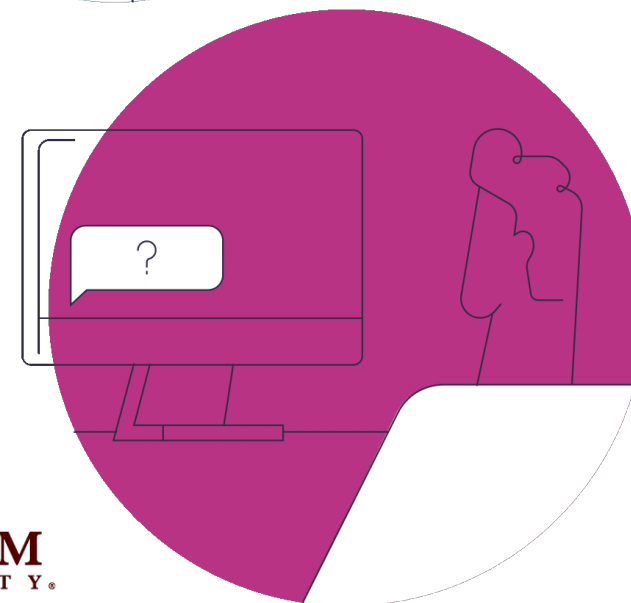
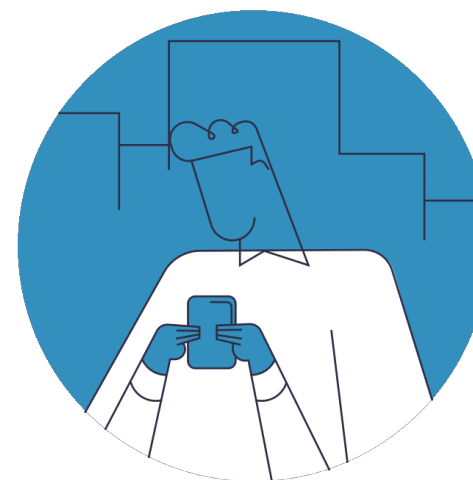


