Relating Monte Carlo particle tracking to Finite Element Degrees of Freedom

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Abstract:
The abstract

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1 Introduction

1.1 Tracklength as a measure of flux

The classical definition of flux is that of the number of particles crossing a unit area, however, the alternate definition is the tracklength per unit volume. Using the latter we can apply Monte Carlo tracking to estimate the average tracklength, $\bar{\ell}$, of N amount of particles traveling through (or in) a computational cell as

$$\bar{\ell} = \frac{1}{N} \sum_{n=0}^{N-1} \ell_n \tag{1.1}$$

The scalar flux, ϕ, is then just the average tracklength divided by the volume of the cell, V_c,

$$\phi = \frac{1}{V_c N} \sum_{n=0}^{N-1} \ell_n. \tag{1.2}$$

We are now interested in the expansion of the flux into, N_D, linear basis functions (one for each DOF) in the form

$$\phi \approx \phi_h = \sum_{j=0}^{N_D-1} b_j \phi_j \tag{1.3}$$

and require that

$$\int_V b_i \left[\phi - \sum_{j=0}^{N_D-1} b_j \phi_j \right] .dV = 0 \tag{1.4}$$

After rearranging the terms we get a linear system

$$\mathbf{A} \phi = \mathbf{y} \tag{1.5}$$

where

$$\begin{aligned} \mathbf{A}_{ij} &= \int_V b_i b_j .dV \\ \phi_i &= \phi_i \\ \mathbf{y}_i &= \int_V b_i \phi .dV \end{aligned}$$

The $\mathbf{A}_{ij}$ terms are normally available from the finite element matrices developed in preperation for diffusion solves. The $\mathbf{y}_i$ terms are determined by first defining a weighted tracklength, $\ell_{n,i}$, for each DOF i with the average weight

$$w_{n,i} = \frac{\int_0^{s_f} b_i(s).ds}{\int_0^{s_f} .ds} \tag{1.6}$$

where $s_f = ||\vec{r}_f - \vec{r}_i||_2$ and s is along the track corresponding to $\vec{r}$ on the line starting at location $\vec{r}_i$ and extending to $\vec{r}_f$ such that

$$s = ||\vec{r} - \vec{r}_i||_2. \tag{1.7}$$

The weighted tracklength is then $\ell_{n,i} = w_{n,i}\ell_n$ but since $\ell_n = \int_0^{s_f} .ds$ we have cancellation and

$$\ell_{n,i} = \int_0^{s_f} b_i(s).ds \tag{1.8}$$

The fluxes corresponding to each DOF i needs to be divided by the volume of trial space i which we will denote with $V_{c,i}$ and is then

$$\int_V b_i \phi.dV = \frac{1}{N} \sum_{n=0}^{N-1} \ell_{n,i} \tag{1.9}$$

1.2 Linear shape functions on 2D triangles

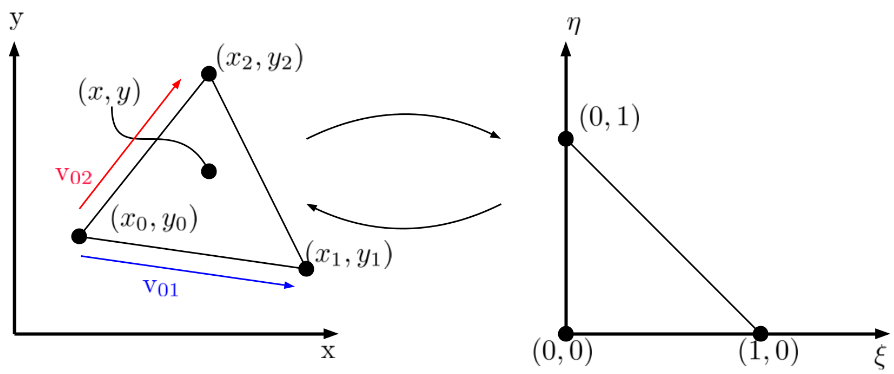

Figure 1: Triangle reference element.

