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1 Introduction

A solid material subjected to mechanical and thermal loading will change its shape and develop internal stress and temperature variations. What is the best way to describe this behavior? In principle, the response of a material (neglecting relativistic effects) is dictated by that of its atoms, which are governed by quantum mechanics. Therefore, if we could solve Schrödinger's equation for all of the atoms in the material (there are about $10^{22} = 10\,000\,000\,000\,000\,000\,000\,000$ atoms in a gram of copper) and evolve the dynamics of the electrons and nuclei over "macroscopic times" (i.e. seconds, hours and days), we would be able to predict the material behavior. Of course, when we say "material," we are already referring to a very complex system. In order to predict the response of the material we would first have to construct the material structure in the computer, which would require us to use Schrödinger's equation to simulate the process by which the material was manufactured. Conceptually, it may be useful to think of materials in this way, but we can quickly see the futility of the approach: the state of the art of quantum calculations involves just hundreds of atoms over a time of nanoseconds.

Fortunately, in many cases it is not necessary to keep track of all the atoms in a material to describe its behavior. Rather, the overall response of such a collection of atoms is often much more readily amenable to an elegant, mathematical description. Like the pocket watch on the cover of this book, the complex and intricate inner workings of a material are often not of interest. It is the outer expression of these inner workings – the regular motion of the watch hands or macroscopic material response – that is of primary concern. To this end, lying at the opposite extreme to quantum mechanics, we find continuum mechanics and thermodynamics (CMT). The CMT disciplines completely ignore the discreteness of the world, treating it in terms of "macroscopic observables" – time and space averages over the underlying swirling hosts of electrons and atomic nuclei. This leads to a theory couched in terms of continuously varying fields. Using clear thinking inspired by our understanding of the basic laws of nature (which have been validated by experiments) it is possible to construct a remarkably coherent and predictive framework for material behavior. In fact, CMT have been so successful that with the exception of electromagnetic phenomena, almost all of the courses in an engineering curriculum from aerodynamics to solid mechanics are simply an application of simplified versions of the general CMT theory to situations of special interest. Clearly there is something to this macroscopically averaged view of the world. Of course, the continuum picture becomes fuzzy and eventually breaks down when we attempt to apply it to phenomena governed by small length and time scales.[1] Those are

[1] Having said that, it is important to note that continuum mechanics works remarkably well down to extremely small scales. Micro electro mechanical systems (MEMS) devices, which are fully functioning microscopic

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exactly the "multiscale" situations that we explore in depth in the companion book to this one titled *Modeling Materials: Continuum, Atomistic and Multiscale Techniques* (MM) [TM11]. Here, we focus on CMT.

Continuum mechanics involves the application of the principles of classical mechanics to material bodies approximated as continuous media. Classical mechanics itself has a long and distinguished history. As Clifford Truesdell, one of the fathers of modern continuum mechanics, states in the introduction to his lectures on the subject [Tru66a]:

> The classical nature of mechanics reflects its greatness: Ever old and ever new, it continues to pour out for us understanding and application, linking a changing world to unchanged law.

The unchanged laws that Truesdell refers to are the balance principles of mechanics: conservation of mass and the balance of linear and angular momentum. Together with the first law of thermodynamics (conservation of energy), these principles lead to a set of coupled differential equations governing the evolution of material systems.[2] The resulting general theory of continuum mechanics and thermodynamics is applicable to arbitrary materials undergoing arbitrarily large deformations. We develop this theory and explore its applications in two main parts. Part I on *theory* focuses on the basic theory underlying CMT, going from abstract mathematical ideas to the response of real materials. Part II on *solutions* focuses on the application of the theory to solve actual problems.

