

3d visualization of atomistic simulations on every desktop

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Abstract.

Once upon a time, after making simulations, one had to go to a visualization center with fancy SGI machines to run a GL visualization and make a movie. More recently, OpenGL and its mesa clone have let us create 3D on simple desktops (or laptops), whether or not a Z-buffer card is present. Today, 3D a la Avatar is a commodity technique, presented in cinemas and sold for home TV. However, only a few special research centers have systems large enough for entire classes to view 3D, or special immersive facilities like visualization CAVEs or walls, and not everyone finds 3D immersion easy to view. For maximum physics with minimum effort a 3D system must come to each researcher and student. So how do we create 3D visualization cheaply on every desktop for atomistic simulations? After several months of attempts to select commodity equipment for a whole room system, we selected an approach that goes back a long time, even predating GL. The old concept of anaglyphic stereo relies on two images, slightly displaced, and viewed through colored glasses, or two squares of cellophane from a regular screen/projector or poster. We have added this capability to our AViz atomistic visualization code in its new, 6.1 version, which is RedHat, CentOS and Ubuntu compatible. Examples using data from our own research and that of other groups will be given.

1. Introduction

Our group carries out atomistic simulations in carbon systems, with an emphasis on geometric structure and vibrations, especially near defects and interfaces. We need to observe the system development, and are often concerned with the structure deep inside the sample, which may not be accessible to non-destructive experiment. Analog models are helpful for gaining insight into 3D structures, but it is hardly practical to construct precise analog models for each timestep frame of a simulation. The next best is a 3D stereo visualization.

We will introduce anaglyphic stereo in the next section, our AViz code in the following one, and conclude with a description of the new AViz 6.1 and some sample results.

2. Anaglyphic stereo

Let us review two early stereoscopic computer visualization approaches: one is the 1965 ORTEP (Oak Ridge Thermal-Ellipsoid Plot Program) software [1, 2] that drew two stereoscopic images using a plotter (predating laser printers and inkjet printers) that were placed side by side in a system with two lenses. One relaxed the focus of ones eyes till they came into a view with depth perception. A single frame of two ORTEP plots from our group's research (M. Sc thesis of A. Silverman [3]) is shown in Figures 1 and 2. The sample shown on the left is of crystalline

silicon and in the center there is an image of an amorphous silicon sample, created from the crystal via a melt and quench using molecular dynamics. The opportunity to see the amorphous structure that would have been hard, if not impossible, to achieve with an analog model was exhilarating way back then, with or without the stereo implementation. This approach was popular for molecules, but the limited number of atoms meant that for simulations of solids, it was not practical. (We were able to draw only 78 atoms of our 216 atom sample). The size restriction of many chemical visualization programs continued to be limiting for applications to solids for a long time.

The second stereo example is the anaglyphic process which uses simple colored glasses or two squares of cellophane. An example of this method is the image of a random walk on a sphere, shown in Figure 3. This was drawn with a FORTRAN/PGPLOT code written in 1993 as part of a graduate Computational Physics class project by Dimitry Gangardt, based on an article by J.C. Sprott[4]. Sprott's original code, was presented in BASIC and won the first annual Computers in Physics Software award. Viewing this and similar anaglyphic images without the two-colored glass shows some red and cyan lines. Unfortunately while showing depth clearly this specific implementation removes the possibility to use color in the images and thus an important route to information is missed.

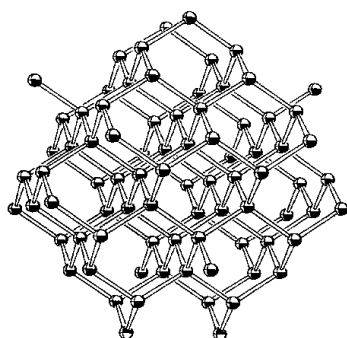


Figure 1. Crystalline silicon with ORTEP.

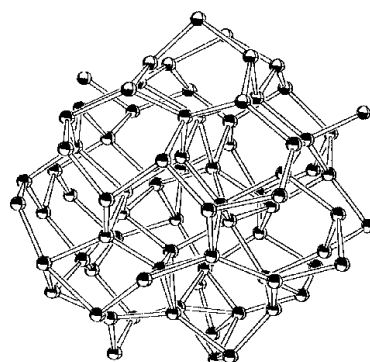


Figure 2. Amorphous silicon with PGPLOT.

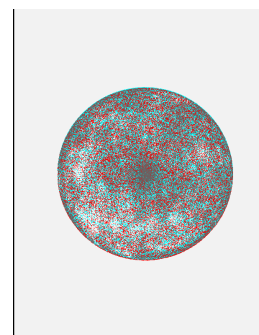


Figure 3. Anaglyphic random walk with PGPLOT.

