CONTINUUM MECHANICS

Constitutive Modeling of Structural and Biological Materials

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CONTINUUM MECHANICS

This is a modern textbook for courses in continuum mechanics. It provides both the theoretical framework and the numerical methods required to model the behavior of continuous materials. This self-contained textbook is tailored for advanced undergraduate or first-year graduate students with numerous step-by-step derivations and worked-out examples. The author presents both the general continuum theory and the mathematics needed to apply it in practice. The derivation of constitutive models for ideal gases, fluids, solids, and biological materials and the numerical methods required to solve the resulting differential equations are also detailed. Specifically, the text presents the theory and numerical implementation for the finite difference and the finite element methods in the Matlab® programming language. It includes thirteen detailed Matlab® programs illustrating how constitutive models are used in practice.

Dr. Franco M. Capaldi received his PhD in Mechanical Engineering from the Massachusetts Institute of Technology. He taught Mechanical Engineering at Drexel University from 2006 to 2011. He is currently an Associate Professor of Civil and Mechanical Engineering at Merrimack College. His research focuses on the modeling of biological and polymeric materials at various length scales.

To Irene, Emma, and Nina with love.

Preface

This textbook is designed to give students an understanding and appreciation of continuum-level material modeling. The mathematics and continuum framework are presented as a tool for characterizing and then predicting the response of materials. The textbook attempts to make the connection between experimental observation and model development in order to put continuum-level modeling into a practical context. This comprehensive treatment of continuum mechanics gives students an appreciation for the manner in which the continuum theory is applied in practice and for the limitations and nuances of constitutive modeling.

This book is intended as a text for both an introductory continuum mechanics course and a second course in constitutive modeling of materials. The objective of this text is to demonstrate the application of continuum mechanics to the modeling of material behavior. Specifically, the text focuses on developing, parameterizing, and numerically solving constitutive equations for various types of materials. The text is designed to aid students who lack exposure to tensor algebra, tensor calculus, and/or numerical methods. This text provides step-by-step derivations as well as solutions to example problems, allowing a student to follow the logic without being lost in the mathematics.

The first half of the textbook covers notation, mathematics, the general principles of continuum mechanics, and constitutive modeling. The second half applies these theoretical concepts to different material classes. Specifically, each application covers experimental characterization, constitutive model development, derivation of governing equations, and numerical solution of the governing equations. For each material application, the text begins with the experimental observations, which outline the behavior of the material and must be captured by the material model. Next, we formulate the continuum model for the material and present general constitutive equations. These equations often contain parameters that must be determined experimentally. Therefore, the textbook has a chapter covering the theory and application of experimental error analysis and simple curve fitting. For each material class, the continuum model is then applied to a specific application and the resulting differential equations are solved numerically. Complete descriptions of the finite difference and finite element methods are included. Numerical solutions are implemented in Matlab® and provided in the text along with flow charts illustrating the logic in the Matlab® scripts.

Contents

1 Mathematics

As scientists and engineers, we make sense of the world around us through observation and experimentation. Using mathematics, we attempt to describe our observations and make useful predictions based on these observations. For example, a simple experimental observation that the distance traversed by an object traveling at a constant velocity is linearly related to both the velocity and the time can be formalized using the relation, $\boldsymbol{d} = \boldsymbol{v}t$, where $\boldsymbol{d}$ is the distance vector, $\boldsymbol{v}$ is the velocity vector, and t is the time. The distance, velocity, and time are physical quantities that can be measured or controlled. Physical quantities such as distance, velocity, and time are represented mathematically as tensors. A scalar, for example, is a zeroth-order tensor. Only a magnitude is required to specify the value of a zeroth-order tensor. In our previous example, time is such a quantity. If you are told that the duration of an event was 3 seconds, you need no other information to fully characterize this physical quantity. Velocity, on the other hand, requires both a magnitude and a direction to specify its meaning. The velocity would be represented using a first-order tensor, also known as a vector. The internal stress in a material is a second-order tensor, which requires a magnitude and two directions to specify its value. You may recognize that the two required directions are the normal of the surface on which the stress acts and the direction of the traction vector on this surface. Tensors of higher order require additional information to specify their physical meaning. In this chapter, we will review the basic tensor algebra and tensor calculus that will be used in the formulation of continuum representations.

