JOINT INSTITUTE FOR NUCLEAR RESEARCH
Laboratory of Information Technologies

FINAL REPORT ON THE SUMMER STUDENT PROGRAM

LAMMPS and VMD – simulating and visualizing molecular dynamics

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Abstract

LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. We will walk through some examples of simulation using this powerful packages that we will visualize with the help of VMD. Visual Molecular Dynamics (VMD) is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and build-in scripting. We used this tool to tackle the problem of clusterization of Al atoms by analysis the distribution of cluster sizes as a dependency of cooling rate. The research stage was finalized through a seminar held in the Laboratory of Information Technologies, JINR, Dubna, Russian Federation.

With the advances in nanotechnology there is a great interest to model the processes that take place at the atomistic level. Knowing and being able to simulate this type of processes could lead to new advances in the field nanomaterials, such as the possibility to obtain new nanomaterials with better physical, chemical and structural properties.

Our aim was to study the clusterization of Al atoms through analysis of cluster size distribution. We approached the problem using the molecular dynamics method. Molecular dynamics is a computer simulation method for studying the physical movements of atoms and molecules, which make it a type of N-body simulation. To perform the simulation we turned to one of the most used open-source packages available – LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) developed by Sandia National Labs and Temple University. For a complete feedback we used VMD (Visual Molecular Dynamics) to visualize and comprehend better our results.

During the research stage at Laboratory of Information Technology we were presented with the capabilities and properties of the heterogeneous computing cluster HybriLIT. We were introduced to parallel libraries such as OpenMPI, OpenMP, CUDA etc. used on the cluster through courses specially designed for beginners.

We used LAMMPS to perform simulation of clusterization of atoms interacting through the Lennard-Jones potential and a Nosé–Hoover thermostat that cools down the system. The visualization of the simulation confirmed that our simulation was good as we could see clusters of different sizes forming at different rates of cooling(Fig.1).

In order to simulate Al atoms we used the adp pair_style in LAMMPS. *adp* computes pairwise interactions for metals and metal alloys using the angular dependent potential (ADP) of (Mishin), which is a generalization of the embedded atom method (EAM) potential. The initial setup is a randomly spreaded set of 100.000 Al atoms in a cubic simulation box with periodic boundary conditions. Initial temperature was set to 3.000 K, the final temperature was set to 50K and the simulation time is set to 100ps. We investigate the distribution of cluster sizes for different temperature dropping rates (Tau). We observe that when Tau=1.000 the cluster sizes are mostly concentrated around low number of atoms, with the largest cluster having a number of 24 atoms(Fig.2). When the cooling is slower, larger Tau, the distribution of cluster sizes is strongly skewed to the right, with only around 13% being individual atoms, with the largest cluster composed of 198 atoms. This result are preliminary and are bound to further checking.

Establishing a connection between temperature drop rate and the cluster sizes is our aim as future work. We would like to extend the study to a set of Cu atoms as a further development.

During the research stage we compose a tutorial for LAMMPS and VMD potential users. A hands-on tutorial was held in the Laboratory of Information Technologies in 7 september, at 10:00, room 407.

Methods

During the research stage we used the infrastructure provided by the heterogeneous computing cluster HybriLIT. LAMMPS was used as a serial program at the beginning and then migrated to the cluster for GPU acceleration. VMD was the tool used for visualization purposes.

Figures

Below are listed the figures mentioned in the text.

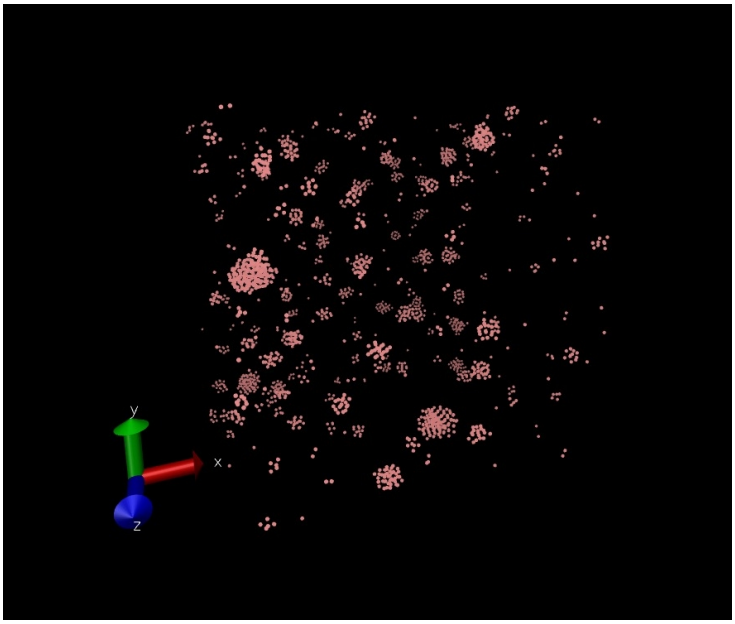

Fig.1. Clusters formed using Lennard Jones potential and a Nose-Hoover thermostat

