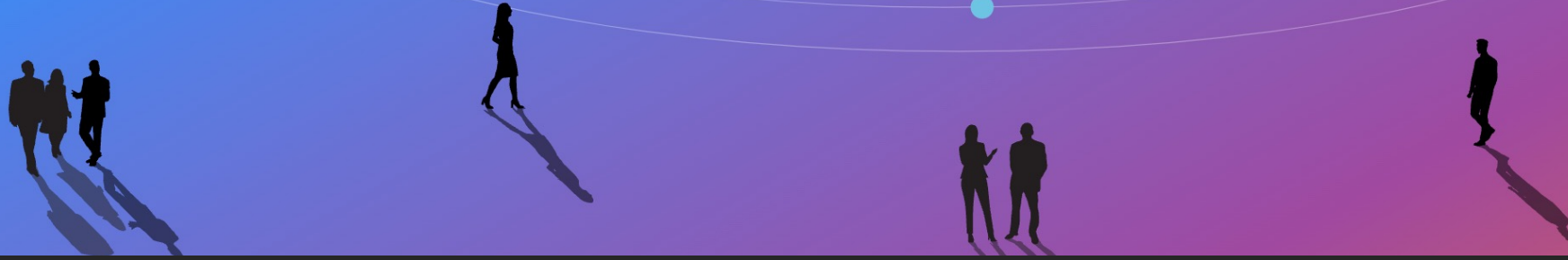


# Extend. Expand. Exemplify.

The SGCI team continues to offer its services AND brings you a new Center of Excellence to Extend Access, Expand the Community, and Exemplify Good Practices for CI through Science Gateways.



## Leveraging Science Gateways for Research Projects and Research Communities

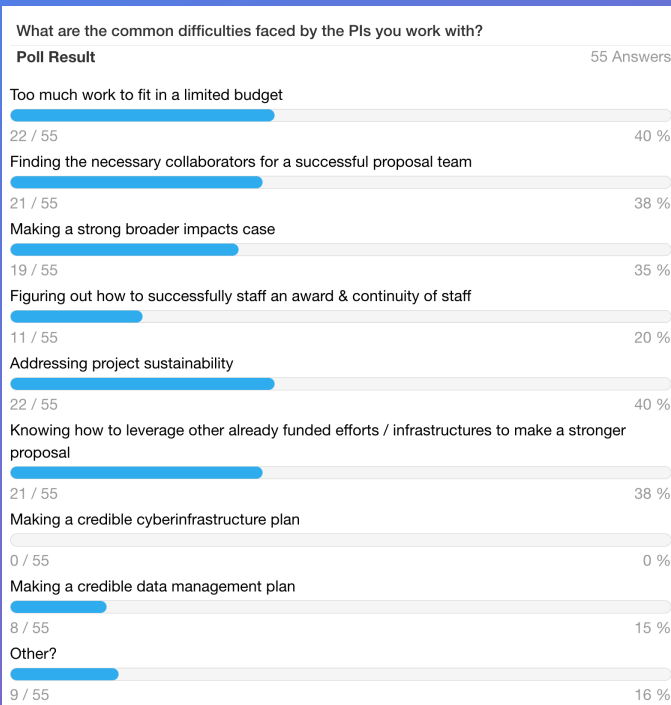
Michael Zentner  
Division Director, Sustainable Scientific Software  
San Diego Supercomputer Center  
University of California, San Diego



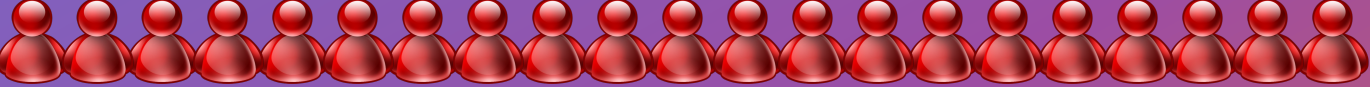
NSF awards  
1547611  
2231406

SGX3 | SGCI

# Poll Results: What are the common difficulties faced by the PIs you work with?



55 Respondents as of 5/8/2023

- Addressing project sustainability  
(22/55) 
- Too much work to fit in a limited budget  
(22/55) 
- Knowing how to leverage other already funded efforts / infrastructures to make a stronger proposal  
(21/55) 
- Finding the necessary collaborators for a successful proposal team  
(21/55) 
- Making a strong broader impacts case  
(19/55) 

# Poll Results: What are the common difficulties faced by the PIs you work with?

- Knowing how to leverage other already funded efforts / infrastructures to make a stronger proposal
  - Making a strong broader impacts case
  - Addressing project sustainability
  - Finding the necessary collaborators for a successful proposal team
  - Too much work to fit in a limited budget
- 
- The diagram consists of a large dark blue rounded rectangle on the right side of the slide. Yellow arrows point from specific items in the left list to items inside this rectangle. An arrow points from 'Knowing how to leverage other already funded efforts / infrastructures to make a stronger proposal' to 'Science Gateways as:'. Three arrows point from 'Making a strong broader impacts case', 'Addressing project sustainability', and 'Finding the necessary collaborators for a successful proposal team' to 'Engines of broader impact', 'Habitats for project sustainability', and 'Agency funded service organizations as:' respectively. Two arrows point from 'Too much work to fit in a limited budget' to 'Expert collaborators' and 'Budget extenders'.
- Science Gateways as:
    - Infrastructures for leverage
    - Engines of broader impact
    - Habitats for project sustainability
  - Agency funded service organizations as:
    - Expert collaborators
    - Budget extenders

# Science Gateways...

An abstract, expressive drawing in black ink with vibrant colors. It features several elongated, vertical shapes that resemble stylized figures or structures, rendered in shades of orange, green, blue, and red. The background is white with scattered black lines and dots, suggesting a network or a complex system. The overall style is dynamic and artistic.

