LAMMPS and its Applications

Molecular and Business Modelling

UCL NatSci Innovation Lab 2020

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29/7/2020

Contents

We encourage readers to read more on LAMMPS in their official website. Most of our information can also be found in this link: http://lammps.sandia.gov/ The source of scientific literature using LAMMPS can be found here: https://lammps.sandia.gov/papers.html

1 Introduction

LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator, develped by Sandia National Laboratories. The software can be run by laptops, desktops, or even supercomputers. It is a classical molecular dynamics code. In short, it takes into account of initial positions and velocities of atoms or molecules, calculates the inter-atomic potentials between atoms using mathematical formulations, and returns the positions and velocities of the input atoms or molecules of later times.

We will be discussing its applications using examples of scientific literature.

2 Applications and advantages

It is good for running atomistic, mesoscale, and coarse-grain simulations. The code itself is material oriented, and contains a wide range of inter-atomic potentials. It is also effective for large scale simulations. We will take a look into (3-4?) papers which used LAMMPS as their modelling software.

2.1 Visualization

While running the simulation, image files are saved using the software's "dump image" command. On the other hand, if you would want to use have high quality and interactive visualisations, you may choose to use

2.1.1 Example using GitHub resources

An example of image from one of the examples given in GitHub is shown below:
The input file, [in.crack], simulates a cracking action. We took the original file from the public LAMMPS repository in GitHub, and ran it using Bash. [1]

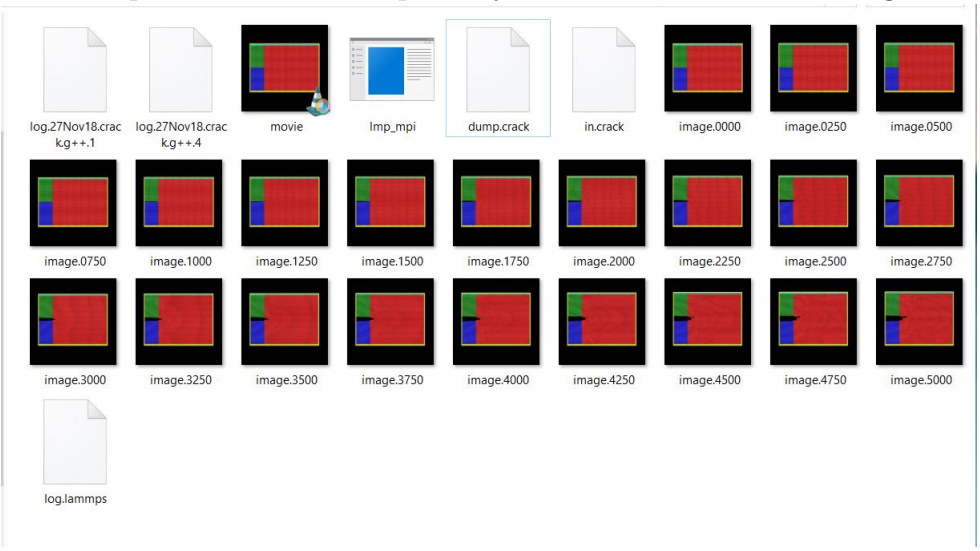

Fig 2.1.1: File contents within the example file
The file contents are shown above in Fig 2.1.1. By using the "dump image" command within the script, images of the simulation and a video file are returned for visualization purposes, without the use of a visualization software.

2.1.2 Example in scientific literature

In this example, this paper from the Physical Review Letters [2] discusses the difference between crater formation mechanism on a target by high-velocity nanoparticles (x 10^{-9}m) and macroparticles (> x 10^{-6}m). In this simulation, a nanometre wide copper sphere impacts a single crystal copper target with a speed of 5km/s [2], and Figure 2 shows the visualisation of the simulation:

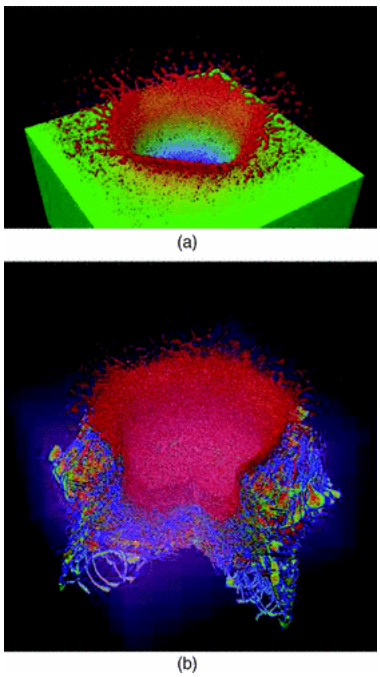

Fig 2: Image of the simulation. Retrieved from [2, 027601-2, FIG. 2]

