molecular graphics & modelling society

MGMS Lecture Tour: Professor Arthur J. Olson

The Scripps Research Institute, La Jolla, California, USA

"Interacting with Protein Interactions"

University of Cardiff, Monday, 7 July 2014

• *Local Host:* Jamie Platts / platts@cardiff.ac.uk

4:00 pm, Cardiff School of Chemistry, University of Cardiff, Main Building, Park Place, Cardiff, CF10 3AT

University of Oxford, Tuesday, 8 July 2014

• *Local Host:* Phil Biggin / philip.biggin@bioch.ox.ac.uk

2:30 pm, Main Seminar Room, Department of Biochemistry, South Parks Road, Oxford, OX1 3QU

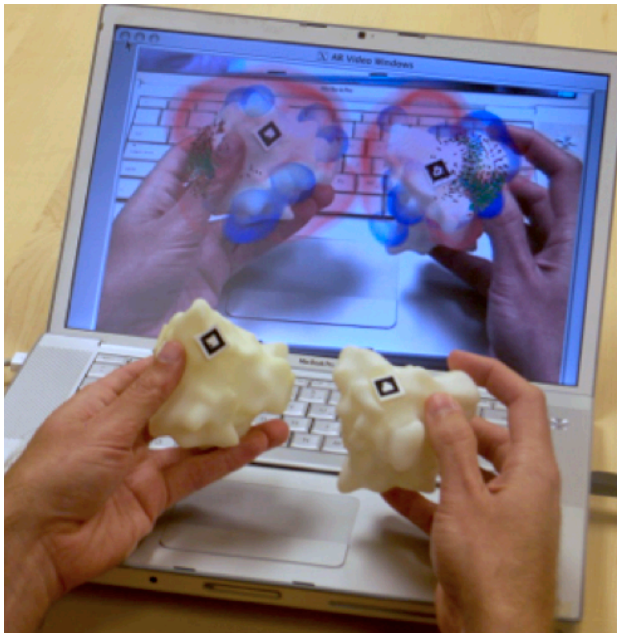
University of Cambridge, Wednesday, 9 July, 2014

Special Event of the Cambridge Cheminformatics Network Meetings

• *Local Host:* Andreas Bender / ab454@cam.ac.uk

4:00 pm, Pfizer Lecture Theatre, Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW

Seminars are free of charge and open to all.



Biology *has become accessible to an understanding of processes that span from atom to organism. As such we now have the opportunity to build a spatio-temporal picture of living systems at the molecular level. In our recent work we attempt to create, interact with, and communicate physical representations of complex molecular environments.*

I will discuss the challenges and demonstrate three levels of interaction with protein interactions: 1) human perceptual and cognitive interaction with complex structural information; 2) interaction and integration of multiple data sources to construct cellular environments at the molecular level; and 3) interaction of software tools that can bridge the disparate disciplines needed to explore, analyze and communicate a holistic molecular view of living systems.

In order to increase our understanding and interaction with complex molecular structural information we have combined two evolving computer technologies, solid printing and augmented reality. We create custom tangible molecular models and track their manipulation with real-time video, superimposing text and graphics onto the models to enhance their information content and to drive interactive computation.

We have recently developed automated technologies to construct the crowded molecular environment of living cells from structural information at multiple scales as well as bioinformatics information on levels of protein expression and other data. We can populate cytoplasm, membranes, and organelles within the same structural volume to generate cellular environments that synthesize our current knowledge of such systems.

The communication of complex structural information requires extensive scientific knowledge as well as expertise in creating clear visualizations. We have developed a method of combining scientific modeling environments with professional grade 3D modeling and animation programs such as Maya, Cinema4D and Blender. This gives both scientists and professional illustrators access to the best tools to communicate the science and the art of the molecular cell.

Gillet, A., Sanner, M., Stoffler, D., Olson, A.J. (2005) Tangible interfaces for structural molecular biology. ***Structure****:13:483-491.*

Johnson, G.T., Autin, L., Goodsell, D.S., Sanner, M.F., Olson A.J. (2011) ePMV Embeds Molecular Modeling into Professional Animation Software Environments. ***Structure*** *19(3):293-303.*

http://mgms.org/lecture_tour.html