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Modeling and visualization of molecular dynamic processes

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- Formulation of the problem
- Modelling of a nanosize metal grain in argon
- Creation of carbon chains from monatomic components (gas)
 - Conclusion
 - References

Formulation of the problem

Two many-particle molecular dynamic problems are regarded within this work . These problems are important in practical applications.

- Modelling of movement of a metal nanosize grain in gas
- Creation of carbon chains from monatomic components

These problems have been investigated in order to check the possibility to solve them by using existing methods and programs and to test the correspondence between computations and theory.

For both problems large systems had been modelled, hence their solution requires large computational resources.

To perform the computations and to visualize the results special software was selected and studied.

Software package LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator ^[1]

- Based on classical molecular dynamics

i.e. it uses classical equations of Newton: $\frac{d^2\vec{r}}{dt^2} = -grad U(\vec{r})$

- Created specially for parallel computer clusters.
- Uses MPI on systems with distributed memory (we can use MPI realization more suitable for current system)
- Coded with C++
- Open source (GPL license)
- Active developing project with technical support (mail list)

Systems we can model using LAMMPS

- Atomic systems
- Charged particle systems
- Polymers, organic molecules, proteins, DNA...
- Metals
- Granular materials
- Coarse mesogrid models
- Ellipsoidal particles
- Point dipoles
- Combination of everything listed above

Setup and start

- LAMMPS is distributed in a source code
- Additionally should be installed
 - *MPI realization (MPICH) for parallel computing*
 - *FFTW - fast Fourier transform*
- Source code is compiled and the created executable file can be used on computers with similar configuration
- To start the computation the following command is used: *mpiexec -n <num_proc> lmp <input.file>*
- Input file (text, 10 -25 lines) contains all the information about the modeled system

Data output

- Text or binary output file:

One big file (2 GB max on 32 bit CPU, limitation of C language)

Many small files (one file per one computational step)

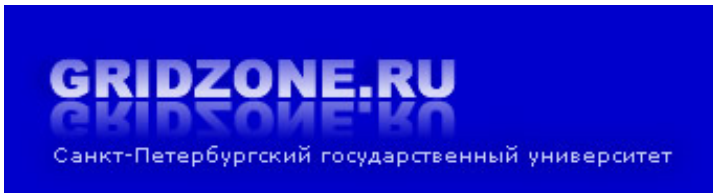
- Different formats (including popular *dcd* – used in CHARMM, NAMD, XPlor; *xtc* – in GROMACS)
- Output information is determined by user and can contain:
 - System thermodynamical parameters
 - Coordinates, speed and other info about every atom
 - Average system parameters (pressure, temperature, etc.)
 - Computing of parameters with an algorithm written by user

Disadvantages

- No graphical interface (only command prompt)
- Inability to create molecular systems (only with other software)
- Inability to determine automatically coefficients of interaction potentials (only for special (AIREBO, EAM for a few metals, etc.))
- Inability to produce a complex analysis of the results
- No built-in software for visualization of results and for building plots

Hardware used for computation

Computations were performed on the basis of the distributed scientific complex of grid technologies at SPbSU



4 computational nodes (parallel)

Server platform Supermicro X7DVL-E/ 1U"

