# Round Table Assignments

**Camacho**

xiaosong wang
Jiyoung Lee
Lexi Morrissey
Elissa Fink
Karolina Mikulska-Ruminska
Fernando Concha-Benavente
Marta Wells
bill hawse
ivet bahar

**Benos/Finn**

Abigail Overacre-Delgoffe
Anda Vlad
Dimitris Manatakis
Amanda Kowalczyk
Jingyu Zhang
Shu Wang
Nathan Clark
Neha Abraham

**Morel/Faeder**

Hongchun Li
xiaojun tian
Brian Dang
Nassima Bouhenni
Christopher Dunstan
Nicole Matamala
Deepa Issar
Nicolas Pabon

**Shlomchik/Liu**

Malcolm Hoffman
Sherry Zhang
robin lee
anne carvunis
Stephen Moore
Hyokyeong Lee
Shuchi Smita

**Vignali/Chikina**

Louise D'Cruz
Kieran Okerstrom
Wayne Mao
Raghav Partha
Connor Higgins
Leonard Watson
Nina Senutovitch
Michelle Patino

**Borghesi**

David Koes
Ketan Maheshwari
Michelle Miller
Tony Cillo
Henry Ma
Bentley Wingert

**Chennubhotla**

James Krieger
Luong Nguyen
Miller Mrosek
Luca Ponzoni
Karl Keat
McKenzie Grundy

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## 1. Carlos Camacho (Structural)

Dr. Carlos J. Camacho, PhD has achieved international recognition for his work in the biophysics of protein interactions, molecular recognition, antigenicity and drug discovery. He developed the first automated method to predict docked proteins "ClusPro" (now licensed to Schrodinger LLC). His lab has also developed novel technologies to predict predict/design novel (ant)-agonists to difficult pharmaceutical targets by searching the largest chemical libraries in the world. In this area, he has ongoing collaboration in disease areas as diverse as leukemia, ovarian, and breast cancers, proteasome and HIV among others. His most recent work involves understanding PD-1 druggability. Dr. Camacho has published more than 80 peer reviewed papers (H-index 39). Full list of publications is listed at https://scholar.google.com/citations?user=vP5B95UAAAAJ&hl=en.

## 2. Takis Benos and Olja Finn (Genomics)

Drs. Finn and Benos are collaborating on a project that aims to elucidate causal relationships in gene expression data sets that can provide mechanistic insight into anti-cancer immunity and help predict responses to cancer vaccines and eventually other forms of immunotherapy. Their first project is on a gene expression data set derived from participants in a large, multicenter trial of a vaccine for cancer prevention. In this round table, we will discuss issues related to the problems of cancer vaccine research and problems related to computational causal discovery in heterogeneous biomedical datasets.

Olivera (Olja) J. Finn, Ph.D. Dr. Finn is University of Pittsburgh Distinguished Professor of Immunology and Surgery and Founding Chair of the Department of Immunology. She is the discoverer of the MUC1 tumor antigen and has published extensively and continuously for the last 30 years on the basic and preclinical work on MUC1 cancer vaccines. She has been a co-investigator on a dozen clinical trials of various MUC1 vaccines in pancreatic, colon, breast, prostate and lung cancer. Her current efforts are on the development and clinical testing of preventative cancer vaccines. She has received many honors the most recent being the American Association of Immunologists Life Time Achievement Award (2016), The American Association for Cancer Research Cancer Immunology Prize (2017) and the National Cancer Institute Outstanding Investigator Award (2016). The NCI Award provides long-term funding for her research in cancer immunoprevention.

Dr. Panayiotis (Takis) Benos is Professor and Vice Chair of the Department of Computational and Systems Biology, University of Pittsburgh School of Medicine. He is also a member of the University of Pittsburgh Cancer Institute (UPCI) and holds joint (courtesy) appointments with the Department of Biomedical Informatics (DBMI) and Department of Computer Science, University of Pittsburgh. His laboratory has developed statistical and machine learning algorithms to model transcriptional and post-transcriptional regulatory networks in disease. In recent years, he has expanded his efforts in the area of causal modeling and discovery, especially from heterogeneous, multi-modal biomedical data. He is a Project Leader in the BD2K Center for Causal Discovery and PI on multiple NIH grants related to algorithmic development and applications of causal discovery methods in diverse biomedical problems.

