PART I

FUNDAMENTALS

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CHAPTER 1

INTRODUCTION

1.1 ERA OF SIMULATION AND COMPUTER AIDED ENGINEERING

1.1.1 A World of Simulation

"Computer simulation" has become a popular terminology in almost all disciplines of science and engineering today. Successful stories of computer simulation on various research projects have been reported in many professional conferences and events. In recent years, many technical journals have emerged dedicating to theories, techniques, and applications of simulations. Simulation shines in almost every aspect of research.

In its final report of 2006, the Blue Ribbon Panel on simulation-based Engineering Science of US National Science Foundation claimed the critical importance of simulation technology in the twenty-first century and considered it as the national priority for tomorrow's engineering and science (available at http://www.nsf.gov/pubs/reports/sbes_final_report.pdf). The working group of scientists of computational mechanics, applied mathematics, and other disciplines has envisioned revolutionizing engineering science through simulation. Simulation is essentially the computational science and engineering. It involves heavily the use of finite element method and other numerical approaches. In the past half century, finite element methods have been used for many engineering applications with the advances of high-speed computing power and software functionality. The evolution of finite element technology has also stimulated the development of computer architectures and technologies. As many physical events are too costly for any type of failure, computer simulation has become a

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highly desired tool to evaluate the process before carrying out the actual procedure. For example, medical doctors can first perform computer simulation on a bypass surgery procedure for treating disease in aorta and iliac artery to assess the potential results without subjecting any human life to danger. These scientific and engineering applications have placed additional importance on numerical simulation to provide precise and accurate information.

Approximate solutions to the differential and/or integral equations from various engineering problems have been in demand for a long time due to the difficulty in obtaining analytical solutions. Courant (1943) constructed the approximate solution to St. Venant torsion problem by triangulation with linear approximation for the minimum potential energy and the Ritz method. In fact, Courant (1943) demonstrated all the basic concepts of the finite element method. In the mid-1950s, Argyris (1954, 1957) and his colleagues extensively developed certain generalization of the linear theory of structures and presented procedures for analyzing complex discrete structures. Turner et al. (1956) analyzed classical elasticity equation and illustrated the triangular element properties for plane stress. Clough (1960) named such an approximation method the "finite element," for the first time. Since then, work and research on the finite element method has grown extensively. While many algorithms and applications of linear problems were still under development, nonlinear analysis has been developed at a significantly faster pace. Oden (1972) among others demonstrated significant achievements in nonlinear applications and provided the basic concepts and algorithms of nonlinear finite element methods.

Following the development of the fundamentals, finite element software was quickly commercialized and further propelled engineering applications. The first software program was delivered by Ed Wilson. The subsequent development became SAP and NONSAP. The first nonlinear commercial software MARC led by Pedro Marcal and ADINA led by Jürgen Bathe were among the early software developed for nonlinear structural dynamics. Finite element then started to be introduced into universities' colloquiums. It is critical that, in accompanying the development of numerical methods and engineering applications, the mathematical theories about interpolation, convergence, and error estimation of the finite element methods have also been heavily developed to provide strong support for the finite element method. The monograph edited by Ciarlet and Lions (1991) is an excellent collection of the mathematical achievements. We agree with the statement by Belytschko (1996) that extending from linear static analysis to nonlinear dynamic analysis greatly increases the level of difficulty. The generally adopted solver for nonlinear problems has been basically a Newton–Raphson procedure or a modified one. These numerical schemes are the foundation of successful engineering applications. For strongly nonlinear problems, however, the Newton–Raphson iteration can fail to converge. The algorithm to obtain a convergent solution within reasonably short time has been a focal point of finite element researches.

1.1.2 Evolution of Explicit Finite Element Method

The explicit finite element method has been successfully applied to various situations of nonlinear transient dynamics in the past decades. It is now widely adopted in the

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manufacturing process as well as in the research activity. As reported in journals and conferences, many problems have been solved by using explicit finite element. The applications involve various industries and manufacturing processes. The following references are just a few examples: Anghileri et al. (2005) and Ho and Smith (2006) for bird strike at the airplane; Xue and Schmid (2005) for train collision; Saha et al. (1995) and Houssini (2006) for automobile crashworthiness; Neumayer et al. (2006) for package drop; Chow and Tai (2000) for sheet metal stamping; Lu and Wu (2006) for forging and extrusion processes; Medvedev (2002) for welding. The list of applications goes on and on. These examples have a common feature, that is, dynamic contact or say impact. We name these applications as impact engineering for late reference.

