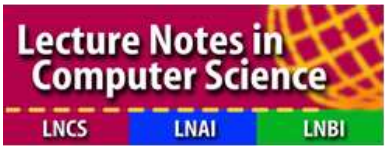
3nd International Symposium on Mathematical and Computational Oncology (ISMCO'21)

October 11-13, 2021, Virtual (Pacific Standard Time – PST)

ISMCO 2021

Contents

Registration Desk Hours: N/A



Monday, October 11th

8:50–9:00	*Welcome* – **George Bebis, University of Nevada, Reno**	
9:00–10:00	*Keynote:* **Eytan Ruppin**, **CDSL, NCI, NIH, USA** Moderator: Russell Rockne	
10:10-11:10	**Statistical and Machine Learning Methods for Cancer Research** Chair: Anne Deslattes Mays	
	10:10	**Kristen Anderson and Sharon Hori**. Image Classification of Skin Cancer: Using Deep Learning as a Tool for Skin Self-Examinations
	10:30	**Hayan Lee, Gilbert Feng, Ed Esplin and Michael Snyder**. Predictive Signatures for Lung Adenocarcinoma Prognostic Trajectory by Multiomics Data Integration and Ensemble Learning
	10:50	**Arnav Solanki, Marc Riedel, James Cornette, Julia Udell, Ishaan Koratkar and George Vasmatzis**. The Role of Hydrophobicity in Peptide-MHC Binding
11:10-11:30	Coffee Break	
11:30-12:10	**Spatio-temporal tumor modeling and simulation I** Chair: Chengyue Wu	
	11:30	**David Bernard, Anthony Kobanda and Sylvain Cussat-Blanc**. Simulating cytotoxic T-lymphocyte & cancer cells interactions : An LSTM-based approach to surrogate an agent-based model
	11:50	**Iurii Nagornov, Jo Nishino and Mamoru Kato**. tugHall version 3.0: a tool to simulate a personal evolution of cancer cells with copy number alterations
12:10-1:30	Lunch Break	
1:30-2:30	*Keynote:* **Elli Papaemmanuil**, **Memorial Sloan Kettering Cancer Center, USA** Moderator: George Bebis	
2:30-3:00	Coffee Break	
3:00-4:30	**Panel Discussion** Moderator: Anne Deslattes Mays (Science and Technology Consulting LLC)	
	Topic: Bringing Mathematical and Computational Methods to the Broader Oncology Community **Panelists** • Soheil Meshinchi, Fred Hutchinson Cancer Center • Ching Lau, The Jackson Laboratory • Adam Resnick, Children's Hospital of Philadelphia • George Vasmatzis, Mayo Clinic Zoom link: **https://us06web.zoom.us/j/81787609784?pwd=UlBFSFJNR1A0WXYzTEQ3MlhyM0lWZz09**	

Tuesday, October 12th

9:00–10:00	*Keynote:* **Paul K. Newton, University of Southern California, USA** Moderator: Ernesto Bueno da fonseca Lima	
10:10-11:10	**General cancer computational biology** Chair: Dinler Antunes	
	10:10	**Julia Udell, Marc Riedel and George Vasmatzis**. Prediction of neoantigenic peptides derived from chromosomal rearrangements in mesothelioma
	10:30	**Tom van den Bosch and Daniel Miedema**. Chromosomal copy number heterogeneity predicts survival rates across cancers
	10:50	**Tina Ghodsi Asnaashari and Young Hwan Chanag**. Strategies to reduce long-term drug resistance by considering effects of differential selective treatments
11:10-11:30	Coffee Break	
11:30-12:30	**Mathematical Modeling for Cancer Research** Chair: Russell Rockne	
	11:30	**Thierry Goudon, Kevin Atsou and Veronique Braud**. A PDE Model for tumor-immune system interctions that captures equilibtium and escape phase
	11:50	**Chloé Colson, Helen M. Byrne and Philip K. Maini**. Mathematical modelling of tumour response to combined treatments of hyperthermia and radiotherapy
	12:10	**Teddy Lazebnik and Svetlana Bunimovich-Mendrazitsky.** Improved Geometric Configuration for the Bladder Cancer BCG-based Immunotherapy Treatment Model
12:30-1:30	Lunch Break	
1:30-2:30	*Keynote:* **Tom Yankeelov, The University of Texas at Austin, USA** Moderator: Kathleen Wilkie	
2:30-3:00	Coffee Break	
3:00-7:00	**Tutorial I**	
	Current methods and open challenges for structural modeling in cancer immunotherapy Instructors: Antunes Dinler, Maurício M. Rigo, Andre Fonseca, Sarah Hall-Swan, Lydia Kavraki Zoom link: **https://riceuniversity.zoom.us/j/96681193182?pwd=MVo3bkt0eW9Vb3NGMm1Ydmt1R1RTUT09**	