GOODLUCK: A Deeper Dive

Julie Ma, Dhruva Chakravorty

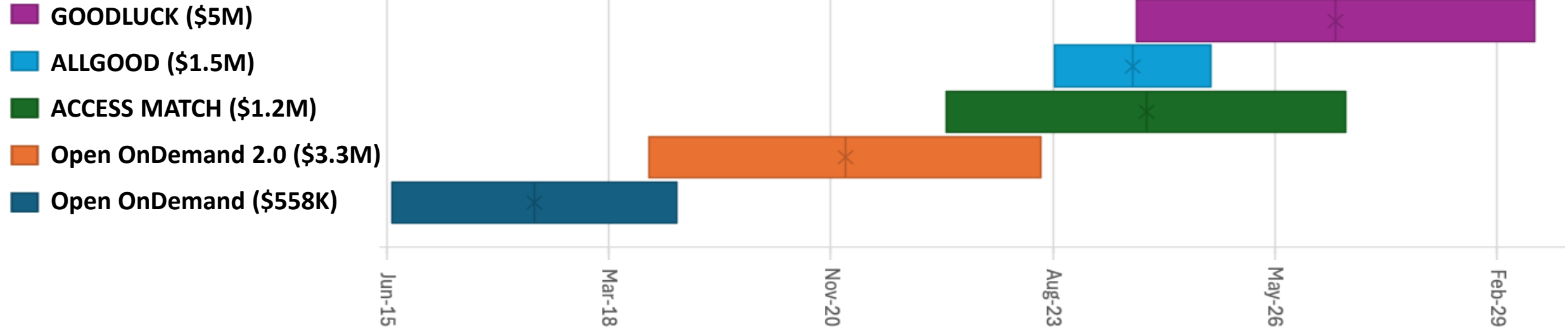
Lissie Fein, Alan Sussman, Karen Tomko



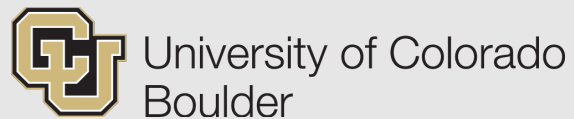
NSF Funding History



OPEN nDemand



COLLABORATORS

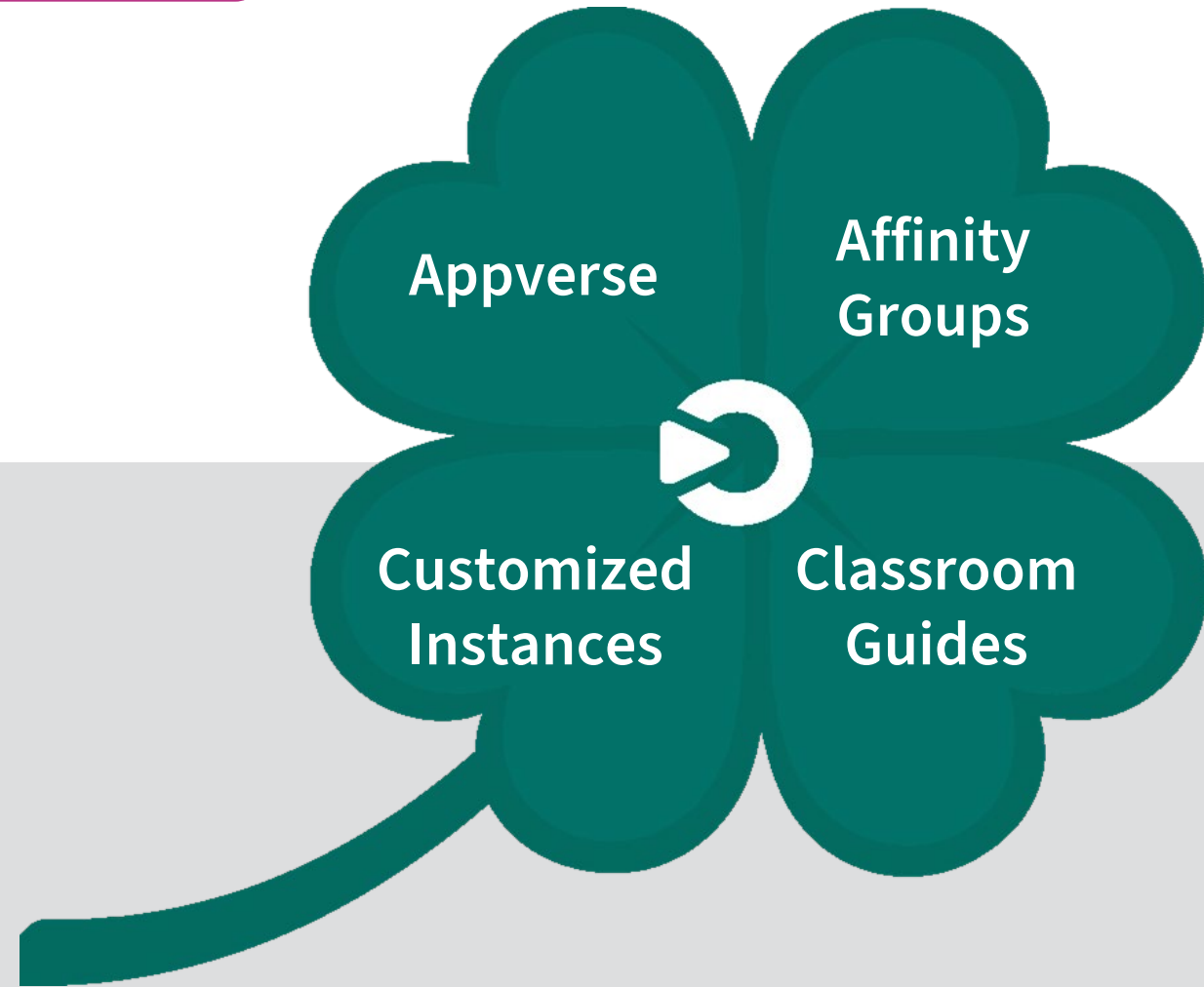


openondemand.org/history

GOODLUCK

Growing Open OnDemand: Leveraging Unified Community Knowledge

Domain solutions for the sciences,
engineering & education



Project Summary

Growing Open OnDemand: Leveraging Unified Community Knowledge (GOODLUCK)

