

CryoCloud JupyterHub for NASA Cryosphere communities: Open science as a process, not a product

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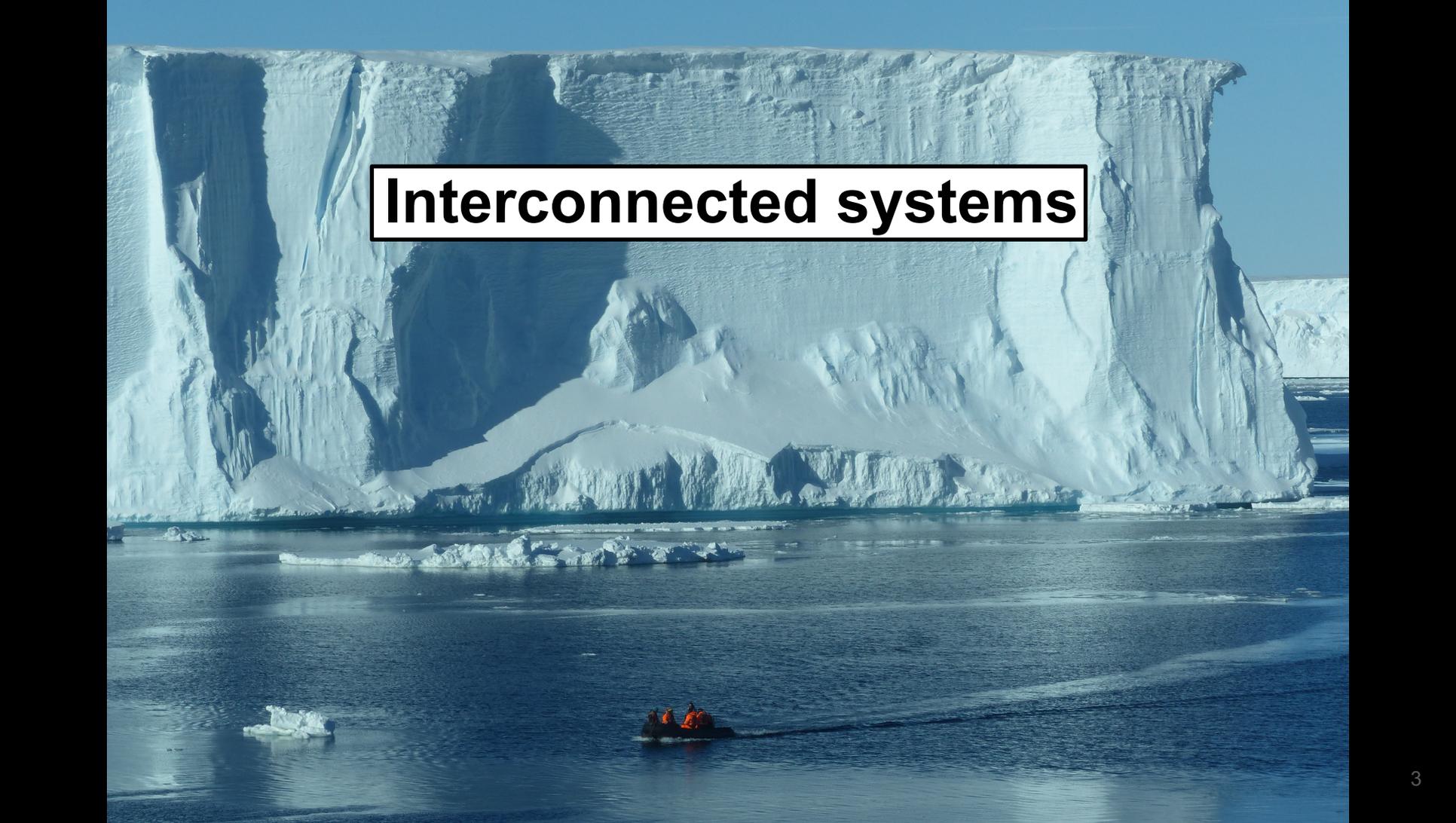
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CryoCloud



A photograph of a massive, towering ice wall, likely a glacier or ice shelf, under a clear blue sky. The ice wall is composed of various textures and colors, from bright white to deep blue. In the foreground, a small boat with several people in orange gear is on the water, providing a sense of scale. The water is dark blue with some ice floes. A white box with a black border contains the text "Interconnected systems" centered over the middle of the image.

Interconnected systems

Open science, community building, and infrastructure for _____ communities

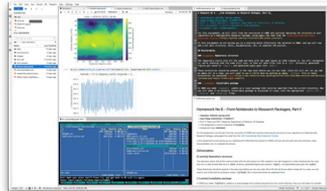
Defining open-source science and values



Models for serving the community



CryoCloud JupyterHub for Cryosphere communities



Lessons learned and outlook



The problem

Science has success in discovery, some limitations in impact

Participation of all society

More informed decision-making

Better localized knowledge and decision-making

The opportunity

Advances in technological & social innovation can boost science

Technological Innovation	Social Innovation
Explains 25% of innovation success	Explains 75% of innovation success

Source: Erasmus University: Competition and Innovation monitor (2006)

Necessity

For a high performing science ecosystem to address global challenges

Misinformation
Climate change
Policy making



Science done in a fundamentally more open way is the future

Principle and practice of making research products and processes available to all, while respecting diverse cultures, maintaining security and privacy, and fostering collaborations, reproducibility, and equity.



Open-source science at the forefront

OPEN-SOURCE SCIENCE INITIATIVE **Overview** Why Do Open Science? Transform to Open Science (TOPS)

Open-Source Science Initiative

NASA is making a long-term commitment to building an inclusive open science community over the next decade. Open-source science is a commitment to the open sharing of software, data, and knowledge (algorithms, papers, documents, ancillary information) as early as possible in the scientific process. The principles of open-source science are to make publicly funded scientific research transparent, inclusive, accessible, and reproducible. Advances in technology, including collaborative tools and cloud computing, help enable open-source science, but technology alone is insufficient. *Open-source science requires a culture shift to a more inclusive, transparent, and collaborative scientific process, which will increase the pace and quality of scientific progress.*

To help build a culture of open science, NASA is championing a new initiative: the Open-Source Science Initiative (OSSI). OSSI is a comprehensive program of activities to enable and support moving science towards openness, including policy adjustments, supporting open-source software, and enabling cyberinfrastructure. OSSI aims to implement NASA's [Strategy for Data Management and Computing for Groundbreaking Science 2019-2024](#), which was developed through community input.



OPEN (TRANSPARENT) SCIENCE
scientific process and results should be visible, accessible, and understandable

OPEN (ACCESSIBLE) SCIENCE
data, tools, software, documentation, and publications should be accessible to all (FAIR)



OPEN (INCLUSIVE) SCIENCE
process and participants should welcome participation by and collaboration with diverse people and organizations

OPEN (REPRODUCIBLE) SCIENCE
scientific process and results should be open such that they are reproducible by members of the community



Transform to Open Science (TOPS)

From 2022 to 2027, TOPS will accelerate the engagement of the scientific community in open science practices through events and activities aimed at:

- Lowering barriers to entry for historically excluded communities
- Better understanding how people use NASA data and code to take advantage of our big data collections
- Increasing opportunities for collaboration while promoting scientific innovation, transparency, and reproducibility.

The TOPS mission is aligned with recommendations from NASA's [Strategy for Data Management and Computing for Groundbreaking Science 2019-2024](#), the National Academies reports on [open science](#), [reproducibility](#), and [scientific software](#), and the 2021 UNESCO [draft Recommendation on Open Science](#) synthesis report.



