

Finite Element Method and Computational Structural Dynamics
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Lecture - 33
Mapped Elements - III

Hello friends. So we had seen how to model distorted a curve geometries using distortion of regular edge finite element standard, finite element, finite elements as we call them as parent elements. And then using the parametric mapping concept to transform these regular geometries into distorted domains of any desired shape. And that allows us the twin advantages of modelling, distortion or modelling, curve geometries very complex geometries, while retaining the advantage of constructing polynomial interpolation as the approximation of primary variable within the element.

So, approximation it is very easy to construct using standard interpolation formula in regular geometries and that advantage is retained while using the parametric mapping concept we can extend these elements to cover curved geometries. And, thereby reducing the problem size in capturing curved or more complex geometries with reasonably large sized elements instead of forcibly using very small element; small size elements to reduce the discretization error.

So, we have seen how distortion effects and wonder what conditions the accuracy, the convergence criteria will be satisfied. And fortunately, for isoperimetric mapping in which the mapping of geometry is done using the same interpolation functions which are used for approximation of the primary variables in the problem. So, if we use those interpolation functions satisfying all the requirements of interpolation functions for approximation interpolation or primary variables, then we found that those necessary conditions for convergence will be satisfied. So, that brings us to the next problem.

So, to say, because the governing differential equations of the problem are of course, defined in terms of Cartesian coordinates or physical coordinates. And the finite element approximation, that we now are talking about are defined in terms of local coordinate. So, every element is bounded by limits of local coordinates ranging from minus 1 to plus 1 for rectangular or hexahedral domains. And area or volume coordinates for triangular and tetrahedral domains ranging from 0 to 1.

So, these are all the local coordinates. And the interpolation functions are defined in terms of these local coordinates, which are defined which are valid within the interior of the element. And this is fine because conceptually the finite element approximation over the whole domain is constructed in such a way that non-zero contribution from an element only happen within the element, outside the element the effect of that element is 0. The interpolation functions are not defined or the approximation within an element is not defined outside the domains, outside the boundaries of that element.

So, this local coordinate system is perfectly fine for defining the approximation over individual elements. And in the physical domain we can define the mesh and these parent elements, regular elements can be mapped on to respective points in the physical space and to models the complete domain. So, now the problem in the physical space involves partial; I mean the differential equation in the physical space is given in terms of physical coordinate system, Cartesian coordinates or cylindrical coordinates or whatever. And accordingly the derivatives are in terms of Cartesian coordinates or physical coordinates and the weighted residual the weak form of the weighted residual statement would also involve derivatives with respect to Cartesian coordinates.

Now we have a problem. In the sense that the primary variable of approximation is defined is now defined in terms of local coordinates ξ , η , ζ which range from minus 1 to plus 1. So, we have a issue here; how to define these domain integrals which are in which involve Cartesian coordinate derivatives and then how to evaluate the domain integrals.

So, we start with the first problem I mean try to solve this 1 by 1. So, local coordinates and Cartesian derivatives. So the, as I said we maintain these two advantages approximation using local coordinates in regular geometries and then mapping these regular geometry into any arbitrary curved shape by using parametric mapping for distortion. But formulation of finite element equilibrium equations require evaluation of domain integrals where the integrands are functions of Cartesian derivatives of primary variables.

So, what to do? The evaluation of these integrals in case of distorted domains poses a minor problem. The interpolated field of primary variables as we discussed are defined in terms of the local coordinates, instead of Cartesian coordinates. But, we also have

another definition the Cartesian coordinates themselves are defined in terms of local coordinates, is not it.

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Local Coordinates and Cartesian Derivatives-1

- ▶ Formulation of finite element equilibrium equations requires evaluation of domain integrals where the integrands are functions of Cartesian derivatives of the primary variables.
- ▶ Evaluation of these integrals in the case of distorted domains poses a minor problem — the interpolated field of primary variable is defined in terms of the local coordinates (ξ , η , and ζ) instead of the Cartesian coordinates (x , y , and z), as:

$$u^{(e)} = \sum_i N_i(\xi, \eta, \zeta) u_i, \quad v^{(e)} = \sum_i N_i(\xi, \eta, \zeta) v_i \quad \text{and} \quad w^{(e)} = \sum_i N_i(\xi, \eta, \zeta) w_i$$
- ▶ The geometry in Cartesian coordinates is also interpolated in terms of local coordinates and hence it should be possible to relate Cartesian derivatives to derivatives with respect to local coordinates.

