



27th Annual CSP Workshops on “Recent Developments in Computer Simulation Studies in Condensed Matter Physics”, CSP 2014

A “Rosetta stone” for AViz

Joan Adler^a, Hila Glanz^a, Nadir Izrael^a

^aPhysics Department, Technion -IIT, Haifa, Israel, 32000

Abstract

The Computational Physics group at the Technion has developed a visualization code, AViz, for atomistic visualization. AViz can visualize atoms, vector spins, quadrupoles, electronic densities, polymers and more. The required input of data files in the standard .xyz format can be prepared from a wide range of private and public domain simulation codes; and in the event that these are not the natural output of the code, conversion can be made. In order to extend its use, especially for industrial simulations, it is highly desirable to simplify the translation from simulation output to visualization input. We describe some steps towards the goal of providing a “Rosetta Stone” for such translation that can lead to better understanding. A recent simulation of liquid crystals is used as an example.

© 2014 The Authors. Published by Elsevier B.V. This is an open access article under the CC BY-NC-ND license

(<http://creativecommons.org/licenses/by-nc-nd/3.0/>).

Peer-review under responsibility of The Organizing Committee of CSP 2014 conference

Keywords: simulation, liquid crystal, visualization

1. Introduction

The triumph of the Rosetta stone is that three languages - ancient Greek, Demotic (an Egyptian language) and Hieroglyphics, provide the same message on a single stone. The Greek is easy to understand, the Demotic (an old Egyptian language) intermediate and the Hieroglyphics was incomprehensible, until then. This is analogous to a visualization being easy to understand, the simulation itself intermediate, and a direct statement of a model or its Hamiltonian somewhat incomprehensible. The issue with AViz is that simulations can be made and understood via their visualizations, but translating the simulation outputs into AViz inputs has until now been more than a little haphazard. Even if a dedicated code with AViz output can be written that outputs data into the desired .xyz format, researchers often want to use strong public domain codes such as LAMMPS or QUANTUM ESPRESSO. These simulations are efficient but their output formats can be confusing.

As part of the EU FP7-NMP (Nanosciences, nanotechnologies, Materials and new Production technologies) initiative a major effort to simplify execution of and understanding from simulation tools for use in an industrial environment is being made. Use of simulation tools is often hampered by a steep learning curve unlikely to be adopted in an industrial setup. The lack of coherent standardized simulation frameworks leads to an unnecessary waste of resources and are a barrier to the broader use of nano-scale simulations. In the FP7-NMP-SimPhoNy project, researchers at the

* Corresponding author. Tel.: +97248293937 ; fax: +97248295755.
E-mail address: phr76ja@tx.technion.ac.il

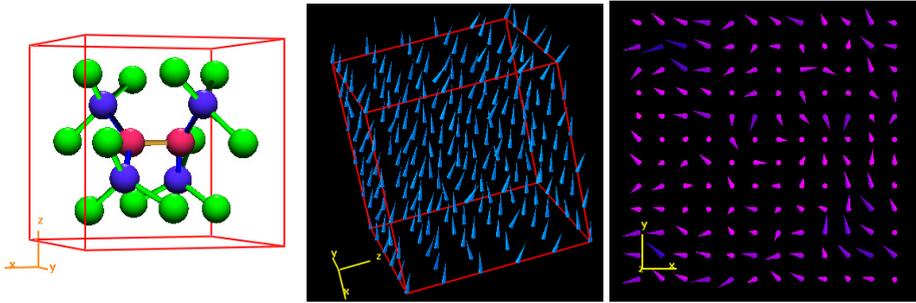


Fig. 1. Far left, from Adler (2003) and Adler *et al.* (2011a) and right, from Hihinashvilli *et al.* (2004) are images drawn from the two datafiles presented in part in the text, the central frame also from Hihinashvilli *et al.* (2004), is from a three dimensional spin simulation.

Technion, and several European Universities and Institutes will prepare a unified environment for such simulations. The Technion part will include python interfaces to their AViz visualization package for both atomistic and electronic density simulations. We have also taken steps, AViz (2013), to improve the ease of installation and implementation.

2. AViz in brief

Our original AViz vision (Adler (2003)) was 3D animation on every graduate student desk, and the code was designed for efficiency and a wide range of options. AViz datafiles are in a simple ASCII format. The first row is an integer number of atoms. The 2nd row is a comment to identify the file. The remaining rows have, at a minimum, atomic type and x , y and z coordinates. The first few lines of the data file for the split interstitial defect (Figure 1, Adler *et al.* (2011a)) are:

```
42
Split interstitial
J 5.3012 5.29852 7.09405 9
H 6.16665 6.12665 8.05686 7
J 5.25262 7.05947 5.22232 9
H 6.17108 8.1017 6.13538 7
J 5.2896 7.08316 8.92685 9
```

In this case the initial letter indicates an atomic type which depends on the number of neighbors of the atom (and of its neighbours) but it is more usually just the atomic species. The bonds are added via the AViz interface for specific distance ranges with their color dependant on the atomic types. This is important for situations where defects distort bond length rather than the simple “one length fits all” prescription of some chemical visualization codes choice of bond lengths.

