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Original Article

Hypervariate constitutive modeling illustrated via aleatory uncertainty in a foundation model

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ABSTRACT

Even if a ceramic's homogenized properties (such as anisotropically evolving stiffness) truly can be predicted from complete knowledge of sub-continuum morphology (*e.g.*, locations, sizes, shapes, orientations, and roughness of trillions of crystals, dislocations, impurities, pores, inclusions, and/or cracks), the necessary calculations are untenably hypervariate. Non-productive (almost derailing) debates over shortcomings of various first-principles ceramics theories are avoided in this work by discussing numerical coarsening in the context of a pedagogically appealing buckling foundation model that requires only sophomore-level understanding of springs, buckling hinges, dashpots, *etc.* Bypassing pre-requisites in constitutive modeling, this work aims to help students to understand the difference between damage and plasticity while also gaining experience in Monte-Carlo numerical optimization via scale-bridging that reduces memory and processor burden by orders of magnitude while accurately preserving aleatory (finite-sampling) perturbations that are crucial to accurately predict bifurcations, such as ceramic fragmentation.

1. Background

Exascale computing is on the horizon, yet the typical vision for using it is a tragically uninspired goal to merely solve traditional governing equations at higher resolutions. Such profound computing power, however, has the potential to replace conventional (deterministic and phenomenological) constitutive models for brittle and ductile media with "organic" (first-principles) theories that explicitly track the net effects of a "swarm" of millions or even trillions of evolving and statistically variable microcracks, dislocations, impurities, fibers, and other micro-morphological entities that interact with each other in moderately simple ways to produce highly complex ensemble (swarm) behavior as a group. Ordinary fast-running constitutive models (of the type ubiquitously available in finite-element software) might have only a few internal variables (*e.g.,* a work-hardening yield strength), whereas potentially more predictive "organic swarm" models are intrinsically hypervariate because they invoke equations that explicitly require attributes of a mob or swarm of entities in order to predict net behavior. Such models would therefore require, in principle, trillions of internal variables in each finite element. As this computational burden is untenable even for exascale hardware, some degree of data decimation (binning) is needed to make the benefits of organic swarm modeling outweigh the costs in comparison to conventional phenomenological constitutive models.

Conventional damage and plasticity models already can predict stress and lateral dilatation in axial compression [1]. Such models, however, are typically tuned to limited empirical data for one material at a time, making them useless for exploring processing effects (*e.g.,* grain size influenced by sintering or chemistry) and unreliable for general loading that deviates by very much from the loading used to calibrate them (*e.g.,* multiple-strikes on armor from different directions). As sketched in Fig. 1, on the other hand, even grossly idealized fracture laws can be applied to predict far more realistic "swarm migration" of a crack population from its initially isotropic state to any nontrivial anisotropic texture. In particular, well-known fracture growth and coalescence theories (*cf.,* [2]) can be applied to evolve the attributes (size and orientation) of each microcrack in a domain. Using updated morphological attributes (size and orientation) for each member of this "crack swarm," homogenization theories (*cf.,* [3,4]) can be applied to find the new overall elastic compliance and directionally dependent strength tensors (which are needed to infer macroscale response to a an arbitrary change in loading direction). To exploit both

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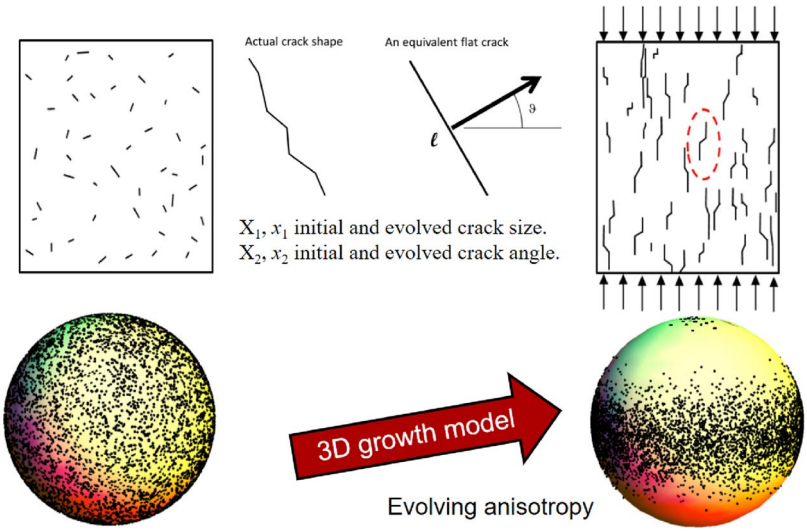

