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MULTISCALE COMPUTATIONAL METHODS FOR FAILURE

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ABSTRACT

Replacing prototype testing by computer simulation is essential for speeding design cycle times. Since a critical requirement in any design is to prevent failure without incurring high cost, the ability to simulate failure is vital in this paradigm shift from testing to computer simulation. The ultimate goal is to be able to predict macroscale failure starting from computations at the atomistic scale with minimal testing. But computational modeling of failure and reliable predictions are still highly problematic and are one the biggest challenges in computational mechanics. In this talk, we will summarize some methods for concurrent and hierarchical multiscale computations. The latter are often called coarse-graining. The emphasis will be on methods for failure analysis. In failure analysis, standard coarse-graining procedures often encounter difficulties. If the material is rate-independent, then in the failure process the deformation localizes to a set of measure zero and any coarse-grained material law will become ill-posed and the solutions become mesh-dependent. Difficulties are also encountered for material models that lose stability, for in that case the localization scale becomes much smaller than the resolution of the coarse-scale model.

Here a coarse-graining theory is described that extracts a discontinuity and a bulk material law from the representative volume element at the finer scale, along with a cohesive law. The application of this method requires the definition of a perforated representative volume element. [1] This is a representative volume element which excludes all subdomains that are cracked or exhibit exponential growth in their response, i.e. a material instability. The theory provides a method for extracting both the amplitude and the direction of the equivalent discontinuity at the coarse scale on the basis of an extension of Hill's formula. The method can account for both nucleation and growth of discontinuities. It has been shown that the method conserves power between the fine scale and the coarse scale. In addition, it has been shown that if all material remaining in the perforated representative volume element is strictly elliptic, then the bulk material at the coarse scale is stable. The method can be applied both in a hierarchical manner, where a constitutive response is passed to a coarser scale, or in a concurrent manner, as in FE^2. It is called the multiscale equivalent aggregating discontinuities (MEAD) method; it has also been called the multiscale aggregating discontinuities (MAD) method.

Some examples of applications of the method will be given, both for passing from the atomistic scale to the continuum scale and from the microscale to the macroscale. An example of a micro/macro analysis is illustrated in Figure 1. In these calculations, the discontinuity extracted from a representative volume element was passed to the macroscale and the discontinuity was modeled by the extended finite element method. [2, 3] The results are compared to a direct numerical simulation, in which the detailed microstructure is modeled in the subdomain through which the crack passes. It can be seen in Figure 2 that the path of the crack as computed by the MEAD method agrees quite well with the direct numerical simulation. A comparison of a reaction force for the MEAD method and direct numerical simulation is also given in Figure 1. It can be seen that there are some discrepancies, but the overall agreement is quite good. The MEAD calculation only required 3% of the computer time of the direct numerical simulation.

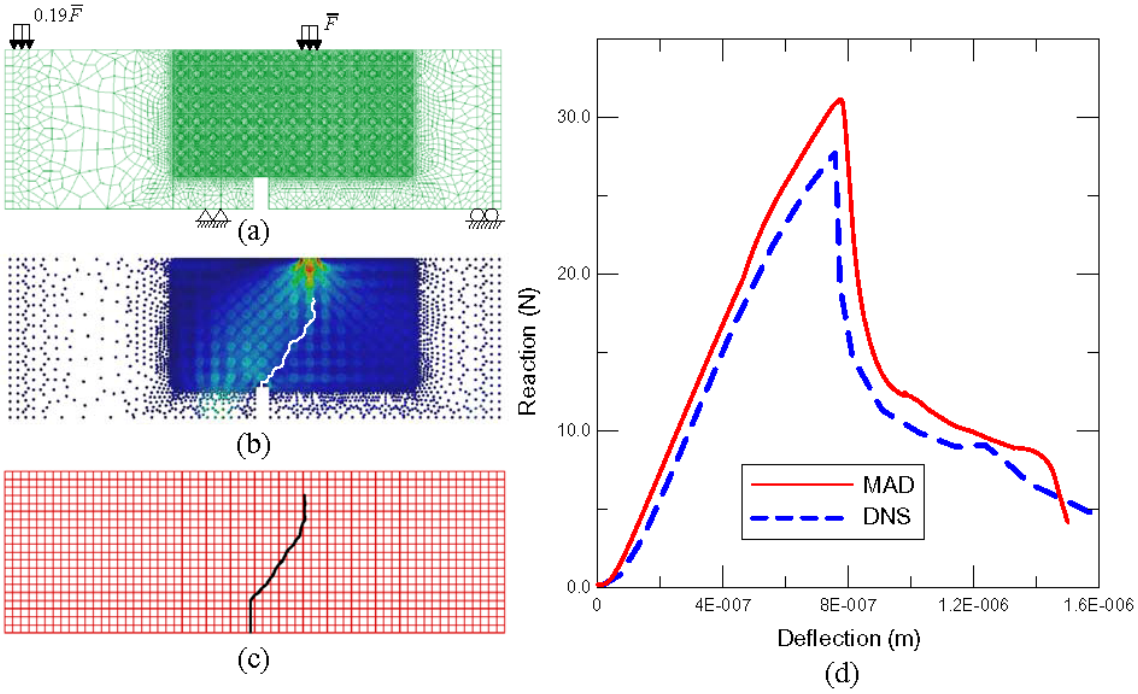

Figure 1. Comparison of the three-point bending results from direct numerical simulation (DNS) and MEAD: (a) the undeformed model for DNS, (b) solution from the DNS, (c) solution from the MEAD, and (d) comparison of the force deflection curves.

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