3D+ Visualization: Avizo, VisIt, and Mathematica via CHEM4581: Mathematical Methods in Chemistry

by Jinghua Ge[1] and Les Butler[2]
MW 11:30-12:30; Friday 11:30-12:30 computer lab time
Frey 101

Course Plan

This is a team-taught class on visualization methods for undergraduates and graduate students. This course builds off two prior offerings of Honors 3035 in 2008 and 2011 "3D Visualization", the capabilities of the Tier 1 Visualization Lab, the CCT HPC, the campus site license for Mathematica, and the experiences of Jinghua, Les, and others (invitations to be extended) with visualization and 3D data acquisition. The use of the CHEM4581 course number will allow both undergraduates and graduate students to take this course and receive credit. For undergraduates, this course can count for honors credit.

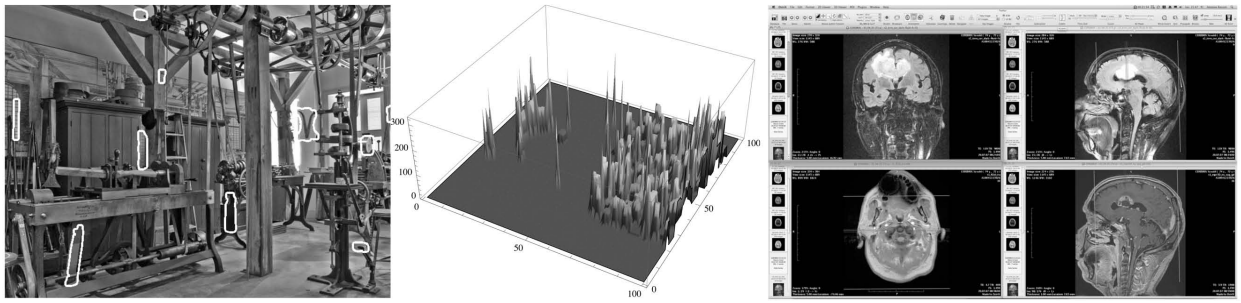

Figure 1: Examples of Mathematica processing and a public-domain MRI data set.

The course objective is to teach about 20 students image processing and data analysis operations in Avizo, VisIt, and Mathematica. Topics include binarization, dilation/erosion, segmentation, connected components analysis, texture, transformations (watershed, distance, Radon, affine), data formats (binary, TIF, DICOM, HDF), scripting (python for VisIt, Tcl/Tk for Avizo), and data analysis with Mathematica. In addition, lectures and demonstrations will cover 3D data acquisition, mainly X-ray tomography and MRI. The course format is lectures on MW and 50-minute lab on Fridays (with informal time extensions). The labs will give students hands-on experience with the Avizo and VisIt software.

There are several justifications for learning three software solutions for image processing. First, we have already observed that students "get it" when the same concept, say the watershed transformation, is presented in two different contexts. Based on recent experience in Honors 3035, when the watershed transformation was presented in both Avizo and Mathematica, there was much better

[1]Center for Computation and Technology: jinghuage@cct.lsu.edu
[2]Department of Chemistry: lbutler@lsu.edu

comprehension by the students. Second, Avizo and VisIt represent two extremes of current visualization software. Avizo (`http://www.vsg3d.com/avizo/overview` is an expensive, commercial product with a friendly user interfacet. VisIt (`https://wci.llnl.gov/codes/visit` is a DOE LLNL product freely available, cross-platform and with an effective backend for running on a computer cluster. Both products are scriptable; VisIt python scripting is particularly well-coupled to a GUI record function.

Approximate Course Outline

Weeks 1-5: Installation on student laptops Mathematica, VisIt, ImageJ, and Filezilla. Lectures on data formats, data import, histograms, threshold and binarization. Labs on introduction to Avizo, VisIt. Mathematica homework on data formats, importing, histograms, image and contour plots, and opacity. 3D data acquisition.

Weeks 6-10: Lectures on erosion/dilation, distance/watershed transformation, and connected components analysis. Labs on segmentation, open/closing operations, label fields, and connected component output. Mathematica homework on erosion/dilation, distance/watershed transformation, connected components, and re-ordering of label fields.

Weeks 11-15: Lectures on inverse Radon transformation, affine transformation, texture, optimization, python scripting. Labs on scripting, affine transformation, brushes for manual editing. Mathematica homework on Radon transformation, affine transformation, optimization.

Grading

Grades will be based on homework, participation in labs, midterm, and final. There will be separating syllabi for undergraduates and graduate students. We have consulted with the Honors College and for the undergraduates, this course can count for honors credit.

Bibliography

Digital Image Processing Using MATLAB, 2nd ed Rafael C. Gonzalez, Richard E. Woods, Steven L. Eddins (La-SIGMA library, 244 Johnson)

Volumetric Image Analysis Gabriele Lohmann (La-SIGMA library, 244 Johnson)

Morphological Image Analysis: Principles and Applications Pierre Soille (La-SIGMA library, 244 Johnson)

Introduction to the Mathematics of Medical Imaging Charles L. Epstein

Strategies for Teaching 3D Visualization in a Multidisciplinary Course Jinghua Ge, Dominique G. Homberger, and Leslie G. Butler, in preparation for submission to ACM Transactions on Computing Education