Separated Temporal and Spatial (SETS) Framework for Stress Calculations in Atomic Models

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The continuum scale modeling of macroscopic phenomena like damage, relaxation, plastic flow, etc. is often motivated by observations from molecular dynamics or ab-initio simulation. Consequently, stress and strain definitions need to be consistently valid across all scales and between scales ranging from a continuum material point which is orders of magnitude larger than atomic scale right up to a continuum material point which is the Wigner-Seitz cell of a single atom. An ensemble average or time average of the free energy is a fundamental way to compute stress and strain for continuum material point of any size. However, we have found that the traditional methods of computation across these scales suffer from significant drawbacks. Certain methods attempt to map entire atomic trajectories with the macroscopic material deformation. For example, a canonical transform[1] falls under this category, however it only maps positions and momenta, while excluding the additional degrees of freedom from the thermostat. Hence, it is insufficient to map trajectories for an NVT ensemble. The other approach is to separate the equilibrium positions of atoms from their vibration about these positions. The phonon gas[2] approach follows along these lines; however it is limited to the quasi-harmonic approximation and sacrifices locality at atomic spatial scale.

We propose formalism called Separated Temporal and Spatial (SETS) which obviates the necessity for canonical transforms while retaining locality at atomic scale and is applicable for continuum material points of all possible sizes. The atomic trajectory is represented using (a) atomic equilibrium position and (b) the second moments of atomic position, which we denote as beta. Accordingly, the Helmholtz free energy of the system is split into four parts representing the static potential energy, dynamic potential energy, kinetic energy and entropy. The continuum scale parameters are the deformation gradient and temperature, which map to the equilibrium positions and to beta. A deformation boundary condition applied to an RVE at finite temperature produces change in equilibrium positions as well as atomic trajectories. In this work, for the first time, we derive expressions for two local strains, corresponding to the change in equilibrium positions and the change in the atomic cloud, represented by beta. Local atomic scale stresses are defined as energetic conjugates to these local strains. They are derived from the Helmholtz free energy of an atom of interest and classified as spatial and dynamic stresses. This is in contrast to the current methods used for atomistic-to-continuum homogenization, where the deformation gradient is mapped to the atomic scale either (a) only in terms of changing the equilibrium positions or (b) in terms of linearly mapping the entire trajectory. We applied our formalism to crystalline Aluminum using NVT ensembles and show that neither of these scenarios realistically represents the motion of individual atoms, even for a homogenous crystal of Aluminum. Our approach captured critical events preceding failure at the atomic scale; for example a zone of high local dynamic stress, representing atoms escaping local potential wells preceded the formation of shear band and eventual failure in crystalline aluminum. The interstitial paths traced by individual atoms reveal insights for improving current continuum theories for failure accounting for dynamic contributions to continuum stress. In summary, the SETS promises (a) to be a robust approach for studying mechanical behavior at high temperatures in a continuum framework and (b) an important add-on to granular micromechanics[3] for application to atomic scale[4].

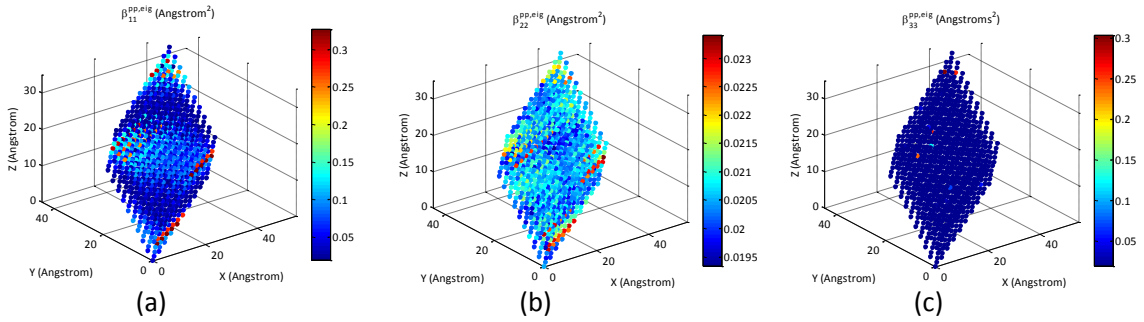

Figure 1 Pseudo-color representation of eigenvalues of (a) β_{11} (b) β_{22} and (c) β_{33} at 11.7505% strain, when the Cauchy-Born rule is first violated.

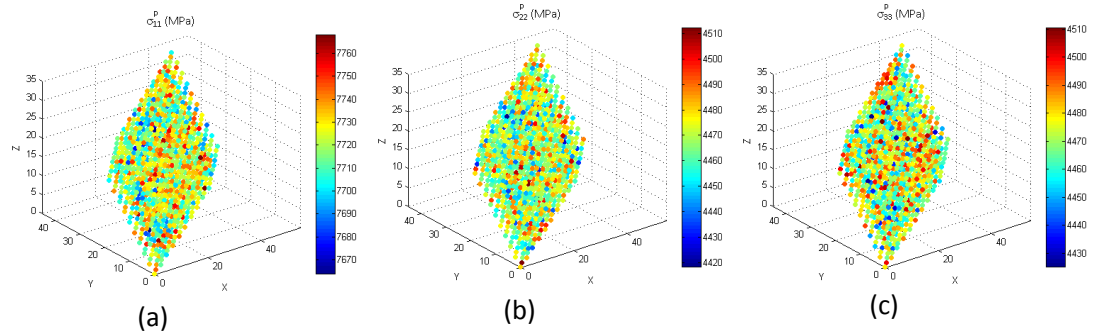

Figure 2 The components of traditionally computed stress (a) σ_{11} (b) σ_{22} and (c) σ_{33} show no obvious failure planes at 11.7505% strain

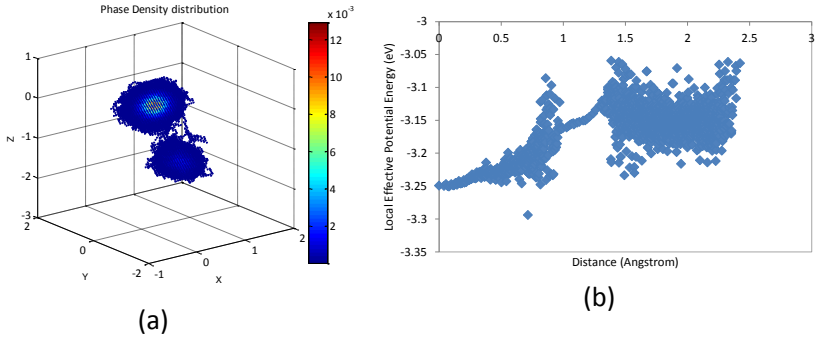

Figure 3 (a) The phase density for a sample atom from the "high β" region shows two distinct clouds indicating (b) a jump into a new potential well at 11.7505% strain

References

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