## Leveraging NSF's Cyberinfrastructure to Support Major Facilities Research

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CI4MF, Long Beach, CA – January 17, 2024

# **Office of Advanced Cyberinfrastructure**

Transform science and engineering research through an integrated cyberinfrastructure ecosystem

#### Advanced Cyberinfrastructure Research

Testbeds (computing, data, networking)

- Software and data infrastructure
- Cybersecurity and networking
- Core research program

Research partnering with other divisions and directorates

#### Nationally available infrastructure and services for the R&E community



Large-scale computing, data and networking infrastructure



Software, services and middleware



Allocations, user support, communities of practice



Training and workforce development



# **OAC investment areas**

Advanced Computing	Production and operational level advanced computing and data capabilities and services	
Networking & Cybersecurity	Advanced networking and security infrastructure, research and communities of practice capabilities	
Learning & Workforce Development	Foster a national research workforce for creating, utilizing, and supporting advanced CI	
Software & Data Cl	Supports development and deployment of robust, reliable and sustainable data and software CI	
Strategic Investments	Special opportunities, cross-cutting and national initiatives, CI for open science and public access	



# Major Facility Cl supported across entire OAC portfolio

OAC has long partnered across NSF to support development of CI capabilities, pathways, and platforms for discovery at major facilities.

These investments span all aspects of the OAC investment area



Data Lifecycle for Facilities

#### In the spotlight:

Enabling new modes of computational- and dataintensive science such as computation at the edge, data discovery and Al-enabled discovery.



## Major Facility Cl supported across entire OAC portfolio



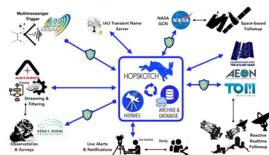
Training and user support







**Communities of practice** 



Software and data infrastructure

**Major Facilities** 



**Advanced computing** 



#### **Networking & Security**

# **Communities of Practice**









Minority Serving Cl Consortium (MS-CC)



