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# Archetype-blending continuum theory

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ABSTRACT

We propose a modular approach for generalized computational mechanics in mesostructured continua, namely the archetype blending continuum (ABC) theory. The theory's modularity derives from its mathematical constructors: archetypes, or building blocks that all multi-component material laws are generated from. These archetypes are the means used to discretize a description of material motion that relies on the fundamental theorem of calculus, an approach that contrasts the Taylor series expansions that underlie previous generalized continuum kinematics. All enhanced continuum methods to date assume embedded scales may be seen as separable material points in larger domains, an assumption that creates unnecessary restrictions on the constitutive modeler and makes the additional stress tensors introduced far less physical. The ABC theory removes that assumption and provides mesostructural basis for higher order stress quantities by attributing them separately to archetypes and their interactions. In this manner, ABC is a bridge between generalized continuum mechanics and micromechanics, two well-established fields. Thus, a multi-component material design space may be probed with the ABC theory by adding and removing archetype modules or by refining archetypes themselves. This work presents the mathematics and ingredients for finite element implementation of the theory so that others may build on the specific demonstrations for solid mechanics explored here: multi-component elasticity and multi-crystal plasticity. Abstract extensions of the ABC theory into stochastic space and multiphysics problems are also briefly propounded.



## 1. Introduction

### 1.1. Motivation and philosophy

Materials are modular. That is, microstructured materials are aggregates of individual components. We hereafter collectively refer to these aggregates as *multi-component* materials. The components define material building blocks, termed *archetypes*,[1] which by different synthesis and processing techniques self-assemble to form a complex mesostructure or *conformation*. In general, archetypes contain their own sub-structures, meaning they are *submorphic*, and their self-assembly generates new mesoscale structures defining material *mesomorphism*. A multi-component material's conformation has a set of apparent properties that depends on the properties of the archetypes, their interactions, and their mesomorphism; this property set has recently been referred to as a material genome [2]. An analogy may be found in Lego building blocks: an archetype corresponds to an individual brick whose interior is described by submorphism. An arrangement of interlocking bricks would correspond to a conformation and the resulting mesoscale pattern to mesomorphism. The entirety of properties of this assembly is the system's genome. The mesoscopic intersection of archetypes is where modern mechanics research opportunities abound: the scale is too large for explicit descriptions but too small for traditional continuum mechanics. Representative examples of archetypes, their conformations, and dependent macroscopic phenomenologies are shown in Fig. 1(a).

Take for example crystals as archetypes. In Fig. 1(a), we see that intermetallic phases segregate from matrix crystals to create a complex mesostructure that controls fracture processes. The different archetypes form in response to a favorable energetic state (meta-stable) during heating and subsequent cooling (heat treatment or processing) of the alloy. In filled elastomers, pure amorphous polymer hydrocarbon chains have random submorphism while the reinforcing fillers like silica, carbon black, or nanoclay have crystalline submorphic order. The nanocomposite self-assembles to form filler networks at the mesoscale. Processing induces in these networks distinct interphase zones whose properties are derivatives of polymer and filler. The interplay of these mesoscale features characterizes nanocomposite failure modes, such as craz-

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[1] For other usage of the term 'archetype' in the context of continuum mechanics see [1].

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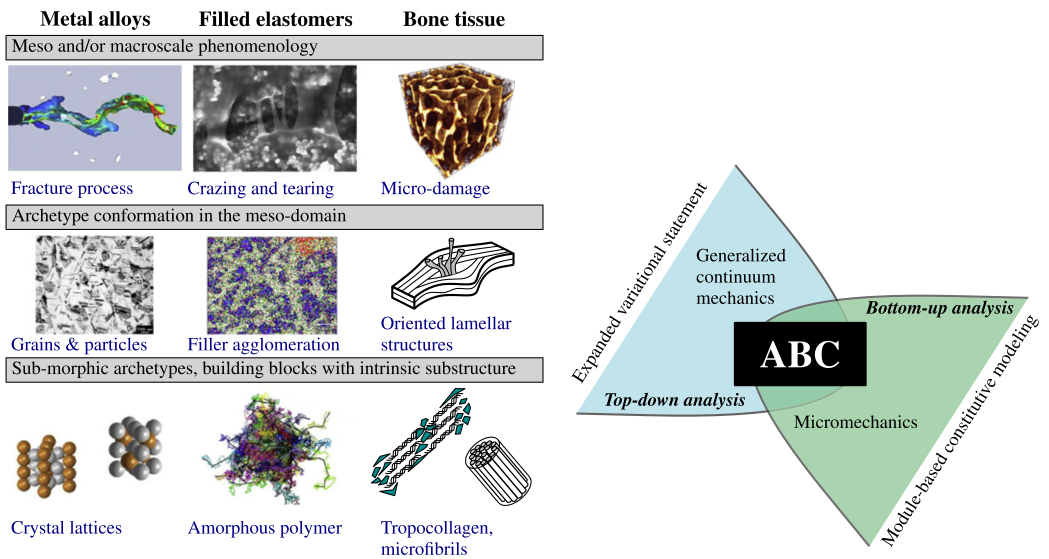


(a) Examples of archetypes and their conformations.