The linear shape functions on the degrees of freedom of the right reference element are

$$\begin{aligned} N_0(\xi,\eta) &= 1 - \xi - \eta \\ N_1(\xi,\eta) &= \xi \\ N_2(\xi,\eta) &= \eta. \end{aligned}$$

From these functions we can interpolate the point (x, y) with the following

$$\begin{aligned} x &= N_0 x_0 + N_1 x_1 + N_2 x_2 \\ y &= N_0 y_0 + N_1 y_1 + N_2 y_2 \end{aligned}$$

We can now express x and y as functions of ξ and η by substituting the expressions for N_0, N_1 and N_2 into the expressions for x and y

$$\begin{aligned} x &= (1 - \xi - \eta)x_0 + (\xi)x_1 + (\eta)x_2 \\ &= x_0 - \xi x_0 - \eta x_0 + \xi x_1 + \eta x_2 \\ &= x_0 + (x_1 - x_0)\xi + (x_2 - x_0)\eta \end{aligned}$$

and

$$\begin{aligned} y &= (1 - \xi - \eta)y_0 + (\xi)y_1 + (\eta)y_2 \\ &= y_0 - \xi y_0 - \eta y_0 + \xi y_1 + \eta y_2 \\ &= y_0 + (y_1 - y_0)\xi + (y_2 - y_0)\eta \end{aligned}$$

In terms of the vectors from vertex 0 to the other two vertices (refer to Figure 1) we can write this as

$$x = x_0 + \mathrm{v}_{01x}\xi + \mathrm{v}_{02x}\eta \tag{1.10}$$

$$y = y_0 + \mathrm{v}_{01y}\xi + \mathrm{v}_{02y}\eta \tag{1.11}$$

which is in the form of a linear transformation and from which we can determine the very important Jacobian matrix

$$\mathbf{J} = \begin{bmatrix} \frac{dx}{d\xi} & \frac{dx}{d\eta} \\ \frac{dy}{d\xi} & \frac{dy}{d\eta} \end{bmatrix} = \begin{bmatrix} \mathrm{v}_{01x} & \mathrm{v}_{02x} \\ \mathrm{v}_{01y} & \mathrm{v}_{02y} \end{bmatrix} = \begin{bmatrix} (x_1 - x_0) & (x_2 - x_0) \\ (y_1 - y_0) & (y_2 - y_0) \end{bmatrix}. \tag{1.12}$$

From which we can determine any transformation

$$\begin{bmatrix} x \\ y \end{bmatrix} = \vec{\mathrm{v}}_0 + \mathbf{J} \begin{bmatrix} \xi \\ \eta \end{bmatrix} = \vec{\mathrm{v}} \tag{1.13}$$

and

$$\begin{bmatrix} \xi \\ \eta \end{bmatrix} = \mathbf{J}^{-1} \begin{bmatrix} \vec{\mathrm{v}} - \vec{\mathrm{v}}_0 \end{bmatrix}. \tag{1.14}$$

Therefore, given any position in cartesian coordinates (i.e. xy), we can use the transformation above to obtain the corresponding natural coordinates ξ and η and subsequently evaluate the value of the shape function. Using this approach we can see the shape functions on a triangle in Figure 2 below.

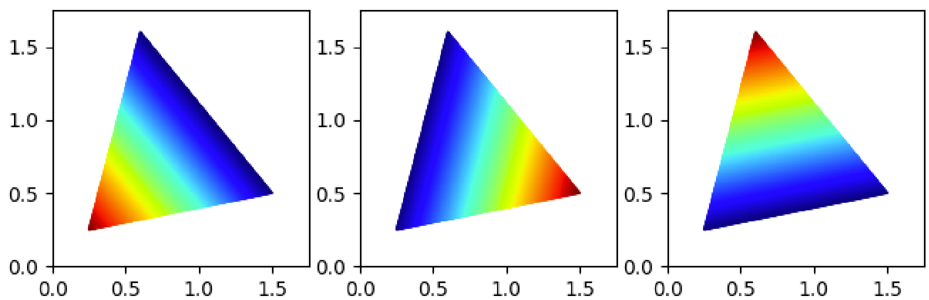

Figure 2: Linear shape functions on a triangle.

References

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