Wednesday, October 13th

9:00–10:00	*Keynote:* **Georg Luebeck, Fred Hutchinson Cancer Research Center, USA** Moderator: Heyrim Cho	
10:10-11:10	**Computational methods for anticancer drug development** Chair: Kathleen Wilkie	
	10:10	**Mauricio M. Rigo, Dinler A. Antunes, Anja Conev, Romanos Fasoulis, Sarah Hall-Swan and Lydia Kavraki**. Molecular Dynamics and Ensemble Generation as a Tool to Study pHLA-I:TCR Interaction Towards Cancer Immunotherapy
	10:30	**Stephanie Owen, Cyrus Nosrati, Dagim Tadele, Jeffrey Maltas, Michael Hinczewski and Jacob Scott**. Ecological epistasis can drastically alter evolutionary trajectories on genotypic fitness landscapes, neutralizing or mimicking genetic selection in evolutionary simulations
	10:50	**Josua Aponte-Serrano and Amit Hagar**. Run for your life – an integrated virtual tissue platform for incorporating exercise oncology into immunotherapy
11:10-11:30	Coffee Break	
11:30-12:10	**Spatio-temporal tumor modeling and simulation II** Chair: Ernesto Bueno da fonseca Lima	
		Nikolaos Dimitriou, Salvador Flores-Torres, Joseph Matthew Kinsella and Georgios Mitsis. Validating hybrid spatiotemporal models of tumour growth with 3D cell culture data
		Jason M. Gray, Stephanie Owen, Michael Hinczewski and Jacob Scott. Simulating Cancer Initiation, Evolution, and Immune Evasion in a Spatial Four Phenotype Model
12:10-1:30	Lunch Break	
1:30-2:30	*Keynote:* **Mona Singh, Princeton University, USA** Moderator: George Vasmatzis	
2:30-3:00	Coffeee Break	
3:00-7:00	**Tutorial II**	
	How can (experimental) data go on tumor growth models? Instructors: Ernesto A. B. F. Lima, Emanuelle A. Paixao Zoom link: **https://utexas.zoom.us/j/91952684049?pwd=NjJUeEFOakJBNDBaUmhTT0JsUzNiUT09**	

KEYNOTE TALK

Monday, October 11, 2021 at 9am

Precision oncology via the tumor transcriptome

Eytan Ruppin
CDSL, NCI, NIH
USA

Abstract: Precision oncology has made significant advances, mainly by targeting actionable mutations and fusion events involving cancer driver genes. Aiming to expand treatment opportunities, recent studies have begun to explore the utility of tumor transcriptome to guide patient treatment. I will introduce a new approach, termed SELECT, which harnesses genetic interactions to successfully predict patient response to cancer therapy from the tumor transcriptome. SELECT is tested on a broad collection of 35 published targeted and immunotherapy clinical trials from 10 different cancer types. It is predictive of patients' response in 80% of these clinical trials and in the recent multi-arm WINTHER trial. In summary, we report the first systematic, transcriptomics-based approach that is predictive across many targeted and immune therapies. The predictive signatures and the code are made publicly available for academic use, laying a basis for future prospective clinical studies. As time permits, I will provide a brief overview of MadHitter, a new approach for guiding precision cancer therapy based on single cell tumor transcriptomics.

Speaker Bio-Sketch: Eytan Ruppin received his M.D. and Ph.D. (Computer Science) from Tel-Aviv University where he has served as a professor of Computer Science & Medicine since 1995, conducting computational multi-disciplinary research spanning a wide variety of topics, including neuroscience, machine learning and systems biology. He joined the University of Maryland in July 2014 as director of its center for bioinformatics and computational biology and moved to the NCI in January 2018 as chief of its newly established cancer data science branch (CDSL). His lab co-identified the first metabolic synthetic lethal (SL) drug target to treat cancer (Nature, 2011), was the first to identify metabolic SLs in cancer in a genome-wide manner (Molecular Systems Biology, 2011) and the first to infer cancer SLs by mining patients tumor data (Cell, 2014). More recently, his research has been focused on developing new computational approaches for SL/transcriptomics based precision oncology (Nat Comm 2018, MSB 2019, Cancer Cell 2019, NCB 2019, Science Advances 2021, Cell 2021) and for immunotherapy (Nat Med 2018, Cell 2018, JAMA Onc 2019, Nat Cancer 2020). Eytan is a co-founder of a few startup companies involved in precision medicine and cancer drug discovery, including Metabomed, Medaware and Pangea Therapeutics an editorial board member of EMBO Reports and Molecular Systems Biology and a fellow of the International Society of Computational Biology (ISCB).