3. AViz basics and history

With no apology, AViz [5, 6, 7] was created in 2001 to meet the visualization needs of the Technion Computational Physics Group, within an opensource, LINUX/HPC oriented framework. There are other systems that could probably supply some of these, and we recommend that everyone uses what suits them. Our visualization needs are many, but the most important requirement from the start has been for cheap, legal, 3D visualization on every group member's desktop, with a system that is robust to the graduation of an individual student. Interactive or postprocessing options, and a way to prepare movies for presentation are also desirable.

There have been three main releases. Original AViz, (4.6, for Red Hat 7.0) prepared by G. Wagner and A. Hashibon, for which A. Sorokin wrote the manual, was replaced by AViz 5.6 in 2002 with an improved interface. Various additional features (sequential polymers etc) were added to specific implementations, and in 2011, Y. Koenka and A. Silverman prepared AViz 6.0 with several major updates and features from the specific implementations[8]. The newest version, described below, is called AViz 6.1 and has been shown to be compatible with Ubuntu, CentOS, and Red Hat Enterprise.

The underlying methodology of all versions is as follows: prepare a data file of atomic site types and locations (or a set of datafiles called a filelist), tune the visualization with the buttons on the interface, and record a set of images. Tuning includes manipulation thru space, changing the size of objects or connecting them with “bonds” or adjusting color or lighting. There is a wide selection of websites giving instructions and examples for specific features. Much of the effort has come from undergraduate course or final projects, where preparation of a website presenting the project has been one of the requirements. A project of consolidation of the explanatory material is now underway.

4. AViz 6.1

The first stereo AViz was prepared by H. Zilken in Juelich. This version was very exciting, but the hardware rendering, projection and manpower demands were not feasible to reproduce at the Technion in even a single realization. This may be possible in the future, but since we are making visualizations for High Performance Computing (HPC) atomistic simulations, in recent months we have focused on creating a hardware environment for parallel HPC, and could not find resources for a powerful visualization system as well. Such a powerful system is not possible for every desktop, and the most effective way to ensure researchers visualize is to enable them to do so from their desktops. Our need for improved 3D insight has become stronger than ever and so we returned to the older style anaglyphic stereo.

AViz 6.1 [9, 10] has incorporated the possibility of Stereo Vision (SV), and although more than two colors are possible there remains some color washout, depending on color selection. SV works by showing a different image to each eye, thus creating the illusion of a 3D image. The SV images generated by AViz, such as those in this paper, are best viewed using red-cyan anaglyphic glasses, Figure 4, or two squares of red (left eye) and cyan (right eye) cellophane. For quick viewing, a cardboard frame of approximately 14 by 5 cm with two 3.5 by 2.5 cm holes whose centers are about 6cm apart, over which cellophane is stuck, can be easily constructed.

In order to operate the SV abilities, 3 buttons in the shape of stereoscopic glasses were added in the bottom of the right hand toolbar of the main AViz viewing window. In order to enable/disable the SV mode, press the “Enable/Disable” button, as shown in Figures 5 (enabled) and 6 (disabled). It is easily seen (even if this paper is printed in black and white) that in the enabled case of Figure 5 there is a double frame and (cyan/red) bleeding from the spheres that is not present in Figure 6. Readers who are viewing this in black and white are recommended to refer to the color versions of the images that can be found together with animations at the website[10]. These images can be enlarged for easier viewing.



Figure 4.
Two-color
glasses.

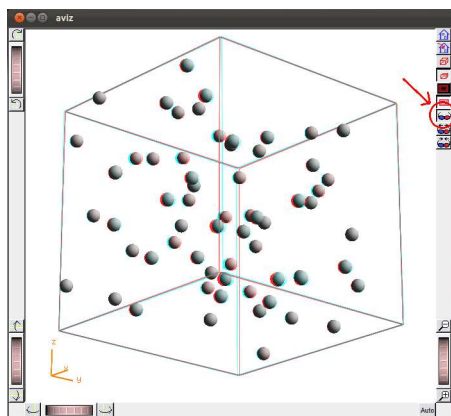


Figure 5. AViz 6.1 interface with
stereo enabled.

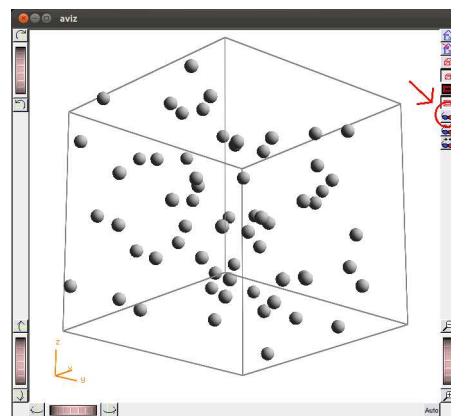


Figure 6. AViz 6.1 interface with
stereo disabled.