1.1 Vectors

A first-order tensor, also known as a vector, is used to represent a physical quantity whose representation requires both direction and magnitude. However, additional requirements must be satisfied. First, two vectors must add according to the parallelogram rule. Second, if a vector is defined within a given reference frame, and a second rotated reference frame is defined, it must be possible to express the components of a vector in one reference frame in terms of the components within another reference frame.

Whereas the physical meaning of a vector, such as the velocity of a car, is independent of coordinate system, the components of a vector are not. If we define a set of ***orthonormal basis vectors***, $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$, we can express a vector as a linear combination of the basis vectors such that

$$\boldsymbol{a} = a_1\boldsymbol{e}_1 + a_2\boldsymbol{e}_2 + a_3\boldsymbol{e}_3,$$

where a_1, a_2, a_3 are scalars representing the components of the vector in the $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, and $\boldsymbol{e}_3$ directions respectively. The ***magnitude*** of a vector, $|\boldsymbol{a}|$, is a measure of the length of a vector and is defined as

$$|\boldsymbol{a}| = \sqrt{(a_1^2 + a_2^2 + a_3^2)}.$$

It is often necessary to compare the relative size of two physical quantities whether they be scalars, vectors, or a general nth-order tensor. In each case, we may compare the ***norm*** of the two tensors. The norm of a scalar is equal to the absolute value of the scalar, whereas the norm of a vector, denoted as $\|\boldsymbol{a}\|$, is equal to its magnitude. Both the magnitude and the norm of a vector are zero if and only if each of the components of the vector is zero.

Whereas magnitude specifies the size of the vector, the direction of the vector may be represented by a ***unit vector***, $\hat{\boldsymbol{a}}$, parallel to the original vector, $\boldsymbol{a}$, such that

$$\hat{\boldsymbol{a}} = \frac{\boldsymbol{a}}{|\boldsymbol{a}|}.$$

This unit vector captures the directional information contained within the vector but discards the magnitude. The magnitude of any unit vector is equal to one. If two vectors, $\boldsymbol{a}$ and $\boldsymbol{b}$, are parallel, one vector can be written as a scalar, α, times the other vector,

$$\boldsymbol{a} = \alpha\boldsymbol{b}.$$

Vector and tensor equations can become quite complicated. It is often possible to use ***index notation*** to simplify and manipulate the representation of vector or tensor equations. Let us begin with the assumption that we are modeling physical quantities in a three-dimensional space that is spanned by the orthonormal basis vectors, $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$. In order to write a vector equation in index notation, we introduce an index, i, which in this case is a variable that can assume the value of 1, 2, or 3. The representation of a vector as a linear combination of the basis vectors can be written in the compact form,

$$\boldsymbol{a} = a_1\boldsymbol{e}_1 + a_2\boldsymbol{e}_2 + a_3\boldsymbol{e}_3 = \sum_{i=1}^{3} a_i\boldsymbol{e}_i.$$

The summation from 1 to 3 over a repeated index is quite common and may be represented in a more compact form using the ***abbreviated summation convention*** which is also termed ***Einstein notation*** as

$$\boldsymbol{a} = a_i\boldsymbol{e}_i. \tag{1.1}$$

The abbreviated summation convention is implied if and only if an index appears exactly twice within the same term of an equation.