KEYNOTE TALK

Monday, October 11, 2021 at 1:30pm

Population genomic approaches for molecular biomarker discovery in clinical oncology

Elli Papaemmanuil
Memorial Sloan Kettering Cancer Center
USA

Abstract: Recent characterization of the genes recurrently mutated in cancer have led to the routine implementation of tumor profiling at diagnosis with the expectation to diagnose and treat patients according to their unique molecular profile - the vision of precision medicine. However, development of molecularly guided clinical decision support tools warrants the delivery of evidence based, data driven, comprehensive models that extend beyond single markers. In my talk I will discuss critical considerations for biomarker characterization, statistical model development, and clinical decision support tool development for clinical adoption.

Speaker Bio-Sketch: Dr. Papaemmanuil got her BSc and MSci in Human Molecular Genetics with Honors at the University of Glasgow and her PhD in Human population genetics at the Institute of Cancer Research in London. She performed her postdoctoral studies at the Wellcome Trust Sanger Center and joined the University of Cambridge as faculty, prior to moving to the Memorial Sloan Kettering Cancer Center. Dr. Papaemmanuil has employed genome profiling methodologies to study the role of acquired mutations in cancer development and how these determine clinical phenotype and response to therapy. More recently she has established high-throughput laboratory profiling approaches and developed statistical modelling methodologies that integrate clinical and molecular parameters to inform patient tailored disease classification and clinical decision support (prognosis and treatment decisions). Her main research motivation is to develop research that helps translate recent cancer genome discoveries into clinical practice. Her current research spans, bioinformatic and algorithmic platform development, biomarker discovery and validation and experimental models of disease biology. Additionally, Dr. Papaemmanuil has a strong interest to understand the effects of treatment in disease progression and genetic drivers of treatment response. Dr. Papaemmanuil leads the Pediatrics Precision medicine initiative for MSK Kids, which sets out to evaluate, validate and deliver a clinical prototype for integrative whole genome and whole transcriptome sequencing analyses to understand mechanisms of disease biology and guide treatment strategies in pediatric cancers.

KEYNOTE TALK

Tuesday, October 12, 2021 at 9am

Three problems in mathematical oncology

Paul K. Newton
Viterbi School of Engineering and Ellison Institute for Transformative Medicine
University of Southern California
USA

Abstract: I will introduce three problems in mathematical oncology all of which involve nonlinear dynamics and control theory. First, I will describe our work using Markov chain models to forecast metastatic progression. The models treat progression as a (weighted) random walk on a directed graph whose nodes are tumor locations, with transition probabilities obtained through historical autopsy date (untreated progression) and longitudinal data (treated) from Memorial Sloan Kettering and MD Anderson Cancer Centers. Then, I will describe our models (both deterministic and stochastic) that use evolutionary game theory (replicator dynamics/Moran processes with prisoner's dilemma payoff matrix) to design multi-drug adaptive chemotherapy schedules to mitigate chemo-resistance by suppressing 'competitive release' of resistant cell populations. The models highlight the advantages of antagonistic drug interactions (over synergistic ones) in shaping the fitness landscape of co-evolving populations. Finally, I will describe our work on developing optimal control schedules (based on Pontryagin's maximum principle) that maximize cooperation for prisoner's dilemma replicator dynamical systems.

