CoS & CoS Research Network Luncheon

Research highlights from the faculty of the College of Computing and the College of Sciences

Friday, October 11, 2024

Georgia Tech

List of Presenters

1. Alexandra (Sasha) Boldyreva; sasha@gatech.edu
2. Elizabeth Cherry; echerry30@gatech.edu
3. Alex Duncan; alex.duncan@gatech.edu
4. Greg Eisenhauer; eisen@cc.gatech.edu
5. Flavio Fenton; flavio.fenton@physics.gatech.edu
6. Ben Freemen; bfreeman47@gatech.edu
7. Anna Ivanova; aivanova7@gatech.edu
8. Joshua Kretchmer; jkretchmer3@gatech.edu
9. Joe Lachance; joseph.lachance@biology.gatech.edu, jlachance6@gatech.edu
10. Karl Lang; karl.lang@eas.gatech.edu, klang37@gatech.edu
11. Anton Leykin; leykin@math.gatech.edu, aleykin3@gatech.edu
12. Meg Millhouse (with Surabhi Sachdev and Laura Cadonati); mmillhouse3@gatech.edu, ssachdev38@gatech.edu, ssachdev38@gatech.edu
13. Steve Mussman; mussmann@gatech.edu
14. Alessandro Orso; mussmann@gatech.edu, ao44@gatech.edu
15. Jeff Young; jyoung9@gatech.edu

Georgia Tech

List of Presenters

16. Zhigang Peng; zpeng@gatech.edu
17. Dana Randall; randall@cc.gatech.edu, dr83@gatech.edu
18. Kexin Rong; krong@gatech.edu
19. David Sherrill; sherrill@chemistry.gatech.edu, cs207@gatech.edu
20. Minoru Shinohara; shinohara@gatech.edu
21. Qi Tang; qtang@gatech.edu
22. Amanda Timmerman; atimmerman3@gatech.edu
23. Cindy Xiong; cxiong@gatech.edu
24. John Wise; jwise@physics.gatech.edu
25. Wei Xu; wei.xu@cc.gatech.edu
26. Yalong Yang; yalong.yang@gatech.edu
27. Saman Zonouz; szonouz6@gatech.edu
28. Amy Bruckman; asb@cc.gatech.edu
29. Vlad Kolesnikov; kolesnikov@gatech.edu
30. Francesca Storici; francesca.storici@biology.gatech.edu

Georgia Tech

Alexandra (Sasha) Boldyreva

School of Cybersecurity and Privacy
sasha@gatech.edu, www.cc.gatech.edu/~aboldyre
CODA S0913

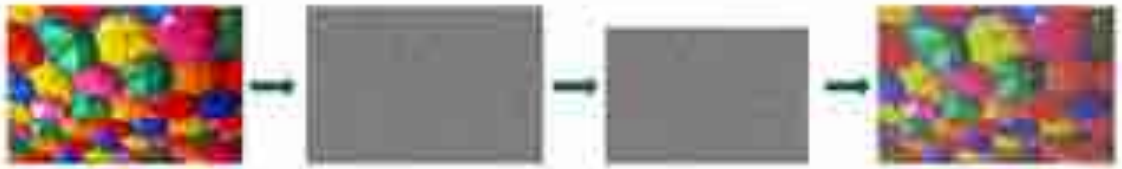
Area of research:

- Cryptography
  - In particular: Practice-oriented provable security

Current projects:

- Searchable encryption for cloud storage
- Biometrics-based crypto secure against brute-force attacks

- Encryption and authentication for images undergoing compression



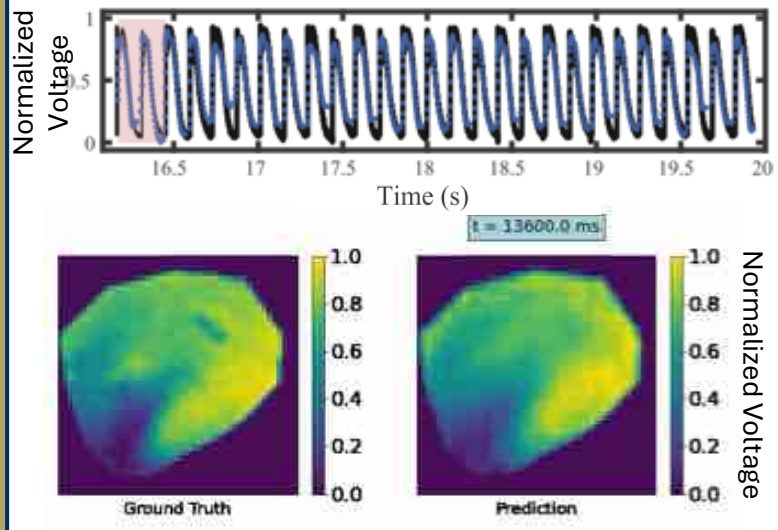
- Fighting misinformation with digital image attestation