...are about web-based  
platforms for scientific  
connections.



```
document.getElementById(div).innerHTML = errMess;
else if (i==2)
{
    var atpos=inputs[i].indexOf("@");
    var dotpos=inputs[i].lastIndexOf(".");
    if (atpos<1 || dotpos<atpos+2 || dotpos>inputs[i].length-1)
    document.getElementById('errEmail').innerHTML = "Error";
    else
    document.getElementById(div).innerHTML = "Success";
}
```



Scientific Software to Supercomputers...



```
document.getElementById(div).innerHTML = errormsg;
else if (i==2)
{
    var atpos=inputs[i].indexOf("@");
    var dotpos=inputs[i].lastIndexOf(".");
    if (atpos<1 || dotpos<atpos+2 || dotpos>inputs[i].length-1)
    document.getElementById('errMsg').innerHTML = "Invalid email address";
    else
    document.getElementById(div).innerHTML = "Valid email address";
}
```



...to massive audiences of  
researchers and students





```
document.getElementById(div).innerHTML += errormsg;
else if (i==2)
{
  div = divs[i];
  var atpos=inputs[i].indexOf("@");
  var dotpos=inputs[i].lastIndexOf(".");
  if (atpos<1 || dotpos<atpos+2 || dotpos>inputs[i].length-1)
  document.getElementById('errEmail').innerHTML += "Invalid email address  

  else
  document.getElementById(div).innerHTML += "Valid email address";
}
```

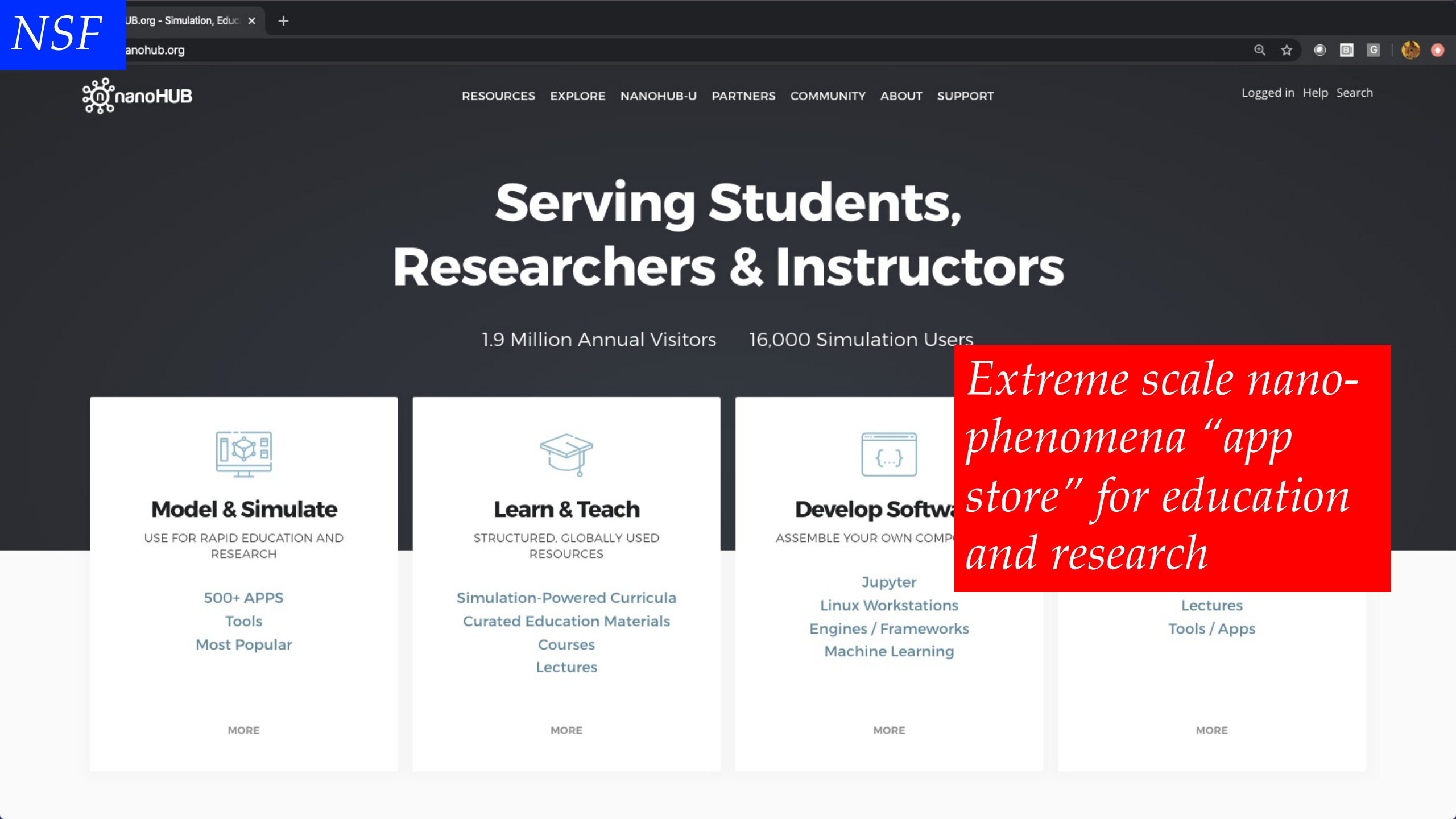


...to expensive instruments









# Serving Students, Researchers & Instructors

1.9 Million Annual Visitors 16,000 Simulation Users



## Model & Simulate

USE FOR RAPID EDUCATION AND RESEARCH

500+ APPS  
Tools  
Most Popular

MORE



## Learn & Teach

STRUCTURED, GLOBALLY USED RESOURCES

Simulation-Powered Curricula  
Curated Education Materials  
Courses  
Lectures

MORE



## Develop Software

ASSEMBLE YOUR OWN COMPONENTS

Jupyter  
Linux Workstations  
Engines / Frameworks  
Machine Learning

MORE

Lectures  
Tools / Apps

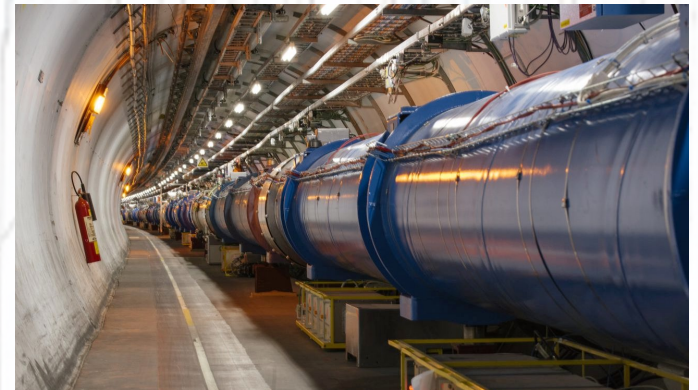
MORE

*Extreme scale nano-phenomena “app store” for education and research*

```
document.getElementById(div).innerHTML += errormsg;
else if (i==2)
{
    var atpos=inputs[i].indexOf("@");
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    if (atpos<1 || dotpos<atpos+2 || dotpos>inputs[i].length-1)
    document.getElementById('errmsg').innerHTML += "Invalid email address";
    else
    document.getElementById(div).innerHTML += "Valid email address";
}
```



