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# On Modeling the Mechanical Behavior of Matter: The Continuum Assumption

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**Abstract**

This paper is dedicated to Dr. Rajagopal, a great scientist, mathematician, and mentor. His excellence in theoretical analysis is at the highest level; yet when combined with his insight into the mechanics of real materials, I think Raj's contributions are destined to be classics. Given my interest in the mechanics of soft tissues and the obvious challenges associated with anisotropic, inelastic, and non-linear behavior; Raj's input, advice, criticism, and encouragement have been invaluable. I can think of no better tribute to Raj than to question our foundational principles and advance the boundary of their application. Moreover, the focus of this work is on the "raw material" of mechanics; the stuff that exists, has mass, and occupies space. The fact of the matter is matter, and how to model its mechanical behavior. Toward this end, we searched for a framework that is tautologically intact for discontinuous materials, and surprisingly, we found continuum mechanics.

## 1 Introduction

This work is, in essence, a new way of arriving at our current state-of-the-art, the use of continuum mechanics for modeling the mechanical behavior of matter. Admittedly, such a result is rather paltry—one that reminds the author of G.K. Chesterton's fictional explorer who thinks he is discovering a new world and foolishly finds his home country (Chesterton, 2004). Insights, nevertheless, arise from this circular inquiry when we consider, explicitly, our reason for departing and how, by further reasoning, we are driven home again to continuum mechanics. As with Chesterton's explorer, it is a comfort to be ready for battle in a foreign land and then, in a mere moment, be home again. It is a comfort for the author because there is no need to change what we have been doing with regard to modeling the behavior of biological tissues. What has changed is the reasoning in doing so. The purpose of this exploration is a firmer foundation, one that is strong enough to be broadened and then applied to biological tissues (and to all materials which are comprised of constituents that have a finite size).

The author's reason for firstly departing from continuum mechanics is, perhaps, sophomoric. In his class in introductory biomechanics, sophomores object when materials or biotissues are considered as entities that are continuously divisible—i.e., as continuous bodies. They already know about cells, extracellular matrix, molecules, and atoms, and hence they know that materials and biotissues are made up of discrete constituents. Why assume that something is continuous when we know, truthfully, that it is not? It violates a tautology to consider that a discontinuous body is continuous. The word "approximately" is anticlimactic to young seekers of truth (old seekers too), and comparing the scale of an object to the scale of its constituents cannot fill this tautological void. Moreover, in biomechanics the scale of the constituents can be on the same order as the organ. With the naked eye, one can see that muscle is marbled. Collections of muscle cells, extracellular matrix, and vessels are appreciated as finitely discrete sub-regions. As a student and now a teacher, the author thought: there has to be a better way forward than assuming what we know to be wrong is somehow right. So the search for a better foundation begins.

## 2 Matter as an Aggregation of Constituents

Let us utilize the word matter in its conventional sense, as compositions of material that are large enough to contain a substantial amount of its constituents, and let the constituents be distributed uniformly (see remark at the end manuscript for comments on heterogeneity). Atoms or molecules are the typical constituents that, in abundance, make up matter. Nevertheless for the purposes of including biotissues and composites such as muscle and epoxy reinforced with fiberglass, let us permit constituents to be finite like cells and fibers. To avoid confusion with the conventional use of the

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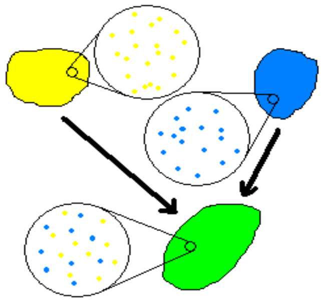

Figure 1: As an illustrative example of an aggregation having a different behavior than its constituents, consider the combination of yellow and blue paint to make green paint that is composed of yellow and blue pigments.

term matter (and with unconventional uses too), let us define the term aggregation as a material collection of a substantial amount of constituents.

We are, in essence, considering a body to be made up of a material that is an aggregation, and the aggregation, in turn, is made up of constituents. Hence, consider an iron bar to be made up of an aggregation, iron matter, with the iron matter being comprised of a substantial amount of its constituents, iron atoms and atomic impurities (let us neglect grains in this example). An iron aggregation is, perhaps, microscopic. Heart muscle (myocardium), on the other hand, is a macroscopic aggregation that makes up a body called the heart. It must be large to include all the constituents that comprise myocardium—i.e., cellular matter, fiber matter, vessel matter and fluid matter.

