IMS-NTU joint workshop on Biomolecular Topology: Modelling and Data

(24 Jun 2024–28 Jun 2024)

Organizing Committee

Co-chairs

Jelena Grbic
University of Southampton

Jie Wu
Yanqi Lake Beijing Institute of Mathematical Sciences and Applications

Kelin Xia
Nanyang Technological University

Members

Fei Han
National University of Singapore

Fengchun Lei
Dalian University of Technology

Zhi Lu
Fudan University

Guowei Wei
Michigan State University

Venue

IMS Auditorium

Institute for Mathematical Sciences

3 Prince George's Park
Singapore 118402

Jointly sponsored by

NANYANG TECHNOLOGICAL UNIVERSITY
SINGAPORE

For more information: https://ims.nus.edu.sg/events/biomolecular-topology-modelling-and-data-analysis/

Workshop

24–28 June 2024

Monday, 24 June 2024

Time	Title	Speaker
0845–0900	Registration	
0900–0910	Opening Remarks	Workshop Organizers
Session Chair: Yasuaki Hiraoka (*Kyoto University)*		
0910–1000	Toward quantum accuracy in protein energy calculations	John Z.H. Zhang *Shenzhen University of Synthetic Biology, China*
1000–1050	The discrete Dirac operator determines the interplay between network topology, geometry and dynamics	Ginestra Bianconi *Queen Mary University of London, UK*
1050–1120	Coffee Break	
1120–1210	Capturing Robust Topology in Data	Bei Wang *University of Utah, USA*
1210–1400	Lunch at IMS	
Session Chair: Ginestra Bianconi (*Queen Mary University of London*)		
1400–1450	scEGOT: Single-cell trajectory inference framework based on entropic Gaussian mixture optimal transport	Yasuaki Hiraoka *Kyoto University, Japan*
1450–1540	The AI Frontier in Protein Design: From Geometric Deep Learning to Large Models	Yuguang Wang *Shanghai Jiao Tong University, China*
1540–1610	Coffee Break	
1610–1700	A Biophysics DNN Model with Topological and Electrostatic Features	Weihua Geng *Southern Methodist University, USA*
1800	*Conference Dinner* The Scholar Chinese Restaurant 9 Kent Ridge Dr, Singapore 119241	

Tuesday, 25 June 2024

Time	Title	Speaker
0850–0900	Registration	
Session Chair: Jason Cantarella (*University of Georgia*)		

Tuesday, 25 June 2024		
Time	Title	Speaker
0900–0950	Chromatic persistent homology	Herbert Edelsbrunner *Institute of Science and Technology (IST), Austria*
0950–1040	Designed self-assembly of molecular knots, links and topological gels	Cristian Micheletti *International School for Advanced Studies (SISSA), Italy*
1040–1110	Coffee Break	
1110–1200	Topological Representation and Uncertainty for Biomedical Images	Chao Chen *Stony Brook University, USA*
1200–1400	Lunch at IMS	
Session Chair: Chao Chen (*Stony Brook University*)		
1400–1450	Generative and Coevolutionary Approaches to Protein Structure	Julie C Mitchell *Oak Ridge National Laboratory, USA*
1450–1540	Can we geometrically sense the shape of a molecule?	Vitaliy Kurlin *University of Liverpool, UK*
1540–1610	Coffee Break	
1610–1700	Geometric structure guided nonnegative matrix factorization model for complete deconvolution of biological data	Duan Chen *University of North Carolina at Charlotte, USA*

Wednesday, 26 June 2024		
Time	Title	Speaker
0850–0900	Registration	
Session Chair: Bei Wang (*University of Utah*)		
0900–0950	Topological Graph Contrastive Learning	Yulia R. Gel *National Science Foundation and University of Texas at Dallas, USA*
0950–1040	Diffusion Models for Molecular Structure Prediction	Jian Tang *HEC Montréal, Canada*
1040–1110	Group Photo & Coffee Break	
1110–1200	Computer vision-inspired graph neural network architectures for molecular property prediction	Binh Nguyen *Victoria University of Wellington, New Zealand*
1200–1400	Lunch at IMS	

Wednesday, 26 June 2024		
Time	**Title**	**Speaker**
1400	*Excursion to Botanic Gardens* One way transfer from IMS - Botanic Gardens https://www.nparks.gov.sg/sbg	

Thursday, 27 June 2024		
Time	**Title**	**Speaker**
0850–0900	Registration	
Session Chair: Henry Adams (*University of Florida*)		
0900–0950	Harmonic Methods for Topological Data	Robert Ghrist *University of Pennsylvania, USA*
0950–1040	On the use of group equivariant non-expansive operators for protein pocket detection	Patrizio Frosini *Università di Bologna, Italy*
1040–1110	Coffee Break	
1110–1200	Geometric data analysis of protein-protein interactions	Jiahui Chen *University of Arkansas, USA*
1200–1400	Lunch at IMS	
Session Chair: Vitaliy Kurlin (*University of Liverpool*)		
1400–1450	The statistical topology theory of aging	Rongling Wu *Beijing Institute of Mathematical Sciences and Applications, China*
1450–1540	Hausdorff vs Gromov-Hausdorff distances	Henry Adams *University of Florida, USA*
1540–1610	Coffee Break	
1610–1700	Linkage and polygon spaces; a test case for TDA?	Jason Cantarella *University of Georgia, USA*

Friday, 28 June 2024		
Time	**Title**	**Speaker**
0850–0900	Registration	
Session Chair: Jie Wu (*Yanqi Lake Beijing Institute of Mathematical Sciences and Applications*)		
0900–0950	Topological Compound Fingerprinting in Computer-Aided Drug Discovery	Yuzhou Chen *Temple University, USA*
0950–1040	Periodic Geometry and Topology-Based Machine Learning Frameworks in Material Design	Chuan-Shen Hu *Nanyang Technological University, Singapore*
1100–1300	Lunch at IMS	

This schedule is accurate as of 26 June 2024 and is subjected to changes.