The structural analysis for the impact engineering such as above is a class of transient dynamics. It is a highly nonlinear system including large deformation, large rotation, nonlinear material, contact, impact, etc. For such a system, usually only numerical solution can be expected. Even with numerical approach, engineers have seen substantial challenges from large deformation in dynamic buckling and postbuckling mode. In this area, the traditional (implicit) approach had not achieved much satisfaction until the explicit finite element method emerged as a powerful tool. The explicit approach provides an alternative problem-solving procedure. It is essentially an incremental method. Apart from the traditional implicit method, explicit approach basically does not form the system stiffness matrix and does not need to invert the large matrix. Hence, the explicit method has avoided certain difficulties of nonlinear programming that the implicit method has.

As described in Belytschko et al. (2000), the explicit finite element software was originated in the United States. Several groups of scientists had worked on the concept of explicit integration for nonlinear transient dynamics. Wilkins (1964) was among the earliest publications on explicit finite element methods. As reported by Constantino (1967), the first explicit software was built in 1964.

Other early developments include HONDO and later PRONTO led by Sam Key; SADCAT, WHAMS, and Super WHAMS led by Ted Belytschko, and DYNA-2D/3D led by John Hallquist. The commercial software boomed in the mid-1980s. We have seen PAMCRASH in the market first, followed by RADIOSS, DYTRAN, and ABAQUS-explicit. In later 1980s, headed by John Hallquist, LS-DYNA was commercialized. In fact, the fast development and implementation of many modern numerical technologies make LS-DYNA distinguished from the pack of commercial software.

1.1.3 Computer Aided Engineering (CAE)—Opportunities and Challenges

As Moore's rule predicted, the computing power increases tenfolds every 5 years. The CAE engineers have witnessed and enjoyed the great advances in computer architectures and software functionalities.

With growing computing power, expectations for more accurate predictive analysis (by the project management) have also risen. Simulation as an important design tool has been built into the manufacturing process. This brings a tough challenge to engineers as they try to assess the reliability of the results predicted by the computer simulation, even before the prototype test is conducted. Being over confident and overly reliant on simulation results have at times led to wrong and costly decisions. In recent years, the concept of verification and validation (V & V) has been proposed; see Oden et al. (2003) and Babuska and Oden (2004) for basic concepts and theories, also Oberkampf and Barone (2004) for engineering practices. Verification and validation is critical for certain types of simulation, whose errors could lead to major disasters. The essential point is how to systematically justify the numerical solutions.

From our years of engineering experiences, the authors strongly feel that it would be helpful for engineers to have a deep understanding of the "back bones" of the software. One of the main objectives of this book is to introduce the related theory and technology for the explicit finite element method. This book can also serve as a textbook for related disciplines in graduate level work and studies. This book identifies certain unresolved issues currently existing in finite element formulation and its implementation in software. It is also the authors' intent to assist researchers to find interesting and challenging topics for their studies that will eventually help engineers make better computer simulations.

1.2 PRELIMINARIES

1.2.1 Notations

Several aspects of applied mechanics, applied mathematics, and numerical methods are involved in this book. Due to the complexity of the course, many physical variables and parameters will be employed. Many of them have components in three-dimensional (3D) space and are time dependent. Notations commonly seen in engineering literatures will be used to identify these variables, in a consistent manner. In case if same symbol is used for different variables in different discipline, we will choose an alternative definition. The following is a partial list of the most important variables in the text:

u	displacement
v	velocity
a	acceleration
ε	strain
σ	stress
t	time
ζ	thickness of plate/shell
h	element size
E	Young's modulus
G	shear modulus
ν	Poisson ratio
λ, μ	Lamé elasticity constants
ρ	mass density
ξ, η	coordinates of reference system

Φ	shape functions of finite element
$(\dot{f})$	first-order time derivative of function f
$(\ddot{f})$	second-order time derivative of function f
$f_{,x}$	a (partial) derivative $\partial f/\partial x$

Exceptions will accompany additional explanations whenever it is necessary.