Speaker Bio-Sketch: Professor Newton received his B.S. (cum laude) degree in Applied Mathematics/Physics at Harvard University in 1981 and his Ph.D. in 1986 from the Division of Applied Mathematics at Brown University. He then moved to the Mathematics Department at Stanford University to work as a post-doctoral scholar under J.B. Keller. He became Assistant (1987) and Associate Professor (1993) in the Mathematics Department at the University of Illinois Champaign-Urbana (UIUC) and at the Center for Complex Systems Research (CCSR) at the Beckman Institute. In 1993 he moved to the Aerospace & Mechanical Engineering Department and the Mathematics Department at the University of Southern California and was promoted to Full Professor in 1998. Trained as an applied mathematician, Professor Newton's work focuses on developing mathematical models for nonlinear dynamical processes in continuum mechanics and biophysics, currently focusing mostly on mathematical oncology and systems biology. He has held visiting appointments at Caltech, Brown, Hokkaido University, The Kavli Institue for Theoretical Physics at UC Santa Barbara, and The Scripps Research Institute where he functioned as head of the mathematical modeling section of the NCI supported Physical Sciences Oncology Center (2009-2014). He is currently a Professor of Applied Mathematics, Engineering, and Medicine in the Viterbi School of Engineering, the Dornsife College of Letters, Arts and Sciences, the Norris Comprehensive Cancer Center in the Keck School of Medicine, and a founding affiliate member of the LJ Ellison Institute for Transformative Medicine of USC. He currently serves as Editor-in-Chief of the Journal of Nonlinear Science (SpringerNature).

KEYNOTE TALK

Tuesday, October 12, 2021 at 1:30pm

Towards optimizing therapy on a patient specific basis via imaging-based mathematical modeling

Tom Yankeelov
Oden Institute for Computational Engineering and Sciences
Livestrong Cancer Institutes
Departments of Biomedical Engineering
Diagnostic Medicine, Oncology
The University of Texas at Austin
USA

Abstract: The ability to accurately predict the response of tumors to therapy, and then use this information to optimize treatment on an individual patient basis, would dramatically transform oncology. In an attempt to move in this direction, we have developed a clinical-mathematical framework that integrates quantitative magnetic resonance imaging (MRI) data into mechanism-based mathematical models to predict the response of locally advanced breast cancer to neoadjuvant therapy. We will present our recent efforts on this topic and then discuss how these methods can be extended to enable patient-specific simulations of treatment response to a range of therapeutic regimens, thereby providing a pathway for optimizing therapy on a patient-specific basis.

Speaker Bio-Sketch: Tom Yankeelov is the W.A. "Tex" Moncrief Chair of Computational Oncology and Professor of Biomedical Engineering, Diagnostic Medicine, and Oncology at The University of Texas at Austin. Dr. Yankeelov is the founding Director of the Center for Computational Oncology, and also serves as co-Director for the Quantitative Oncology Research Program and Director of Cancer Imaging Research within the Livestrong Cancer Institutes at UT Austin. The overall goal of Dr. Yankeelov's research is to develop tumor forecasting methods by integrating advanced imaging technologies with predictive, multi-scale models of tumor growth to optimize therapy. This is accomplished by dividing his efforts into approximately equal parts mathematical modeling, pre-clinical development, and implementation in clinical trials.

KEYNOTE TALK

Wednesday, October 13, 2021 at 9am

Barrett's Esophagus: efficient design of multiscale simulations for surveillance and treatment

Georg Luebeck
Fred Hutchinson Cancer Research Center
USA

Abstract: Barrett's Esophagus (BE), a metaplastic tissue alteration associated with gastroesophageal reflux, predisposes to esophageal adenocarcinoma (EAC). Endoscopic screening of patients with persistent symptomatic reflux aims to identify patients with BE at risk of progressing to cancer. Such patients are recommended to undergo follow-up examinations for dysplasia or small cancers in the earliest stages. This is useful because the prognosis for EAC detected at an early stage is dramatically better than for advanced stages that are mostly lethal. Thus, endoscopic surveillance of BE, in which multiple biopsies are routinely examined for preneoplastic changes and/or early neoplastic lesions, will increase patient survival compared with patients diagnosed with EAC without prior BE surveillance. However, over-diagnosis is a major concern because the annual rate of progression from BE to EAC is less than 1% overall but depends on age, gender, race/ethnicity, BE segment length, history of gastroesophageal reflux and other life-style factors. Multiscale models that include these factors have been developed but suffer computational bottlenecks and are technically demanding. In this talk I will discuss how mathematical insights and multitype branching process theory can be used to significantly speed up simulations to assess and evaluate various screening modalities in a large number of individuals.

Speaker Bio-Sketch: Georg Luebeck is a member in the Herbold Computational Biology Program at the Fred Hutchinson Cancer Research Center and Affiliate Professor in Applied Mathematics (University of Washington). Inspired by the pioneering work of Moolgavkar, Venzon, and Knudson (MVK), he has made significant contributions to stochastic models of cancer and its precursors based on principles of multistage carcinogenesis. Among them, the development of mathematical and computational tools to facilitate the application of stochastic multistage clonal expansion (MSCE) models to cancer screening, intervention, and prevention, in particular for colorectal cancer and esophageal adenocarcinoma. His recent work focuses on age-related epigenetic drift and its impact on aging and cancer development in colon and esophagus. In Luebeck et al., Cancer Res. 2019 vol 79(3), he explored the implications of epigenetic drift in colorectal tissues and its potential role as a selective force in neoplasia. Similarly, he and his colleagues identified significant effects of differential epigenetic drift in Barrett's esophagus (BE) associated with biological tissue aging and silencing of genes that are known to repress endogeneous retroviruses.