2 x Intel Xeon 3.0GHz/1333/4MB (Dual Core) EM64T

2 x 2048MB DDR ECC REG

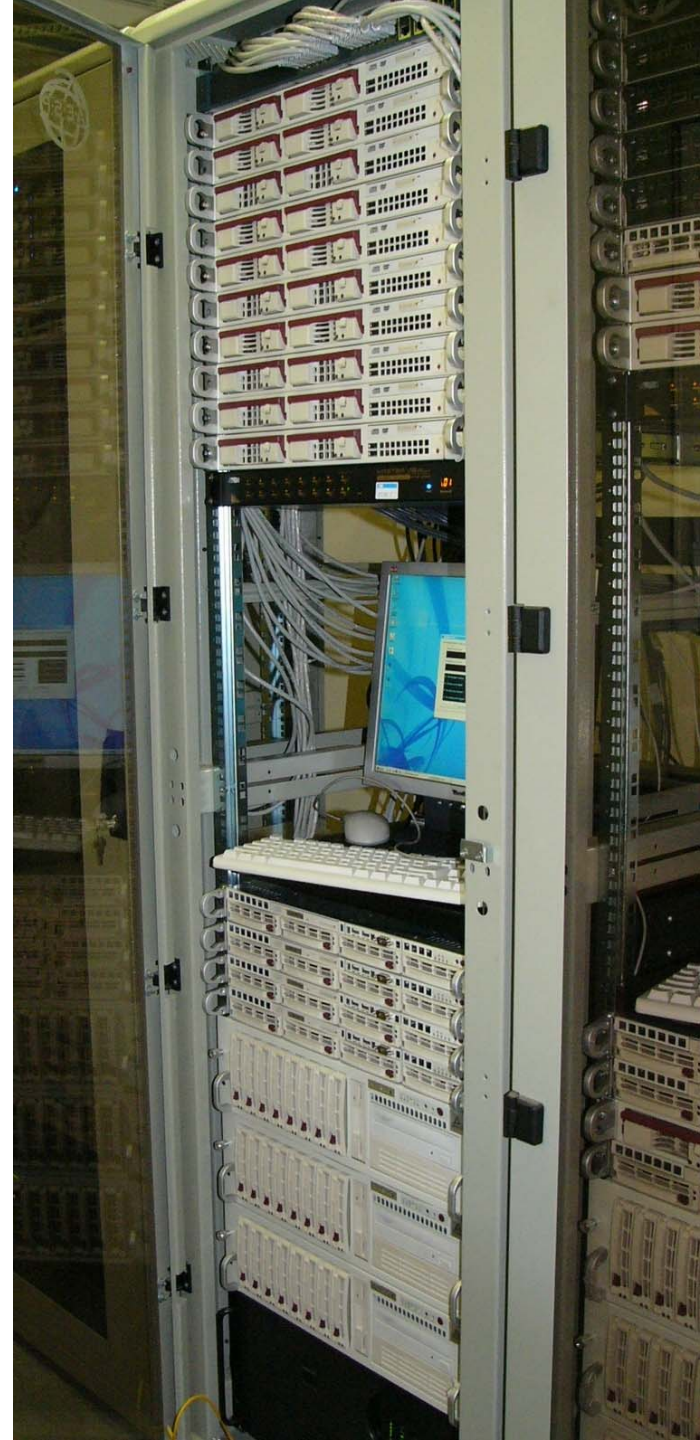
2 x SATA Raid 0,1/2x160G / LAN 1G

Lan GigEthernet

Cisco Catalyst 4506

Cisco Catalyst 2969G

OS: Scientific Linux 4.6, 5.2



Visualization

2 packages were used for visualization

VMD – freeware software for visualizing of modeling results of different programs including LAMMPS (can be improved using Tcl scripts). Works only with graphical interface, high quality visualizations [2].

GNUPlot – open source program for building 2D and 3D plots, works with graphical interface and command prompt, output in many popular formats (gif, jpeg, png etc.) [3].

Modelling of movement of a nanosize metal grain in argon (2 dimensions)

Problem: to model a movement of a metal grain in inert gas, to observe a track of the grain and a gas distribution in this track.

Note: The size of the grain and the free path of argon atoms are of the same order of magnitude, so we cannot use the usual principals of aero- or hydrodynamics in our case, we have to solve equations of molecular dynamics!

This is only a 2 dimensional model and computations are rather boring. The real problem is a 3 dimensional one, so it would require 100 times more time to compute it in the case considered.

System parameters

Medium: argon (Ar)

Free path – 750 Å

Temperature – 300 K

Pressure – 101 kPa

Atomic mass Ar – 39.948 g/mole

Number of atoms $\approx 550\,000$

Grain: nickel (Ni)