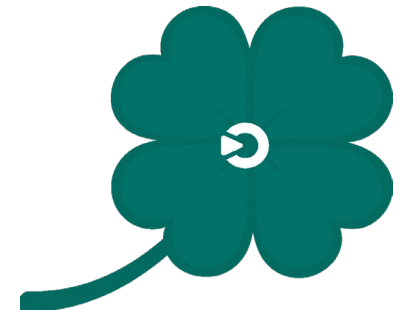
Provide tools and processes for researchers to enhance Open OnDemand use, analysis, and result sharing.

Intellectual Merit

- Service providers will provide scalable and accessible resources with a low barrier to entry
- Researchers, industry professionals, and students will tackle diverse science and engineering challenges
- Open OnDemand enables new opportunities, and accelerates scientific innovation

Broader Impacts

- Broader resource adoption across science domains and underrepresented communities
- Improved collaboration/consistency among researchers conducting “team science”
- Engagement with students (future clients of service providers)



Initial Science Drivers

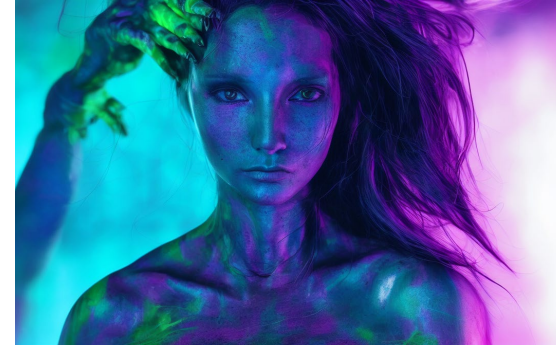
Proposed Focus Areas for Year 1



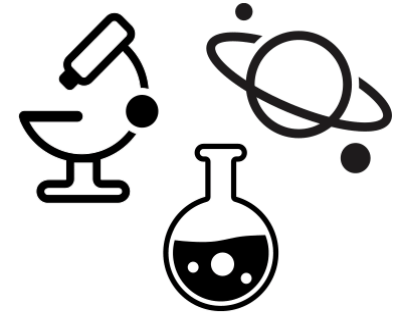
**Cryo-EM
(MGHPCC POC)**



**Alloy Discovery
(Texas A&M – POC)**



**Art Design
(OSC POC)**



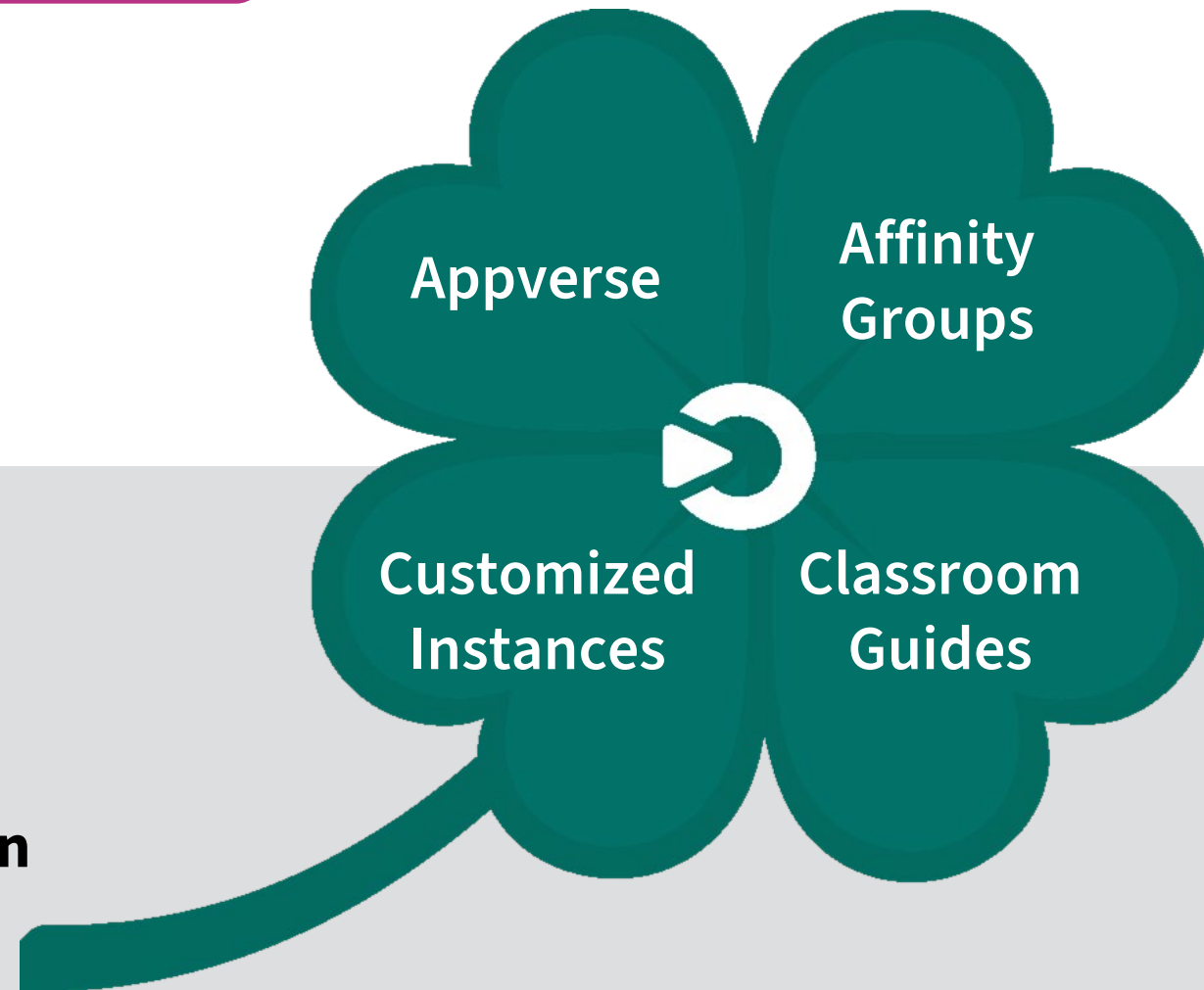
**Rotorcraft Development
(UMD POC)**

GOODLUCK Community

Growing Open OnDemand: Leveraging Unified **Community** Knowledge

Community input is key to our efforts!

