Pittsburgh Supercomputing Center Overview

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Pittsburgh Supercomputing Center

Enabling discovery since 1986

The **Pittsburgh Supercomputing Center (PSC)** provides advanced research computing capability, education, and expertise to the national research community.

Since 1986, PSC has provided university, government, and industry researchers with access to some of the most powerful systems available for high-performance computing, enabling discovery across all fields of science.

OUR AREAS OF EXPERTISE

- high-performance and data-intensive computing
- data management technologies
- software architecture, implementation, and optimization
- enabling ground-breaking science, computer science, and engineering
- user support for all phases of research and education
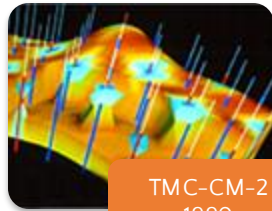- STEM outreach in data science, bioinformatics, and coding
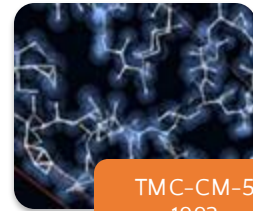
Enabling discovery since 1986
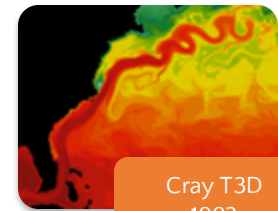

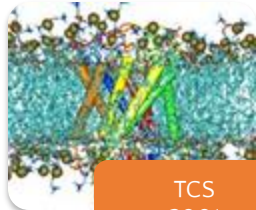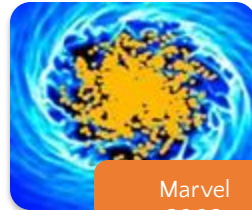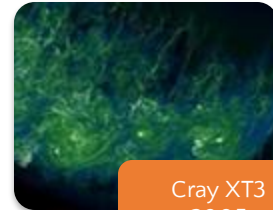Cray X-MP 1986 → Cray Y-MP 1989 → TMC-CM-2 1990 → TMC-CM-5 1992 → Cray C90 1992 → Cray T3D 1993
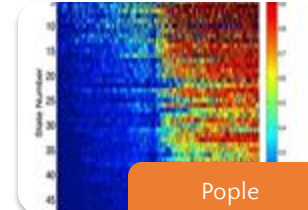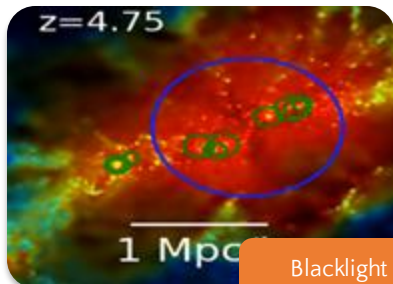
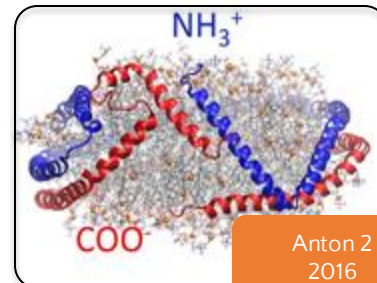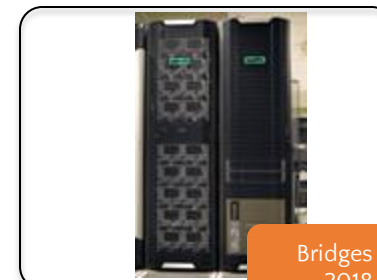Cray T3E 1996 → TCS 2001 → Marvel 2003 → Cray XT3 2005 → Pople 2008 → Anton 2010

Blacklight 2010 → Bridges 2016 → Anton 2 2016 → Bridges AI 2018

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Providing world–class computing resources

Bridges-2

Provides transformative capability for rapidly evolving, computation-intensive and data-intensive research, creating opportunities for collaboration and convergence research.

Neocortex

Highly innovative platform for larger and faster artificial intelligence research.