KEYNOTE TALK

Wednesday, October 13, 2021 at 1:30pm

Integrative methods for deciphering cancer networks

Mona Singh
Princeton University
USA

Abstract: Networks of molecular interactions underlie virtually all functions executed within a cell. Networks thus provide a powerful foundation within which to interpret a wide range of rapidly accumulating biological data. In this talk, I will present formulations and algorithms that leverage the structure and function of biological networks in order to analyze cancer genomes and discover cancer-relevant genes. This is a difficult task, as numerous somatic mutations are typically observed in each cancer genome, only a subset of which are cancer-relevant, and very few genes are found to be somatically mutated across large numbers of individuals. I will introduce a framework that can rapidly integrate multiple sources of information about molecular functionality in order to discover key interactions within a network that tend to be disrupted in cancers. Crucially, our approach is based on analytical calculations that obviate the need to perform time-prohibitive permutation-based significance tests. Next, I will describe algorithms that consider both prior and newly collected data within a network context in order to uncover cancer-relevant subnetworks. Overall, our work showcases the versatility and power of a network viewpoint in advancing biomedical discovery.

Speaker Bio-Sketch: Mona Singh obtained her AB and SM degrees at Harvard University, and her PhD at MIT, all three in Computer Science. She did postdoctoral work at the Whitehead Institute for Biomedical Research. She has been on the faculty at Princeton since 1999, and currently she is Professor of Computer Science in the computer science department and the Lewis-Sigler Institute for Integrative Genomics. She received the Presidential Early Career Award for Scientists and Engineers (PECASE) in 2001, and is a Fellow of the International Society for Computational Biology and a Fellow for the Association for Computing Machinery. She is Editor-In-Chief of the Journal of Computational Biology. She has been program committee chair for several major computational biology conferences, including ISMB (2010), WABI (2010), ACM-BCB (2012), and RECOMB (2016), and has been Chair of the NIH Modeling and Analysis of Biological Systems Study Section (2012-2014).

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Sadanandam	Anguraj	Institute of Cancer Research (ICR)
Satagopam	Venkata Pardhasaradhi	University of Luxembourg and ELIXIR-Luxembourg
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Textor	Johannes	Radboud University
Tian	Xiaojun	Arizona State University
Trucu	Dumitru	University of Dundee
Tuller	Tamir	Tel Aviv University
Ushizima	Daniela	Lawrence Berkeley National Laboratory
Vakil	Vahideh	Rutgers University
Vasmatzis	George	Mayo Clinic
Viossat	Yannick	Université Paris-Dauphine
Wass	Mark	University of Kent
Xu	Yanji	Rare Disease Informatics, NIH
Yamaguchi	Rui	Aichi Cancer Center Research Institute
Yuan	Bo	Harvard University
Zehavi	Meirav	Ben-Gurion University
Zelikovsky	Alex	Georgia State University

Discussion Panel

Bringing Mathematical Methods to the Broader Oncology Community

Moderator

- Deslattes Mays Anne, Science and Technology Consulting, LLC

Panelists

- Soheil Meshinchi, Fred Hutchinson Cancer CenterChen Ken, MD Anderson
- Ching Lau, The Jackson Laboratory
- Adam Resnick, The Children's Hospital of Philadelphia
- Lincoln Stein, Ontario Institute for Cancer Research
- Jinghui Zhang, St. Jude Children's Research Hospital

Tutorials

(1) Current methods and open challenges for structural modeling in cancer immunotherapy - 3rd Edition

Instructors:

- Antunes Dinler, Rice University, USA
- Fonseca Andre, University of Houston, USA
- Hall-Swan Sarah, Rice University, USA
- Lydia Kavraki, Rice University, USA
- Rigo Mauricio, Pontifical Catholic University of Rio Grande do Sul, Brazil

(2) How can (experimental) data go on tumor growth models?

Instructors:

- Ernesto Lima, The University of Texas at Austin, USA
- Emanuelle A. Paixao, National Laboratory of Scientific Computing (LNCC), Brazil