Shamrock highlights strategies and mechanisms to facilitate your participation



Five year NSF award #2411375



Supercomputer
Center



TEXAS A&M
UNIVERSITY



UNIVERSITY OF
MARYLAND

Leadership Team



**Alan
Chalker**

**Ohio
Supercomputer
Center**

*Project direction
& oversight*

Customization



**Dhruva
Chakravorty**

**Texas A&M
University**

Appverse



**Julie
Ma**

**Massachusetts
Green High
Performance
Computing
Center**

Community



Alan Sussman

**University of
Maryland**

Customized
Instances



Karen Tomko

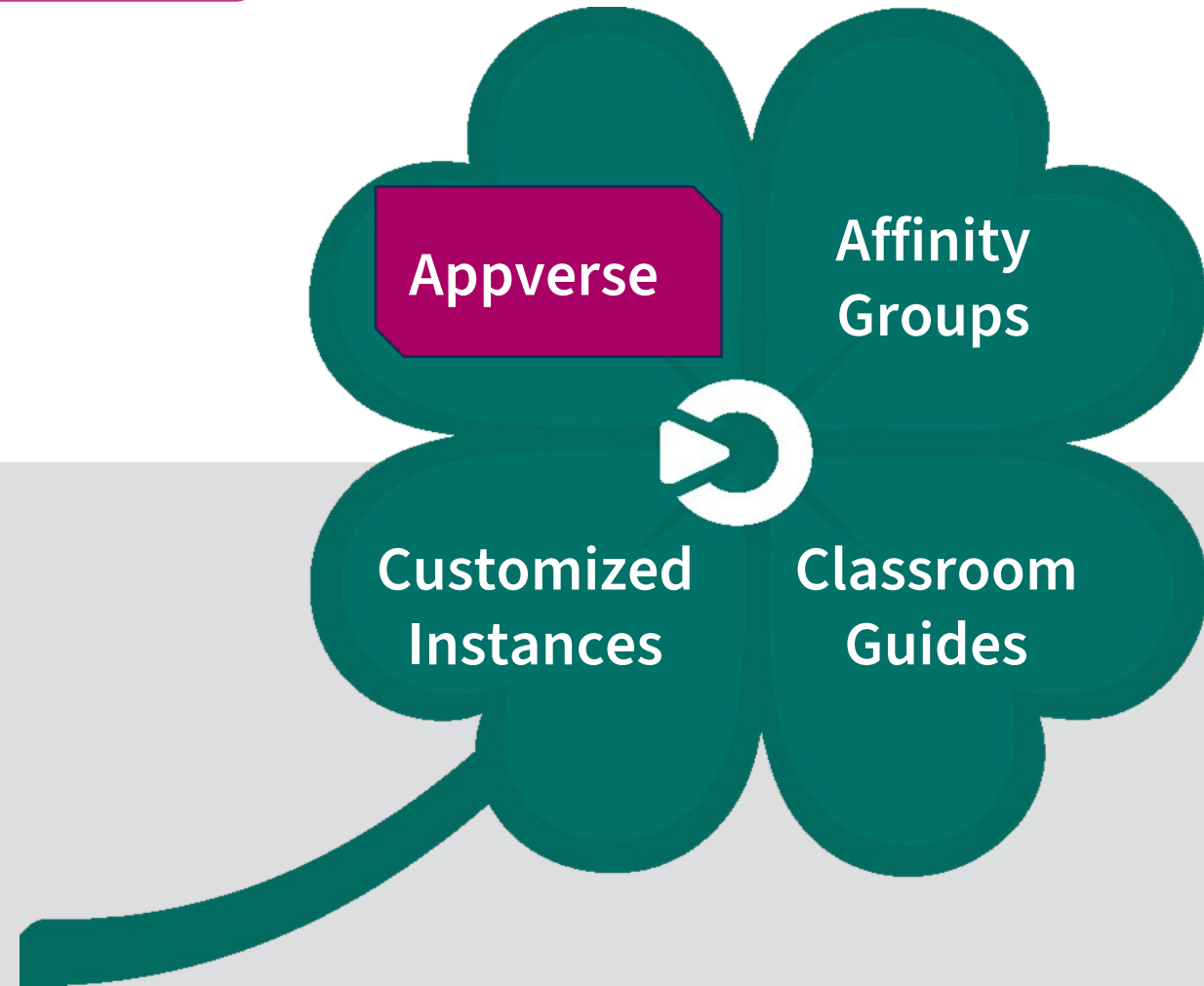
**Ohio
Supercomputer
Center**

Classroom

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Domain solutions for the sciences,
engineering & education



The OOD Appverse

Apps for scientific applications by developers, and researchers

KEY FEATURES

- Build and share apps for your OOD instance (GitHub)
- Central repository for apps
- Apps can be for research or IT functions
- Tiered structure - validated and sponsored apps
- Curation process – maintenance, updates, and training
- AI app integration
- Affinity Groups will publicize the Appverse



Stable Diffusion
System Installed App



Classroom Jupyter
System Installed App



Classroom RStudio
System Installed App



Blender
System Installed App



QGIS
System Installed App



IQmol
System Installed App



Jupyter + Spark
System Installed App

Sessions to watch out for

3/20 Thursday at 1130 AM

"Using a Passenger App for Displaying GPU Node Configuration and Resource Availability"

Michael Dickens

<https://cfp.openondemand.org/2025/talk/M3EWSU/>



3/20 Thursday at 12 PM

"Drona Workflow Engine"

