NCSA Fellows 2023-24 Idea Acceleration Workshop

October 7, 2022

Welcome!
We will begin shortly.

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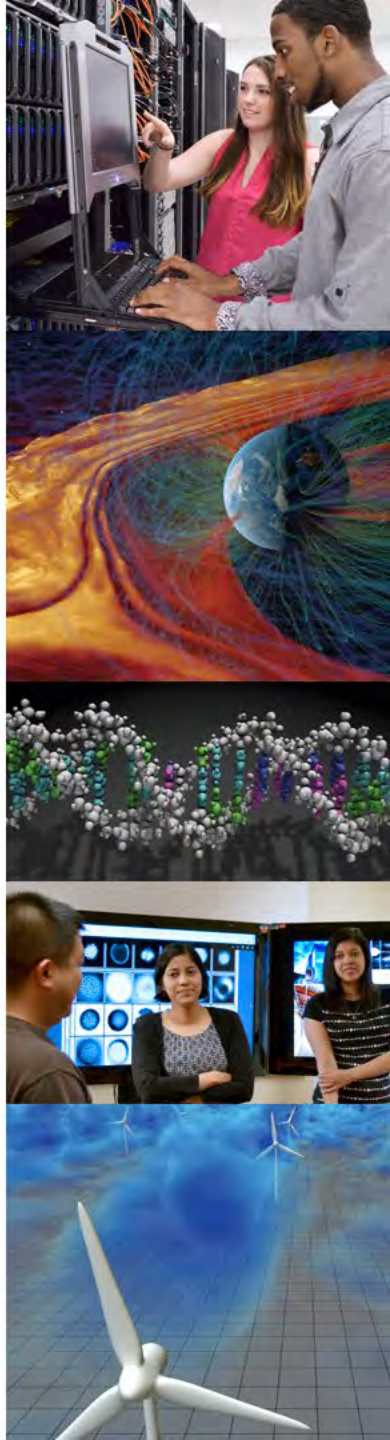
Agenda

- Opening remarks - John Towns, Executive Associate Director, Engagement, NCSA

- Brief Overview of NCSA Fellows program - Olena Kindratenko, Senior Research Coordinator, NCSA

- NCSA Staff presentations from 11:05 am – 11:45 am
  - Seid Koric: Research Consulting Directorate
  - Xiaoxia Liao: Data Analytics
  - Christina Fliege: Genomics
  - Gregory Bauer: Science and Engineering Application Support Group
  - Kenton McHenry: Software
  - Volodymyr Kindratenko: Center for AI Innovation
  - Daniel Lapine: Innovative Systems Laboratory
  - John MacMullen: Midwest Big Data Hub
  - Jeff Carpenter: Visualization Program Office
  - Maria Jaromin: Healthcare Innovation Program Office
  - Matthew Hudson: Center for Digital Agriculture



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Agenda (cont.)

- Faculty presentations from 11:45 am – 12:30 pm
  - Sean Mullen, Department of Kinesiology and Community Health
  - Juan Salamanca, School of Art and Design
  - Vadim Zharnitsky, Department of Mathematics
  - Jinhui Yan, Civil and Environmental Engineering
  - Nancy McElwain, Department of Human Development and Family Studies
  - Yilan Xu, Department of Agricultural and Consumer Economics
  - Haohan Wang, School of Information Sciences
  - Ramez Hajj, Department of Civil and Environmental Engineering
  - Yilang Feng, Gies College of Business
  - Nickvash Kani, Department of Electrical and Computer Engineering
  - Han Zhao, Department of Computer Science
  - Darko Marinov, Department of Computer Science
  - Rich Sowers, Mathematics, Industrial and Enterprise Systems Engineering
  - Howard Gritton, Department of Comparative Biosciences
  - Yongjoo Park, Department of Computer Science

- Networking session in Zoom breakout rooms from 12:30 pm – 1:00 pm

  This session is a speed match-making event that helps potential fellowship applicants find NCSA staff and other researchers with whom to collaborate and build successful proposals.

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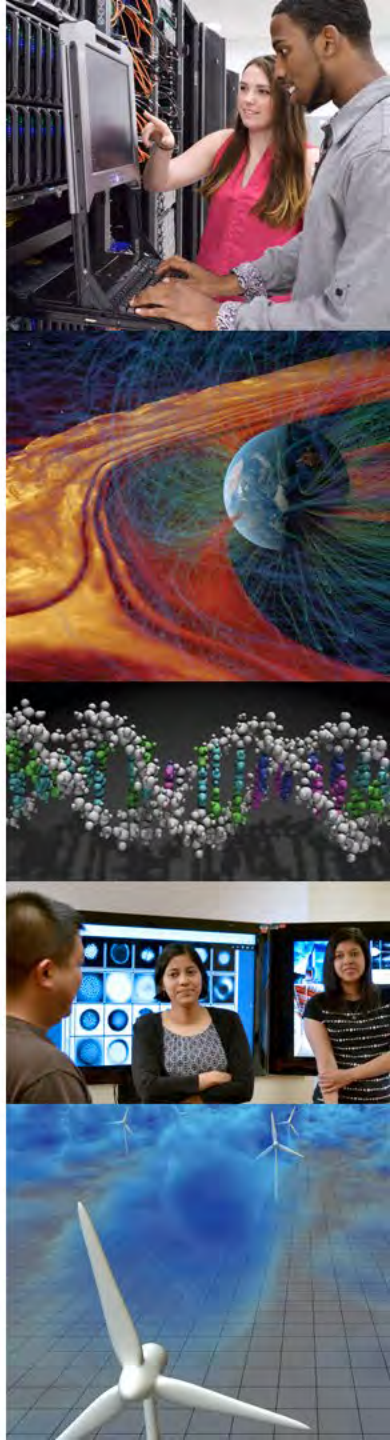


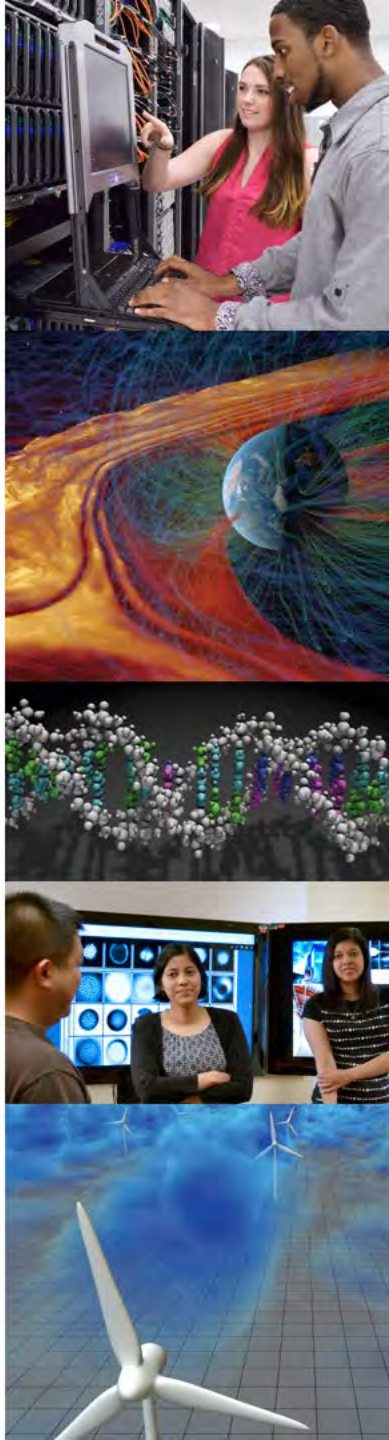
NCSA Fellows Program (est. 1999)

- Competitive program provides seed funding (up to $25K/award) for demonstration, start-up projects, workshops, and/or other activities with the potential to lead to longer-term collaborations and externally funded activities around research and development
  - Anticipate funding from the NCSA's Director's Office for 5-6 projects for the 2023-2024 cohort
  - Additional projects may be funded by other NCSA programs if they match the research interests

Important Dates

- **October 31, 2022**: Deadline to submit to the NCSA Fellows Program –Link to submit will be posted on our NCSA wiki webpage following the Idea Accelerator Workshop
- **By February 1, 2023**: Target date for decisions
- All information from NCSA Fellows Kick-off meeting and the Idea Acceleration workshop will be available on the NCSA Wiki via NCSA Fellows website: https://www.ncsa.illinois.edu/about/fellowships-internships/ncsa-fellows-program/

NCSA staff presentations



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Research Consulting Directorate and Confluence of Numerical Modeling Methods and Artificial Intelligence

Seid Korić
koric@Illinois.edu
Technical Associate Director-NCSA
Research Professor –The Grainger College of Engineering
University of Illinois at Urbana-Champaign

National Center for Supercomputing Applications
UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

Ideas Acceleration Workshop, October 7, 2022

Research Consulting at NCSA

ENABLING ACADEMIC & INDUSTRY RESEARCH

User Support

- Help desk
  - Access, sys. monitoring
- Business IT
  - Desktop Support, Event Services, CMDB, Savannah, Tableau, Conference Room and Virtual Meeting Support
- Computing environments
  - Compilers, libraries, I/O
  - Allocations
- Jobs
  - Scripts, queues, web interfaces
- Training & documentation