Introducing capabilities to accelerate artificial intelligence, machine learning, and data analytics.
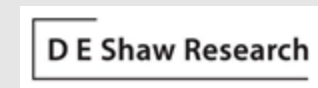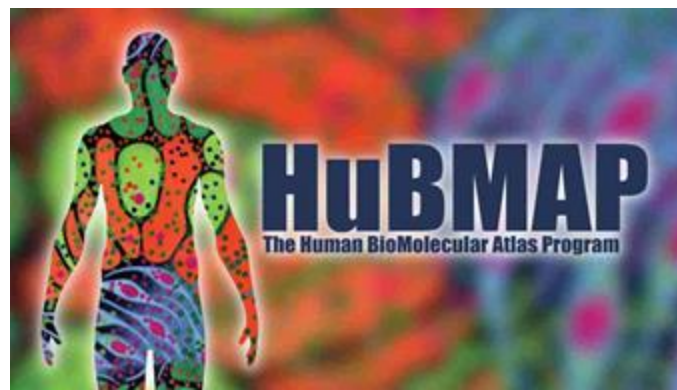
Anton 2

Enables breakthrough research in areas such as medicine, biology, and biochemistry.

Custom designed hardware for simulating biological molecules at the atomic level with molecular dynamics orders of magnitude faster than standard computers.

PSC Collaborations
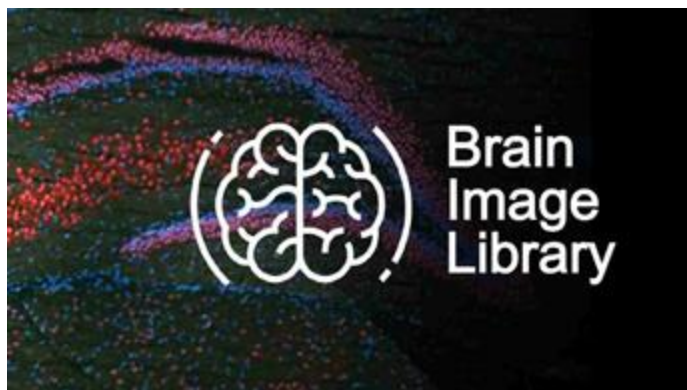
National AI Research Resource

NAIRR is an NSF initiative that will support a shared research infrastructure facilitating access to compute, software, datasets, models, training and user support for researchers and students.

- PSC is part of the pilot program as a 'resource provider'
- NAIRR seeks to strengthen and democratize the US AI innovation ecosystem
- Launched in response to the President's Executive Order on Trustworthy AI
- Inter-agency collaborative effort – NSF, NIH, DOE, NASA, NOAA