What is sought herein is a framework that enables the quantification of the mechanical behavior of an aggregation. The behavior of constituents like molecules, fibers, and cells is, of course, critical to the behavior of an aggregation. Yet we need to first define the behavior of an aggregation before we can understand how the behavior of an aggregation arises from the behavior of its constituents.

Consider an illustrative example of how the behavior of an aggregation may be distinctly different from that of the constituents. Shown in the top of Figure 1 is yellow paint (composed of yellow pigments in a white base) and blue paint (composed of blue pigments in a white base). When they are mixed together, the result is green paint (composed of yellow and blue pigments in a white base). In our terminology, the figure depicts:

1) a yellow aggregation with yellow pigments and white base as the constituents,
2) a blue aggregation with blue pigments and white base as the constituents, and
3) a green aggregation with yellow pigments, blue pigments and white base as the constituents.

Now consider the following two statements:

a) The combination of yellow matter and blue matter make green matter (yellow + blue = green).
b) The combination of yellow pigments in white base and blue pigments in white base results in a mixture of yellow and blue pigments in white base (yellow + blue = yellow + blue).

Statement (a) is an accurate description of observed phenomenon. Statement (b) is factually correct, but it is “too true” in the sense that the concept of green is absent. The most intriguing result is the transcendence of scales—i.e., the combination of yellow and blue pigments makes a green aggregation. To arrive at this result we need to know the behavior of the constituents (the yellow pigment is yellow and the blue pigment is blue) AND we need to know the behavior of the aggregation (it is green). However, if we utilize a continuum model for the green aggregation and start dividing it, we find that sub-regions become yellow, blue, or white. If we divide it enough, none of the sub-regions of the green aggregation are green. So we ask, is the green aggregation green?

If we do not have a framework that permits us to establish that green matter is green, then children in kindergarten may be wiser than scientists when we consider the combination of blue matter and yellow matter. They will see that yellow + blue = green, and we will state that yellow + blue = yellow + blue. The point here is that the behavior of the aggregation is a separate entity than the behavior of the constituents. For a mechanical example, note that the behavior of gaseous matter is different than the behavior of gas atoms. The former may be PV=nRT, and the latter may be a Maxwell-Boltzman distribution. Likewise, the behavior of iron matter is different than the behavior of iron atoms. Rather, the behavior of iron matter depends on the behavior of iron atoms (and on impurities). To establish how the behavior of iron matter depends on its constituents, it is necessary to define the behavior of iron matter in a manner that is distinct and quantifiable. Art class, ideal gasses, and iron matter are, of course, already on a firm foundation. How about myocardium with its finitely sized constituents? Does myocardium have a behavior that is definable? If so, we may ask, how does the behavior of myocardium depend on the behavior of its constituents? If not, then we should ask, what is this thing called myocardium? Can it be a substance if it does not have mechanical behavior?

## 3 Modeling the Mechanical Behavior of Matter

In our search for a framework to define the mechanical behavior of an aggregation, specifying how to model the behavior is helpful. Consider a very simple model for an aggregation wherein all sub-regions of the model behave like the aggregation behaves—the result will be a model that behaves as the aggregation behaves. For example, let all sub-regions of a model for green matter be green, and in so doing green matter will be modeled appropriately as green. Likewise, for all sub-regions of a model for iron matter, let the behavior be like that of iron matter, and in so doing our model for iron matter will behave like iron matter behaves. Clearly, such a model of an aggregation is only good for representing the aggregation—i.e., it is not appropriate for modeling the constituents. An atomic model would be needed for representing the behavior of the constituents of iron matter. Now for myocardium, consider a model for myocardium wherein all sub-regions behave as myocardium behaves. The result would be a model that behaves, tautologically so, as myocardium behaves.