...to data





## Welcome

Deposit

Search

Visualize

Analyze

Download

Learn

## A Structural View of Biology

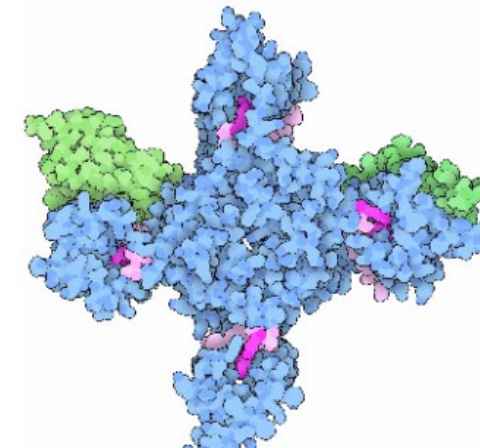
This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

COVID-19  
CORONAVIRUS  
Resources

## March Molecule of the Month

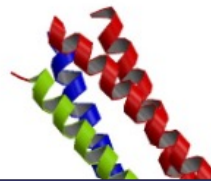


Voltage-

>204,000 structures

## Latest Entries

As of Tuesday Feb 25 2020



## Features & Highlights

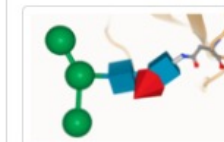


### Improve Your Coordinates, Keep Your ID (Phase II)

PDB versioning, which enables depositors to update entries while retaining their original PDB ID, is now available for all structures.

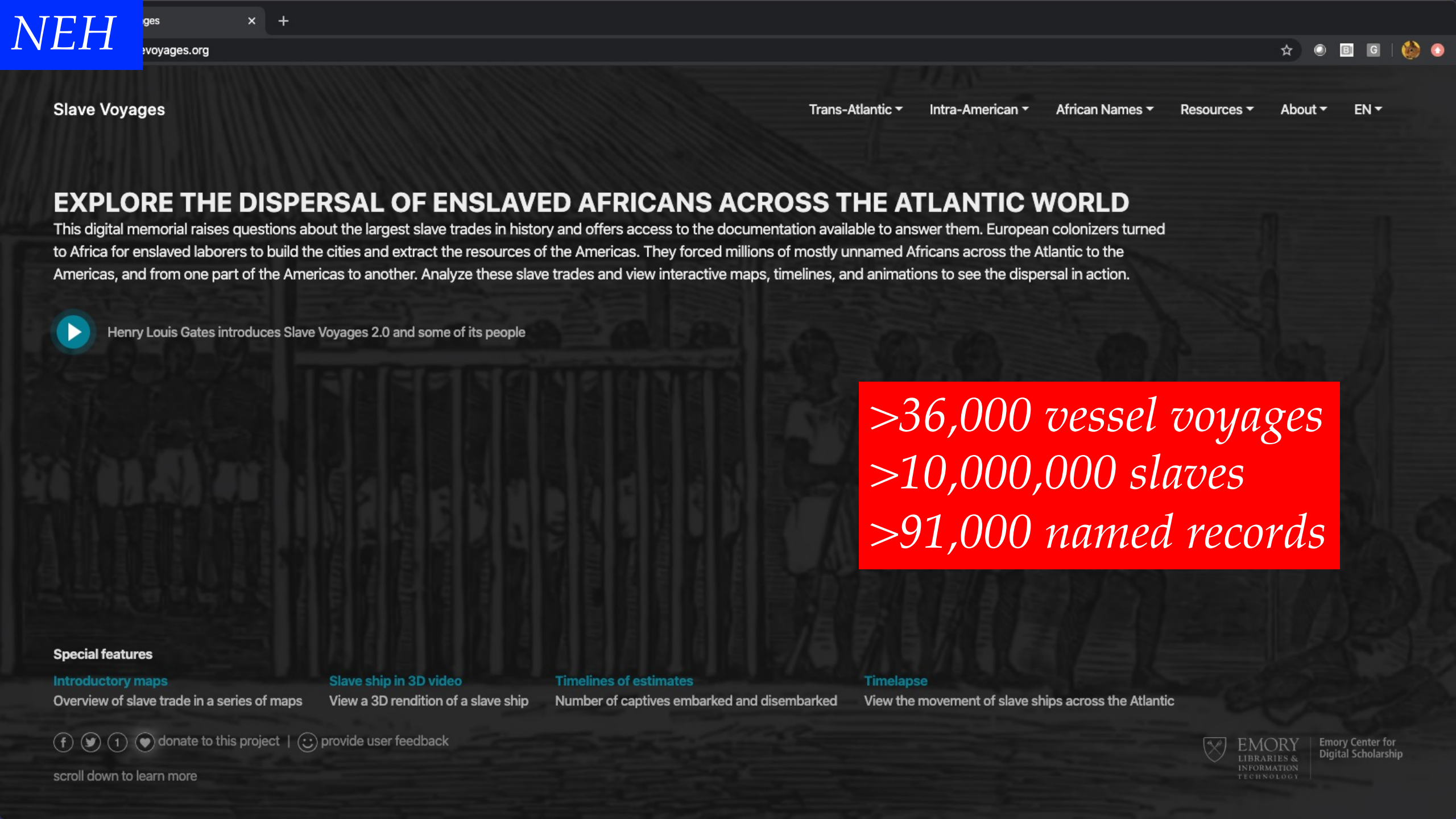
## News

Publications



### Improving carbohydrates in the PDB for 2020

To improve the ability to search for these structures and their complex chemistry (e.g., stereo-isomers, anomeric configurations, hydrogen bonding, etc.)



# EXPLORE THE DISPERSAL OF ENSLAVED AFRICANS ACROSS THE ATLANTIC WORLD

This digital memorial raises questions about the largest slave trades in history and offers access to the documentation available to answer them. European colonizers turned to Africa for enslaved laborers to build the cities and extract the resources of the Americas. They forced millions of mostly unnamed Africans across the Atlantic to the Americas, and from one part of the Americas to another. Analyze these slave trades and view interactive maps, timelines, and animations to see the dispersal in action.

