

The 4th International Conference on Mathematical and Computational Medicine



**Conference Check-in and Social Mixer
Monday, December 3, 2018
6:00 PM - 8:00 PM**

Please join us for a casual get together in the Lobby Bar with beverages and captivating conversation. Enjoy the nostalgia of old friends, the intrigue of new ones, and the tropical paradise of Cancun!

This is also a perfect time for attendees to get their name badges and other conference materials: Conference check-in will resume at 8:00 a.m. the following morning, December 4, 2018.

Hope to see you there!

Welcome to Cancun!

(Please scroll down for complete Conference Agenda)

**The 4th International Conference on
Mathematical and Computational Medicine**

Tuesday, December 4, 2018

Day 1

8:00 – 8:30 **Registration/Check-in**

8:30 – 8:45 Jayajit Das - WELCOME & OPENING REMARKS

**Session 1
Immunology
Chair: Das**

8:45 – 9:10 Amber Smith, PhD –
“Modeling Disease Progression During Influenza.”

9:10 – 9:35 Avner Friedman, PhD – Ohio State University
“Using Mathematical Models to Conduct Cancer Clinical Trials.”

9:35 – 10:00 Elsje Pienaar, PhD – Purdue University
“Systems Pharmacology Approaches to Tuberculosis Treatment.”

10:00 – 10:15 **Break**

10:15 – 10:40 Jayajit Das, PhD – Ohio State University
“Mechanisms of Activation and Tolerance in Natural Killer Cells.”

10:40 – 10:55 Darren Wethington, Research Associate– Nationwide Children’s Hospital
“Mechanistic Modeling of Respiratory Syncytial Virus (RSV) in Cotton Rats.”

**Session 2
Gene Regulation**

10:55 – 11:20 Ilya Ioshikhes, PhD – University of Ottawa
“Matching Nucleosome Patterns to the Complexity of the Organism.”

11:20 – 11:45 Remo Rohs, PhD – University of Southern California
“How DNA Shape Advanced our Understanding of Gene Regulation.”

11:45 – 5:00 **Break**

**Session 2 (cont.)
Gene Regulation
Chair: Kloczkowski**

5:00 – 5:25 Marek Grabowski, PhD – University of Virginia
“Data Sharing in Structural Biology: Advances and Challenges.”

5:25 - 5:50 Oliver Lichtarge, PhD – Baylor College of Medicine
“Computing Disease Driver Genes with a Calculus of Fitness Landscapes.”

5:50 - 6:15 Cristi Galindo, PhD – Vanderbilt University Medical Center
“RNASeq for the Biologist: Sometimes Less is More.”

6:15 – 6:30 **Break**

6:30 – 6:55 Richard Joh, PhD – Massachusetts General Hospital Cancer Center
“Gene Clustering Drives Co-regulation of Disparate Biological Pathways in Eukaryotes.”

6:55 - 7:20 Zbyszek Otwinowski, PhD – University of Texas
“Title”

7:20 - 7:35 Virginia Ma, Student – Columbus Academy
“An In-silico Design for Evaluating Cell-type Deconvolution Methods - Application to Pancreatic Cancer.”

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Wednesday, December 5, 2018

Day 2

Session 3

Protein

Chair: Wlodek Minor

- 8:30 – 8:55 Jinbo Xu, PhD – Toyota Technological Institute Chicago
“Fast and Accurate Protein Folding by Deep Learning.”
- 8:55 – 9:15 Ulrich Hansmann, PhD – University of Oklahoma
“Conformational Transitions in Proteins and Amyloids”
- 9:15 – 9:40 Agnieszka Karczynska, PhD – University of Gdansk
“Protein-protein Docking by Simulations with the Coarse-grained UNRES Force Field.”
- 9:40 – 10:05 Wlodek Minor, PhD – Virginia
“Reproducibility in Structural Biology.”
- 10:05 – 10:20 **Break**
- 10:20 – 10:45 Emilia Lubecka, PhD – University of Gdansk
“Contact- and Data-assisted Modeling of Protein Structure with the UNRES Force Field.”
- 10:45 – 11:10 Sebastian Kmiecik, PhD – University of Warsaw
“Title”
- 11:10 – 11:35 Vsevolod “Seva” Katritch, PhD – University of Southern California
“New Computational Tools for GPCR Thermo-Stabilization.”
- 11:35 – 12:00 Grzegorz A. Rempala, PhD – Ohio State University
“Classification Problem for Genetic Risk Prediction in Longitudinal Studies.”
- 12:00 - 5:00 **Break**

Session 4

Protein

Chair: Eshel Faraggi

- 5:00 – 5:25 Sergei Grudinin, PhD – National Institute for Research in Computer Science and Control
“Artificial Intelligence for Learning Protein Interactions.”
- 5:25 - 5:50 Maksim Kouza, PhD – Ohio State University
“All-atom Simulations of Peptide Aggregation.”
- 5:50 - 6:15 Marek Cieplak, PhD – Institute of Physics, Polish Academy of Science
“Folding of Knotted Proteins Under Nascent Conditions and Unfolding of Entangled Neurotoxic Polypeptides in Proteasomes.”
- 6:15 – 6:30 **Break**
- 6:30 – 6:55 Eshel Faraggi, PhD – IUPUI
“Title”
- 6:55 - 7:20 Andrzej Kloczkowski, PhD – Ohio State University
“Title”
- 7:30 – **GALA DINNER**

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Thursday, December 6, 2018

Day 3

Session 5 Human Genetics Chair: Stewart

- 8:30 – 8:55 David Bickel, PhD – University of Ottawa
“Title”
- 8:55 – 9:15 Saonli Basu, PhD – University of Minnesota
“Title”
- 9:15 – 9:40 Timothy Thornton, PhD – University of Washington
“Challenges and New Approaches for Large-Scale Whole-Genome Analysis in Multi-Ethnic Populations.”
- 9:40 – 10:05 Shilpa Pathak, PhD – Ohio State University
“Proven Epilepsy Gene Extends Healthy Life Span in Inbred Mice.”
- 10:05 – 10:20 **Break**
- 10:20 – 10:45 Jaroslaw (Jarek) Meller, PhD – University of Cincinnati
“Sig2Lead: Combining Pharmacogenomics and Cheminformatics Towards Compound Identification.”
- 10:45 – 11:10 Shili Lin, PhD – Ohio State University
“Partial Likelihood for Detecting the Effects of Two Epigenetic Factors on Complex Diseases.”
- 11:10 – 11:35 Qin Ma, PhD – South Dakota State University
“Algorithm Design and Tool Development for Gene Regulation Elucidation from Single-cell RNA-Seq data.”
- 11:35 – 12:00 William Stewart, PhD – Ohio State University
“Title”
- 12:00 – 5:00 **Break**

Session 6 Computational Medicine Chair: Bartlett

- 5:00 – 5:25 Andrzej Joachimiak, PhD – Argonne National Laboratory/University of Chicago
“X-ray and Cryo-EM Structures of Hsp 104 Disaggregase That Antagonizes Diverse Proteotoxic Misfolding Events.”
- 5:25 – 5:50 Maga Rowicka, PhD – University of Texas
“Title”
- 5:50 – 6:15 Samuel Handelman, (MD) PhD – University of Michigan
“Title”
- 6:15 – 6:30 **Break**
- 6:30 – 6:55 Christopher Bartlett, PhD – Ohio State University
“Formalisms of Quantum Computation in Genetic Analysis.”
- 6:55 - 7:10 Andrzej Kloczkowski - “Closing remarks”**