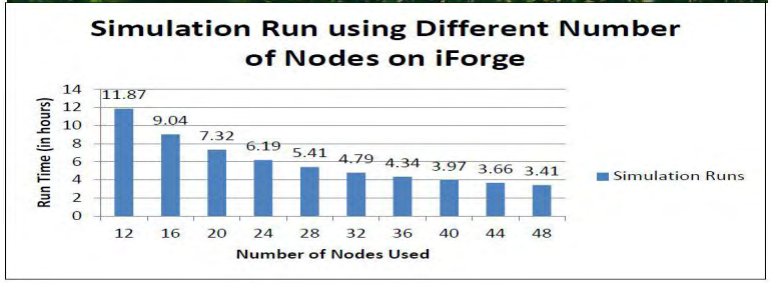
Research Solutions

- Code dev. & improvements
  - Debugging, profiling, development
- Software & apps
  - Installs, maintenance, validations, benchmarks
- Advanced support
  - Numerical methods, accelerated computing, advanced programming
- Domain expertise and consulting
  - Modeling/Simulation, Genomics, Data Analytics, Machine Learning, GIS, Physics, Engineering, Astronomy

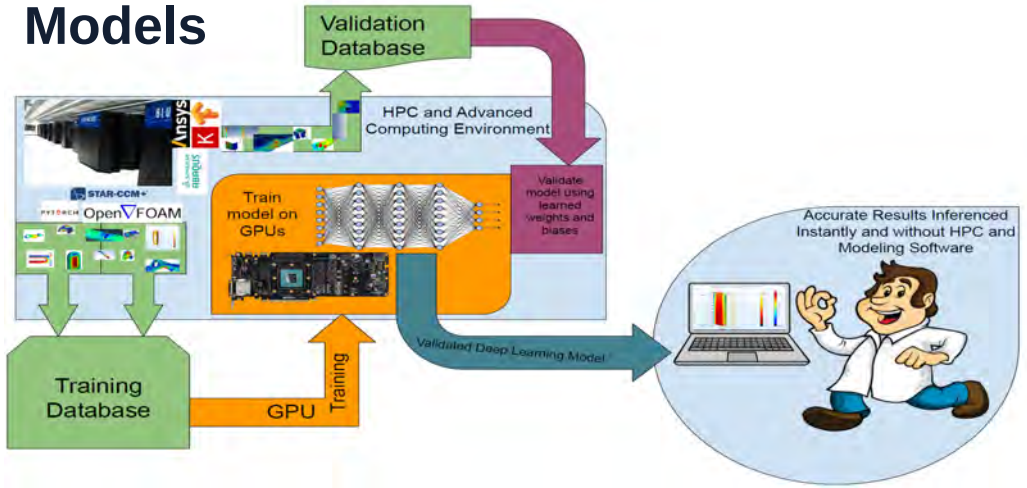
Outreach

- Academic and industry collaboration and partnership
- Grant development
- Student talent & workforce development

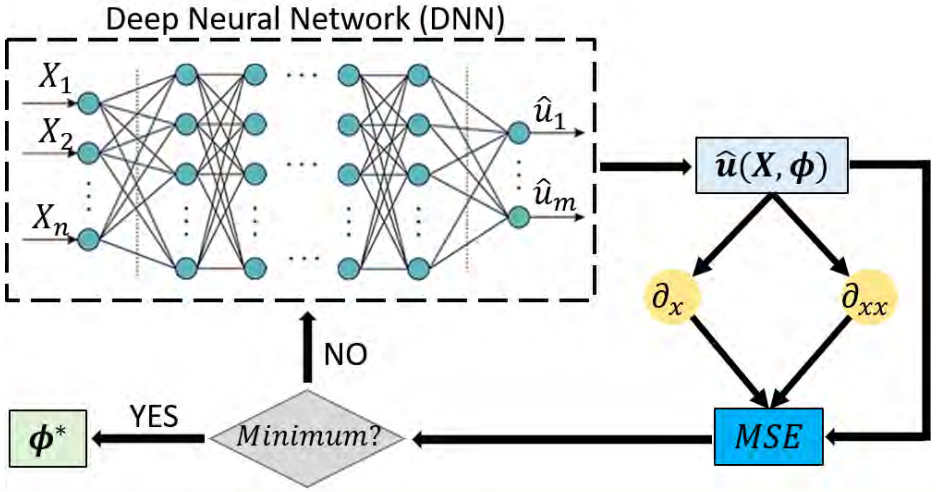
Classical Statistical Models + HPC



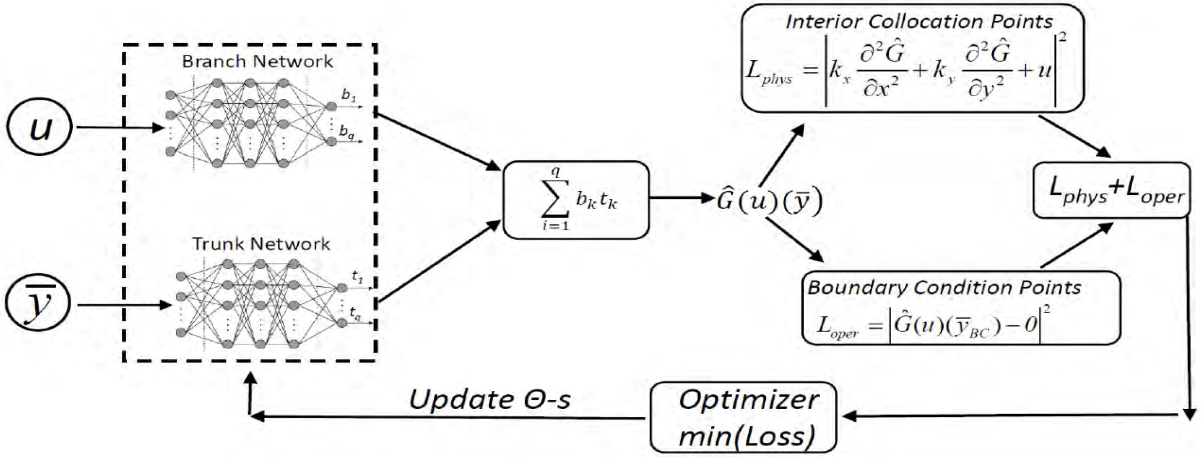
Data-Driven Surrogate Deep Learning Models



Physics-informed Neural Networks



Deep Operator Networks (DeepONets)



Data Analytics

Xiaoxia Liao

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Introduction

- Data engineering
- Apply ML/DL/Programming for problem solving
- Domain expertise: CS, Physics, GIS, MechEng
- Industry project consulting
- Contribute to our university’s world-class research

