Visualization of MD and MC Simulations for Atomistic Modeling

Joan Adler¹, Adham Hashibon¹, Nir Schreiber¹,
Anastasia Sorkin¹, Slava Sorkin¹ and Geri Wagner¹

¹Technion - Israel Institute of Technology, Haifa 32000, Israel

Abstract

We discuss the role of visualization in atomistic modeling, presenting arguments in favor and noting that visualization facilitates discussion with experimental collaborators and presentation. The MC and MD calculations made in the Computational Physics Group at the Technion include modeling of diamond/graphite systems and aluminium/alumina interfaces, as well as studying defects in copper and vanadium. Some examples of new physics results obtained with visualizations of simulation samples are given. Our new AViz package is introduced and examples of AViz' applications such as modeling the creation of interstitial defects in diamond, and the behaviour of a 50,000 atom drop of aluminium on an alumina surface are presented. Some tricks for enhancing 3D perception, such as highlighting atoms with changed coordination numbers and bonds as well as their implementation in AViz will be described. Visualization of spin systems is also possible with AViz, as is the preparation of animations and movies.

Key words: atomistic simulations, visualization, molecular dynamics, Monte Carlo

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1. Motivation for visualization in atomistic simulations

Visualization is essential for both development and presentation. In the debugging stages complicated solid structures and boundary conditions are best tested by the human eye. Once a simulation program is prepared and run, visualization of interim and final states helps understand what is happening within the sample and helps identify phenomena suitable for quantitative study. For experimental collaborators the visualizations provide a common language, and for discussion between collaborators and for presentation: "A picture is worth a thousand words". In addition to these research-related positive aspects of visualization, students with visualization skills and experience are always in demand for industry, and judicious use of visualization is a great way to grab the attention of undergraduate students, especially in service courses. For the MTV generation it is good to add a little activity into physics classes.

Arguments against visualization usually include "it is too expensive" or state that some individuals find three-dimensional visualization difficult to achieve or claim that the startup time and transfer time between students could be better used. As is described below we are making an on-going effort to address these valid but solvable objections.
2. Behind the AViz package

Two recent papers from our group describe our earlier routines for 3D visualization [1] and visualization over Internet2, methods of collaboration with experimentalists and our push-server [2]. We developed our present version of our (A)tomistic (Viz)ualization package as a result of trying to simplify our own research in atomistic and spin simulations, by maximising sharing within our group and minimising effort in transferring know-how and individual student start-up times.

There are lots of other excellent ways to visualize; but we found none that exactly suited our needs, which are for an interactive graphics system which is cheap both in terms of no software costs and requires minimal hardware support to run on each student’s desktop. We also need the option to switch between interactive and post-calculation viewing, 3D, efficiency at drawing large numbers of atoms and bonds and the ability to highlight selected configurations at will. We believe in (legally) free software and open source code-sharing. Hence AViz sources and instructions are freely available, under a GNU General Public License, copyrighted by Geri Wagner and Adham Hashibon [3].

3. Systems that we study and visualize

We use Molecular Dynamics (MD) and Simulated Annealing with both classical and tight-binding potentials and (if needed) ab-initio, and also model spin systems. Most projects are in collaboration with experimental groups at the Technion, and visualization is an important tool for exchanging information with and presenting results to our collaborators. We review here both older projects where we used our earlier visualization codes whose inconveniences provided motivation for the AViz package and and recent studies that were test beds for AViz. In many cases results were first “seen on the screen” and then qualitatively analysed. (We note that in none of the above projects it would have been possible to obtain results in such close agreement with experiment with simple potentials of the Lennard-Jones type.)

Materials that interest us include carbon [4-9]. In [4] we studied the formation of split interstitials, in [5] we studied the graphitization of larger areas of diamond under irradiation with multiple atoms, in [6] we considered sulphur as a potential dopant for n-type diamond and in [7] we used MD to simulate thermal stress at the (001) diamond surface. More details on [4,5] are given below in the context of AViz’ ease in implementing tricks for enhancing 3D perception, see also [8] where a diamond sample with an amorphous region inside is being studied with tightbinding MD to determine its band structure.

Sometimes visualization leads us into utterly unexpected scenarios. In [9] we used tight-binding molecular dynamics, inserting a hydrogen atom into diamond and watching where it went. To our total surprise it found a new type of interstitial site (which we called the ET (equilateral triangle site)) that does not occur for hydrogen in silicon.

