# Data Workflow and Visualization: X-Ray Interferometry, Vistrails and IPad/Android Collaboration

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**Abstract:** X-ray interferometry is providing new insights into processes such as flame retardant protection of polymers and in situ examination of lithium-ion battery performance. The data processing is intricate, requiring decisions about stepped grating settings, single-shot grating referencing, phase unwrapping thresholds, rotation stage centering, choice of tomography reconstruction algorithm, and more. VisTrails is a workflow solution that has the potential to partially automate the process, but retain user input and log critical parameters into an XML database. Then, the exciting results demand informal presentations. We are considering the iPad/Android application KiwiViewer by KitWare. However, the app is at an early development stage; we discuss possible upgrades to the app—an SBIR is in preparation—that will aid our informal science discussions.

**Keywords:** scientific visualization, workflow, provenance, collaboration, tomography

## 1. Introduction

Traditional X-ray imaging is based on absorption. A new imaging method is based on refraction and has two main advantages: less radiation dose to the patient and two new image contrast mechanisms. Recently, we have collaborated with the Advanced Photon Source (Argonne) X-ray optics test beamline to use X-ray grating-based interferometry to acquire differential phase contrast and diffraction images of a bird feather [1], a foraminifera [2], *in situ* lithium-ion battery operation, and burning flame retardant/polymer blend samples [3]. We plan to implement one variation of X-ray interferometry, single-shot [4], at the LSU CAMD tomography beamline soon after the 2013 wiggler upgrade is completed.

X-ray interferometry has problems with workflow, visualization, and collaboration. *Workflow*: At present, we use individual Mathematica notebooks record the workflow provenance for each sample; this is effective, but cumbersome. *Visualization*: Each imaging mode has its own information content: absorption conveys concentration of high-*Z* elements, differential phase contrast reveals domain boundaries, and diffraction shows presence of X-ray scattering centers such cracks with dimensions much smaller than pixel resolution. *Collaboration*: Traditionally, imagers have collaborated by sharing jpeg and movies in media such as PowerPoints. However, key features such as drilling into the data and making annotations are lacking. Years

ago, the cafe "paper napkin" was a key collaboration tool. Now, we would like the "cloud-based 4D paper napkin". Herein, we give a status report on the quest for this "napkin".

## 2. Visualization Tools and Accomplishments

Briefly, we list the important tools and their developments over the past year.

- An NSF MRI (DMR-0923440) funded upgrade of the LSU CAMD synchrotron will give tomography 10x flux, X-ray energy increase from 30 keV to over 60 keV, and more phase coherent radiation. The upgraded started in May and should be completed by Fall, 2013.
- X-ray interferometry data analysis: In collaboration with LIGO, we developed a fast, robust algorithm [2,5]. Stepped-grating interferometry yields sinusoidal data which can be fitted with a Levenberg-Marquardt least squares analysis, effective, but slow, ~0.5 yr. The new LIGO algorithm takes a few minutes.
- X-ray interferometry application: We acquired 2D phase contrast X-ray movies of burning flame retardant/polymer blends and static 3D phase contrast tomography. The successful flame retardants show distinctive protective char layer development [4]. A new lithium-ion battery was imaged with phase contrast at 36 keV; more experiments at higher X-ray energy and with worn batteries are needed to develop this procedure.
- To teach visualization methods, traditional coursework material has been converted into an iPad iBook format.
- VisTrails is an open-source workflow/provenance visualization tool. In our hands, we have incorporated some of our Mathematica codes into a VisTrails workflow. More details are given in Section 4.
- KitWare KiwiViewer is an iOS/Android app for visualization of 3D data. At present, tomography data import is unreliable, the data set sizes must be small, there is no provision for 4D data, and collaborative annotation such as dropping a pin on a special feature is not possible. We are planning a DOE SBIR project with KitWare to enhance the KiwiViewer app to better meet our needs. More details are presented in Section 5.

## 3. The iPad iBook on Scientific Visualization

Jinghua Ge (CCT LSU) and Les Butler (Chemistry, LSU) have taught scientific visualization for three semesters. and have developed a key set of notes describing the use of Avizo Fire, LLNL VisIt, Python scripting, ImageJ, and Mathematica. PDF lecture notes do not effectively convey the visualization procedures and results. Experienced high school science teachers, Chris Hynes and Shawn Liner, have transformed some notes into an iPad iBook. Some screen shots—codes, definitions, movies, and dynamic 3D objects—are shown in Fig. 1.