Engage in the open science community on the Transform to Open Science (TOPS) GitHub



TOPS. (2021). Creative Commons Attribution 4.0 License. <https://doi.org/10.5281/zenodo.5225076>



Open Science Curricula: **OpenCore**

<https://nasa.github.io/Transform-to-Open-Science/>

NASA (and US+): 2023 the Year of Open Science

YEAR OF
OPEN
SCIENCE

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“...I realized that open science isn’t just about tools. Open-science innovation is being driven by a global community with diverse perspectives. The scientific questions are more interesting and nuanced, the solutions better.” - Chelle Gentemann

open.science.gov



NIST



USGS
science for a changing world



Open science values

Intellectual generosity

Intellectual humility

Right to participate in science

Everyone deserves to be treated with dignity and respect

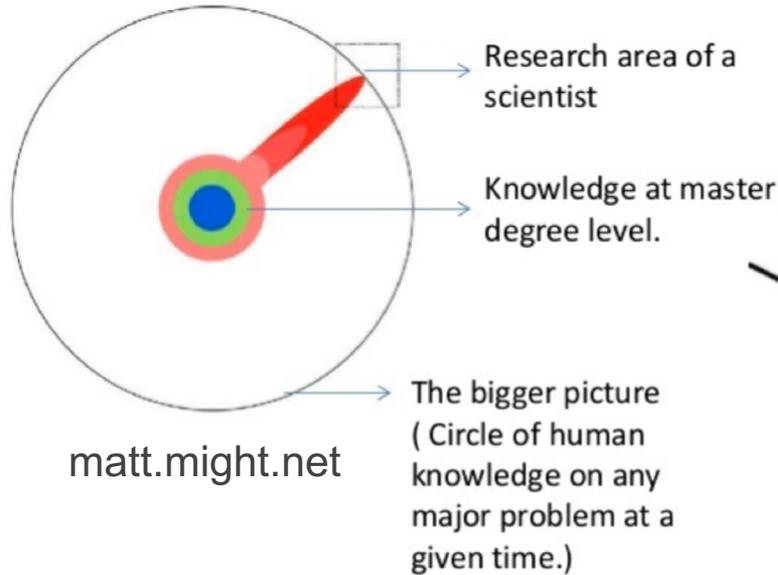
Intellectual generosity

Sharing ideas, advancing other's understanding

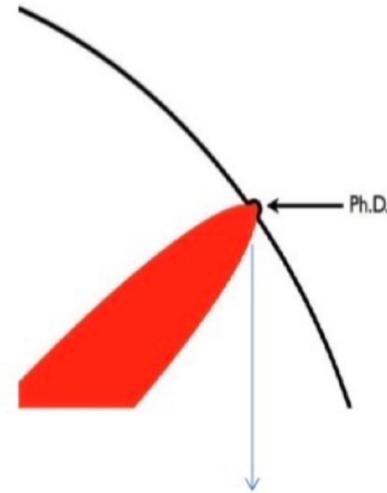
Reduce competition and enhance collaboration



Intellectual humility



Our contributions are small relative to the body of knowledge

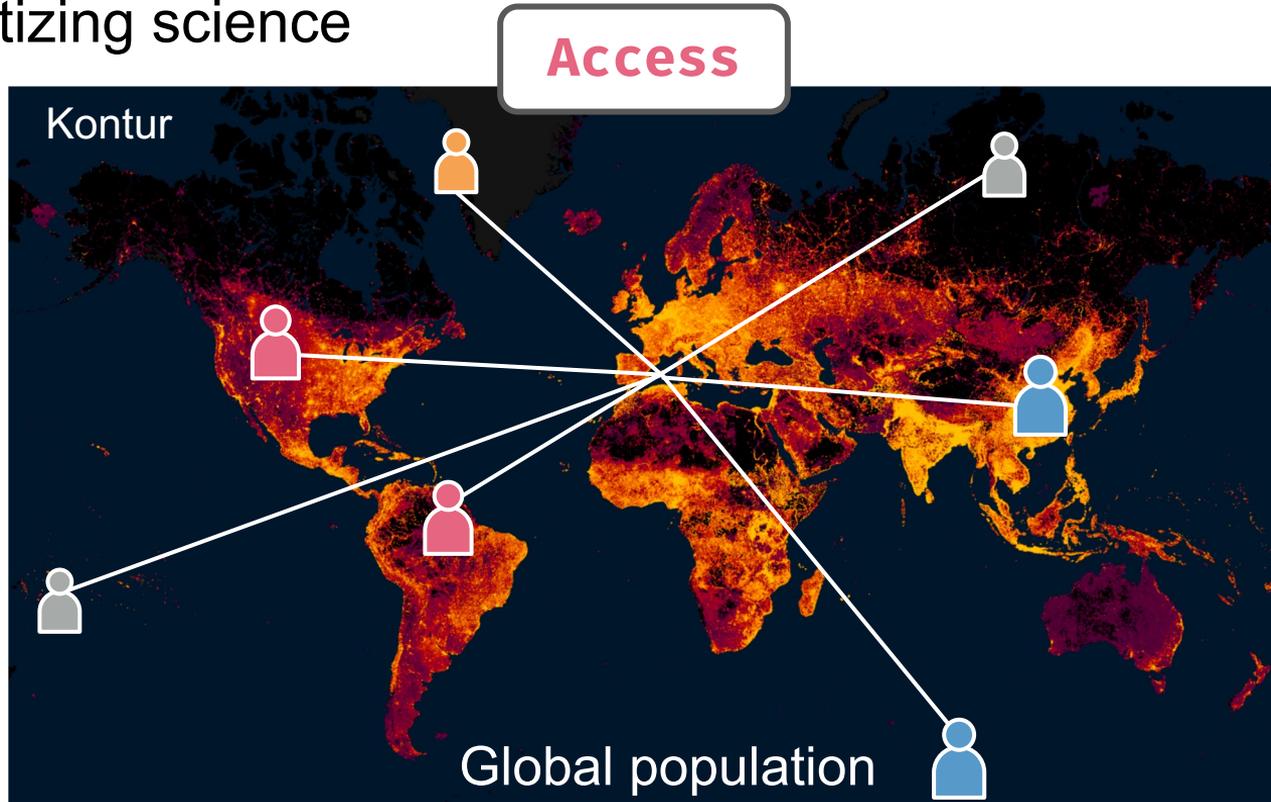


The dent a scientist makes at the boundary of human knowledge on any major problem.