Elizabeth Cherry – School of Computational Science and Engineering

Interests:

- Scientific computing
- Computational modeling
- High-performance computing
- Scientific machine learning
- User-friendly scientific software
- Nonlinear dynamics & math bio

Machine learning: predictions of time series (cardiac voltage data, single cell and tissue)

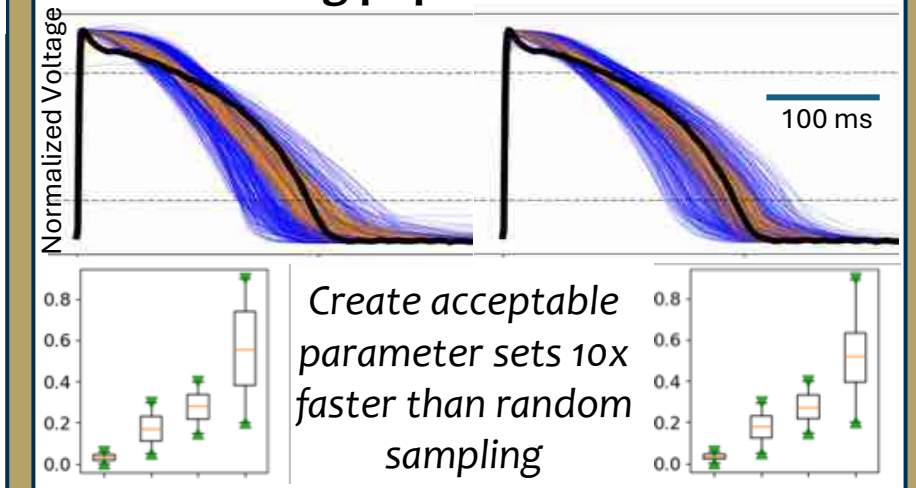


Explanted human heart: predictions over ~2.4s (11.2 s training, 2.4s validation)

Browser-based, GPU-accelerated optimization tool

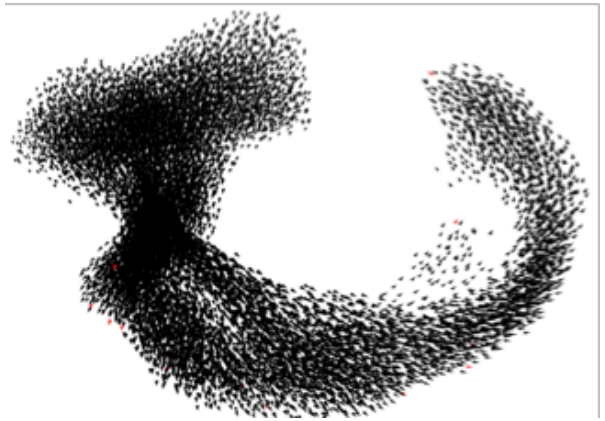
Can fit up to ~30 parameters for 4 coupled differential equations in ~30 seconds

