Graphene, the two-dimensional allotrope of carbon, is an excellent thermal conductor with highly unusual electronic properties. To better understand thermal conduction in graphene at the atomic scale, we perform quantum Green’s function calculations of phonon transport through graphene nanoconstrictions. To mimic phonon decay and generation due to anharmonic interactions and thermal fluctuations, all atoms are coupled to local Langevin heat baths [1]. The temperatures of the heat baths, which can be suitably interpreted as local atomic temperatures, are determined self-consistently by demanding that the average heat current to the baths vanishes.

The solution of the stochastic equations of motion leads to a non-linear system of equations for bath temperatures, which is solved by the Newton-Raphson method. The carbon-carbon interaction is modeled by the fourth-nearest-neighbor force constant model [2]. We study the validity of linearizing the self-consistent equations and compare the full quantum temperature profiles to the classical results. Our model and results provide new insight to phonon transfer in graphene and can help in the design of efficient devices.

Figure 1: Left: Graphene nanoconstriction. The system extends infinitely to the left and right, but the temperatures are determined self-consistently only in the shown region. In the non-visible parts of the left and right leads, the temperatures are set to $T_L$ and $T_R$, respectively. Right: Self-consistent bath temperature profile (K) in the constriction. The leads are at temperatures $T_L = 300$ K and $T_R = 280$ K. Phonon scattering time is set to $\tau = 1$ ps.