Marinus Pennings

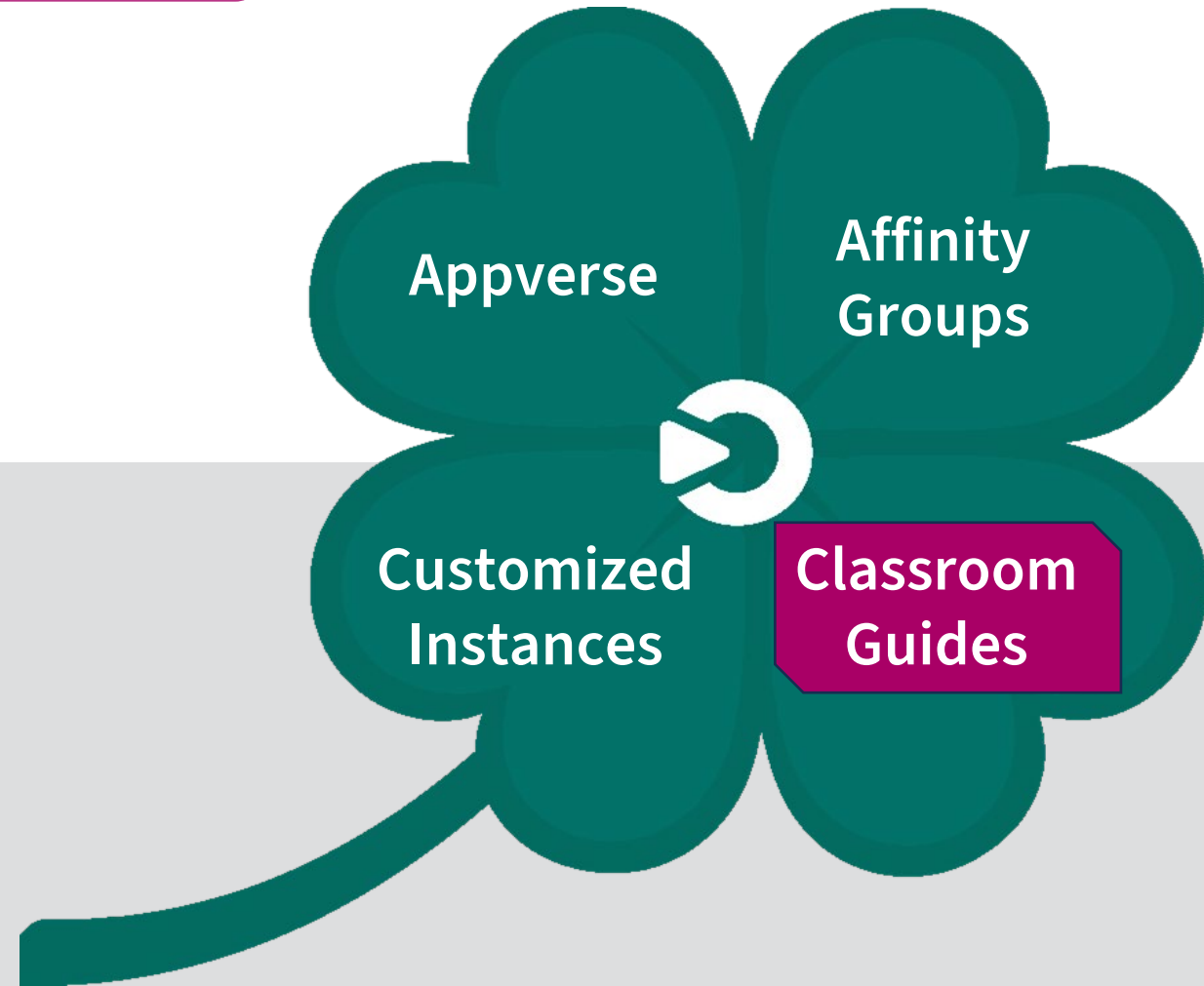
<https://cfp.openondemand.org/2025/talk/8XZYTIX/>



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Domain solutions for the sciences,
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Classroom Guides