Facility data lifecycle

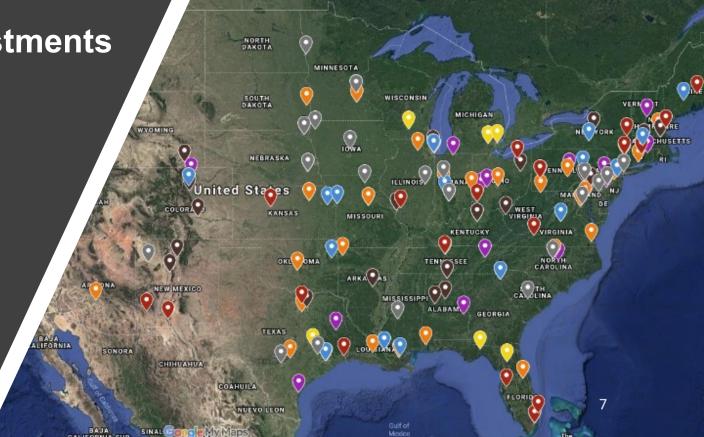




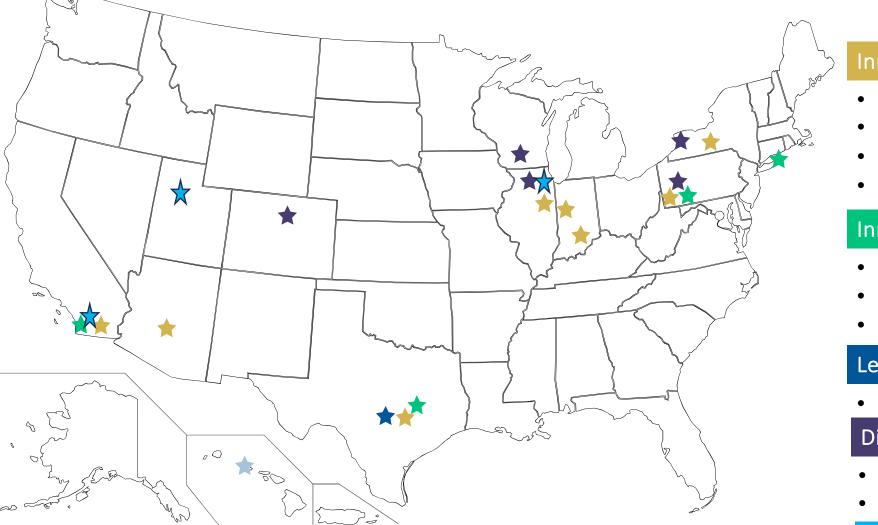


#### **Networking & Cybersecurity Investments**

- Networking as a fundamental layer and underpinning of CI Continuum
- CC\* Campus Cyberinfrastructure
- IRNC International R&E Network Connections
- CICI Cybersecurity Innovation for Cyberinfrastructure
- FABRIC Adaptive Programmable Research Infrastructure for CS and Science Applications



### NSF-supported Advanced Computing Resources



#### Innovative Production Systems

- Anvil
- Bridges 2
- Delta
- Delta Al

- Expanse
- Jetstream 2
- Stampede 2
- Stampede 3

#### Innovative Prototypes/Testbeds

- Neocortex
  NRP
  - Voyager ACES
  - Ookami

#### Leadership-class

• Frontera

Distributed Services

- PATh / Open Science Grid
- ACCESS

#### Cloud Technologies/Access

- Cloudbank
- Chameleon Lab

Cloudlab

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# Advanced Computing and Data systems: GPU and CPU based systems available for your research

**Advanced Computing Systems** 



U. Of Illinois



U of Texas, Austin



UC San Diego



J of Indiana





CMU

U. Wisconsin OUDBank Facilitates access to cloud resources





What is available? advanced computing and data systems, services and support (at no cost)

Who is eligible? academic and govt researchers, students, and educators

*How to get access?* <u>https://access-</u> <u>ci.org/about/get-started/#start</u>

#### Welcome to ACCESS.

Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support

GET STARTED

## Cyberinfrastructure of Sustained Scientific Innovation (CSSI) Data and Software infrastructure

#### Core Cyberinfrastructure

- MVAPICH-TAO Integration
- FZ Lossy Compression Software
- gem5 simulator

#### **Open Science**

- ARXIV
- Reproducible permafrost geomorphology analysis
- Science-i Cyberinfrastructure for Forest Ecosystem Research

#### Al Infrastructure

- Diamond (Neural Network Training on NSF HPC systems)
- Homomorphic Encrypted ML on FPGA
- Benchmarking framework for Causal Learning

#### Al for Sciences

- Machine Learning framework for Political Scientists
- Foundational AI framework for Material Sciences
- ML toolkit for NOAA water column data
- Nuclear physis with Neural Deconvolution

#### Sustaining Community CI

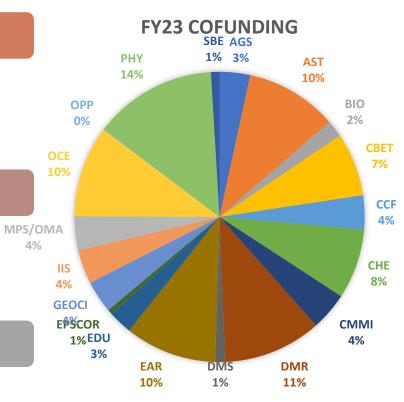
- ARGOVIS
- Open SciServer
- Community Atmospheric Model (CAM)
- SimVascular

#### Data Cl

- Solid Mechanics Benchmark Datasets
- Citizen Science Photometry
- ProDM Data Management for Exascale Computational Science

Exp and Obs science

Project Class	Awards	Funding
Elements	32	18.7M
Frameworks	15	54.2M
Sustainability	3	2.7M



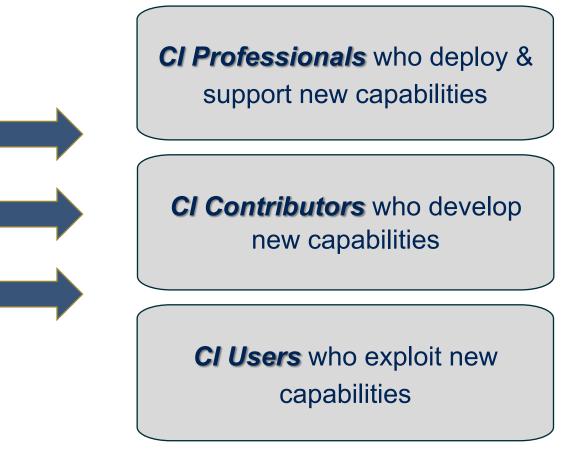
# Exemplar recent CSSI awards to enable and accelerate experimental and observational science