## 4 Defining the Mechanical Behavior of Matter

Upon specifying how to model the mechanical behavior of an aggregation, let us consider the mechanical behavior of an aggregation as that which makes our model of the aggregation correct for the aggregation. Resulting definition: let the mechanical behavior of an aggregation be the behavior that arises from an accurate model with all sub-regions of the model behaving in the same manner. In similar fashion for our illustrative example, let the color of an aggregation be the color that arises from an accurate model of the aggregation with all sub-regions of the model having the same color. In so doing, green matter will have a green color whether it is made up of green pigments or of a combination of blue and yellow pigments. Forthwith a way to define the color of an aggregation, we can conclude that a combination of blue and yellow pigments will yield green matter. As for mechanical behavior, consider a model of iron matter wherein all sub-regions behave in the same manner. Using continuum mechanics for the model and upon requiring the model to yield the observed behavior of iron matter (as for example, tests on iron bars within the elastic limits), we will conclude that iron matter behaves as conventionally defined with appropriate bulk and shear moduli for iron. Now consider myocardium. Let us define the behavior of myocardium as that which would be needed in a continuum model of myocardium so that the model behaves as myocardium behaves. Such a definition may appear too circular to be useful, and yet are we not already doing this? We can conceive (and already have constructed) models of myocardium that behave as the overall tissue behaves for laboratory tests that we perform on the myocardium. Alas, we have "discovered" our home country.

## 5 A "New" Approach

Consider two approaches to modeling the mechanical behavior of a material substance that is an aggregation of constituents:

1) Continuum Mechanics: Let us assume that an aggregation is a continuous body and let us model it as such. In so doing, the accuracy of assumption improves when the length scale of the constituents is small relative to the length scale of the body.
2) Aggregation Mechanics: Let us consider a model of an aggregation with all sub-regions of the model behaving in the same manner and behaving such that the model behavior is an accurate representation of the mechanical response of the aggregation over time scales, length scales, and stimuli of interest (i.e., for the process class of interest). Moreover, let us define the mechanical behavior of an aggregation as that which arises from the model. In so doing, we obtain a model that behaves as the aggregation behaves, and we permit quantification of the mechanical behavior of the aggregation.

The end result of both approaches is to use a continuum mechanics framework with an aggregation represented as a continuous body. That said, our journey away from continuum mechanics and back again results in an approach that is tautologically appropriate for an aggregation. Consider the mechanical behavior of myocardium again, as it is the material that is of most interest to the author. Approach 1 raises significant objections to the use of continuum mechanics because the constituents are finite and on the same order as the spatial variation in stress and strain fields in the heart. For approach 2, however, we do not assume the aggregation is a continuous body per se; rather, we define the behavior of an aggregation as that of a continuous body with the same overall behavior as the aggregation. By definition, the model and the aggregation have the same mechanical behavior. The model, of course, cannot represent the constituents, but if the aggregation is sub-divided into constituents, then it is no longer an aggregation anyway.

By demonstration (i.e., we already utilize continuum models of aggregations that accurately represent the behavior of aggregations) our "new" approach is sufficient for defining the behavior of an aggregation, and it permits measurement and modeling of it. Whether or not such an approach is necessary is an open question. Myocardium is an aggregation that occupies space, and it has critical mechanical behavior (you would be dead without its mechanical action). How else can we answer the question, "what is the mechanical behavior of myocardium?" Further considerations, criticisms, and alternatives are more than welcome.

## 6 Remark on accuracy

In the realm of characterizing the mechanical behavior of real matter, an exact representation is a non-realizable ideal. Behaviors such as ideal gas, ideal fluid, Newtonian fluid, and linear elastic solid are easily shown to be insufficient for real substances. After some time in the laboratory, it is now the opinion of the author that the behavior of real substances is not analytical—i.e., an infinite number of parameters or terms would be needed to define, exactly, the mechanical behavior of a material within its entire range of strain, strain-rate, and strain history. Consequently, the question becomes what accuracy is good enough, and this question is only answered by considering the application for which a representation is needed. If the application at hand is to design a strong enough bridge for an expected range of loads, then an elastic model for steel and concrete will be accurate enough for estimating the stresses and strain because they, in the final design, will be well below yield limits—otherwise fatigue would be noticeable sooner (minutes) rather than later (centuries). When safety factors are increased to provide for inaccuracies in material behavior, ideal representations are often accurate enough. We have sought a framework to define the behavior of real matter with an emphasis on making it logically permissible. What tests are needed and to what precision? How many terms should be included in the constitutive relation? These are questions that must be answered after we have chosen an application and have asked: What accuracy is needed for this application? What behaviors need to be included (e.g., fracture, fatigue, viscous damping, etc.) for this application?

