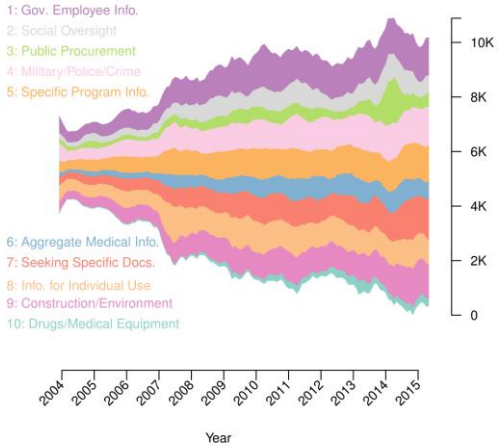

University of Delaware
Research Office
DELAWARE
Data Science
SYMPOSIUM
MAY 12, 2017

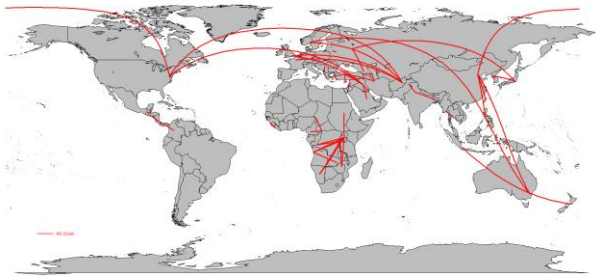
Text as data

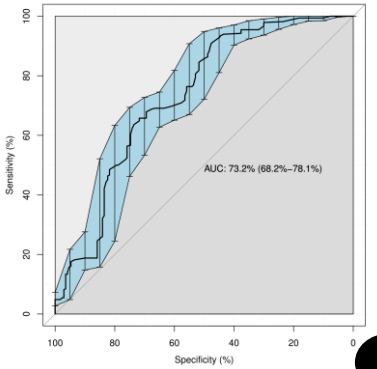
- Proliferation of political text
- New Opportunities
- New Challenges



Analysis of event data

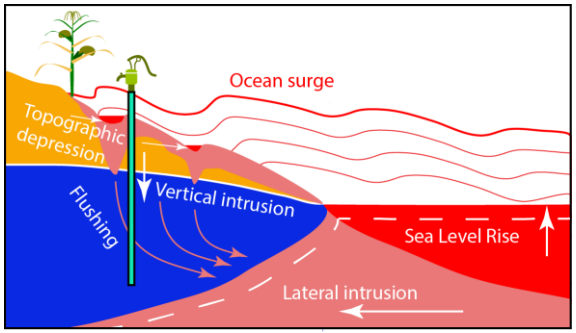
- Who did what to whom (where/when)
- High volume w/complex linkages
- Spatio-temporal analysis/forecasting



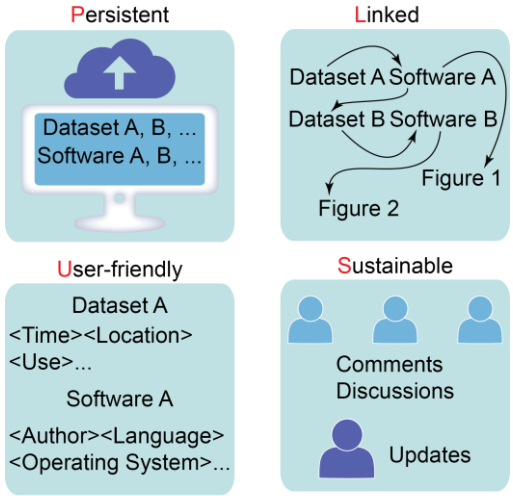


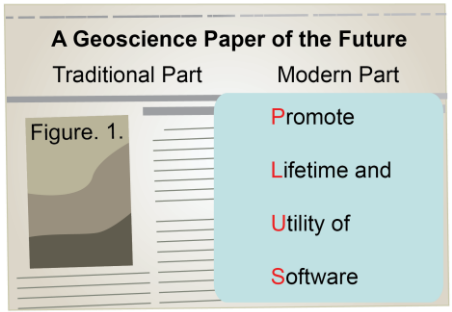
Data Management in Geoscience Papers

---Xuan Yu Dept. Geological Sciences



- Sea-level Rise Rate
- Topography
- Geology
- Tides
- Soil
- Hydrogeologic field observation





Presenter: Dr. Xiaoke Zhang, Assistant Professor of Statistics.

The world is dynamic in time and space. **So is data!**

Functional data: data from a sample of random functions (i.e., stochastic processes).
∞−dimensional data.

Easy availability and extensive applicability: Time: finance, transportation, clinical trials. Space: agriculture, ecology, epidemiology.
Time+Space: climatology, neuroscience.

Functional data analysis (FDA): a branch of statistics that analyzes functional data.
Representative topics: function estimation, regression, dimension reduction, classification, clustering, network, etc.

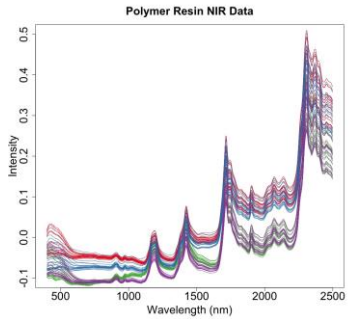
Shanshan Ding
Assistant Professor of Statistics

- **High-dimensional statistical learning for big data -Dimension reduction, sufficient dimension reduction (SDR), feature screening**
  1. Dimension folding PCA and PFC (neuroimaging data)
  2. Tensor sufficient dimension reduction (neuroimaging data)
  3. SDR with simultaneous variable selection in ultra-high dimension (genomic studies)

  (e.g. biomarker and disease related brain region identification)
- **Parsimonious and efficient statistical modeling and inference-Envelope models and methods**
  1. Envelope matrix-variate regressions (neuroimaging, temporal and spatial data)
  2. Envelope quantile regression (health and behavioral studies)
- **Statistical applications - biosciences, health and behavioral sciences, environmental studies**

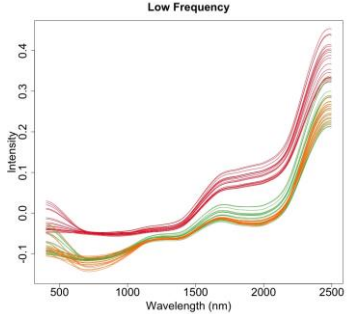
  Neuroimaging (EEG, MRI, fMRI), genomic data (RNA-seq, microarray), temporal and spatial, longitudinal data, time series, etc.