3. AViz vizualizations for diverse models

AViz has capabilities far beyond simple atomic systems. Options include additional flags such as number of neighbours or the spin direction if the object is a vector spin. Some of the additional rows require additional calculations post simulation. An example of 6 out of 144 rows of a datafile for vector spins prepared for the 2004 CSP workshop, from Hihinashvilli *et al.* (2004), is shown; this is for the rightmost image of Figure 1.

```
144
# 12x12 Heisenberg ferromagnet
Sp 1.0000 1.0000 1.0000 -0.5489 0.2497 0.7978
Sp 1.0000 2.0000 1.0000 -0.5951 0.2954 0.7474
```

```
Sp 1.0000 3.0000 1.0000 -0.4631 0.1305 0.8767
Sp 1.0000 4.0000 1.0000 -0.5206 0.0163 0.8536
```

Other objects that can be represented are cylinders (quadrupoles or liquid crystals from Adler and Cohen (2010)) and atoms joined in a chain such as polymers, from Shyuv (2006).

4. Transforming simulation output into AViz input

If the code producing the data is entirely self-written it is straightforward to output the additional information direct to the AViz input files. If this is not the case, and especially if it is a “canned” code that outputs in specific formats, wrappers must be written to make the required conversions. Selected existing wrappers are listed in the next two subsections; they work, but are in an unwieldy collection of languages.

4.1. Electronic density

- As presented in Adler *et al.* (2007), the first attempt to use AViz to visualize electronic density was made to show orbitals of the hydrogen atom. These are based on its exact solution (in polar coordinates), expanded in MATHEMATICA, converted to a rectangular grid, where the value of each grid point was expressed with dots whose number was based on the density value, located randomly in the volume of the grid point and whose color was loosely binned. The MATHEMATICA code gave output in the form of AViz .xyz files.
- This was extended by Or Cohen in Adler *et al.* (2011b) for simple atoms and molecules where the density was calculated with PCGAMESS (Firefly) and a C# code was used to prepare AViz input files.
- The next development was made with the cooperation of Valentino Cooper who kindly calculated the electronic density around a nanotube from our strained nanotube coordinates from Pine *et al.* (2014) with QUANTUM ESPRESSO at Oakridge National laboratory. The wrappers to transform this output to AViz input were written at the Technion in FORTRAN.
- A calculation made last year by Meytal Krief, reported on in Adler *et al.* (2014), extended the hydrogen atom calculation to use Dan Peled’s (Peled *et al.* (2013)) analoglyphic stereo. Her study contains simplified and improved MATHEMATICA instructions.

4.2. Atomistic applications

- The oldest wrapper programs date from the beginning of AViz when FORTRAN codes were written to transform the data formats of the visualization codes (Vi3d) we used at that time into the current .xyz format. They are downloadable from the AViz website, Wagner and Hashibon (2001). The program includes writing the characters needed to label the atoms.
- C++ code wrappers used for LAMMPS to AViz in student project by Koren Schrieber in Adler *et al.* (2014).
- Pavel Aharonov carried out a Computational Physics class project on transferring AFM images to AViz. The AFM output was in hdf format and he wrote a C++ code to transform to AViz .xyz input, Aharonov (2005). hdf output can be obtained from many of the codes which we plan to use, thus this will be extended to hdf5.
- A notable atomistic application is presented in Mazvovsky *et al.* (2012) which provides fortran code to create nanotubes and output .xyz files ready for visualization.

5. A new AViz implementation for Liquid Crystals

Our RBNI Nanotechnology Institute had a visit by Professor Shunsuke Kobayashi, (Kobayashi *et al.* (2013)) from Japan, who spoke about how colloids could change the optical and electrical properties of liquid crystals This phenomena may be relevant for Liquid crystal television screens. AViz had a liquid crystal option, (proposed by Mike Allen, quite a while ago) that had been used for quadrupole simulations, but never for liquid crystals. There is an extensive literature, see Antypov and Cleaver (2004), on simulations of liquid crystal defects surrounding colloid impurities, but less information about the affect of colloids on liquid crystal conductivity issues. In addition, it has become clear