Fig. 1. A nominally isotropic micro-cracked medium acquires "induced anisotropy" under axial loading in which cracks kink to become effectively vertical [2], causing initially uniform crack orientations to migrate towards the equator of the orientation sphere.

concurrent and hierarchical multi-scale methods, however, it is recognized that even exascale computing would require some degree of coarse graining. The million or trillion internal variables for evolving crack sizes and orientations must be "binned" down to a representative sub-population that is small enough to be computationally tractable *yet large enough to accommodate acceptably accurate swarm-based evolution of material properties*. Numerous sophisticated methods already exist for scale bridging (*cf.*, [5] for a review), so this paper limits its scope to a pedagogically simple (intentionally idealized) context of a foundation built from springs and buckling hinges. By avoiding any need for prerequisite knowledge of constitutive modeling, this foundation theory is suitable as a "concept familiarization" activity that can help undergraduate students, graduate interns, and professional analysts gain a first exposure to differences between plasticity and damage while simultaneously learning methods of hypervariate systems. This simpler context, a foundation theory, is designed to share many key features with inelastic constitutive models (brittle, ductile, and/or viscous), and it furthermore illustrates how statistical variability in morphology can produce significant changes in homogenized behavior (such as reduction in peak strength) even in the continuum limit.

Pursuing accurate solutions to almost laughably idealized "first-principles" constitutive models helps to form a foundation upon which to eventually introduce more realistic features. Models for micro-cracked ceramics, for example, often rely on unrealistic axioms, such as penny-shaped frictionless cracks that are dilutely distributed in a homogeneous linear-elastic matrix, leading to well-established formulas (*cf.,* [6,3]) that express the fourth-order elastic compliance tensor as the sum of the matrix compliance plus extra terms arising from crack opening and/or sliding. These extra terms involve a summation over all possible crack sizes and crack orientations. The intimidating complexity of fourth-order multi-index tensor projectors and other physical details cause other *equally important* issues pertaining to numerical evaluation (and practical verification) to become lost in the noise.

To explore issues and numerical methods associated with hypervariate systems, one needs only a function that takes a large number of inputs to produce a relatively small number of outputs. We will use a foundation model for that purpose because its output is a force–displacement response that is homogenized from the combined action of many simple components (springs, dashpots, and buckling hinges), each of which is understood by freshman students. The foundation model in this paper provides (1) features that allow students to learn the difference between damage and plasticity, (2) statistical perturbation of the geometrical properties of the foundation components in order to give students a first exposure to aleatory uncertainty, and (3) an opportunity to decimate or "bin" an unmanageably large number of foundation components down to an optimized representative subset. By favoring simple idealizations over premature complexity, this approach is faithful to the scientific method.[4]

Algorithms for efficient approximation of properties of micro-cracked media have already appeared in the literature (*cf.,* [7]), but the impact of such work is lessened by constitutive details that distract from more basic concepts of numerically evaluating ensemble behavior of large numbers of components, whether they be microcracks in a ceramic, humans in a dense crowd, or any other hypervariate population of variables. This paper addresses that shortcoming by considering an idealized analog problem that purposely sets aside constitutive details in favor of very simple rules of a foundation composed of parallel components made from elementary parts (spring, dashpots, *etc.*). This idealization, however, includes the complication of "aleatory uncertainty," which refers to statistical variation in the geometric micro-morphology (such as foundation spring lengths, number of foundation components per area, *etc.*) and is therefore highly relevant to ceramics modeling for which aleatory uncertainty arises as a result of natural variation in crack morphology. The idealized foundation is designed to exhibit many of the features one sees in stress–strain curves for ceramics, but it is cast in a way that helps students to understand the physical origins of those features, while also teaching them how to use smart binning to efficiently approximate the summation of tens of thousands of individual component response functions in a way that preserves effects of the natural perturbations in foundation properties that come from aleatory uncertainty in morphology at a scale too small to model explicitly. If this topic were to be confined to realistic constitutive models, such concepts would be needlessly inaccessible to undergraduates.

We are broadly interested in ways to approximately evaluate a function, $h(x_1, x_2, \ldots, x_N)$ in the "hypervariate" case that the number of inputs, N, is too enormous for practical direct evaluation. We furthermore require approximate evaluation methods to capture perturbations in the output that arise from statistical variation in the N inputs. The scope of this investigation presumes that the original function of N

[4] Ballistics, for example, was founded on a willingness to first thoroughly understand the "unrealistic" case of a point mass moving in a constant gravity field in a vacuum without drag.