Diameter – 520 Å

Atomic mass Ni $m=4201.78$ g/mole

Grain mass: $M = 4.52 \cdot 10^{-18}$ g

Speed: 325-1625 m/s

Number of atoms ≈ 700

Model volume – orthogonal box, size 75000 by 30000 Å

Boundary conditions – periodical

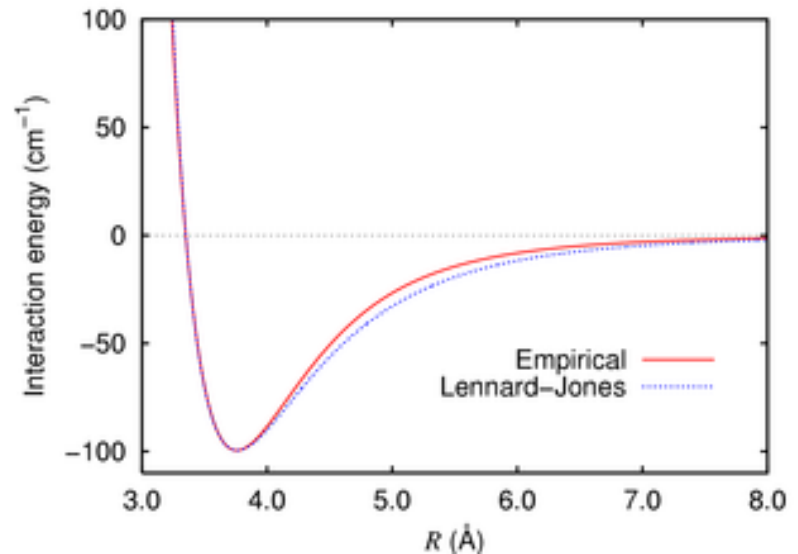
Note: Nickel atoms form not a grain, but a hollow sphere (for faster computing), that is why we introduce strange atomic mass. The mass of the sphere is equal to the mass of the grain. Atoms do not move with respect to each other, but travel as a whole in the direction of X axis.