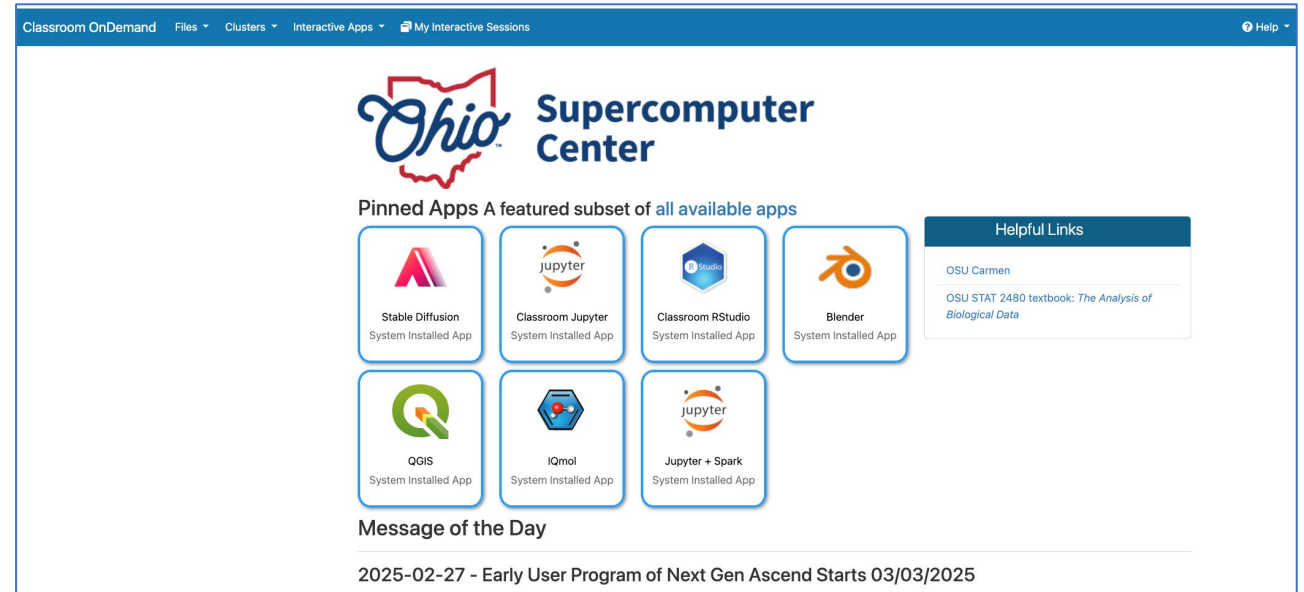
Resources for supporting classroom use of shared CI

Requirements for classroom

- Intuitive user interface
- Access from anywhere
- Responsiveness
- Scalability
- Repeatability

OSC's Approach

- OOD customizations
- Kubernetes managed resources
- Processes to customize allocation/project setup
- Processes and tools for creating isolated software environments
- Support for file sharing and homework submission



OSC's class.osc.edu

Challenge: Generalizing OSC's approach for broader adoption

General OOD configuration

App customizations

- BC apps for Jupyter, Rstudio
- Entries in cluster.d/cluster.yml

Kubernetes managed resources

- Jupyter and Rstudio sessions
- Supports interactive use during class
- Resources based on configuration in cluster.yml

OSC specific processes and tools

Processes to customize allocation/project setup

- Classroom intake process to gather input for customizations
- Self service account creation for students

Processes and tools for creating isolated software environments

- Documentation and scripts to setup custom environments
- Managing paths to isolate environments in student and instructor accounts

Support for file sharing and homework submission

- Instructor scripts for creating submission directory
- Student scripts for copying homework

Classroom Guides

More details:

“Managing the software environment for a
classroom deployment of OOD”

