Electrostatic calculations on GPUs

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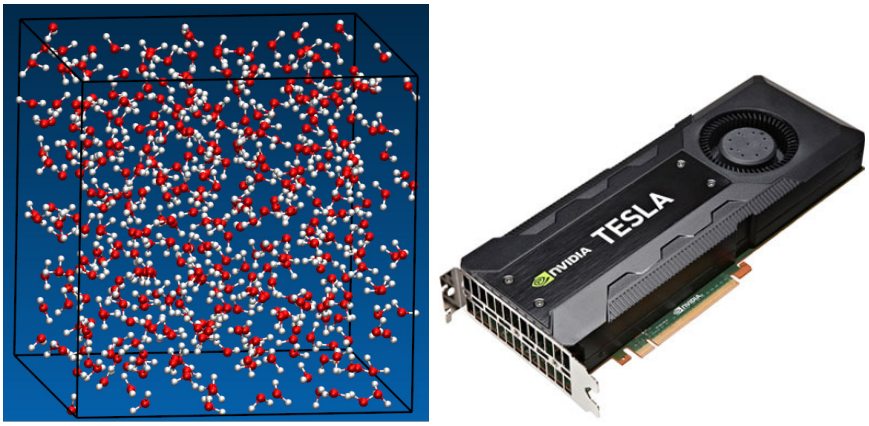

Figure 1: Left: A system of water molecules. Right: An example of a GPU accelerator. A TESLA K40 with 4.29 Tflops peak single precision floating point performance.

During the last decades, Molecular dynamics (MD) simulation has become an important tool to study many-body problems such as lipids and proteins. The presence of modern computers and especially the heterogenous systems including CPU and Graphics Processing Unit (GPU) clusters, has made simulation of bigger systems more feasible. GPU clusters accelerate the compute-intensive problems and are therefore well suited to use in molecular dynamics calculations. In MD simulations, the electrostatic computation is a major bottleneck of the simulation as it constitute the most time consuming part. In this project we want to implement a GPU version of an existing CPU code for computing electrostatic interactions using C-CUDA for NVIDIA GPUs.