Undergrad Winter Vacation Scholarship Project

Porting Smooth Particle Hydrodynamics LAMMPS package to GPUs.

Project start date: Preferably by 1st July. Earlier start is possible.

Project duration: 4 weeks minimum.

Payment per week: $500.

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Department: Materials Science and Engineering

Project description:

As part of the MineAlloy ARC Research Centre, we are developing simulation tools to simulate the wear resistance of ductile materials used in the mining industry. Materials submitted to wear experience large deformation and damage which we are simulating.

Usually, the simulation of materials and structures subjected to macroscopic deformations is done using well established Finite Element Methods (FEM). In FEM, a solid is divided into finite elements constituting a mesh onto which linearised partial differential equations are solved. As the accuracy of FEM decreases with the distortion of the mesh elements, when large deformations occur complex remeshing processes are required. In this case, particle based methods are preferred. Indeed, instead of discretising a solid into a mesh, they do it using an ensemble of particles. In the case of the oldest particle based method, Smooth Particle Hydrodynamics (SPH), particles interact with each other through a smooth kernel function. This enables the possibility to simulate large deformations. This is why for the simulation of wear we are using SPH.

Our simulations make use of a user package for the worldwide used Molecular Dynamics simulator LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) (see https://lammps.sandia.gov/). As its name indicates, LAMMPS is a massively parallel software that uses MPI, OpenMP, and CUDA as parallelisation
options. MPI is used by default and, if the package used supports it, it can be paired with CUDA (or OpenMP). As of today, the SPH package supports only MPI, and your task would be to help us port it to CUDA.

**Pre-requisites:** You must have taken FIT3143 or FIT5170 courses on parallel computing, you should be Linux proficient, have a good knowledge of Git, and know well C/C++ and CUDA.

**Extra information:** If shortlisted, you will be interviewed at a mutual convenient time.