Give and receive criticism with grace

Right to participate in science

Democratizing science



Everyone deserves to be treated with dignity and respect

Objective and constructive discourse

DIVERSITY



of people and perspectives

EQUITY



in policy and practice

INCLUSION



of all voices and visions

Open science values

Intellectual generosity

Intellectual humility

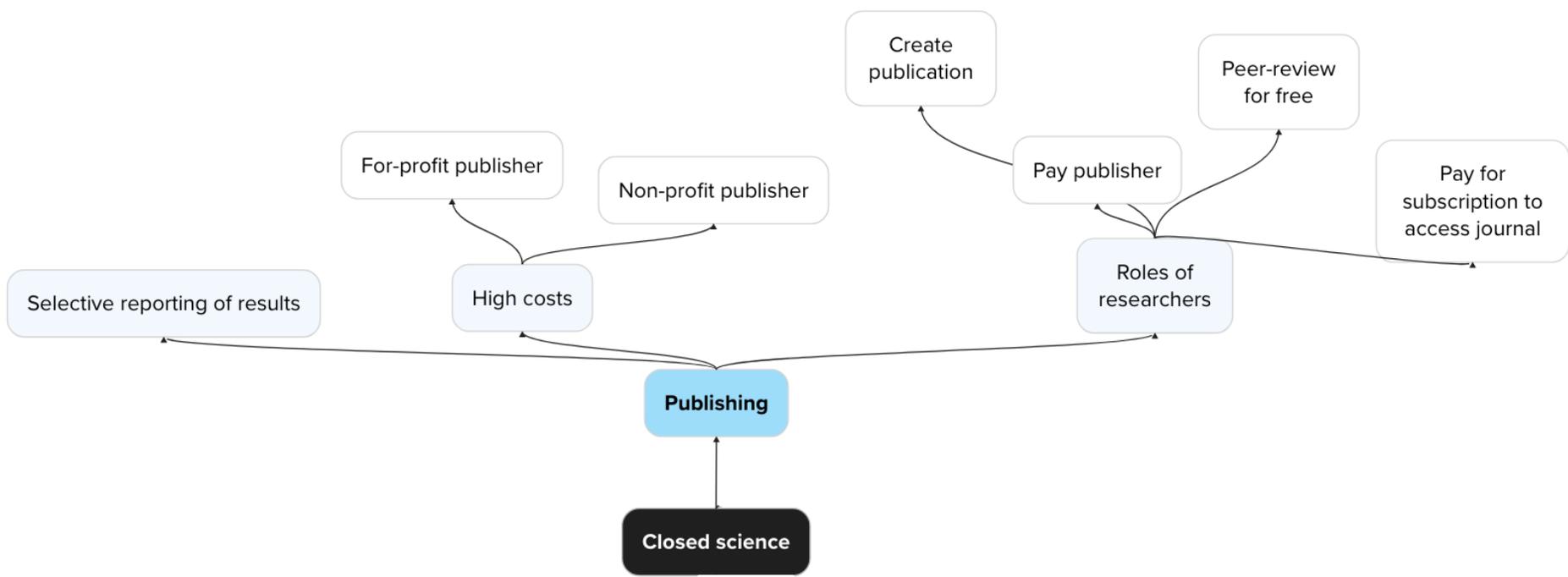
Right to participate in science

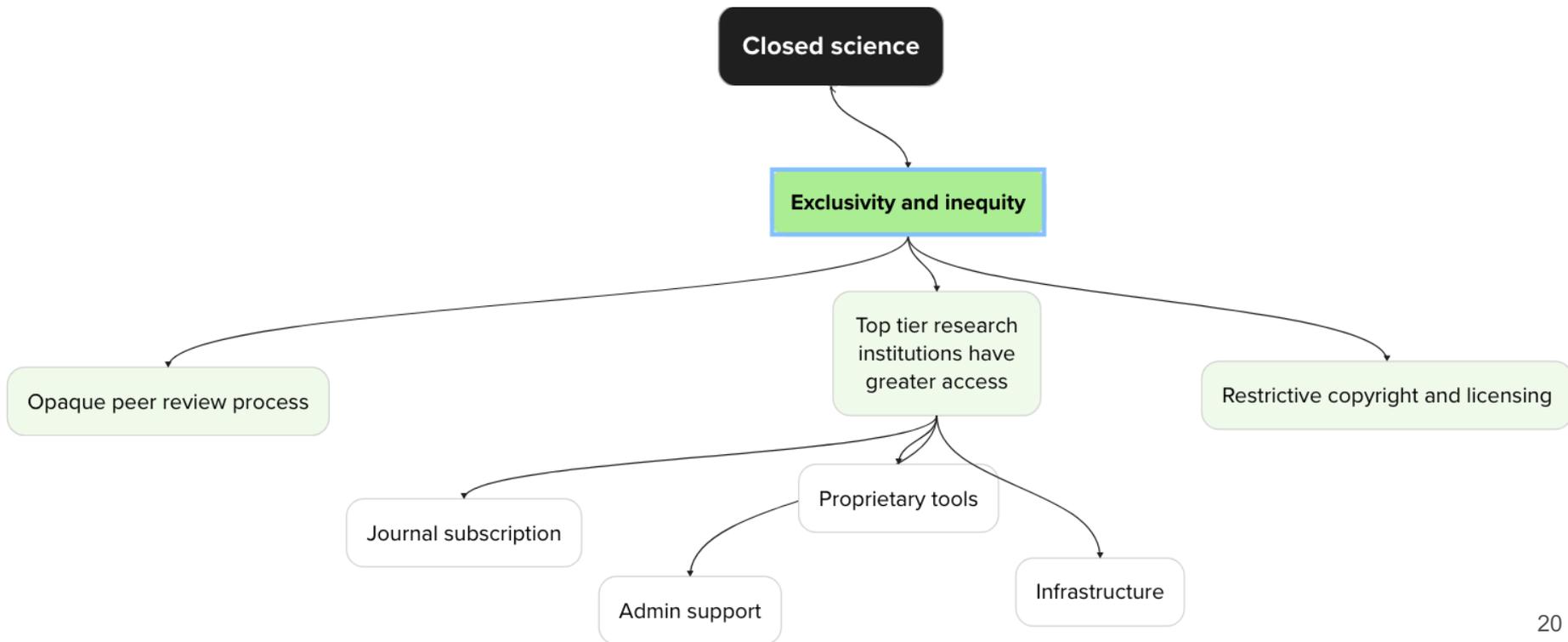
Everyone deserves to be treated with dignity and respect

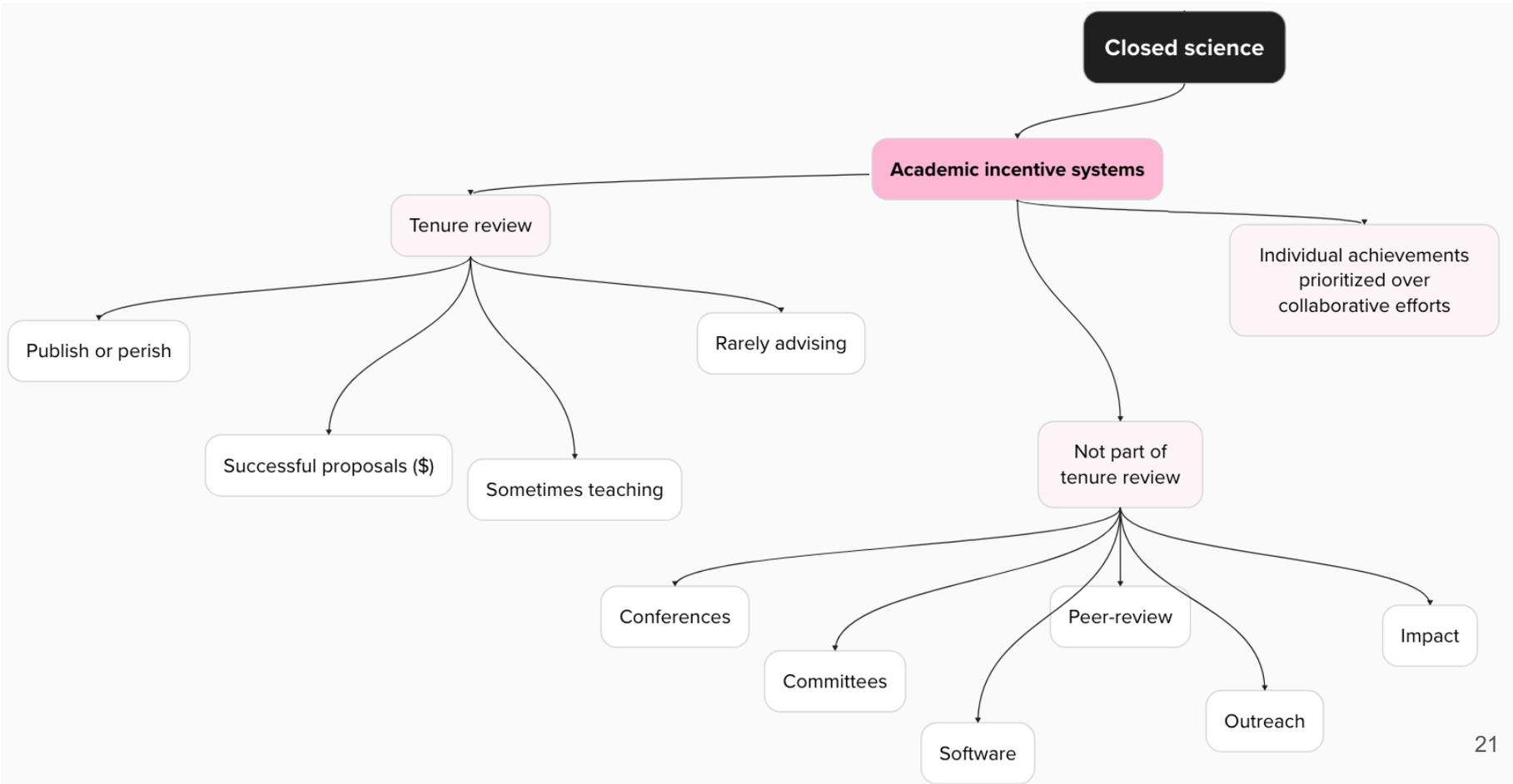
Open science as a process, not a product

The challenge:

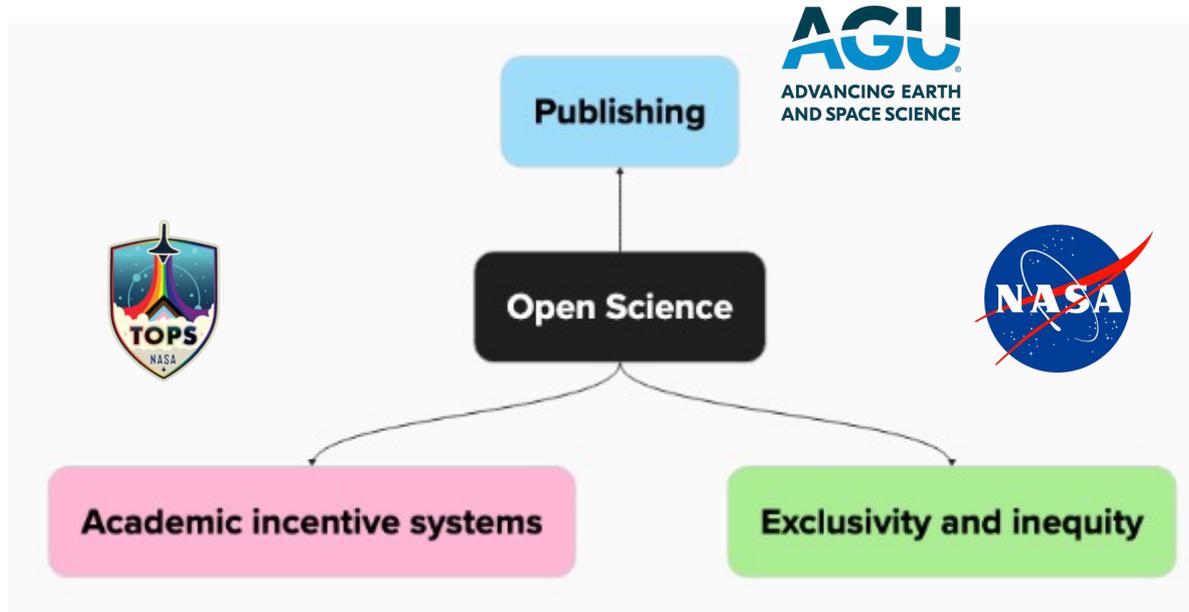
Closed science



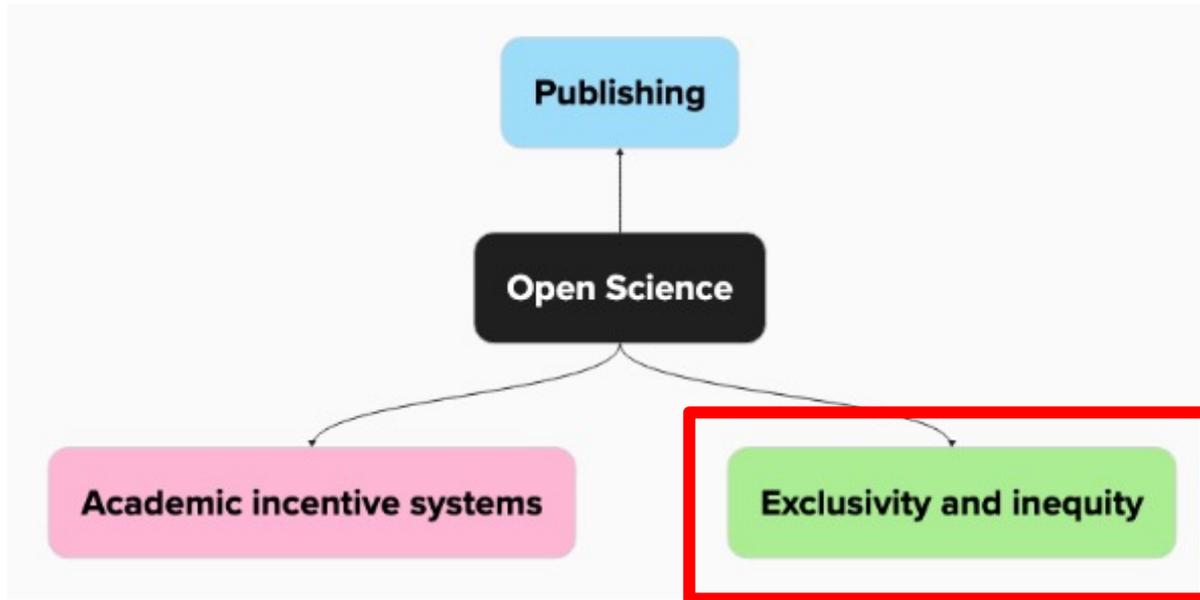




Finding solutions

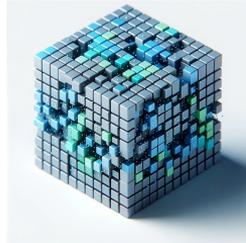


Our piece of the puzzle



Solutions through computing

Research requires computing capabilities



Research computing requires infrastructure that may not be trivial to access



We need certain computing resources to produce impactful results

Produce solutions



Conduct research

ChatGPT

On usable timeframes

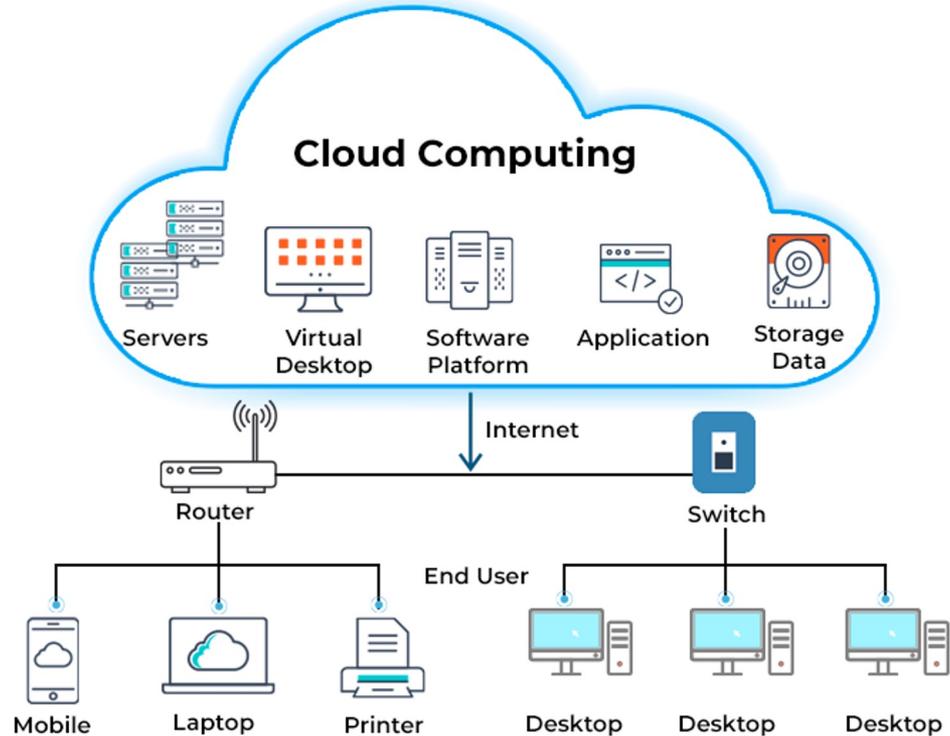


ChatGPT

Collaborative, reproducible, open science in the
cloud

What is the cloud?

CLOUD COMPUTING ARCHITECTURE



C. L. Gentemann^{1,2} , C. Holdgraf^{3,4} , R. Abernathey^{3,5} , D. Crichton⁶ , J. Colliander^{3,7,8} ,
E. J. Kearns⁹ , Y. Panda³ , and R. P. Signell¹⁰ 



 [ChelleGentemann](https://twitter.com/ChelleGentemann)

Key Points

Science stands at the cusp of a new, open science, cloud-enabled era

Advances in data, software, and computing are enabling transformational, interdisciplinary science, **changing the realm of possible questions**

Deliberately designed open science communities can **advance science and inclusivity simultaneously**



<https://agupubs.onlinelibrary.wiley.com/doi/10.1029/2020AV000354>

AGU Advances

RESEARCH ARTICLE

Science Storms the Cloud

10.1029/2020AV000354



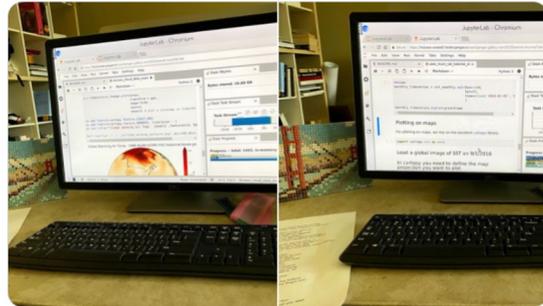
ChelleGentemann

Process massive amounts of data from a \$36 computer...