- 2311263, Elements: Portable Machine Learning Models for Experimental Nuclear Physics
- 2311323, Elements: The TARDIS radiative transfer framework A modeling toolkit for transients
- 2311355, Frameworks: SCiMMA: Real-time Orchestration of Multi-Messenger Astrophysical Observations
- 2209655, Collaborative Research: Elements: A task-based code for multiphysics problems in astrophysics at exascale
- 2209852, Frameworks: Target and Observation Manager Systems for Multi-Messenger and Time Domain Science
- 2103662, Framework: An A+ Framework for Multimessenger Astrophysics Discoveries through Real-Time Gravitational Wave Detection
- 2103741, Collaborative Research: Frameworks: Seismic COmputational Platform for Empowering Discovery (SCOPED)
- 2103682, Elements: Scaling MetPy to Big Data Workflows in Meteorology and Climate Science
- 2114582, Collaborative Research: Frameworks: Einstein Toolkit Ecosystem: Enabling fund. research in era of multi-messenger Astrophysics
- 2103963, CSSI Elements: EWMS Event Workflow Management Service (IceCube Neutrino Observatory)
- 2103889, Elements: Machine Learning Quark Hadronization
- 2209720, Elements: Scalable Bayesian Software for Interpreting Astronomical Images
- 2004645, Collaborative Research : Elements : Extending physics reach of LHCb by developing & deploying algorithms ...
- 1931469, Collaborative Research: Frameworks: Machine learning and FPGA computing for real-time apps in big-data physics experiments
- 1836650, S2I2: Institute for Research and Innovation in Software for High Energy Physics (IRIS-HEP)

# Learning and Workforce Development

NSF 23-520: Training-based Workforce Development for Advanced Cyberinfrastructure (CyberTraining)

NSF 23-521: Strengthening the Cyberinfrastructure Professionals Ecosystem (SCIPE)



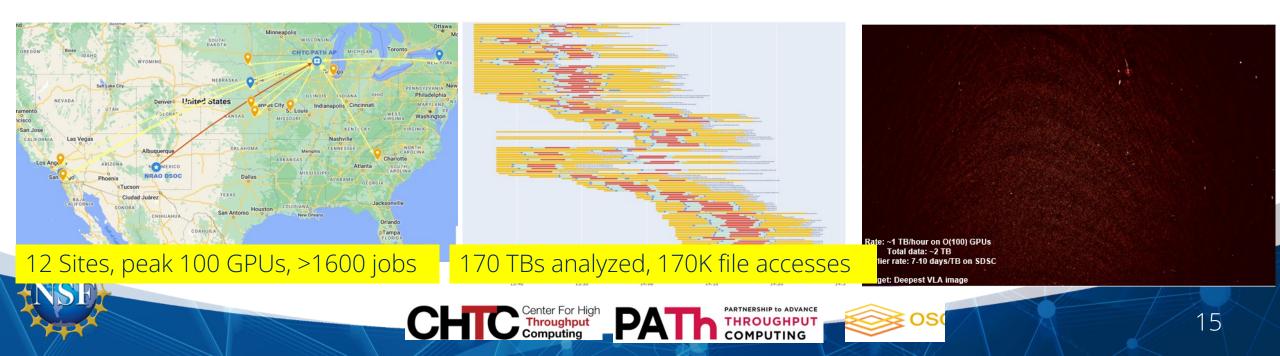


# Supporting Facilities Examples and Highlights

## NRAO Large Scale Distributed Data Analysis

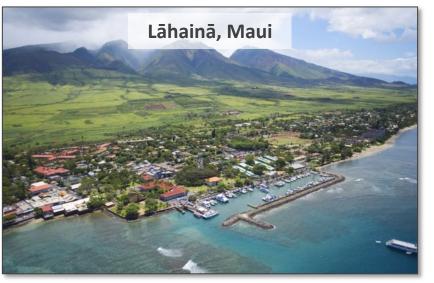


- NRAO data set had not been analyzed for 10 years: wide-band image at radio frequencies of the Hubble Ultra-Deep Field
- Important for understanding parameters of universe evolution including spectral behavior of emissions from distant galaxies
- NRAO team partnered with PATh and CTHC to develop a distributed data analysis algorithm using HTCondor
- Dec 2023 data analysis run resulted in deepest image by VLA