Xiaoxia Liao

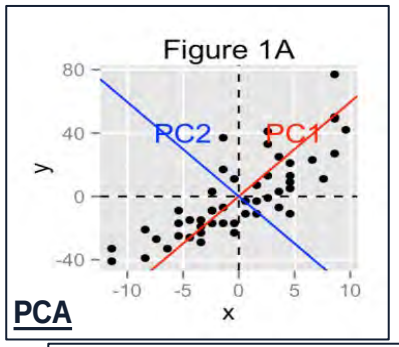
Dr. Aiman Soliman

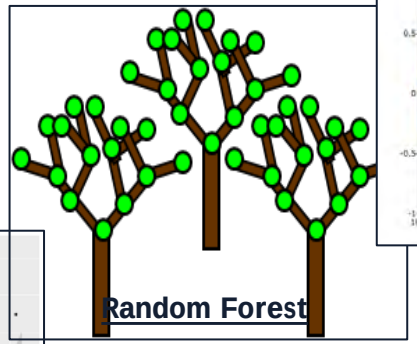
Yifang Zhang

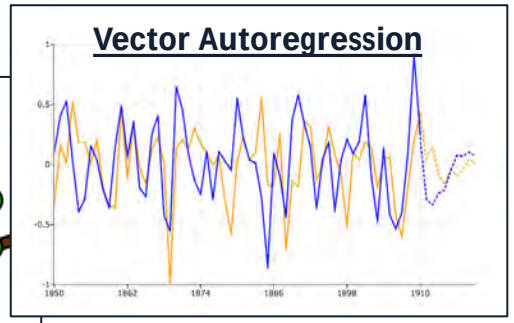
Dr. Shirui Luo

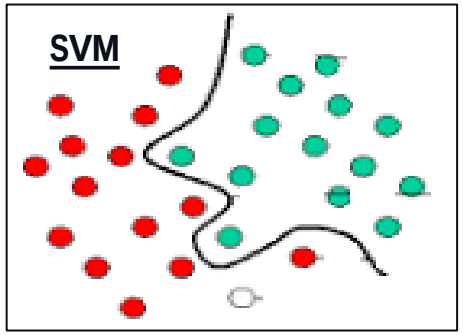
Dr. Matt Krafczyk

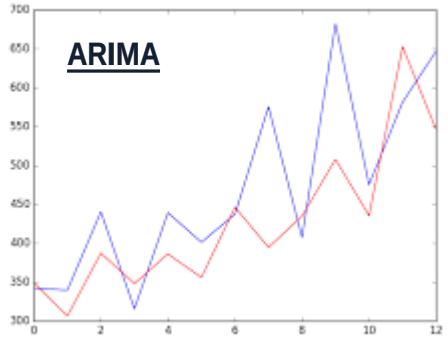
Implemented Many ML/DL Algorithms

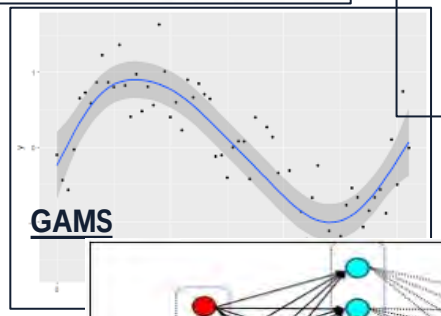


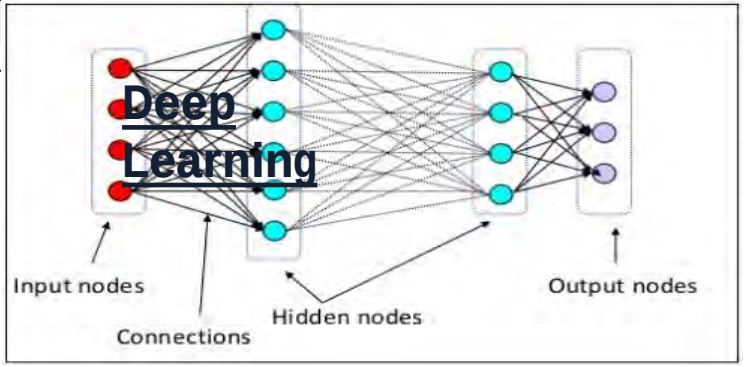


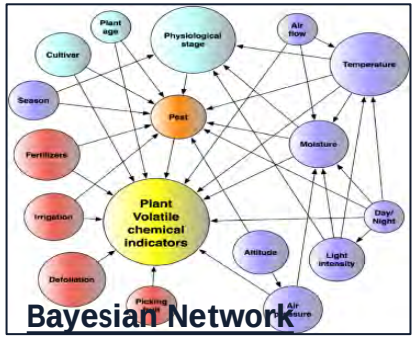


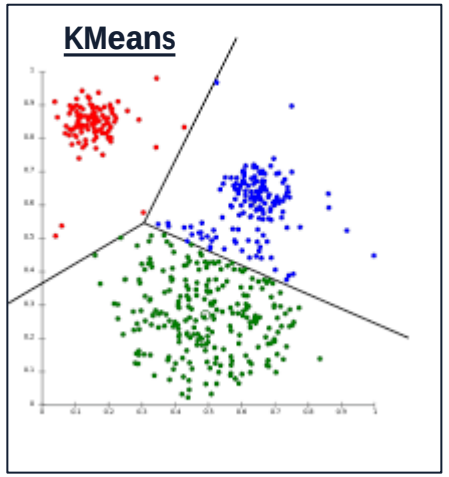


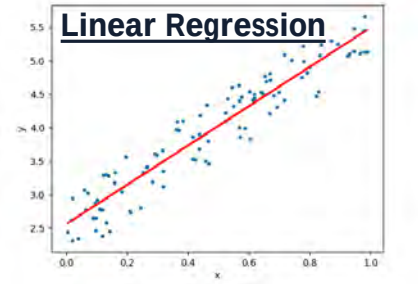




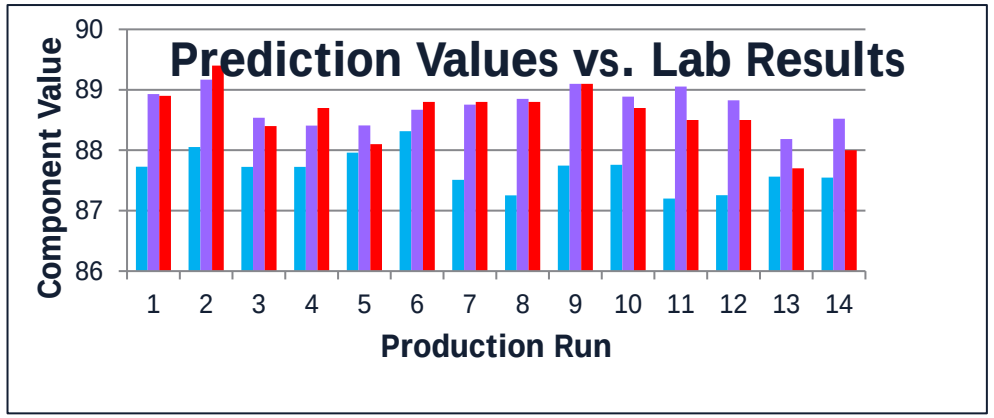




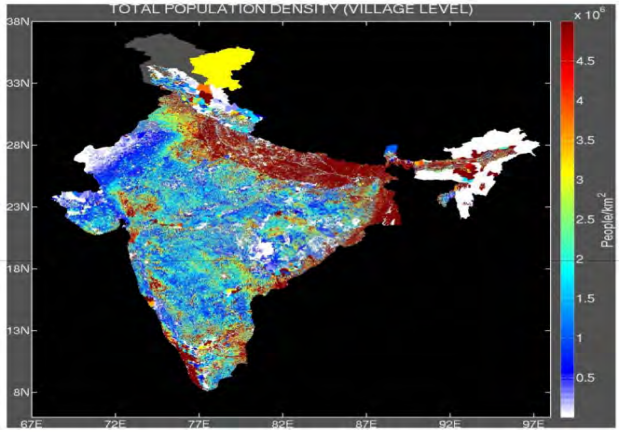




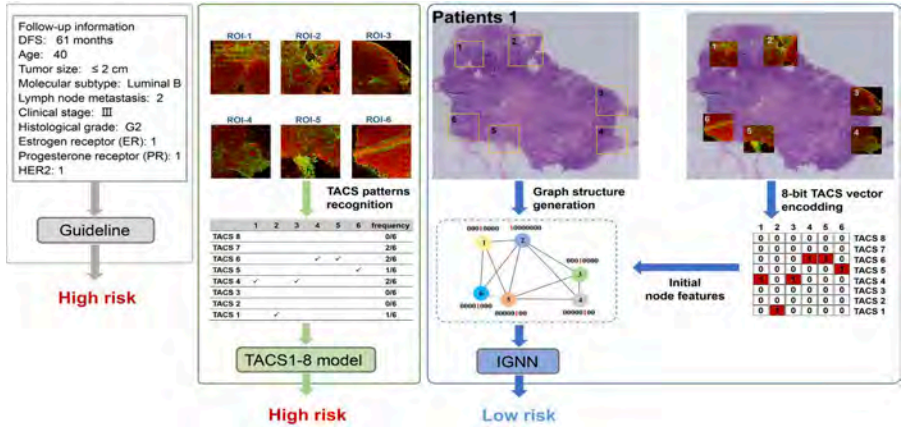
Example Projects



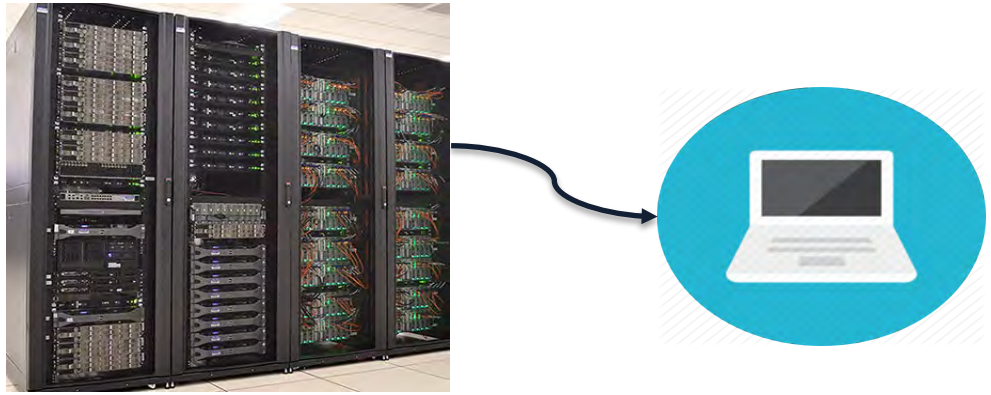
ML for Manufacturing



Data Science in Geospatial, Social, Economics



Bioimage Deep Learning



HPC Application and User Support

Genomics

Christina Fliege
cfliege2@illinois.edu

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Genomics

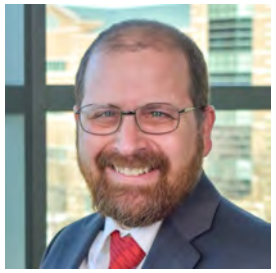
Genomics workflow development
tool selection, performance optimization, refactoring, porting, productionize, introduction of new features

Genomics software and algorithm development, cancer and evolutionary development software

Benchmarking and Analysis of new Biological sofware

Machine-Learning and Modeling of Biological Data sets

Biological Biomedical and Agricultural Domain Expertise


Joshua Allen
Python debugging, optimization, and performance analysis, Genomics workflows for clinical production, HPC: scheduling, optimizing, automating, New approaches to bioinformatics problems and algorithm development

David Bianchi, Ph.D
Biological Data Science and Bioinformatics Analysis, Scientific HPC, GPU programming and Code Profiling, Metabolic and Kinetic Modeling of Biological Pathways

Weihao Ge, Ph.D
R, Python, Machine-learning, Epidemiological Modeling, Statistics, Molecular Dynamics

Mohith Manjunath, Ph.D
cancer genomics, workflow development, Google Cloud Platform (GCP), Python & R, computational mechanics

