Heat Flow Studies for Large Temperature Gradients By Molecular Dynamics Calculation

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We derived a molecular dynamics algorithm capable of simulating heat flow in fluids beyond the linear regime. The method is simple and easily applicable to any molecular model used at present in computer simulations. Unlike the synthetic Evans method, our algorithm establishes real temperature differences between two regions of the model system by pumping heat continuously into the high temperature region and taking it away from the low temperature region. Since there is no solid phase present, the generated density variation is small. The heat flow can be calculated from the energy input and output of the thermostat or can be measured by the method of planes (MOP). We performed extensive calculations to study the performance of the algorithm and compared the determined heat conductivity coefficients to results obtained by the synthetic method. For the studied simple fluid model the conductivity was found practically independent of the size of the temperature gradient.