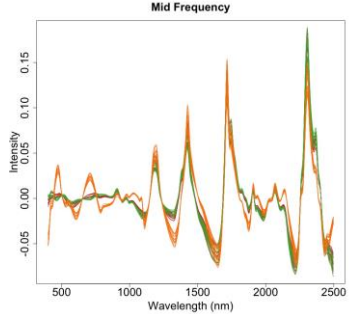
Robust Regression Models in Unseen Domains by Wavelet Scale Projection Research in the Laboratory for Chemometrics

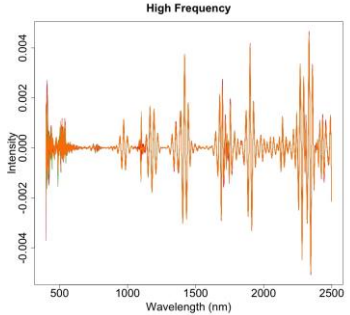


wavelet transform

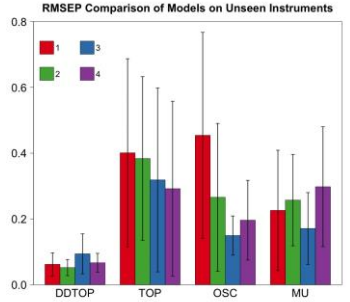
orthogonal projection



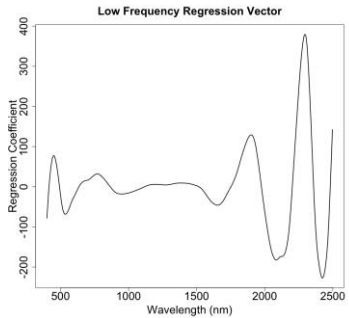


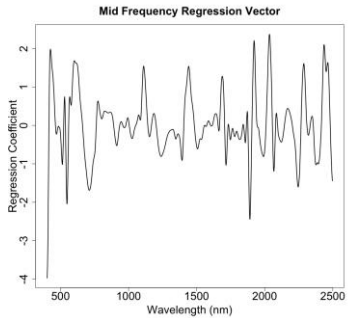


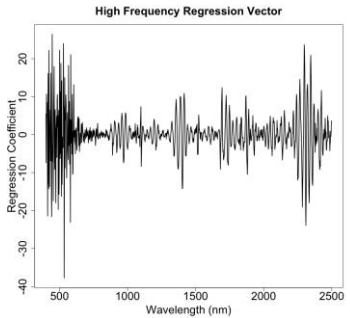
latent variable regression model on each scale



high stability and performance in unseen domains



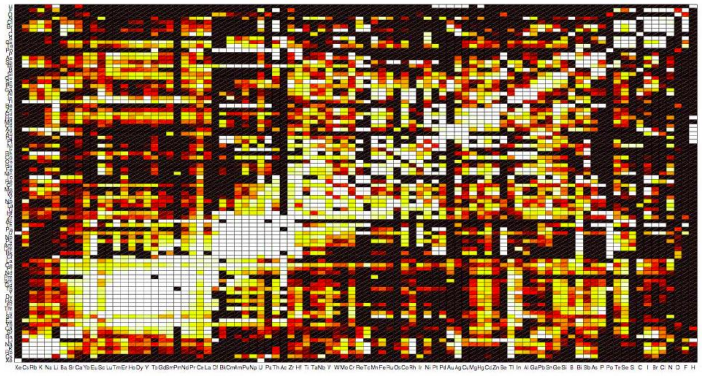


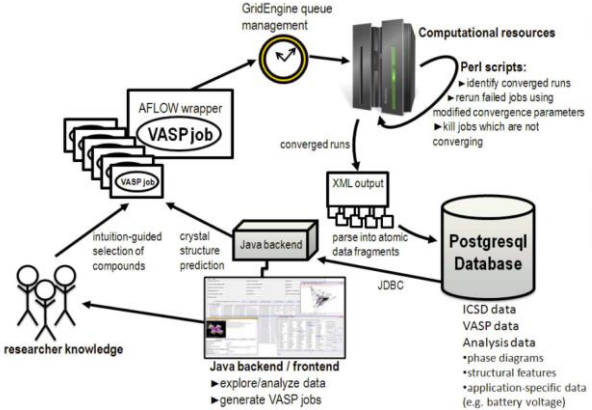


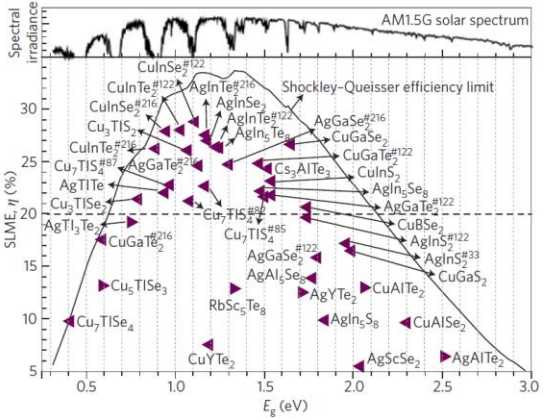
Research funded by NSF grant 1506853

Big Data for Designing Amazingly Useful Materials

Branislav K. Nikolić, Department of Physics & Astronomy, https://wiki.physics.udel.edu/qttg

