Computer Simulating Movements of Atoms

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Introduction

Molecular dynamics (MD) is the study of movements of atoms and molecules using computer simulations.

When a ball is thrown in the air, its path through space and the forces acting on the ball are known. The path is deterministic, so there is only one possibility for where the ball will land given the initial conditions of the toss. Molecular movement is more random, but there are patterns within their movement that can be modeled.
This research models the movement over time by calculating the potential energy from intermolecular forces, and then computing solutions for Newton's equations of motion to find each atom's changing position and speed at each time interval. However, even today's computers are not fast enough to calculate all these interactions for millions of atoms at once, so lots of statistical techniques are used to remove unnecessary information and speed up processing time.

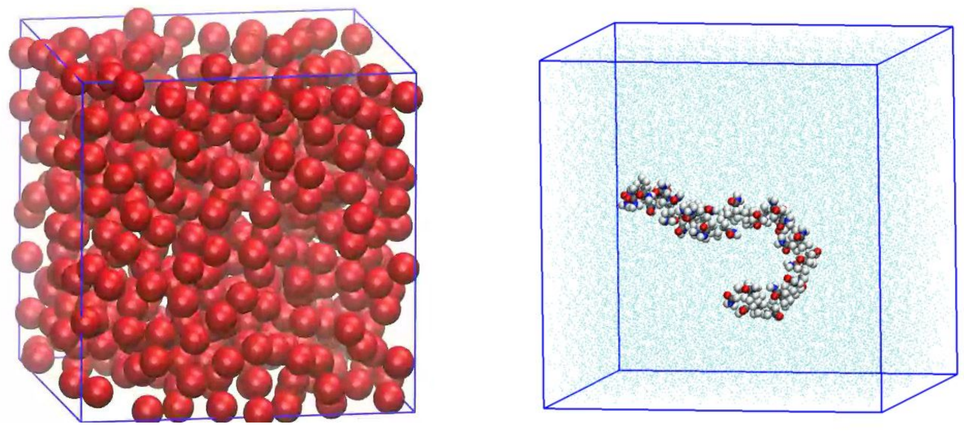
These microscopic interactions are responsible for macroscopic properties we observe in materials at the human scale. Computer simulations of atoms moving around can explain why materials have the properties they do, leading to the discovery of new drugs, more efficient fuels, improved nanomaterials, and a better understanding of the proteins, cells, and molecules that are critical for everyday life.

Materials and Methods

This project used the open source software LAMMPS to simulate the motion of noble gases (simple, inert systems of one atom), water molecules (multiple atoms with bond energy), and proteins under different initial conditions.

When a simulation runs, the atoms are changing position each time the model is looped over the next time interval, creating a path of the atom's movement called a trajectory. These trajectories were viewed in open source software VMD and OVITO, like a movie of the system developing.

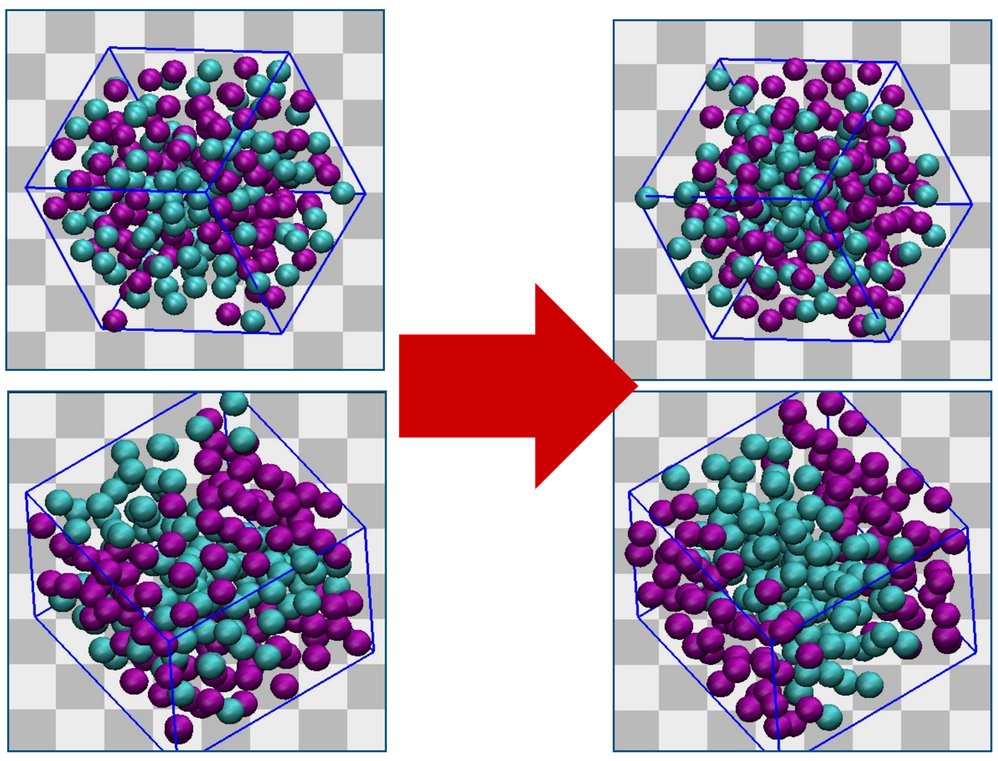
Simulations are calculating more than just trajectories. The potential energy from intermolecular forces (modeled as the Lennard-Jones Potential), kinetic energy, temperature, and other parameters can be analyzed or compared to experimental results to confirm a model's accuracy.



Demonstrations of molecular dynamics. On right is simulated Argon atoms in a box. On left is a simulated protein in a solvent. Image credit: Oak Ridge National Laboratory.

Results

Shown below are the first and final snapshots of two different atoms interacting inside a box. In the first row, the atoms start randomly distributed and remain diffused throughout the box at the end of the simulation. In the second row, the atoms were changed to prefer their own species. By the end of the simulation, the atoms were sorting into distinct regions of different particles. This is an example of how scientists can adapt the model to match experimental results.



Conclusions

This project showed it is possible to run complete MD simulations on a personal computer, opening up the possibility for observing atomic interactions in a high school classroom. Using free software on a base-model computer, multiple simulations were completed on models showing single atoms, bonded atoms, and proteins and their trajectories displayed.

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