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So, the geometry in Cartesian coordinates is also interpolated in terms of local coordinates. And hence, it should be possible to relate Cartesian derivatives to the derivatives with respect to local coordinates. Because primary variables are defined in terms of local coordinates, Cartesian coordinates are defined in terms of local coordinates. So, we can compute the derivatives of Cartesian coordinates in terms of local coordinates, we can compute the derivatives of primary variables in terms of local coordinates.

So, using these it should be possible to relate these two results to what we need that is the Cartesian derivatives. How do we do this? So, since the Cartesian coordinates are defined in parametric form we resort to the definition of total derivative, we try to find what is total derivative with respect to a local coordinate will be.

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Local Coordinates and Cartesian Derivatives-2

Since the Cartesian coordinates are defined in parametric form, total derivatives with respect to local coordinates are:

or, in matrix form:

$$\begin{aligned}\frac{\partial}{\partial \xi} &= \frac{\partial x}{\partial \xi} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \xi} \frac{\partial}{\partial y} + \frac{\partial z}{\partial \xi} \frac{\partial}{\partial z} \\ \frac{\partial}{\partial \eta} &= \frac{\partial x}{\partial \eta} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \eta} \frac{\partial}{\partial y} + \frac{\partial z}{\partial \eta} \frac{\partial}{\partial z} \\ \frac{\partial}{\partial \zeta} &= \frac{\partial x}{\partial \zeta} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \zeta} \frac{\partial}{\partial y} + \frac{\partial z}{\partial \zeta} \frac{\partial}{\partial z}\end{aligned}$$

$$\begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial \zeta} \end{pmatrix} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}$$

$$= J \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}$$

$x = \sum_i N_i(\xi, \eta, \zeta) x_i$, $y = \sum_i N_i(\xi, \eta, \zeta) y_i$, and $z = \sum_i N_i(\xi, \eta, \zeta) z_i$ define the mapping of local coordinates onto Cartesian coordinates and J is known as the Jacobian matrix of this local to Cartesian coordinate transformation.



Total derivative can be derived can be defined in terms of respective derivatives with respect to other coordinate directions. So, these derivatives can also be calculated. We are talking of 3 dimensional domains here, for 2 dimensional domain we just take the first two terms. So, the idea is, in these equations or let us write these in matrix form it becomes easier to appreciate.

So, in the matrix form we have these derivatives with respect to local coordinates given as a product of this matrix. So, these matrix of partial derivatives can be computed, it can be evaluated at each point within the domain. And then these are the derivatives partial derivatives with respect to Cartesian coordinates.

So, this matrix of derivatives of Cartesian coordinates with respect to local coordinates is known as the Jacobian of transformation. So, it relates how the local coordinates are mapped to Cartesian coordinates or the global physical coordinates x, y and z. So, this defines the transformation relationship between the two coordinate systems. And when we have this, once we have this mapping known, so this Jacobian can be evaluated at any point.

So, and as I said earlier last time that element distortions have to be moderate and all those convergence criteria that we said hold in case of distorted domains those hold only under the conditions of moderate distortions. So, that moderate distortion is the keyword; key operating word. Now how do; at that time I had mentioned if there are severe distortions which do not ensure, do not relate, to do not preserve one to one mapping

between each point in parent domain to each point in the distorted domain. Then the analysis cannot progress and these convergence conditions will not be satisfied.

And that is indicated or that is detected by this Jacobian of transformation, if there is one to one mapping then this Jacobian will always be a positive definite matrix. So, the determinant of this Jacobian will be positive at every point within the domain; interior of the domain element distorted domain. And if the distortions are severe such that one to one correspondence is lost, so there is no longer one to one mapping. For example, if the domain parent element wraps back on to itself, then there is no one to one mapping between parent element and the distorted element. In this case the Jacobian of transformation will be negative definite; will be negative. And that can be computed and that of course has to be evaluated during the computation, the Jacobian of the determinant of this Jacobian matrix.

So, it will be detected very easily that there is something wrong with the distortion or the parametric mapping of the elements and the analysis cannot progress. And the, if any such event happens then the message is usually flagged and the analysis stops at that point. So, that is a very very important point to be noted of the mapping and the measure of the adequacy of mapping is the positive definiteness of this Jacobian of transformation.

