U.S. National Science Foundation
Directorate for Technology, Innovation and Partnerships

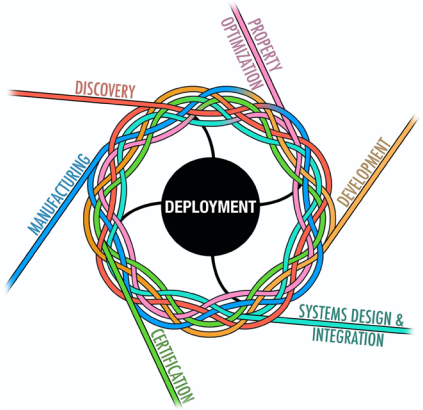
NSF Test Bed: Toward a Network of Programmable Cloud Laboratories

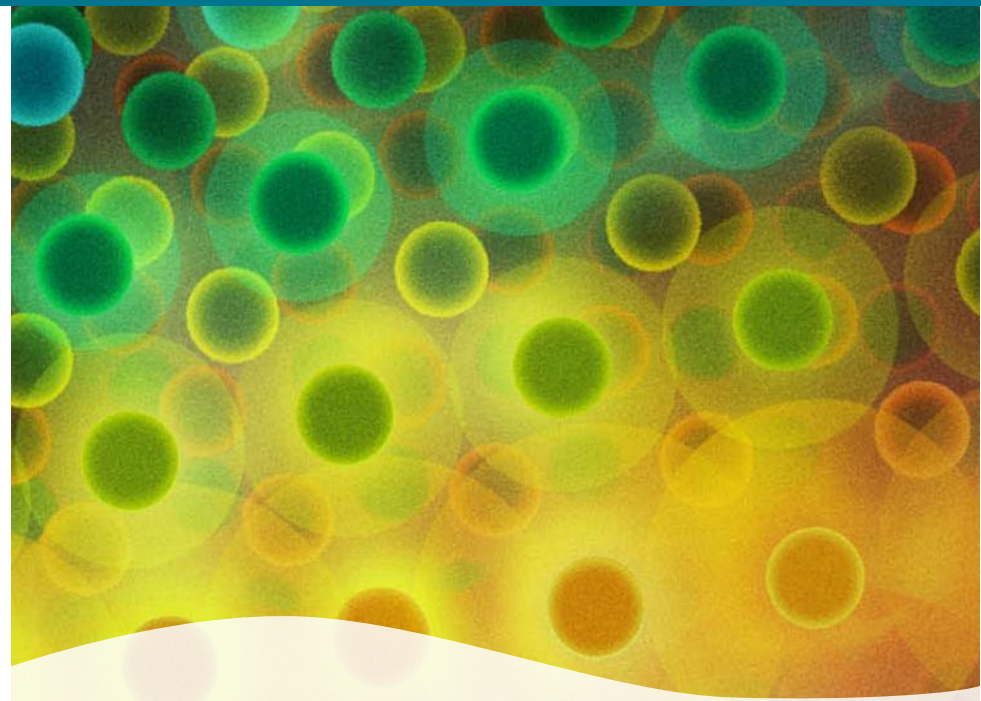
(NSF PCL Test Bed)

Presenters: Chaitan Baru, Alex Vadati, TIP Directorate

The U.S. National Science Foundation Test Bed: Toward a Network of Programmable Cloud Laboratories (NSF PCL Test Bed)

This program will seed and cultivate an autonomous laboratory ecosystem across the U.S. to unleash the potential of the American innovation ecosystem. These laboratories will combine technological and human capacity to enable integration, testing, evaluation, validation, and translation of cutting-edge technology solutions in automated science and engineering.





Opportunity available to:

- Academia
- Business & Industry
- Nonprofits

MISSION

PROMOTE the progress of science

ADVANCE the national health, prosperity, and welfare

SECURE the national defense

NSF's strategic priorities

Strengthening established NSF

with **investments that expand the frontiers of knowledge and discovery**

Create opportunities and access for all Americans

Using **capacity building and interventions** that enhance and broaden participation for all Americans everywhere