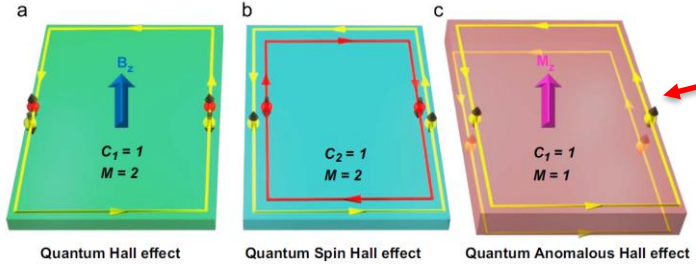




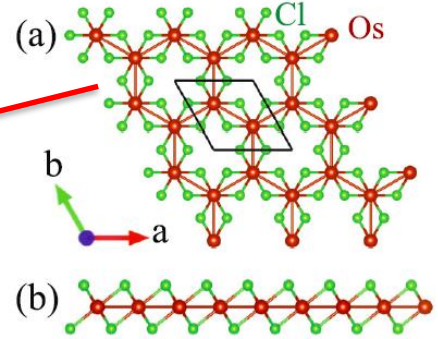


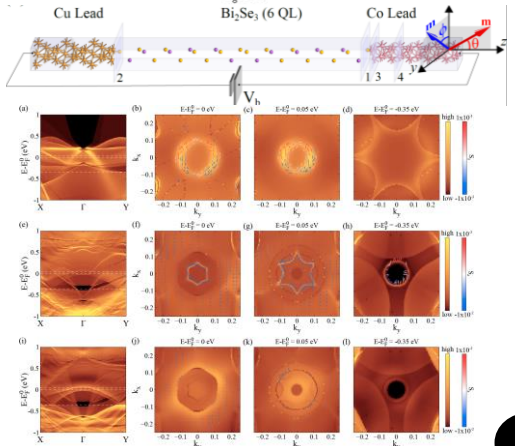
Zunger group, PRL **108**, 068701 (2012)

Examples of topological materials



Nikolić group, PRB **95**, 201402(R) (2017)



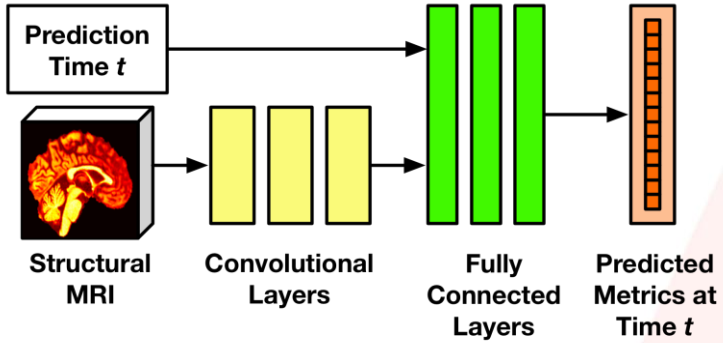


Nikolić group, https://arxiv.org/abs/1701.00462

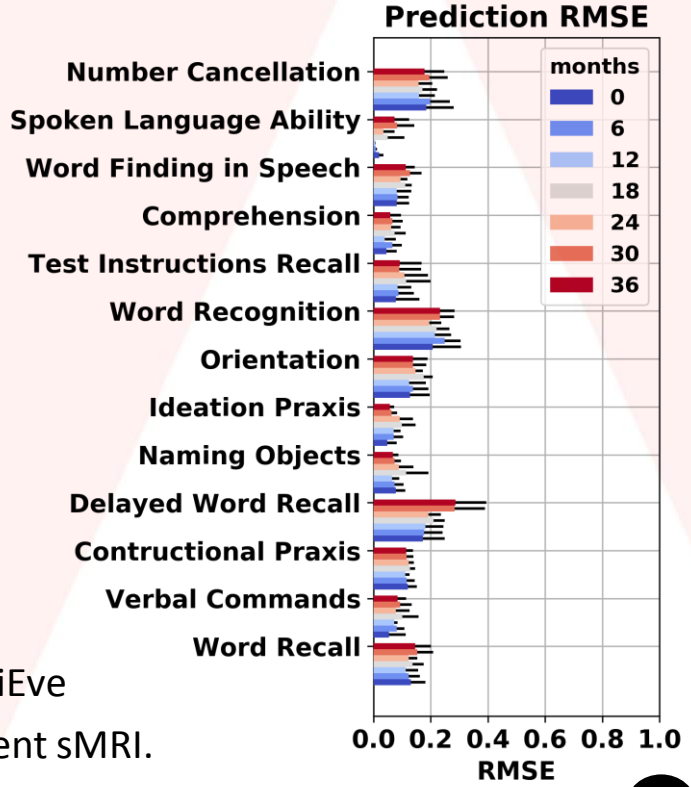
Mul$variate Cogni$ve Metric Trajectory Predic$on in Alzheimer's Disease

Lev E. Givon

- Huge, growing AD dataset*: 1650 paEents/controls, > 100 biomedical data types, mulE-year longitudinal data.
- Goal: discover interrelaEonships between mulEple biomarker trajectories that shed light on progression of AD.



- CogniEon = learning, memory, language, praxis, orientaEon, …
- ADNI-trained ConvNet architecture can predict 13 normalized cogniEve metrics up to 3 years into future from minimally preprocessed current sMRI.



Joint work with L.J. Mariano, A.R. Schneider, D. O'Dowd, J.M. Irvine, & Alzheimer's Disease Neuroimaging IniEaEve*

DRAPER

Charles Boncelet, ECE Dept, boncelet@udel.edu, 831-8008

Conducting research on machine learning applied to

- Information Security, esp. steganography and steganalysis.
- Electric Grid, control and resiliency.
- Signal processing.
- Algorithms for machine learning, e.g., graph based learning and entropy based methods.

Research highlights:

- Completed textbook, Probability, Statistics, and Random Variables.
- Working on new book, Python for Signal Processing.
- Many highly cited papers in information security.
- Expert in data compression.

Analyzing Biological Networks Via Machine Learning

Li Liao
Computer & Information Sciences

Biological networks, including Protein-protein interactions (PPI) networks, play critical roles in many biological processes in the cell. Reconstructing and analyzing these networks from the huge amount of data generated from high throughput technologies present tremendous challenges as well as opportunities in both our efforts toward understanding the basic biology and translational research that can impact on human health. Our current research is focused on developing computational methods based on machine learning that can integrate data of different types and overlay multiple layers of mapping onto incomplete network to gain insights and make useful inference and detection of network related properties.

