AIM for Blender

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Introduction

Blender is a free and open source 3D animation suite[1], supporting (amongst other things) modelling, animation and rendering of 3D scenes. Blender also provides an API for Python scripting, allowing the writing of extensions to the program's functionality. This document describes one such extension (termed an *Add-On*), which allows the user to read a file containing a set of objects constituting the topology of a scalar function of the chemical wavefunction of a system (the electron density $\nabla\rho(\mathbf{r})$ being the canonical example) and creates corresponding 3D objects for manipulation in Blender. This functionality allows the full power of Blender to be applied in creating images and animations of such topologies.

Things AIM for Blender Does Not Do

AIM For Blender is *not* able to perform topological analysis of $\nabla\rho(\mathbf{r})$ for a wavefunction. It starts from a provided description of the topology to be rendered. For topological analysis, an external program is required, and a list of such programs is provided below.

Describing Topology: The .top File

Given the variety of programs available for topological analysis of scalar functions computed from chemical wavefunctions, it seems apt to provide a generic file definition into which the output files of each program can be converted. This filetype can then be read by A4B and no dependence on the underlying analysis programs is introduced. The extension '.top' will be used for these files.

Components of a Topology

A topology consists of various objects, each with different 3D representations. Critical points (CPs) are points in space (described by a position vector $\mathbf{r}_{\mathrm{cp}}$ and a rank and signature (ω, s) which depend on the behavior of the function around that point), and are typically rendered as spheres with different colors for different (ω, s). Atomic Interaction Lines (AILs) are paths through the scalar field with particular properties, and are in general rendered as curves. Interatomic Surfaces (IASs) are boundaries between basins and are rendered as surfaces, typically colored by the element of their associated nucleus.

References

1. http://www.blender.org.