Accelerating technology and innovation

through innovative, **cross-cutting partnerships** and programs

NSF TIP's core message

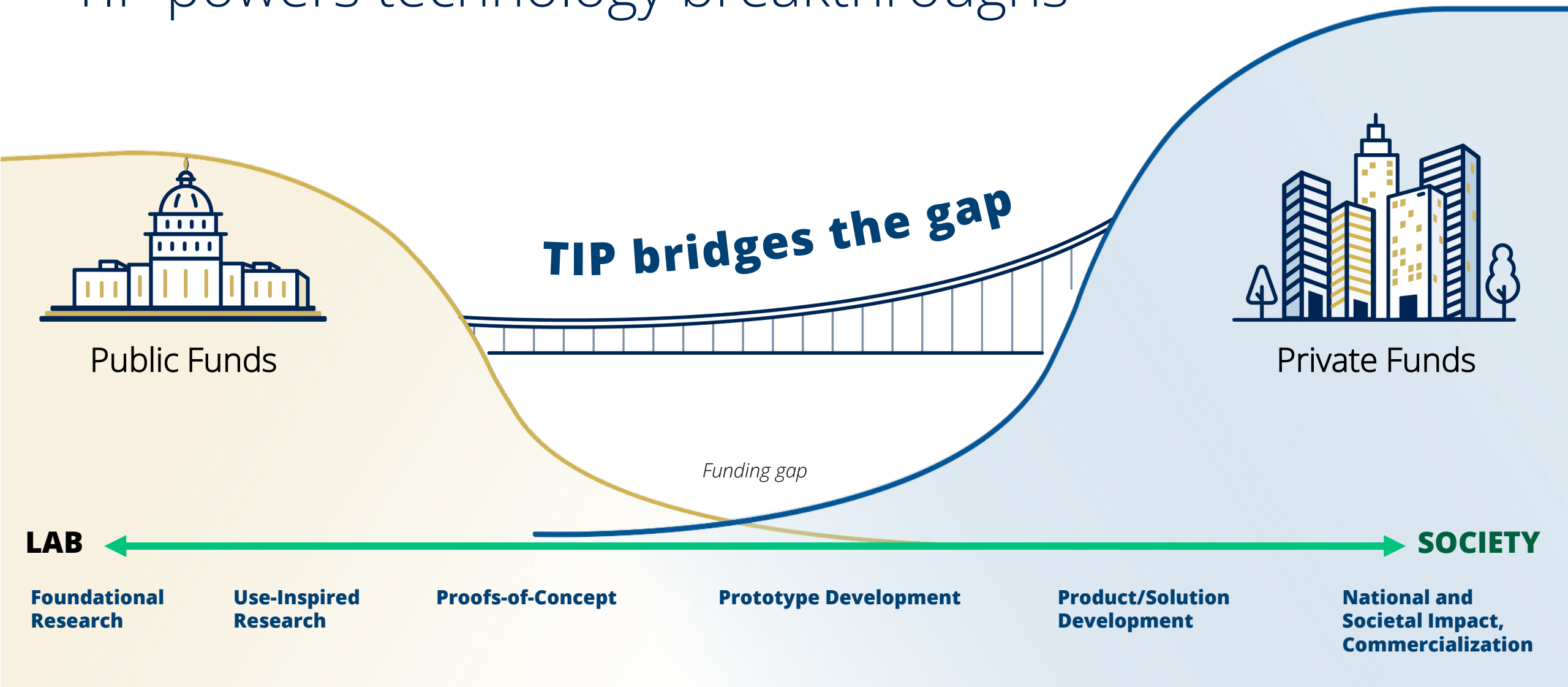
NSF TIP advances U.S. competitiveness and societal impact by nurturing partnerships that drive and accelerate:

Regional Innovation and Economic Growth

Technology Translation and Development

Workforce Development

TIP powers technology breakthroughs



Vision for the NSF PCL Test Bed program

- Accelerate laboratory science and discovery

  Support automated experiments with artificial intelligence (AI) in the loop to shorten experiment cycles and speed discovery

- Support programmable experiments

  Enable execution of bespoke, programmable laboratory workflows

- Provide remote access

  Remove geographic barriers and provide cloud-based access to laboratories including expensive, specialized instruments, to academia and industry

- Facilitate collaboration

  Establish, metadata, data, process, and AI standards to create a PCL ecosystem that facilitates collaborations

