Penn Institute for Computational Science

The Penn Institute for Computational Science (PICS) is a cross-disciplinary institute for the advancement, integration, and support of Penn research via the tools and techniques of high-performance computing. Because scientific computing stretches across all areas of science, engineering, medicine and increasingly the humanities, PICS impacts the entire university. PICS promotes research through a regular seminar series, an annual conference, by hosting joint research projects and through researcher and student training.

PICS enables computational research by providing an ongoing series of short technical "how to" workshops or bootcamps for Penn researchers and graduate students. Beginning in Fall 2015, PICS will offer a Masters (MSE) of Scientific Computing that may be pursued as a stand-alone masters degree or in conjunction with PhD programs within the disciplines. It provides multifaceted graduate training in the fundamentals and applications of scientific computing through a comprehensive curriculum including numerical methods, algorithm development, high-performance computing, data science, and applications within the science and engineering.

PICS provides an administrative home for interdisciplinary computation-centric projects that span across departments and/or schools. The PICS staff works with faculty to aid the preparation of group proposals, organizing meetings, working with business offices, and coordination of reports in support of sponsored research. PICS maintains a conference room (325 LRSM) for the use of PICS faculty.

PICS advises the administration of schools and the university on issues related to computation-centric research. In addition, PICS works with campus computing organizations to improve campus computational and network infrastructure through advising and external grants for infrastructure enhancement.

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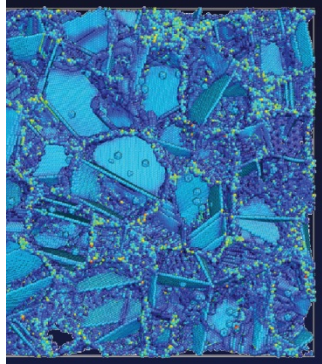
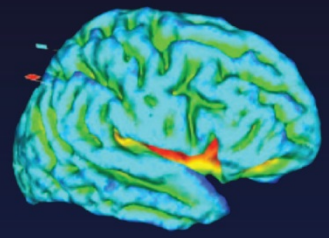
PICS Penn Institute for Computational Science

D³: Deformation, Defects, Diagnosis

May 28 and 29, 2015





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This symposium is made possible by the Provost Interdisciplinary Seminar Fund and support from the School of Engineering and Applied Science.

D^3: Deformation, Defects, Diagnosis

The Penn Institute for Computational Science (PICS), the Graduate Group in Applied Mathematics and Computational Science (AMCS), and the University of Pennsylvania are hosting a one and one-half day symposium on the computational and mathematical issues associated with describing the deformation of data sets and ordered structures and identifying defects within these. This issue has long been studied in the context of materials and condensed matter physics as it applies to mechanical deformation and the defects that contribute to this, as well as electronic properties. At the same time, medical diagnostics depend on imaging modalities in which large data sets have to be deformed and registered with respect to normative anatomical templates. A key question is whether defects that are observed are a result of the deformation or are of anatomical origin. A recent development in computer graphics is the mapping of volumetric images conforming to one surface onto another surface– e.g., the change in the shape of a muscle or jawbone between two distinct animals (or animation characters). These three apparently distinct research areas share an underlying mathematical structure and computational methodologies, yet each has developed largely independently. The intellectual focus of this conference will be the building of bridges between these disparate research areas by clarifying their shared (and distinct) mathematical and computational foundations. Recent developments in scientific computing are opening up exciting directions in D^3research. A key challenge in all of these areas is the enormous data associated with seemingly countless numbers of defects. Another is that the configurational space tends to evolve continuously with deformation. Since knowledge of defect configurations can provide key diagnostics in many applications, there is great and growing interest in knowing the defect states with high resolution. Clearly, large-scale simulation is a powerful tool for D^3research.

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PICS Symposium – D^3: Deformation, Defects, Diagnosis

May 28 – 29, 2015, Wu & Chen Auditorium, Levine Hall
University of Pennsylvania

Thursday, May 28

8:15 AM Registration and Continental Breakfast

9:00 AM **Welcome Remarks**
Eduardo Glandt
Nemirovsky Family Dean
School of Engineering and Applied Science
University of Pennsylvania

Session 1 **Chair:** John Bassani

9:15 AM **From Sorcery to Science: How Hollywood Physics Advances Computational Engineering**
Eitan Grinspun
Computer Science, Columbia University

9:55 AM **Fast Implicit Euler Time Integration**
Ladislav Kavan
Computer and Information Science, University of Pennsylvania

10:20 AM Coffee Break

Session 2 **Chair:** Ravi Radhakrishnan

10:40 AM **Bringing Together Physics, Biology, and Medicine to Hit HIV Where it Hurts**
Arup K. Chakraborty
Chemical Engineering, Massachusetts Institute of Technology