Part I begins with Chapter 2 on scalars, vectors and tensors and the associated notation used throughout the book. This chapter deals with basic physical and mathematical concepts that must be understood before we can discuss the mechanics of continuum bodies. First and foremost we must provide basic definitions for *space* and *time*. Without such definitions it is meaningless to speak of the positions of physical objects and their time evolution. Newton was well aware of this and begins his *Principia* [New62] with a preface called the *Scholium* devoted to definitions. In many ways Newton's greatness lies not in his famous laws (which are based on earlier work) but in his ability to create a unified framework out of the confusion that preceded him by defining his terms.[3] Once space and time are agreed upon, the next step is to identify suitable mathematical objects for describing physical variables. We seek to define such things as the positions of particles, their velocities and more complex quantities like the stress state at a point in a solid. A key property of all such variables is that they should exist independently of the particular coordinate system in which they are represented. Variables that have this property are called *tensors* or *tensor fields*. Anyone with a mathematical or scientific background will have come across the term "tensor," but few really understand what a tensor is. This is because tensors are often

machines smaller than the diameter of a human hair ($\sim$100 microns), are for the most part described quite adequately by continuum mechanics. Even on the nanoscale where the discrete nature of materials is apparent, continuum mechanics is remarkably accurate to within a few atomic spacings of localized defects in the atomic arrangement.

[2] The second law of thermodynamics also plays an essential role. However, in the (standard) presentation of the theory developed here it does not explicitly enter as a governing equation of the material. Rather, it serves to restrict the possible response to external stimuli of a material (see Chapter 6).

[3] Amazingly, more than 300 years after Newton published *Principia*, the appropriate definitions for space and time in classical mechanics remain controversial. We discuss this in Section 2.1.

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defined with a purely rules-based approach, i.e. a recipe is given for checking whether a given quantity is or is not a tensor. This is fine as far is it goes, but it does not lead to greater insight. The problem is that the idea of a tensor field is complex and to gain a true and full understanding one must immerse oneself in the rarefied atmosphere of differential geometry. We have placed ourselves squarely between these two extremes and have attempted to provide a more nuanced fundamental description of tensors while keeping the discussion as accessible as possible. For this reason we mostly adopt the Cartesian coordinate system in our discussions, introducing the more general covariant and contravariant notation of curvilinear coordinates only where necessary.

Our next step takes us away from the abstract world of tensor algebra and calculus to the description of physical bodies. As noted above, we know that in reality bodies are made of material and material is made of atoms which themselves are made of more fundamental particles and – who knows – perhaps those are made of strings or membranes existing in a higher-dimensional universe. Continuum mechanics ignores this underlying discrete structure and provides a *model* for the world in which a material is infinitely divisible. Cut a piece of copper in two and you get two pieces of copper, and so on ad infinitum. The downside of this simplification is that it actually becomes *more* complicated to describe the shape and evolution of bodies. For a discrete set of particles all we need to know is the positions of the particles and their velocities. In contrast, how can we describe the "position" that an evolving blob of material occupies in space? This broadly falls under the topic of *kinematics of deformation* covered in Chapter 3. The study of kinematics is concerned exclusively with the abstract motion of bodies, taking no consideration of the forces that may be required to impart such a motion. As a result, kinematics is purely the geometric, descriptive aspect of mechanics, phrased in the language of *configurations* that a blob of material can adopt. In a sense one can think of a configuration being the "sheet music" of mechanics. The external mechanical and thermal loading are what ultimately realize this configuration, just as the musicians and their instruments ultimately bring a symphony to life.

A continuum body can take on an infinity of possible configurations. It is convenient to identify one of these as a *reference configuration* and to refer all other configurations to this one. Once a reference configuration is selected, it is possible to define the concept of *strain* (or more generally "local deformation"). This is the change in shape experienced by the infinitesimal environment of a point in a continuum body relative to its shape in the reference configuration. Since it is shape change (as opposed to rigid motion) that material bodies resist, strain becomes a key variable in a continuum theory. An important aspect of continuum mechanics is that shape change can be of arbitrary magnitude. This is referred to somewhat confusingly as "finite strain" as if contrasting the theory with another one dealing with "infinite strain." Really the distinction is with theories of "infinitesimal strain" (like the theories of strength of materials and linear elasticity taught as part of an engineering curriculum). This makes continuum mechanics a nonlinear theory – very general in the sort of problems it can handle, but also more difficult to solve.