The sum of two vectors, $\boldsymbol{b}$ and $\boldsymbol{c}$, is equal to a vector such that

$$\boldsymbol{a} = \boldsymbol{b} + \boldsymbol{c}.$$

The addition of two vectors is both communitive, $\boldsymbol{b}+\boldsymbol{c}=\boldsymbol{c}+\boldsymbol{b}$, and consistent with the parallogram rule. The components of the vectors $\boldsymbol{b}$ and $\boldsymbol{c}$ parallel to the same basis vector can be added. Vector addition can be written in terms of components such that

$$a_1\boldsymbol{e}_1+a_2\boldsymbol{e}_2+a_3\boldsymbol{e}_3=(b_1+c_1)\boldsymbol{e}_1+(b_2+c_2)\boldsymbol{e}_2+(b_3+c_3)\boldsymbol{e}_3.$$

This gives three separate equations for the components of the vector $\boldsymbol{a}$,

$$a_1=b_1+c_1,$$
$$a_2=b_2+c_2,$$
$$a_3=b_3+c_3.$$

In index notation, this set of three equations is represented as

$$a_i=b_i+c_i,$$

where i can take on a value of 1, 2, or 3. The subscript i, termed a ***free index***, appears exactly once in each of the terms in the equation. In contrast, the subscript i, appears twice in the right term in Equation (1.1). In that equation, the subscript is termed a ***dummy index*** which signifies a summation from 1 to 3 over the repeated indices.

The scalar valued ***dot product***, also known as a ***scalar product*** or ***inner product***, of two vectors is defined as

$$\boldsymbol{a}\cdot\boldsymbol{b}=|\boldsymbol{a}||\boldsymbol{b}|\cos\theta_{\boldsymbol{ab}}=a_1b_1+a_2b_2+a_3b_3=a_ib_i,$$

where $\theta_{\boldsymbol{ab}}$ is the angle between the two vectors. There are no free indices in this equation, but there is a single dummy index, i. When written in index notation, a scalar-valued function will have no free indices, and a vector valued function will have a single free index. In the general case, an nth-order tensor-valued function will have n free indices. From the definition of the dot product, we can see that the dot product of two perpendicular vectors ($\theta_{\boldsymbol{ab}}=90°$) is equal to zero. In addition, the dot product of a vector with itself gives the magnitude of the vector squared, $|\boldsymbol{a}|^2=\boldsymbol{a}\cdot\boldsymbol{a}$. The dot product of a unit vector with itself will then be equal to one, $\boldsymbol{e}_1\cdot\boldsymbol{e}_1=1$. An ***orthonormal basis set*** has the property that each basis vector is perpendicular to the others. Therefore, the dot product of each basis vector with all other basis vectors is zero and the dot product of each basis vector with itself is equal to one giving

$$\boldsymbol{e}_i\cdot\boldsymbol{e}_j=\delta_{ij},$$

where we have introduced the ***Kronecker delta***, δ_{ij}, which has the property

$$\delta_{ij}=\begin{cases}0 & if \quad i\neq j\\ 1 & if \quad i=j\end{cases}. \tag{1.2}$$

The components of a vector, $\boldsymbol{a}$, along the direction of a unit vector $\boldsymbol{e}_1$, is given by

$$\boldsymbol{a}\cdot\boldsymbol{e}_1=|\boldsymbol{a}|\cos\theta_{a\boldsymbol{e}_1}=a_1,$$

where $\theta_{a\mathbf{e}_1}$ is the angle between vector **a** and the basis vector $\boldsymbol{e}_1$.

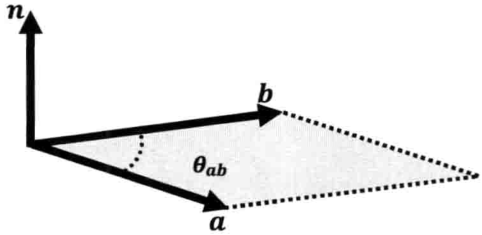

Figure 1.1. Illustration of a parallelogram bounded by vectors $\boldsymbol{a}$ and $\boldsymbol{b}$.

The result of the ***vector product*** or ***cross product***, $\boldsymbol{c}$, of two vectors, $\boldsymbol{a}$ and $\boldsymbol{b}$, is a vector that is perpendicular to each of the original vectors. The cross product is written as

$$\boldsymbol{c} = \boldsymbol{a} \times \boldsymbol{b} = (a_2 b_3 - a_3 b_2)\boldsymbol{e}_1 + (a_3 b_1 - a_1 b_3)\boldsymbol{e}_2 + (a_1 b_2 - a_2 b_1)\boldsymbol{e}_3.$$

The magnitude of the cross product is equal to

$$|\boldsymbol{c}| = |\boldsymbol{a}||\boldsymbol{b}|\sin\theta_{ab},$$

where θ_{ab} is the angle between the two vectors.