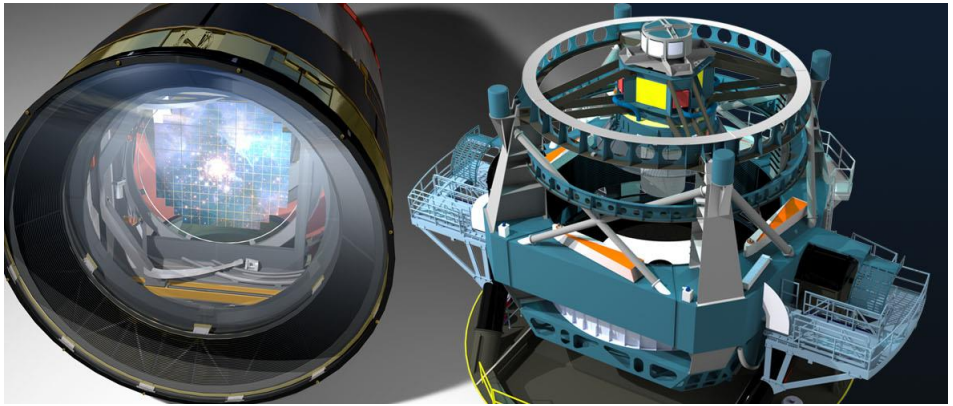
Specifically, we showcase several such methods that address the following: a) assessment of network evolution; b) inference of *de novo* edges; and c) detection of disease related nodes.

Astronomy: New Era of Petascale Data Science

John Gizis

Co-Chair, LSST Stars, Milky Way & Local Volume Science Collaboration

- Major new *NASA* space and *NSF* ground surveys
- *LSST*: 10 year survey of the sky, 15 Tb/night, 37 billion stars and galaxies

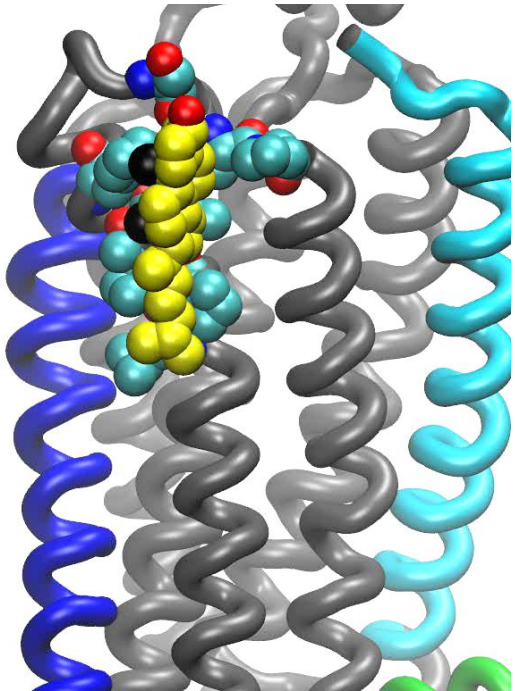


- Open Data Policy puts premium on data science collaborations and computational resources.

Molecular simulation of membranes with the Anton2 special purpose machine

Anton is 100x faster than commodity machines for “all-atom” classical MD

Cholesterol interacting with a Parkinson’s target



Lyman research group
Physics and Astro, Chem and Biochem

Our interests:

- Modeling membranes w/ SoA HPC resources
- Fast, scalable algorithms for hydrodynamics
- Petascale HPC for drug binding kinetics

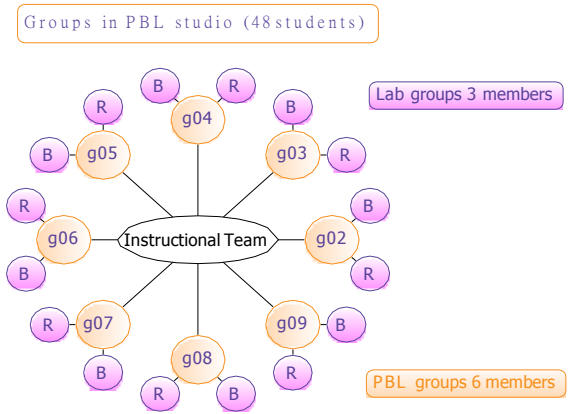
Data Driven Instruction and Assessment of Learning

Banjo. Oriade, PhD, adebanjo@udel.edu (Dept. of Physics and Astronomy | Dupont Interdisciplinary Science Learning Laboratories)

This work is directed at data driven instructional environment design, implementation, and formative assessment for effective student centered learning - evidencing the journey to course learning goals (critical thinking, problem solving, and collaboration skills).

Some results:

1. Successfully guiding instruction using item analysis of, in the synchronous case, student clicker responses, and in asynchronous case, quiz/exam responses. Measures for analysis include choice frequency (distractors), difficulty index, and discrimination index.
2. Creation of about 15 hands on guided inquiry activities for SCEN 101 Physical Science; and new course SCEN 115 Origami Science.
3. Learning tool for Physics teacher training,"Making the tacit explicit:..." (Oriade PhysTEC Conference,**62**, 2, Session P3, Feb. 2017).



It takes a village, the SCEN 101 instructional team, to implement student-centered learning and provide students with just-in-time formative feedback.

THANKS TEAM!

- Data collected from multiple sources including (1) rubrics in course LMS, (2) homework site, (3) deliverables from individual and group student work, (3) student clickers, and (4) from semester long multi-part projects.
- Design principles inspired by Goldberg et. al. (AJP **78**, 1265 (2010)), and we focus on the necessity of tools and the need for others/peers for learning. Tools were created, and others (high and low tech.) adapted. Figure on the left shows group topology. There are eight PBL groups (max. 6 members). Each PBL group is split into two experiment based learning (EBL) groups. Inter- and intra- group conversations enrich the learning experience.
- Work in progress: Analytics driven constructions for automated individual and group feedback and email prompts - based on a cost function and training set built from past metrics of student performance.