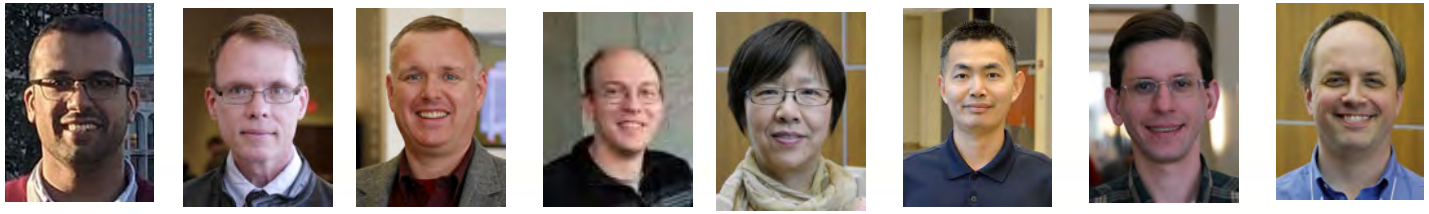
Research Consulting Science and Engineering Application Support

Gregory Bauer

National Center for Supercomputing Applications
UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

Science and Engineering Application Support

- Help with porting, debugging, performance analysis, scaling studies, acceleration, code improvements, workflows.
- Assist with implementation of programming models: MPI, OpenMP, OpenACC.
- Design and development of computational algorithms.
- AI, ML and DL method development
- NCSA Delta and Nightingale, NFI Hydro
- Domain expertise



- Diab Abueidda, PhD
  - AI applications, ML/DL, Materials Engineering.
- Galen Arnold
  - Performance Tuning, Debugging, HPC, Python
- Robert Brunner
  - HPC runtimes (Charm++), NAMD/VMD, HPC
- Jing Li, PhD
  - Numerical algorithms and methods
- Qiyue Lu, PhD
  - Finite Element, Iterative Methods, HPC, Mech Eng.
- Ryan Mokos
  - Porting, Debugging, Workflows, Network Simulation,
- Craig Steffen, PhD
  - Accelerators, IO, Exp. Particle Physics
- Roland Haas, PhD
  - Numerical Relativity, HPC, Python

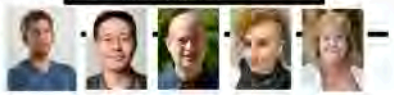
NCSA Software

- Scientific software development
  - Data management, data analysis & machine learning, workflows, science gateways, …
  - Reusable software tools & frameworks
- Bridging and amplifying efforts across different projects

US RSE

Software Program Office
- *Kenton McHenry*
- *Jong Lee*
- *Dan Katz*
- *Katie Naum*
- *Lisa Yanello*

Management Committee







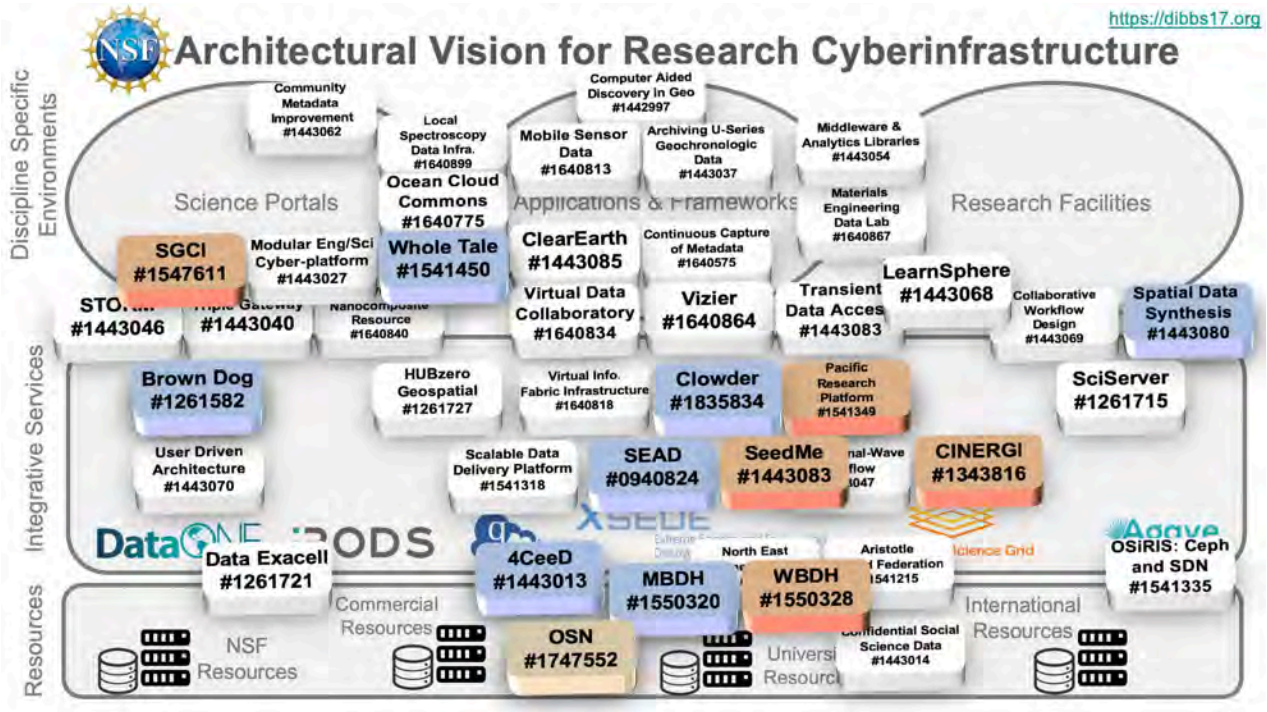
Software Applications and Data Lab (SADL)
- *Luigi Marini*
- *Max Burnette*
- *Chen Wang*
- *Todd Nicholson*
- *Vismayak Mohanarajan*
- *Mikolaj Kowalik*
- *Dippanita Dey*

Research Software Applications and Learning Technologies (ReSALT)
- *Chris Navarro*
- *Sandeep Puthanveetil Satheesan*
- *Bing Zhang*

Software Design Delivery and Deploy (SD3)
- *Rob Kooper*
- *Ben Galewsky*
- *Yong Wook Kim*
- *Sara Lambert*
- *Mike Bobak*
- *Doug Freidel*
- *Minu Mathew*

Visual Analytics (VA)
- *Matt Berry*
- *Lisa Gatzke*
- *Charles Blatti*
- *Chad Olson*
- *Jessica Saw*
- *Fangyu Zhou*
- *Santiago Nunez-Corrales*

Tools for Research Institutes and Infrastructure (TRI)
- *Nathan Tolbert*
- *Steven Peckins*
- *Rebecca Eveland*
- *Camille Goudeseune*
- *Michael Shapiro*



Center for AI Innovation

Volodymyr Kindratenko

National Center for Supercomputing Applications
UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

Center for AI Innovation (CAII)

Volodymyr Kindratenko (kindrtnk@illinois.edu)

1. **Research (Academic)**
2. **Scholarship (Students)**
3. **Industry (Companies)**
4. **Technology (Systems)**

- Bring together University AI research community for opportunities to collaborate
- Align academic research with industry challenges and opportunities
- Provide students with opportunities to learn and work in AI domain
- Partner with leading researchers and technology developers to bring state-of-the-art AI capabilities to the University research community

AI Systems Innovation Lab

- HAL
  - 16 IBM Power9 servers with 4x NVIDIA V100 GPUs
  - DDN parallel file system
- HALL-I
  - Cerebras CS-2 Wafer Scale Engine with 850K AI optimized compute cores
- HAL-DGX
  - 8 NVIDIA A100 GPUs
- NVIDIA Arm HPC Developer Kit
  - 2 NVIDIA A100 GPUs
- FPGA systems
  - IBM AC 922 server with CAPI2.0 Nallatech card
  - IBM IC 922 server with OpenCAPI AlphaData card
  - x86 server with Xilinx u250 card

Innovative Systems Lab (ISL)