Generating populations of models



Create acceptable parameter sets 10x faster than random sampling

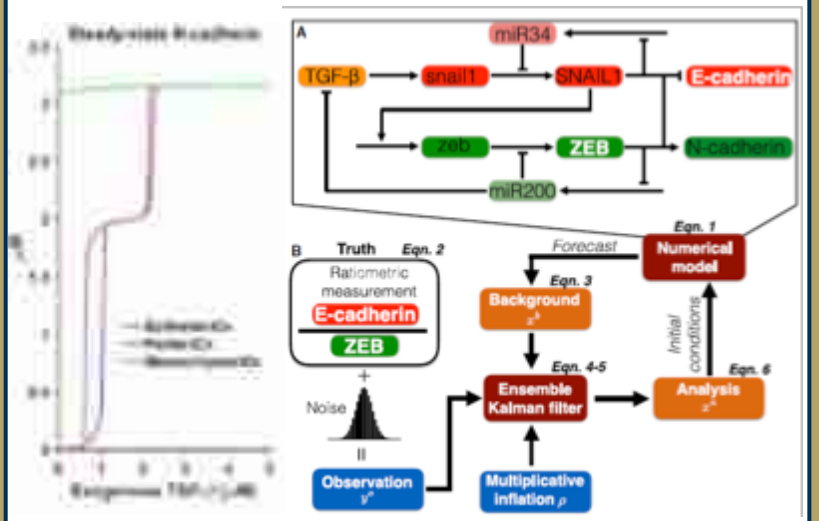
GPU-accelerated simulations of 10^4 bird flocks in 3D



Turn dynamics

Effects of leaders, predators

Data assimilation



Epithelial-mesenchymal transition: can predict current state and transition

Alex Duncan
Senior Director of OMSCS

Learning at Scale
- Peer advising
- Peer review
- Broad trends in learning at scale

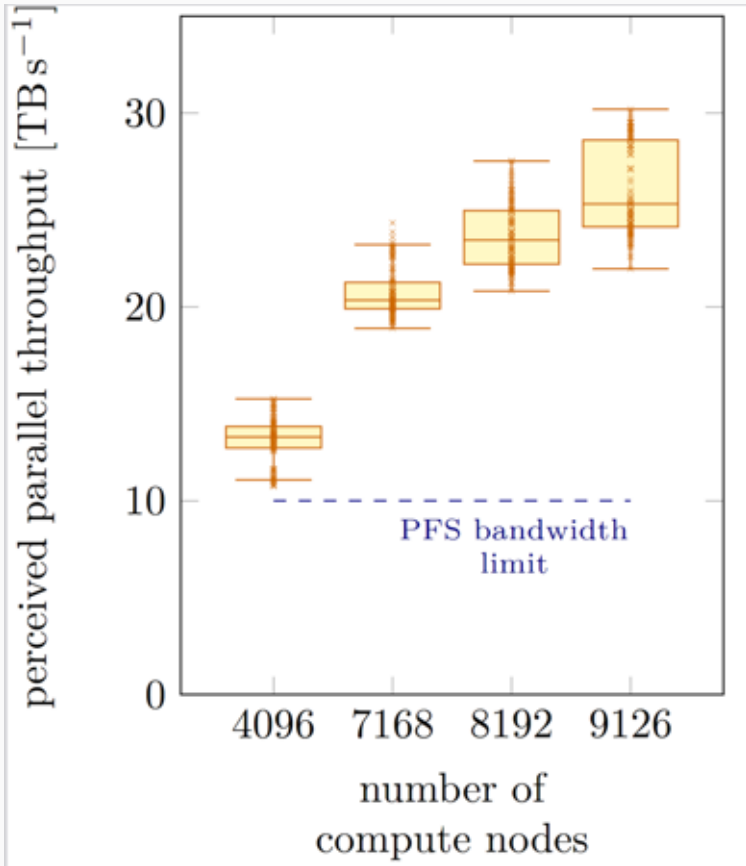
Student Experience
- Student obstacles
- Perceptions of digital proctoring
- Student life

Online Learning and CS Education
- Enrollment motivations/goals
- Prep for OMSCS
- Trends in OMSCS

Georgia Tech

High Speed I/O and Application Coupling at Exascale

- How do you get data out of large-scale scientific simulations?
  - Long term storage
  - Transfer to analysis or visualization
- Work with Oak Ridge National Lab
- ADIOS I/O system
  - Self-describing application-friendly data model
  - N-dimensional arrays decomposed across MPI ranks
  - No requirement that read decomposition matches write
  - Portable write performance
- Newest work
  - Stream data directly between running HPC applications without changes using the same APIs
    - Avoid slow filesystem
  - Semantic remote data access
    - Move metadata, not data
    - Analyze portions of a dataset without moving it all



Greg Eisenhauer – eisen@cc.gatech.edu

Georgia Tech College of Computing
School of Computer Science

Georgia Tech

CHAOS LAB

Complex Heart Arrhythmias and other Oscillating Systems

Flavio H. Fenton

School of Physics

Interest:

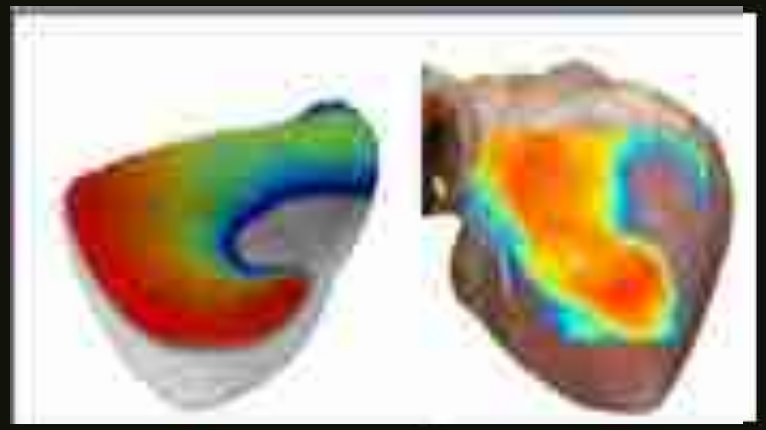
- Anything that oscillate
- Dynamical & Nonlinear Systems
- Chaos and Chaos Control
- High-Performance computing with GPU
- Computational Physics
- Outreach

I use a combined
Theoretical + Experimental + Numerical approach

Main interest are:
+Heart Dynamics
+Arrhythmia Mechanism
+ Control/termination of Arrhythmias.
+Pattern Formations

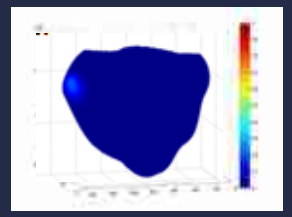
Zebra Fish Heart

Spiral waves of electrical dynamics → Tachycardia



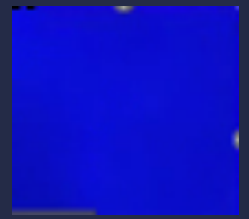
Topological dynamics of spiral waves in 3D

Defibrillation Studies

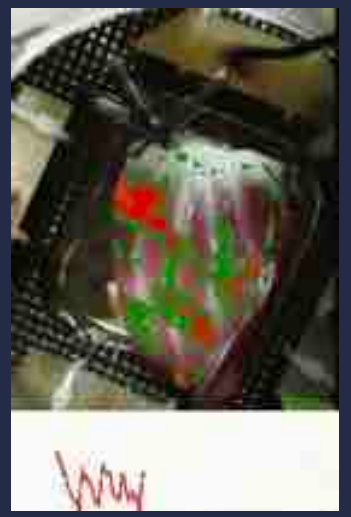


1 shock

LEAP: 5 low energy shock



Defibrillation Studies
In-vitro Optical Mapping



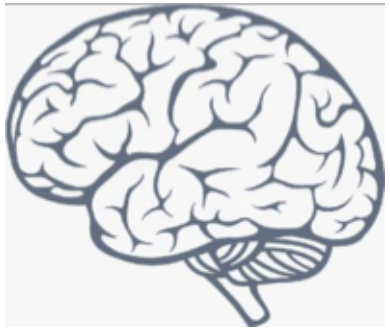
ECG from in vivo
LEAP Experiments

Species on the move: how warming temperatures have set in motion an “escalator to extinction”

Ben Freeman, Biology

What is the relationship between language and knowledge/reasoning?

in the human brain

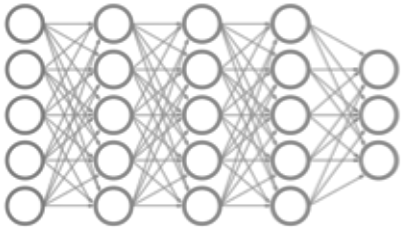


```
validation['cid']=0
if sum(validation.values())==7:
    print('yes')
    count+=1
```