#### RAPID – an Evaluation of an Artificial Intelligence-enhanced Edge Sensor System for Multi-Hazard Monitoring and Detection (Award #2346568)

Jason Leigh, Tom Giambelluca, Chris Shuler- University of Hawai'i Peter Beckman - Northwestern University



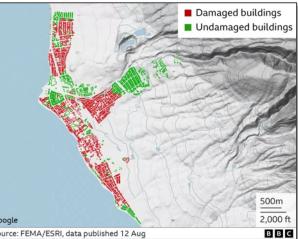
- Estimated recovery will cost
  \$5.5B and years
- RAPID builds upon 3 OAC activities – Hawai'i Mesonet, Sage, and SAGE3
- Data gathering to aid in recovery efforts & contribute as a proof-of-concept for future hazard monitoring scenarios – especially in the Pacific

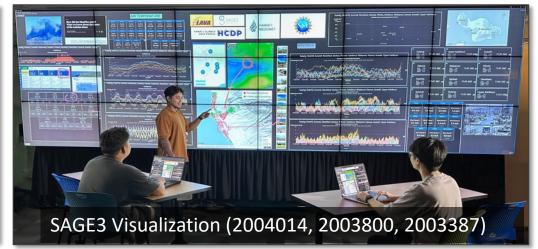




#### Hawai'i Climate Data Portal (EPSCoR Change Hawai'i 2117975)







Catalytic chain of rapid OAC investments in community planning for CI in Multimessenger Astrophysics

SCIMMA y planning for Scalable Cyberinfrastructure to support Multi-Messenger

Workshop: Cyberinfrastructure for Multi-**Messenger Astrophysics** Funders: PHY + OAC, PHY-1838082, May 2018

"Workshop will consider how multi-messenger astrophysics can be enabled by enhanced cyberinfrastructure."

**Collaborative Research: Community Planning for** Scalable Cyberinfrastructure to Support Multi-Messenger Astrophysics (SCiMMA) Funders: OAC + MPS/AST, MPS/PHY, MPS/OMA, OAC-1841625 + 12 collab awards, Sept 2018

"This project seeks to carry out community planning for scalable cyberinfrastructure to support MMA."

Framework: An A+ framework for multimessenger astrophysics discoveries through real-time gravitational wave detection Funders: OAC + PHY,

OAC-2103662, May 2021. *"this project targets the development of a* software framework for the real-time discovery of gravitational waves"

A Framework for Data Intensive Discovery in Multi-messenger Astrophysics Funders: OAC with NSF HDR-Frameworks, OAC-1934752, Sept 2019.

*"This is the conceptualization phase for a Scalable" Cyberinfrastructure Institute for Multi-Messenger* Astrophysics (SCIMMA)."

# A look forward: integration is a key theme

# Defining, advancing, and interconnecting the broad CI ecosystem

#### OAC supports highly innovative, distributed systems, services and expertise

#### Challenges

- OAC portfolio of systems and services are hard for non-insider to understand
- While ACCESS has focused coordination of many resources, others are not included
- Difficult for stakeholders to understand portfolio in aggregate, capabilities, users and workload that could inform future directions

## NSF Advanced Computing in Chips and Science Act (Summarized Sec. 10374)

- Computing Needs Gather information about the computational needs of NSF funded projects and publish reports every 2 years
- Set roadmaps that set priorities and guide strategic investments every 5 years
  - Describes resources that would fully meet anticipated project needs including major facilities
  - Draws on community input
  - Reflects technology trends
  - Addresses needs of historically underrepresented groups and geographic regions

## National Discovery Cloud for Climate (NDC-C)

In FY 2023, CISE will invest. . .in the development of a National Discovery Cloud (NDC) for Climate. This resource will federate advanced compute, data, software and networking resources, democratizing access to a cyberinfrastructure ecosystem that is increasingly necessary to further climate-related S&E. The NDC for Climate will serve as a pilot for future efforts to enable equitable access to an NDC across all fields of S&E. **-- NSF FY 2023 Budget Request** 