Daniel Lapine

October 2022

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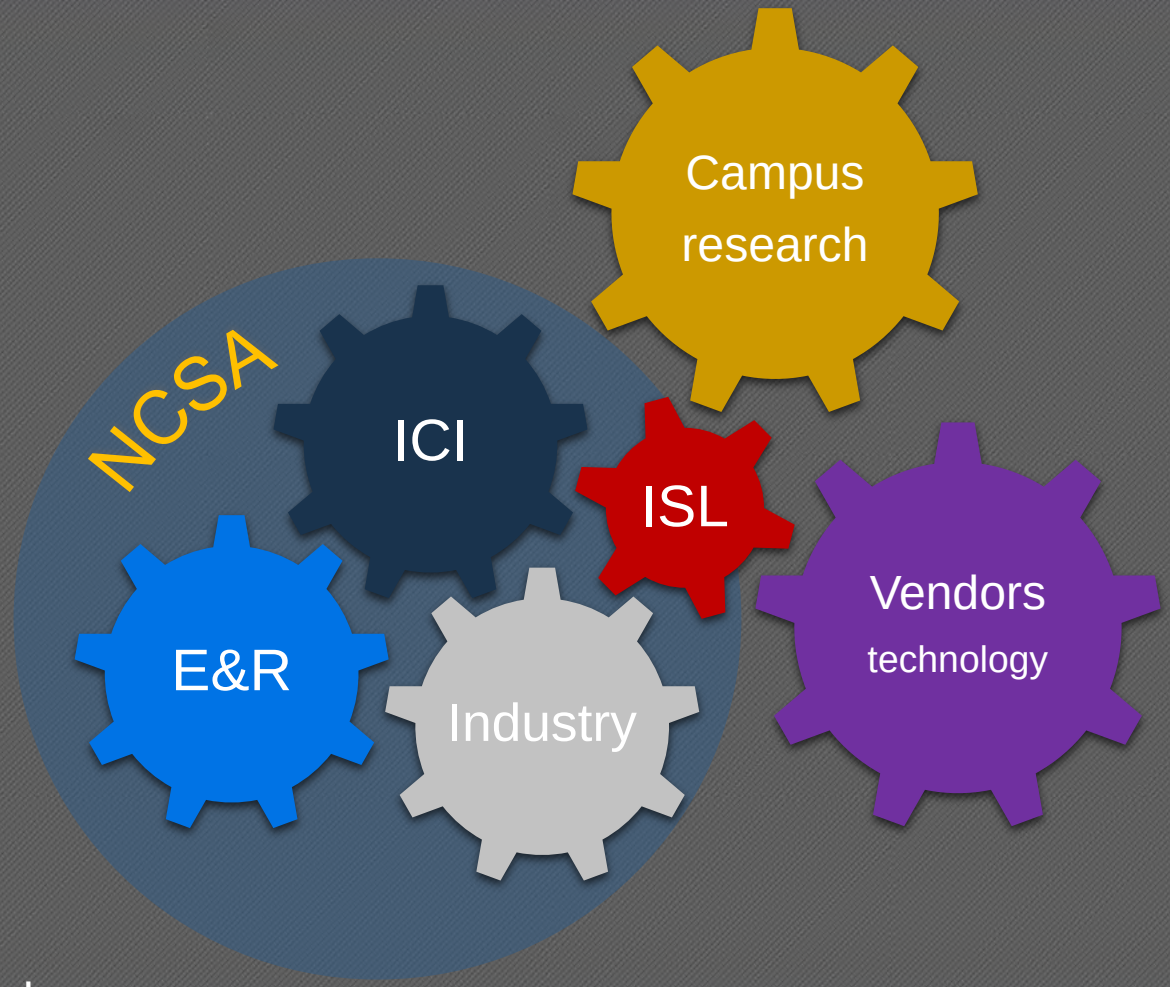
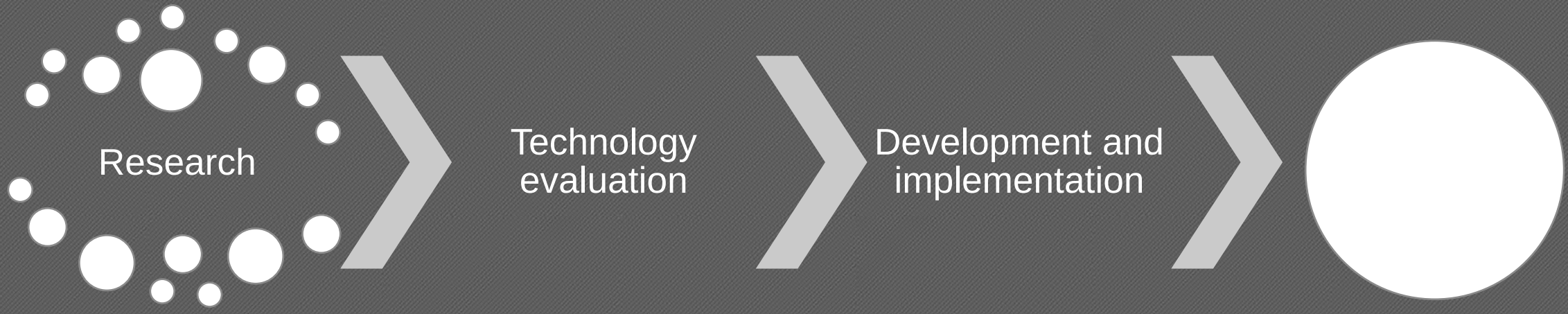
ISL Vision: Opportunity Engine for NCSA

- **Joining New Research**
  - Special projects
  - Connection to campus
  - Business development
- **Discovering Technologies**
  - R&D vehicle for new technologies
  - Addressing mid- and long-term needs in core technology areas
  - R&D agenda setup by technical leadership, input from faculty and staff
  - Connection to outside research and vendors



ISL's Research-to-Production Pipeline



Research at industry/academia leads to technology development which may or may not be suitable for scientific computing

ISL engages at the early stages of technology development to evaluate its suitability for future use in NCSA production environments

ISL puts together components necessary for the technology to become usable in production environments

As technology becomes mature, the larger community starts to sustain the effort

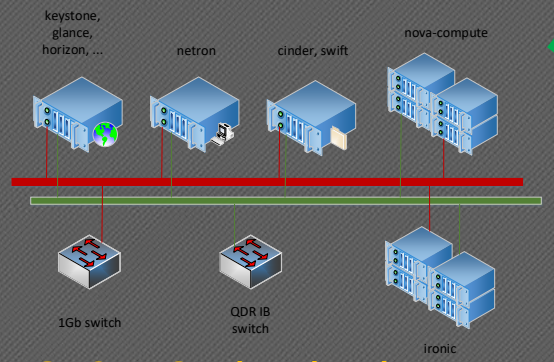
ISL Impact Examples

ISL FPGA- GPU Cluster, 2008-2021

~$1.5M in NSF-funded research

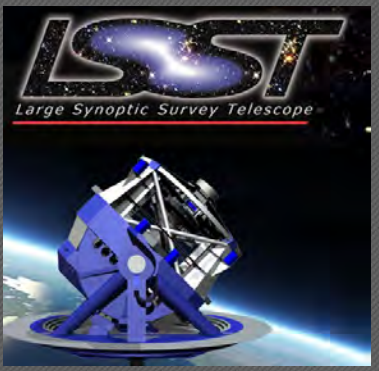
Blue Waters

Delta



ISL OpenStack and Hadoop clusters, 2012-2013

Radiant



Nebula

List of ISL Systems

https://wiki.ncsa.illinois.edu/display/ISL20/Systems

Midwest Big Data Innovation Hub (MBDH)

Priority Areas & Cross-Cutting Themes

- Advanced Materials and Manufacturing
- Big Data and Health
- Digital Agriculture
- Smart and Resilient Communities
- Water Quality
- Data Science Education and Workforce Development
- Cyberinfrastructure, Data Access, and Use

Working Groups and Projects

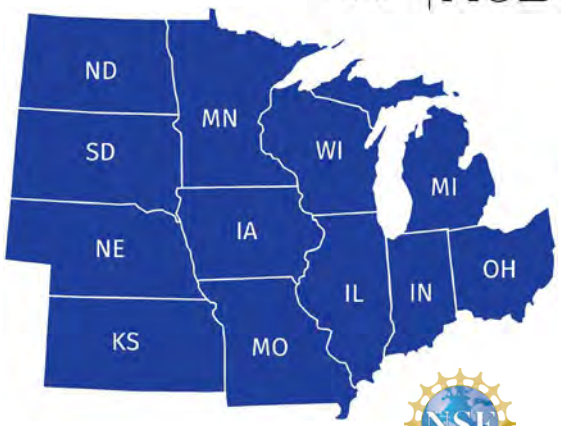
- IEEE working group on best practices for ag supply chain data interoperability
- Midwest Carpentries Community
- Data Science Student community and National Student Data Corps Midwest chapter
- COVID Information Commons community

Goals

- Build and cultivate diverse, multi-discipline, cross-sector **Communities** around data challenges and cyberinfrastructure resources
- Foster innovative activities across our **Priority Areas**
- Increase **Education and Training** around data science, particularly in small institutions and under-represented populations
- Incubate new regional initiatives through our **Community Development and Engagement** program

Join Us!

- Community Data Needs Assessment (Community DNA) research activities
- Collaboration Café monthly webinar
- Data Science Education Working Group
- Cyberinfrastructure and Data Sharing Working Group (national monthly call)



MidwestBigDataHub.org | wjohn@illinois.edu

1550320
1916613

NCSA Visualization Program Office (VizPO)

Name: Jeff Carpenter

Visualization Designer

Advanced Visualization Lab

ILLINOIS

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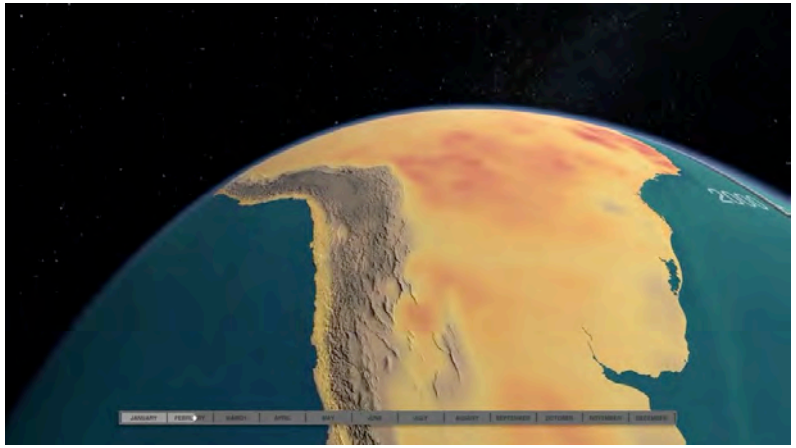
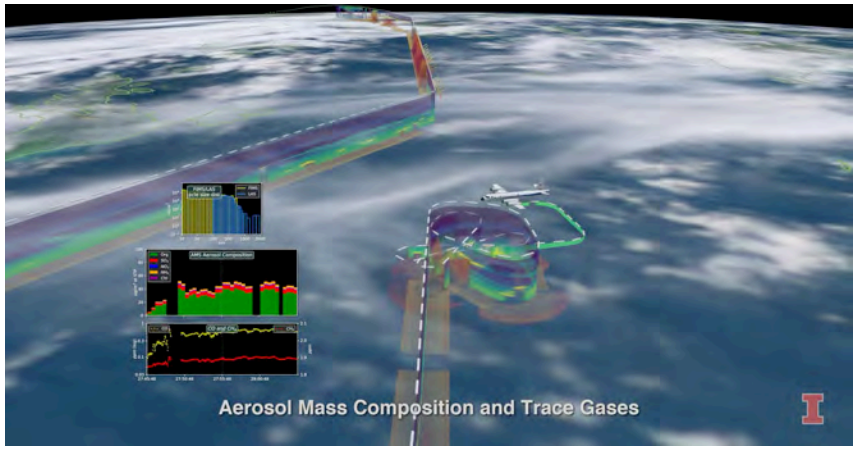
Advanced Visualization Lab (AVL)

Advanced Visualization Lab (AVL) focuses on cinematic scientific visualization for public outreach, and has contributed to many documentary films, planetarium and museum experiences, and live performance.