Having laid out the geometry of deformation, we must next turn to the laws of nature to determine how a body will respond to applied loading. This topic naturally divides into two parts. Chapter 4 focuses on this question from a purely mechanical perspective. This

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means that we ignore temperature and think only of masses and the mechanical forces acting on them. At the heart of this description are three laws taken to be fundamental principles in classical mechanics: conservation of mass and the balance of linear and of angular momentum. Easily stated for a system of particles, the extension of these laws to continuous media leads to some interesting results. The big name here is Cauchy, who through some clever thought experiments was able to infer the existence of the stress tensor and its properties. Cauchy was concerned with what we today would call the "true stress" or for obvious reasons the "Cauchy stress." This is the force per unit area experienced by a point in a continuum when cut along some plane passing through that point. The notion of configurations introduced above means that the stress tensor can be recast in a variety of forms that, although lacking the clear physical interpretation of Cauchy's stress, have certain mathematical advantages. In particular, the first and second Piola–Kirchhoff stress tensors represent the stress relative to the reference configuration mentioned above.

The second set of the laws of nature that must be considered to fully characterize a continuum mechanics problem are those having to do with temperature, i.e. the laws of thermodynamics discussed in Chapter 5. In reality, a material is not just subjected to mechanical loading which leads to stresses and strains in the body; it also experiences thermal loading which can lead to an internally varying temperature field. Furthermore, the mechanical and thermal effects are intimately coupled into what can only be described as thermomechanical behavior. Thermodynamics is for most people a more difficult subject to understand than pure mechanics. This is another consequence of the "simplification" afforded by the continuum approximation. Concepts like temperature and entropy that have a clear physical meaning when studied at the level of discrete particles become far more abstract at the macroscopic level where their existence must be cleverly inferred from experiments.[4] The three laws of thermodynamics (numbered in a way to make C programmers happy) are the *zeroth law*, which deals with thermal equilibrium and leads to the concept of temperature, the *first law*, which expresses the conservation of energy and defines energy, and the *second law*, which deals with the concept of entropy and the direction of time (i.e. why we have a past and a future). Unlike a traditional book on thermodynamics, we develop these concepts with an eye to continuum mechanics. We do not talk about steam engines, but rather show how thermodynamics contributes a conservation law to the field equations of continuum mechanics, and how restrictions related to the second law impact the possible models for material behavior – the so-called "constitutive relations" described next.

The theory we have summarized so far appears wonderfully economical. Using a handful of conservation laws inferred from experiments, a very general theoretical formulation is established which (within a classical framework) fully describes the behavior of materials subjected to arbitrary mechanical and thermal loading. Unfortunately, this theory is not closed. By this we mean that the theoretical formulation of continuum mechanics and thermodynamics possesses more unknowns than equations to solve for them. If one thinks about this for a minute, it is not surprising – we have not yet introduced the particular nature

[4] A student wishing to truly understand thermodynamics is strongly encouraged to also explore this subject from the perspective of statistical mechanics as is done in Chapter 7 of [TM11].

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of the material into the discussion. Clearly the response of a block of butter will be different than that of steel when subjected to mechanical and thermal loading. The equations relating the response of a material to the loading applied to it are called *constitutive relations* and are discussed in Chapter 6. Since we are dealing with a general framework which allows for arbitrary "finite" deformation, the constitutive relations are generally nonlinear. Continuum mechanics cannot predict the particular form of the constitutive relations for a given material – these are obtained either empirically through experimentation or more recently using multiscale modeling approaches as described in MM [TM11]. However, continuum mechanics *can* place constraints on the allowable forms for these relations. This is very important, since it dramatically reduces the set of possible functions that can be used for interpreting experiments or multiscale simulations. One constraint already mentioned above is the restrictions due to the second law of thermodynamics. For example, it is not possible to have a material in which heat flows from cold to hot.[5] Another fundamental restriction is related to the *principle of material frame-indifference* (or "objectivity"). Material frame-indifference is a difficult and controversial subject with different, apparently irreconcilable, schools of thought. Most students of continuum mechanics – even very advanced "students" – find this subject quite difficult to grasp. We provide a new presentation of material frame-indifference that we feel clarifies much of the confusion and demonstrates how the different approaches mentioned above are related and are in fact consistent with each other. A third restriction on the form of constitutive relations is tied to the symmetry properties of the material. This leads to vastly simplified forms for special cases such as isotropic materials whose response is independent of direction. Even simpler forms are obtained when the equations are linearized, which in the end leads to the venerable (generalized) Hooke's law – a linear relation between the Cauchy stress and the infinitesimal strain tensor.