## **Components of an NDC-C**

Advanced Compute	Open Platforms	Data Resources	<b>Broad Engagement</b>
New Climate Cl	Sustainable Climate Cl	Security/Resiliency	Cloud Resources

**Opportunities DCL:** <u>https://www.nsf.gov/pubs/2024/nsf24024/nsf24024.jsp</u>

NSF

**Further Information:** <u>ndcc-queries@nsf.gov</u>

## **NDC-C Prototype Investments**

#### Advanced Compute

- DeltaAl
- Stampede3
- ACCESS/RAMPS

#### New Climate Cl

- Glaciology, Ice Sheet
  Modeling
- Oceanographic
  Modeling
- Forest Ecosystems
- Permafrost
  Geomorphology

#### Security/Resiliency

 Securing Hazard Workflows

#### **Open Platforms**

• Pelican/OSDF

•

•

- National Data Platform
  Pilot
- Edge Computing Sage

#### Sustainable Climate Cl

- Atmospheric physics modeling
- Marine data access

#### **Data Resources**

- NCAR/OSDF
- QGreenland-Net
  - NOAA Sonar Data
- Campus Storage (EnviStor)

#### Key Data Challenges and Research Directions

- Democratizing access to datasets
- Enabling AI ready datasets
- Creating data pipeline tools and expertise
- Cybersecurity of complex workflows
- New modes of interacting with data and managing the data lifecycle

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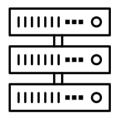


#### **Cloud Resources**

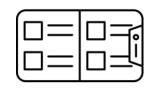
- CloudBank
- CloudLab
- Chameleon

## Vision for the National AI Research Resource

**A widely-accessible, national research infrastructure** that will advance the U.S. AI R&D environment, discovery, and innovation by empowering a diverse set of users through access to:









Secure, high-performance, privacy-preserving **computing** 

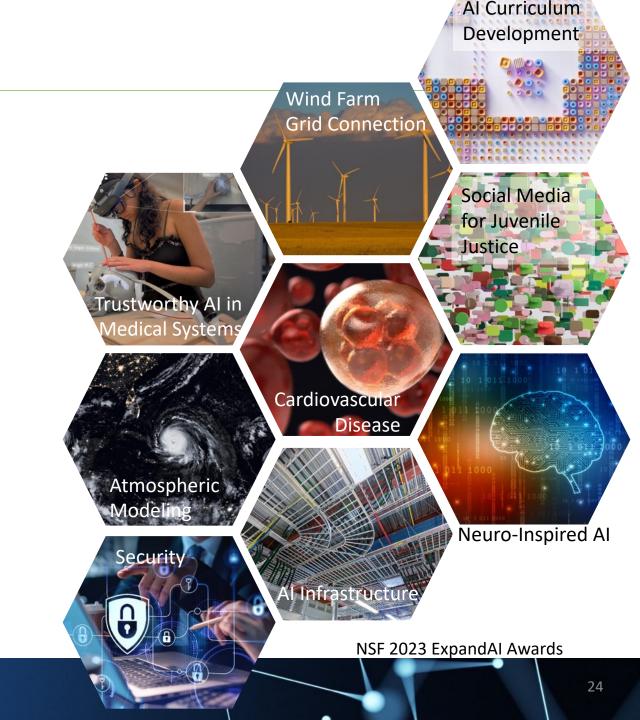
High-quality datasets

Catalogs of testbeds and Training tools and user educational materials support mechanisms



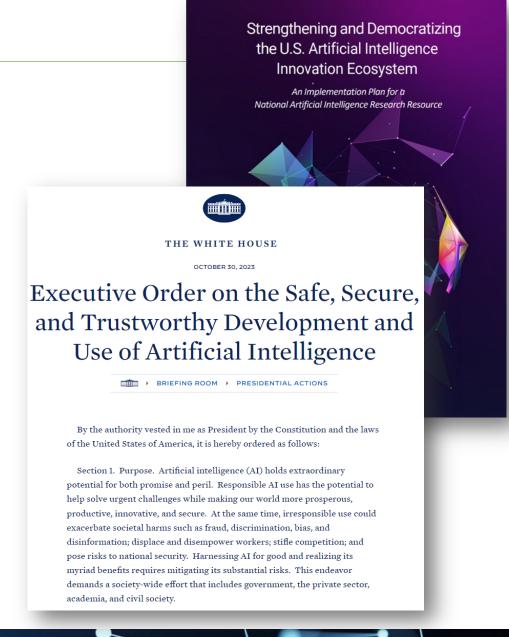
## Why do we need a NAIRR?

