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Research domain(s), discipline(s)/sub-discipline(s)

chemistry; materials science; X-ray and neutron tomography; interferometry

Title of Response

X-ray and Neutron Tomography for Materials Science

Abstract

This response describes the data volume of advanced X-ray and neutron tomography, enhanced with interferometry. The cyber challenges are data volume, data security, collaborative visualization software, and instruction of their use.

Question 1 (maximum 400 words) – Data-Intensive Research Question(s) and Challenge(s). Describe current or emerging data-intensive/data-driven S&E research challenge(s), providing context in terms of recent research activities and standing questions in the field. NSF is particularly interested in cross-disciplinary challenges that will drive requirements for cross-disciplinary and disciplinary-agnostic data-related CI.

I use and build X-ray and neutron tomography systems. I use beamlines at the Advanced Photon Source. With a W.M. Keck Foundation grant, I built an interferometry/tomography system at LSU, incorporating some ideas from the NSF-supported LIGO project. I am contracted to build a neutron interferometry system for ORNL HFIR CG-1D beamline. The data volume is tomography (2k^3 voxels) x interferometry (3-fold increase) x time series (1-10) x multiple samples (1-10). The X-ray applications include polymer science (NSF GOALI with Albemarle Corp on flame retardants in 3D printing) and biomedical (brown adipose tissue in mice). The neutron interferometry applications include early crack detection in stressed additive manufactured stainless-steel components (four recent publications). The cybersecurity applications include counterfeit detection in additive manufacturing (proposal pending). Our startup company, Refined Imaging LLC, has received NSF I-Corps and SBIR Phase I funding. The X-ray and neutron interferometry/tomography community is, in my opinion, wonderfully open and sharing at the international level. In 2019, I used German neutron imaging facilities, German micro fabrication facilities, and presented our work at meetings in Switzerland and Japan. An approved Los Alamos LANSCE beam time proposal that I led included co-PIs from Germany. I've talked at length with Chinese researchers about electron-beam-based neutron sources for imaging applications. I am preparing an NSF supplement request for international collaboration with a Swedish researcher.

Question 2 (maximum 600 words) – Data-Oriented CI Needed to Address the Research Question(s) and Challenge(s). Considering the end-to-end scientific data-to-discovery (workflow) challenges, describe any limitations or absence of existing data-related CI capabilities and services, and/or specific technical and capacity advancements needed in data-related and other CI (e.g., advanced computing, data services, software infrastructure, applications, networking, cybersecurity) that must be addressed to accomplish the research question(s) and challenge(s) identified in Question 1. If possible, please also consider the required end-to-end structural, functional and performance characteristics for such CI services and capabilities. For instance, how can they respond to high levels of data heterogeneity, data integration and interoperability? To what degree can/should they be cross-disciplinary and domain-agnostic? What is required to promote ease of data discovery, publishing and access and delivery?

Sneaker-net still dominates international, national, corporate, and on-campus research collaborations. I do not know how to begin to collaborate on the cybersecurity/counterfeiting project, which already involves two universities in Louisiana and a corporate research lab in New York; these three units have signed the legal non-disclosure paperwork, include a PhD in cybersecurity, and still data collaboration is problematic. The collaborative visualization tools are lacking. My colleagues use NIH ImageJ (freeware), which has about 5% of the needed capabilities for this research. I use and teach

Mathematica, which has the power, but as they say, "one of the best user interfaces of the 1980s". We write our papers in Overleaf (Latex in the Cloud), but it can't handle intensive graphics (chokes a >1Mb images). I spend $4k/yr on Avizo (best in class visualization software, but modest market penetration); Avizo has no collaborative/cloud tools. The DOE-supported LLNL VisIT project is interesting, but is optimized for computer generated volumes, not experimentally measured volumes. Some brilliant, but small projects come out of the "Open Chemistry" Kitware, Inc. project. Here's one blue sky suggestion: Task Kitware "Open Chemistry" with mashing ImageJ, Avizo, LLNL VisIt, Mathematica, and Overleaf.

Question 3 (maximum 300 words) – Other considerations. Please discuss any other relevant aspects, such as organization, processes, learning and workforce development, access and sustainability, that need to be addressed; or any other issues more generally that NSF should consider.

In Fall 2019, I taught first semester freshman chemistry MWF 7:30AM to initially 120 students, with 85 surviving to take the final. It's a flipped classroom with the Pearson suite of MasteringChemistry and LearningCatalytics. I observed some students like videos (youtube instruction, Khan academy). I used the Microsoft Stream to make new videos for my class; it's mostly good, except the audio transcription is not science enabled; it cannot handle scientific notation. I predict the future of tomography and visualization instruction will need a suite of videos for the next generation of STEM workers. Let's fix the problem of accurate audio transcription.

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