Potential used for simulation

Lennard Jones potential describes interaction between argon atoms (Ar-Ar), between argon and nickel (Ar-Ni).

I.e. it holds for those atoms, that do not participate in chemical reactions.

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$



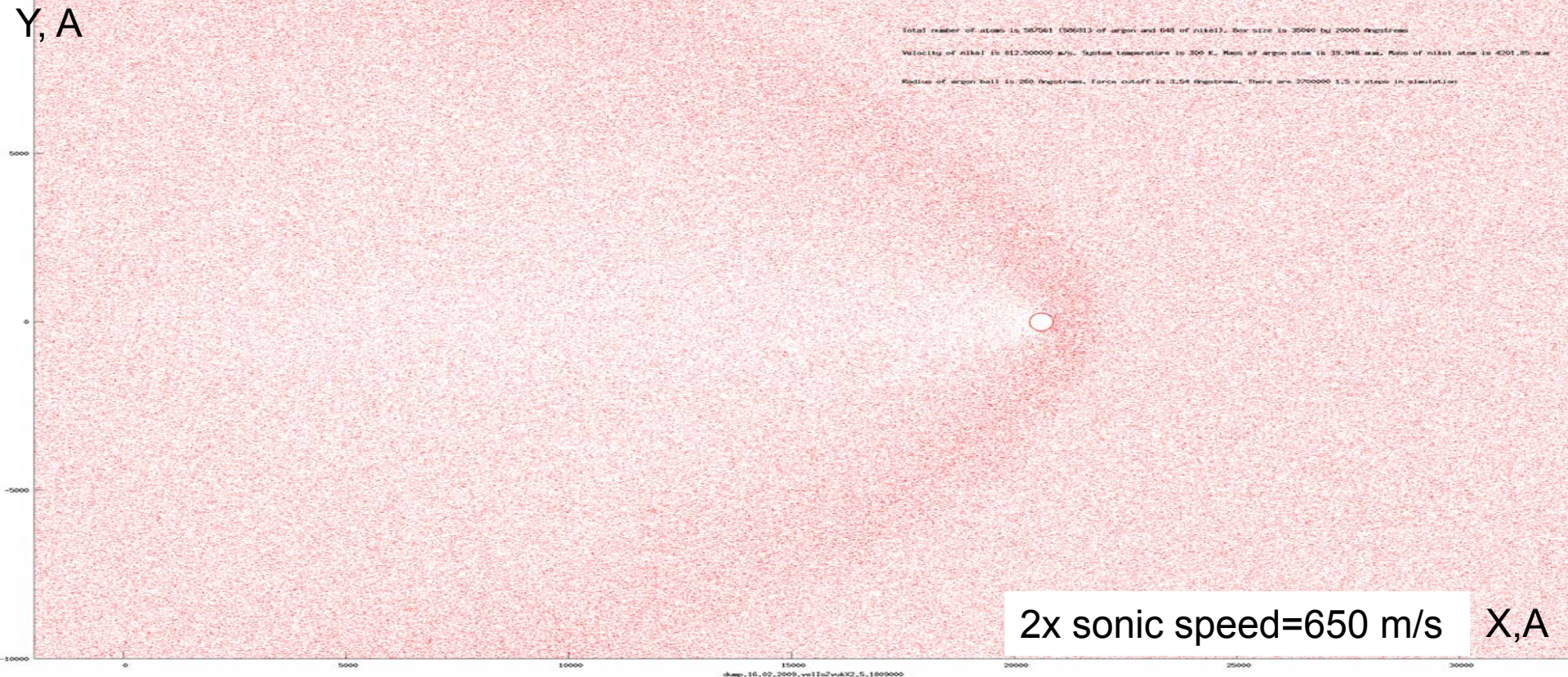
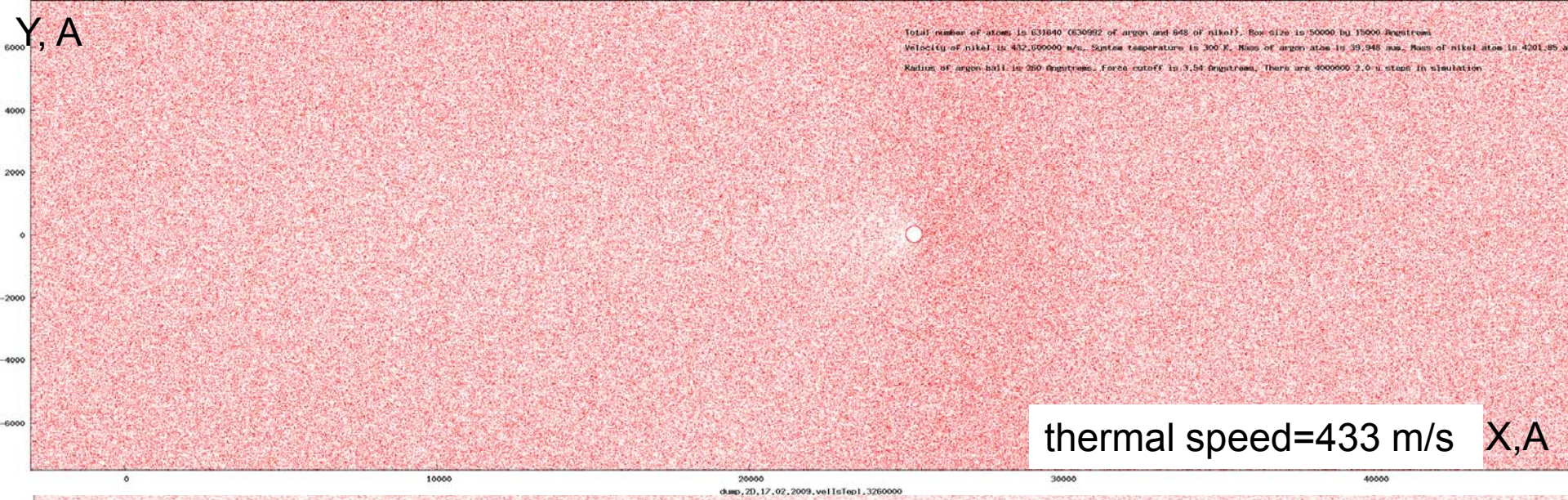
ϵ here is a characteristic interaction energy,