## 7 Remark on constitutive relations based on the behavior of constituents

When defining the constitutive behavior of a material, it is critical to distinguish between the behavior of the material and that of its constituents—so that we may appropriately investigate how the behavior of a material depends on the behavior of its constituents. For an example of what not to do (author's opinion), consider what is commonly done to represent the behavior of solid-like materials that undergo large deformations: 1) investigate the microstructure (i.e., the constituents), 2) assume a behavior for the constituents and 3) derive the constitutive relation for the material or biotissue. The most common occurrence of this approach in biomechanics is to restrict a material response to be the sum of a matrix component plus a fiber component because it appears that the tissue is composed of fibers within an isotropic matrix. Such approaches are often successful in that a representation can be found that has an acceptable accuracy for the application at hand. Nevertheless, we are not truly representing the behavior of the aggregation. We are saying that yellow + blue = yellow + blue. To arrive at yellow + blue = green, the behavior of the aggregation needs to be definable in a manner that is separate from its constituents. Upon so doing, we can compare a phenomenological model for the aggregation with a model built upon the behavior of the constituents, and consequently, we may be able to transcend scales and determine how the behavior of an aggregation arises from the behavior of its constituents. Without a method to independently define the behavior of an aggregation, then such a multi-scale investigation is ill-conceived because of an inability to validate results. Basically, when we assume that the constitutive behavior of an aggregation is a sum of matrix behavior plus fiber behavior, then we should expect that the resulting constitutive relation will be a sum of matrix behavior plus fiber behavior—c.f., yellow + blue = yellow + blue.

## 8 Remark on heterogeneous aggregations

The concepts above were developed for the case of aggregations with the constituents distributed uniformly, so that we can permit all sub-regions of the model to behave as the aggregation behaves. When constituents are not distributed homogeneously, we need to have a framework that permits heterogeneity in aggregation behavior. Biological tissues are, frankly, heterogeneous. The compositions of collagen and matrix materials are different on the inner wall of the heart versus the outer wall, on the inner wall of arteries versus the outer wall, on the inner wall of the femur versus the outer wall. To account for heterogeneities, let us take a similar approach to our homogeneous case and define the mechanical behavior of an aggregation as that which makes our model of the aggregation correct for the aggregation. Yet instead of proposing a homogeneous model, consider a heterogeneous one—i.e., consider a heterogeneous model that is appropriate for accurately representing the aggregation of interest and let the behavior of the aggregation be that which is needed to have the model accurately represent the aggregation. Is this a new approach that is perhaps too circular to be useful? No, we already do it. For myocardium we typically have material properties, such as fiber direction, vary throughout the heart with cubic interpolation in the radial dimension and linear interpolation in the hoop and apex-base dimensions. Moreover, we can consider increasing orders of heterogeneous behavior for aggregations: zero-order heterogeneity would be homogeneous behavior, first order heterogeneity would be linear variation in behavior, second order heterogeneity would be quadratic variation, and etcetera. Discontinuous heterogeneity (i.e., two separate aggregations making up a tissue or body) is perhaps dealt with as a contact problem between two separate bodies rather than as an infinite order of heterogeneity. The focus here is on a tractable framework for modeling the mechanical behavior of real matter. The question at hand is, for example, what order of heterogeneity is needed for the heart wall? Perhaps one way to find out is to start with zero order and increase the order until there is no significant gain in doing so—similar to mesh refinement in finite element analysis. The order needed for the heart is thus the lowest order that meets our "accurate enough for this application" supposition. Of course, there are many open questions about uniqueness for representations when, for example, a zero-order model with many terms in the constitutive relation may fit the same behavior as a first-order model with fewer terms. As evidenced by the author's works in mechanics, there is much work to be done in the realm of building constitutive frameworks that permit unique solutions (Criscione et al, 2000-2008).

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