

GSoC 2011 – VTK Project: Chemistry Visualization

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1 Project Details

From the VTK/GSoC wiki:

Addition of new data types, mappers and visualizations for chemistry visualization. VTK has already been used in several open source chemistry applications, but lacks specialized support for this area. Features such as marching cubes, GPU accelerated volume rendering and glyph mappers could be leveraged here, along with BSD licensed projects such as OpenQube to read in a wider range of inputs. A CML reader could also improve general chemistry I/O. This could also make use of existing work in infovis and 2D charting to display numerical output.

2 Motivation

My motivation in pursuing this project is centered on bringing the features of VTK to Avogadro ¹, an open-source 3D molecular editor. Another popular tool, SCM's ADF-GUI ², already uses VTK and would be improved by adding native chemical visualization to the library.

3 Expected Outcome

This project will result in, at minimum, a native implementation of the tools necessary to visualize chemical structures in VTK. The ability to render the electronic structure of molecules will also be implemented. If time permits, additional functionality such as plotting molecular orbital diagrams, visualizing spectroscopic tensors, animating geometry optimizations, rendering periodic crystal structures, etc will be added (there is certainly no shortage of useful things to render or plot in chemistry!). Current and potential users of VTK in the chemistry field will be contacted, and their input will help guide the work done in the second half of the project.

4 Tentative Timeline

Frequent communication with the mentor will occur throughout the summer. I expect to spend at least 40 hours per week working on this project.

April 25 - May 22: *Preparation Period*

- Introduce myself on VTK mailing list and IRC.
- Visit Kitware if time permits.
- Become familiar with the VTK workflow and source code, learn Kitware's coding style.
- Contact Avogadro and ADF-GUI/SCM developers to discuss which features would be most useful for them.

May 23 - July 12: *First Half of GSoC Timeline*

- Design and implement molecular structure data type in VTK.
- Implement simple molecular visualization (atoms, bonds, etc).
- Interface with existing libraries (OpenQube) for obtaining and processing cube data.
- Decide on supported file formats, write serialization code

July 12 - July 19: *Mid-term*

- Evaluate progress and finalize any incomplete work from first half.
- Check in with Avogadro and ADF developers, decide which requested functionality is possible to implement in the remaining time

¹<http://avogadro.openmolecules.net>

²<http://www.scm.com>

July 15 - August 14: *Second Half of GSoC Timeline* Implement advanced features:

- Molecular orbital rendering
- Electron density calculation and rendering
- Support for extended systems (e.g. crystals, surfaces, etc)
- Community requested features

August 15 - August 22: *Wrap Up Period*

- Clean up code and submit any remaining patches to Gerrit

5 About Me

I am a Ph.D. student in Dr. Zurek's theoretical chemistry research group at SUNY Buffalo. I have used Linux and open-source software since high school, and started contributing to open-source projects during my undergraduate studies. I've enjoyed writing code to process and visualize data for a long time; the first useful library I wrote was a Python module that I used in my courses to process experimental data, produce plots with matplotlib, and fit functions to data.

My first contribution to an open-source project added support for special-characters to Kile, a \LaTeX editor for the KDE desktop environment. Shortly after completing this work, I discovered the Avogadro project, which was still rather young and under heavy development. Around this time I began independently learning quantum chemistry and computational methods under the guidance of one of my professors, as my institution did not offer a course in quantum chemistry. In one of my inorganic chemistry courses, we synthesized several compounds that had unique experimentally determined vibrational spectra. My first non-trivial contribution to Avogadro was the Spectra extension, which I wrote to compare the experimental spectra with those calculated by NWChem on our physics department's new computer cluster. In the course of writing the Spectra extension, I ported an existing plot widget from the KDE libraries to pure Qt and added several new features, turning the widget from a static display of points to an interactive plot supporting mouse navigation and selection. I have continued Avogadro development for the last two years and still contribute frequently, most recently with my Crystallography extension. Since my first contribution in March 2009, I have committed 317 patches to Avogadro, 7.04% of all commits to the project.

Our research group specializes in the prediction of novel crystal structures under extreme conditions, such as high pressures. In contrast to other fields of chemistry, there is relatively little understanding of the forces at play, and chemical intuition does not offer much in the prediction process. Thus, we use automated search techniques. My work in the group centers on one such technique, using a genetic algorithm to "evolve" stable structures from randomly generated configurations or seeded guesses. I wrote an initial version of my C++/Qt genetic algorithm "XtalOpt"³ in about one month, and I've been the sole maintainer/developer for the past two years. The XtalOpt sources currently contain over 30,000 lines of original code. Our group has developed novel search techniques and shared them through publication⁴ and the code itself, which is publicly available under the GPL. XtalOpt is supported on both Windows and Linux, and we have tracked over 100 downloads of our windows installer. The number of additional users who have obtained the code through git clones or sharing installers is unknown. I will continue to work part-time on XtalOpt and Avogadro development if accepted for this Google Summer of Code position, although I do not expect these commitments to limit my ability to work on VTK full-time.

The majority of my studies have been in chemistry and physics, and last semester I took a course in high-performance computing. The latter exposed me to various parallelization APIs and focused on writing fast, efficient code.

I have read the VTK tutorials and made a few "Hello world"-type applications with the C++ library. I would like to be a part of bringing the features of VTK into Avogadro, which is a large part of my motivation in applying to develop native VTK chemistry tools. I have significant experience manipulating and visualizing data sets and possess the mathematical background to understand and develop 3D data visualization techniques.

I believe I am an excellent candidate to add native chemistry visualization support to VTK. My background in chemistry has provided the intuition to know what chemists expect from a high quality chemical visualization, and I am confident in my ability to write code that will meet these expectations. My experiences processing and visualizing data sets in Python and C++ will be useful while working on VTK, and my dedication to open-source software will fit well with the atmosphere at Kitware.

³<http://xtalopt.openmolecules.net>

⁴Lonie DC, Zurek E. Comp. Phys. Comm. 2011 182(2) p372-387