Both indices and bold faces will be used to represent the vectors, matrices, and tensors. Indices will be used for the components of vector variables, for example, f_j indicates the j-component of variable f. Regarding coordinates, usually 1, 2, and 3 are for the x-, y-, and z-directions, respectively. Indices are also used for matrices, tensors, and other variables. For example, u_j^N will be used later for x_j-component of displacement of node N. To avoid any possible confusion with the sequence of matrix multiplications, or the multiplication with tensors of order 3 and higher or variables with multiindices, the index notation will be used more often. Bold-faced variables will also be used, when their number of components is easy to understand and their operation will not be confused.

The lower-case indices are most likely used for spatial components, with Latin indices for 3D variables and Greek indices for two-dimensional (2D) variables. Capital Latin indices are often used for nodal variables of finite elements.

Simple tensor operations will be used for shorthand writing purposes, which should be easily understood by readers without extensive knowledge of tensor analysis. Cartesian coordinate system will be used exclusively, except in special situations where additional explanations are provided. Hence, there is essentially no difference for superscripts and subscripts or contravariant and covariant components of the tensors. In particular, $u_{i,j}$ simply means a partial derivative $\partial u_i/\partial x_j$.

The commonly used convention of summation on repeated indices is adopted. The convention of summation only applies to paired variables with the same indices. Summation of tripled or more variables will use the traditional notation Σ. This convention is also extended to summation involving nodal values of finite elements. For instance,

$u_j v_j = \sum_j u_j v_j$:	a dot product of two vectors $\boldsymbol{u} \cdot \boldsymbol{v}$.
$a_{ij} b_j = \sum_j a_{ij} b_j$:	a multiplication of a matrix with a vector $\boldsymbol{Ab}$.
$u_N \Phi_N = \sum_N u_N \Phi_N$:	interpolation formula with finite element nodal values and the shape functions.

Note that the number of components in above examples is not critical and easy to understand. The pair of indices in the summation is called dummy index, which can be replaced by any character. This is a necessary practice when an index would appear to be triple or more but summation is really acting on two variables only. Some differential operators can be expressed using the convention of summation:

$u_{j,j} = \nabla \bullet \boldsymbol{u}$:	divergence of vector $\boldsymbol{u}$.
$w_{,jj} = \nabla^2 w$:	Laplacian of function w.

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Special tensors and their functionalities are adopted:

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} : \quad \text{Kronecker delta,}$$

$$\in_{ijk} = \begin{cases} 0 & \text{if any two indices are equal} \\ 1 & \text{if } i, j, k = 1, 2, 3 \text{ or } 2, 3, 1 \text{ or } 3, 1, 2 \\ -1 & \text{if } i, j, k = 3, 2, 1 \text{ or } 2, 1, 3 \text{ or } 1, 3, 2 \end{cases} : \quad \text{3D permutation tensor.}$$

Part of their operational functionalities is listed below for later reference:

$$\delta_{ij} u_j = u_i,$$

$$\delta_{jj} = 3, \quad \delta_{ij}\delta_{jk} = \delta_{ik}, \quad \delta_{ij}\delta_{ij} = \delta_{jj} = 3,$$

$$\in_{ijk}\in_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}, \quad \in_{ijk}\in_{ijn} = 2\delta_{kn},$$

$$c_k = \in_{ijk} a_i b_j : \ \boldsymbol{c} = \boldsymbol{a} \times \mathbf{b} : \quad \text{vector product of two vectors in 3D space,}$$

$$\in_{ijk} a_i b_j c_k = \boldsymbol{a} \times \boldsymbol{b} \bullet \boldsymbol{c} : \quad \text{mixed product of three vectors in 3D space.}$$

This threefold summation represents a mixed product of three vectors, which is equivalent to the volume framed by the vectors $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$.

The 2D Kronecker delta and permutation tensor are defined with α and β ranging from 1 to 2:

$$\delta_{\alpha\beta} = \begin{cases} 0 & \text{if } \alpha \neq \beta \\ 1 & \text{if } \alpha = \beta \end{cases} : \quad \text{2D Kronecker delta,}$$

$$\in_{\alpha\beta} = \begin{cases} 0 & \text{if } \alpha = \beta \\ 1 & \text{if } \alpha, \beta = 1, 2 \\ -1 & \text{if } \alpha, \beta = 2, 1 \end{cases} : \quad \text{2D permutation tensor.}$$

The related properties are, for example,

$$\delta_{\beta\beta} = 2,$$
$$\in_{\alpha\beta} a_\alpha b_\beta = a_1 b_2 - a_2 b_1 = \begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix} : \quad \text{2D determinant,}$$
$$\in_{\alpha\beta} \psi_{,\beta} : (\psi_{,2}, -\psi_{,1}) : \quad \text{differential operator of curl on a scalar function.}$$