In the figure above, image (a) represents a normal impact of the particle to the target, while image (b) shows the same system, but only the dislocations of the target[2]. The simulation is compared to an experimental image(Fig 3) as shown below:

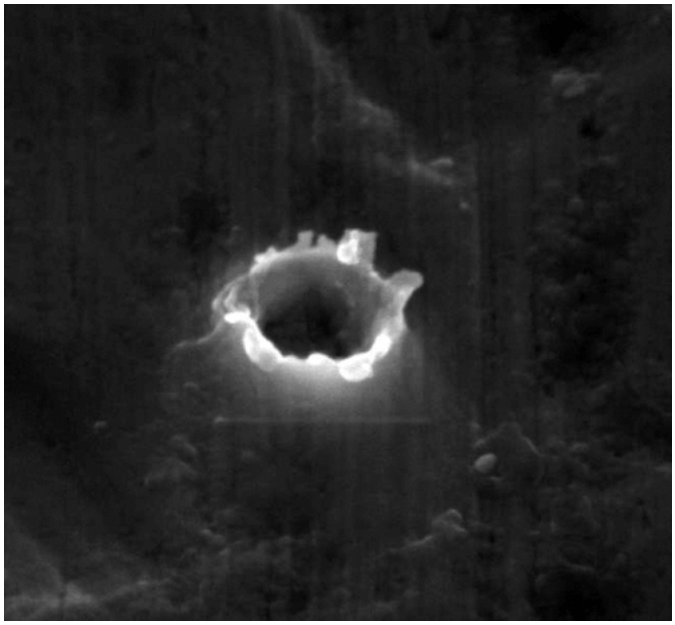

Fig 3: Experimental image. Retrieved from [2, 027601-2, FIG. 3]

This image is a secondary electron image, which is a result of detecting inelastic collisions of electrons and the target[3, 4]. This time, a high speed particle from comets is collided with an aluminium target from the Stardust mission[2]. For more information about the Stardust mission, check here:
https://stardust.jpl.nasa.gov/home/index.html

The study [2] addresses that the ratio of the volume of target's crater per atomic volume to energy of the particle(such ratio is named *crater efficiency*, denoted as "a"), changes slowly with the cluster size. The simulation allowed the researchers on how the effect of "plastic flow", which is the permanent change of shape of a body once the applied stresses satisfy the yield critereon[5], can increase the cratering efficiency, as the effective target strength decreases. The visualization using LAMMPS gives us a tangible concept of an expected experimental image, which is clearly an advantage using the software.

2.2 Adaptability

LAMMPS is a very versatile software amongst the scientific community. We will discuss the interdisciplinary uses of LAMMPS in the following section.

2.2.1 Example in Materials Science

Material science is the study of materials and their physical behaviours. LAMMPS is widely used in material science, while classical molecular dynamic models aid in running simulations. For example, there is a paper on the behaviour of coal ash effected by calcium oxide and magnesium oxide in a blast furnace[7], and the oxygen defects on stabalizing the crystal structure of $MgAl_2O_4$[**?**].

Crater efficiency (from 2.1.2) In Section 2.1.2, we already covered the study regarding plastic flow and crater creation on materials. The study gives us more

understanding on how materials will act in times of collision in a nano and macro scale, and the practical behaviour on crater efficiency. As stated in the paper [2], when crater efficiency is reduced, it will provide improved nanostructural designs, as well as modification techniques.

Mechanical properties of TMDs Another example will be on the study [6] on a kind of 2D materials, known as monolayer ternary transitional metal dichalogenides (TMDs). The stated example will be $MoS_{2x}MoTe_{2(1-x)}$, where the mechanical properties of this newly synthesized material, such as its fracture behaviours and Young's modulus at different temperatures, are studied by classical molecular dynamics simulations using LAMMPS.

