UNCLASSIFIED

Information Science and Technology Seminar Speaker Series

Marcus D. Hanwell
Kitware

Scalable Approaches to Immersive Data Storage, Visualization and Analysis

Wednesday, July 17, 2013

3:00 - 4:00 PM

TA-3, Bldg. 215, Rm. 182 (Physics Auditorium)

Abstract: As computational power and storage capabilities grow we need to move beyond simply storing data and towards scalable techniques for indexing, visualizing, and interacting with our data. This requires a variety of techniques, from metadata abstraction, powerful search algorithms, client-server based data processing pipelines using flexible frameworks, and domain-specific approaches. Some of the building blocks common to different areas will be covered, along with several approaches explored for chemical data and how that might be expanded for general materials simulations and data. The Open Chemistry project will be described as it concerns the complete simulation lifecycle, and how it has reused several projects developed at Kitware and from the wider community. We will focus on the use of MongoDB and related technologies in the Open Chemistry project, and how that same technology is being applied in other areas such as the DARPA XDATA project. We will touch on the development of several related projects such as XDATA and ParaViewWeb and how they are being incorporated in the Open Chemistry project to provide a simple solution for chemists who want to store, search, collaborate, and share their data with the wider community.

Biography: Dr. Marcus D. Hanwell is a Technical Leader at Kitware, where he leads the Open Chemistry project and play a critical role in developing new workflows in Git, performing Gerrit code review, and contributing to next generation build systems in the VTK, ITK, and Titan projects. Dr. Hanwell is the Principal Investigator on the Open Chemistry project, which focuses on developing open-source tools to for chemistry, bioinformatics, and materials science research. He was inspired to pursue the development of computational chemistry tools while working on his experimental/computational Physics PhD and postdoctoral studies, when he realized how outdated and cumbersome current tools are for handing the scale of data required by chemists. In his spare time, Dr. Hanwell is an active member of the KDE open-source communities, and of the KDE e.V. He is one of the core developers of Avogadro, an open-source, 3D, cross-platform molecular visualization and editing application/library; this work was featured by Trolltech as an instance of “Qt in Use.” Dr. Hanwell has also won a Blue Obelisk award for his work in Open Chemistry, and continues to develop and promote open approaches in chemistry and related scientific fields.

For more information contact the technical host Curt Canada, cvc@lanl.gov, 665-7453 or James Ahrens, ahrens@lanl.gov, 667-5797.

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