ETH zürich

Master / Semester Thesis

Computational acceleration of rejection-free kinetic Monte Carlo simulations

Background

Many physical and chemical processes can be modelled efficiently on the atomistic level using a simulation approach called rejection-free Kinetic Monte Carlo. In this type of simulation, the computational domain is described in terms of a set of events between atoms, each of which has a certain frequency of occurring. At each simulation step, there is a stochastic event selection process, execution of the selected event, and re-generation of the event list (Fig. 1). This method can be used to describe the evolution of large atomic structures at timescales which are computationally inaccessible to conventional methods (such as Molecular Dynamics).

Project scope

We have developed a rejection-free kinetic Monte Carlo code in C++/CUDA to simulate atomistic processes similar to dielectric breakdown in oxides, and are now building a distributed-memory implementation of the simulation modules. The goal is this project is to investigate optimal ways to distribute the Monte Carlo event selection module (Fig. 2). It will involve testing optimal data structures to build and store the event list (array vs. binary tree), methods of memory-management (updating vs. re-computing the events), and investigating different communication patterns to exchange information between MPI processes. If you are interested in accelerating physics simulations, applying principles of High Performance Computing (HPC), and contributing to a actively-used code, please feel free to contact us for more details!

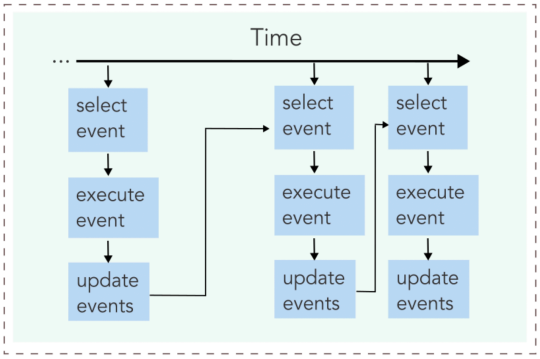

Fig 1: Timeline of a rejection-free Kinetic Monte Carlo simulation, showing only the event selection/execution module.

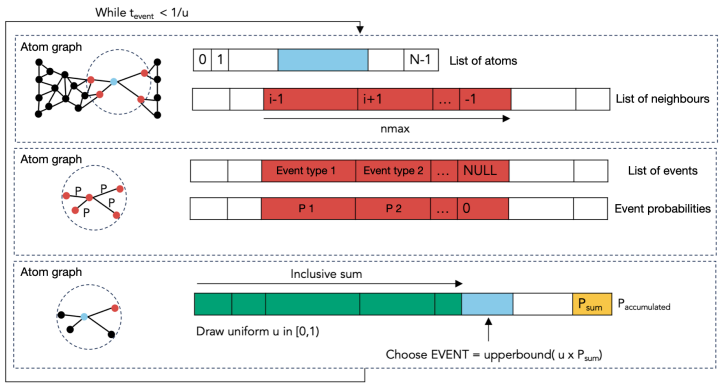

Fig 2: Schematic representation of the rejection-free Monte Carlo event selection step. The diagrams on the left side show sub-sections of the atom graph

Prerequisites

- (Required) Coding experience in C++, knowledge of the HPC principles through coursework
- (Optional) Experience in writing MPI code to distribute computation across nodes
- (Optional) Experience accelerating scientific code with CUDA

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