NSF TIP Workshops

https://events.mcs.cmu.edu/ac-sdl_workshop/

https://research.ncsu.edu/futurelabsworkshop/

A network of programmable cloud laboratories

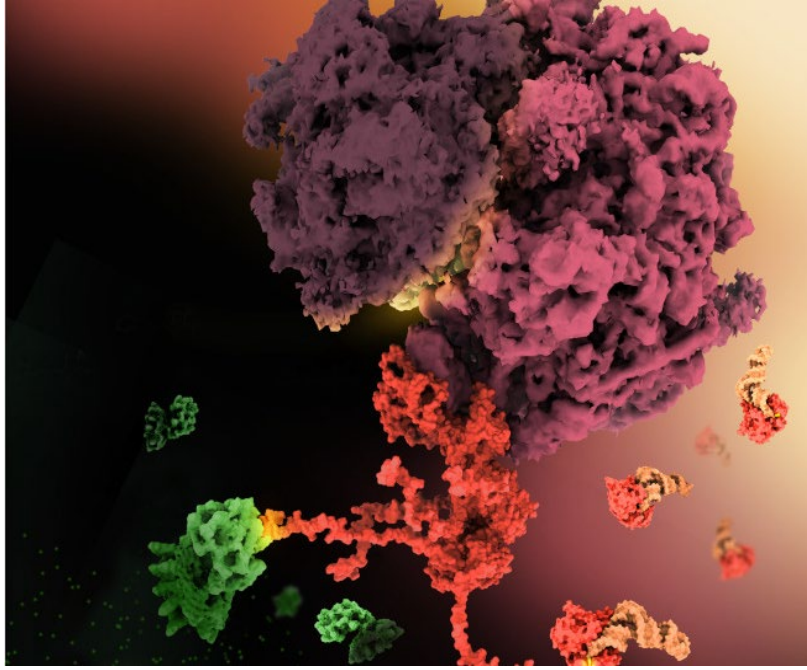
Individual PCL nodes are linked together via common experiment protocols, data standards, and AI tools

Common experimental design protocols, laboratory protocols, and metadata and data standards

Image credits: Argonne National Lab

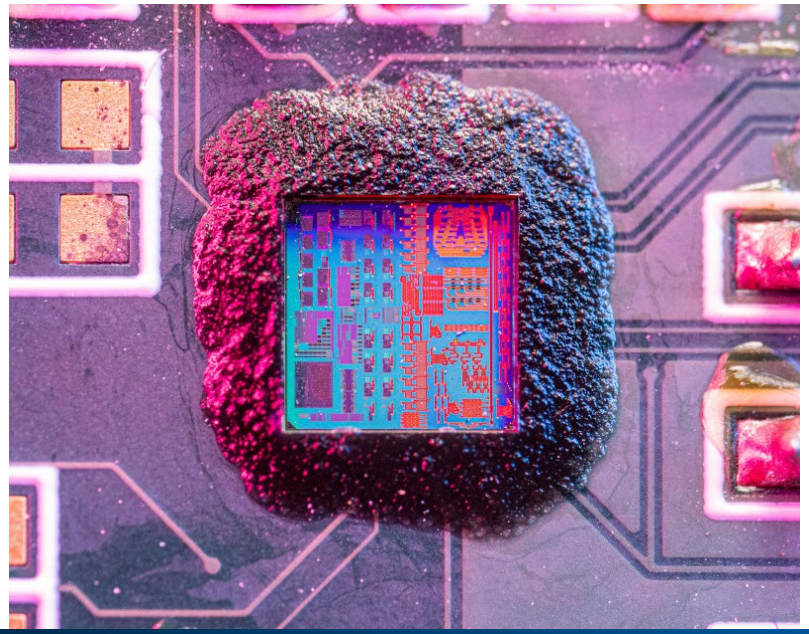
Accelerate scientific advancement

Each proposal should include a clear description of one or more specific science drivers that will provide a framework for the development of the PCL node

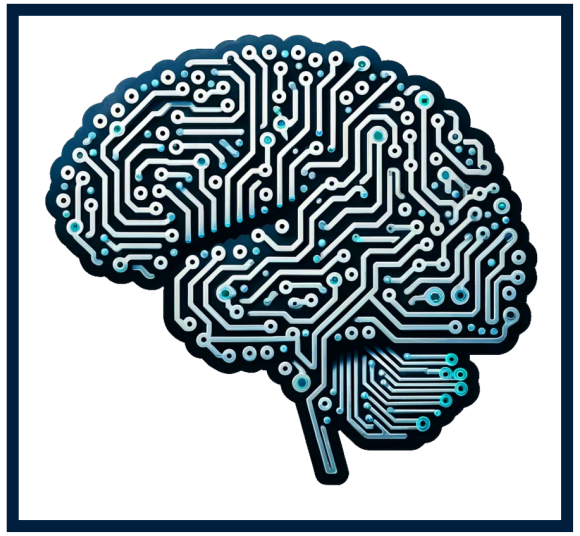


Example science drivers

- **Advanced materials:** materials science, materials synthesis and characterization
- **Biotechnology:** high-throughput characterization services for the bioeconomy supply chain

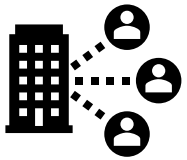


Data and AI Capabilities



- Demonstrated expertise in data management and curation and state-of-the-art AI methods.
- Creation of AI models to support the efficient and effective use of the node and Test Bed.
- Use of AI for coordination across nodes.