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ADAPT PA & Summer Internships
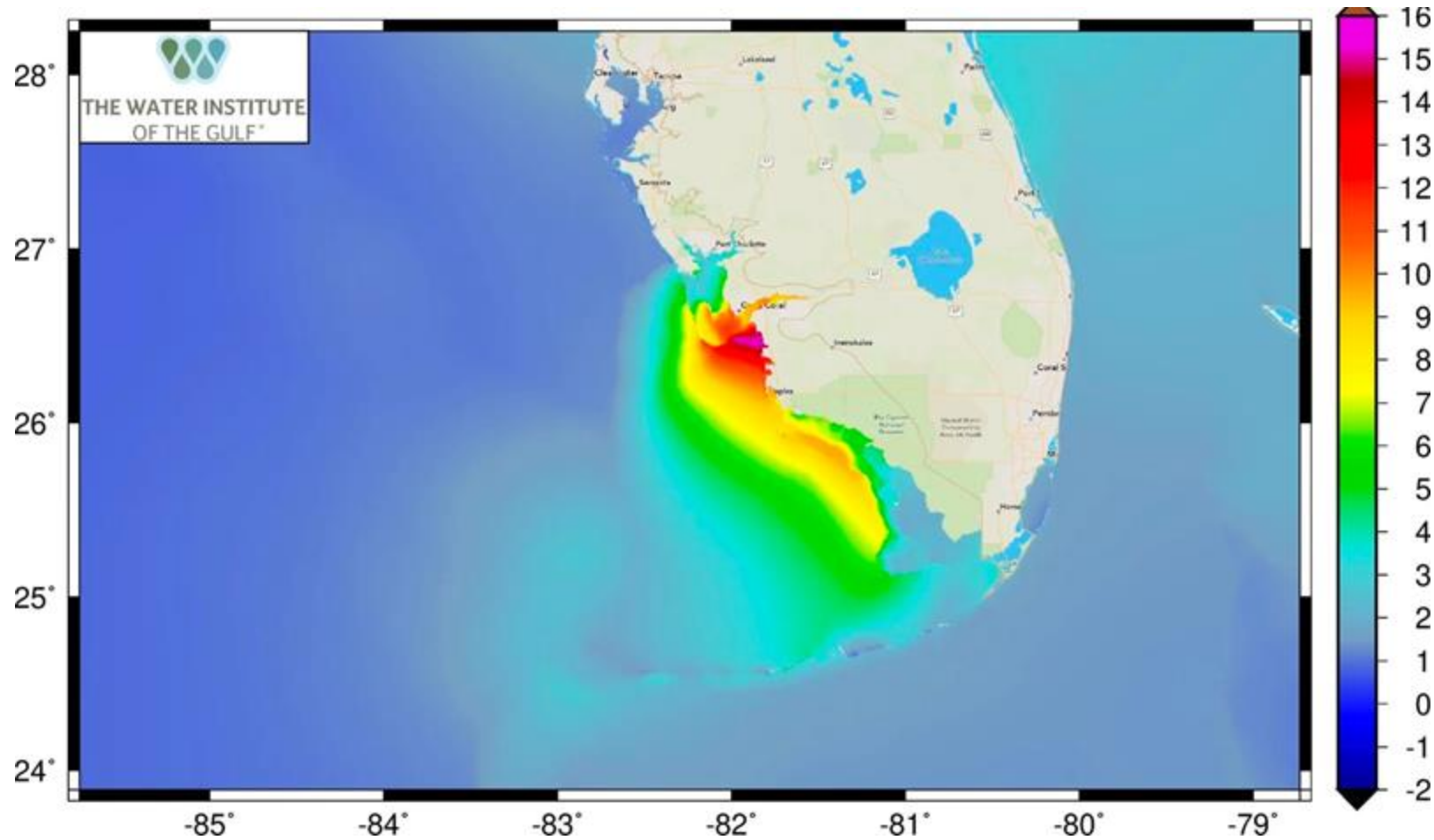
Community Colleges & PASSHE
- Curriculum development
- Teacher training
- Incorporation of PSC tools (Bridges-2) into the classroom

Areas of focus
- data analytics
- machine learning
- additive manufacturing

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Storm Surge Model on Bridges-2 Predicts Hurricane Ian's Flooding Impacts

Fast storm surge predictions led by scientists at the University of North Carolina, Chapel Hill, and The Water Institute of the Gulf, running for the first time on PSC's Bridges-2, gave accurate real-time predictions to emergency management decision makers.

This aided decision-makers in evacuation and disaster-response decisions related to Hurricane Ian that may have saved lives.

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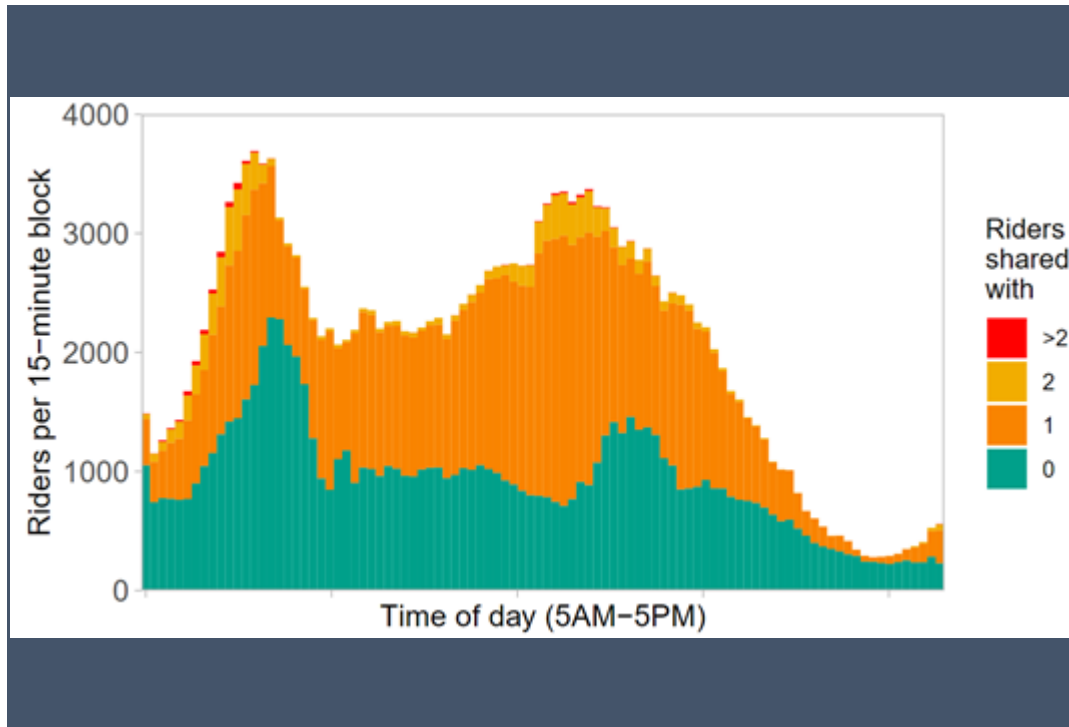
Riders per 15-minute block who have a private ride (0 riders shared with) or who overlap with other riders in the same car (>0 riders shared with).