- AI holds potential to help solve critical societal and global challenges
- Many potential contributors lack access to requisite R&D resources
- It is critical to provide the infrastructure for researchers investigating AI to serve the public interest and to train the next generation of researchers

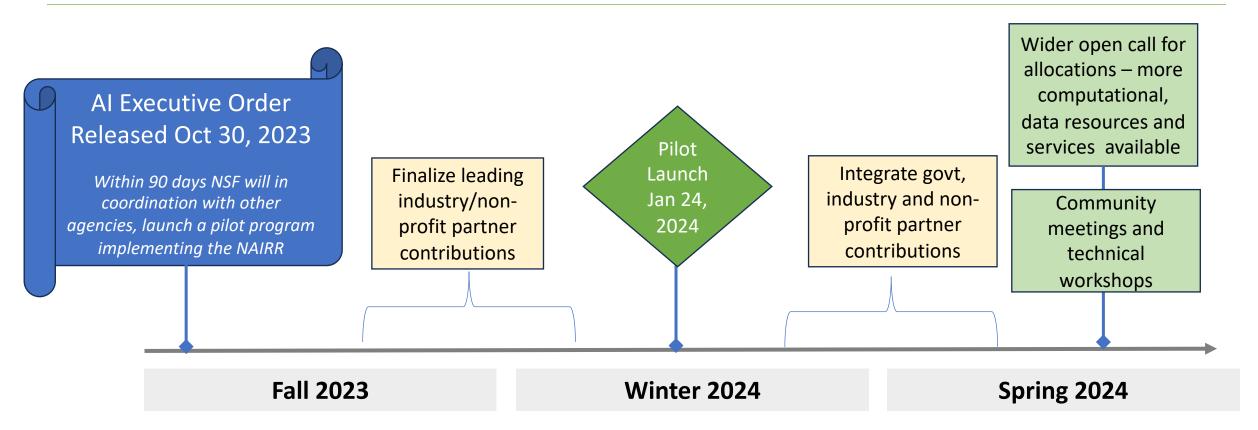


## How did we get here?

- June 2021 NAIRR Task Force launched to examine the feasibility of a NAIRR
- January 2023 Task Force final report provides roadmap for NAIRR implementation including an optional pilot
- March 2023 NAIRR Interagency Working Group led by OSTP & NSF with 14 agencies is established
- October 30, 2023 President's Executive Order on Trustworthy AI directs NSF and collaborating agencies to launch NAIRR pilot within 90 days



## Near-term NAIRR Pilot Timeline



Evolve to tighter governance, integration and allocations model over the two-year pilot

## NAIRR Pilot Goals

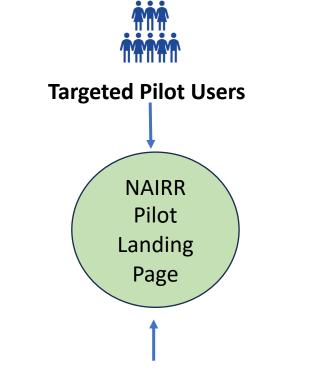
- 1. Demonstrate the value & impact of the NAIRR concept.
- 2. Support novel & transformative AI research and education with participation from broad communities.
- 3. Gain initial experience to advance and refine the NAIRR design in preparation for a full NAIRR implementation.



The pilot will demonstrate or investigate all major elements envisioned in the NAIRR, but at a *limited* scale: A best effort, *proof of concept* approach leveraging agencysupported resources and in-kind contributions from industry and non-profits.

