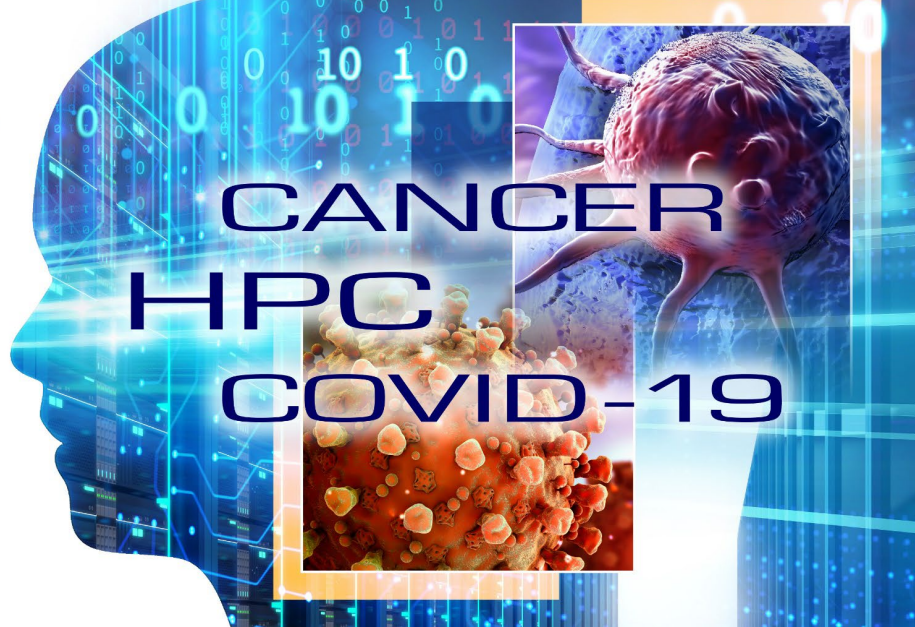


COMPUTATIONAL APPROACHES FOR CANCER WORKSHOP

CAFCW20

November 13, 2020



Program

Friday, November 13, 2020, 10:00 a.m.–6:30 p.m.

Proceedings can be viewed with a Workshop registration (deadline to purchase is Dec. 7, 2020) at <https://www.eventscribe.net/2020/SC20/index.asp?presTarget=1473834>; recording timestamps are listed in blue.

- 10:00 a.m.–10:10 a.m. **Welcome — Sixth Computational Approaches for Cancer Workshop (CAFCW20)**
Eric Stahlberg, PhD, Frederick National Laboratory for Cancer Research
- 10:10 a.m.–11:00 a.m. **Keynote: *Data Science Initiatives at the National Cancer Institute***
(4:32) Norman “Ned” Sharpless, MD, National Cancer Institute Director
Introduced by Sean Hanlon, PhD, National Cancer Institute
- 11:00 a.m.–11:45 a.m. **Panel: *HPC, Cancer and COVID-19***
(58:15) Organizer and Moderator: Patricia Kovatch, Icahn School of Medicine, Mount Sinai
Panel:
Jim Brase, Lawrence Livermore National Laboratory
Diane Del Valle, Icahn School of Medicine at Mount Sinai
Sacha Gnjatic, PhD, Icahn School of Medicine at Mount Sinai
Sharon Nirenberg, MD, Icahn School of Medicine at Mount Sinai
Carlos Simmerling, PhD, Stony Brook University
- 11:45 a.m.–12:00 p.m. ***Scalable Human Pharmacokinetics Property Prediction for Cancer Drug Discovery at ATOM***
(107:10) Presenter: Benjamin Madej, PhD, Frederick National Laboratory for Cancer Research