 Henry Louis Gates introduces Slave Voyages 2.0 and some of its people

>36,000 vessel voyages  
>10,000,000 slaves  
>91,000 named records

## Special features

### Introductory maps

Overview of slave trade in a series of maps

### Slave ship in 3D video

View a 3D rendition of a slave ship

### Timelines of estimates

Number of captives embarked and disembarked

### Timelapse

View the movement of slave ships across the Atlantic

    donate to this project |  provide user feedback

scroll down to learn more



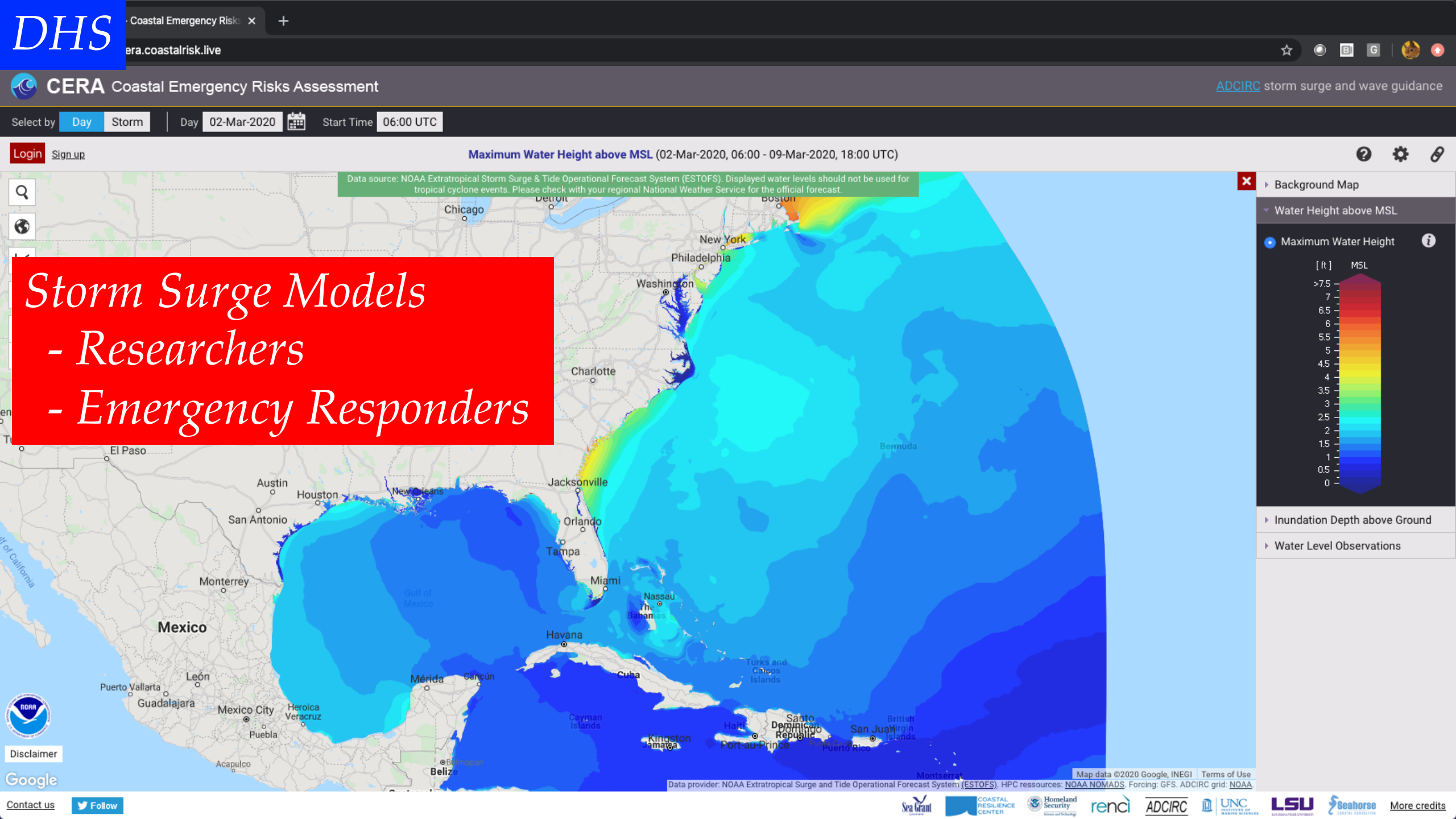
EMORY  
LIBRARIES &  
INFORMATION  
TECHNOLOGY

Emory Center for  
Digital Scholarship











[ABOUT](#)[PROJECTS](#)[TEACHERS](#)[SCIENTIST MENTORS](#)[STUDENTS](#)[DONATE](#)

*Linking 1000's of  
high school students  
with 1000's of  
professional mentors*

STUDENT TEAMS DOING  
**REAL SCIENCE**  
COLLABORATING ONLINE WITH  
**SCIENTIST MENTORS**  
FROM AROUND THE WORLD

## FEATURED POST

Kaymar  
Oct 25, 2019

Plant Update :

1.

The carbonated water  
plants turned out a bit

## HELP US GROW!



Your  
contribution at  
any level will  
go directly  
toward  
increasing  
capacity to

serve more teachers and  
students and it will help to

## \*SEEKING TEACHERS\*

Interested in expanding open  
inquiry opportunities in the  
classroom?



## FEATURED TEAMS STAR TEAMS

Each week we feature some of  
the best projects of the current  
session here. Go to the [Star  
Projects Gallery](#) to see all the  
excellent work by star teams in  
past PlantingScience sessions.



# Welcome to NCI Community Hub

A resource for NCI collaboration and sharing of data, tools, and standards among the cancer research community.

GET STARTED

*130 collaborating  
groups in a HIPAA  
safe environment*

Are you a part of an NCI project or program?

Join NCI Community Hub today to create your own collaboration space or  
join one of the many active communities on the hub!



# The University of Texas COVID-19 Modeling Consortium

## COVID-19 Mortality Projections for US States

These graphs show both the reported and projected number of COVID-19 deaths per day across the US and for individual states. We use local data from mobile-phone GPS traces to quantify the changing impact of social-distancing measures on "flattening the curve." Code syntax and daily updates of our forecasts are available on our [UT-COVID GitHub repository](#).