## NAIRR Pilot launch is next week

- 1. NAIRR Pilot Portal goes live
- 2. Call for allocations on initial set of high-performance computing systems
- 3. Initial datasets
- 4. RFI Survey of Researcher and Educator use cases



Computing, testbeds, datasets, models, software, outreach



### NAIRR Pilot Users



#### **AI Researchers**



Domain Scientists Applying Al



Students and Educators

#### US Based Institutions including:

- Academic institutions
- Non-profits
- Federal agencies or federally-
- funded R&D centers
- State, local, or tribal agencies
- Startups and small businesses with Federal grants

## Initial Focus Areas

#### Initial themes will frame the 2024 open call for proposals and scope activities

#### • Safe, Secure, and Trustworthy AI

- Mature methods for AI testing, evaluation, verification, and continuous monitoring
- Improve accuracy and reliability of model performance
- Advance the ability to assure model behavior and align with human values and safety guardrails

#### • Healthcare

- Cancer treatment
- Individual health outcomes

#### Environment and infrastructure sustainability

- Advance resilience and optimization of agricultural, water, and grid infrastructure
- Address earth, environmental, and climate challenges via integration of diverse data and models

#### • AI Education

• Enable training and education of a cohort of scholars at universities across the country in Al technologies and their responsible use



# Tent poles to organize the NAIRR Pilot effort







Enable open Al research and access to diverse Al resources via a central portal and coordinated allocations

Enable AI research needing privacy and security-preserving resources. Assemble exemplar privacy preserving resources. Facilitate use of Al software, platforms, tools and services across systems



Reach new communities through education, training, user support and outreach



## NAIRR Pilot Opportunities and how you can help

- We will be seeking your help to get the word out, particularly to underserved communities
  - Call for user NAIRR pilot allocations
  - RFI Survey on Researcher and Educator Use Cases
- The first NAIRR Pilot aligned opportunity has already been released
  - Encourages submissions of high impact proposals that advance AI education
  - Supports computing/data/ networking infrastructure needed for AI education
- NAIRR Pilot will host a series of community meetings and technical workshops



Find Funding & Apply ~ M

Manage Your Award V Focu

#### ← Search for more funding opportunities

Important information for proposers

All proposals must be submitted in accordance with the requirements specified in this funding opportunity and in the NSF <u>Proposal & Award Policies & Procedures Guide (PAPPG)</u> that is in effect...

#### Dear Colleague Letter

# Advancing education for the future Al workforce (EducateAl)

December 1, 2023

Encourages the submission of novel and high impact proposals that advance inclusive computing education that prepares preK-12 and undergraduate students for the AI workforce.

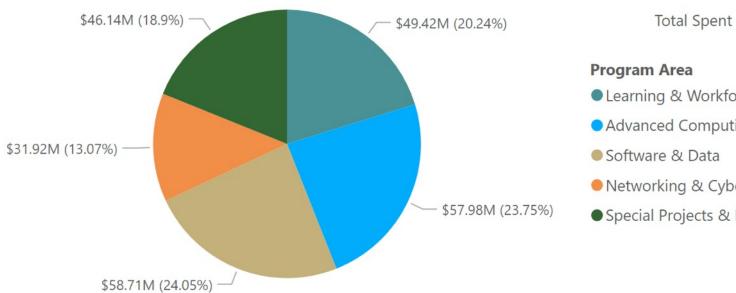
#### Dear Colleagues:

Artificial Intelligence (AI) is transforming the ways in which citizens navigate their daily lives, researchers make discoveries, educators teach their students, students learn both individually and collaboratively, and manufacturers build products. As new Al-driven discoveries and capabilities emerge, it is critical to promote responsible innovation, competition, and collaboration to unlock the technology's potential to solve some of society's most difficult challenges and maintain U.S. leadership in applying AI to address critical global challenges.