Chelle-ter in Place
@ChelleGentemann

On my kids @Raspberry_Pi running @TeamKano #OpenSource OS I'm analyzing @GCPcloud #cmip6 climate data and @awscloud MUR SST from @podaac. A \$36 computer running processes on both AWS and GCP with over 80 workers and 245GB. #openscience! @NASAEarth



1:18 PM · Mar 1, 2020 · Twitter Web App

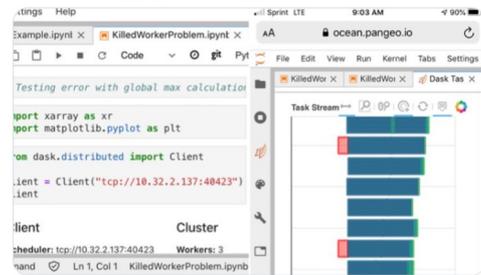
...or from your cell phone or on a flight



Julius Busecke @JuliusBusecke · Feb 6
I am analyzing #CMIP6 on the train on MY PHONE!



Goddamn it, @pangeo_data is amazing! This has literally been the only time I have wanted a bigger phone screen 😭



2 13 66

Replies



Thomas Moore @SurfTasmania · Feb 6
Replying to @JuliusBusecke and @pangeo_data
Nice! That's way cooler than spinning up a @pangeo_data HPC cluster on your laptop from 35,000 feet up. 🚀

Image credits: Chelle Gentemann



Key Points

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advance science

<https://agupubs.onlinelibrary.wiley.com/doi/10.1029/2020AV000354>

The Digital Watering Hole (in the cloud)

An opportunity shaped by:

- Open, FAIR and CARE Data
- Scalable computation next to the data
- Modular tools for exploration/narrative



To tackle challenges that

- go beyond disciplinary silos...
- require analysis of *really* big data
- integration of disparate data...
- *participation* of disparate, diverse communities...
- to ultimately connect with society and impact critical decision making.

Proofs of concept

Exoplanet analysis: two orders of magnitude faster in the cloud

Retention of an exoplanet's atmosphere as it orbits close to a star

Analysis per planet:

- 5 hours on local computer
- 5-10 min in the cloud

With a few lines of code that gave cloud access to data archives





Berkeley
UNIVERSITY OF CALIFORNIA

Stat 159 by Fernando Pérez ([course site](#))

AQ Project Jupyter Book

Exploring the Air Quality of the San Francisco Bay Area using OpenAQ

ANALYSIS NOTEBOOKS

- Exploring and Visualizing OpenAQ Data
- Los Angeles Exploration & Visualization
- Analyzing the dark day over San Francisco (Sep 9 2020)
- Predicting Concentrations of PM 2.5

Powered by **Jupyter Book**

Exploring the Air Quality of the San Francisco Bay Area using OpenAQ

STAT 159/259 Final Project

Authors: Wesley Darling, Gyuhyeon Seo, Ram Kripa, Jae Hee Koh

Project Motivation

On September 9th, 2020, in the midst of the COVID-19 pandemic and wildfires up and down the State of California, residents of the San Francisco Bay Area woke up to a shocking sight:

JupyterBook based site



"Main Paper"

Analysis II: Predicting Concentrations of PM_{2.5}

In the Data Exploration and Visualization sections above, it is clear that there are multiple sensor locations that do not measure PM_{2.5}. Can we infer these values for an entire city, the goal of...

Long Short-Term Memory (LSTM) and other recurrent neural networks (RNNs) are used to solve the remaining problem faced by recurrent neural networks (RNNs). In RNNs, there are two major update gates, reset gate. These gates have hidden state from the previous sequence as input to the layer or neuron cells. During the training process, RNNs learn how to learn parameter compared to LSTM. It helps them filter the most relevant information.

A first prediction model using Global Document Unit Neural Network was developed using only air quality data to predict the PM_{2.5} concentration based on the concentration of CO, NO₂, and O₃. First the air quality data were scaled and made stationary using the following technique as shown in the figure below.

Supporting code & tests

```

82 lines (33 slots) 3.11 KB
wesley-darling inside pip installable Latest commit a942778 on May 11 History
A1 contributor
1 from pandas import read_csv as vc
2 import openaq
3 import pandas as pd
4 import geopandas as gpd
5 import os
6 import pytest
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```



Berkeley
UNIVERSITY OF CALIFORNIA

Stat 159 by Fernando Pérez ([course site](#))

Exploring the Air Quality of the San Francisco Bay Area using OpenAQ

AQ Project Jupyter Book

Search this book...

Exploring the Air Quality of the San Francisco Bay Area using OpenAQ

ANALYSIS NOTEBOOKS

Exploring and Visualizing OpenAQ Data

Los Angeles Exploration & Visualization

Analyzing the dark day over San Francisco (Sep 9 2020)

Predicting Concentrations of PM_{2.5}

Powered by Jupyter Book

STAT 159/259 Final Project

Project Motivation

Introduction

Data Exploration

Visualization of SF Bay

Authors: Wesley Darling, Gyuhyeon Seo, Ram Kripa, Jae Hee Koh

Project Motivation

On September 9th, 2020, in the midst of the COVID-19 pandemic in the State of California, residents of the San Francisco Bay Area woke up to a dark day over the city.

50-2000 students working in the cloud for \$1 to \$2 per student per semester

Analysis II: Predicting Concentrations of PM_{2.5}

In the Data Exploration and Visualization sections above, it is clear that there are multiple sensor locations that do not measure PM_{2.5}. One key requirement for a model for air quality, the goal of the second analysis is to predict these PM_{2.5} concentrations using only the data from the sensors that do measure PM_{2.5}. This is a classic machine learning problem to predict the concentration of a variable based on other variables. In this analysis, we will use a recurrent neural network (RNN) to predict the concentration of PM_{2.5} based on the data from the sensors that do measure PM_{2.5}.

Cated Recurrent Unit (GRU)

```

# Create the time series and reshape it to be 1D
time_series = FigureAxisLocation_Frames[CA_Frames_2].copy()
time_series.index = time_series.index.tz_convert('UTC')

# Save Frame
plt.savefig(filename)
plt.close()

with open(os.path.join('figures', filename), 'w') as writer:
    for i in range(0, time_series.shape[0]):
        time_series.index = time_series.index + pd.Timedelta(days=1)
        writer.write(time_series[i].to_json())

with open('figures/01_line_landscape_gif', 'w') as file:
    writer.write(time_series.to_json())

```

Exploring the OpenAQ API

Visualizing the available period

