Discrete Element Modelling with LAMMPS Developed for High Performance Computing by HECToR dCSE Team

Catherine O'Sullivan, George Marketos, Imperial College London (ICL)
HECToR CSE Team, Numerical Algorithms Group Ltd (NAG)

An HPC expert from ICL, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, has successfully enabled highly-scalable Discrete Element Modeling (DEM) simulations to be performed on HECToR. While DEM is widely used to simulate the response of granular materials for civil, process, or chemical engineering applications, its adaptation to high-performance computing (HPC) by the DEM user community remains small in comparison to the use of HPC for other molecular dynamics (MD) applications. Consequently the impact of current DEM simulations on industry and in basic science is currently limited. The Large-scale Atomic/Molecular Massively Parallel Simulator, LAMMPS, is widely used in MD, and is a very good platform for DEM simulations, but while the resultant code is highly scalable, it lacks the necessary functionality for the majority of DEM applications.

The key objective of this dCSE project was to add needed functionality to granular LAMMPS by implementing new C++ classes that would significantly increase the type and number of highly-scalable DEM simulations that can be performed on HECToR, enabling simulation of routine laboratory tests used in geomechanics and other fields. Two sets of new boundary conditions and a new contact model for the bonding between two grains were developed. The new boundary conditions enable dealing with rigid stress controlled boundaries and the inclusion of membrane boundaries with greater accuracy. An inter-grain interaction model for the bonding between two grains was also developed. This implemented a model widely used in other codes to simulate bonded material such as porous rocks.

Commenting on the dCSE project success, *Dr Catherine O'Sullivan of the Civil and Environmental Engineering Department at ICL said: "The support provided via the dCSE mechanism has allowed development of the LAMMPS code to enable Discrete Element Method simulations (DEM) of granular materials to be run in a high performance computing environment. Discrete Element Method simulations model granular materials at the particle scale and provide a vast amount of information about the material response. They also enable failure mechanisms to be studied in detail. A central consideration in DEM simulations is the need to include representative numbers of particles. Hitherto, these simulations have typically used serial code and this has limited the numbers of particles to 100,000 or less. This funding has facilitated a step change in the size of simulations engineers can now consider; the first simulation of a geo-engineering problem involving 1.4 million particles was successfully completed."*

The stress-controlled demonstration was the first known DEM simulation for geomechanics where more than 1,000,000 particles were compressed in a controlled manner.

HECToR

HECToR is managed by EPSRC on behalf of the participating Research Councils with a mission to support capability science and engineering in UK academia. The Cray XE6 supercomputer, located at the University of Edinburgh, is managed by UoE HPCx Ltd. The CSE Support Service is provided by NAG Ltd and ensures users have access to appropriate HPC expertise to effectively exploit advanced supercomputers for their science. A critical feature of the CSE Support Service is the distributed CSE (dCSE) programme which, through lightweight peer review, delivers dedicated performance and scalability projects on specific codes in response to proposals from users. The dCSE programme now consists of over 70 focused projects complementing the traditional HPC user applications support and training also provided by NAG.

The dCSE projects completed so far have delivered outstanding examples of the cost savings and new science that can be enabled through dedicated CSE effort. The LAMMPS project reported here adds to these success stories with a successful performance improvement.

Project Background

Typically, Discrete Element Method (DEM) simulations have been run on serial code by the UK-based DEM user community. A previous EPSRC-funded research project (EP/G064180/1) identified granular LAMMPS as the most suitable open-source parallelised code for large-scale DEM simulations. However, to enable full advantage to be taken of the opportunities posed by using HPC facilities such as HECToR for DEM simulations it was necessary to develop the boundary conditions implemented in Granular LAMMPS. The first modification was to allow rigid wall movement, and so allow for strain controlled simulations. The second step was to implement full stress-controlled rigid boundaries and membrane boundaries. This allows more realistic simulations of laboratory tests, which are routinely confined by latex membranes. As this feature is not currently available in any other open-source code, and requires a computationally expensive Voronoi diagram calculation, it is expected that this will increase the adoption of Granular LAMMPS and High-Performance Computing by the DEM user community.

Dr Catherine O'Sullivan of the Civil and Environmental Engineering Department at ICL was the Principal Investigator for the project. Dr George Marketos, also of ICL carried out the 7 person-month project, in close collaboration with the NAG CSE team.

Project Results

To develop granular LAMMPS for moving and rigid stress controlled boundaries, modifications were made to the FixWallGran C++ class. For the addition of the membrane boundary condition, an algorithm based on the weighted Voronoi graph method was implemented by calling the external package, Voro++ package within the FixMembraneGran class.

To develop the new contact model for the bonding between two grains, a non-linear elastic contact spring model was implemented as the new class. Another new class was developed to add the new bonding model. And the LAMMPS input script was also updated to enable specifying the new functionality. The new code was verified against results from the commercial code PFC^{3D}.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/LAMMPS-DEM/

For more information contact: HECToR CSE Team
The Numerical Algorithms Group Ltd, Wilkinson House, Jordan Hill Road, Oxford, OX2 8DR, United Kingdom
Telephone: 01865 511 245 Email: hector-cse@nag.co.uk Web: http://www.hector.ac.uk/cse/