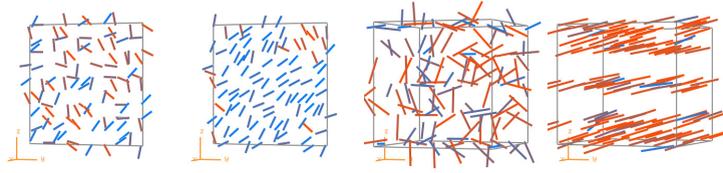


Fig. 2. Far left to far right images from the Liquid crystal simulations of an initial disordered 2d liquid crystal, and low temperature 2d ordered phase, then of an initial 3d disordered phase and a final 3d ordered phase.

that very few of our Technion physics students know much about liquid crystals, as they had not been part of any of our courses. Thus an educational project about simulations of liquid crystals in their own right as well as a prelude to simulations of the electrical properties with colloids began. We have prepared websites, Glanz-Izrael (2013), that present a simulated annealing codes for liquid crystals, and include an AViz visualization option. Looking towards python wrappers for AViz, this project was carried out entirely in python. The code can also be used for simulating similar systems including Ising or Potts models; in general dimension.

The Gay-Berne (GB, a generalized Lennard-Jones (LJ) potential for anisotropic potentials, Gay and Berne (1981)) is used. The usual LJ potential is:

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

where σ , the separation of the particles when $U_{ij} = 0$, is also known as the collision diameter and ϵ is the depth of the potential well at the minimum in U_{ij} . The molecules of the GB system have translational and orientational degrees of freedom. The potential is given by

$$U_{ij}^{GB} = 4\epsilon_0 \left[\epsilon(\hat{u}_i, \hat{u}_j) \right]^{\nu} \left[\epsilon'(\hat{u}_i, \hat{u}_j, \hat{r}_{ij}) \right]^{\mu} \times \left[\left(\frac{\sigma_0}{r_{ij} - \sigma(\hat{u}_i, \hat{u}_j, \hat{r}_{ij}) + \sigma_0} \right)^{12} - \left(\frac{\sigma_0}{r_{ij} - \sigma(\hat{u}_i, \hat{u}_j, \hat{r}_{ij}) + \sigma_0} \right)^6 \right]$$

where σ , the intermolecular separation at which the attractive and repulsive terms cancel is now:

$$\sigma(\hat{u}_i, \hat{u}_j, \hat{r}_{ij}) = \sigma_0 \left[1 - \frac{\chi}{2} \left\{ \frac{(\hat{r} \cdot \hat{u}_i + \hat{r} \cdot \hat{u}_j)^2}{1 + \chi(\hat{u}_i \cdot \hat{u}_j)} + \frac{(\hat{r} \cdot \hat{u}_i - \hat{r} \cdot \hat{u}_j)^2}{1 - \chi(\hat{u}_i \cdot \hat{u}_j)} \right\} \right]^{-\frac{1}{2}}$$

The shape anisotropy parameter χ is $\chi = \frac{\kappa^2 - 1}{\kappa^2 + 1}$, $\kappa = \sigma_{ee}/\sigma_{ss}$ and σ_{ee} (σ_{ss}) are the separation(s) when the molecules are end to end (side by side). The depth of the well is expressed as $\epsilon(\hat{u}_i, \hat{u}_j, \hat{r}_{ij}) = \epsilon_0 \epsilon^{\nu}(\hat{u}_i, \hat{u}_j) \epsilon'^{\mu}(\hat{u}_i, \hat{u}_j, \hat{r})$ where $\epsilon(\hat{u}_i, \hat{u}_j) = \left(1 - \chi^2 (\hat{u}_i \cdot \hat{u}_j)^2 \right)^{-\frac{1}{2}}$ and

$$\epsilon'(\hat{u}_i, \hat{u}_j, \hat{r}_{ij}) = 1 - \frac{\chi'}{2} \left\{ \frac{(\hat{r} \cdot \hat{u}_i + \hat{r} \cdot \hat{u}_j)^2}{1 + \chi'(\hat{u}_i \cdot \hat{u}_j)} + \frac{(\hat{r} \cdot \hat{u}_i - \hat{r} \cdot \hat{u}_j)^2}{1 - \chi'(\hat{u}_i \cdot \hat{u}_j)} \right\}$$

The parameter χ' is related to the anisotropy in the well depth via

$$\chi' = \frac{1 - \kappa'^{\frac{1}{\mu}}}{1 + (\epsilon_{ee}/\epsilon_{ss})^{\frac{1}{\mu}}}$$

where $\kappa' = \epsilon_{ee}/\epsilon_{ss}$ is the ratio of well-depth for end to end to side by side. \hat{u}_i and \hat{u}_j are the orientation vectors of the two molecules, r_{ij} is the vector joining the two centers, \hat{r}_{ij} is the unit vector and ϵ_0 and σ_0 are scaling parameters.