- 12:00 p.m.–12:15 p.m. **CAFCW20 Morning Break**
- 12:15 p.m.–12:30 p.m. *Scaffold-Induced Molecular Subgraphs (SIMSG): Effective Graph Sampling Methods for High-Throughput Computational Drug Discovery*
(121:13)
Rick Stevens; Ashka Shah; Arvind Ramanathan, PhD; Max Zvyagin; Austin Clyde
Presenters: Ashka Shah, University of Chicago, and Max Zvyagin, Argonne National Laboratory
- 12:30 p.m.–12:45 p.m. *Causal Deconvolution of a Mechanistic Model of EGFR and ERK Signaling Explains Adaptive and Genetic Resistance in Melanoma*
(135:56)
Presenter: Fabian Fröhlich, PhD, Harvard Medical School
- 12:45 p.m.–1:00 p.m. *An Efficient, Data-Driven Approach to Model Specific Cancer Cell Lines*
(150:44)
Peter Balogh, PhD; John Gounley, PhD; Amanda Randles, PhD
Presenter: Peter Balogh, PhD, Duke University
- 1:00 p.m.–1:15 p.m. *Deep Learning Based Prediction of the Temporal Behavior of RAS Protein Conformations on Simulated Cell Membrane Surfaces*
(167:03)
Brian C. Van Essen, PhD; James Glosli, PhD; Sam Adé Jacobs. PhD; Timothy S. Carpenter, PhD; Peer-Timo Bremer, PhD; Harsh Bhatia, PhD; Helgi I. Ingólfsson, PhD; Gautham Dharuman, PhD; Adam Moody
Presenter: Adam Moody, Lawrence Livermore National Laboratory
- 1:15 p.m.–2:00 p.m. **Panel #2: Digital Twins for Cancer Care**
(182:11)
Organizers: Emily Greenspan, PhD, National Cancer Institute and Eric Stahlberg, Frederick National Laboratory for Cancer Research
Moderator: Eric Stahlberg, PhD, Frederick National Laboratory for Cancer Research
Panel:
Richard Arthur, GE Research
Emily Greenspan, PhD, National Cancer Institute
Tina Hernandez-Boussard, PhD, Stanford University
- 2:00 p.m.–3:20 p.m. **Posters available at cafcw20.virtualpostersession.org;
password: cafcw20
Poster and Presenters**

A Multistaged Hyperparallel Optimization of the Fuzzy-Logic Mechanistic Model of Molecular Regulation, Paul Aiyetan, MD, Frederick National Laboratory for Cancer Research

Analyzing Tracking Graphs to Better Understand RAS Diffusion, Torin McDonald, Scientific Computing and Imaging Institute, University of Utah

Analyzing Tumor Heterogeneity thru Advanced Proteogenomic Bioinformatic Approaches, Don Johann, MD, University of Arkansas for Medical Science

Bayesian Deep Learning for Robust Information Extraction from Cancer Pathology Reports, Devanshu Agrawal, University of Tennessee at Knoxville

Developing Predictive Random Forest Models of MRP3 and MRP4 Transporter Inhibition, Amanda Paulson, PhD, Accelerating Therapeutics for Opportunities in Medicine (ATOM) Consortium

Exploring Strengths and Weaknesses of PQSAR 2, Stewart He, PhD, Lawrence Livermore National Laboratory

Large-Scale Photoacoustic Tomography: A Trade-off Between Image Quality and Computational Cost, Gabriel Bordovský, Brno University of Technology

Leveraging a Hybrid and Multiscale Model to Assist Androgen Deprivation Therapy in Recurrent Prostate Cancer Patients, Mengdi Tao, University of Pennsylvania

Long Time Evolution of Lipid Membranes, Tomas Ooppelstrup, Lawrence Livermore National Laboratory

Machine Learning for Detection of Circulating Tumor Cells by Optical Imaging without Label, Yaling Liu, PhD, Lehigh University

Making the Most of Genomic Data for Small and Medium-Sized Data Commons, Jong Cheol Jeong, PhD, University of Kentucky

Molecular Classification of Pediatric High-Risk Leukemias Using Expression Profiles of Multimodally Expressed Genes, Sneha Jariwala, University of California, Santa Cruz

Neural Collaborative Filtering Method for IC50 Prediction of drug compounds, Sookyoung Kim, PhD, Lawrence Livermore National Laboratory

Performance Evaluation of Graph Convolutional Networks for Information Extraction from Cancer Pathology Reports, Hong-Jun Yoon, PhD, Oak Ridge National Laboratory

- Probabilistic-based Interactive Machine Learning for Tomogram Segmentation and Annotation*, Talita Perciano, PhD, Lawrence Berkeley National Laboratory
- System for High Intensity Evaluation During Radiation Therapy (SHIELD-RT): A Prospective Randomized Study of Machine Learning-Directed Clinical Evaluations During Outpatient Cancer Radiation and Chemoradiation*, Julian Hong, MD, University of California, San Francisco
- Training Data Error Impacts on Deep Neural Networks for Classifying RNA-seq Gene Expressions*, Rajeev Jain, Argonne National Laboratory
- 3:20 p.m.–3:25 p.m.
(229:25) **Afternoon Welcome**
Patricia Kovatch, Icahn School of Medicine, Mount Sinai
- 3:25 p.m.–3:40 p.m.
(231:20) ***Machine Learning Driven Importance Sampling Approach for Multiscale Simulations***
Presenter: Harsh Bhatia, PhD, Lawrence Livermore National Laboratory
- 3:40 p.m.–3:55 p.m.
(246:34) ***A Metapath Approach to Predicting Drug Response in Cancer Cell Lines***
Judith D. Cohn, PhD, Los Alamos National Lab; Benjamin H. McMahon, PhD, Los Alamos National Lab; Nicholas W. Hengartner, PhD, Los Alamos National Lab; Marian Anghel, PhD, Los Alamos National Lab; Tudor Oprea, MD, PhD, University of New Mexico School of Medicine
Presenter: Judith D. Cohn, PhD, Los Alamos National Laboratory
- 3:55 p.m.–4:10 p.m.
(264:00) ***Towards a Data-Driven System for Personalized Cervical Cancer Screening***
Presenter: Geir Severin Elvatun Rakh Langberg, Cancer Registry of Norway
- 4:10 p.m.–4:40 p.m.
(278:00) ***Integration of Domain Knowledge Using Medical Knowledge Graph Deep Learning for Cancer Phenotyping***
Presenter: Mohammed Alawad, PhD, Oak Ridge National Laboratory
- 4:40 p.m.–4:55 p.m. **Afternoon Break**
- 4:55 p.m.–5:10 p.m.
(312:05) ***Deciphering Hallmarks of Resistance in Breast Cancer***
Presenter: Amrita Basu, PhD, University of California, San Francisco