The magnitude of the cross product is a measure of the area within a parallelogram defined by the two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$, Figure 1.1. The unit normal perpendicular to the parallelogram is defined by the direction of the cross product, $\boldsymbol{n} = \frac{\boldsymbol{a}\times\boldsymbol{b}}{|\boldsymbol{a}\times\boldsymbol{b}|}$. Two parallel vectors will have a cross product equal to zero.

In this textbook, we will always employ a ***right-handed orthonormal basis set***, which has the properties that each basis vector is perpendicular to the other two, the magnitude of each basis vector is equal to one, and the basis vectors are related according to $\boldsymbol{e}_1 \times \boldsymbol{e}_2 = \boldsymbol{e}_3$. If these conditions are satisfied, the cross product between any two unit vectors can be written as

$$\boldsymbol{e}_i \times \boldsymbol{e}_j = \varepsilon_{ijk}\boldsymbol{e}_k,$$

where ε_{ijk} is the ***Levi-Civita symbol***, also known as the ***permutation symbol*** or the ***alternating symbol.*** The Levi-Civita symbol has the values

$$\varepsilon_{ijk} = \begin{cases} 1 & \text{if} \quad ijk = 123, 231, \text{or } 312 \\ -1 & \text{if} \quad ijk = 132, 213, \text{or } 321 \\ 0 & \text{for repeated indices} \end{cases}.$$

A commonly used identity relating the permutation symbol and the Kronecker delta is

$$\varepsilon_{ijk}\varepsilon_{ipq} = \delta_{jp}\delta_{kq} - \delta_{jq}\delta_{kp}. \tag{1.3}$$

EXAMPLE 1.1. *Determine whether each term in the following equation is a scalar, vector, or tensor and identify the free and dummy indices.*

$$B_{ij} = a_m a_m I_{ij} + \beta C_{ij}.$$

Solution:
The indices i and j both appear exactly once within each term of this equation. They are each free indices. The index m appears exactly twice within the second term. This is a dummy index and signifies a summation over the index m. The summation may be expanded to obtain

$$B_{ij} = (a_1a_1 + a_2a_2 + a_3a_3)\,I_{ij} + \beta C_{ij}.$$

The variable, a_m, has a single index which signifies that a_m is the scalar component of the vector $\mathbf{a}$. The variable, B_{ij}, has two indices, which means B_{ij} is a scalar component of the second-order tensor, $\mathbf{B}$. The variable β has no index and is therefore a scalar.

EXAMPLE 1.2. *Find the value of* δ_{ii}.

Solution:
Expanding this equation using the summation convention, we find that

$$\begin{aligned}\delta_{ii} &= \sum_{i=1}^{3} \delta_{ii}\\ &= \delta_{11} + \delta_{22} + \delta_{33}\\ &= 3.\end{aligned}$$

EXAMPLE 1.3. *Show that* $\delta_{ij}a_i = a_j$.

Solution:
In this equation, there is both a dummy index, i and a free index, j. Therefore, this is a compact representation of the following three equations:

$$\begin{aligned}\delta_{i1}a_i &= \delta_{11}a_1 + \delta_{21}a_2 + \delta_{31}a_3\\ &= 1 \times a_1 + 0 \times a_2 + 0 \times a_3\\ &= a_1,\\ \delta_{i2}a_i &= \delta_{12}a_1 + \delta_{22}a_2 + \delta_{32}a_3\\ &= 0 \times a_1 + 1 \times a_2 + 0 \times a_3\\ &= a_2,\\ \delta_{i3}a_i &= \delta_{13}a_1 + \delta_{23}a_2 + \delta_{33}a_3\\ &= 0 \times a_1 + 0 \times a_2 + 1 \times a_3\\ &= a_3.\end{aligned}$$

This result can be compactly written as

$$\delta_{ij}a_i = a_j.$$