

# 2018 Workshop on Computational Structural Bioinformatics

Wednesday, August 29, 2018  
JW Marriott Washington DC, Salon D (A-B)  
<http://www.cs.odu.edu/~bioinfo/csbw.html>

Workshop Co-chairs: Filip Jagodzinski, Brian Y. Chen, Kevin Molloy  
Each talk is allotted ~ 25 minutes + 5 for questions. Keynote : 1 hour.

<b>8:00-10:00 am – Morning Session 1 – Focus : Cryo-EM</b> Session Chair: Filip Jagodzinski
<b>Opening Remarks</b>
<i>EMNets: A Convolutional Autoencoder for Protein Surface Retrieval Based on Cryo-Electron Microscopy Imaging</i> , Jingjing Yang, Renzhi Cao and Dong Si
<i>A Method for Fully Automated Particle Picking in Cryo-Electron Micrographs based on CNN</i> , Ting Da, Jianzhong Ding, Liang Yang and Gregory Chirikjian
<i>Exploratory Studies Detecting Secondary Structures in Medium Resolution 3D Cryo-EM Images Using Deep Convolutional Neural Networks</i> , Devin Haslam, Tao Zeng, Rongjian Li and Jing He
<i>A Probabilistic Anomaly Detection Method for Protein Structures Derived from Cryo-EM Density Maps</i> , Salim Sazed, Maytha Alshammari, Rayshawn Walker, Jing He and Lin Chen
<b>Coffee break 10:00-10:30, Capital Foyer</b>
<b>10:30-11:00 am – Morning Session 2</b> Session Chair: Kevin Molloy
<i>Community Detection for Decoy Selection in Template-free Protein Structure Prediction</i> , Liban Hassan, Zahra Rajabi and Amarda Shehu
<b>11:00am – noon Keynote</b> Session Chair: Brian Chen
Brian Pierce, Assistant Professor Institute for Bioscience & Biotechnology Research, University of Maryland, NIST
<i>High Resolution Modeling and Design of Immune Recognition</i>
After graduating from Duke University with a double major in Physics and Computer Science in 2000, Brian worked for two years at a software development company, then entered graduate school at Boston University where he received his Ph.D. in Bioinformatics in 2008, under advisor Prof. Zhiping Weng. He then took a Senior Scientist position at Pfizer for two years, leading computational modeling and design in the Vaccine Research group in their La Jolla laboratories. Dr. Pierce returned to academia in 2010 as a research faculty at University of Massachusetts Medical School, before joining the University of Maryland Institute for Bioscience and Biotechnology Research (IBBR) in 2014, where he is presently a tenure-track Assistant Professor (Department of Cell Biology and Molecular Genetics). His research is focused on molecular recognition and protein design, with a particular interest in biotherapeutics and immunology.

**Lunch noon – 1:00pm**

**1:00-2:30 pm – Afternoon Session 1 – Focus : Protein Structure**

Session Chair: Nasrin Akhter

*MAPS: Analyzing Peptide Binding Subsites in Major Histocompatibility Complexes*, Jinbu Wang and Brian Y. Chen

*Peptide-Binding Site Prediction From Protein Structure via points on the Solvent Accessible Surface*, Radoslav Krivak, Lukáš Jendele and David Hoksza

*Modeling the Tertiary Structure of a Multi-domain Protein*, Fahad Almsned, Gideon Gogovi, Nicole Bracci, Kylene Kehn-Hall, Estela Blaisten-Barojas and Amarda Shehu

**2:30-3:00 pm – Poster Session**

Poster boards and easels will be available in the workshop room.

**Coffee break 3:00-3:30, Capital Foyer**

**3:30-5:00 pm – Afternoon Session 2 – Focus : Modeling, Machine Learning**

Session Chair: Lin Chen

*Sub-Class Differences of pH-dependent HIV gp120-CD4 Interactions*, Nicholas Majeske, Scott Morton, Jonathan Howton and Joshua Phillips

*Low Rank Smoothed Sampling Methods for Identifying Impactful Pair-wise Mutations*, Nicholas Majeske, Filip Jagodzinski, Brian Hutchinson and Tanzima Islam

*Deep Learning for Resolution Validation of Three Dimensional Cryo-Electron Microscopy Density Maps*, Todor Avramov and Dong Si

*Dimensionality Estimation of Protein Dynamics Using Polymer Models*, Joshua Phillips, Michael Colvin and Shawn Newsam