σ is a characteristic interaction distance.

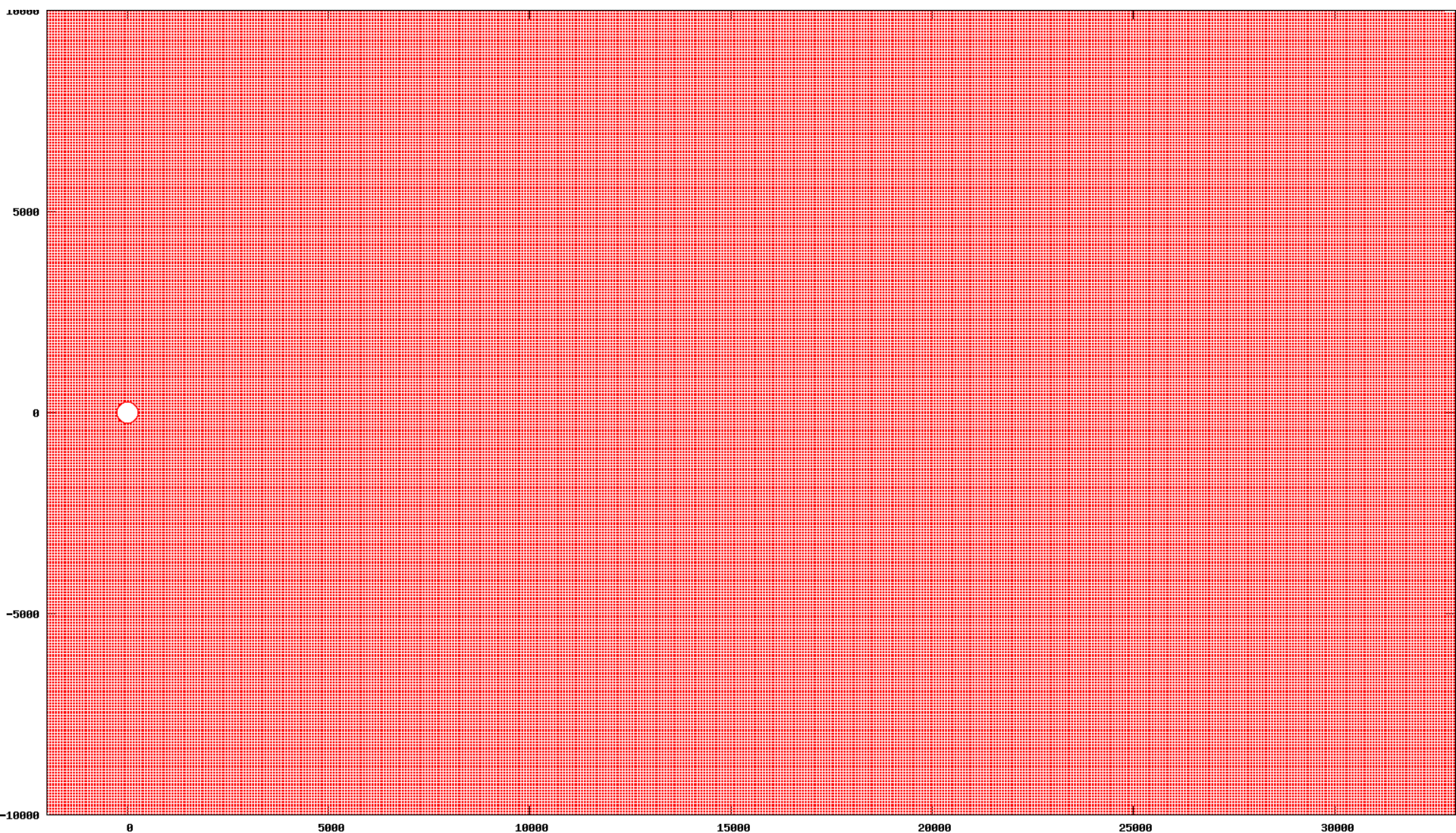
We use also a cut parameter - maximum distance where potential is crucial.

Potential parameters

- We use Lennard Jones potential:
 - Argon-argon interaction $\epsilon=0.185$ kcal/mole; $\sigma=3.54\text{\AA}$; $\zeta=3.54\text{\AA}$ [4];
 - Argon-nickel interaction $\epsilon=1.842$ kcal/mole; $\sigma=3.04\text{\AA}$; $\zeta=3.04\text{\AA}$ [5];
 - Nickel atoms are fixed with respect to each other
 - ϵ here is a characteristic interaction energy,
 - σ is a characteristic interaction distance.
 - ζ is a cut parameter.



Y, A



5x sonic speed=1625 m/s (moving)

X, A

Used resources, output and visualization

Computing time for a model with one grain speed value:
10 hours for 3.5 mln. steps, 1.5 fs each

Output data:

200 - 300 text files containing coordinates of atoms (one file per 10000 steps, one step in a file), 3.5 GB HDD space used.

Note: such output method was chosen because of output limitation of C language (2GB per one file on 32 bit processor)

Visualisation:

Gif images were produced by GNUPlot.

Although VMD is simpler and gives better pictures, it works only with graphical interface, so it was impossible to make pictures on a remote server (where output files were stored), and we used GNUPlot 4.2.

A bash-script was written to read a text file and draw gif images in GNUPlot (one image per a text file).

Creation of carbon chains from monatomic components (gas)

Problem: modelling of breaking covalent bonds in carbon molecules and creation of carbon chains on the basis of usage of AIREBO potential.

1. Modelling methane (CH_4) in a box
2. Modelling diamond
3. Creation of carbon chains from monatomic components (microcanonical ensemble)
 - 3.1 without buffer gas
 - 3.2 with buffer gas (argon)
4. Creation of carbon chains from monatomic components (canonical ensemble, fixed temperature)

Note: All these problems were computed in case of small systems (10 000 atoms) to test possibilities of computational methods.

For interactions with buffer gas usual LJ potential was used.

AIREBO (adaptive intermolecular reactive empirical bond-order) potential [5][6]

is used to model reactions between carbon and hydrogen.