In order to achieve a proper prediction of how the model would look for each eye, the parameter of the distance between the two eyes, known as the pupillary distance (PD), needs to be set. In reality the PD is almost fixed for everyone, but since the models shown in AViz are re-scaled to fit the screen, the pre-configured PD may not be right for all models. Therefore, the 2 buttons may be pressed continuously to increase/decrease the PD as a function of time, and to increase/decrease the 3D effect.

Links to the source code as well as installation instructions for several Ubuntu, RedHat, and CentOS versions of LINUX can be found on the AViz 6.1 website[9]. On this site some animated 3D movies can also be viewed.

5. Results

A selection of still stereo realizations are given in Figures 7-9. Figures 7 and 8 show two different views of a nanotube. The third figure presents data from an off-label implementation of AViz 6.1, [11] extending our visualizations of the electron density of a hydrogen atom to the stereo case.

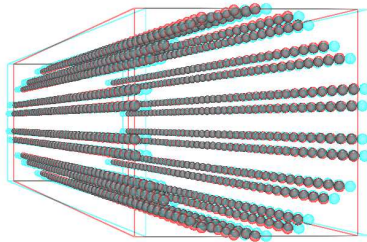


Figure 7. Nanotube side-view.

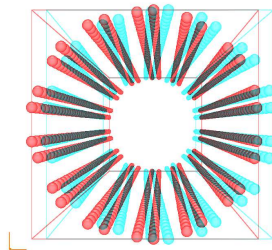


Figure 8. View along the axis of a nanotube.

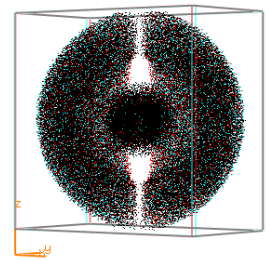


Figure 9. Orbital electronic density of the (3,1,0) state of the hydrogen atom.

The next set of images, in Figures 10 -12, use the dataset for the split interstitial published in [7, 8], but the center one shows a larger number of atoms in order to provide relative bond thicknesses. In [7] and [8], instructions are given for visualizations of this dataset with earlier AViz implementations using different colors (AViz 5.6) and different bond widths (AViz 6.0) respectively. The new image was prepared as described above. It shows that a substantial amount of color is retained. The final image, Figure 13, shows some 5120 atoms of an implanted diamond sample[12].

Acknowledgments

We thank H. Zilken of Juelich for developing the first stereo AViz, and the Juelich-Technion-Aachen Umbrella project for enabling our collaboration. The new code was written as an undergraduate project by D.P. based on earlier visualizations by previous members of the Computational Physics Group at the Technion. Some of the data used in the testing of AViz 6.1 was generated by researchers and students at CiNaM, CNRS, Marseilles and J. A. thanks A. Saul for hospitality there. We also thank R. Kreiselman and Y.Katz for assistance in clarifying and enhancing the installation instructions.

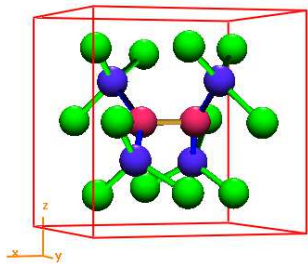


Figure 10. Split interstitial from [7] using color for differently coordinated atoms and the bond between them.

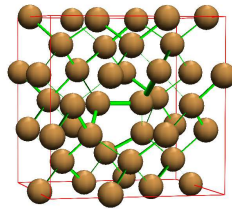


Figure 11. Split interstitial from [8] with variable bond thickness.

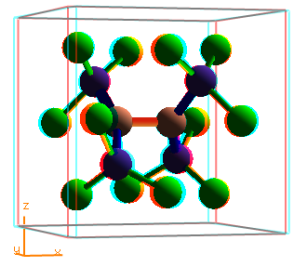


Figure 12. Split interstitial from AViz 6.1 showing that this type of anolyglyphic stereo can retain much of the color.

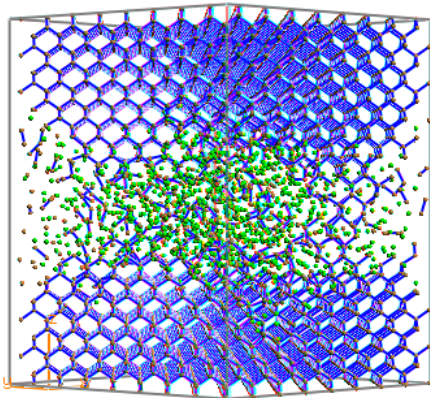


Figure 13. Stereo rendering of data from [12] of an implanted diamond sample modelling creation of a diamond membrane, showing some 5120 atoms.

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