CONTINUUM FIELDS IN DYNAMICALLY DEFORMING ATOMISTIC PARTICLE SYSTEMS

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The continuum interpretation of dynamics of a system of atomic particles demands consideration of the discrete atomic force fields at the atomic length scales and the effects of non-local interactions. Many "interpretation techniques" have been used that are based on the management of boundary conditions that permit the matching of a macroscopic region with a microscopic region based on respective macroscopic long-range and atomic short-range deformation gradients. However, in all these techniques a true continuum corresponding to the temporal and the spatial evolution of dynamically deforming atomistic particle system is not considered. We use a recently developed formulation for complete dynamic equivalence between an atomistic system and the corresponding continuum in order to define continuum kinetics and kinematics fields, which follow the temporal evolution of the discrete MD system. Formulation of equivalent continuum is based on (1) conservation of the internal, external and inertial work rates (2) conservation of mass and (3) conservation of linear and angular momentum. Only non-polar materials are considered for the implementation, thereby placing an underlying assumption of only central inter-atomic interactions. Calculations are carried out on a block of copper atoms which is subjected to various loading conditions. The continuum fields corresponding to stress, strain rate, traction and density distributions are obtained for respective loading conditions. Results demonstrate that the work equivalent stress is equal to the force part of virial stress used in atomistic calculations. This confirms that only inter-atomic forces are responsible for stresses in a dynamically deforming MD particle system. The symmetry obtained in the stress solutions, even without explicit consideration of the conservation of angular momentum, demonstrated the symmetry of the work equivalent stress thereby confirming the equivalent continuum theory. Additionally, it is possible to observe local behavior in a truly non-local system through the definition of corresponding true continuum kinetic and kinematic fields.