11:20 AM **Enabling Data-Driven Discovery and Diagnosis at Community-Scale**
Zachary G. Ives
Computer and Information Science, University of Pennsylvania

11:45 AM **It's Not About Big Data in Marketing: It's About Big Data Compression**
Eric T. Bradlow
Wharton Marketing Department, University of Pennsylvania

12:10 PM Lunch

Session 3 **Chair:** Charles Epstein

1:30 PM **Bayesian Inverse Problems for Spacial Random Fields**
George Biros
Institute for Computational Engineering and Science
University of Texas, Austin

2:10 PM **Modeling Normal and Abnormal Anatomies via Template Deformations and Residuals**
Christos Davatzikos
Radiology, University of Pennsylvania

2:35 PM **Similarity Matching: A New Framework for Neural Computation**
Dmitri Chklovskii
Neuroscience, Simons Center for Data Analysis

3:15 PM **How You Think: Structural Network Mechanisms of Human Brain Function**
Danielle S. Bassett
Bioengineering, University of Pennsylvania

3:40 PM Coffee Break

Session 4 **Chair:** Celia Reina

4:00 PM **High-Throughput Screening of Crystalline Porous Materials**
Christopher H. Rycroft
Applied Mathematics, Harvard University

4:40 PM **Inherent Structure Landscape Analysis of Defects in Crystals**
Talid R. Sinno
Chemical and Biomolecular Engineering
University of Pennsylvania

5:05 PM **How Disordered Solids Flow**
Andrea J. Liu
Physics and Astronomy, University of Pennsylvania

6:30 PM **Banquet**
Lower Egyptian Gallery
Museum of Archeology and Anthropology
University of Pennsylvania, 3260 South Street

Friday, May 29

8:30 AM Continental Breakfast

Session 5 **Chair:** Randy Kamien

9:00 AM **Materials Cartography: Representing and Mining Material Space Using Structural and Electronic Fingerprints**
Stefano Curtarolo
Mechanical Engineering and Materials Science
Duke University

9:40 AM **Seeing and Sculpting Nematic Liquid Crystal Textures**
Bryan Chen
Lorentz Institute for Theoretical Physics
University of Leiden

10:05 AM Coffee Break

Session 6 **Chair:** David Srolovitz

10:25 AM **Hierarchical Probabilistic Graphical Models for the Detection and Segmentation of Multiple Sclerosis Lesions in Brain MRI**
Tal Arbel
Electrical and Computer Engineering, McGill University

11:05 AM **Simulating the Dynamics of a Photoexcited System: Cheap and Dirty Approximations to Solve Exponentially Difficult Problems in a Reasonable Amount of Time**
Joseph E. Subotnik
Chemistry, University of Pennsylvania

11:30 AM **Computing at the Large Hadron Collider: The Discovery of the Higgs Boson**
Elliot Lipeles
Physics and Astronomy, University of Pennsylvania

12:00 PM **Lunch**

Adjourn

Abstracts and Speaker Bios

From Sorcery to Science: How Hollywood Physics Advances Computational Engineering
Eitan Grinspun, Columbia University

Abstract: Blockbuster films depend on computational physics. The focus is on models that capture the qualitative, characteristic behavior of a mechanical system. Visual effects employ mathematical and computational models of hair, fur, skin, cloth, fire, granular media, and liquids. This is scientific computing with a twist. But techniques developed originally for film can also advance consumer products, biomedical research, and basic physical understanding.

I will describe computational models based on discrete differential geometry (DDG). The focus is on the formal geometric structure of a mechanical system. We build a discrete (hence readily computable) geometry from the ground up, mimicking the axioms, structures, and symmetries of the smooth setting. Problems addressed via DDG include dynamic evolution of thin visco-elastic structures, granular media, and the tying of tight knots.

Bio: Eitan Grinspun is Associate Professor of Computer Science at Columbia University. He was Professeur d'Université Invité at l'Université Pierre et Marie Curie in 2009, a Research Scientist at the Courant Institute of Mathematical Sciences from 2003-2004, a doctoral student at the California Institute of Technology from 1997-2003, and an undergraduate in the Engineering Science program at the University of Toronto from 1993-1997.

He received the National Science Foundation CAREER Award in 2007, the Alfred P. Sloan Research Fellowship in 2010, He was named one of “Ten Brilliant Scientists” by Popular Science Magazine in 2011, and among the “Most Creative People in Business and Innovation” by Fast Company Magazine in 2013.

Eitan investigates the connections between geometry, mechanics, and algorithms, with an eye to physical simulation techniques. The technologies developed by his lab are used today at major film studios, consumer software, and in various disciplines of academic research, spanning biology, engineering, graphics, mechanics, and medicine.