Average Daily Temp
2000 vs 2100

The Tao of Bach

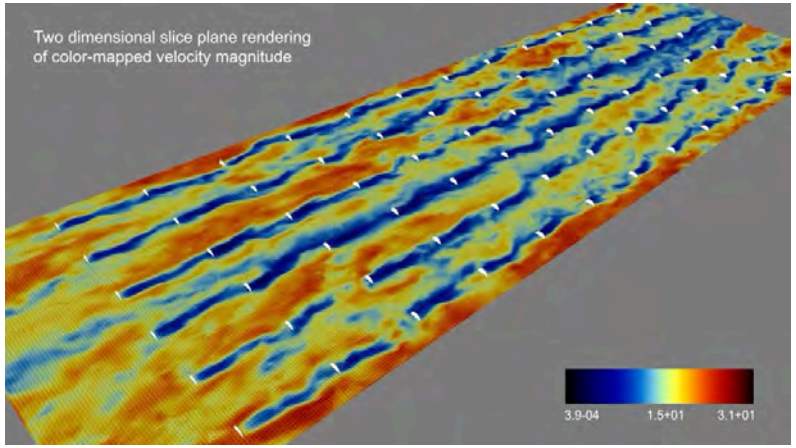


Camp2Ex Dashboard

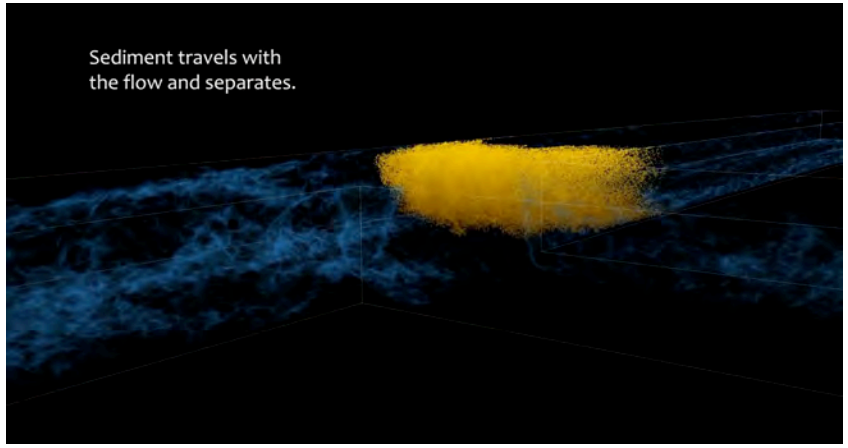
Data Analytics and Visualization (DAV)

Data Analytics and Visualization

- Originated as the combination of Blue Waters and XSEDE visualization support
- The team has experience working with Augmented Reality/Virtual Reality, High Performance Computing, parallelization & optimization running on advanced hardware systems



Large Eddy Sim of Wind Farms



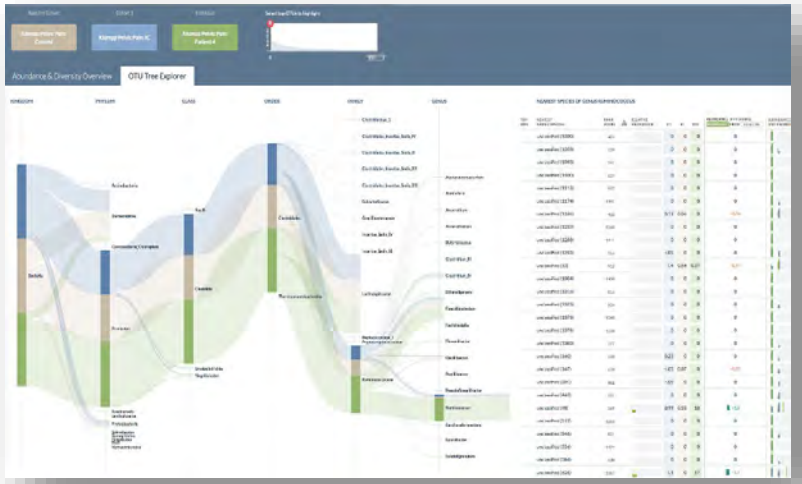
Bulle Effect at River Bifurcations

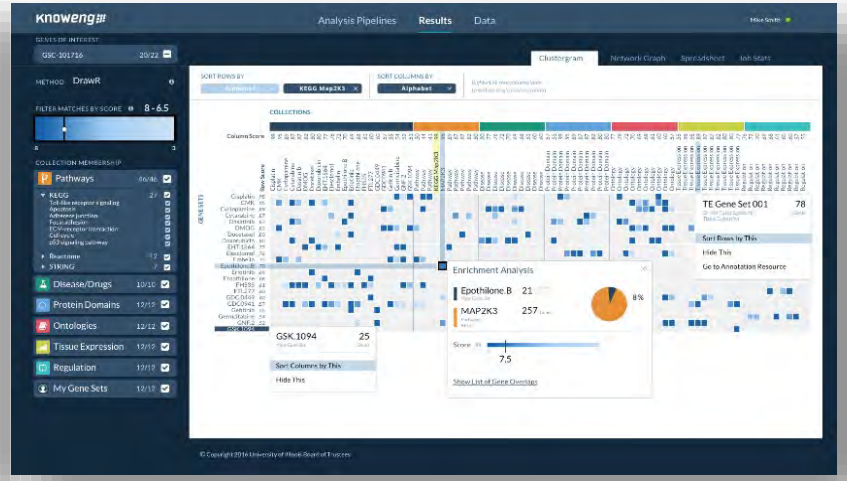
Football training in VR

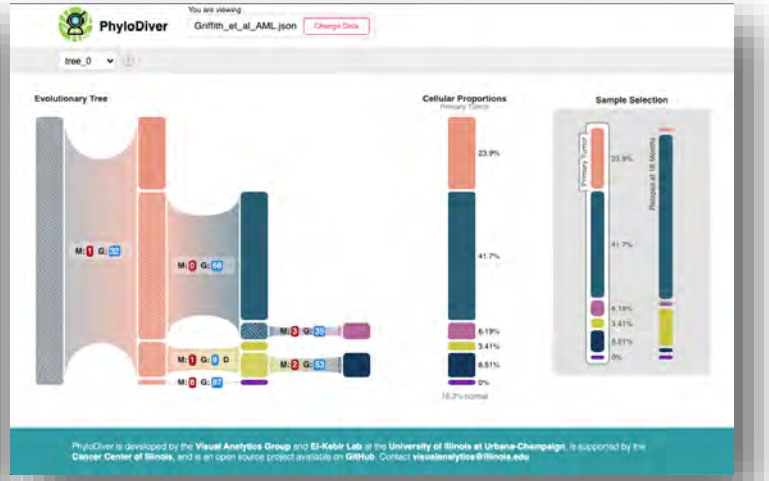
The Visual Analytics Group (VA Group)

The Visual Analytics Group makes complex data more accessible to researchers, healthcare providers, and community members.

We create innovative software tools that combine visualization and UX design with new analytical approaches and pixel-perfect implementation to address global challenges in healthcare and beyond.





