The first aspect of my research is called stochastic homogenization. The conductance of a material can be highly heterogeneous at a molecular level (see picture), and therefore any direct simulation is computationally undesirable since the variations on small scales need to be addressed. However, if we further assume the material to have some spatial homogeneity in statistical information, then we may make approximations by simulating some homogeneous material, so that computational cost can be significantly reduced. In the first part of my thesis, which is joint work with professors Jianfeng Lu and Felix Otto, we study the approximation of three-dimensional infinite material, and give an optimal algorithm that successfully captures the correct scaling of error induced by truncation and randomness.

The second part of my thesis, which consists of joint works with Yu Cao (former Duke math PhD student) and Jianfeng Lu, is about sampling from a target distribution, which has profound relationship with optimization, statistics, molecular dynamics and machine learning. A popular approach to sampling consists of using continuous time Markov Chain Monte Carlo processes: after running a stochastic process for a long time, its distribution will be close to the target. Therefore, studying the convergence rates of these processes is important for applied mathematicians, since processes that converge fast have a practical advantage. In the second part of the thesis, we give sharp estimates on the convergence rates of several sampling processes, including the underdamped Langevin dynamics, randomized Hamiltonian Monte Carlo, the zigzag process and the bouncy particle sampler. Our results in underdamped Langevin dynamics improve on previous results of many great mathematicians including Cédric Villani.