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Local Coordinates and Cartesian Derivatives-3

The Jacobian matrix is computed as:

$$J = \begin{bmatrix} \frac{\partial N_1}{\partial \xi} & \dots & \frac{\partial N_m}{\partial \xi} \\ \frac{\partial N_1}{\partial \eta} & \dots & \frac{\partial N_m}{\partial \eta} \\ \frac{\partial N_1}{\partial \zeta} & \dots & \frac{\partial N_m}{\partial \zeta} \end{bmatrix} \begin{bmatrix} x_1 & y_1 & z_1 \\ \vdots & \vdots & \vdots \\ x_m & y_m & z_m \end{bmatrix}$$

where, m denotes the total number of nodes in the element. Thus, the Cartesian derivatives may be obtained as:

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = J^{-1} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial \zeta} \end{pmatrix} \quad (1)$$

which exist if and only if the Jacobian matrix of the transformation is positive definite, i.e., $|J| > 0$ everywhere in the domain.

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So, Jacobian matrix can be calculated now for each point. So, if there are m number of nodes in the element then each term of this Jacobian would involve.

So, then the Jacobian matrix can be calculated as this summation of the approximation, derivative of the geometry approximation. And once we have this calculated at different points then it can be calculated the derivative, the Cartesian derivative can be simply evaluated as inverse of this Jacobian multiplied by derivatives with respect to local coordinates pretty simple.

And this, these local coordinate derivatives can always be computed very easily, because everything all the primary variables, all the approximation are in terms of these local variable, local coordinate systems, local coordinates. So, these derivatives can be calculated and when pre multiplied by the inverse of this Jacobian at respective locations evaluated at the with this node coordinates the derivatives with respect to Cartesian coordinates can be evaluated as required.

So, this J inverse or this derivative with respect to Cartesian coordinate or this relationship for that matter the one-to-one relationship between derivatives with respect to Cartesian coordinates to the derivatives with respect to local coordinates exist only if the Jacobian of transformation is positive definite. That is determinant of J is greater than 0 should be greater than 0 everywhere in the domain. So, throughout the element the determinant of this Jacobian matrix should be greater than 0; should be positive. So, as long that is a very important check and all finite element analysis codes they maintain this check.

And whenever Jacobian is singular or it is even 0 or very close to 0 a message is flashed that it is near singular the errors in the results may be erroneous. And if it is negative then the analysis stops right away. There is no point in progressing further there has been the results if at all we proceed beyond this point then the results are going to be useless anyway. So, how do we evaluate the domain integrals then? So, the domain integrals we found that Cartesian derivatives can be expressed in terms of local derivative. So, that problem is solved.

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So, now, we have a function of xi eta and zeta which have to be evaluated which this integrated over the domain which is defined in physical domain; physical coordinates. So, dx dy integration with respect to x and y over some domain boundary. Now the next step that needs to be done is to transform this domain of integration also into in terms of local coordinates.

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Evaluation of Integrals in Distorted Domains
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Evaluation of Domain Integrals-1

- ▶ After transformation of variables, the domain of integration is also transformed to a regular bounded domain: $d\Omega = dx \cdot dy \cdot dz = |J| d\xi \cdot d\eta \cdot d\zeta$
- ▶ The integrands in terms of Cartesian coordinates can be transformed in terms of local coordinates by appropriate substitution of parametric mapping: $G(x, y, z) \rightarrow \bar{G}(\xi, \eta, \zeta)$.
- ▶ The domain integral can be evaluated as:

$$\iiint_{\Omega_e} G(x, y, z) dx dy dz = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 \bar{G}(\xi, \eta, \zeta) |J| d\xi d\eta d\zeta$$

$$\approx \sum_{i=1}^{n_\xi} \sum_{j=1}^{n_\eta} \sum_{k=1}^{n_\zeta} (W_i W_j W_k \bar{G}(\xi_i, \eta_j, \zeta_k) |J(\xi_i, \eta_j, \zeta_k)|)$$

which is of the standard form of Gauss-Legendre numerical quadrature.

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And that is achieved by using again the simple rule of transformation. So, the domain of integration is calculated as shown in slide.