- Integrating AI with lab experiments at every stage to enhance precision, insight and impact:
  - Pre-experiment stage: Use AI to assist in designing optimal experimental setups or determine if AI can simulate outcomes to predict the most promising approaches.
  - Experiment stage: Use AI to monitor real-time data through sensors or imaging tools, control experimental conditions autonomously and make real-time adjustments to maintain accuracy or respond to anomalies.
  - Post-experiment stage: Use AI to recommend follow-up experiments or accelerate data analysis and visualization.



Node and Test Bed usage models

1. Power users.
2. High-throughput users.
3. First-time automated lab users.
4. Prototyping users.
5. Industry users.
6. Educational.
7. Research.

Eligibility

- Only organizations with *pre-existing instrument facilities* are eligible to apply to the program to be a PCL node.
- Proposals must include at least one **co-principal investigator** with relevant expertise in **data management and AI** to support the activities described in the proposal.
- Each PCL Node will be funded up to $5 million/year for four years, for a total budget not to exceed $20 million per PCL node.

Multi-institutional proposals: For projects involving a collaboration among multiple institutions, the proposal must be submitted by a **single lead institution** with funding for all other participating institutions made through **subawards**.

Proposals submitted as separately submitted NSF "collaborative proposals" as described under PAPPG Chapter II.E.3.b will be returned without review.

Types of organizations that can apply

- **Institutions of higher education (IHEs)** - two- and four-year IHEs (including community colleges) accredited in, and having a campus located in the U.S., acting on behalf of their faculty members.

- **For-profit organizations** - U.S.-based commercial organizations, including small businesses, with strong capabilities in scientific or engineering research or education and a passion for innovation.

- **Non-profit, non-academic organizations** - Independent museums, observatories, research labs, professional societies, community organizations, and similar organizations located in the U.S. that are directly associated with educational or research activities or that bring relevant expertise/perspectives

NSF review criteria

All NSF proposals are evaluated using the following two criteria:

- **Intellectual merit**: The intellectual merit criterion encompasses the potential to advance knowledge.
- **Broader impacts**: The broader impacts criterion encompasses the potential to benefit society and contribute to the achievement of specific, desired societal outcomes.

The NSF PCL Test Bed program has additional review criteria…

Additional Review Criteria

Science drivers. What science drivers will help transform the science/engineering areas, while driving the development of the PCL Node

Data and AI capabilities and expertise represented at the PCL Node.

Node capabilities. Include an In*strument Inventory Table,* node expertise, partnerships, access control, user recruitment plan, research security.

Cross-node collaborations. Collaborations may occur in a range of areas, e.g., metadata, data, and data sharing standards; AI model development and use.

Training and education. In areas represented by the science drivers, relevant AI, and test bed technologies.

New users/user communities. Plans for bringing in new users/user communities to the PCL Test Bed and automated science and engineering.

Metrics to evaluate PCL Node usage and user satisfaction.

Management plan. A strong management structure will be necessary to successfully execute on all the aspects of this project

Plan for post-award continued operation to establish a test bed that can sustain itself.

Budget preparation. Ensure budget covers all necessary aspect: node operations and resources, science driver support, data and AI support, on-boarding new users, any acquisition of new instruments and/or other lab resources, support for annual PI meeting

