High throughput multi-scale modelling of the thermal conductivity

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Since the last few years it is possible to perform multi-scale ab initio computations of the lattice thermal conductivity of semiconductors and insulators. The basic idea is to perform quantum mechanical computations of the physical properties at the atomic scale, and then transfer those properties at the meso and macro scale to study heat transport in an actual device.

At the scale of devices, the transport equations are solved using a Monte Carlo method which allow to include the effects of boundary conditions, and study the dependence of the thermal conductivity as a function of the size and the shape of the device. What is the optimum size, shape and chemical composition for a given target, like the cooling of nano devices as shown in Fig 1, are actual questions we wish to answer during this thesis.

To answer those questions, high performance computing and the use of intelligent algorithms are needed to search the complicated optimization space. Therefore, the above-mentioned procedure for solving the transport equations must be fully automatic. In the first part of the thesis, based on existing code, a python solver will be implemented to solve the transport equations using a Monte Carlo method. The second part of the thesis will be devoted to use this code coupled with artificial intelligent algorithms to optimize heat transport in nano-cooling applications.

The recruited student will be under the supervision of Laurent Chaput and David Lacroix, and will be based in Nancy, France. We are looking for a highly motivated student, with background in physics and mathematics, and very strong programming skills in Python. Experience with coding in FORTRAN would be appreciated too.

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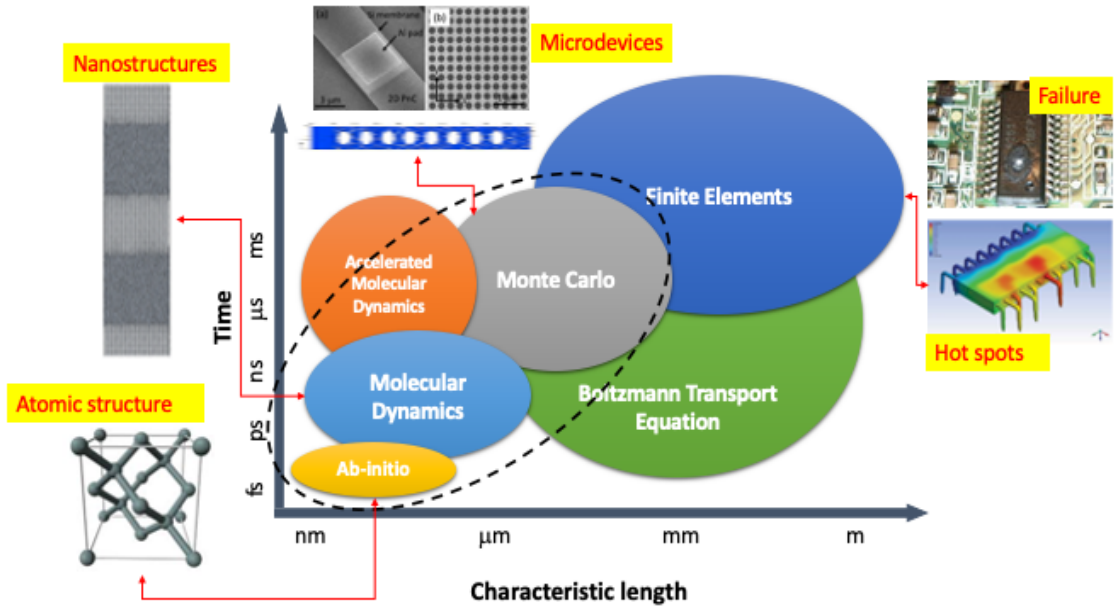

Figure 1: Multi-scale modeling of Heat transport