Fast Implicit Euler Time Integration
Ladislav Kavan, University of Pennsylvania

Abstract: In this talk I will describe a new numerical procedure for implicit Euler time integration, useful for simulating mass-spring systems or continuum-based elastic materials. We express the widely used implicit Euler method as an energy minimization problem and introduce special auxiliary variables which allow us to decouple the task into many small non-convex problems and a large convex quadratic problem. The Hessian of the quadratic problem is constant and therefore we can pre-compute its sparse Cholesky factorization, allowing for very fast iterations. Our method typically converges to the same final result as would be obtained by solving the standard form of implicit Euler using Newton's method. Although the asymptotic convergence of Newton's method is faster than ours, the initial ratio of work to error reduction with our method is much faster than Newton's. This makes our approach perfectly suitable for applications where low latency is critical, such as computer games, virtual reality, or surgical simulators.

Bio: Ladislav Kavan is an Assistant Professor of Computer and Information Sciences at the University of Pennsylvania. He is Deputy Director of the SIG Center for Computer Graphics. He received his Ph.D. in Computer Science in 2007 from Czech Technical University, in Prague.

Ladislav explores new approaches to real-time computer graphics and animation. In his most recent work, he studied how to take a standard physics-based deformation model and transform it into a geometric "deformer," i.e., a simple closed-form algorithm that can produce virtually the same result, several orders of magnitude faster than the original formulation. In his previous work, he applied techniques from abstract and linear algebra, spectral methods and finite elements to improve upon technology used in the game and film industries.

Bringing Together Physics, Biology, and Medicine to Hit HIV Where It Hurts
Arup Chakraborty, Massachusetts Institute of Technology

Abstract: HIV is a highly mutable virus, which evades natural and vaccine-induced immune responses and is the causative agent for the AIDS epidemic. I will describe methods, rooted in statistical physics, which aim to determine the fitness landscape of HIV – i.e., a definition of the collective sets of mutations that allow the virus to maintain fitness and evade immunity, and those combinations of mutations that cripple it. The “Hamiltonian” that describes this fitness landscape is analogous to the Hopfield Hamiltonian for associative memory in neural networks. I will show how this Hamiltonian reveals encoded “memories” in the HIV population of host-pathogen riposte won by the virus, and scaling laws that describe this phenomenon. I will also present how evolutionary dynamics with our inferred fitness landscape can predict HIV evolution in individual patients, and how we have harnessed this

knowledge, along with other experimental tests, to design a therapeutic vaccine against HIV which is being advanced to pre-clinical trials.

Bio: Arup K. Chakraborty is the Robert T. Haslam Professor of Chemical Engineering, Chemistry, Physics, and Biological Engineering at MIT. He is the founding Director of MIT's Institute of Medical Engineering and Science. He is also a founding member of the Ragon Institute of MIT, MGH, and Harvard, which is focused on multi-disciplinary approaches to understand human immunology and develop a vaccine against HIV and other scourges on the planet. After obtaining his PhD in chemical engineering at the University of Delaware, and postdoctoral studies at the University of Minnesota, he joined the faculty at the University of California at Berkeley in December 1988. He rose through the ranks, and ultimately served as the Warren and Katherine Schlinger Distinguished Professor and Chair of Chemical Engineering, Professor of Chemistry, and Professor of Biophysics at Berkeley. He was also Head of Theoretical and Computational Biology at Lawrence Berkeley National Laboratory. In September 2005, Arup moved to MIT. The central theme of his research is the development and application of theoretical/computational approaches, rooted in physics and engineering, to aid the quest for mechanistic principles in immunology and harness this understanding to aid the design of vaccines against mutable pathogens. A characteristic of his work is the impact of his studies on experimental immunology and clinical studies (he collaborates extensively with leading immunologists). Arup's work at the interface of the physical, life, and engineering sciences has been recognized by many honors that include a *NIH Director's Pioneer Award*, the *E.O. Lawrence Memorial Award for Life Sciences*, the *Allan P. Colburn and Professional Progress* awards of the American Institute of Chemical Engineers, a *Camille Dreyfus Teacher-Scholar* award, a Miller Research Professorship, and a *National Young Investigator* award. Arup is a member of the National Academy of Engineering and a Fellow of the American Academy of Arts & Sciences and the American Association for the Advancement of Science. He is also a member of the US Defense Science Board.

Enabling Data-Driven Discovery and Diagnosis at Community-Scale
Zachary G. Ives, University of Pennsylvania

Abstract: The Big Data era promises to usher in a revolution in medicine and the life sciences: via large volumes of data, statistical and machine learning techniques, and computational resources, it is envisioned that scientists will make more effective discoveries, better substantiate hypotheses, and ultimately even make real-time diagnoses. However, to reach that vision, we need the data to first be made accessible for processing, made searchable to find the relevant results among thousands of other entries, and made integrated such that it can be processed in a uniform way by Big Data tools and algorithms. Each of these aspects involves critical challenges -- some political, some scientific, some technical -- that tend to be almost universally underrated and under-addressed. I will describe our collaborative effort to change data sharing for the neurosciences (and beyond) via a cloud-hosted data sharing portal called IEEG, including the underlying software platform Habitat.