## 3. Penny Morel and Jim Faeder (Systems Modeling)

In the last several years Drs. Faeder and Morel have been actively collaborating on understanding the basis of how TCR signal strength controls T helper cell fate. This computational model led to some testable predictions, which have opened new research directions.

James R. Faeder, PhD, is Associate Professor of Computational and Systems Biology at the University of Pittsburgh School of Medicine. His research focuses on the development of novel computational methods and tools for the modeling and simulation of cell regulatory networks, as well as their application to specific systems of basic and biomedical relevance including immune regulation, cancer, and chemo-sensing in bacteria. Dr. Faeder is the co-leader of the Cell Modeling component of the NIH P41 center for Multiscale Modeling of Biological Systems (MMBioS) at the University of Pittsburgh, which supports development of the MCell simulation platform for simulation of spatially realistic 3-D cellular models. His group also leads the development of the BioNetGen software for rule–based modeling of biochemical systems and is currently working on the integration ofrule-based and spatial modeling. Dr. Faeder has worked on a number of projects involving immune receptor signaling and has active collaborations with

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several members of the Immunology Department, including Penny Morel, Sarah Gaffen, and Dario Vignali. Each of these projects involves the development of predictive models of immunoreceptor signaling with the goal of determining the mechanisms that affect cell fate decisions.

Penelope A. Morel, MD, is Professor of Immunology with a secondary appointment in Medicine, Division of Rheumatology. Dr. Morel's work focuses on basic immunological mechanisms in the context of autoimmune disease as well as normal immune responses. She has a longstanding interest in the use of computational and mathematical models for the deeper understanding of immunological processes, and her lab was among the first to use mathematical modeling to better understand immune responses with initial studies focused on Th1/Th2 cross regulation.

## 4. Mark Shlomchik and Bing Liu (TLRs & Systems modeling)

In this round table, Dr Shlomchik will lead the discussion on the distinct roles of Toll-like receptors in systemic autoimmunity. Dr Liu will share his experience on using systems-level modeling to elucidate how TLR pathway crosstalk enables macrophages to fine-tune their responses to multiple, temporally separated infection events. Future collaborations will also be discussed.

Dr. Mark J. Shlomchik, PhD received his medical and doctoral degrees in 1989 from the University of Pennsylvania, where he also completed residency training in pathology and laboratory medicine. After postdoctoral work at Fox Chase Cancer Center in Philadelphia, again working with Martin Weigert, he joined the faculty at Yale University, rising to the rank of full professor in 2004. In July 2013, he was named Chair of Department of Immunology, Pitt School of Medicine. Dr. Shlomchik's lab investigates B cell immune responses and the pathogenesis of systemic autoimmune diseases, especially lupus. The origins of SLE have been a longstanding interest dating back to Dr. Shlomchik's PhD thesis, which helped to elucidate how the process of clonal expansion and selection led to the generation of autoantibodies. His lab has contributed to the understanding of distinct roles of Toll-like receptors in systemic autoimmunity. The role of antigen presentation to T cells in autoimmunity has been a particular area of interest. Dr. Shlomchik helped elucidate the unique roles of B cells in this process, and more recently has dissected the roles of DCs in tissue pathogenesis. His lab also works on understanding the development of high affinity antibody responses and immune memory, which are fundamental to vaccine responses and long-lived immunity to pathogens.

Dr. Bing Liu, PhD is a Research Assistant Professor at the Department of Computational and Systems Biology, University of Pittsburgh. His research focuses on the development of computational modeling, simulation and analysis techniques for the study of biological systems. He has developed probabilistic approximation techniques for capturing the dynamics of biological networks and a suite of advanced algorithms for calibrating mathematical models, discovering new biology, and predicting therapeutic strategies. As an integral part of his research, he works closely with biologists to study various biological pathways related to innate immunity and cell death. His work contributed to the understanding of regulatory mechanisms of complement systems and also revealed STAT1-mediated TLR3-TLR7 pathway crosstalk which confers innate immune memory and homeostasis.

## 5. Dario Vignali and Maria Chikina (Genomics)

Drs. Vignali and Chikina have been collaborating on the analysis of gene expression datasets of tissue lymphocytes from tumor and autoimmunity model systems. Our round table discussion will focus on what we have learned about working with small cell numbers and complex mixtures of multiple cell types, and what technical and quality control measures need to be considered and utilized in order to obtain robust datasets.

