MECHANICS OF RANDOM AND FRACTAL MEDIA

Allocation: Illinois/50 Knh
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EXECUTIVE SUMMARY:

One of the grand challenges to engineering (as identified by the National Academy of Engineering) is America's aging and failing infrastructure. A major barrier to deciding if a structure is safe or needs to be repaired or replaced is an accurate assessment of the damage state of a given load-bearing material or structure. Complex damage (crack and defect) patterns in natural and man-made materials often lead to consideration of their fractal and disordered structures. To properly understand the damage state of load-bearing materials and structures and assess the associated failure hazard, the multiscale geometry of existing damage has to be considered.

A challenge in health science that requires similar methodology is the modeling and simulation of mild traumatic human brain injury. Given a brain's complex structure, the key idea is to run computer models based on the MRI-resolved 3D images of human heads.

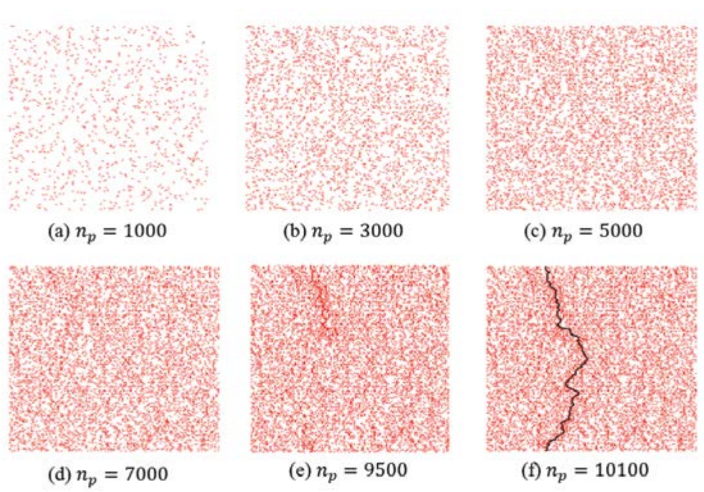

FIGURE 1: Failed springs at different loading stages. The final crack leading to macroscopic failure is shown as black line in (e). Localization of damage only took place as the peak load was reached.

INTRODUCTION

Conventional continuum solid mechanics hinges on the assumption of homogeneous material properties. However, almost all natural (inanimate and biological) and man-made materials contain some microstructure(s) and exhibit spatially distributed randomness (material defects, impurities, etc.) and even fractal patterns. As a result, in elasto-plastic materials under macroscopically uniform and monotonic loading boundary conditions, 'weaker' material grains and regions plasticize first and gradually spread in a cooperative fashion throughout the whole body. In elasto-brittle materials, nano- and microscale cracks form and then coalesce into mesoscale cracks, then grow and result in global failure of the material and structure. If we consider biomechanics of the human head under impact loading conditions, the stress waves (and possible localized damage) represent the true response of the entire brain patterns. Problems of this type can be run to greater resolution and more efficiently on Blue Waters than on any other computer.

METHODS & RESULTS

1. Scale-dependent homogenization [1] was used to estimate the effective elastic shear moduli (or effective conductivity) of 2D two-phase materials with Gaussian correlated isotropic microstructures. The microstructural randomness inherent in these materials motivates a study of homogenization from a statistical volume element to a representative volume element. This finite-size scaling, studied in terms of material responses under two uniform boundary conditions (displacement and traction), obtained at a wide range of mesoscales for a wide range of contrasts in elastic moduli of both phases. The mesoscale is defined as the ratio of domain size to the grain size. A study involving Monte Carlo sampling of many realizations of spatially correlated microstructures, each solved by finite elements, led to scale-dependent bounds and a universal normalized scaling function.

2. Large-scale lattice model simulations are computationally demanding as the system of linear equations is solved after each lattice bond fails or yields (fig. 1). The number of bonds at final failure (n_f) for elastic brittle transition scales with L as $n_f \sim O(L^{1.8})$ in 2D and $n_f \sim O(L^{2.7})$ in 3D [2–4]. Moreover, as the system approached macroscopic failure there was a critical slowdown of iterative solvers. The computational cost further increased because a significant number of realizations were required to obtain good statistics. To this end, we used algorithms involving conjugate gradient and massive parallelization to implement the elastic plastic brittle 2D and 3D code.

