

AViz – Atomistic Visualization

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AViz, is a C++ and OpenGL/mesa based public domain package designed to visualize large numbers of atoms, vector spins, quadrupoles and other solid objects. Its application in dot mode to the visualization of electronic density is described in a companion abstract, here we concentrate on visualization of three dimensional systems of solid objects, whose locations and (where applicable) directions or polymer connections are calculated in advance or in parallel with a wide range of simulation or enumeration tools.

AViz differs from many other excellent existing visualization tools in that it was created by physicists interested in the study of defects, amorphous systems and sample melting with the philosophy that no predefined bond lengths, connections or angles exist. Bonds are actually concentrations of high electronic density, but the basic information concerns object locations (and directions if the object is a spin or a quadrupole). Cylindrical bonds can and are constructed as a guide to the eye for depth comprehension, or drawn to aid recognition of local atomic coordination, but are only one of many tools for helping to understand sample structures.

The latest version of AViz can be found on the SimPhoNy Github pages and a new website contains examples and tutorials. Within the framework of SimPhoNy effort has already gone into streamlining the source compilation process, and in material to support installers who may not be systems experts. Tutorials both on general AViz' use and on applications to nano-materials such as nanotubes are being developed,

AViz has many options, and is especially useful for projects with interaction between computational experts and laboratory experimentalists, because it enables translation between different worldviews with the universal language of visualization. However, until now it is only available in LINUX, and its installation was a little complex. In the framework of SimPhoNy, efforts have been made to clean up the code and simplify the installation, with files on Github. Plans to provide versions for other systems are on track.