1.2.2 Constitutive Relations of Elasticity

Elasticity is the foundation of structural mechanics. Here we summarize the constitutive relations for later reference, but we would not provide detailed review for elasticity as we focus on nonlinear problems. For 3D solid material, let u_i be the components of displacement. The strain of small deformation is

$$\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2. \tag{1.1}$$

The corresponding stresses are determined by the generalized Hooke's law:

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}. \tag{1.2}$$

Here, $\boldsymbol{E}$ is called the elasticity tensor. The inverse relation is expressed with the compliance tensor $\boldsymbol{C}$:

$$\varepsilon_{ij} = C_{ijkl}\sigma_{kl}. \tag{1.3}$$

For the general elasticity, both $\boldsymbol{E}$ and $\boldsymbol{C}$ are symmetric with

$$E_{ijkl} = E_{klij} = E_{jikl} = E_{ijlk},\ C_{ijkl} = C_{klij} = C_{jikl} = C_{ijlk}. \tag{1.4}$$

For isotropic elastic materials, there are only two independent material parameters. The elasticity tensor can be expressed with Young's modulus E and Poisson ratio ν, or using Lamé elasticity constants λ and μ. We have

$$E_{ijkl} = \frac{E\nu}{(1+\nu)(1-2\nu)}\delta_{ij}\delta_{kl} + \frac{E}{1+\nu}\delta_{ik}\delta_{jl} = \lambda\delta_{ij}\delta_{kl} + 2\mu\delta_{ik}\delta_{jl}, \tag{1.5a}$$

$$C_{ijkl} = -\frac{\nu}{E}\delta_{ij}\delta_{kl} + \frac{1+\nu}{E}\delta_{ik}\delta_{jl} = -\frac{\lambda}{2\mu(3\lambda+2\mu)}\delta_{ij}\delta_{kl} + \frac{1}{2\mu}\delta_{ik}\delta_{jl}, \tag{1.5b}$$

$$\begin{aligned} \sigma_{ij} &= \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij}, \\ \varepsilon_{ij} &= -\frac{\nu}{E}\delta_{ij}\sigma_{kk} + \frac{1}{2\mu}\sigma_{ij}. \end{aligned} \tag{1.6}$$

The elasticity constants are related with the following formulae:

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)},\ \mu = \frac{E}{2(1+\nu)}. \tag{1.7}$$

We also use $G = \mu$, called shear modulus. Besides, we define the bulk modulus K with

$$\begin{aligned} K &= \frac{E}{3(1-2\nu)} = \frac{2(1+\nu)\mu}{3(1-2\nu)} = \frac{3\lambda+2\mu}{3}, \\ \sigma_{jj} &= 3K\varepsilon_{jj}. \end{aligned} \tag{1.8}$$

Plane stress or the generalized plane stress state is of particular interest, where $\sigma_{33} = 0$, and other stress components are independent of the thickness. We have

$$\varepsilon_{33} = -\frac{\lambda}{\lambda + 2\mu}\varepsilon_{\delta\delta}, \tag{1.9}$$

$$\begin{aligned} \sigma_{\alpha\beta} &= \frac{E}{1-\nu^2}(\nu\delta_{\alpha\beta}\varepsilon_{\eta\eta} + (1-\nu)\varepsilon_{\alpha\beta}), \\ \varepsilon_{\alpha\beta} &= -\frac{\nu}{E}\delta_{\alpha\beta}\sigma_{\eta\eta} + \frac{1}{2\mu}\sigma_{\alpha\beta}, \end{aligned} \tag{1.10}$$

$$\begin{aligned} \sigma_{11} &= E_1(\varepsilon_{11} + \nu\varepsilon_{22}),\ \varepsilon_{11} = (\sigma_{11} - \nu\sigma_{22})/E, \\ \sigma_{22} &= E_1(\varepsilon_{22} + \nu\varepsilon_{11}),\ \varepsilon_{22} = (\sigma_{22} - \nu\sigma_{11})/E, \\ \sigma_{ij} &= 2\mu\varepsilon_{ij}, i \neq j,\ \varepsilon_{ij} = \sigma_{ij}/2\mu, \quad i \neq j, \end{aligned} \tag{1.11}$$

$$E_1 = \frac{E}{1-\nu^2}. \tag{1.12}$$