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Variance Reduced Monte Carlo Simulations of Phonon Transport in Semiconducting Materials[1] JEAN-PHILIPPE PERAUD, Department of Materials Science and Engineering, MIT, COLIN LANDON, NICOLAS HADJICONSTANTINOU, Mechanical Engineering Department, MIT — We present a class of variance reduction methods for drastically reducing the statistical uncertainty associated with Monte Carlo simulations of phonon transport in semiconducting materials. The variance reduction is achieved using a control variate approach, with a nearby equilibrium serving as the control. The resulting simulation methods exhibit drastically reduced statistical uncertainty that is proportional to the deviation from equilibrium; in other words, arbitrarily small signals can be simulated, because, as the signal decreases, the statistical uncertainty also decreases proportionally. The lower statistical uncertainty significantly reduces the cost associated with simulations of systems close to equilibrium (e.g. for calculating thermal conductivity). The computational gains enable efficient and essentially noise-free simulation of three-dimensional problems. Application of our methodology to the investigation of the effect of engineered porosity patterns on the thermal conductivity of silicon as well as the transient response of thin films subject to laser irradiation will be presented and discussed.

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