Bio: Zachary Ives is a Professor and Markowitz Faculty Fellow at the University of Pennsylvania. He received his PhD from the University of Washington. His research interests include data integration and sharing, managing "big data," sensor networks, and data provenance and authoritativeness. He is a recipient of the NSF CAREER award, and an alumnus of the DARPA Computer Science Study Panel and Information Science and Technology advisory panel. He has also been awarded the Christian R. and Mary F. Lindback Foundation Award for Distinguished Teaching. He serves as the Director for Penn's Singh Program in Networked and Social Systems Engineering, and he is a Penn Engineering Fellow. He is a co-author of the textbook Principles of Data Integration, and received an ICDE 2013 ten-year Most Influential Paper award. He has been an Associate Editor for Proceedings of the VLDB Endowment (2014) and a Program Co-Chair for SIGMOD (2015).

It's Not About Big Data in Marketing: It's About Big Data Compression
Eric Bradlow, University of Pennsylvania

Abstract: While most scholars who focus on big data in Marketing are concerned with the explosion in the number of rows, bigger gains can be had by cleverly collecting "better columns" of data and compressing them using principles of sufficiency. In this talk, I will discuss some recent research that makes big data smaller, without losing much of the information.

Bio: Eric T. Bradlow is currently Chairperson, Wharton Marketing Department, Vice-Dean and Director, Wharton Doctoral Programs, The K.P. Chao Professor, Professor of Marketing, Statistics, and Education and Co-Director of the Wharton Customer Analytics Initiative at The Wharton School of the University of Pennsylvania. He earned a Bachelor of Science in Economics from The Wharton School in 1988, an A.M. in Mathematical Statistics in 1990 and a Ph.D. in Mathematical Statistics in 1994 from Harvard University. He joined the Wharton faculty in 1996.

From 2008 - 2011, Eric was Editor-in-Chief of *Marketing Science,* the premier academic journal in Marketing. He was recently named one of eight inaugural University of Pennsylvania Fellows, a Fellow of the American Statistical Association, a Fellow of the American Education Research Association, a Fellow of the Wharton Risk Center, a Senior Fellow of the Leonard Davis Institute for Health Economics, is past chair of the American Statistical Association Section on Statistics in Marketing, is a statistical Fellow of Bell Labs, and was previously named DuPont Corporation's best young researcher. His academic research interests include Bayesian modeling, statistical computing, and developing new methodology for unique data structures with application to business problems, education and psychometrics and health outcomes. He has won research awards in Marketing,

Statistics, Psychology, Education and Medicine. His personal interests include his wife Laura, his sons Ethan, Zach, and Ben, and his love of sports and movies.

Bayesian Inverse Problems for Spacial Random Fields
George Biros, University of Texas at Austin

Abstract: Remote sensing, image analysis, subsurface characterization, coarse-graining, and inverse scattering are examples of problems in which we seek to reconstruct a spatial field given noisy and incomplete information. In Bayesian inverse problems we need to construct likelihood and prior probability density functions. I will present a methodology that combines supervised learning with classical Gibbs measures for likelihood and smoothness priors to construct likelihood and prior functions. The overall methodology has several components, including optimal transport control problems, matrix approximation using high-dimensional N-body methods, and multiscale modeling of non-stationary random fields. I will discuss the computational challenges in working with such problems and will present experimental results for segmentation of medical images.

Bio: George Biros is the W. A. "Tex" Moncrief Chair in Simulation-Based Engineering Sciences in the Institute for Computational Engineering and Sciences and has appointments with the departments of Mechanical Engineering and Computer Science (by courtesy) at the University of Texas at Austin.

From 2008 to 2011, he was an Associate Professor in the School of Computational Science and Engineering at Georgia Tech and The Wallace H. Coulter Department of Biomedical Engineering at Georgia Tech and Emory University. From 2003 to 2008, he was an Assistant professor in Mechanical Engineering and Applied Mechanics at the University of Pennsylvania. He received his BS in Mechanical Engineering from Aristotle University Greece (1995), his MS in Biomedical Engineering from Carnegie Mellon (1996), and his PhD in Computational Science and Engineering also from Carnegie Mellon University (2000). He was a postdoctoral associate at the Courant Institute of Mathematical Sciences from 2000 to 2003. Biros was among a team of researchers that won the IEEE/ACM SC03 and SC10 Gordon Bell Awards for special Achievement.