Ivanova et al, 2020, eLife

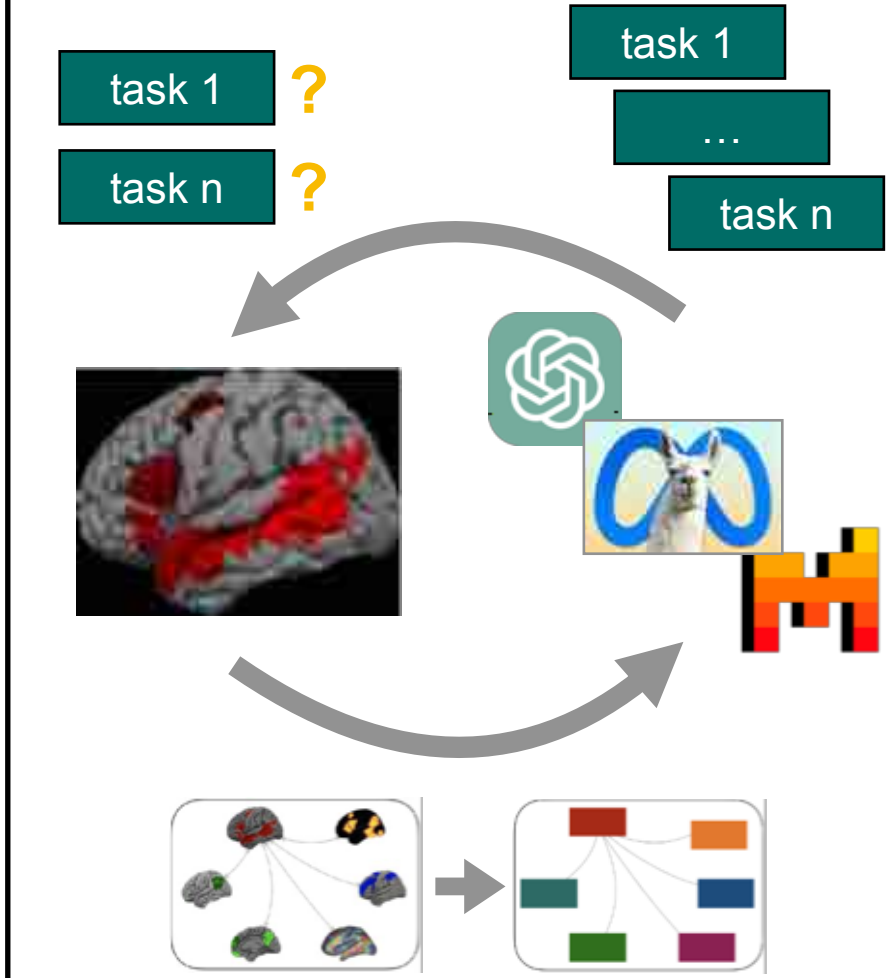
Ivanova et al, 2021, NoL

in AI models (LLMs)



Kauf, Ivanova et al, 2023, CogSci

Ivanova et al, in review



Mahowald, Ivanova et al, 2024, TiCS

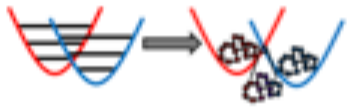
Kretchmer Group: New simulation methods for electron dynamics in complex environments

Method Development

Multi-faceted research group working at the interface of electronic structure and quantum dynamics

Classically Isomorphic Methods

Map a complicated quantum system to a computationally tractable classical system



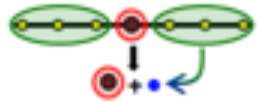
Quantum mechanics

Classical mechanics

Real-Time Electronic Structure

Solve the time *dependent* Schrödinger equation – Quantum embedding

Subsystem coupled to *large* environment

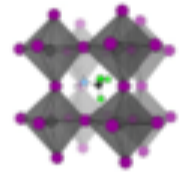


Subsystem coupled to *small* environment

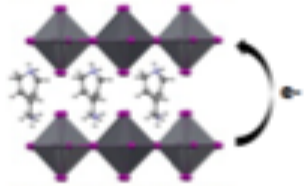
Electron Transport in Correlated Materials

Examine electron-nuclear and electron-electron interactions in governing the non-equilibrium transport of electrons