And the domain boundaries are always limited by the local coordinates; local coordinates only vary between -1 to + 1 for rectangular and hexa hexagonal domain right and for triangular and volume tetrahedron they would vary from 0 to 1. So, the boundary boundaries of integral also change to very regular limits.

So, coming back, so this integrands in terms of the Cartesian coordinates can be transformed in terms of local coordinates by appropriate substitution of parametric mapping. So, essentially any general function of x , y and z can be transformed into a corresponding equivalent function of ξ , η and ζ . So, and that becomes the new integrand and the domain integral which integrates over the element domain. So, $G(x, y, z)$ integrated over this domain is evaluated in terms of local coordinates by this new integrand which is transformed integrand.

So, these are the local coordinates and the limits of the local coordinates are between -1 to + 1. Now this format is perfectly matched, perfectly suited for numerical evaluation of this, integral. And we discuss this numerical evaluation of integral while discussing the numerical quadrature definite integral numerical evaluation of definite integral. So, this is what it is. In that, we have discussed the use of Gauss quadrature. So, it is essentially weighted summation. So, I evaluate this integrand at sample eta different point and certain pre defined points and there are weights associated with those points. So, this integral is simply some of the weighted values sampling of the integrand at those points.

So, if I evaluate at ξ_i there is associated with it is associated with weight W_i , if I evaluate it at η_j there is weight associated at corresponding to that point that is called W_j . So, i, j, k they all vary with respect to different points which are I mean number of points for the evaluation of quadrature. So, how many samples are to be taken with respect to each coordinate direction. So, n_ξ is the number of sampling points in along the ξ direction, n_η is the number of sampling points along η direction and n_ζ is the number of sampling points along ζ direction. And the weighting coefficients would of course vary according to the number of sampling points and the position of sampling points.

So, this entire integrand is evaluated at each of those sampling points multiplied by appropriate weighting coefficient and then sum is accumulated and that accumulated sum is equal to this domain integral that is required. And once we have this the element

equilibrium equations are established I mean mostly; except the boundary term. We have still not discussed the boundary term, but all the domain integrals they can be evaluated in this way. And Gauss quadrature is normally we take same number of sampling points in all coordinate directions. So, if that is the usual process, but there can be situation in which we take different orders or different integration rule different orders of integration rule for different directions maybe or for different components, for different integrals are evaluated according to different rules.

So, how are these number of sampling points evaluated, or now how do I take a call how many sampling points do I need to evaluate these integrals sufficiently accurately? Because you see this is approximation. So, everything anything that we will compute is an approximation and we are trying to approximate these definite integral by a weighted sum. So, we can get a very close approximation, but that depends on how many number of sampling points I have choose and what is the nature of this integrand. For polynomials it may be it is a standard result for 1 dimensional quadrature, Gauss-Legendre numerical quadrature is the most efficient quadrature rule for integrating polynomials. And our approximation is of course, polynomial 3-dimensional quadrature rule I mean this most efficient result that Gauss-Legendre quadrature are the most efficient quadrature rule for polynomial integrand. It is only proved in case of 1-dimensions, 1-dimensional quadrature and we just hope that it holds for higher I mean 2-dimensional integrals and 3-dimensional integrals although there is no standard result which proves that.

Now, an n point Gauss quadrature rule. So if I sample the integrand at n number of points then we can exactly integrate a polynomial of degree $2n - 1$. So, if the integrand is of degree $2n - 1$ then i would need an n point quadrature. So, that is the basic rule for evaluating deciding number of quadrature, number of order of the quadrature rule and different domains, different domain integrals will of course have different degree of polynomial in the integrand and those need to be looked at.

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Evaluation of Integrals in Distorted Domains
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Evaluation of Domain Integrals-2

- ▶ An n point Gauss-Legendre quadrature can integrate exactly a polynomial of degree $2n - 1$.
- ▶ The coefficients n_ξ , n_η and n_ζ denote the order of quadrature along respective coordinate directions.
- ▶ The choice of an appropriate order of quadrature is very important in finite element computations. While using a high order quadrature rule ensures accuracy of numerical computations at the cost of a significant increase in computational costs, choice of a very low order quadrature leads to numerical instability.
- ▶ The desired order of quadrature rule is one which facilitates exact evaluation (same as analytical integration) of the elements of element stiffness matrix ($K_e = \iint_{\Omega_e} B^T D B d\Omega$) when the element is in regular, or undistorted shape.