The addition of constitutive relations to the conservation and balance laws derived before closes the theory. It is now possible to write down a system of coupled, nonlinear partial differential equations that fully characterize a thermomechanical system. Together with appropriate boundary conditions (and initial conditions for a dynamical problem) a well-defined *(initial) boundary-value problem* can be constructed. This is described in Chapter 7. Special emphasis is placed in this chapter on purely mechanical static problems. In this case, the boundary-value problem can be conveniently recast as a variational problem, i.e. a problem where instead of solving a complicated system of nonlinear differential equations, a single scalar energy functional has to be minimized. This variational principle, referred to as the *principle of minimum potential energy* (PMPE), is of great importance in continuum mechanics as well as more general multiscale theories such as those discussed in MM [TM11]. A key component of the derivation of the PMPE is the theory of stability, which is concerned with the conditions under which a mechanical system is in *stable* equilibrium as opposed to *unstable* equilibrium. (Think of a pencil lying on a table as opposed to one balanced on its end.) We only give a flavor of this rich and complex theory, sufficient for our purposes of elucidating the derivation of PMPE.

[5] This is true for thermomechanical systems. However, if electromagnetic effects are considered, the application of an appropriate electric potential to certain materials can lead to heat flow in the "wrong" direction without violating the second law.

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The discussion of stability and PMPE concludes the first part of the book. At this stage, we are able to write down a complete description of any problem in continuum mechanics and we have a clear understanding of the origins of all of the equations that appear in the problem formulation. Unfortunately, the complete generality of the continuum mechanics framework, with its attendant geometric and material nonlinearity, means that it is almost always impossible to obtain closed-form analytical solutions for a given problem. So how do we proceed? There are, in fact, three possible courses of action, which are described in Part II on *Solutions*. First, in certain cases it *is* possible to obtain closed-form solutions. Even more remarkably, some of these solutions are *universal* in that they apply to all materials (in a given class) regardless of the form of the constitutive relations. In addition to their academic interest, these solutions have important practical implications for the design of experiments that measure the nonlinear constitutive relations for materials. The known universal solutions are described in Chapter 8.

The second option for solving a continuum problem (assuming the analytical solution is unknown or, more likely, unobtainable) is to adopt a numerical approach. In this case, the continuum equations are solved approximately on a computer. The most popular numerical approach is the *finite element method* (FEM) described in Chapter 9. In FEM the continuum body is discretized into a finite set of domains, referred to as "elements," bounded by "nodes" whose positions and temperatures constitute the unknowns of the problem.[6] When substituting this representation into the continuum field equations, the result is a set of coupled nonlinear algebraic equations for the unknowns. Entire books are written on FEM and our intention is not to compete with those. We do, however, offer a derivation of the key equations that is different from most texts. We focus on static boundary-value problems and approach the problem from the perspective of the PMPE. In this setting, the FEM solution to a general nonlinear continuum problem corresponds to the minimization of the energy of the system with respect to the nodal degrees of freedom. This is a convenient approach which naturally extends to multiscale methods (like those described in Chapter 12 of [TM11]) where continuum domains and atomistic domains coexist.

The third and final option for solving continuum problems is to simplify the equations by linearizing the kinematics and/or the constitutive relations. This approach is discussed in Chapter 10. As noted at the start of this introduction, this procedure leads to almost all of the theories studied as independent subjects in an engineering curriculum. For example, few students understand the connection between heat transfer and elasticity theory. The ability of continuum mechanics to provide a unified framework for all of these subjects is one of the reasons that this is such an important theory. Most students who take a continuum mechanics course leave with a much deeper understanding of engineering science (once they have recovered from the shell shock). We conclude in Chapter 11 with some suggested *further reading* for readers wishing to expand their understanding of the topics covered in this book.

[6] It is amusing that the continuum model is introduced as an approximation for the real discrete material, but that to solve the continuum problem one must revert back to a discrete (albeit far coarser) representation.

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PART I

THEORY

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2 Scalars, vectors and tensors

Continuum mechanics seeks to provide a fundamental model for material response. It is sensible to require that the predictions of such a theory should not depend on the irrelevant details of a particular coordinate system. The key is to write the theory in terms of variables that are unaffected by such changes; *tensors*[1] (or *tensor fields*) are the measures that have this property. Tensors come in different flavors depending on the number of spatial directions that they couple. The simplest tensor has no directional dependence and is called a *scalar invariant* to distinguish it from a simple scalar. A *vector* has one direction. For two directions and higher the general term *tensor* is used.