For more information, please visit our [model FAQ](#).

Select your area in the dropdown menu below

Bringing science to policy makers

Via Cisco Webex  
Austin, TX  
6:32 AM CT



**CORONAVIRUS PANDEMIC**

**NEW MODEL USES CELL PHONES TO FORECAST VIRUS SPREAD**

Lauren Ancel Meyers | Professor of Integrative Biology, Statistics & Data Sciences, UT Austin

**CORONAVIRUS PANDEMIC**

**GLOBALLY**

TOTAL CASES  
2,580,729

DEATHS  
178,371

**IN THE UNITED STATES**

TOTAL CASES  
825,306

DEATHS  
45,075

SOURCE: JOHNS HOPKINS UNIVERSITY

**LIVE**

**CNN**

AM ET 4:32

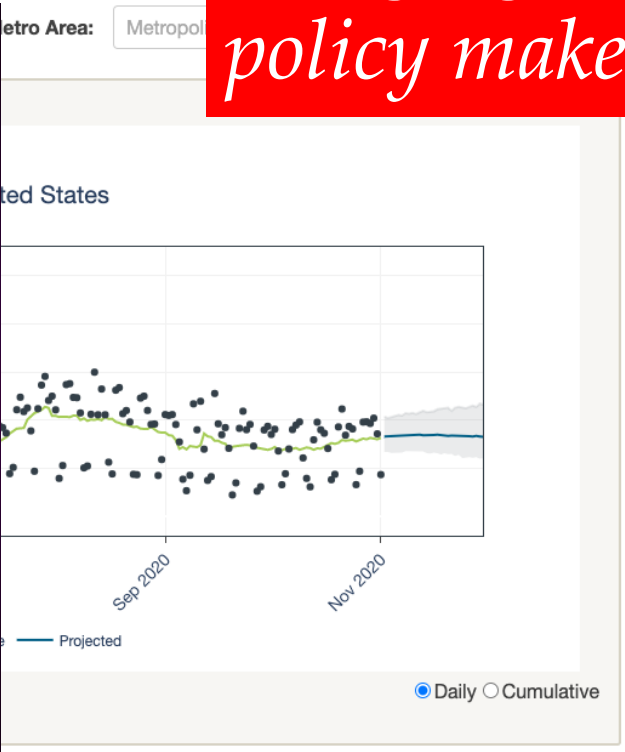
RIGHT NOW

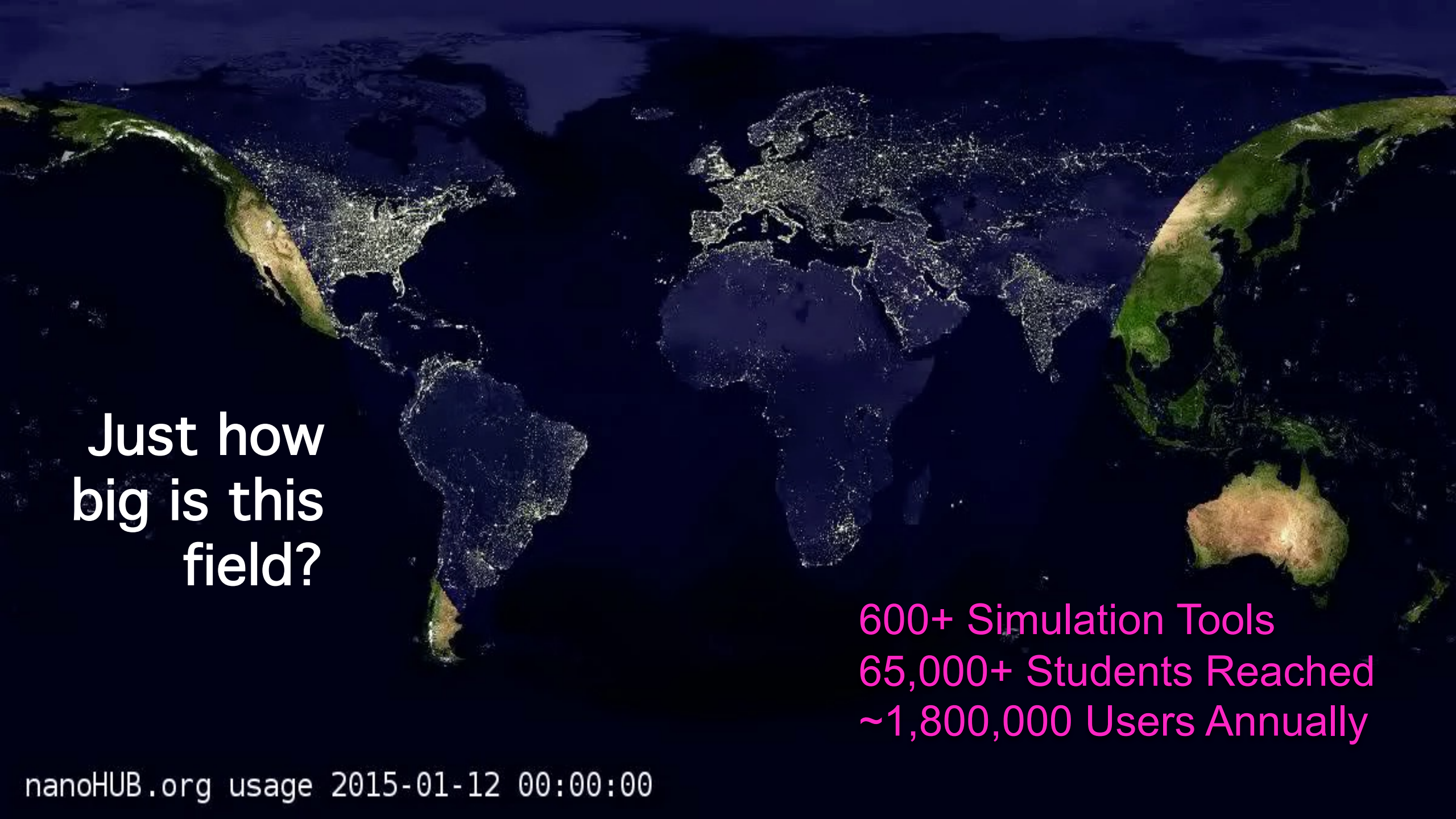
BOSTON 34°

NEW YORK 36°

PHILADELPHIA 37°

NEW DAY





Just how  
big is this  
field?