5:10 p.m.–5:40 p.m.
(330:27)

Why I'm Not Answering: Understanding Determinants of Classification of an Abstaining Classifier for Cancer Pathology Reports

Sayera Dhaubhadel; Benjamin McMahon, PhD

Presenter: Sayera Dhaubhadel, Los Alamos National Laboratory

5:40 p.m.–6:25 p.m.
(358:32)

Panel #3: Translating Cancer Research Advances in Artificial Intelligence into Clinical Practice

Organizer and Moderator: Sally Ellingson, PhD, University of Kentucky

Panel:

Douglas W. Blayney, MD, Stanford University Medical Center

Cody Bumgardner, PhD, University of Kentucky

Stephanie Harmon, PhD, National Cancer Institute

Yaling Liu, PhD, Lehigh University

6:25 p.m.–6:30 p.m.
(403:20)

CAFCW20 Wrap-Up

Keynote



Norman "Ned" Sharpless, MD, National Cancer Institute

Dr. Ned Sharpless has served as the director of the National Cancer Institute since October 2017. Previously, Dr. Sharpless served as acting commissioner of the U.S. Food and Drug Administration, director of the University of North Carolina Lineberger Comprehensive Cancer Center and on the faculty of Harvard Medical School.

Dr. Sharpless earned his medical degree from UNC and completed his internal medicine residency at Massachusetts General Hospital and a hematology/oncology fellowship at Dana-Farber and Partners Cancer Care.

Dr. Sharpless is a member of the Association of American Physicians as well as the American Society for Clinical Investigation (ASCI), the nation's oldest honor society for physician–scientists. He served on the ASCI council from 2011 to 2014. He has written more than 150 original scientific papers, reviews and book chapters and holds 10 patents. He co-founded two clinical-stage biotechnology companies: G1 Therapeutics and HealthSpan Diagnostics.

In addition to serving as Director of NCI, Dr. Sharpless is Chief of the Aging Biology and Cancer Section in the National Institute on Aging's Laboratory of Genetics and Genomics, where he continues his research on the biology of the aging process that promotes the conversion of normal self-renewing cells into dysfunctional cancer cells. Dr. Sharpless has made pivotal contributions to the understanding of the relationship between aging and cancer and in the preclinical development of novel therapeutics for melanoma, lung cancer and breast cancer.

Thank you to our CAFCW20 Program Committee:

Frank Alexander, PhD, Brookhaven National Laboratory

Orly Alter, PhD, University of Utah

John Baldoni, PhD, Integral Health, Inc.

Jeff Buchsbaum, MD, PhD, National Cancer Institute

Fernanda Foertter, BioTeam

Emily Greenspan, PhD, National Cancer Institute

Ryuji Hamamoto, PhD, National Cancer Center Japan/RIKEN, Tokyo

Abdul Hamid Halabi, NVIDIA

Florence Hudson, Northeast Big Data Innovation Hub, Columbia University

Steven Litster, PhD, Amazon Web Services

Michael McManus, PhD, Intel

William Richards, PhD, Brigham and Women's Hospital, Harvard Medical School

Ilya Shmulevich, PhD, Institute for Systems Biology

Thomas Steinke, PhD, Zuse Institute Berlin

Kristin Swanson, PhD, Mayo Clinic Arizona

George Zaki, PhD, Frederick National Laboratory

CAFCW20 Organizing Committee:

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Sean Hanlon, PhD, National Cancer Institute

Sally Ellingson, PhD, University of Kentucky

Patricia Kovatch, Icahn School of Medicine, Mount Sinai

Petrina Hollingsworth, Frederick National Laboratory for Cancer Research

Lynn Borkon, Frederick National Laboratory for Cancer Research