This potential is called empirical, because almost all its components came from fitting experimental results and not from theory.

Here are some formulae:

$$E = E^{REBO} + E^{LJ} + E^{tors}$$

Bond-order part is a short-range potential and describes covalent bonds.

$$E_{ij}^{REBO} = V_{ij}^R(r_{ij}) + b_{ij}V_{ij}^A(r_{ij})$$

It consists of repulsive and attractive pairwise potentials. Indexes *i* and *j* correspond either to hydrogen or to carbon.

b_{ij} is a bond-order term. A variety of chemical effects that affect the strength of covalent bonding interaction are all accounted for in this term.

$$E_{ij}^{\text{LJ}} = S(t_r(r_{ij}))S(t_b(b_{ij}^*))C_{ij}V_{ij}^{\text{LJ}}(r_{ij}) + [1 - S(t_r(r_{ij}))]C_{ij}V_{ij}^{\text{LJ}}(r_{ij}),$$

$$V_{ij}^{\text{LJ}}(r_{ij}) = 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$

The LJ component consists of LJ potential and spline (S) and cosine (C) switch functions which depend on the distance between atoms and presence of neighbouring atoms. Switches make less or switch off LJ repulsion if a bond is created.

$$E^{\text{tors}} = \frac{1}{2} \sum_i \sum_{j \neq i} \sum_{k \neq i, j} \sum_{l \neq i, j, k} w_{ij}(r_{ij})w_{jk}(r_{jk})w_{kl}(r_{kl}) \times V^{\text{tors}}(\omega_{ijkl}).$$

$$V^{\text{tors}}(\omega) = \epsilon \left[\frac{256}{405} \cos^{10} \left(\frac{\omega}{2} \right) - \frac{1}{10} \right].$$

Torsional potential describes bond interactions, it depends on dihedral angle constructed by 4 neighboring atoms. It contains bond weights (cosine spline switches (w)) varying from 0 to 1.

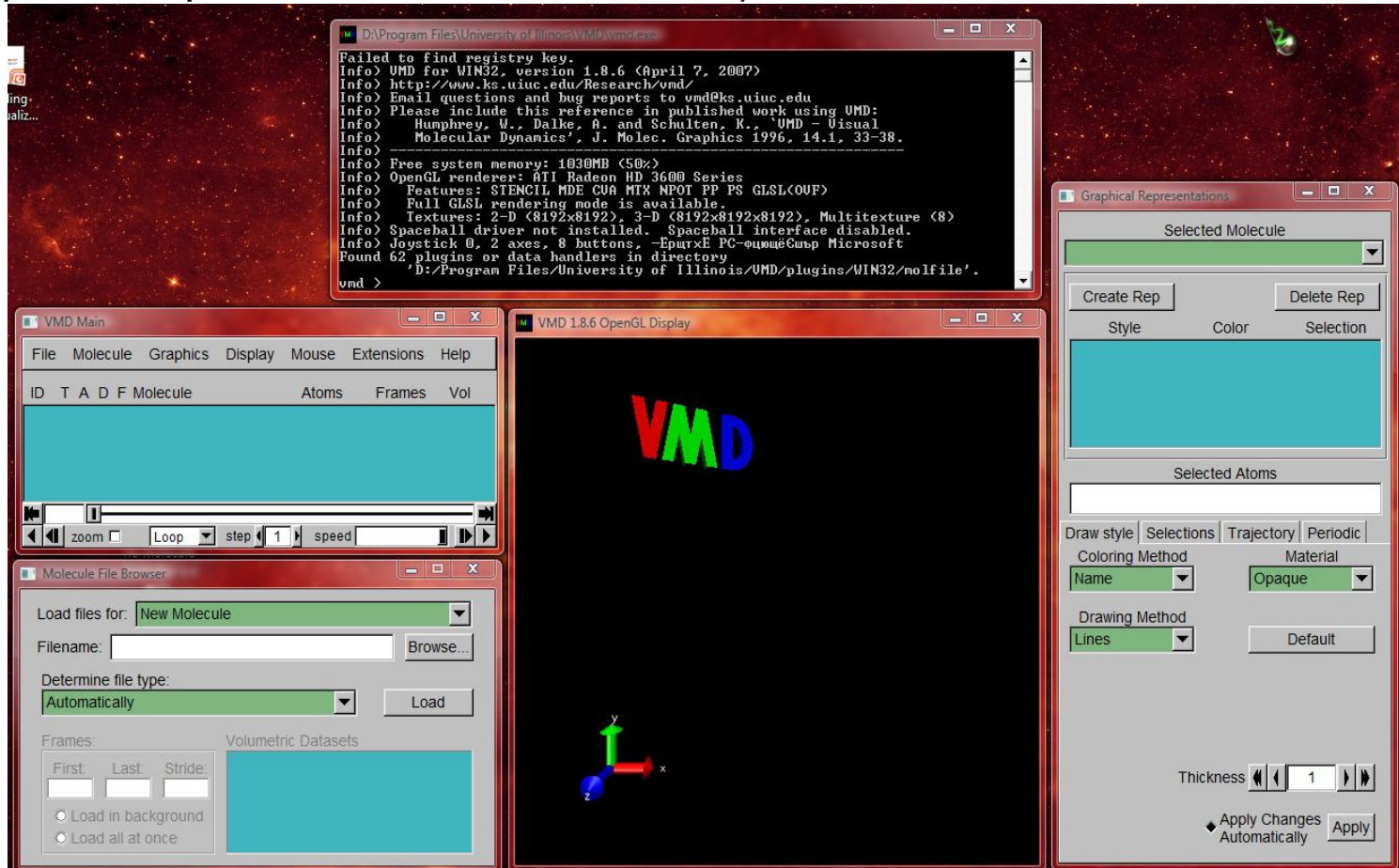
All switches are selected in a way to make the whole potential as smooth as possible during the creation and breaking of covalent bonds.