Modeling Normal and Abnormal Anatomies via Template Deformation and Residuals
Christos Davatzikos, University of Pennsylvania

Abstract: The field of computational anatomy has developed schemes for mapping anatomical templates onto individual scans, and hence obtaining quantitative descriptions of anatomical characteristics. However, there can be infinitely many ways of deforming a template to an individual, each one leading to a different residual. We approximate these pairs of (transformation, residual) by a morphological appearance manifold, and derive an optimal position on this manifold by minimizing group variance, aiming to find the optimal deformation that allows us to detect differences between healthy and diseased individuals. We also present approaches utilizing sparse decompositions of a patient's anatomy to a set of deformed templates, thereby detecting abnormalities as deviations from this decomposition.

Bio: Christos Davatzikos is the Wallace T. Miller Sr. Professor of Radiology, with secondary appointment in Electrical and Systems Engineering and joint appointments with the Bioengineering and Applied Math graduate groups at Penn. He received his undergraduate degree by the National Technical University of Athens, Greece, in 1989, and Ph.D. from Johns Hopkins University, in 1994. He joined the faculty at the Johns Hopkins School of Medicine as Assistant Professor (1995) and later Associate Professor (2001) of Radiology. In 2002 he moved to Penn to direct the Section for Biomedical Image Analysis, and in 2013 he established the Center for Biomedical Image Computing and Analytics. His interests are in the field of medical image analysis. Earlier in his career, Davatzikos focused on image registration and computational neuroanatomy. In the more recent years he has focused on the application of machine learning and pattern analysis methods to medical imaging problems. Davatzikos is an IEEE Fellow and member of various editorial boards.

Similarity Matching: A New Framework for Neural Computation
Dmitri Chklovskii, Simons Foundation

Abstract: Despite our extensive knowledge of the biophysical properties of neurons, there is no commonly accepted algorithmic theory of neuronal function. Here we explore the hypothesis that a neuron performs online matrix factorization of the streamed data. By starting with a matrix factorization cost function we derive an online algorithm, which can be implemented by neurons and synapses with local learning rules. We demonstrate that such network performs feature discovery and soft clustering. The derived algorithm replicates many known aspects of sensory anatomy and biophysical properties of neurons. Thus, we make a step towards an algorithmic theory of neuronal function, which should facilitate large-scale neural circuit simulations and biologically inspired computing.

Bio: Dmitri "Mitya" Chklovskii is an inter-disciplinary scientist with contributions to neuroscience, physics, engineering, and computer science. He holds a PhD in Theoretical Physics from MIT and was a Junior Fellow at the Harvard Society of Fellows. He transitioned to theoretical neuroscience at the Salk Institute and founded the first theoretical neuroscience group at Cold Spring Harbor Laboratory, where he was an Assistant and then Associate Professor. From 2007 to 2014 he was a Group Leader at the Janelia Farm Research Campus of the Howard Hughes Medical Institute where he led a team that assembled the largest-ever connectome. As Group Leader for Neuroscience at the Simons Center for Data Analysis, Chklovskii leads an effort to understand how the brain analyzes complex datasets streamed by sensory organs, in an attempt to create artificial neural systems.

How You Think: Structural Network Mechanisms of Human Brain Function
Danielle S. Bassett, University of Pennsylvania

Abstract: Cognitive function is driven by dynamic interactions between large-scale neural circuits or networks, enabling behavior. Fundamental principles constraining these dynamic network processes have remained elusive. I will discuss a recent application of network control theory to human neuroimaging data that provides new insights into the structural network mechanisms of human brain function. Using diffusion spectrum imaging data, we build a structural brain network with 234 nodes (brain regions) connected by weighted edges (number of white matter streamlines linking brain regions). We employ a simplified noise-free linear discrete-time and time-invariant network model of neural dynamics in which the state of brain regions depends on the connectivity between them. We interrogate this model to determine the role of brain regions in different control strategies. Our results suggest that densely connected areas, particularly in the default mode system, facilitate the movement of the brain to many easily-reachable states. Weakly connected areas, particularly in cognitive control systems, facilitate the movement of the brain to difficult-to-reach states. Areas located on the boundary between network communities, particularly in attentional control systems, facilitate the integration or segregation of diverse cognitive systems. As a whole, this body of work suggests that structural network differences between the default mode, cognitive control, and attentional control systems dictate their distinct roles in controlling brain network function. More generally, our results support the view that macroscale structural design underlies basic cognitive control processes via the fundamental mechanism of network controllability.

Bio: Danielle S. Bassett is the Skirkanich Assistant Professor of Innovation in the Department of Bioengineering at the University of Pennsylvania. She is most well-known for her work blending neural and systems engineering to identify fundamental mechanisms of cognition and disease in human brain networks. She received a B.S. in physics from the Pennsylvania State University and a Ph.D. in physics from the University of Cambridge, UK. Following a postdoctoral position in the Complex Systems Group at the University of California Santa Barbara, she was a Junior Research Fellow at the Sage Center for the Study of the Mind. In 2012, she was named American Psychological Association's `Rising Star' and given a Alumni Achievement Award from the Schreyer Honors College at Pennsylvania State University for extraordinary achievement under the age of 35. In 2014, she was named an Alfred P Sloan Research Fellow and received the MacArthur Fellow Genius Grant.