600+ Simulation Tools  
65,000+ Students Reached  
~1,800,000 Users Annually

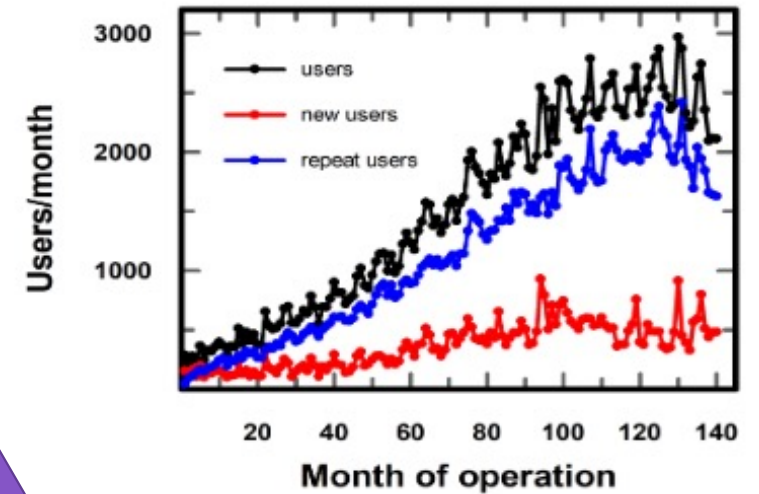
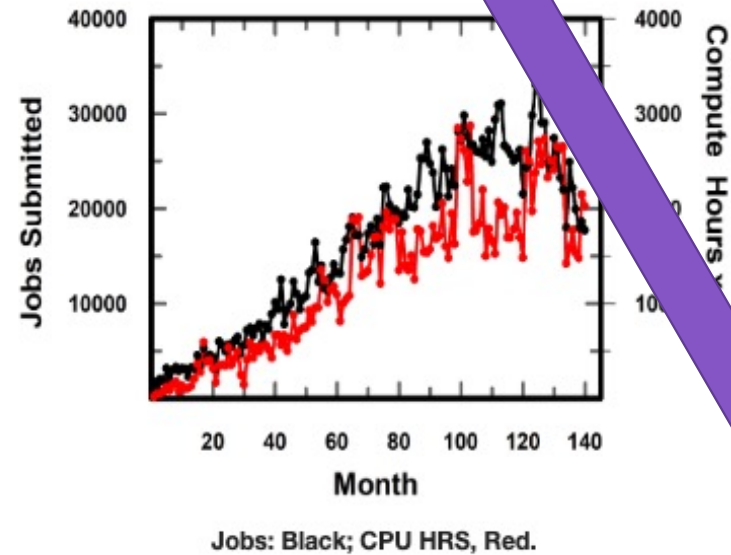


Does it  
matter?

Gateways  
have direct  
science  
impact

## CIPRES Science Gateway Usage Statistics 12/1/2009 - 9/30/2021

- 2.29 million TeraGrid/XSEDE jobs submitted by 52,026 unique users.
- Average of 549 new XSEDE users registered in each of the last 12 months.
- 166 million core hours of TeraGrid/XSEDE time distributed to scientists.
- Used for curriculum delivery by at least 114 instructors.
- Supported at least 9,700 publications



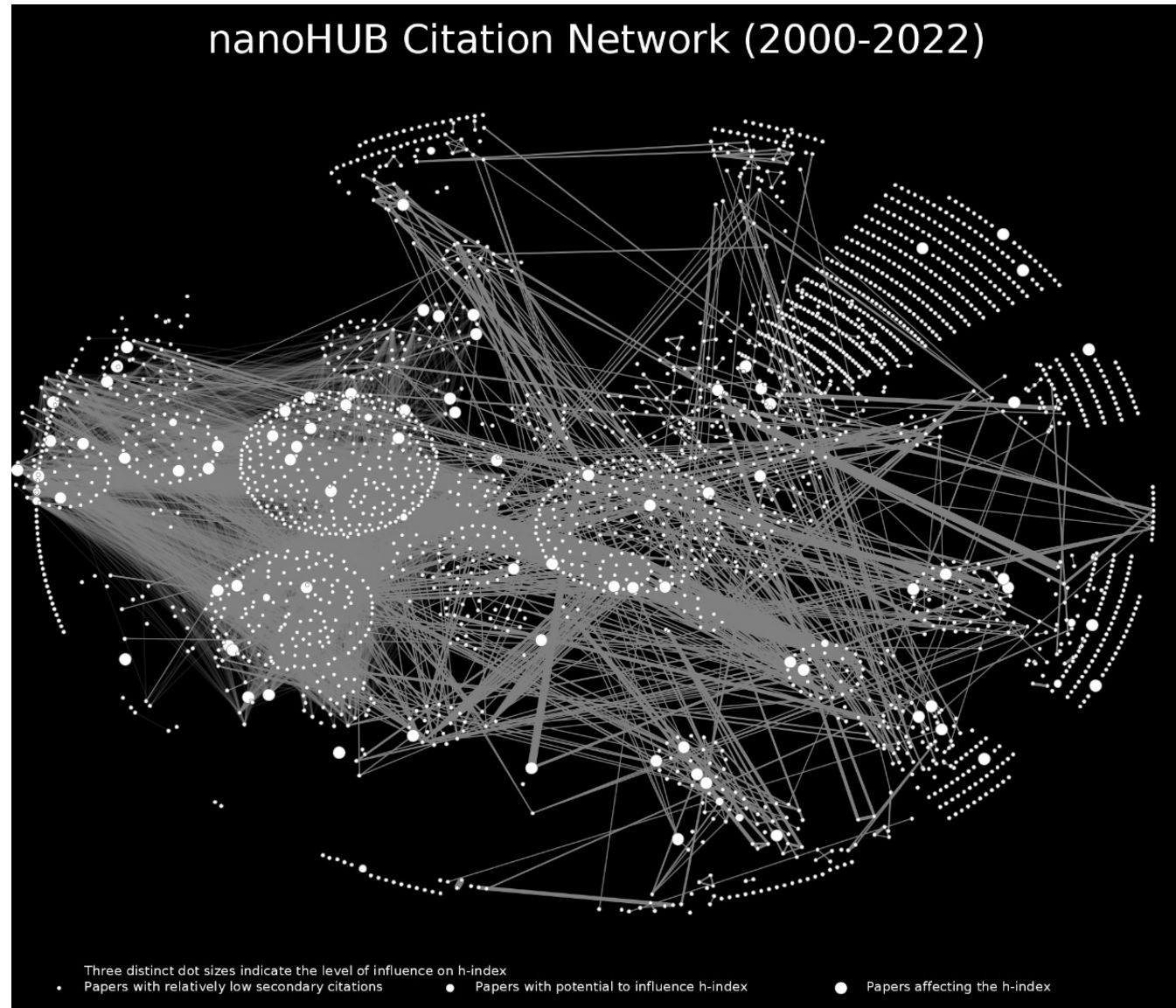
- **Supported at least 9,700 publications.**

Does it  
matter?