The samples were cooled with variants of simulated annealing based on Metropolis Monte-Carlo. Explicit results for several cooling schedules in both dimensions are given on the site, and instructions for different, larger samples are



Fig. 3. Taken from the website, Glanz-Izrael (2013) - at left, energy of a 2d liquid crystal sample as a function of the temperature, and at right the visualization at a temperature value selected from the energy graph.

also provided. In Figure 2 on the left two two-dimensional samples are shown (initial disordered and cooled relatively ordered) and in Figure 2 on the right two three-dimensional realizations are given. Once simulation data is entered into specific file locations, and interactive web interface for analysis and presentation is provided. An example of this page is given in Figure 3. The AViz instructions include an explanation of how to invoke the color changing that indicates angular direction, thereby reinforcing visual identification of orientational order. The sites include downloadable code for the simulation, as well as careful instructions for its implementation and extension.

Acknowledgements

Supported in part by FP7-NMP-604005 SIMPHONY. Discussions with Shunsuke Kobayashi are acknowledged with thanks as is support of RBNI, Technion for his visit. Discussions with A. Hashibon on AViz wrappers provided useful input for this project.

References

- Adler J., 2003. Visualization in Atomistic and Spin Simulations, *Computers in Science and Engineering*, **5**, pp. 61-65.
- Adler, J., Fox, J., Kalish, R., Mutat, T., Sorkin, A., and Warszawski, E., 2007. The essential role of visualization for modeling nanotubes and nanodiamond, *Computer Physics Communications*, **177** pp. 19-20.
- Adler, J. and Cohen, O., 2010. Solid Hydrogen - New twists on an old problem in "Recent Developments in Computer Simulation Studies in Condensed Matter Physics, X", edited by D. P. Landau, S. P. Lewis and B. Schuttler, *Physics Procedia* **6**, pp. 2-6.
- Adler, J., Koenka, Y. and Silverman, A., 2011. Adventures in carbon visualization with AViz, *Physics Procedia*, **15**, pp. 7-16.
- Adler, J., Zaffran, J., Silverman, A., Sorkin, A., Cohen, O. and Kalish, R., 2011. Simulation and visualization of nanodiamond and nanographite, *Computer Physics Communications*, **182**, 2009.
- Adler, J., Artzi, Y., ben Bashat, L., Izraeli, T.Y., Kreif, M., Lavi, I., Leibenzon, A., Levi, A., Schlesinger, I., Toledano, E., Peretz, U., Weisler, Y. and Yagil, A., 2014. How do I simulate problem X? *IOP Conference Series*, to appear 3rd Quarter 2014.
- Antypov, D., and Cleaver, D.J., 2004. *J. Phys.: Condens. Matter*, **16** S1887.
- Aharonov, 2005 - <http://phelafel.technion.ac.il/~pavela>
- AViz, 2001 - <http://phycomp.technion.ac.il/~aviz>
- AViz, 2013 - <http://phycomp.technion.ac.il/~aviz/describe.html>
- Gay, J.G. and Berne, B.J., 1981. Modification of the overlap potential to mimic a linear site site potential, *Journal of Chemical Physics*, **74** pp. 3316-3319.
- Glanz-Izrael, 2013 - <http://phelafel.technion.ac.il/~hilag> and <http://phelafel.technion.ac.il/~nadir>
- Hihinashvili, R., Adler J., Tsai, S.H. and Landau, D.P., 2004. Visualization of vector spin configurations, for "Recent Developments in Computer Simulation Studies in Condensed Matter Physics, XVII", edited by D. Landau, S. P. Lewis and B. Schuttler, Springer, pp. 169-73.
- Kobayashi, S., Shiraishi, Y., Sawai, H., et al., 2013. Optical properties of NTN-FSC-LCD and ECB cells with the doping of nanoparticles, *Proceedings of SPIE Vol. 8642* 86420M.
- Mazvovskiy, D., Halious, G., and Adler, J., 2012. The role of projects in (Computational) Physics Education, *Physics Procedia*, **34**, pp. 1-5.
- Peled, D., Silverman, A. and Adler, J., 2013. 3D visualization of atomistic simulations on every desktop, *IOP Conference Series*, **454**, 012076.
- Pine, P., Yaish, Y. and Adler, J., 2014. Vibrational analysis of thermal oscillations of single-walled carbon nanotubes under axial strain, *Phys. Rev. B*, **89** 115405.
- Shyuv, 2006 - <http://phycomp.technion.ac.il/~shyuv>