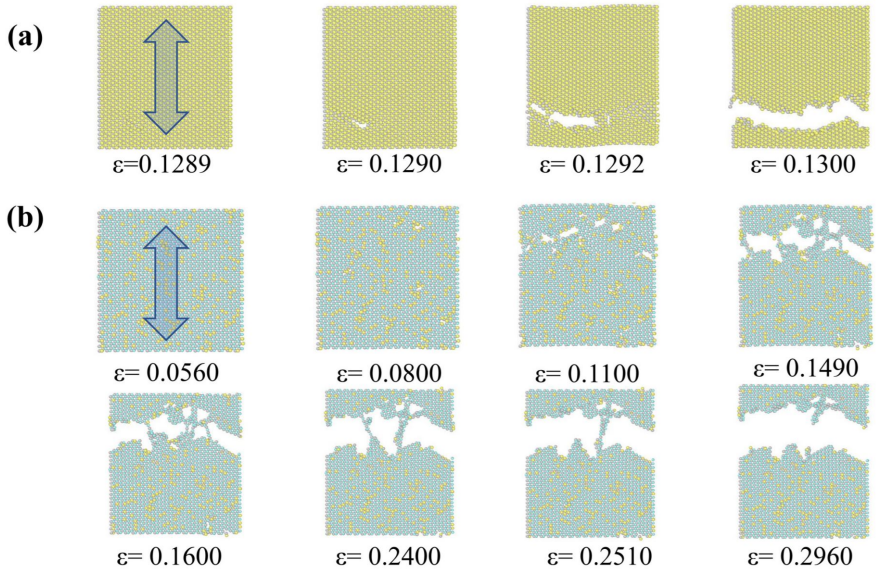

Fig 4: Image of the simulation. Retrieved from [6, J. Appl. Phys. 126, 215105-10 (2019); doi: 10.1063/1.5122264]

Here we see examples stated in the paper[6]. Both underwent simulations of tensile loading along the zigzag location. In Fig4(a), it shows the brittle fracture in MoS_2 nanosheets at 300K; Fig4(b) shows the ductile fracture in $MoS_{0.4}Te_{1.6}$ nanosheets at 500K[6]. The ε denotes ratio of the material's extension to its original length, i.e. its strain.

To conclude, the simulation using LAMMPS provided calculations and visualizations of mechanical properties of the TMDs, using equations regarding such properties, as well as molecular dynamics.

You can see more of the results in the paper here:[6]

2.2.2 Example in Physical Chemistry

Physical chemistry is the subject where physics is used in systems of chemistry. I will use an example published quite recently (Dec 31, 2019) in the LAMMPS website.

Simulation of SnO_2 nanoparticle In this paper[9], cavitation behaviours of a nanoparticle, tin(IV) dioxide (SnO_2) immersed in water was being investigated. In this case, the term cavitations is a hydrodynamic phenomenon, which can be seen as having a small "hole", or a cavitation void, in a liquid due to negative pressure, without forming an air bubble. [10]

The paper concluded that cavitations will only occur when the nanoparticle is within the water, together with am alteration of a local electric field, that induces the cavitation.
Using LAMMPS, molecular dynamic simulations of a 1.5 nm SnO_2 immersing in water were done, with and without the presence of an electric field .

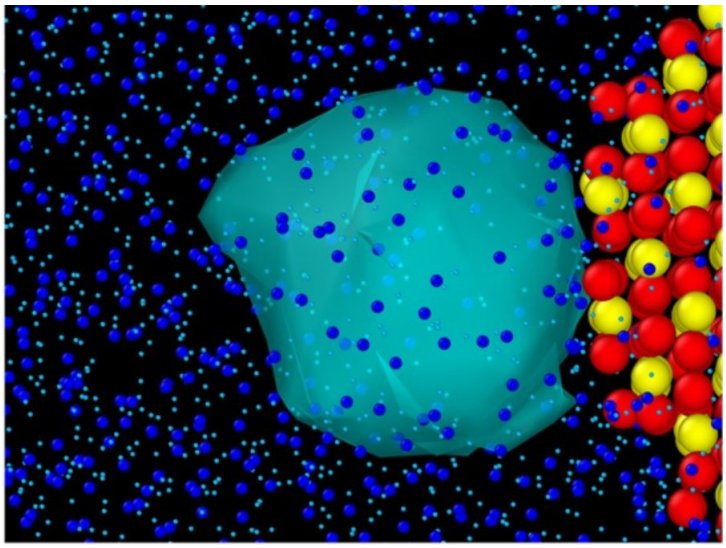

Fig 5: Image of the system just after cavitation. Retrieved from [9, Figure 2(a) ACS Omega. 2019 Dec 31; 4(27): 22274–22279.Published online 2019 Dec 18. doi: 10.1021/acsomega.9b00979]
In the simulation, many formulas, mathematical models, as well as the various properties of the stated molecules have been implemented and calculated accordingly to give results. For example, energy required for generation of a spherical void[11], magnitudes of electric field strengths, properties of bulk crystals SnO_2, relevant force field calculations, and vice versa.
Do go and check out their paper[9], which will give you an exciting insight on how LAMMPS assist in our understanding of physical chemistry, as well as fluid dynamics.

2.2.3 Example in Biophysics

Biophysics uses the knowledge of physics to model or explain biological systems, for example bacterial movements in fluid flows [12], modelling of magnetic particles in blood flow[13], and single cell mechanics simulations[14].

3 Common uses

There are some common features using LAMMPS as a tool.

1. Multidisciplinary researches
2. Building lattices
3. Include various variables and equations for repetitive calculations
4. Support theories related to research
5. Simulating data, and comparing results with experimental data
6. Visualisation of systems

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