Dare to be first.
UNIVERSITY OF DELAWARE

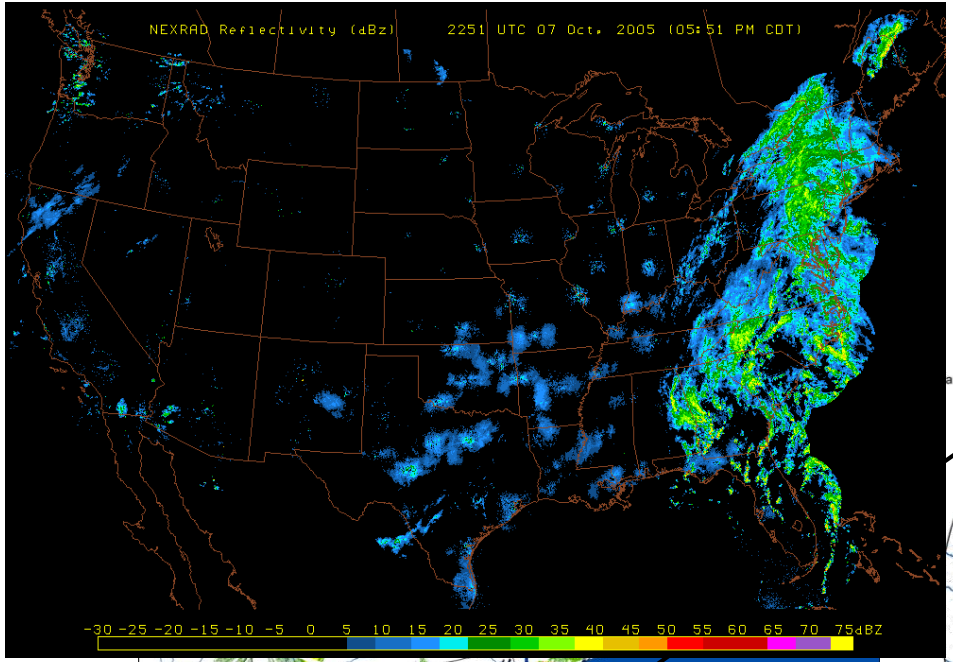
NEXRAD – Weather Surveillance Radar

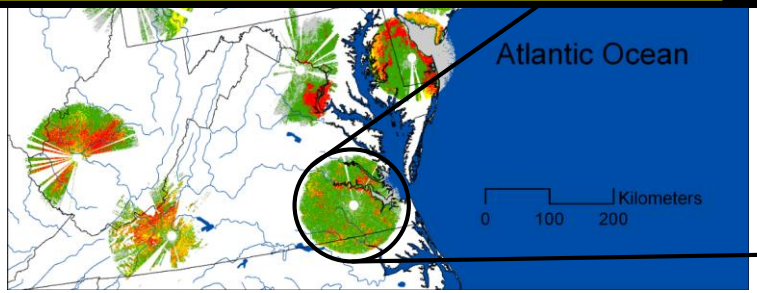
Jeffrey Buler, Ph.D.
Department of Entomology and Wildlife Ecology

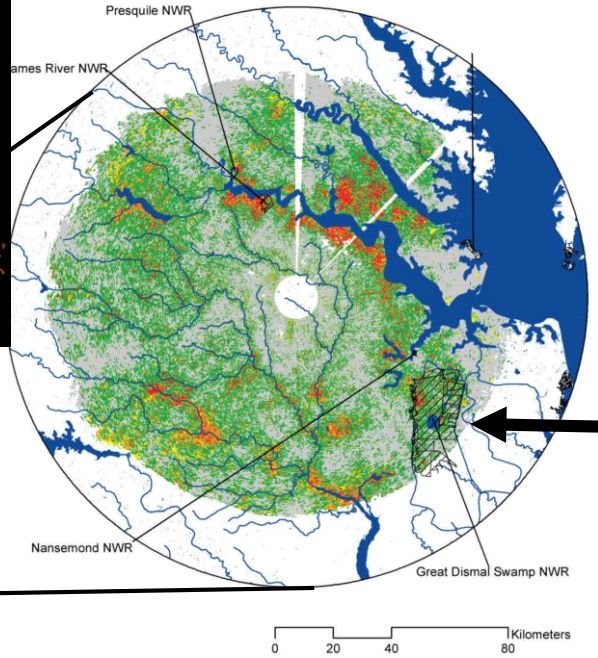
Aeroecology Program @ University of Delaware

- Mapping migratory bird distributions with NEXRAD
- Need to automate real-time processing

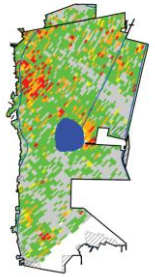
amazon web services







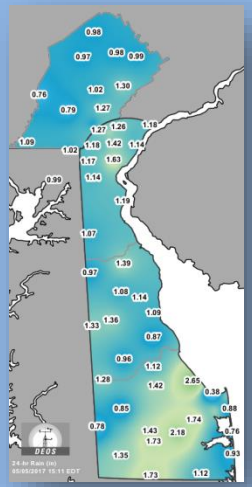
- Macroecology
- Conservation Biology
- Sustainability



CEMA: Center for Environmental Monitoring and Analysis

- Develop, operate, and maintain real-time environmental monitoring resources for Delaware
- Create and maintain value-added environmental data applications for all sectors of the Delaware economy
- Provides environmental data expertise, particularly in weather and climate, for Delaware.

