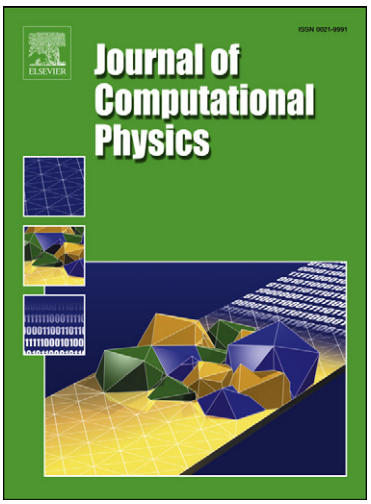

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Thermal parameter identification for non-Fourier heat transfer from molecular dynamics

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Abstract

Fourier's law leads to a diffusive model of heat transfer in which a thermal signal propagates infinitely fast and the only material parameter is the thermal conductivity. In micro- and nano-scale systems, non-Fourier effects involving coupled diffusion and wavelike propagation of heat can become important. An extension of Fourier's law to account for such effects leads to a Jeffreys-type model for heat transfer with two relaxation times. We propose a new *Thermal Parameter Identification* (TPI) method for obtaining the Jeffreys-type thermal parameters from molecular dynamics simulations. The TPI method makes use of a nonlinear regression-based approach for obtaining the coefficients in analytical expressions for cosine and sine-weighted averages of temperature and heat flux over the length of the system. The method is applied to argon nanobeams over a range of temperature and system sizes. The results for thermal conductivity are found to be in good agreement with standard Green-Kubo and direct method calculations. The TPI method is more efficient for systems with high diffusivity and has the advantage, that unlike the direct method, it is free from the influence of thermostats. In addition, the method provides the thermal relaxation times for argon. Using the determined parameters, the Jeffreys-type model is able to reproduce the molecular dynamics results for a short-duration heat pulse where wavelike propagation of heat is observed thereby confirming the existence of second sound in argon. An implementation of the TPI method in MATLAB is available as part of the online supplementary material.

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