In 2015, she received the IEEE EMBS Early Academic Achievement Award, and was named an ONR Young Investigator. She is the founding director of the Penn Network Visualization Program, a combined undergraduate art internship and K-12 outreach program bridging network science and the visual arts. Her work has been supported by the National Science Foundation, the National Institutes of Health, the Army Research Office, the Army Research Laboratory, the Alfred P Sloan Foundation, the John D and Catherine T MacArthur Foundation, and the University of Pennsylvania. She lives with her husband and two sons in Wallingford, Pennsylvania.

High-Throughput Screening of Crystalline Porous Materials
Christopher Rycroft, Harvard University

Abstract: Crystalline porous materials, such as zeolites, contain complex networks of void channels that are exploited in many industrial applications. A key requirement for the success of any nanoporous material is that the chemical composition and pore topology must be optimal for a given application. However, this is a difficult task, since the number of possible pore topologies is extremely large: thousands of materials have been already been synthesized, and databases of millions of hypothetical structures are available.

This talk will describe the development of tools for rapid screening of these large databases, to automatically select materials whose pore topology may make them most appropriate for a given application. The methods are based on computing the Voronoi tessellation, which provides a map of void channels in a given structure. This is carried out using the software library Voro++, which has been extended to account for three-dimensional non-orthogonal periodic boundary conditions. Algorithms to characterize and screen the databases will be described, and an application of the library to search for materials for carbon capture and storage will be discussed.

Bio: Chris Rycroft is an assistant professor of applied mathematics in the Harvard School of Engineering and Applied Sciences. He is interested in mathematical modeling and scientific computation for interdisciplinary applications in science and engineering. He is particularly interested in the mechanics of materials, numerical methods, and geometry. He has released several software libraries, including Voro++ for three-dimensional computations of the Voronoi tessellation, a technique in computational geometry that has a wide range of applications.

Prior to his appointment at Harvard, Rycroft was a Morrey Assistant Professor in the Department of Mathematics at the University of California, Berkeley. While in Berkeley, he was part of the Bay Area Physical Sciences–Oncology Center (PS–OC), where he investigated how cancer cells mechanically interact with each other and their environment. Rycroft is a visiting faculty scientist at the Lawrence Berkeley Laboratory, where he has worked on several projects relating to energy production and efficiency. He obtained his PhD in Mathematics in 2007 from the Massachusetts Institute of Technology.

Inherent Structure Landscape Analysis of Defects in Crystals
Talid Sinno, University of Pennsylvania

Abstract: The interplay between entropic and energetic forces makes the analysis of microstructure in crystals at high temperature unexpectedly difficult. A particular challenge is the calculation of free energies that requires consideration of multiple, distinct configurations whose relative importance depends on temperature and pressure. The tool of inherent structure landscape analysis is shown to be exceptionally well-suited for this purpose. While the notions of potential energy landscapes and inherent structures are in routine use in the thermodynamic and kinetic analysis of glasses and supercooled liquids, they have been only sparsely applied in the context of defect and microstructure thermodynamics in crystalline materials. Using crystalline silicon as a backdrop, the aim of this talk is to apply these concepts to study the high-temperature thermodynamics and structural characteristics of point defect (self-interstitials and vacancies) clusters, and their roles in crystal melting.

Inherent structure analysis is carried out by repeated quenching of instantaneous configurations generated during long-time molecular dynamics simulations of defect clusters, from which probability distribution functions and density-of-states distributions are constructed. Coupled with detailed structural observations, a comprehensive and quantitative thermodynamic and morphological picture for point defect clusters is described. In particular, it is shown that configurational and vibrational entropy both play important roles in setting the behavior of defect clusters, resulting in a rich diversity of structures whose selection depends on processing conditions, namely temperature and pressure. Moreover, the inherent structure analysis quantitatively explains the link between processing conditions and defect structure, and provides a powerful approach for computing temperature-dependent free energies of these complex entities.

Bio: Talid Sinno received his B.S. in Chemical Engineering and B.A. in Chemistry from the University of Pennsylvania (1991). He received a Ph.D. (1998) in Chemical Engineering from M.I.T, where he subsequently spent another year as a postdoctoral researcher and lecturer. He has been a member of the faculty of the Department of Chemical and Biomolecular Engineering at Penn since 1999, and is currently Professor of Chemical and Biomolecular Engineering and also holds a secondary appointment in the Department of Mechanical Engineering and Applied Mechanics.

Talid's research interests are in the broad area of computational materials science with specific focus on multiscale modeling and simulation of nucleation, aggregation, and crystallization processes in a wide range of material systems. Example areas of current focus include microstructure and defect evolution in semiconductor silicon crystals, multiscale modeling of deposition processes on silicon and silicon-germanium substrates, crystallization of DNA-functionalized colloidal particles, and platelet cell aggregation in blood flow. His group develops and applies numerous computational techniques to study these problems including molecular dynamics, Monte Carlo, and continuum modeling.