Charge-transport in 3D and 2D perovskites



Explicit electron in fully atomistic simulation

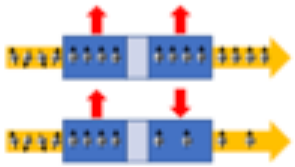


Interlayer ET

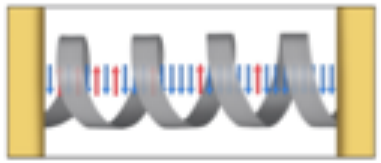
Spin Dynamics Across Interfaces

Examine how spin-spin and spin-orbit interactions govern interfacial spin-transport

Magnetic Tunnel Junctions

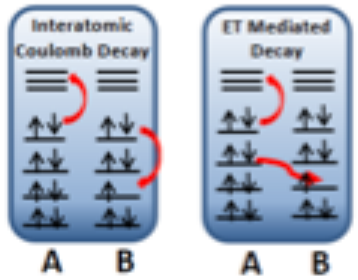


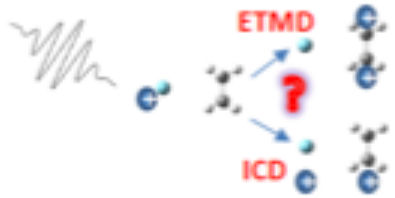
Chirality-Induced Spin Selectivity



Electron Relaxation in Weakly Bound Systems

Ionization of a core electron initiates competing ultrafast electronic processes that lead to fragmentation in VdW and H-bonded systems





Joe Lachance
Doc Blanchard Associate Professor
School of Biological Sciences

Motivating question:

Why do genetic disease risks vary across human populations?

Automatic feature detection for accessible geochronology

NSF proposal pending, potential for CS student funding

Problem: Radiometric dating is fundamental earth science, but most methods (e.g. U-Pb) are expensive and limited to select, wealthy labs.
How can we make radiometric dating more accessible to everyone?

Solution: image-based analysis of ^{238}U fission tracks is a cheap way to date minerals - requiring only access to a computer (and some time).

Catch: image-based analysis is still time consuming and error-prone.
How can we automatic detection of fission tracks from image stacks?

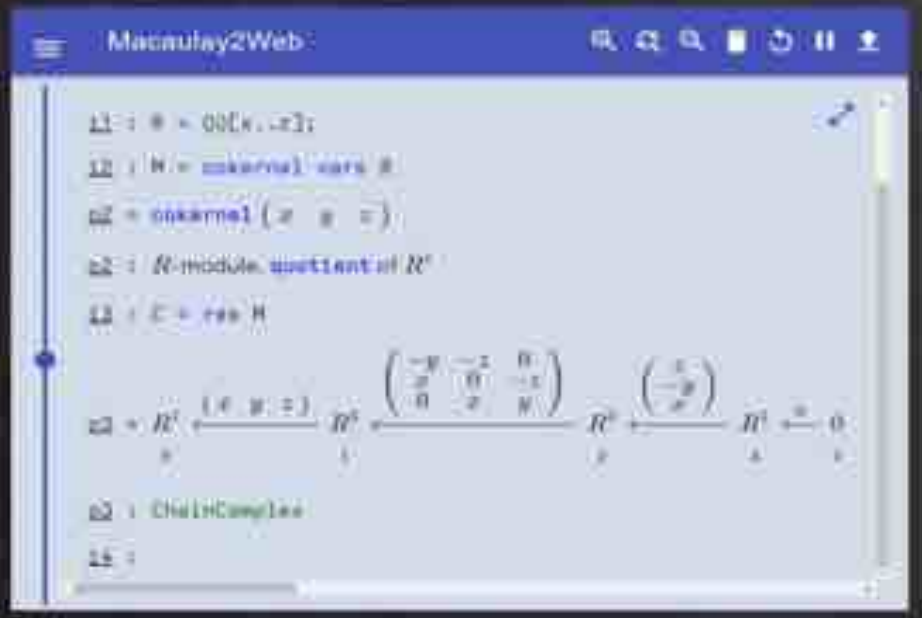
Collaboration: looking for help in **image processing, machine learning (YOLO), Java based app development in ImageJ/Fiji**