Tensors are tricky things to define. Many books define tensors in a technical manner in terms of the rules that tensor components must satisfy under coordinate system transformations.[2] While certainly correct, we find such definitions unilluminating when trying to answer the basic question of "what is a tensor?". In this chapter, we provide an introduction to tensors from the perspective of linear algebra. This approach may appear rather mathematical at first, but in the end it provides a far deeper insight into the nature of tensors.

Before we can begin the discussion of the definition of tensors, we must start by defining "space" and "time" and the related concept of a "frame of reference," which underlie the description of all physical objects. The notions of space and time were first tackled by Newton in the formulation of his laws of mechanics.

2.1 Frames of reference and Newton's laws

In 1687, Isaac Newton published his *Philosophiae Naturalis Principia Mathematica* or simply *Principia*, in which a unified theory of mechanics was presented for the first time. According to this theory, the motion of material objects is governed by three laws. Translated from the Latin, these laws state [Mar90]:

1 The term "tensor" was coined by William Hamilton in 1854 to describe the norm of a polynome in his theory of quaternions. It was first used in its modern sense by Woldemar Voigt in 1898.

2 More correctly, tensors are defined in terms of the rules that their components must satisfy under a *change of basis*. A rectilinear "coordinate system" consists of an origin and a basis. The distinction between a basis and a coordinate system is discussed further below. However, we will often use the terms interchangeably.

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I *Every body remains in a state, resting or moving uniformly in a straight line, except insofar as forces on it compel it to change its state.*
II *The [rate of] change of momentum is proportional to the motive force impressed, and is made in the direction of the straight line in which the force is impressed.*
III *To every action there is always opposed an equal reaction.*

Mathematically, Newton's second law (also called the *balance of linear momentum*) is

$$\boldsymbol{F}^{\text{ext}} = \frac{d}{dt}(m\boldsymbol{v}), \tag{2.1}$$

where $\boldsymbol{F}^{\text{ext}}$ is the total external force acting on a system, m is its mass and $\boldsymbol{v}$ is the velocity of the center of mass. For a body with constant mass, Eqn. (2.1) reduces to the famous equation, $\boldsymbol{F}^{\text{ext}} = m\boldsymbol{a}$, where $\boldsymbol{a}$ is acceleration. (The case of variable mass systems is discussed further on page 13.)

Less well known than Newton's laws of motion is the set of definitions that Newton provided for the fundamental variables appearing in his theory (force, mass, space, time, motion and so on). These appear in the *Scholium* to the *Principia* (a chapter with explanatory comments and clarifications). Newton's definitions of space and time are particularly eloquent [New62]:

Space "Absolute space, in its own nature, without reference to anything external, remains always similar and unmovable."
Time "Time exists in and of itself and flows equably without reference to anything external."

These definitions were controversial in Newton's time and continue to be a source of active debate even today. They were necessary to Newton, since otherwise his three laws were meaningless. The first law refers to the velocity of objects and the second law to the rate of change of velocity (acceleration). But velocity and acceleration relative to what? Newton was convinced that the answer was *absolute space* and *absolute time*. This view was strongly contested by the *relationists* led by Gottfried Leibniz, who as a point of philosophy believed that only relative quantities were important and that space was simply an abstraction resulting from the geometric relations between bodies [DiS02].

Newton's bucket The argument was settled (at least temporarily) by a simple thought experiment that Newton described in the *Principia*.[3] Take a bucket half filled with water and suspend it from the ceiling with rope. Twist the rope by rotating the bucket as far as possible. Wait until the water settles and then let go. The unwinding rope will cause the bucket to begin spinning. Initially, the water will remain still even though the bucket is spinning, but then slowly due to the friction between the walls of the bucket and the water, the water will begin to spin as well until it is rotating in unison with the bucket. When the

[3] The story of this experiment and how it inspired later thinkers such as Ernst Mach and Albert Einstein is eloquently told in Brian Greene's popular science book on modern physics [Gre04].

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