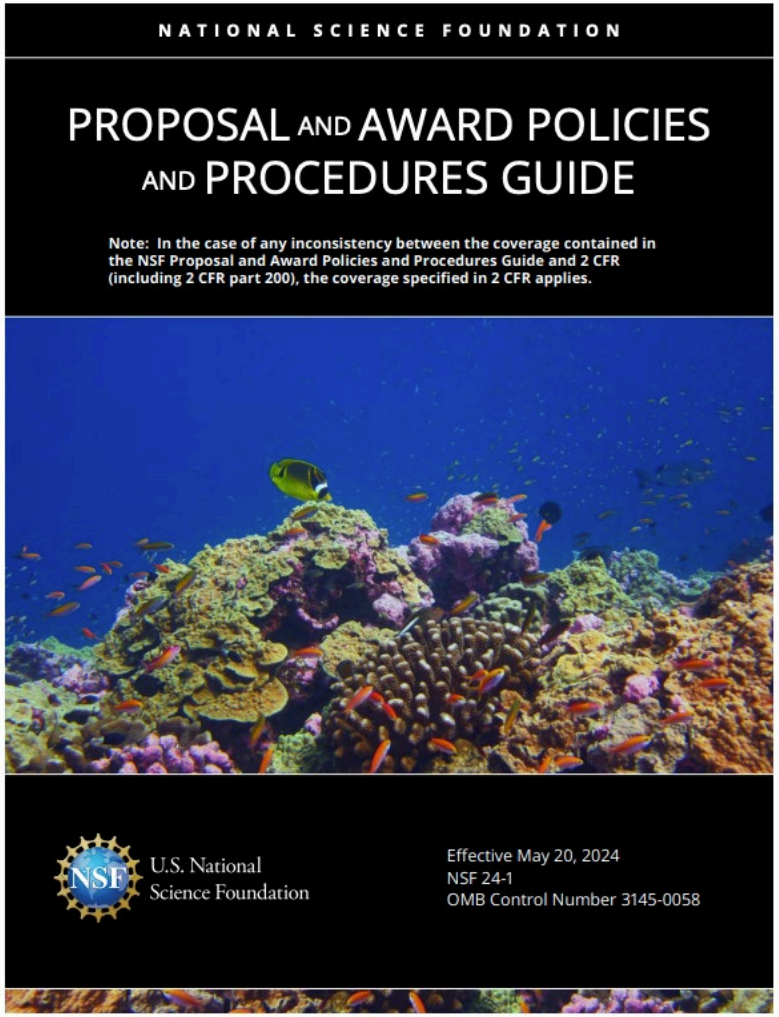
Details can be found in Section V. PROPOSAL PREPARATION AND SUBMISSION INSTRUCTIONS of the PCL solicitation

Be sure to review the PAPPG…

https://www.nsf.gov/policies/pappg/24-1

and additional guidance on NSF's priorities and executive order implementation

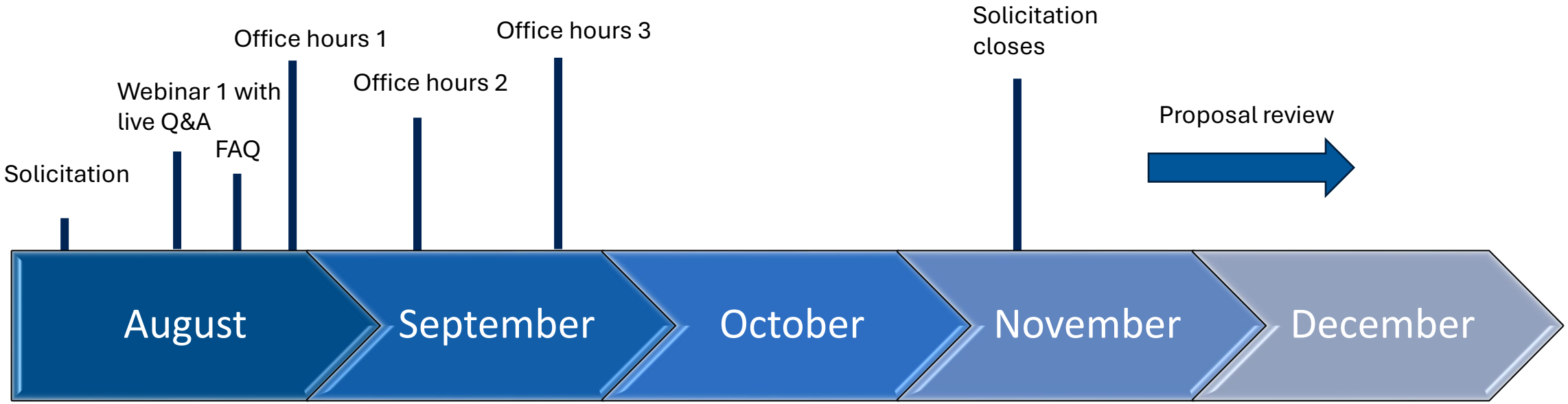
https://www.nsf.gov/executive-orders#information-for-proposers-611



Not able to propose but interested in being a reviewer for the NSF PCL Test Bed program?