Acknowledgements

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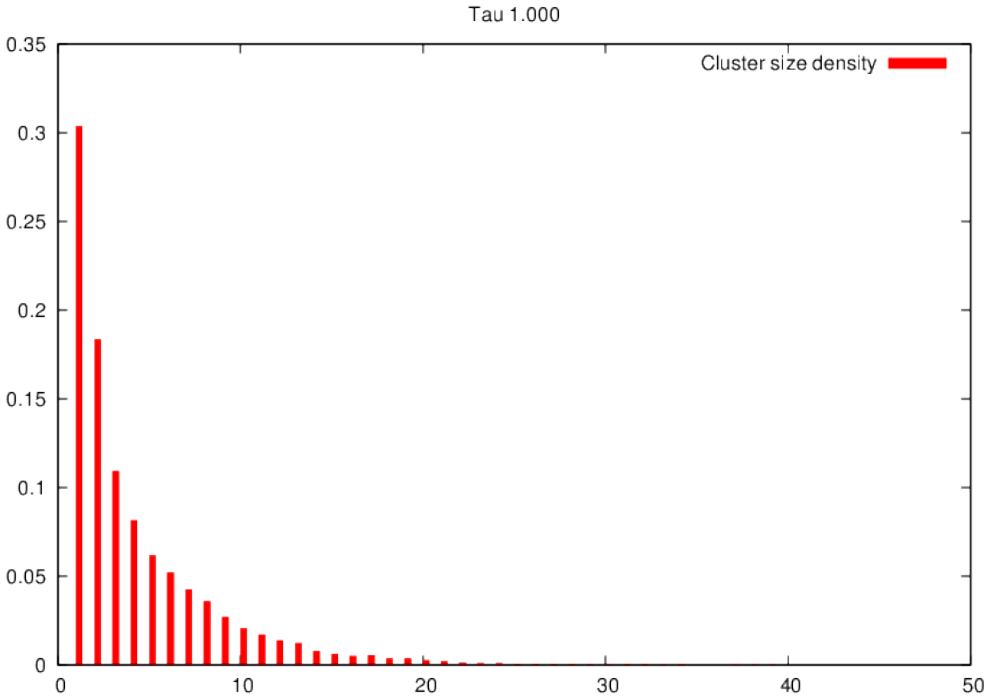

Figure 2.: Cluster size density for a temperature drop rate of 1.000 timesteps

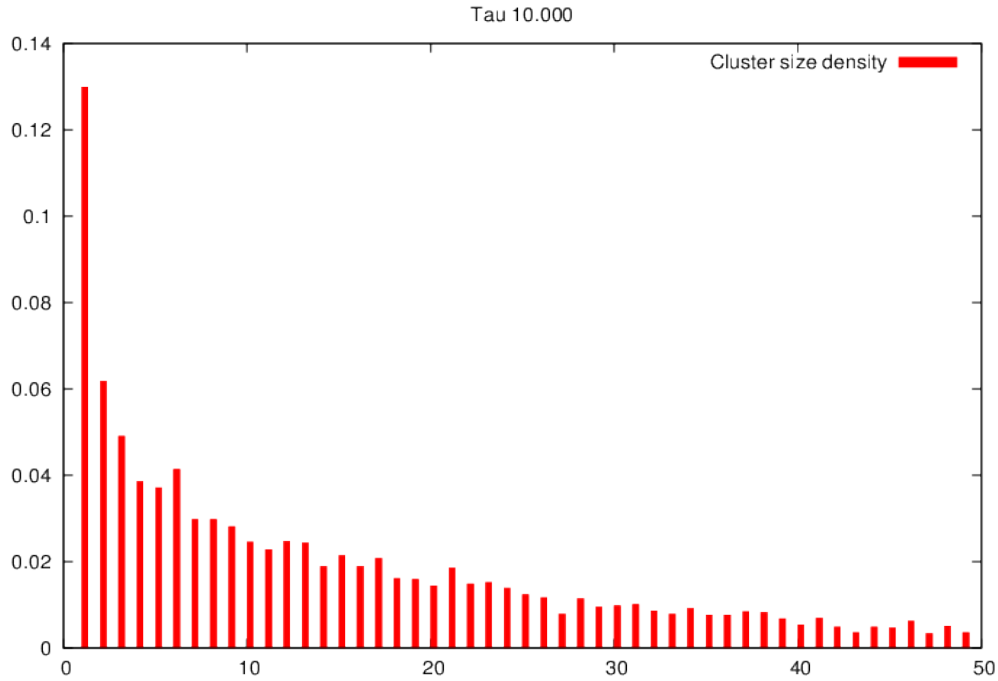

Figure 3: Cluster size density for a temperature drop rate of 10.000 timesteps