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Thermomechanical Continuum Representation of Atomistic Deformation at Arbitrary Time and Size Scales

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A thermomechanical equivalent continuum (TMEC) theory for the deformation of atomistic particle systems at arbitrary size and time scales has recently been developed. The description of coupled thermomechanical continuum behavior is derived directly from the ground up, using molecular dynamics concepts. This theory is a further advancement from a pure mechanical equivalent continuum (EC) theory developed recently. These new theories provide fully dynamic continuum interpretations of atomistic deformation with different resolutions for atomic particle motion.

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