Gateways  
have science  
collaboration  
impact

2,724 vetted  
citations

68,310  
secondary  
citations





# Does it matter?

## Gateways have financial impact

PDB Archive contains >1 TB of Structure Data for Proteins, DNA, and RNA

### The PDB Archive

- Grows at the rate of nearly 10% per year
- Used to download >2 million structure data files per day
- Managed by International collaboration US-Asia-Europe
- Manages "Big Data" as global Public Good

### PDB Data

- Enable research in subject areas from Agriculture to Zoology (Analysis)
- Contributed data to nearly >1 million published research papers
- Used by >400 biological data resources

The cost to replicate the contents of the PDB archive is estimated at  
**\$16 billion (USD)** (Analysis)

### PDB Data Impact

- Basic and applied research
- Patent applications
- Discovery of lifesaving drugs
- Innovations that can lead to new product development and company formation
- STEAM education: PDB-101 provides curricula and online tools for teachers and students

**>1,000,000** Data Consumers worldwide served every year

Researchers, scientists, educators, students, curious public, medical professionals, patients, and patient advocates

Public and Private sectors, including pharmaceutical and biotechnology companies

Generates return on investment of  
**~1,500 times federal funding** (Analysis)

The cost to replicate the contents of the PDB archive is estimated at  
**\$16 billion (USD)** (Analysis).

Generates return on investment of  
**~1,500 times federal funding** (Analysis).

**Science Gateways are  
engines of Broader  
Impact...**



**...because they democratize  
access and engage large,  
diverse audiences.**





**Science Gateways are sustainability habitats for scientific applications, scientific data sets, their creators, their users...**

**...because they are places many can pool together to address sustainability as a group.**



# A PI may find a Science Gateway beneficial if:

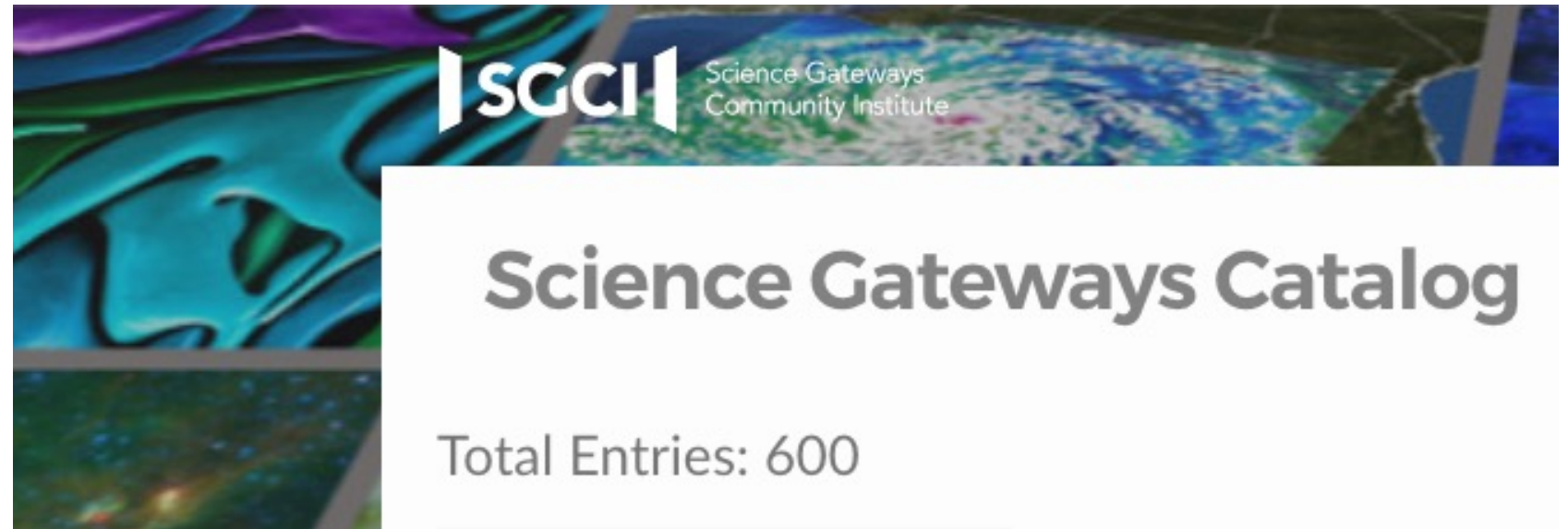
- They want to reach a broad and diverse audience
- They want to work with others to create a place for research results to live and be sustained
- They want others to be able to reproduce results
- They want their results to be FAIR
- They are a community builder and need a community platform

So, how do you find or build a gateway?



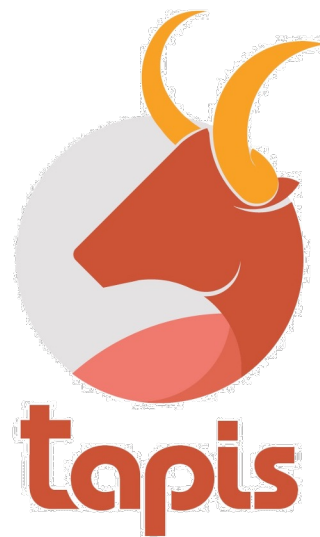


Fortunately  
you are not  
alone.