```

62 lines (33 slots) 3.11 KB
1 from pathlib import Path as vu
2 import openaq
3 import pandas as pd
4 import geopandas as gpd
5 import os
6 import pytest
7
8 npl = openaq.OpenAQ()
9 pytest.shared = pd.DataFrame()
10
11 def test_location_filter():
12     df = vu.location_filter(npl.locations(country='US'), df=True, limit=50000)
13     assert df.shape == (133, 14)
14     pytest.shared = df
15
16
17 def test_shared_data_per_loc_per_day():
18     df = vu.shared_data_per_loc_per_day(npl.locations(country='US'), df=True, start_date='2020-09-07', end_date='2020-09-08')
19     assert df.shape == (648, 14)
20     pytest.shared = df
21
22 def test_shared_data_per_loc_per_day():
23     gdf = vu.shared_data_per_loc_per_day(npl.locations(country='US'), df=True, start_date='2020-09-07', end_date='2020-09-08')
24     assert gdf.shape == (648, 21) and gdf.index.dtype == 'datetime64[ns]'
25     pytest.shared = gdf
26
27
28 def test_shared_data_per_loc_per_day():
29     gdf = vu.shared_data_per_loc_per_day(npl.locations(country='US'), df=True, start_date='2020-09-07', end_date='2020-09-08')
30     assert gdf.shape == (648, 138)
31     pytest.shared = gdf

```

Exploring the Air Quality of the San Francisco Bay Area using OpenAQ

Project Motivation

On September 9th, 2020, in the midst of the COVID-19 pandemic in the State of California, residents of the San Francisco Bay Area woke up to a dark day over the city.

Location	Country	City	State	Postal Code	Latitude	Longitude	Altitude	Timezone
San Francisco	US	San Francisco	CA	94102	37.7749	-122.4194	16	America/Los_Angeles
San Jose	US	San Jose	CA	95128	37.3382	-121.8883	121	America/Los_Angeles
San Diego	US	San Diego	CA	92101	32.7157	-117.1617	16	America/Los_Angeles



github.com/UCB-stat-159-s22/hw07-group13



New spaces and organizational models are needed

Cloud computing and ICESat-2 science

Cloud computing and open science concerns from the May 2022 ICESat-2 Science Team Meeting

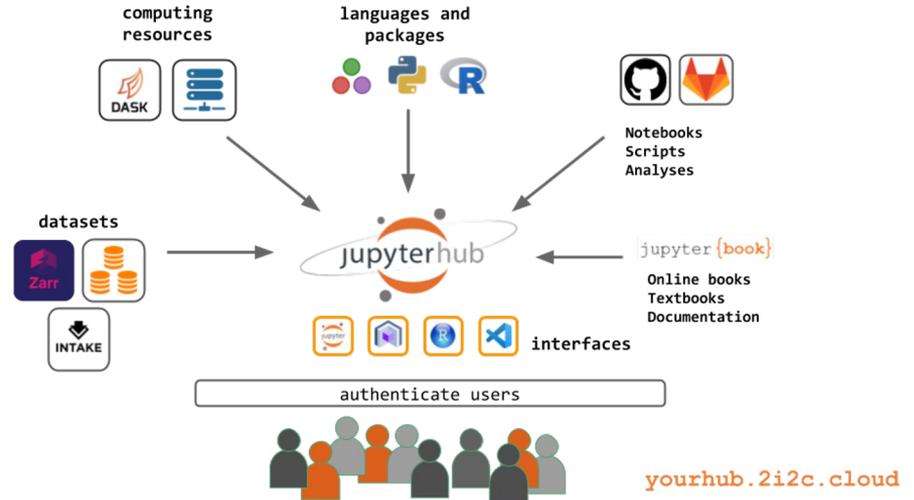
- Non-intuitive pricing structures, computing options, infrastructure
- Poor documentation
- Costly to use
- Not obviously more collaborative or faster



This didn't ring true to our experience in the cloud!

The International Interactive Computing Collaboration

- **Non-profit.**
- **Service provider** for interactive computing infrastructure.
- An R&D team that **contributes back to open source** communities.





: A cloud-computing platform with *bumpers*

Goal: Simple and cost effective managed cloud environment for training and transitioning new users to cloud workflows and determining community best practices

Built and developed for cryosphere scientists by software professionals at **2i2c** to make it possible to:

- Process data faster
- Minimize downloading
- Democratize science





: A cloud-computing platform with *bumpers*

Cryo**Cloud**

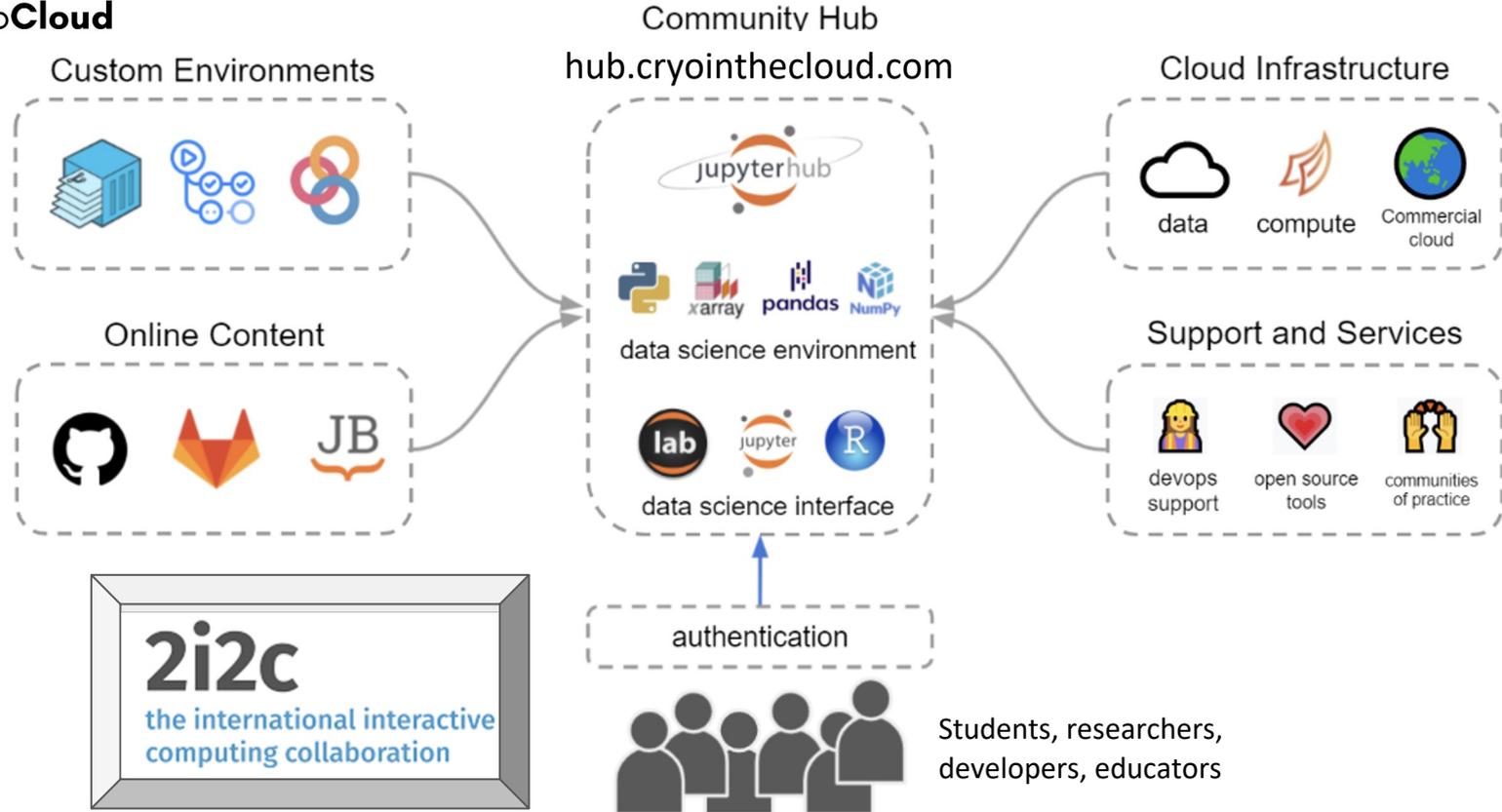
- Persistent for (at least) three years
- Small servers (32 Gb / 4 CPU) for all users, option to bring own cloud credits to access larger servers
- New tool development
 - Personal cost-monitoring tool
 - Intra- and inter-hub collaboration tools
- Helping 2i2c scale with community surveys, feedback, and guidance



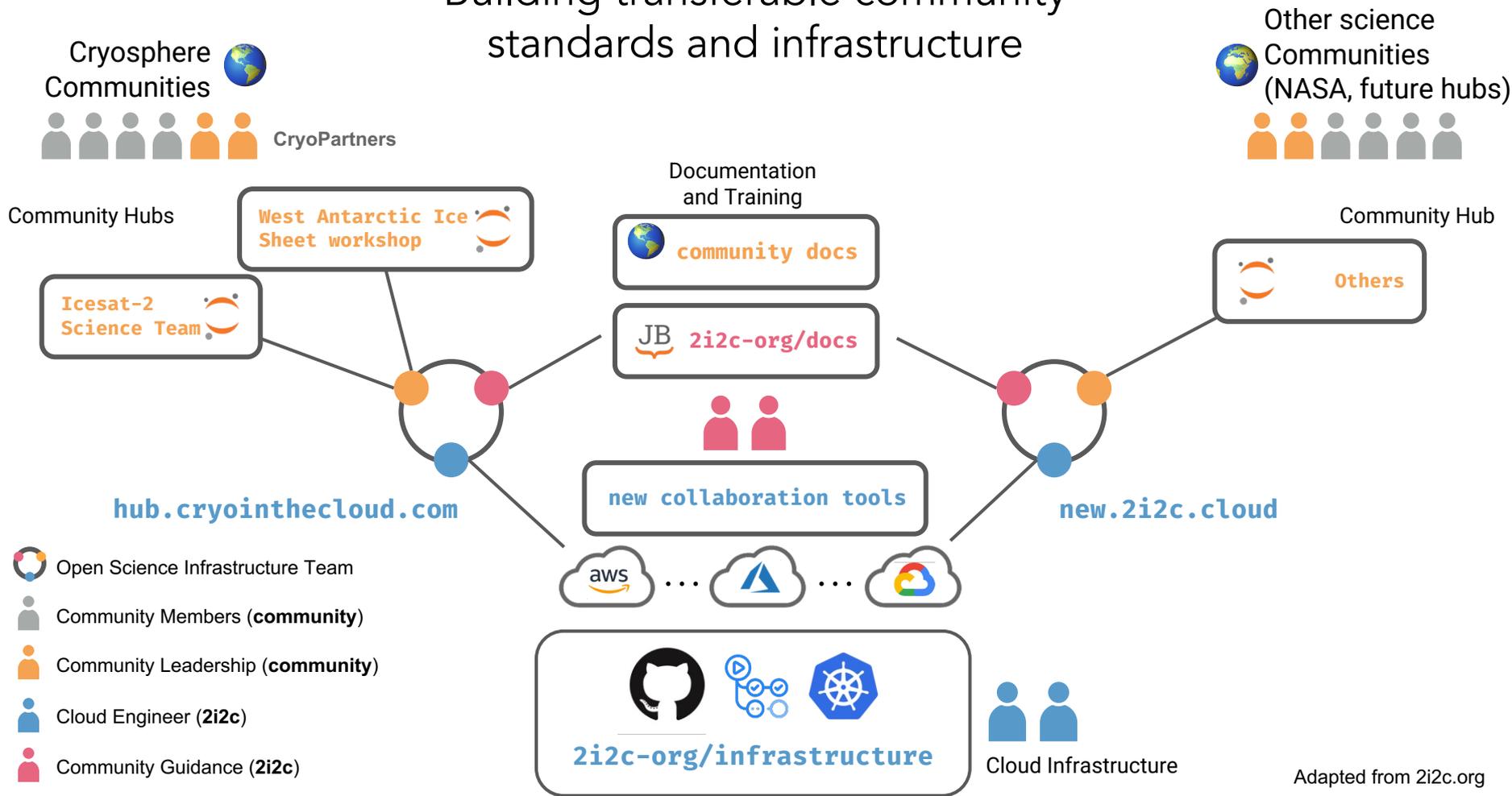


Cryo**Cloud**

: accelerate discovery and enhance collaboration



Building transferable community standards and infrastructure



CryoCloud documentation & community building

cryointhecloud.com

- CryoCloud Github:
github.com/cryointhecloud

- CryoCloud Slack
- Community office hours
- Training, tutorials, and resources
- Bring in Cryosphere communities and share in infrastructure ideation and construction



CryoCloud JupyterBook

All the content! More about us, resources, training, and tutorials all found here!



CryoCloud

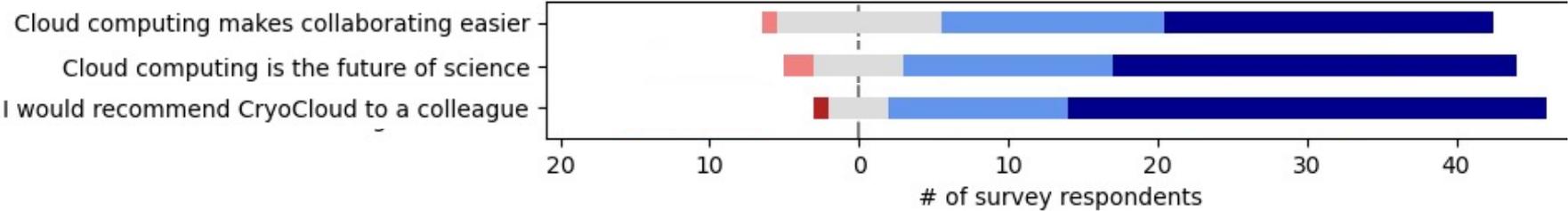
CryoCloud JupyterHub

Get onto the cloud. Our shared cloud platform for NASA Cryosphere communities.

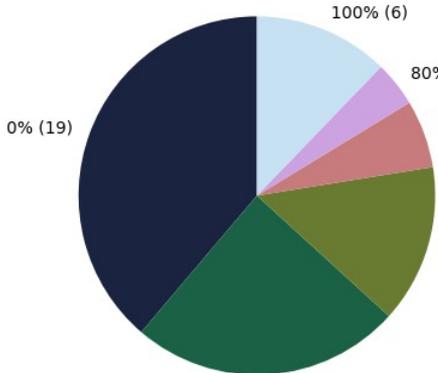
Advantages to a community platform



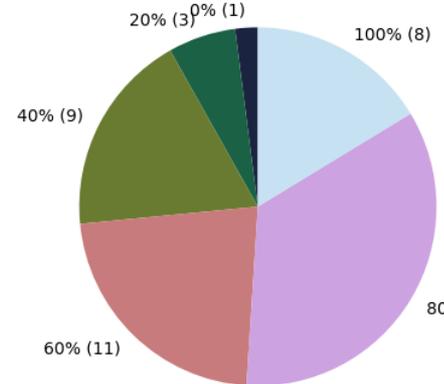
CryoCloud community feedback integral to building community best practices



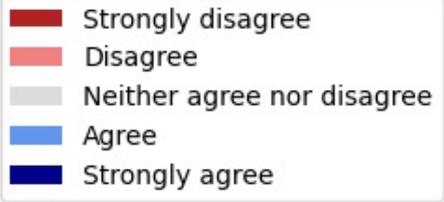
What percentage of your research computing to you perform in the cloud



Today



5 years from now



CryoCloud helps accelerate science and makes open science easy

Faster – No manual data handling, faster data read-ins

Easy to use, customizable – same software as on personal computer

Collaboration made easy – co-coding, shared tools

Eliminates technology bottlenecks – shared challenges

No software expertise needed – cloud-computing as a service



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Versatile choice of computer language and server size

Server Options

- **Small: up to 4 CPU / 32 GB RAM**

Start a container with at least a chosen share of capacity on a node of this type

Image

R

Node share

~1 GB, ~0.125 CPU

Medium: up to 16 CPU / 128 GB RAM

GPU: up to 4 CPU / 16 GB RAM

Julia (soon!)

Matlab

✓ Python

R

Other...

✓ ~1 GB, ~0.125 CPU

~2 GB, ~0.25 CPU

~4 GB, ~0.5 CPU

~8 GB, ~1.0 CPU

~16 GB, ~2.0 CPU

~32 GB, ~4.0 CPU

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Different kinds of users in one place accelerates feedback and collaboration

The screenshot shows a JupyterLab environment. On the left is a file browser with a search bar and a list of files and folders. The main area contains a code editor with the following Python code:

```
fig, ax = plt.subplots(figsize=(6,6))  
image.sel(band='blue').plot()  
plt.plot(ISlons,ISlats,color = 'green')  
plt.plot(ATMlons,ATMlats,color = 'orange')
```

Below the code is a plot titled "Figure 4" showing a satellite image of a region. The plot has a color scale on the right ranging from 15000 to 40000. The y-axis is labeled "latitude (degrees_north)" and ranges from 69.15 to 69.30. The x-axis is labeled "band = blue, time = 2019-05-07T14:53:54.971000,..." and ranges from 09.30 to 09.30. A terminal window at the bottom shows a warning message:

```
WARNING: No ICDS were found. Either,  
- Install a conda package providing a OpenCL implementation (pocl, oclgrind, intel-compute-  
- Make your system-wide implementation visible by installing ocl-icd-system conda package.  
(notebook) jovyan@jupyter-tsnow03:~$
```

Datasets



Tools and Developers



earthaccess
A Python Library for NASA Earthdata

CryoCloud helps accelerate science and makes open science easy

Faster – No manual data handling, faster data read-ins

Easy to use, customizable – same software as on personal computer

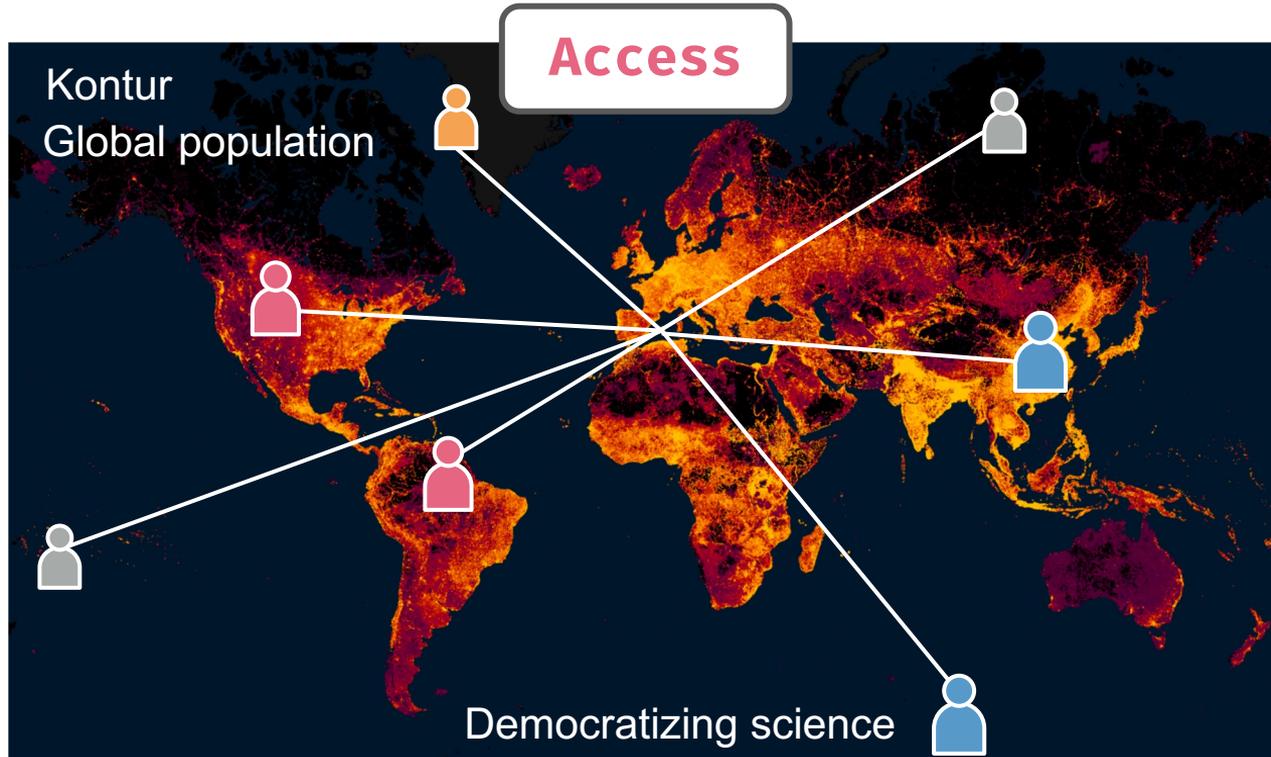
Collaboration made easy – co-coding, shared tools

Eliminates technology bottlenecks – shared challenges

No software expertise needed – cloud-computing as a service



Early careers, underrepresented groups, and non-R1 academic institution researchers benefit the most



CryoCloud helps accelerate science and makes open science easy

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A consistent platform provides a place where individuals and communities can rapidly mobilize when need arises

- ICESat-2 Science Team pre-launch training: Dec 2022
- FOGGS: March 2023
- ICESat-2 Hackweek: Aug 2023
- WAIS: Sept 2023
- ICESat-2 Science Team Meeting: Oct 2023
- AGU Year of Open Science: Dec 2023

*Norwegian ML Workshop (Apr), QGreenland Workshop (May),
NSIDC User Working Group (Sept), GeoSmart Hackweek (Oct)*



ICESAT-2



Cost to run a workshop in the cloud

Case study: QGreenland Workshop

Standing up own hub for 1 month

\$4500 for hub

\$75 in cloud credits

Science experts to advise in constraining hub needs

2-4 work weeks - Build and maintain hub



With CryoCloud

\$75 in cloud credits

2 hours to 2 work days - Science and/or tech experts to advise on user & infrastructure needs

Shared resource community model – expertise and technology



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Matt Fisher (he) 1:22 PM

Indeed! And not to mention the intangible savings. \$75 dollars is feels like \$0 when I think about what I'm buying -- not having to deal with anyone else's weird computer problems!

Some of that was quality-of-life stuff that I hope get shared among other hubs so that time cost should ideally have been a one-time thing instead of recurring.



QGreenland

+



CryoCloud

cloud

s - Science
advise on
needs

community
technology

Self-sustaining ecosystem generated once have a critical mass of experts who drank the coolaid

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Ongoing challenges

Data not in the cloud or cloud-optimized formats

Boundaries of what a community is

Imagining new social and logistical structures

- Models for contributing to sustain the infrastructure and costs
- Interconnection between computing systems



Vision for the future

Open science values

Intellectual generosity

Intellectual humility

Right to participate in science

Everyone deserves to be treated with dignity and respect



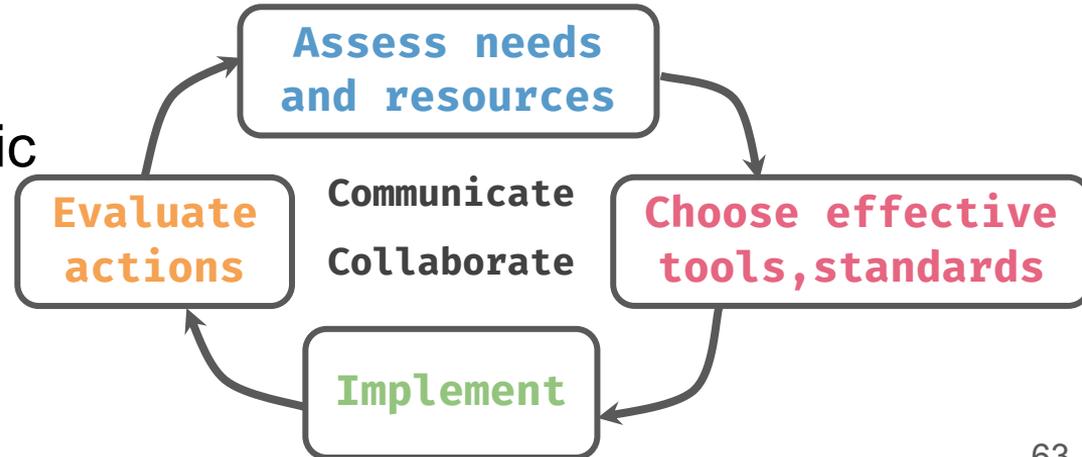
open.science.gov

Guiding practices

Avoid vendor lock-in



Active engagement of scientific community in building new community models



Driving social and technological innovation forward

Open science as a process, not a product

Technological Innovation	Social Innovation
Explains 25% of innovation success	Explains 75% of innovation success

Source: Erasmus University: Competition and Innovation monitor (2006)

A photograph of a massive, vertical ice wall, likely a glacier or ice shelf, under a clear blue sky. The ice wall shows various textures and shadows, indicating its thickness and structure. In the foreground, a small boat with several people in orange gear is moving across the dark blue water, leaving a white wake. Several smaller ice floes are scattered in the water. Two text boxes are overlaid on the image, one above the other, both containing text in a bold, black, sans-serif font.

Interconnected systems

Interconnected researchers



cryointhecloud.com



Cryo**Cloud**

Thank You!



[tsnow03.github.io](https://github.com/tsnow03)

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 @TashaMSnow

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