DEOS Network



70 real-time platforms

Weather

Hydrology

Wave Buoy

Satellite

- Emergency Management
- Transportation
- Natural Resource Managers
- Agriculture
- Public Health
- Researchers
- Consultants

Real-time Snow Monitoring Network

Delaware Water Quality Data Portal

Delaware Irrigation Management System

Coastal Flood Monitoring System

Lima Bean Downy Mildew Risk Tool

Data ⟷ *Stakeholders* ⟷ *Applications*

Graph Blue Noise and Graph Signal Processing

Gonzalo R. Arce

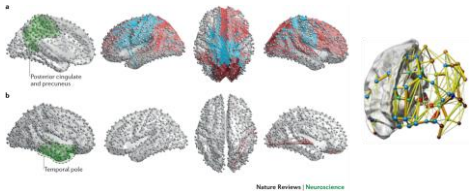
Institute of Financial Services Analytics. University of Delaware

Motivation

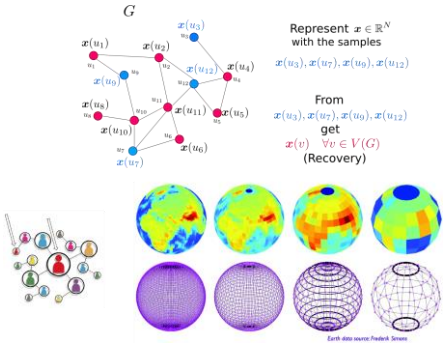
- Network Topology Inference
- Sampling
- Compress signals in irregular domains

- Spectral analysis
- Filtering
- Predict evolution of a network process

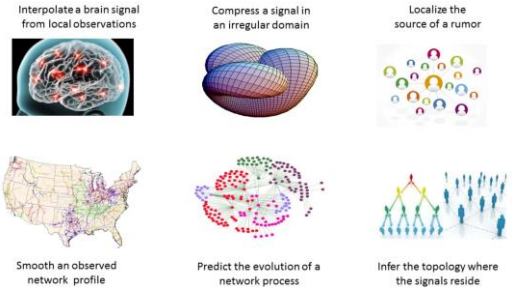
Network Topology Inference



Sampling



Graph Signal Processing



Collaborators: **Alejandro Parada-Mayorga (UD), D. Lau (U. Kentucky)**, S. Segarra (MIT).

Geometric Networks and Graph Limits

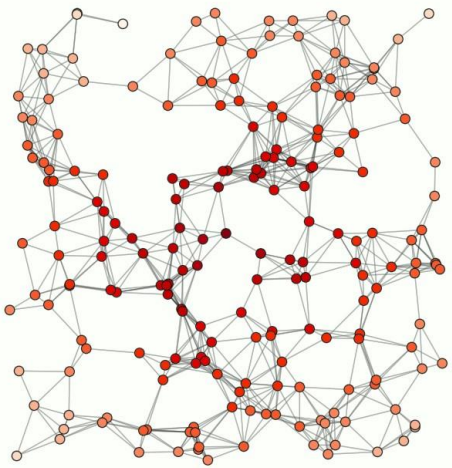
Mahya Ghandehari, Department of Mathematical Sciences

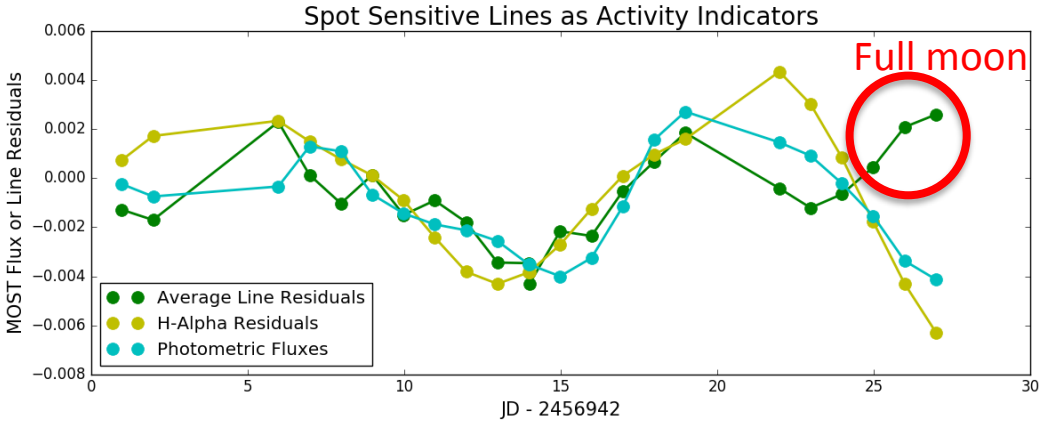
In geometric networks nodes embed in X

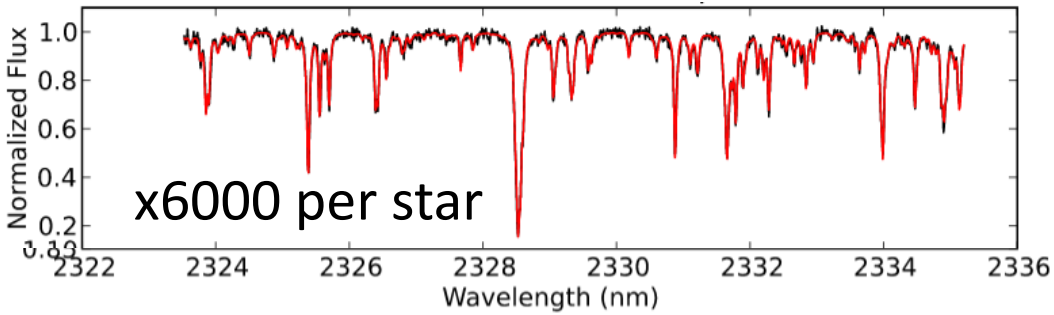
$$u \sim v \text{ iff } d(\pi(u), \pi(v)) \leq 1.$$

Ex. Social, biological and neural networks, . . .

- Question: How to retrieve the geometric reality of a network?
  e.g. metric space, geometric placement?
- Method: Graph limit theory.
- Results: Good "measure" of geometricity.
  Computable, robust to noise, continuous.
- Significance: Identify nearly geometric networks and uniformity of their processes.







