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Coupling Classical Molecular Dynamics Simulations to Continuum Current and Heat Flow Equations: Application to Frictional and Resistive Heating of Nanoscale Metal Contacts CLIFFORD PADGETT, DAVID SCHALL, DONALD BRENNER, North Carolina State University — To reproduce experimental heat flow rates and to model resistive heating, atomic kinetic energies in a molecular dynamics (MD) simulation are coupled via an ad hoc feedback loop to continuum current and heat transfer equations that are solved numerically on a finite difference grid (FDG). For resistive heating, the resistance in each region of the FDG is calculated from the experimental resistivity and atomic density, and a network of resistors is established from which the potential at every FD point is calculated given an applied voltage. The potential difference between connected FDG regions and the resistance are then used to calculate the current between the two points, the heat resulting from that current, and the magnetic and electrical force between grid regions. This information is then added back into the atomic simulation. To illustrate this method, simulations of the frictional and resistive heating of a nanoscale metal contract will be presented. This work was funded by MURI Project No. N00014-04-1- 0601.

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