# **Questions and Discussion**

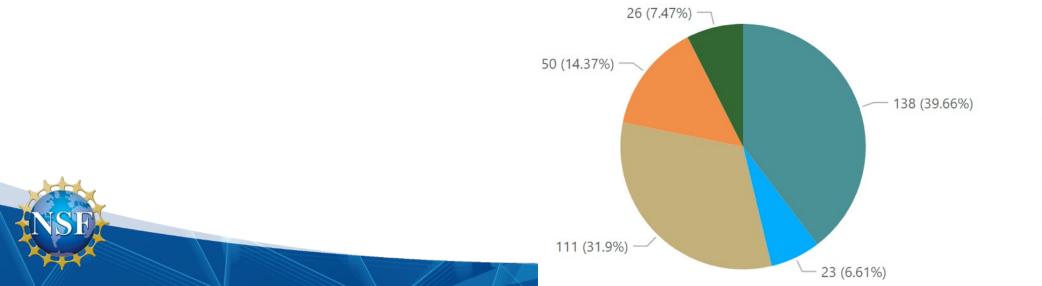
# Backup slides

# OAC FY23 by the numbers



\$246.46M

- Learning & Workforce Develop.
- Advanced Computing
- Networking & Cybersecurity
- Special Projects & DD Reserve



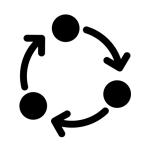
#### 351

**Total Award Count** 

#### **Program Area**

- Learning & Workforce Develop
- Advanced Computing
- Software & Data
- Networking & Cybersecurity
- Special Projects & DD Reserve

Transform science and engineering research through an integrated cyberinfrastructure ecosystem



Defining, advancing and interconnecting broad CI ecosystem



Growing and developing human infrastructure expertise



Enabling discovery through data & software infrastructure

#### NAIRR

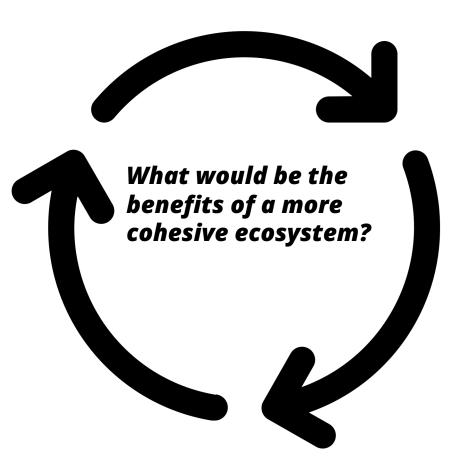
Infrastructure for AI

Investing in and transitioning to new technologies



Developing partnerships for long-term US leadership in research Cl

## OAC Retreat addressed this topic



### **Potential Benefits**

- Easier on-ramp for new communities to understand and access the portfolio of systems, services and capabilities
- Clear pathways for communities to transition from local and regional systems to national, cloud or other agency resources based on science need
- A single currency that can be exchanged for multiple types of resources
- Deeper understanding of the portfolio of OAC investments and workload

#### A National-Scale Testbed Supporting AI Research Spanning the Computing Continuum

Connect AI at the edge with NSF HPC centers to support end-to-end AI workflow research

Explore AI-enabled, nowcasting analysis of hazards



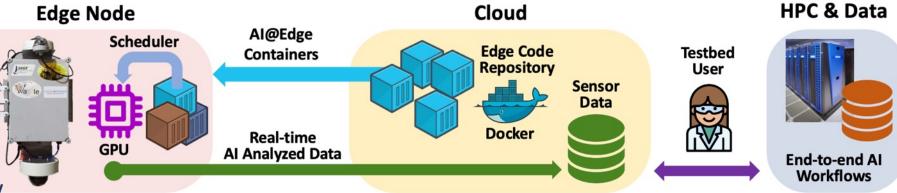
Students from Chicago State Univ. deploying AI-enabled infrastructure

Understanding hazards

#### Institutional Lead:

Northwestern Univ. **Partners:** UCSD; University of Illinois Chicago, Colorado State, U. of Oregon, U. of Utah

This research is part of the National Discovery Cloud for Climate. NSF Award #2331263



Leverages the Sage MSRI-1 open source research infrastructure

## How to get access to the NSF CI ecosystem?

- ACCESS <u>https://access-ci.org/about/get-started/#start</u>
- Frontera allocations <u>https://frontera-</u> portal.tacc.utexas.edu/allocations/
- PaTh High Throughput computing credits <u>https://path-cc.io/</u>
- Cloudbank <u>https://www.cloudbank.org/options-requesting-cloud-</u> resources
- Cloudlab <u>https://cloudlab.us/</u>
- Chameleon experimental testbed <u>https://chameleoncloud.org/</u>