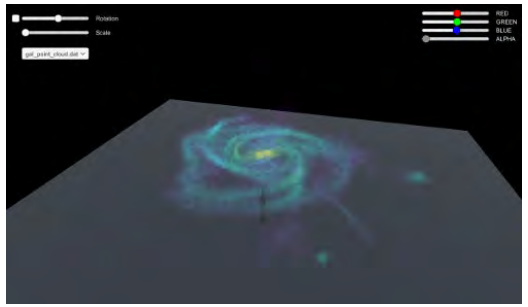


Data Exploration Lab (DXL)

Data Exploration Lab focuses on visualization for research

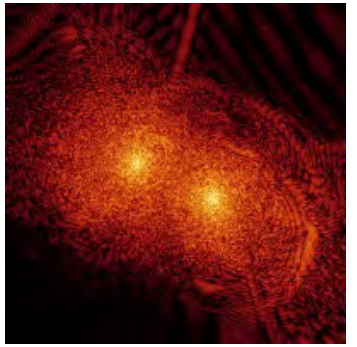
- Philosophy of Projects Make it easier to access, analyze, and understand data.
- Specialize in volumetric data, astrophysics
- Are the primary developers of the open-source software yt. https://yt-project.org/

Whole Tale



VR for SciViz

Crops in Silico



Gamer

YT &
YT Hub

NCSA Visualization Program Office

Questions about NCSA's visualization services?
https://www.ncsa.illinois.edu/expertise/visualization/

Kalina Borkiewicz
Director, Visualization Program Office
Lead, Advanced Visualization Lab
kalina@illinois.edu

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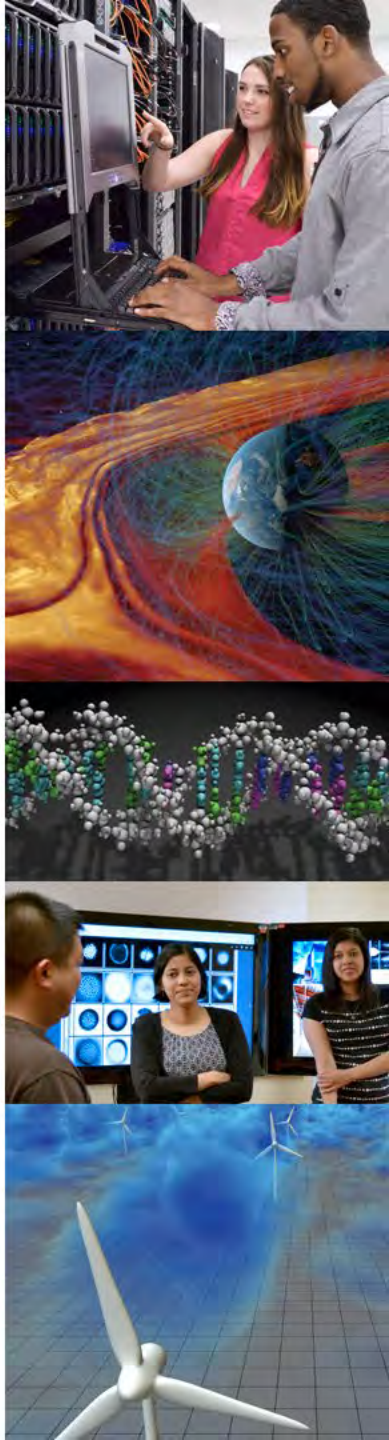


Healthcare Innovation Program Office & Nightingale Cluster

Maria Jaromin
Senior Research Coordinator
mjaromin@illinois.edu

National Center for Supercomputing Applications
UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

Healthcare Innovation Program Office

Healthcare Innovation brings cohesion to the many health projects at NCSA.

Objective

Provide powerful methods, tools and ecosystems for translational research and innovation in support of healthcare advancement

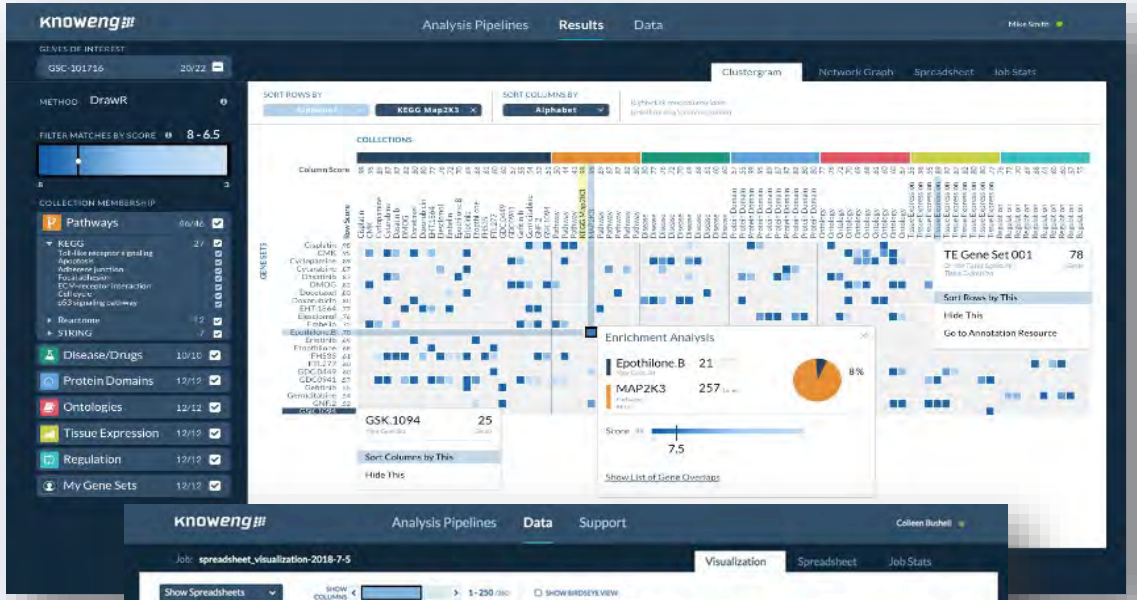
Expertise & Resources

Software development, analysis, visualization, user-experience design, data, compute resources, and cyberinfrastructure

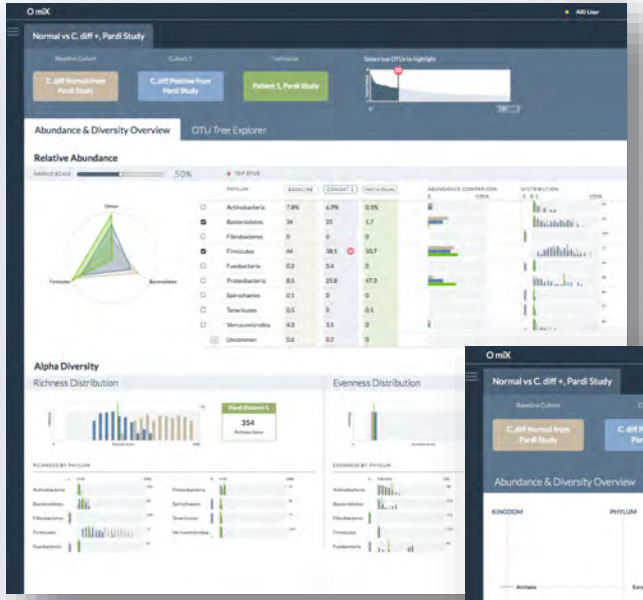
Example Areas	
Visual Analytics Software/Frameworks	*KnowEng, OmiX, PixSure*
Data Analysis	*Biomarker Discovery, Health Disparities*
Image Analysis	*Deep Learning, Annotation, Validation*
Voice Analysis, Remote Sensors	*Timeseries Analysis, Telemedicine*
Cyberinfrastructure	*Nightingale, Data Movement, Storage*
Computational Genomics	*Assembly, Variant Calling, Performance*
User Engagement	*Consultation, Training, User Requirements*
Data Driven Decision Support	*Monitoring, Prediction, Information Design*
Mobile Patient Support, Monitoring	*Mobile Apps, Backend Safer Illinois App*
Augmented Reality/Virtual Reality	*Surgery Prep, Student Training*
Crowd Sourcing	*Lyme Disease*

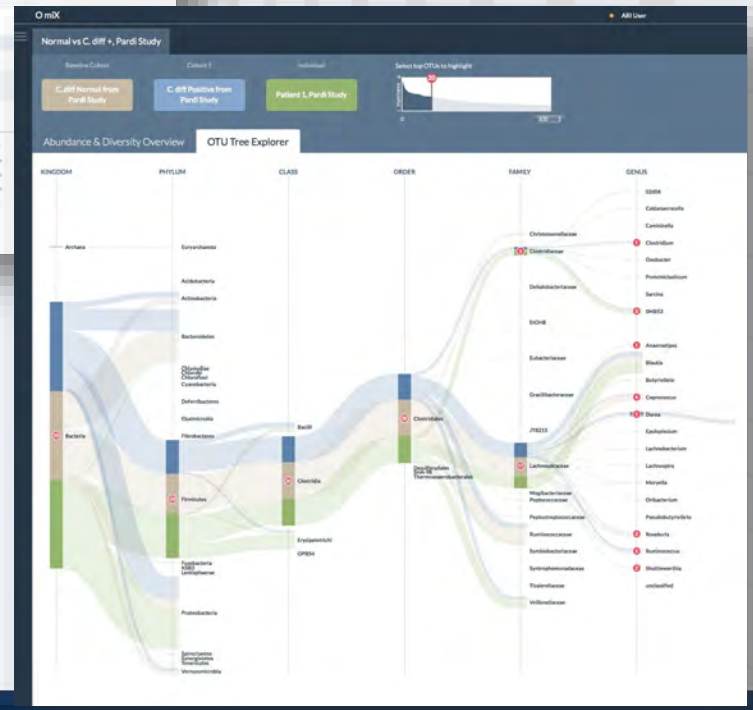
Example Visual Analytics Software/Frameworks

Genomics Analysis Tools – KnowEng



Microbiome Analysis Tools - OmiX





Source: Visual Analytics, NCSA

Nightingale Cluster

High-performance computing environment for storing and processing sensitive, regulated data.