Aperture Photometry Tool (APT), v. 2.4.5

100 Earths project

Goal is to discover 100 Earthlike planets

Humans need to look at every spectrum

Solution: undergrad data analysis lab

*Always remember the **First Rule of Data: Look at the data!** Doing this and using this software will make you an "apt" astronomer.*

Multiscale Complex Fluids Modeling and Simulations

Antony N. Beris, UD Chemical and Biomolecular Engineering

High performance computations and data analysis of Non-Newtonian flows

Direct Numerical Simulations of viscoelastic turbulence using Spectral methods

Karhunen-Loeve, Principal Component Analysis of the results

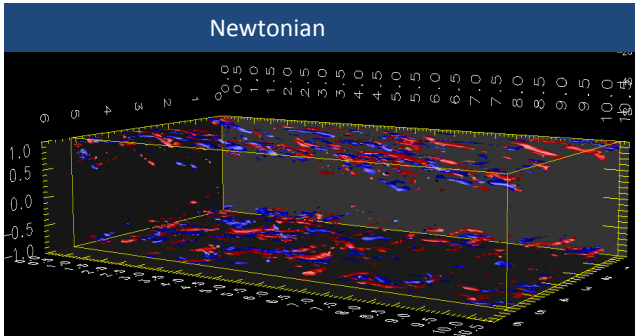
Analysis, modeling and simulation of viscoelastic porous media flows

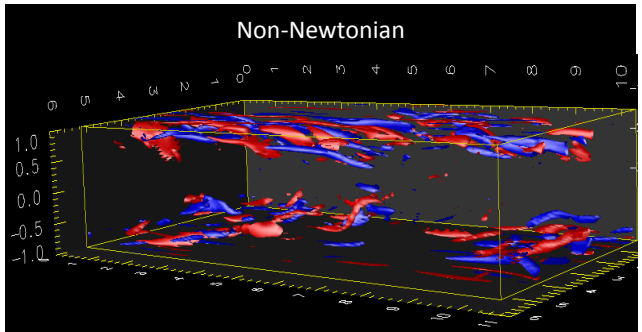
Macroscopic modeling of the flows of multiphase systems, like emulsions and suspensions

Modeling and simulation of thixotropic flows

Evaluation of yield stress and time-dependent hysteresis in aggregating suspensions

Modeling of blood rheology and multiscale simulations of blood arterial flow





Multiscale transport modeling using mesoscopic methods

Lian-Ping Wang, UD Mechanical Engineering

Data-intensive scalable computational methods

Boltzmann-equation based mesoscopic methods (lattice-Boltzmann, gas kinetic schemes)

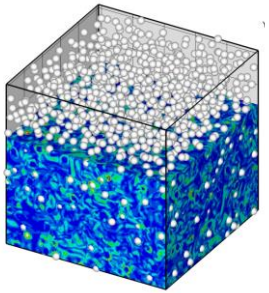
Computationally scalable and physically flexible

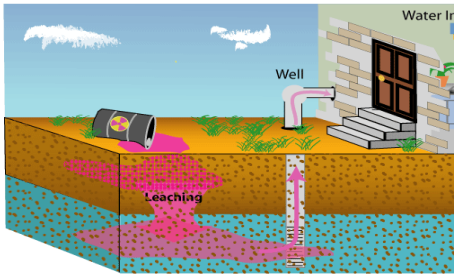
Research questions related to the water cycle and water quality

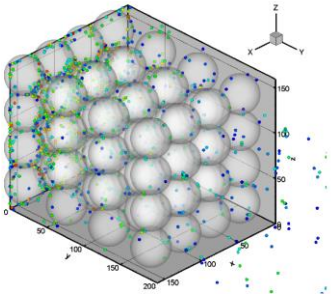
How does air turbulence affect the collision rates of cloud droplets (warm rain initiation)?

What is the fate of contaminants when released to the soil environment?

How to model transport and retention of contaminants?







KEY MESSAGE

Making sense of Big Data is even more important than the data itself

We convert Data to meaning via System-Level Models:

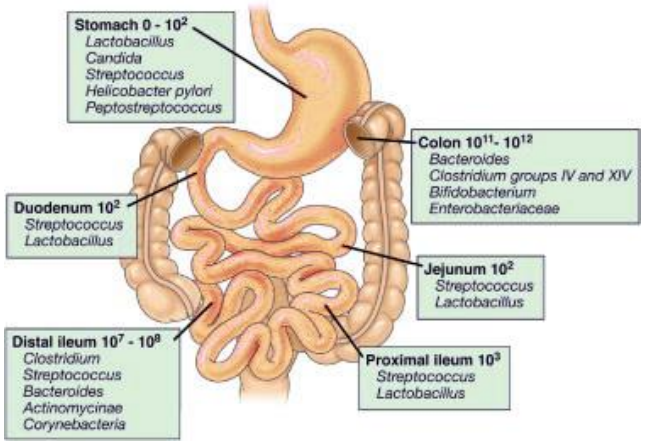
Connectivity maps, Math Models, Artificial Intelligence, other tools

Petrochemical Refinery Data

50,000 data points every millisecond

Human Gut Microbiome

100 trillion cells, 3 million genes



Prasad Dhurjati, Professor of Chemical & Biomolecular Engineering, UD
http://www.che.udel.edu/dhurjati

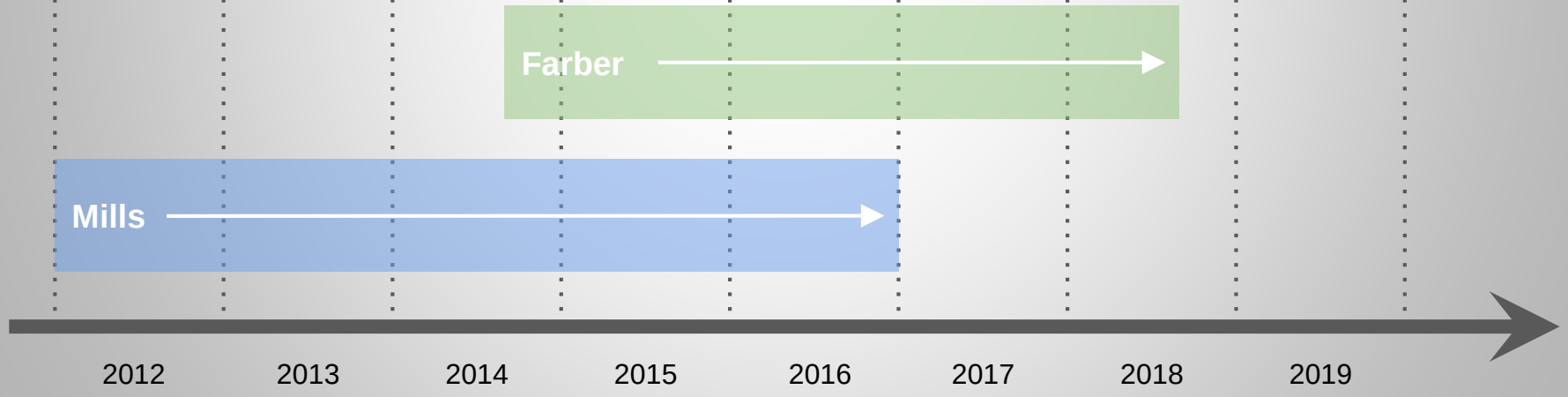
Research on Process Analytics since 1982, Health Analytics since 1995