How Disordered Solids Flow
Andrea Liu, University of Pennsylvania

Abstract: All solids flow at high enough applied stress and melt at high enough temperature. Crystalline solids flow and premelt via localized particle rearrangements that occur preferentially at structural defects known as dislocations. The population of dislocations therefore controls both how crystalline solids flow and how they melt. In disordered solids, there is considerable evidence that localized particle rearrangements induced by stress or temperature occur at localized flow defects but all attempts to identify them directly from the structure have failed. Here we introduce a novel application of machine learning data mining methods to diagnose flow defects, or "soft" particles from their local structural environments. We follow the softness of each particle as it evolves under deformation or temperature. Our results show that machine learning methods can be used to gain a conceptual understanding that has not been achieved with conventional approaches.

Bio: Andrea J. Liu is the Hepburn Professor of Physics in the Department of Physics and Astronomy of the University of Pennsylvania. She is a theoretical soft matter physicist who works on the mechanics of jamming and flow in disordered solids, and on the mechanics of biological processes. From 1994 to 2004, Dr. Liu was on the faculty of the Department of Chemistry and Biology of the University of California, Los Angeles. She received her A.B. in Physics from the University of California, Berkeley in 1984, and her Ph.D. in Physics from Cornell University in 1989.

Materials Cartography: Representing and Mining Material Space Using Structural and Electronic Fingerprints
Stefano Curtarolo, Duke University

Abstract: In this presentation, we show how to use on-line resources to search for novel thermoelectrics [1,2,3] topological-insulators, magnets, and binary/ternary [4,5,6] phase diagrams [7,8], for energy applications. Research sponsored by DOD/DOE. [1] Appl. Phys. Lett. 105, 101907 (2014). [2] Adv. Funct. Mater. doi=10.1002/adfm.201401201 (2014). [3] Phys. Rev. X 4, 011019 (2014). [4] Phys. Rev. X 3, 041035 (2013). [5] Phys. Rev. X 1 (2), 021012 (2011). [6] Phys. Rev. B 78 (5), 054105 (2008). [7] Jour. Am. Chem. Soc. 133 (1), 158-163 (2010). [8] Comp. Mat. Sci. 93, 178-192 (2014).

Bio: After studying Electrical Engineering and Physics in Padova, Italy, Stefano Curtarolo received his PhD in Materials Science from MIT in 2003. Since then, he has been faculty of Materials Science and Physics at Duke University. During his time at Duke, Stefano received the ONR-Young-Investigator, the NSF-Career, the Presidential PECASE Awards, the International Union of Pure and Applied Physics - Young Scientist Prize in Computational Physics, the Stansell Research Award and the 2013 MURI Award for strategies in element replacement. Dr. Curtarolo was promoted to Associate in October of 2008 and to Full Professor in February of 2012. Currently he has more than 100 refereed publications and more than 160 invited departmental seminars and talks in national and international conferences. At Duke University, the SC group started and maintains the “on-line ab-initio aflowlib.org" consortium containing free energy information and electronic characterization of more than 700,000 entries/compounds.

Seeing and Sculpting Nematic Liquid Crystal Textures
Bryan Chen, Leiden University

Abstract: Nematic liquid crystals are the foundation for modern display technology and also exhibit topological defects that can readily be seen under a microscope. Recently, experimentalists have been able to create and control more and more interesting defect textures, including controllably knotted defect lines around colloids (Ljubljana) and the "toron", a pair of hedgehogs bound together with a ring of double-twist between them (CU Boulder). I will review work applying the Thom construction from algebraic topology which allows us to visualize 3 dimensional molecular orientation fields as certain colored surfaces in the sample. These surfaces turn out to be a generalization to 3dimensions of the dark brushes seen in Schlieren textures of two-dimensional samples of nematics. Manipulations of these surfaces correspond to deformations of the nematic orientation fields, giving a hands-on way to classify liquid crystal textures which is also easily computable from data and robust to noise.

Bio: Bryan Chen is a soft condensed matter theorist interested in geometry, topology, and statistical mechanics. He received his Ph.D. in physics from the University of Pennsylvania in 2012 with a dissertation titled "Topological defects in nematic and smectic liquid crystals" under the supervision of Randy Kamien. Since then he has been working at the Instituut-Lorentz at Leiden University as a postdoc with Vincenzo Vitelli on topological mechanical systems.

