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Thermodynamically accurate particle-based mesodynamics ALEJANDRO STRACHAN, BRAD HOLIAN, Theoretical Division, Los Alamos National Laboratory — Particle-based mesoscopic approaches, where groups of atoms are represented by a single *mesoparticle*, are widely used to achieve length- and time-scales beyond what is possible with atomistic modeling. I will present **a new mesodynamical approach that describes the energy exchange between mesoparticles and their internal degrees of freedom** in a thermodynamically accurate way. In our approach, energy exchange is done through particle coordinates, rather than momenta, resulting in Galilean invariant equations of motion; the total linear momentum as well as total energy (including the internal energy of the mesoparticles) are conserved and no coupling occurs when a mesoparticle is in free flight.The parameters entering our mesodynamics are easily obtained from first-principles and its results are in excellent agreement with all-atom simulations. Furthermore, our approach enables for a quantum mechanical description of the thermal properties of the implicit degrees of freedom (all-atom MD is always classical) and is generally applicable to many problems of materials science, chemistry, and biology.

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