

Conference Program

The Third Conference on Computational and Mathematical Bioinformatics and Biophysics

Tsinghua Sanya International Mathematics Forum

December 20 – 24, 2020, (Beijing Time)
December 19 – 23, 2020, (US Central Time)

Zoom Meeting ID: 981 2055 6545

Password: CMBB

Zoom Link:

<https://uasystem.zoom.us/j/98120556545?pwd=OXJhZENITDhpaUsrNDQ5a2NvQVNudz09>

Organizing Committee:

Stephen Shing-Toung Yau, Tsinghua University, China

Guowei Wei, Michigan State University, USA

Changchuan Yin, University of Illinois at Chicago, USA

Shan Zhao, University of Alabama, USA

DAY 1

December 20, 2020, (Beijing Time)

December 19, 2020, (US Central Time)

Beijing Time	US Central Time	Session Chair: Shi-Jie Chen, University of Missouri, USA
8:45 – 8:55 AM	6:45 – 6:55 PM	Zoom Registration
8:55 – 9:00 AM	6:55 – 7:00 PM	Welcoming Remark Stephen Shing-Toung Yau, Tsinghua University, China
9:00 – 9:25 AM	7:00 – 7:25 PM	Shi-Jie Chen , University of Missouri, USA Energy-guided iterative approach to computational prediction of ligand-RNA interaction
9:30 – 9:55 AM	7:30 – 7:55 PM	Jiali Gao , Shenzhen Bay Laboratory, China Importance of quantum effects in biomolecular simulations
10:00 – 10:25 AM	8:00 – 8:25 PM	Duc Nguyen , University of Kentucky, USA Opportunities and challenges for AI and Math in drug discovery
10:30 – 10:55 AM	8:30 – 8:55 PM	Xinqi Gong , Renmin University of China Functional multi-body protein interaction supercomplex structure prediction
11:00 – 11:25 AM	9:00 – 9:25 PM	Jinqiao Duan , Illinois Institute of Technology, USA Xi Chen , Xi'an University of Finance and Economics, China Target search of a protein on DNA in the presence of position-dependent bias

DAY 2

December 21, 2020, (Beijing Time)

December 20, 2020, (US Central Time)

Beijing Time	US Central Time	Session Chair: Jinbo Xu, Toyota Tech Inst at Chicago, USA
8:50 – 9:00 AM	6:50 – 7:00 PM	Zoom Registration
9:00 – 9:25 AM	7:00 – 7:25 PM	Jinbo Xu , Toyota Tech Inst at Chicago, USA Latest development of protein structure prediction by deep learning
9:30 – 9:55 AM	7:30 – 7:55 PM	Qunfeng Dong , Loyola University Chicago, USA A Bayesian Framework for Estimating the Risk Ratio of Hospitalization for People with Comorbidity Infected by the SARS-CoV-2 Virus
10:00 – 10:25 AM	8:00 – 8:25 PM	Yongshuai Jiang , Harbin Medical University, China The framework for population epigenetic study
10:30 – 10:55 AM	8:30 – 8:55 PM	Zhaoming Wang , St. Jude Children's Research Hospital, USA Genetic risk for subsequent breast cancer among female survivors of childhood cancer
11:00 – 11:25 AM	9:00 – 9:25 PM	Lily He , Beijing University of Civil Engineering and Architecture, China A novel alignment-free method for HIV-1 subtype classification

DAY 3

December 22, 2020, (Beijing Time)

December 21, 2020, (US Central Time)

Beijing Time	US Central Time	Session Chair: Robert Krasny, University of Michigan, USA
8:50 – 9:00 AM	6:50 – 7:00 PM	Zoom Registration
9:00 – 9:25 AM	7:00 – 7:25 PM	Robert Krasny , University of Michigan, USA A GPU-Accelerated Fast Summation Method for Electrostatics of Biomolecules
9:30 – 9:55 AM	7:30 – 7:55 PM	Dexuan Xie , University of Wisconsin-Milwaukee, USA Advances in Poisson–Nernst–Planck Ion Channel Models and Finite Element Solvers
10:00 – 10:25 AM	8:00 – 8:25 PM	Xiaoqin Zou , University of Missouri - Columbia, USA Dissimilar Ligands Bind in a Similar Fashion: A Guide to Ligand Binding Mode Prediction
10:30 – 10:55 AM	8:30 – 8:55 PM	Zhan Chen , Georgia Southern University, USA Variational interface models for implicit solvation of biomolecules
11:00 – 11:25 AM	9:00 – 9:25 PM	Shenggao Zhou , Soochow University, China Variational implicit-solvent predictions of the dry–wet transition pathways for ligand–receptor binding and unbinding kinetics

DAY 4

December 23, 2020, (Beijing Time)

December 22, 2020, (US Central Time)

Beijing Time	US Central Time	Session Chair: Huan-Xiang Zhou, University of Illinois at Chicago, USA
8:50 – 9:00 AM	6:50 – 7:00 PM	Zoom Registration
9:00 – 9:25 AM	7:00 – 7:25 PM	Huan-Xiang Zhou , University of Illinois at Chicago, USA Correlated Segment and Fuzzy Membrane Association of Intrinsically Disordered Proteins
9:30 – 9:55 AM	7:30 – 7:55 PM	Qiang Cui , Boston University, USA Multi-scale models for ESCRT driven membrane remodeling
10:00 – 10:25 AM	8:00 – 8:25 PM	Jing-an Cui , Beijing University of Civil Engineering and Architecture, China Final size relation and control for epidemic model with heterogeneous mixing
10:30 – 10:55 AM	8:30 – 8:55 PM	Shaojun Pei , Tsinghua University, China A novel numerical representation for proteins: Three-dimensional Chaos Game Representation and its Extended Natural Vector
11:00 – 11:25 AM	9:00 – 9:25 PM	Duan Chen , University of North Carolina at Charlotte, USA Fast stochastic compression algorithms for biological data analysis

DAY 5

December 24, 2020, (Beijing Time)

December 23, 2020, (US Central Time)

Beijing Time	US Central Time	Session Chair: Ruhong Zhou , Zhejiang University, China and Columbia University, USA
8:50 – 9:00 AM	6:50 – 7:00 PM	Zoom Registration
9:00 – 9:25 AM	7:00 – 7:25 PM	Ruhong Zhou , Zhejiang University, China and Columbia University, USA Immunotherapy Modeling: Molecular Interaction and Recognition of MHC/peptide/TCR Complexes
9:30 – 9:55 AM	7:30 – 7:55 PM	Yaoqi Zhou , Griffith University, Australia RNA secondary structure prediction by Evolutionary Profile and Mutational Coupling
10:00 – 10:25 AM	8:00 – 8:25 PM	Qi Wang , University of South Carolina, USA Collective dynamics of active particles on surfaces
10:30 – 10:55 AM	8:30 – 8:55 PM	Zixuan Cang , University of California Irvine, USA Spatial signaling in single-cell data via optimal transport
11:00 – 11:25 AM	9:00 – 9:25 PM	Kelin Xia , Nanyang Technological University, Singapore Persistent representation based machine learning models for drug design

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