Me: Karl Lang, EAS Asst Prof.
email: karl.lang@eas.gatech.edu
office: Ford 3242

TECH tonics research group

Computer Algebra

Macaulay2: software for commutative algebra, algebraic geometry,

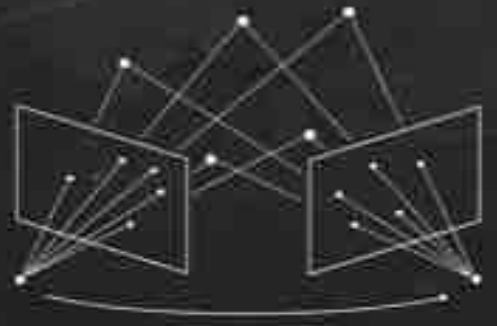


macaulay2.math.gatech.edu

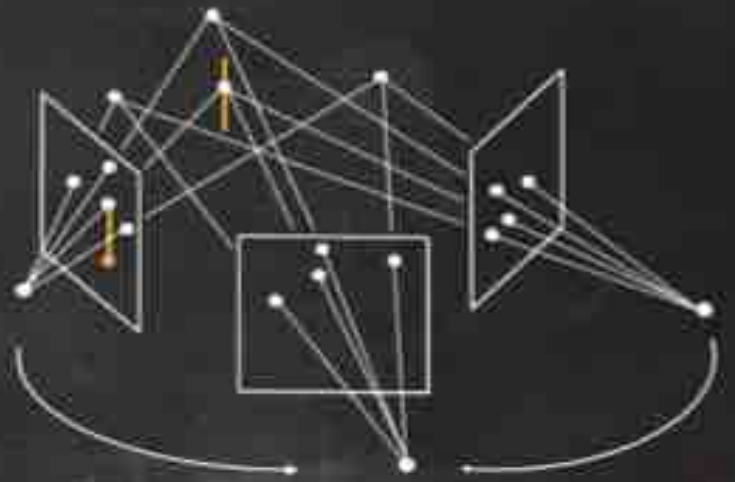
numerical algebraic geometry, nonlinear algebra and applications

Anton Leykin

(CoS/SoM/ACO/ARC/CSE)



Computer Vision



Hruby, Duff, L., Pajdla.
Learning to Solve Hard Minimal Problems.
CVPR 2022 (best paper)

↑

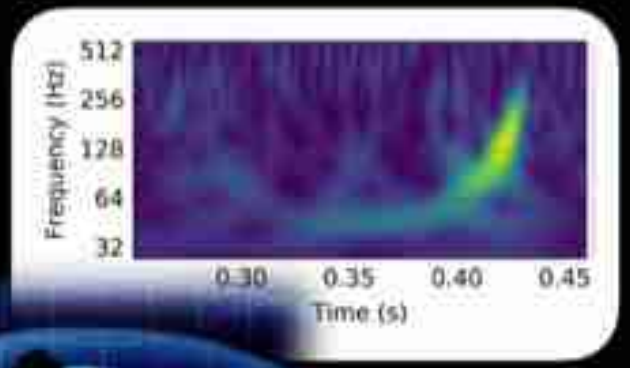
pandemic

↑

Duff, Kohn, L., Pajdla.
PLMP: point-line minimal problems in complete multi-view visibility.
ICCV 2019 (best student paper)

Gravitational-wave data analysis

Meg Millhouse, Surabhi Sachdev, Laura Cadonati — Center for Relativistic Astrophysics



Inspiraling compact objects (black holes, neutron stars) emit ***gravitational waves***

Measured by the Laser Interferometer Gravitational-wave Observatory (**LIGO**)

Our primary research areas:

Detector data quality:
- Identify and remove transient noise artifacts than can negatively affect other analyses

Signal agnostic analysis:
- Reconstruct signals with minimal a priori assumptions on signal type
  - Can be used to find new sources