Hierarchical Probabilistic Graphical Models for the Detection and Segmentation of Multiple Sclerosis Lesions in Brain MRI
Tal Arbel, McGill University

Abstract: Probabilistic graphical models have been shown to be effective in a wide variety of segmentation tasks in the context of computer vision and medical image analysis. However, segmentation of pathologies can present a series of additional challenges to standard techniques. In the context of lesion detection and segmentation in brain images of patients with Multiple Sclerosis (MS), for example, challenges are numerous: lesions can be subtle, heterogeneous, vary in size and can be very small, often have ill-defined borders, with intensity distributions that overlap those of healthy tissues and vary depending on location within the brain. In this talk, recent work on multi-level, probabilistic graphical models based on Markov and Conditional Random Fields (MRF/CRF) will be described to accurately detect and segment (1) lesions and healthy tissues in brain images of patients with MS, and (2) “active” (enhancing) lesions in MRI of patients injected with contrast agents (e.g. Gadolinium). Robustness and accuracy of the methods are illustrated through extensive experimentation on very large, proprietary datasets of real, patient brain MRI acquired during multicenter clinical trials. The methods have also been successfully adapted to other domains such as brain tumour and heart pathology segmentation.

Bio: Tal Arbel is an Associate Professor in the Department of Electrical and Computer Engineering at McGill University, Montreal, Quebec, Canada. She is a member of the Centre for Intelligent Machines, where she is the Director of the Probabilistic Vision Group and the Medical Imaging Lab. Her expertise lies in the development of probabilistic and machine learning methods in computer vision and in medical image analysis, particularly in neurology and neurosurgery. Dr. Arbel received her B.Eng, M.Eng and Ph.D. degrees from the Department of Electrical Engineering at McGill University, where she performed graduate studies and research in the field of computer vision. She then completed a postdoctoral fellowship in the Brain Imaging Centre at the Montreal Neurological Institute. Her recent community activities include: Area Chair of IEEE Conference on Computer Vision and Pattern Recognition (CVPR); Lead guest editor for the Computer Vision and Image Understanding (CVIU) journal, special issue on: "Probabilistic Models for Biomedical Image Analysis"; Co-organizer, "BAMBI: Bayesian and grAphical

Models for Biomedical Imaging Workshop", held in conjunction with MICCAI 2014 & 2015 conferences; Co-organizer for the MICCAI 2017 conference.

Simulating the Dynamics of a Photoexcited System: Cheap and Dirty Approximations to Solve Exponentially Difficult Problems in a Reasonable Amount of Time

Joseph Subotnik, University of Pennsylvania

Abstract: I will discuss the problem of how to calculate frictional effects in photoexcited systems and I will introduce a current solution (known as surface hopping). I will highlight computational challenges in making dynamical predictions for electronically excited systems, and I will also show what physical effects can be successfully modeled today through large simulations.

Bio: Joseph Subotnik received his BA in physics and math from Harvard in 2000 and his Ph.D. in chemical biophysics from Berkeley in 2006. He completed his Ph.D. under the supervision of Martin Head-Gordon and focused on local correlation theory, which is a computational approach for solving Schrodinger's equation in a linear amount of time by exploiting the locality of many electron correlations. From 2007-2009, he was an NSF international postdoctoral fellow, working with Abe Nitzan in Tel-Aviv University and jointly collaborating with Mark Ratner at Northwestern University. The fellowship research focused on understanding the role of electron-electron correlations in non-equilibrium phenomena, including molecular conduction and electron transfer. He joined Penn chemistry as a junior faculty member in July of 2010, and was made associate professor in July, 2014.

Computing at the Large Hadron Collider: The Discovery of the Higgs Boson

Elliot Lipeles, University of Pennsylvania

Abstract: The Large Hadron Collider (LHC) produces of billions of proton-proton collisions per second. At one of the collision points, the particles emerging from the collisions pass through the ATLAS detector resulting in a data stream that is on the order of 80 Terabytes per second. This extreme data volume is processed through a series of computing systems which filter it down to a recordable tens of terabtyes per day which are then processed and simulated in detail. I will give an overview of the processing steps and computing challenges faced by the experiment and how they are handled.

Bio: Elliot Lipeles is an Associate Professor of Physics in the Department of Physics and Astronomy at the University of Pennsylvania. Elliot received his B.A. in Physics and Math from the University of Chicago in 1995, and a Ph.D. in Physics from the California Institute of Technology in 2004. His research interests include many outstanding questions in particle physics such as: What is dark matter? What prevents quantum corrections from raising the Higgs mass much higher than the observed mass? What drives the matter-antimatter asymmetry in the universe? Elliot Lipeles' research group looks for answers to these questions using particle colliders. They are currently focused on the ATLAS experiment at the Large Hadron Collider. Particular projects include contributing to the observation of the Higgs boson using the Higgs to WW decay channel, searching for the Higgs decaying to dark matter or other long-lived weakly interacting particles, and super-symmetry motivated searches for new particles decaying to multiple leptons. Elliot Lipeles is also involved in the operation of the ATLAS trigger system and the design of the ATLAS upgrade trigger system and ATLAS upgrade silicon strip detector.