Data Types

- ✓ Electronic Protected Health Information (ePHI)
- ✓ Controlled Unclassified Information (CUI)
- ✓ Other types of data (incl. PII, FERPA)

Benefits

- ✓ Housed on campus at the NCSA National Petascale Computing Facility and operated by NCSA
- ✓ Experienced NCSA technical staff
- ✓ Extensive user support
- ✓ Resource to foster relationships between various collaborators

Visio and Overview

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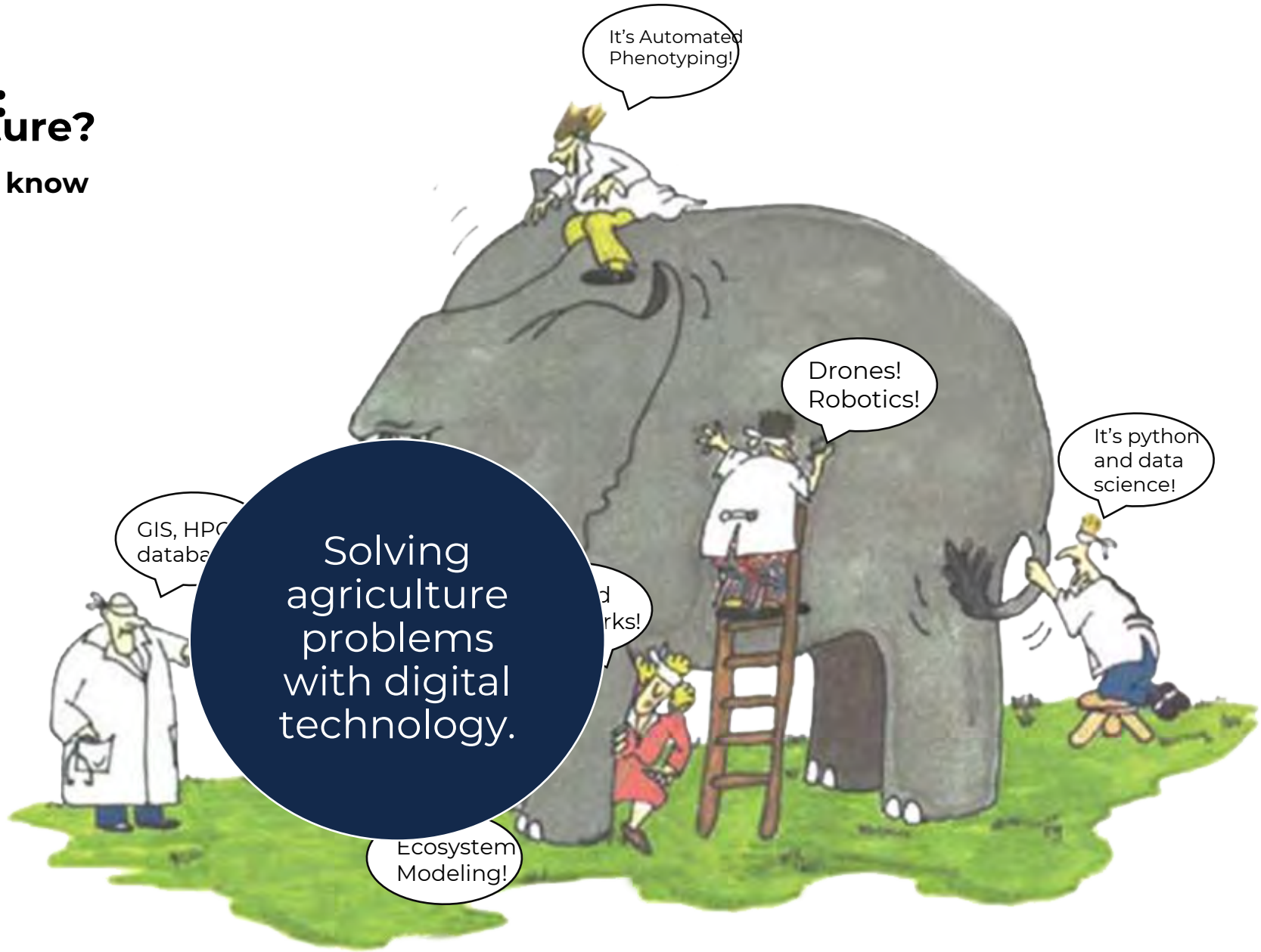
Center for Digital Agriculture

udson
kram Adve

Co-Directors

Digital Agriculture:
What is Digital Agriculture?

… nobody seems to know



Why Now?

Illinois has extensive experience in Digital Agriculture

1 We originated key internet technologies (eg web browser, Apache at NCSA)

2 Now looking to do same for rural internet, agricultural research and tech

3 Projects involving Digital Ag:
TERRA-REF, CABBI (DoE), Big Data Hub (NSF), CCBGM (NSF), Blue Waters (NSF), etc..

AIFARMS

Artificial Intelligence for Future Agricultural Resilience, Management, and Sustainability

A National AI Institute for Agricultural Innovation

Funded by

USDA National Institute of Food and Agriculture

ILLINOIS Center for Digital Agriculture

ILLINOIS NCSA | National Center for Supercomputing Applications

cropps Center for Research on Programmable Plant Systems

Medicine Phoenix

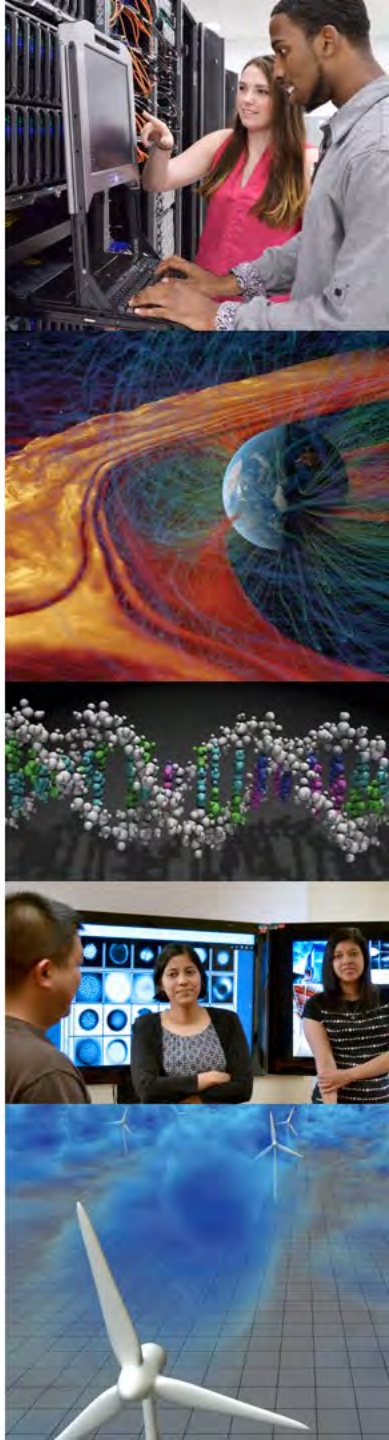
i-FARM Farm of the Future

i-FARM TESTBED

Funded by

USDA National Institute of Food and Agriculture

Networking session in breakout rooms



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- NCSA staff presenters will be moved to their respective Zoom breakout rooms automatically.
- NCSA staff will stay in their rooms and wait for their next visitor.
- Faculty will be able to join any breakout room for 3-5 minutes to have a one-on-one interaction with NCSA staff.
- Faculty will need to use the **Chat** box to indicate what room they would like to visit. NCSA event services will be helping faculty move between the rooms.

Breakout rooms:
Seid Koric: Research Consulting Directorate (RCD)
Xiaoxia Liao (Data Analytics)
Christina Fliege (Genomics)
Gregory Bauer: Science and Engineering Application Support Group (SEAS)
Kenton McHenry: (Software)
Volodymyr Kindratenko: Center for AI Innovation (CAII)
Daniel Lapine: Innovative Systems Laboratory (ISL)
John MacMullen: Midwest Big Data Hub (MBDH)
Jeff Carpenter: Visualization Program Office (VizPO)
Maria Jaromin: Healthcare Innovation Program Office (HIPO)
Matthew Hudson: Center for Digital Agriculture (CDA)

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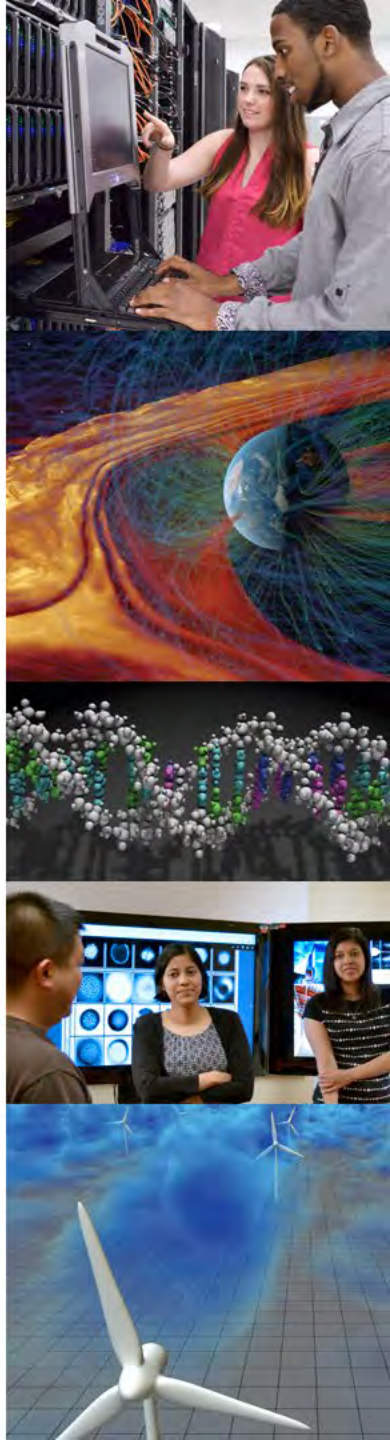

Thank you!

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