Fortunately  
you are not  
alone.



hubzero



UNfortunately  
you are not  
alone.



hubzero



GenApp

Science Gateways Catalog

Total Entries: 600



APACHE  
AIRAVATA





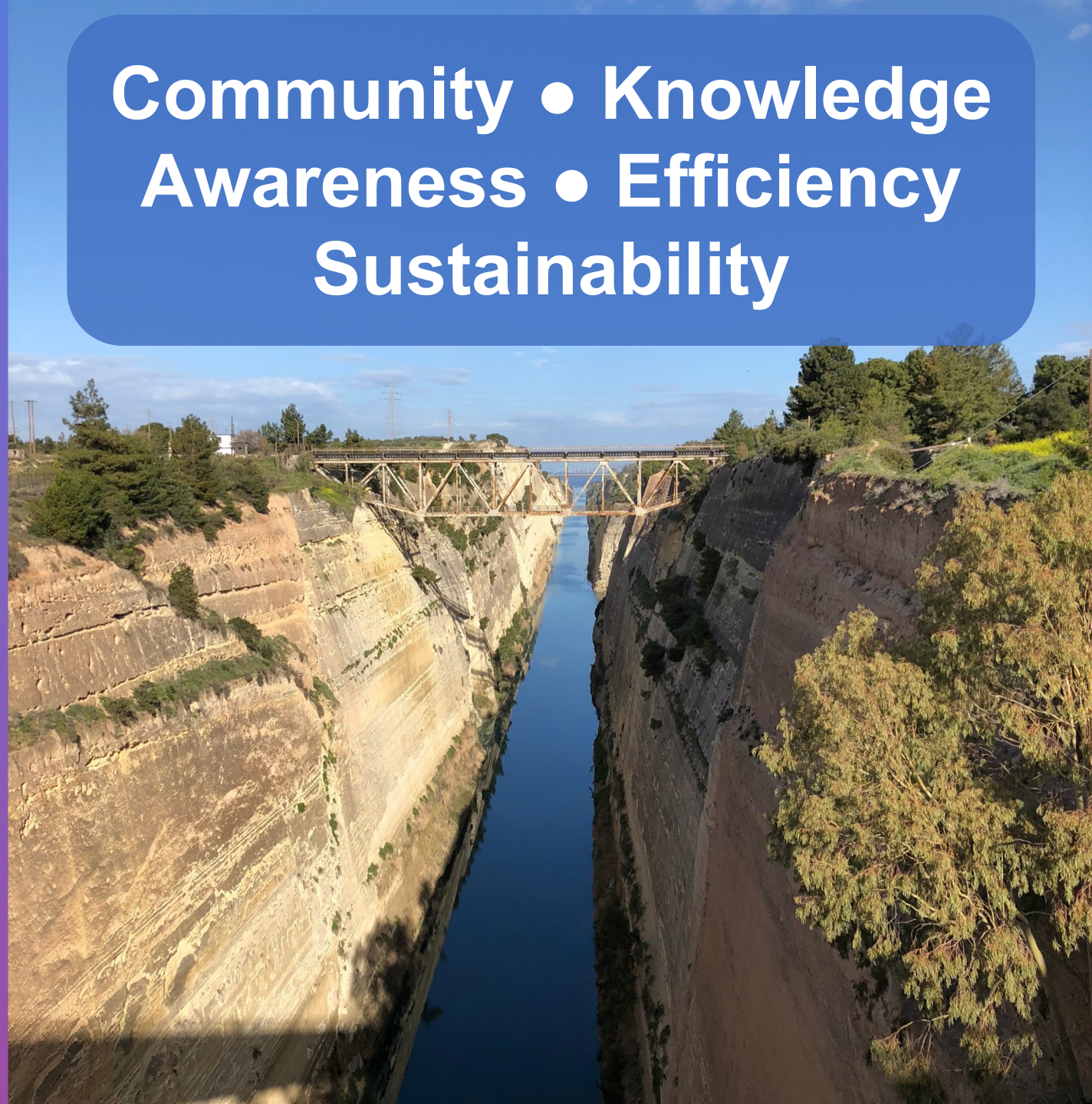
“How hard can it be? It’s just a web site.”



The formation of  
an Institute and a  
Center of  
Excellence...

...to bridge gaps  
and institutionalize  
best practices

**Community • Knowledge  
Awareness • Efficiency  
Sustainability**





# SGX3

A Center of Excellence and a Software Institute to  
serve the Science Gateways Community.

An advisory and community  
building entity



A full-service consulting  
organization

# SGX3

SGX3 – NSF Funded

- ✓ Technology advice (architecture, gap analysis)
- ✓ Workforce development (intern placement)
- ✓ Sustainability training
- ✓ Conference (Gateways 2023 in October)
- ✓ Finding gateway partners
- ✓ User experience consulting



SGCI – Client Funded

- ✓ Hands-on technology development
- ✓ Software team augmentation / outsourcing
- ✓ Professional science gateway operations
- ✓ In-depth sustainability analysis and strategy development



# Impactful Partner

- Broader Impact
  - 161 engagements
  - 1258 students served
  - 3604 attendees at events
- Scholarly Impact
  - 58,520 Citations of our Gateway clients
- Financial Impact
  - Approximately a 7x acceleration in development



**BUT WAIT**



**THERE'S MORE**





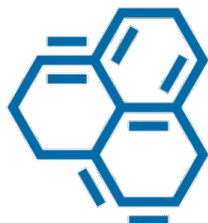
# Alliance for Cyberinfrastructure

NSF-Funded Centers to Help

[mzentner@ucsd.edu](mailto:mzentner@ucsd.edu) – [help@sciencegateways.org](mailto:help@sciencegateways.org)



Science Gateways Community Institute & Center of Excellence: for when you want to build or place content on a science gateway (**[sciencegateways.org](http://sciencegateways.org)**)



Trusted CI: a Cybersecurity Center of Excellence for when you need a review and consultation of cybersecurity issues in research (**[trustedci.org](http://trustedci.org)**)



CI Compass: a Data Lifecycle Center of Excellence for when you need assistance with implementing data management best practices (**[ci-compass.org](http://ci-compass.org)**)



RCD Nexus: a Research Computing and Data Center of Excellence for when you need tools, practices, and professional development resources (**[rcd-nexus.org](http://rcd-nexus.org)**)

# hubzero

A framework for building science gateways that serves millions of users annually and has been operating for 20 years.



A group of software engineers available for hire to implement and maintain research software with professional development processes.

(**[hubzero.org](http://hubzero.org)**)

[info@hubzero.org](mailto:info@hubzero.org)