Used resources, output and visualization

Computing time: 15 min – 2 hours for 150 000 steps 1.0 fs each (depends on the number of atoms).

Output: one large text file (1.5 GB).

Visualization: for these problems VMD was chosen (much less atoms compared with a previous problem, hence one text file).

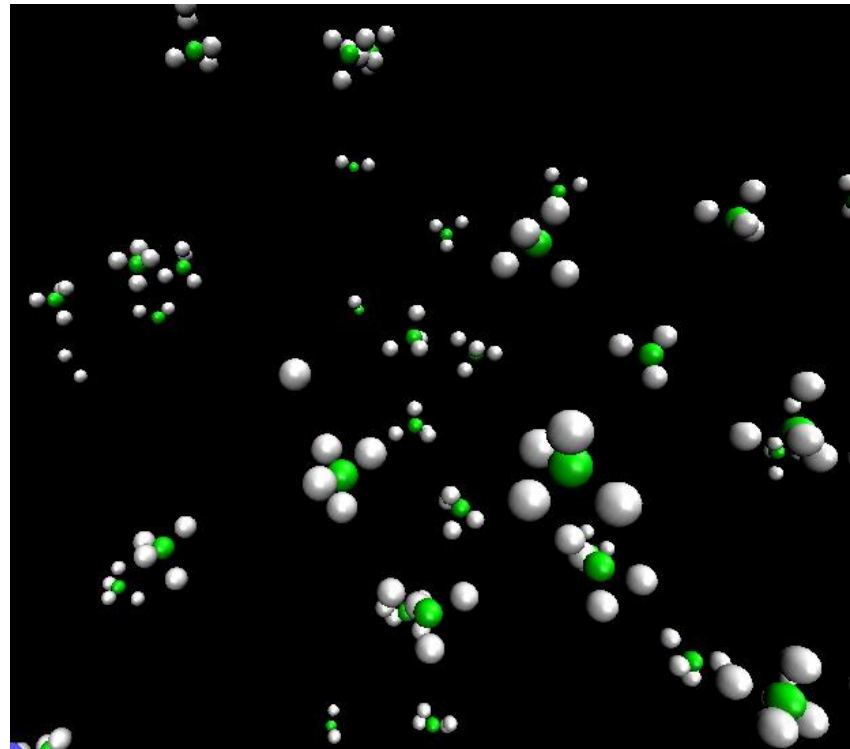
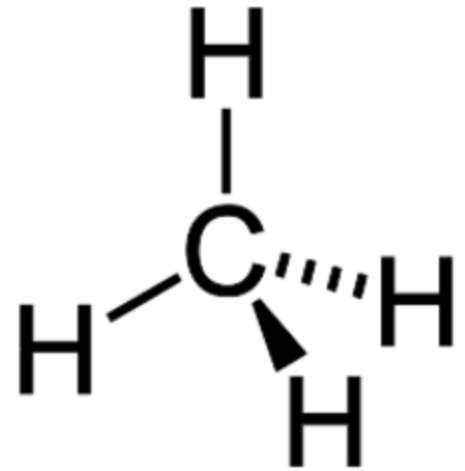


