

**A Material Frame Approach for Evaluating Continuum Variables
Within Atomistic Simulations**

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We will present a material frame formulation whereby expressions for continuum mechanical variables like stress and heat flux are derived from atomic scale quantities intrinsic to molecular simulation. We derive expressions for the 1st Piola-Kirchhoff (P-K) stress tensor and for the material frame-based heat flux vector. Atomistic simulation results are used to compare the stress expression with both the system virial and the Cauchy stress expression developed by Hardy. Our results show that the P-K stress tensor represents a full and consistent measure of stress. We will also present an expanded formulation to define continuum variables from micromorphic continuum theory, and will show this expanded formulation is both suitable and necessary for the analysis of materials represented by directional bonding at the atomic scale.

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