A key limitation of the iPad iBook as shown in Fig. 1 is the lack of high-performance computing. We are in the process of addressing this limitation with a backend for the iPad; access to an HPC cluster with on-demand image processing. An NSF MRI (CNS-1126739) has funded an HPC which we are configuring to support VisTrails. We have tested HTML5 imbedded in an iBook calling a VisTrails workflow running on a server, then returning image data to the iPad. The migration from workstation to the HPC is complex, hence we are also collaborating with the authors of VisTrails, Profs. Claudio Santos and Juliana Freire at New York University. Jinghua Ge

visited them in January and several of us (Ge, Butler, Ham, Beaird, Santos, and Freire) submitted an NSF SI2-SSI proposal in March; the goal is to enhance VisTrails to better meet our needs.

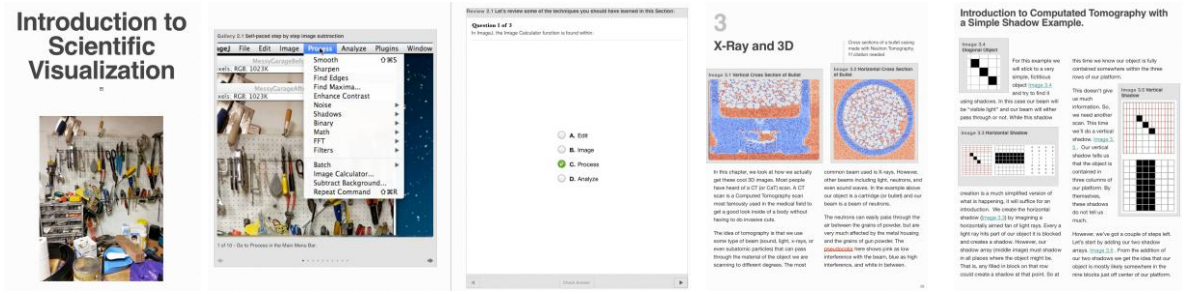
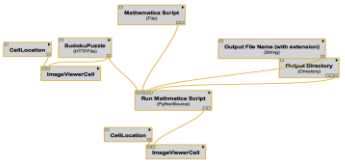



Fig. 1. Some representative screen shots from one of the iPad iBooks.

## 4. VisTrails

What is VisTrails? It is partially described at its website, vistrails.org. Shown in Fig. 2 and 3 are some example workflows we have developed. Fig. 2 shows a sketch of a workflow solving a Soduku puzzle; the puzzle enters the workflow as a scanned image, Mathematica OCR partially interprets the image (we intentionally use imperfect OCR parameters), the user input (VisTrails module) corrects the OCR errors, the puzzle is solved (Mathematica module), and the results displayed.

**Figure 2.** VisTrail flowchart of Sudoku puzzle (under development). The workflow will have image import, initial OCR (based on Mathematica code in a Python wrapper), display for user correction of the OCR, and solution module (Mathematica). This simple workflow illustrates key aspects of image analysis: import, processing, and user interaction.



## 5. KitWare KiwiViewer

KiwiViewer is based on the popular open-source VTK package developed by KitWare. KiwiViewer is a remarkably fluid and engaging app for showing off 3D visualizations. We think KiwiViewer could be a wonderful collaborative tool for discussion of data sets coming from a VisTrails workflow. However, KiwiViewer needs a few new features to enable true collaboration. In a recent video conference with a KitWare developer, we discussed plans for a DOE SBIR project to improve KiwiViewer. Of course, there is jargon to overcome. The KitWare develop describes a future of an "immersive collaborative environment". Is there a difficult learning curve for this environment? For comparison, the chemist describes an improved KiwiViewer as a "digital paper napkin". Are we talking about the same future? Yes. Does "napkin" easily connote a system with a very simple learning curve? We hope so.

## 6. Conclusions

Grating-based X-ray interferometry results are briefly presented, including a novel data analysis algorithm; the experiment has a raw data rate up to 25 GB/h. We are working towards efficient workflow data processing with VisTrails, education of scientific visualization with iPad iBooks, and collaborative informal scientific exchanges with Kitware's KiwiViewer.

## 7. Acknowledgments

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