3. The mechanisms underlying mild traumatic brain injury need to be understood from the standpoint of stress wave patterns taking place in the brain. Fine spatial meshes are needed to properly describe such patterns and resolve the highly heterogeneous brain structure (with a fractal brain surface) [5]. This was accomplished with an MRI-based computational model, previously validated by tagged MRI and a harmonic phase imaging analysis technique on *in-vivo* human brain deformation data [6]. Computer simulations were carried out for various impacts with the cerebrospinal fluid layer explicitly modeled as a viscous or viscoelastic fluid (fig. 2).

WHY BLUE WATERS?

The objective was to introduce spatial material heterogeneity and disorder/randomness into realistic large-scale models of conductive and elastic plastic brittle man-made and natural (i.e. biological) materials, and study the growth of multiscale/fractal material systems in the presence of evolving and interacting defects/cracks or the ensuing wave patterns. In general, we needed to be able to handle very large domains in 2D and then extend the simulations to 3D. Given major computational challenges (number of degrees of freedom and, hence, memory and CPU requirements), this research can only be done on Blue Waters. At a subsequent stage, our large-scale simulations will be extended to other scenarios: anisotropic yield criteria, 2D versus 3D, coupled field (e.g., thermo-mechanical, electro-magneto-mechanical) fields, and head models with more anatomical detail.

PUBLICATIONS

Kale, S., A. Saharan, S. Koric, and M. Ostoja-Starzewski, Scaling and bounds in thermal conductivity of planar Gaussian correlated microstructures. *J. App. Phys.*, 117 (2015), 104301, doi:10.1063/1.4914128.

Kale, S., S. Koric, and M. Ostoja-Starzewski, Stochastic continuum damage mechanics using spring lattice models. *Second Int. Conf. on Damage Mechanics*, Troyes, France, July 8–11, 2015.

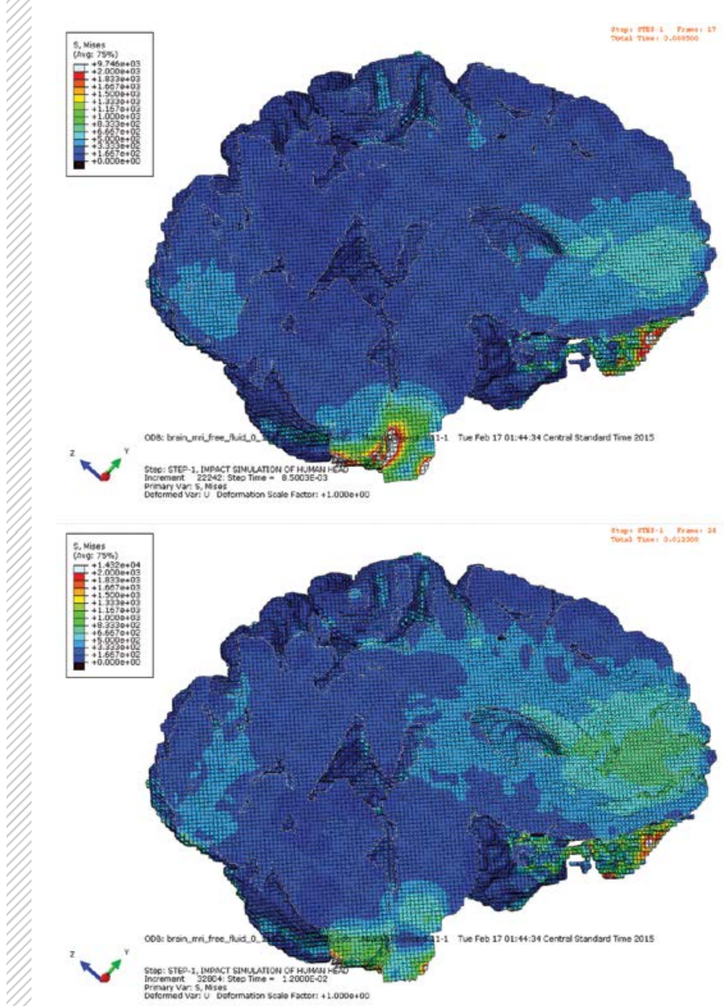

FIGURE 2: Two frames of the evolution of the von Mises stress distribution in the human brain (mid-sagittal view) during a 15 ms frontal impact (forehead) simulation; the cerebrospinal fluid layer was explicitly modeled as a Stokesian fluid.