Dario Vignali, PhD is the Frank Dixon Chair in Cancer Immunology, Vice Chair and Professor of Immunology in the Immunology Department, University of Pittsburgh School of Medicine. He is also co-Leader of the Cancer Immunology Program and co-Director of the Tumor Microenvironment Center in the UPMC Hillman Cancer Center. His research focuses on molecular and cellular aspects of negative

regulatory immune mechanisms including regulatory T cells, inhibitory receptors, and inhibitory cytokines. His lab was instrumental in uncovering the role of Lag3 in mouse models of cancer, tolerance, autoimmunity and immune regulation. His lab discovered the inhibitory cytokine IL35 and the Nrp1:Sema4a axis, which are key regulators of intratumoral Treg stability and function. The majority of his work focuses on analysis of these pathways in murine models of cancer and numerous human tumors. He also studies regulatory mechanisms in autoimmunity, especially and type 1 diabetes. He has published over 160 papers with over 20 as senior or co-author in high impact journals (Nature, Cell, Science, Nature Immunology, Nature Biotechnology, Nature Methods, Immunity, Science Immunology and EMBO).

Maria Chikina, PhD is an Assistant Professor of Computational and Systems Biology, University of Pittsburgh School of Medicine. Her research interests include analyzing pathway and composition effects in gene expression, integration and consistency analysis of clinical datasets and molecular evolution. She has had a specific interest in immunology for several years and her previous immunology related experience involves postdoctoral research in a systems immunology group and participation in automated flow cytometry analysis (FlowCAP) competitions.

## 6. Lisa Borghesi (tSNE projections from flow cytometry)

Drs. Borghesi and Maheshwari are collaborating on a project that exploits newly available algorithmic population discovery methods to analyze immune cell subsets across immunologic tissues within individual humans and between different people. Their first project applies computational tools to large-scale multidimensional flow cytometry data for the study of B lymphocytes. Most of what we know about human B cells comes from peripheral blood, thus our basic knowledge of the humoral component of the human immune system across different tissues is very limited. In this round table, we will discuss the tools of computational flow modeling that are (1) available in the FlowJo software, and (2) the in-progress computational flow pipeline we are implementing on Pitt's high performance cluster.

Dr. Lisa Borghesi, Ph.D. is an Associate Professor in the Department of Immunology. Her laboratory focuses on hematopoiesis and B cell fate choice using murine and humanized mouse models. She is Scientific Director of the Unified Flow Cytometry Core in the School of Medicine and has garnered more than $1.2 million in NIH funding to advance core instrumentation. Her new efforts to combine state-of-the-art high throughput flow cytometry technology with cutting edge computational methods are funded by a CTSI grant (2017).

Dr. Ketan Maheshwari, Ph.D. is a Research Assistant Professor in the Department of Chemistry. Ketan is interested in computational applications of science and engineering, both pure and interdisciplinary. He has expertise in developing, porting, debugging and documenting applications over HPC architectures. He is a technologies enthusiast and likes to wrestle with Python, R, and Linux. Ketan is currently actively collaborating with Prof. Borghesi developing computational techniques to process cytometry data, a research funded by the above CTSI grant.

## 7. Chakra Chennubhotla (Imaging)

Tumor heterogeneity and cell-cell communication in tumor microenvironments play a critical role in drug resistance and metastasis. There is a lack of systematic approach for studying cancers as integrated heterocellular systems, and a critical knowledge gap on how different cell types in a tumor microenvironment simultaneously collaborate to drive invasion/metastasis and therapeutic resistance phenotypes. The discussion will evolve around: 1) Developing and optimizing innovative system biology platforms that may be broadly applicable to studies of intratumor heterogeneity in different tumor types; 2) Designing novel biomarkers that might be useful for guiding patient stratification, therapy selection, and eventually changing clinical practice.

Dr. Chakra Chennubhotla, PhD is an Associate Professor in the Department of Computational and Systems Biology, University of Pittsburgh School of Medicine. He is also a member of the Department of Biomedical Informatics (DBMI) and Department of Computer Science, University of Pittsburgh. His group leads the efforts in computational spatial tumor pathology as part of the ongoing NIH grant on quantifying spatial intratumor heterogeneity.

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