Optimize a fleet of TNC (rideshare) vehicles to satisfy ride demand in Chicago, using public TNC travel data, and compare results when optimizing the fleet for (1) minimum private costs and (2) minimum social costs, including external costs to society of congestion, collisions and emissions.

Research achievements:

- Completed data processing and exploratory data analysis on high–volume Uber & Lyft ride data (>100M rows)

- Developed and benchmarked parallel processing simulation code (C++, OpenMP, Intel Thread Building Blocks)

- Completed an initial set of model runs and developed early policy findings

- In progress: additional model runs and sensitivity tests

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Anton 2, Bridges-2 Simulations Explain Life-Critical Protein in the Brain

Scientists do not fully **understand the iGluR protein in the brain**, which underlies some serious forms of epilepsy. There's only one drug approved for problems with iGluR, *perampanel*. While it helps many people with seizure disorders, it can sometimes cause addiction. Doctors would like to have more choices for treating iGluR-based seizures. For that, we need to better understand iGluR. To uncover the workings of this protein complex and help design better drugs to treat its dysfunctions, a team of computational chemists from Carnegie Mellon University (CMU) employed simulations on PSC's Anton 2 and Bridges-2 systems. Together, these simulations **revealed a step-by-step activation of iGluR that can help identify future drug targets**.
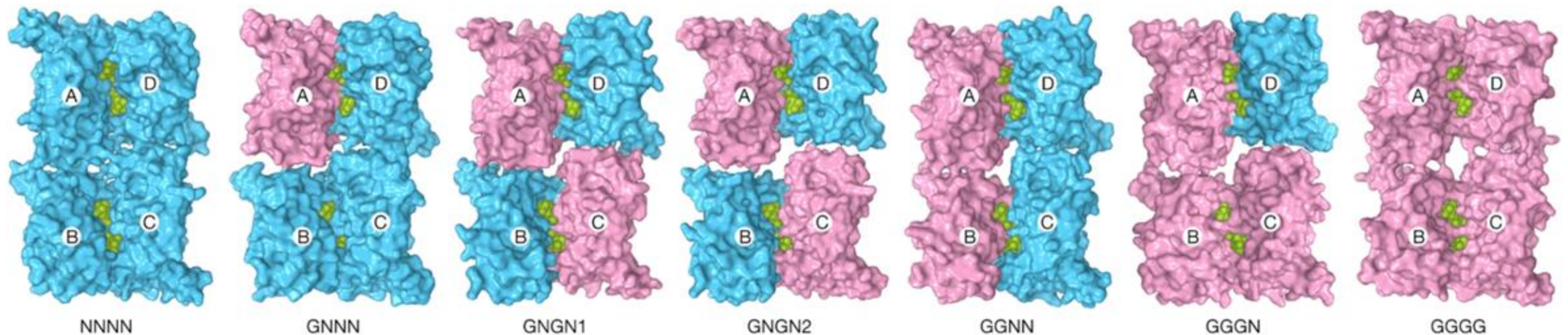
Summary

- PSC serves the national research community
- We're 100% free for open science research
- We have active research projects and a wide array of collaborators
- If you have potential research projects that could leverage PSC, let's talk!

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Thank you!

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