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THERMAL AND MECHANICAL FIELD DECOMPOSITION IN NONEQUILIBRIUM MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

Many physical processes under mechanical deformation including bond breaking, frictional sliding, and dislocation motions generate considerable amount of heat energy that raises the temperature of the whole system dramatically [1,2]. Such systems must be treated by nonequilibrium molecular dynamics (NEMD) simulation. In NEMD, the thermal and mechanical fields, both macroscopic continuum concepts, are indistinguishable because they both manifested themselves as atomic motion. In order to separate the thermal and mechanical fields that are each governed by separate continuum equations in solid, it is necessary to know the relationship between the three dynamical variables in the macroscopic conservation laws (displacement, velocity, and temperature) and the two variables in molecular dynamics (displacement and velocity) that contain all the information about the system under investigation. If the relationship is known, the mechanical part can be separated from the thermal part of the microscopic displacement and velocity fields. Hence, the macroscopic temperature field may be determined from MD to capture heat generation. At the same time, localized mechanical motion is captured by the mechanical part of the microscopic variables.

Attempt to derive macroscopic conservative laws from molecular dynamics in solid is a difficult and challenging task. In contrast to gas, it is hard to treat solid due to the strong interaction between particles. In gas, macroscopic conservation laws (hydrodynamics) can be derived from molecular dynamics [3]. Our theory is motivated by the kinetic theory of gas to link microscopic quantities to macroscopic quantities. In an ideal gas, by making certain assertions on the macroscopic conservations laws derived from the Boltzmann transport equation, the concept of local equilibrium can be established and temperature can be defined as a function of the fluctuating microscopic displacement and velocity field. In solids, by assuming that the fluctuating microscopic displacement field is uncorrelated with the fluctuating velocity field, an approximate yet simple equilibrium probability distribution, a Gaussian distribution, is obtained for the fluctuating microscopic displacement. This approximate equilibrium distribution is further employed for the approximation of a solid system in local equilibrium so that temperature is well defined locally. Since the local fluctuating displacement field has a local Gaussian distribution, the problem of separating the fluctuating thermal part of the

total microscopic displacement from the deterministic mechanical part is a classical problem in statistics most often called signal estimation from data with locally stationary Gaussian noise.

Over the last fifty years, many methods have been developed to treat the Gaussian noise model. We compare three widely-used denoising methods: 1) moving average filter, 2) Fourier-based Wiener filter, and 3) wavelet-based thresholding estimator [4] by applying them to denoise four artificial signals corrupted with thermal fluctuation generated in MD simulation at temperature 100 K and 1000 K [5]. These artificial signals contained features commonly observed in MD displacement and velocity fields that include cusps, corners, and waves of varying frequencies. By comparing the mean absolute errors and mean square errors, we show that wavelet-based thresholding estimator outperforms the other methods. The wavelet-based thresholding estimator is then applied to two nonequilibrium problems simulated in MD to determine the mechanical and thermal fields. The first problem consists of a Mode II crack nucleated and propagated in a hexagonal lattice, and the second one is a nano-indentation problem on a similar lattaice system. From the two problems, the lack of adaptivity can clearly be observed in the filtered velocity time history by a moving average window, which either undersmoothes or oversmoothes different parts of the time history. In contrast, the wavelet thresholding estimate acheives appropriate piecewise smoothness everywhere while keeping gross features of the data intact. The local temperature time history is then calculated from the fluctuating velocity time history, that is, the difference between the total velocity and the filtered velocity. Our results show that the temperature difference can be as high as 20% between the moving average estimate and the wavelet thresholding estimate. Figure 1 shows some preliminary results.

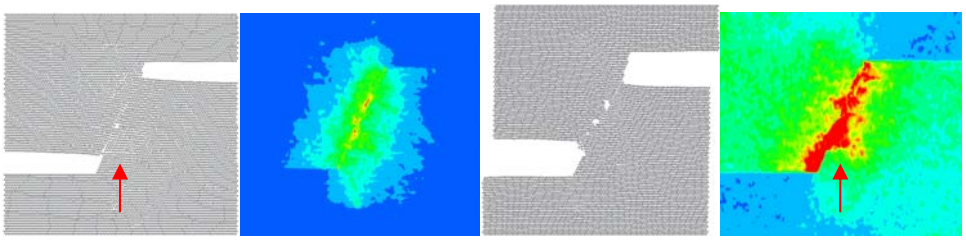

Figure 1. Molecular dynamics simulation of a mode II crack and its corresponding temperature field calculated by the current method. Much heat is generated due to frictional sliding along the crack. Note that the sub-crack (red arrow) serves as a heat diffusion barrier, which is according to our physical understanding of cracks.

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