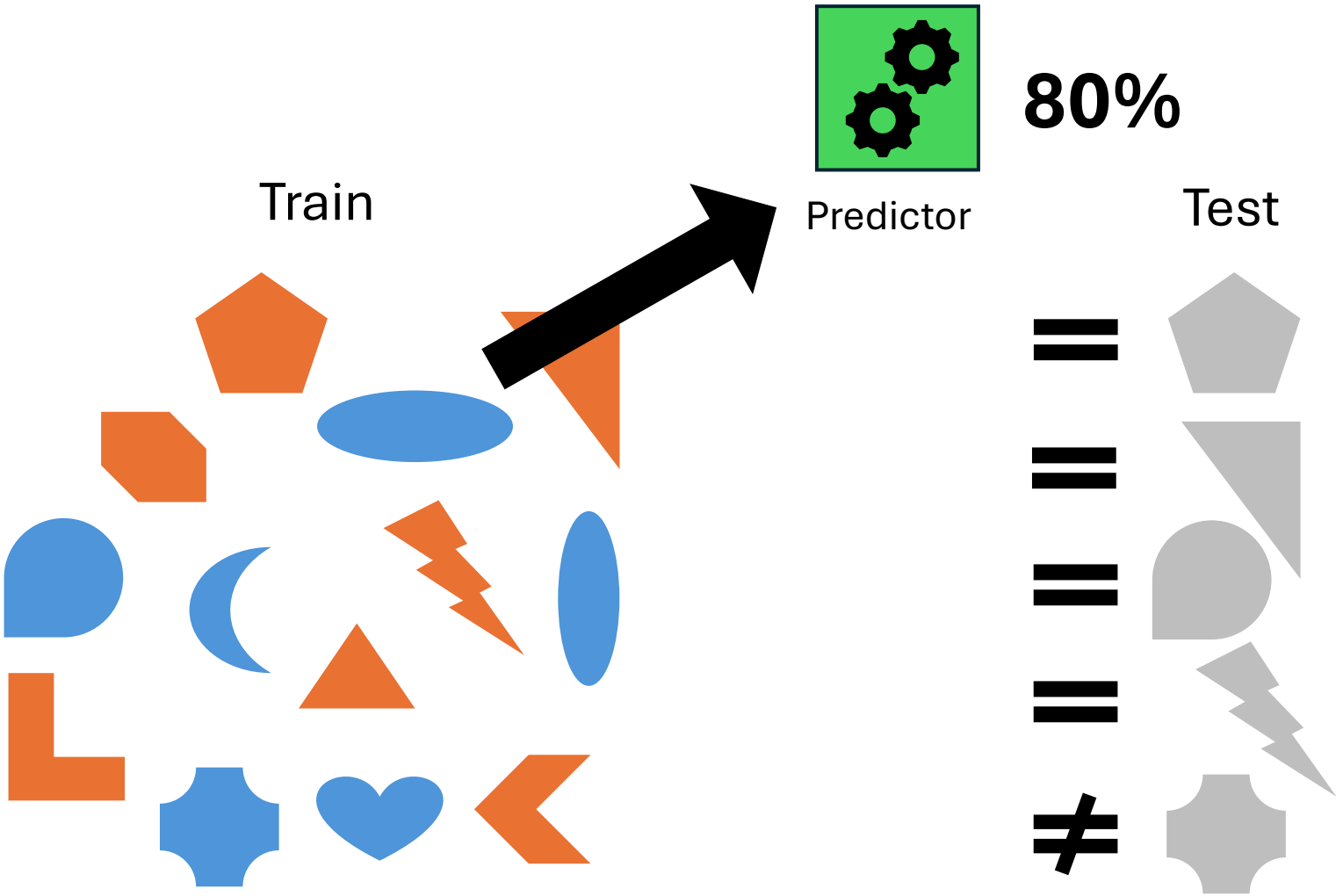
Low-latency detection:
- Rapidly identify GW events in detector data
  - Important for sending alerts to astronomers to follow events up with other observatories

Parameter estimation:
- Infer physical parameters of system, such as masses and spins of objects

Steve Mussmann

Data-centric machine learning

How to build and validate an ML system?



1. Collect
2. Split
3. Train
4. Predict
5. Compare

CSSE: Center for Scientific Software Engineering

https://ssecenter.cc.gatech.edu/

History: Created in December 2021 as part of Schmidt Futures' $40M Virtual Institute for Scientific Software

Mission:

- CSSE will advance and support scientific research by applying modern software engineering practices, cutting-edge technologies, and modern tools to the development of scientific software within and outside GT
- CSSE will also engage with students and researchers to train the next generation of SW engineering leaders

Team: 6 professional software engineers with a combined 61 years of industry experience

CSSE and CoS: CSSE can help CoS researchers with their research projects and research proposals

Vision:

Georgia Tech Software Engineering Center

Alessandro Orso
Jeff Young

Georgia Tech College of Computing
Center for Scientific Software Engineering