to eliminate the dependent variable ξ_2.

Next, consider the problem of a bilinear form involving a derivative:

$$(A)(i, j) = \int_E n_i(\xi_1, \xi_2) \frac{\mathrm{d}n_j(\xi_1, \xi_2)}{\mathrm{d}x} \mathrm{d}x \tag{10}$$

In this case it is necessary to change coordinates in both the integral and the derivative:

$$\mathrm{M}(i, j) = \int_0^1 n_i(\xi_1, 1 - \xi_1) \frac{\mathrm{d}n_j(\xi_1, \xi_2)}{\mathrm{d}\xi_1} \frac{\mathrm{d}\xi_1}{\mathrm{d}x} \frac{\mathrm{d}x}{\mathrm{d}\xi_1} \mathrm{d}\xi_1 \tag{11}$$

where we have deliberately avoided cancellations which are not possible for more complex cases. If, as we suggest above, we can write $n_j(\xi_1, \xi_2) = n_{j,1}(\xi_1) n_{j,2}(\xi_2)$ then we can further expand the derivative into:

$$\mathrm{M}(i, j) = \int_0^1 n_i(\xi_1, \xi_2) \left(n_{j,2}(\mathbf{x}_2) \frac{\mathrm{d}n_{j,1}(\xi_1)}{\mathrm{d}\xi_1} + n_{j,1}(\mathbf{x}_1) \frac{\mathrm{d}n_{j,2}(\xi_2)}{\mathrm{d}\xi_2} \frac{\mathrm{d}\xi_2}{\mathrm{d}\xi_1} \right) \frac{\mathrm{d}\xi_1}{\mathrm{d}x} \frac{\mathrm{d}x}{\mathrm{d}\xi_1} \mathrm{d}\xi_1 \tag{12}$$

The effect of these expansions is to reduce the integral to single variable functions and derivatives. The integral can therefore be evaluated using single variable functions in the local coordinate space combined with the cross derivative term:

$$\frac{\mathrm{d}x}{\mathrm{d}\xi_1} \left(= \frac{\mathrm{d}\xi_1}{\mathrm{d}x}^{-1} \right) \tag{13}$$

In more than one dimension, the transformation becomes a Jacobian matrix. For example in two dimensions:

$$J = \begin{bmatrix} \frac{d\xi_1}{dx_1} & \frac{d\xi_1}{dx_2} \\ \frac{d\xi_2}{dx_1} & \frac{d\xi_2}{dx_2} \end{bmatrix} \tag{14}$$

the change of variables for the integral then becomes $\det\left(J^{-1}\right)$ so that, for example, the mass matrix is:

$$\mathrm{M}(i,j) = \int_0^1 \int_0^1 n_{i,1}(\xi_1)n_{i,2}(\xi_2)n_{i,3}(\xi_1)n_{j,1}(\xi_1)n_{j,2}(\xi_2)n_{j,3}(\xi_1)\det\left(J^{-1}\right)\mathrm{d}\xi_1\mathrm{d}\xi_2 \tag{15}$$

6 Quadrature

Consider the problem of integrating a function on the unit integral:

$$I = \int_0^1 f(x)dx \tag{16}$$

If we have an analytic expression for f it might be possible to perform this integral analytically. However if, as is generally the case in finite element problems, f is a product of basis functions then this approach rapidly becomes expensive and complex. Instead, we can construct numerical approximations to the integral.

The simplest approximation to this integral is given by:

$$I \approx f(0.5) \tag{17}$$

This piecewise constant approximation has an error of $O\left(h^2\right)$ where h is the length of the interval. A better approximation is given by the trapezoidal rule:

$$I \approx \frac{1}{2}\left(f(0) + f(1)\right) \tag{18}$$

which has an error of $O(h^3)$. The error term in quadrature is particularly significant in integrating polynomials: $O(h^n)$ accurate quadrature is exact for polynomials of degree $O(h^{n-1})$. Finite element integrals are typically products of polynomial basis functions so for sufficiently high order quadrature, the integrals will be exact.

More generally, quadrature rules are sets of pairs $\{(\mathbf{x}_i, w_i)|i = 1\ldots G\}$ where $\mathbf{x}_i$ is a point in the reference element and w_i is a weight associated with that point. The integral of a function over the element is therefore given as:

$$\int_\mathrm{E} f(\mathbf{x})dV \approx \sum_{i=1}^G w_i f(\mathbf{x}_i) \tag{19}$$

Here, as elsewhere in scientific computing, there is a trade off between cost and accuracy: higher accuracy quadrature rules require more points per element. The most straightforward approach is to require full quadrature. That is, to have a sufficiently high degree quadrature that all integrals are exact. However, it should always be borne in mind that there are errors of known degree caused by the finite element discretisation so it may be the case that complete quadrature delivers no improvement in accuracy for an additional cost. It may therefore be advisable to employ a degree of quadrature somewhat below that required for completeness.

6.1 Bilinear forms and quadrature

If we return to the mass matrix, then we can apply quadrature to its integration as follows:

$$\mathrm{M}(i,j) \approx \sum_{gi=1}^G n_i(\mathbf{x}_{gi})n_j(\mathbf{x}_{gi})\left(\det(J^{-1})|_{\mathbf{x}=\mathbf{x}_{gi}}\right)w_{gi} \tag{20}$$

We can see from this expression that it is only necessary to store the value of each basis function at each quadrature point on the reference element. Similarly the derivatives of the basis functions need only be stored at the quadrature points: this is sufficient to evaluate both derivatives which occur in the bilinear form and the Jacobian.