IT HPC — Community Clusters

Dare to be first.
UNIVERSITY OF DELAWARE

1st Community Cluster
- AMD processors
- 200 nodes, 5000+ cores
- 40 Gbps InfiniBand network
- 256 TB high-performance storage (Lustre)
- **Currently end-of-life**

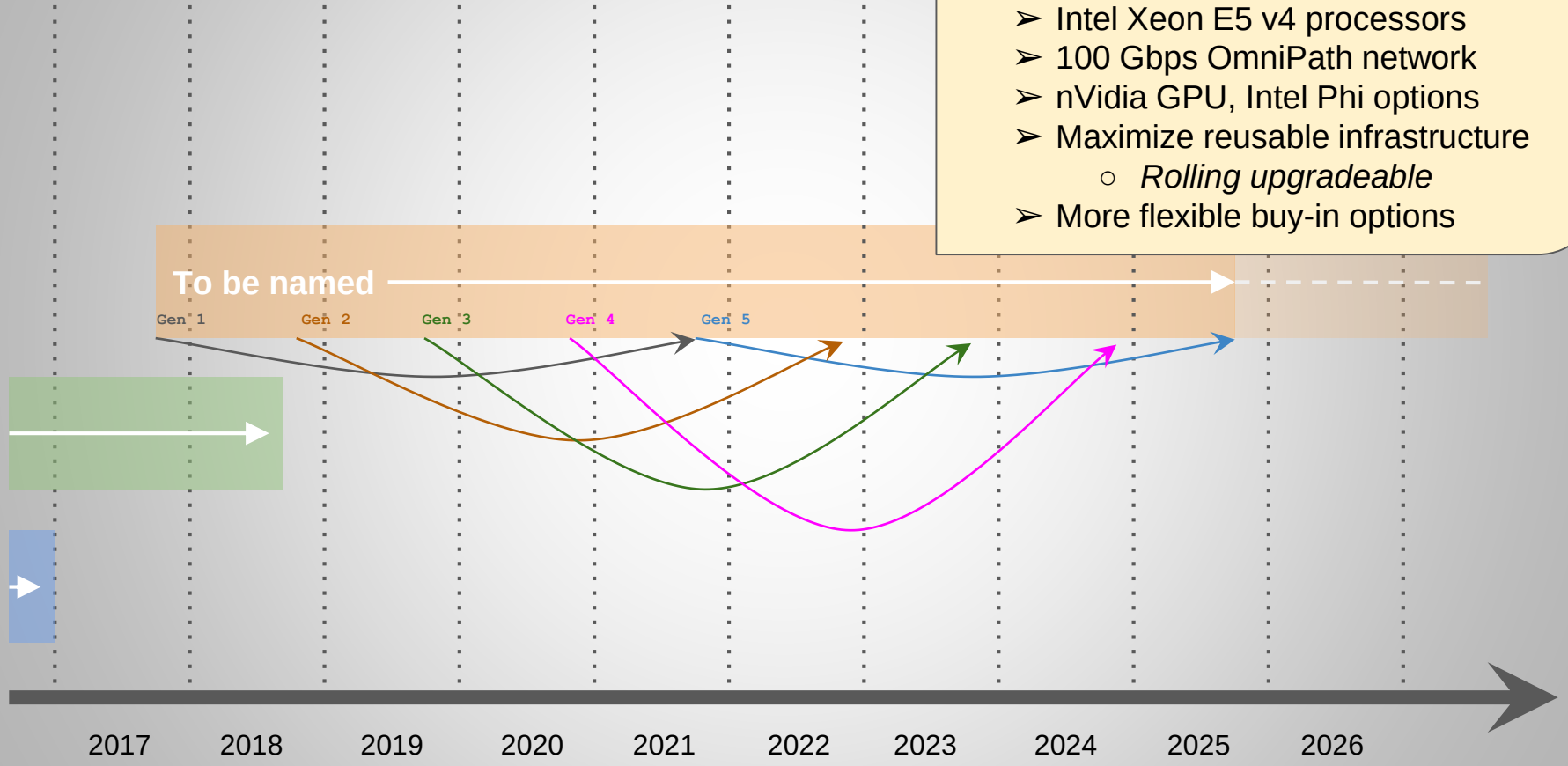
2nd Community Cluster
- Intel Xeon E5 v2 processors
- 192 nodes, 3300+ cores
- 56 Gbps InfiniBand network
- 256 TB high-performance storage (Lustre)
- nVidia GPU, Intel Phi options
- In year 3 of 4 year lifespan



IT HPC — Community Clusters

3rd Community Cluster

- Higher-density construction
- Intel Xeon E5 v4 processors
- 100 Gbps OmniPath network
- nVidia GPU, Intel Phi options
- Maximize reusable infrastructure
  - *Rolling upgradeable*
- More flexible buy-in options



IT HPC — Community Clusters

Dare to be first.
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- Make your voice heard! Let us know **you** need:

  http://www.udel.edu/003818

  http://www.udel.edu/research-computing/contact/

  it-hpc-interest@udel.edu

- For information on Research Computing at the University:

  http://www.udel.edu/research-computing/