Molecular Simulations and Visualization

Faraday Discussion 169

7-9 May 2014
Nottingham, UK

Programme

Wednesday 7 May

11:00	Registration, Tea and Coffee	
12:00	Lunch	
12.45	**Welcome and Introductions** Marc Baaden	
12.55	**Outline of Discussion Format** *Faraday Discussions*, Publishing Editors	
13.00	**Introductory Lecture:** Helmet Grubmüller *Max Planck Institute of Biophysical Chemistry, Germany*	**Paper 1**
	Session 1: Virtual and augmented reality immersive molecular simulations Session Chair: **Art Olson**	
14:00	**3D molecular models of whole HIV-1 virions generated with cellPACK** Graham Johnson*, David Goodsell, Ludovic Autin, Stefano Forli, Michel Sanner, Arthur Olson *University of California, San Francisco, USA*	**Paper 2**
14:05	**Innovative interactive flexible docking method for multi-scale reconstruction elucidates dystrophin molecular assembly** Anne-Elisabeth Molza, Nicolas Férey, M. Czjzek, Elisabeth Le Rumeur, Jean-Francois Hubert, Alex Tek, Benoist Laurent, Marc Baaden, Oliver Delalande* *University of Rennes, France*	**Paper 3**
14:10	Discussion	
15:00	Afternoon Tea	
15:30	**A GPU-accelerated immersive audio-visual framework for interaction with molecular dynamics using consumer depth sensors** David Glowacki*, Michael O'Connor, Gaetano Calabro, James Price, Philip Tew, Thomas Mitchell, Joseph Hyde, David Tew, David Coughtrie, Simon McIntosh-Smith *University of Bristol, UK*	**Paper 4**
15:35	**Studying chemical reactivity in a virtual environment** Moritz Haag and Markus Reiher* *ETH Zurich, Switzerland*	**Paper 5**

15:40	**Exaviz: a flexible framework to analyse, steer and interact with molecular dynamics simulations** Matthieu Dreher*, Jessica Prevoteau-Jonquet, Mikael Trellet, Marc Piuzzi, Marc Baaden, Bruno Raffin, Nicolas Ferey, Sophie Robert, Sébastien Limet *INRIA, France*	**Paper 6**
15:45	Discussion	
17.00	Lightning sessions	
17:30	Poster Session and Wine Reception	
19:30	Dinner	

Thursday 8 May

	Session 2: Advanced visualization and visual analytics Session Chair: **Mark Sansom**	
09:00	**Visual analysis for space-time aggregation of biomolecular simulations** Thomas Ertl*, Michael Krone, Stefan Kesselheim, Katrin Scharnowski, Guido Reina, Christian Holm *University of Stuttgart, Germany*	**Paper 7**
09:05	**Visualising intrinsic disorder and conformational variation in protein ensembles** Julian Heinrich*, Michael Krone, Sean O'Donoghue, Daniel Weiskopf *University of Stuttgart, Germany*	**Paper 8**
09:10	**RiboVision suite for visualization and analysis of ribosomes** Chad Bernier, Anton Petrov*, Chris Waterbury, James Jett, Fengbo Li, Larry Freil, Xiao Xiong, Lan Wang, Blacki Migliozzi, Eli Hershkovits, Yuzhen Xue, Chiaolong Hsiao, Jessica Bowman, Steve Harvey, Martha Grover, Zachary Wartell, Loren Williams *Georgia Institute of Technology, USA*	**Paper 9**
09:15	Discussion	
10:30	Morning Tea	
11:00	**NRas slows the rate at which a model lipid bilayer phase separates** Elizabeth Jeffreys, Mark Sansom, Philip Fowler* *University of Oxford, UK*	**Paper 10**
11:05	**Density based visualization for molecular simulation** Dmitri Rozmanov*, Svetlana Baoukina, Peter Tieleman *The University of Calgary, Canada*	**Paper 11**
11:10	Discussion	
12:00	Lunch	
	Session 3: Computing power revolution and new algorithms: GP-GPUs, clouds and more Session Chair: **Simon McIntosh-Smith**	
13:00	**GPU-accelerated analysis and visualization of large structures solved by molecular dynamics flexible fitting** John Stone*, Ryan McGreevy, Barry Isralewitz, Klaus Schulten *University of Illinois at Urbana-Champaign, USA*	**Paper 12**
13:05	**Visualising and controlling the flow in biomolecular systems at and between multiple scales: from atoms to hydrodynamics at different locations in time and space** Evgen Pavlov, Makoto Taiji, Arturs Scukins, Anton	**Paper 13**

	Markensteijn, Sergey Karabasov, Dimirty Nerukh* *Aston University, UK*	
13:10	**Allosteric pathway identification through network analysis: from molecular dynamics simulations to interactive 2D and 3D graphs** Ariane Allain, Isaure Chauvot de Beauchêne, Florent Langenfeld, Yann Guarracino, Elodie Laine, Luba Tchertanov*, *ENS Cachan, France*	**Paper 14**
13:15	Discussion	
14.30	Afternoon Tea	
15:00	**Haptic-driven, interactive drug design: implementing a GPU-based approach to evaluate the induced fit effect** Athanasios Anthopoulos, Gaia Pasqualetto, Ian Grimstead, Andrea Brancale* *Cardiff University, UK*	**Paper 15**
15:35	**Accelerating electrostatic pair methods on graphical processing units to study molecules in supercritical carbon dioxide** John Baker*, Jonathan D. Hirst *University of Nottingham, UK*	**Paper 16**
15:40	**A real-time proximity querying algorithm for haptic-based molecular docking** Georgios Iakovou*, Stephen Laycock, Steven Hayward, *University of East Anglia, UK*	**Paper 17**
15:45	Discussion	
16.30	Poster Session and Demo's	
17:30	Close of sessions	
19:00	Pre-Dinner Drinks	
19:30	Conference Dinner	

Friday 9 May

	Session 4: Applications and serious games: from docking to protein folding Session Chair: **Sean O'Donoghue**	
09:00	**Immune Attack players perform better on a test of cellular immunology and self confidence than their classmates who play a control video game** Melanie Stegman *Federation of American Scientists, USA*	**Paper 18**
09:05	**Udock, the interactive docking entertainment system** Guillaume Levieux, Guillaume Tiger, Stéphanie Mader, Jean-Francois Zagury, Stéphane Natkin, Matthieu Montes* *CNAM, France*	**Paper 19**
09:10	Discussion	
10:00	Morning Tea	
10:30	**Exploring genomes with a game engine** Jeremiah Shepherd, Lingxi Zhou, William Arndt, Yan Zhang, W. Jim Zheng*, Jijun Tang *University of Texas Health Center at Houston, USA*	**Paper 20**
10:35	**Methodologies for the analysis of instantaneous lipid diffusion in md simulations of large membrane systems** Matthieu Chavent*, Tyler Reddy, Joseph Goose, Anna Caroline Dahl, John Stone, Bruno Jobard, Mark Sansom *SBCB, University of Oxford, UK*	**Paper 21**
10:40	**Rapid decomposition and visualisation of protein-ligand binding free energies by residue and by water** Christopher Woods*, Maturos Malaisree, Julien Michel, Ben Long, Simon McIntosh-Smith, Adrian Mulholland *University of Bristol, UK*	**Paper 22**
10:45	Discussion	
12:00	**Concluding remarks** Frederick Brooks *University of North Carolina at Chapel Hill, USA*	**Paper 23**
12:45	**Acknowledgements**	
13:00	**Close of meeting**	