Another system of interest is the ceramic metal interface, for example alumina/aluminium. Metal/ceramic interfaces such as these have important industrial applications, and can be viewed in electron microscopes, and we may (and do) compare our visualizations with electron micrographs of members of the group of W. Kaplan. We have used embedded atom [10] potentials for aluminium [11] and now are starting with [12] to implement improved potentials for aluminium alumina and copper/alumina. A drop of aluminium on an alumina (sapphire - aluminium oxide) must wet the surface in order to adhere, and this wetting is a complicated and delicate process. Initially [11] we used a model of aluminium atoms, some fixed in the locations of alumina atoms and some free to move in the alumina drop. We investigated density profiles near the surface as functions of crystallographic orientation and found direct correlations between amount of ordering and substrate orientation. Visualization was essential both for debugging the complex geometries and for identifying regions of order and disorder.

The influence of point defects on the melting temperature of copper and vanadium is another project in our group. Our experimental partner here is Emil Polturak and the initial experimental system was helium (where a dramatic decrease
in the shear resistance occurred just prior to the bcc-hcp transition). This led us towards more general questions on the relationship between defects and melting and eventually to simulations with a “tight-binding” potential in copper [13] to show that interstitials reduce the elastic coefficients while vacancies do not. We are now [14] using vanadium to test whether the results were material or lattice structure dependent and have found that simulated tempering is a useful algorithm for these systems.

4. AViz details

The hardware costs are minimal, AViz runs on a basic pentium + very little extra disk. The software costs are zero. There are a lot of tricks to enhance three-dimensional perception - rotation of still samples, change in relative sizes of atoms, animation, adding or removing borders, highlighting bonds, slicing samples that can help 3D visualization and change of perspective. AViz does all these from the interactive interface.

The AViz homepage [15] contains examples, sample datafiles and downloadable installation files (including rpm format for Linux Redhat 7 and source tar files for general UNIX) and a manual. Installation instructions (divided into parts for systems people and parts for individual users) as well as the sample files should minimise startup time. The datafiles are in a exceedingly simple ASCII format which includes at a minimum atomic type and x, y and z coordinates, with options for additional flags such as number of neighbours.

Once AViz is installed you can make your first visualization by downloading a sample datafile from our website (e.g. audrop.xyz which was generated by the code of [11] and contains 50,000 atoms), loading it thru the simple point and click interface and in 2 seconds you will see an image where each atom is represented by a dot. You can rotate this image and when you find a viewing angle that you like, you will be looking at something similar to Fig. 1 (where the colours were selected for a black and white figure from the “colors” option). Then press the “spheres” button and in 2 secs for low quality or another 8 secs for high quality you will view Fig. 2. All this for 50,000 (!) atoms in seconds on a 700MHZ laptop.

AViz can present visualizations of updates of a simulation in real time, using the -watch option and is also designed to create animations from a “filelist” of multiple .xyz files. By pressing either the “snap” button for a still or “autosnap” button for a series of snapshot .png files are created which can then be edited into a .mpg or video movie.

5. An example illustrating some tricks for 3D viewing

This example is based on the formation of interstitials [4]. Let us briefly review the physics behind this model. Carbon exists in two common forms - graphite and diamond. Graphite is a conductor and diamond an insulator. Graphite is soft and diamond is hard. When diamond samples are sufficiently damaged by irradiation, and then an-
nealed, they turn into conductors. Diamonds are used as insulators in industry; so if they are damaged and turn to conductors delicate equipment becomes useless.

We need to understand the damage process to know how to avoid it. Rafi Kalish and collaborators hypothesized that the irradiation damage followed by annealing turns diamond into graphite in small regions. At a sufficient concentration these regions percolate and make a conducting path thru the sample. To explore this further [4] we irradiated diamond samples with a single atom, and found that a single irradiated atom leads to a split interstitial defect. Previous ab initio studies had shown this to be the most stable defect, no one knew how it developed.

We identified this defect in the computer sample with visualization techniques. Specifically we highlighted the expected bond angles of different defects and a split interstitial just jumped out of the 5120 atom sample. (This was originally done with our older code, where each attempt to adjust the visualization required new programming and recompilation, in AViz all these enhancements can be entered interactively thru the interface.) Using color coding to highlight the three-fold coordinated atoms, we found substantial relaxation into this coordination near the place where one atom was displaced. The extent of this relaxation was a surprise. In Fig. 3 there is a snapshot from an animation of the irradiation process, made with AViz. To understand this better you may look at a colored version [16]. The color coding draws attention to the area where the action is, and presenting the bonds helps in depth perception. Rotating the samples also aids depth perception.
6. Spin Visualization

For studying two-dimensional Ising models, simple black/white colored squares give adequate visualization possibilities, and for Potts models or Ising models in three dimensions colored spheres could be used. But, for the study of spin dynamics, visualization of spins that can orient in three dimensions is very useful. The animation and rotation features of AViz enable us to view from all directions as the waves and perturbations pass thru the spins [17].

7. Summary

Visualization helps debugging, understanding and presentation and is very good for sharing results with experimental collaborators. Visualization of atomistic simulations can be cheap and easy. Options such as highlighting bonds and slicing samples thru the AViz interface aid in 3D visualization.

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References