Please reach out to pcl-testbed@nsf.gov with your name, organization, and information on your areas of expertise and we will be in touch!

Timeline


Solicitation
Webinar 1 with live Q&A
FAQ
Office hours 1
Office hours 2
Office hours 3
Solicitation closes
Proposal review
August
September
October
November
December

U.S. National Science Foundation
Directorate for Technology, Innovation and Partnerships

Questions?

Email: pcl-testbed@nsf.gov

Research.gov Help Desk e-mail: rgov@nsf.gov
Grants.gov Contact Center: e-mail: support@grants.gov

NSF PCL Test Bed

Outline (for planning)

- NSF/TIP intro (no need for NSF, right?)
- Overview of the program
  - How this fits into TIPs larger goals + building on NSCEB and MGI
  - Summary of workshops
  - Long term vision for investment – ecosystem development – networking across systems
- Program specifics
  - Who is eligible?
  - PCL Node v Testbed
  - Science drivers
  - AI/ ML/ data
  - Outreach to users

- Merit review and selection
- Timelines

including office hours

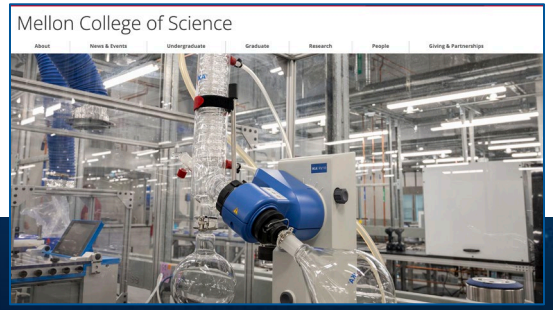
A New “Horizontal”: Strengthen, Scale Use-Inspired and Translational Research

Integrative Activities

International Science & Engineering

Context

- **National Academies of Science, Engineering, ad Medicine** Workshop on AI and Automated Laboratories for Biotechnology: Leveraging Opportunities and Mitigating Risks, **March 2024**: Emerald Cloud Lab: Remote Controlled Life Sciences Lab, emeraldcloudlab.com.
- **Nature Synthesis, June 2023**: The rise of self-driving labs in chemical and materials sciences, Abolhasani & Kumacheva.
- **Argonne Labs, April 2023**: Argonne's self-driving lab accelerates the discovery process for materials with multiple applications.
- **Nature, June 2022**: Cloud labs: where robots do the research, A host of companies provide a remote, automated workforce for conducting experiments around the clock.
- **NASEM, Nov 2022**: Autonomous Materials Discovery and Optimization: A DMMI Workshop.



Analogy to Early Supercomputer Center

- Capability computing → Capability Experiments
  - Use the full capabilities of the resource to solve the largest and most demanding problems.
- Capacity computing → Capacity Experiments
  - Using efficient cost-effective computing power to solve a few somewhat large problems or many small problems
- Vendor embedding
  - Early supercomputer centers “embedded” vendor technical staff at the centers, e.g., Cray, IBM, Sun, SGI, …
- Technical papers. Early supercomputer staff wrote papers on low-level performance of the machines, e.g.,
  - Moore, Reagan W., "UNICOS Performance Dependence on Submitted Workload," Proceedings, Twenty-seventh Semiannual Cray User Group Meeting, London, Great Britain (April 1991).
  - Schroeder, Wayne, Michael Wan, "Experience with the UNICOS 6.1 Memory Scheduler," Proceedings, Twenty-ninth Semiannual Cray User Group Meeting, Berlin, Germany (April 1992).
- Vendors conducted annual User Groups meetings, e.g., CUG, IBM, SGI, …

The Vision: Programmable Cloud Labs

- **Accelerate data collection and discovery:** remote bespoke high-throughput experiments will expedite data collection across a range of field
- **Enable self-driving experiments**: automated laboratories will allow for the incorporation of AI into experimental planning
- **Reduce geographic barriers:** experiments requiring expensive and specialized instruments will be accessible throughout the country to support cutting edge research
- TIP Workshops
  - Workshop on Creating a National Network of Cloud and Self-Driving Labs, October 23-25, 2023, CMU, Pittsburgh PA
  - Foundation for Unmanned Technological Utilization, Research, and Exploration (FUTURE) Lab Workshop, January 11-12, 2024, NCSU, Raleigh, NC