1. Modelling methane (CH₄) in a box.

Parameters:

- cubic box 100 Å
- pressure 4MPa
- temperature 300 K
- 512 molecules
- time 200 fs

[video](#)

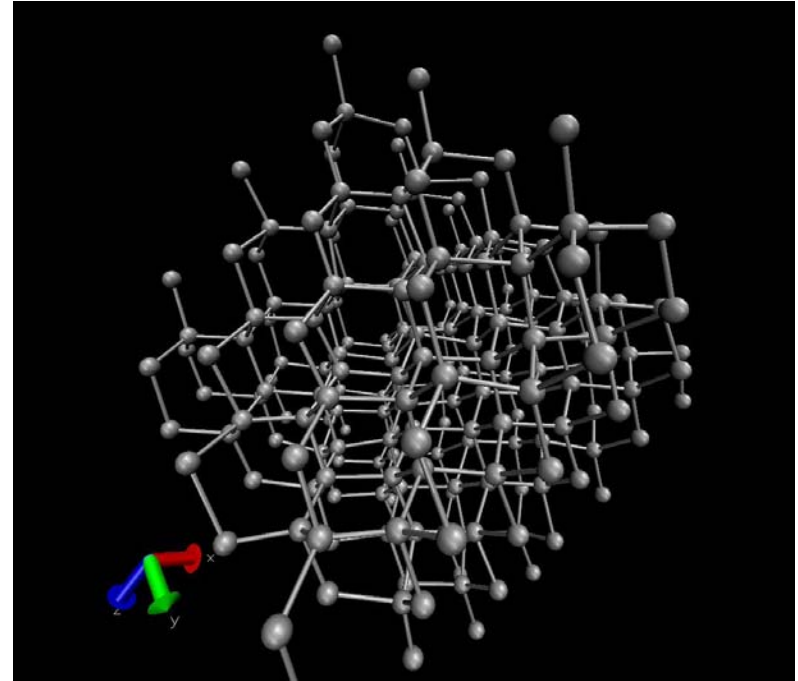


Diamond

Parameters:

- cubic box 10 Å
- lattice 3.35 Å
- temperature 300 K
- 216 atoms
- time 1000 fs

[video](#)



2. Creation of carbon chains from monatomic components (microcanonical)

2.1 without buffer gas

initial parameters:

temperature 100 K

760 hydrogen +760 carbon atoms

pressure 5 MPa

box – 80*40*40 Å

boundary – periodical

time – 150 ps

[video](#) [picture](#)

2.2 with buffer gas (argon)

initial parameters:

temperature 100 K

7260 argon +2904 carbon atoms

pressure 5MPa

box – cube 260 Å

boundary – periodical

time – 150 ps

[video](#) [picture](#) [picture](#) [picture](#)

Note: In these two simulations the total energy of the system is fixed. When new bonds are created, an extra energy is emitted, so the system is heated up.

If we have no energy receiver (buffer gas), the extra energy breaks bonds of neighbouring atoms, so the bonds are unstable.

Buffer inert gas receives extra energy hence the bonds are not breaking (they are more stable).

3. Creation of carbon chains from monatomic components with buffer gas (canonical ensemble, fixed temperature)

initial parameters:

temperature 100 K (fixed)

7260 argon + 2904 carbon atoms

pressure – 5MPa

box – cube 260 Å

[video](#) [picture](#) [picture](#)

Note: In this simulation temperature is fixed and energy is not, so the total system energy decreases.

Canonical ensemble computations are provided by special NVT (number of atoms, volume and temperature) fixing function in LAMMPS (it performs constant NVT integration to update positions and velocities at each timestep for atoms in the group using a *Nose/Hoover temperature thermostat*) [8].

Buffer gas is used here only as an atmosphere rather than a heat receiver.

Conclusion

1. A parallel version of LAMMPS was installed, investigated and adjusted on the computer cluster.
2. A proper software for visualization was chosen.
3. This software was used to solve applied problems:
 - A. Modelling of movement of a nanosize grain in a gas
 - B. Creation of carbon chains from monatomic components

This research will be continued and results will be applied to another problem in nanophysics

References

- [1] <http://lammmps.sandia.gov/features.html>
- [2] <http://www.ks.uiuc.edu/Research/vmd/>
- [3] <http://www.gnuplot.info/>
- [4] A perturbed Lennard-Jones chain equation of state for liquid metals.
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