(b) ABC theory as the connection between micromechanics and generalized continuum mechanics.

**Fig. 1.** The applicability and overarching philosophy of the ABC theory.

ing or tearing. A pronounced structural hierarchy also exists in bone tissue [3,4] that arises from the subsequent assembly of tropocollagen macromolecules, impure hydroxyapatite minerals, and non-collagenous organic material (archetypes) to form the structural levels: microfibrils, fibril arrays, oriented lamellar structures similar to fiber-reinforced composites with a pseudo-random stacking structure, and porous spongy networks or haversian systems (depending on the type of bone tissue) that underlie the macroscopic bone. These complex mesostructures are what give rise to a bone that is simultaneously light and tough [5].

The same logical picture extends to all other heterogeneous materials. The theory we propose herein transforms this abstract picture of materials – archetypes and their conformations – to a mathematically rigorous but simple generalized continuum mechanics theory suitable for many applications in science and engineering. The proposed archetype-blending continuum (ABC) theory connects micromechanics and generalized continuum mechanics (Fig. 1(b)), a simple concept but vitally important. By doing so, limitations in each field are overcome, and new opportunities for predictive continuum modeling of complex materials abound.

The broad field of micromechanics essays to predict bottom-up apparent properties of a material through analysis and *blending* (i.e., homogenization) of its components and their interfaces (or discontinuities), as it is well known that heterogeneous materials derive their suitability for application from these two entities. A fiber-reinforced composite can have a strong matrix and stiff fibers, yet if cohesion is lost at their interface, the material is weakened and rendered unsuitable. The reader is referred to [6–10] for more extended discussions of micromechanical methods. A common thread to micromechanics theories is that they condense all mesostructural information into a single constitutive law, which is variationally conjugate to a single mesoscale velocity field representing the blend. Micromechanics thus limits its predictive reach for multi-component materials by assigning a single mesoscale kinetic energy for the homogenized mesostructure, thereby losing the ability to track energy distributions within the deforming blend. Simply put, there are too few degrees of freedom to represent a complex mesoscale for any detailed dynamic analysis. More general continuum theories are thus of interest.

Generalized continuum mechanics is a broad field that attempts to introduce structural information into a continuum model without its explicit representation. It is assumed that a continuum cloak overlays the complex material structure. The complexity of the material is accounted for by an enhanced variational statement that includes additional degrees of freedom and/or derivatives thereof to offer a continuum summary of material motion at different length scales. Gradient elasticity theories of the mid 1900's (e.g., [11–14]) and gradient-based research thereafter in both nonlinear elasticity [15,16] and plasticity [17–21] represent generalizations of the variational statement to include higher derivatives of kinematic variables. Kröner [22] has provided inspiring discussion on physical interpretation of the torque stresses that arise in high gradient theories as reactions against lattice bending or torsion. Besides these *high gradient* theories, *nonlocal theories of the integral type* [23,24] have been introduced to provide both a microstructural basis to damage and use deformation surrounding a point to influence that point's constitutive law. Finally, a separate class of enriched continuum theories are the *high order* type, i.e., those with additional kinematic variables.

High-order continua began with the transformative work by the Cosserat brothers [25], who introduced additional couple stresses by postulating local micro-rotations independent of the macro-rotations. Micromorphic extensions that represent more general hidden deformabilities of a material point then ensued [26–31]. Additional fields allow the modeler to maintain the computational efficiency congenital to continuum descriptions and compete with direct numerical simulation (DNS) methods in modeling complex material behavior across multiple length scales. These theories act to both improve predictive capability in situations where size effects exist [32,18,33–35, eg.] and improve numerical properties of the governing equations by alleviating mesh sensitivity to localization phenomena [36,31,37]. High-order theories are particularly useful when the scales of stress variation and mesostructure intersect, with application in high-frequency wave propagation [38,39], localization and failure (shear bands, fracture modes) in metals [30,31,40–44], granular materials [37], brittle composites [45], and filled [46] or porous [47] elastomers.

Though these theories mean to overcome micromechanics limitations by introducing additional degrees of freedom, a disconnect