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Coefficients n_ξ , n_η and n_ζ denote the order of quadrature along respective coordinate directions. And choice of appropriate quadrature is very important in finite element computations. While using a high order quadrature rule ensures accuracy of numerical computation. Obviously, if I use more and more sampling points, I would go on approximating it closer and closer approximating the definite integral closer and closer, but that comes at the cost of increased computation.

And this is an very expensive operation sampling the integrand, each integrand if you look is a very complex term. It involves this transformation, involves computation of this determinant of the Jacobian matrix and then carrying out these products of all the terms, right. So, in all these evaluation of this domain integral by using Gauss quadrature is one of the most expensive numerical operations in finite element analysis. And therefore, this decision of the order of quadrature rule is not to be taken lightly. So, the choice of appropriate order of quadrature is very important. And if the choice of a very low order quadrature can lead to numerical instabilities, the matrix, the system of equations may not admit a unique solution.

So, what is the balance point? The desired order of quadrature rule is one which facilitates exact evaluation same as the analytical integration of the elements of stiffness matrix. Again I refer back to the domain integral from solid mechanics applications. So, that strain displacement matrix b transpose d constitutive relation matrix and b is again strain displacement matrix.

So, if I evaluate this when the element is in regular undistorted shape. So, there is no distortion whatsoever and when I do this calculation. So, that means, the parent geometry is same as the distorted geometry, so they go one-to-one. So, a rectangle remains exactly a rectangle no change.

So, if that happens then under what conditions, what is the order of quadrature that is required in the integral for exactly evaluating this integral; because in that case there will not be any Jacobian determinant coming into picture, because there is one to one mapping. So, x is directly related to ξ , y is directly related to η and z is directly related to ζ . So, it is dx, dy, dz is same as $d\xi, d\eta, d\zeta$.

So, there is no Jacobian determinant coming in picture. And therefore, this analytical integral can be evaluated and numerical integral can be evaluated and whichever order gives us the correct solution based on this enter this first point $2n - 1$ degree polynomial requires n number of sampling points.

So, we can evaluate what is the degree of polynomial d matrix is of course constant. The polynomial terms only involve elements of matrix b , strain displacement matrix. So, for example, in case of four-node rectangle matrix b contains linear terms x and y because of the presence of x, y term in the displacement approximation. So, the first derivative would contain either x or y . So, the product would contain x^2 or x, y or y^2 .

So, when we compute this total product the highest degree of polynomial term that we have is x^2, x, y and y^2 . So, what is the highest order of derivative that will be required for second degree polynomial? So, $2n - 1$ is 2 that is second degree polynomial. So, that makes it n is equal to 1.5. So, a 2 point Gauss quadrature is sufficient for this purpose; is the quadrature rule which will correctly integrate this integrand.

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Evaluation of Integrals in Distorted Domains
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Evaluation of Domain Integrals-3

- ▶ In the case of four-node rectangle the integrand B^TDB involves second degree polynomial terms as B comprises constants and linear polynomial terms.
- ▶ A 2×2 quadrature rule is necessary to exactly integrate the second degree polynomial terms in the integrand.
- ▶ Similarly, integrand involves fourth degree polynomial terms in the case of eight-node serendipity element which requires a 3×3 quadrature rule for exact integration.

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So, in case of four-node rectangle the integrand B^TDB involves second degree polynomial terms as b comprises constants and linear polynomial terms. And 2 by 2 quadrature rule is necessary to exactly integrate the second degree polynomial terms in the integrand. Similarly fourth degree polynomial terms are encountered while using eight-node serendipity element and which will require a 3 by 3 quadrature rule for exact integration.

So, this order of quadrature is referred to as full integration or full quadrature. Similar formulations for numerical integration of transformed integrands can be developed for triangular and tetrahedral domains in terms of area or local coordinates that is l_1, l_2, l_3 or v_1, v_2, v_3, v_4 in case of tetrahedron. Rest of the procedures are more or less similar and you can refer to standard text books for more details; the basic concepts are exactly identical to what we have discussed.

So, with this we end our discussion on this domain integrals. We will resume discussion on remaining part that is the boundary integral in our next lecture.

Thank you.