Acta Cryst. (2002). A**58** (Supplement), C218

COMPONENT-BASED SOFTWARE DEVELOPMENT, APPLICATIONS TO STRUCTURAL MOLECULAR BIOLOGY

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A few years ago we have adopted the Python programming language as the development platform for our software needs at the Molecular Graphics Laboratory (MGL) of the Scripps Research institute. We have developed software components that deal with different aspects of our daily work, including: MolKit, for the computational representation and manipulation of macromolecules, DejaVu, for the visualization of 3-D geometry, mslib, for molecular surfaces calculations etc. These components have been assembled to rapidly develop applications such as the Python Molecule Viewer (PMV) and ADT a graphical user interface to our automated docking code AutoDock. The uniqueness of these tools comes from their component-based architecture as well as from their features. We will describe our general software development philosophy as well as specific components such as MolKit, DejaVu and ViewerFramework which are key components of PMV. We will also give a live demonstration of PMV to illustrate its main concepts and features. In addition, we will present our latest addition to our set of components: the NetworkEditor. This component enables the graphical representation of entities (as nodes) and relationships between these entities (as connections). We will demonstrate ViPEr a visual programming environment which was developed using the NetworkEditor. ViPEr enables a user to drag-and-drop computational nodes onto a canvas and connect them to create a computational network. A live demonstration of this program will enable us to demonstrate many of ViPEr's design concepts and the high level of code re-use that we were able to achieve. We will conclude by discussing the pros and cons of using Python for implementing our strategy for software development.

Acta Cryst. (2002). A**58** (Supplement), C218

TANGIBLE INTERFACES IN MOLECULAR BIOLOGY

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As biology and computation become more enmeshed, issues of software use for the study of complex molecular biological systems become central. On the human side, complex structural biological systems must be visualized and communicated at the molecular level for understanding and scientific progress. New modes of human-computer interaction could facilitate this progress.

This talk will focus on our latest approaches to this issue. We are investigating the application of computer-driven autofabrication and augmented-reality to develop novel tangible interfaces for the study of biomolecular structure and interaction. Natural and multi-modal interactions with physical objects, offer an expanded view of molecular structure, and an intuitive interface for manipulation and query. We are exploring the representational repertoire of a 'solid printer', which is capable of producing full color solid models of molecular structures with a variety of physical characteristics.

We are also enabling the connections between these physical molecular models, and their computer representations by integrating augmented or 'mixed' reality software with our molecular modeling environment.

I will discuss and demonstrate these interactive visualization technologies and applications of these technologies to the study of protein structure and interactions in areas such as drug design and biomolecular assembly.

Acta Cryst. (2002). A**58** (Supplement), C218

NEUTRON DIFFRACTION STUDIES ON TRANSITION METAL HYDRIDE COMPLEXES

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Neutron diffraction has played an invaluable and essential role in the characterization of metal-hydrogen interactions. Over the years, we have studied terminal M-H bonds, bridging M-H-M and M-H-B bonds, as well as hydrogen atoms situated on the edges, faces and interstitial cavities of metal cluster complexes. In this talk we will summarize some of our most significant contributions in this area, together with a presentation of some recent results.

Keywords: TRANSITION METAL HYDRIDES NEUTRON DIFFRACTION

Acta Cryst. (2002). A**58** (Supplement), C218

SINGLE CRYSTAL PULSED NEUTRON DIFFRACTION STUDIES OF TRANSITION METAL HYDROGEN INTERACTIONS

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The time-of-flight (TOF) Laue technique for single crystal neutron diffraction measurements at pulsed neutron sources has been used to analyze various types transition metal coordination complexes with hydride and hydrogen ligands. Precise location of hydrogen atoms in the presence of transition metals is often crucial to understanding the electronic structure and the relevant chemistry. At the IPNS, the types of interactions which have been characterized include agostic C-H···metal bonds (C-H = 1.19 Å), terminal and bridging hydrides, and dihydrogen complexes. In the latter case, the effect of varying other ligands on the activation of the coordinated molecular dihydrogen has been studied in a series of osmium complexes with H-H distances of 1.01 to 1.30 Å.

Work supported by US Department of Energy, Basic Energy Sciences-Materials Science, under Contract No. W-31-109-ENG-38.

Keywords: TRANSITION METAL HYDRIDES PULSED NEUTRON DIFFRACTION MOLECULAR DIHYDROGEN COMPLEXES