KEYNOTE TALK

TBD

Estimating the Structure and Motion of Biomolecules at Atomic Resolutions

David Fleet University of Toronto & Google DeepMind Canada

Abstract: One of the foremost problems in structural biology concerns the inference of the atomicresolution 3D structure of biomolecules from electron cryo-microscopy (cryo-EM). The problem, in a nutshell, is a form of multi-view 3D reconstruction, inferring the 3D electron density of a particle from large sets of images from an electron microscope. I'll outline the nature of the problem and several of the key algorithmic developments, with particular emphasis on the challenging case in which the imaged molecule exhibits a wide range of conformational variation (or non-rigidity). Through single particle cryo-EM, methods from computer vision and machine learning are reshaping structural biology and drug discovery.

This is joint work with Ali Punjani.



Speaker Bio-Sketch: David Fleet is a Research Scientist at Google DeepMind (since 2020) and a Professor of Computer Science at the University of Toronto (since 2004). From 2012-2017 he served as Chair of the Department of Computer and Mathematical Sciences, University of Toronto Scarborough. Before joining the University of Toronto, he worked at Xerox PARC (1999-2004) and Queen's University (1991-1998). He received the PhD in Computer Science from the University of Toronto in 1991. He as awarded an Alfred P. Sloan Research Fellowship in 1996 for his research on visual neuroscience. He received research paper awards at ICCV 1999, CVPR 2001, UIST 2003, BMVC 2009, and NeurIPS 2022. In 2010, with Michael Black and Hedvig Sidenbladh he

received the Koenderink Prize for fundamental contributions to computer vision that withstood the test of time. In 2022, with Ali Punjani, he received the Paper of the Year Award from the Journal of Structural Biology for work on cryo-EM. He served as Associate Editor of IEEE Trans PAMI (2000-2004), as Program Co-Chair for CVPR (2003) and ECCV (2014), and as Associate Editor-In-Chief for IEEE Trans PAMI (2005-2008). He was Senior Fellow of the Canadian Institute of Advanced Research (2005-2019), and currently holds a Canadian CIFAR AI Chair. His current research interests span computer vision, image processing machine learning and computational biology.