Wednesday at 10:00am

Belfer Case Study Room

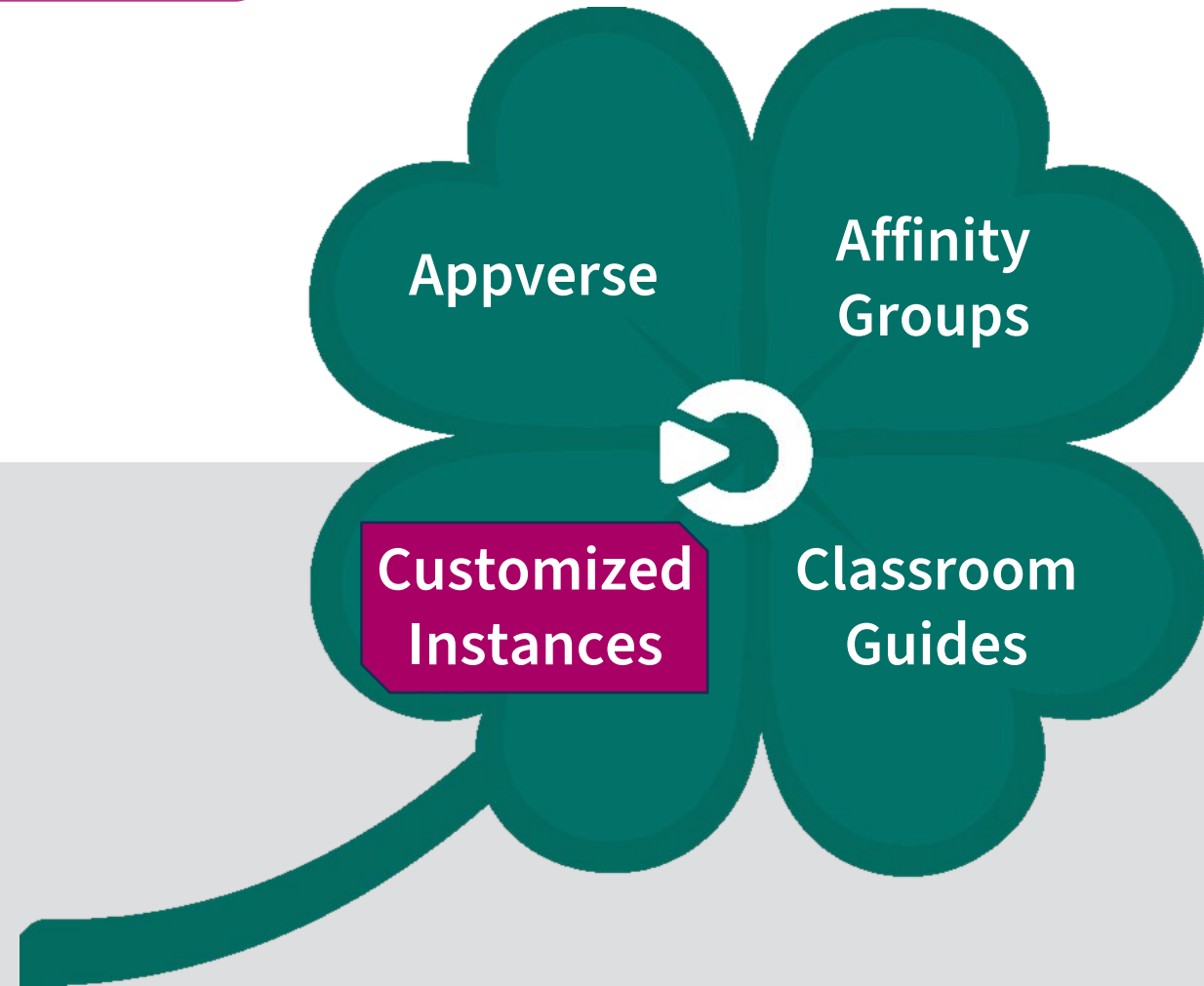


<https://cfp.openondemand.org/2025/talk/TGUZM9/>

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Customized Instances

Challenge: Enabling groups of users to create customized instances of OOD

For groups of researchers and for classroom use

Within a group of researchers (e.g., a faculty member's research group)

- Share applications, workflows, etc. (from Appverse or developed locally) through your OOD instance
- Without sysadmin intervention or privileges

For a class, workshop, tutorial, hackathon, etc.

- Enable a faculty member, or a presenter, to share applications with a set of students or attendees

Initial effort is to develop and disseminate *Project Manager* functionality within OOD

- Focus on one application partner, test new functionality within a moderate sized research group
- Both simulation and data analysis tools developed and used within the group

Customized Instances

Application focus areas include

- Cryogenic electron microscopy (MGHPCC) – viral action mechanisms
- Materials science – alloy discovery and design (TAMU)
- Art design using generative AI (OSU)
- Rotorcraft design – drone design via CFD and structural dynamics (UMD)
- Talk to us if you are interested in testing this functionality in the not-too-distant future

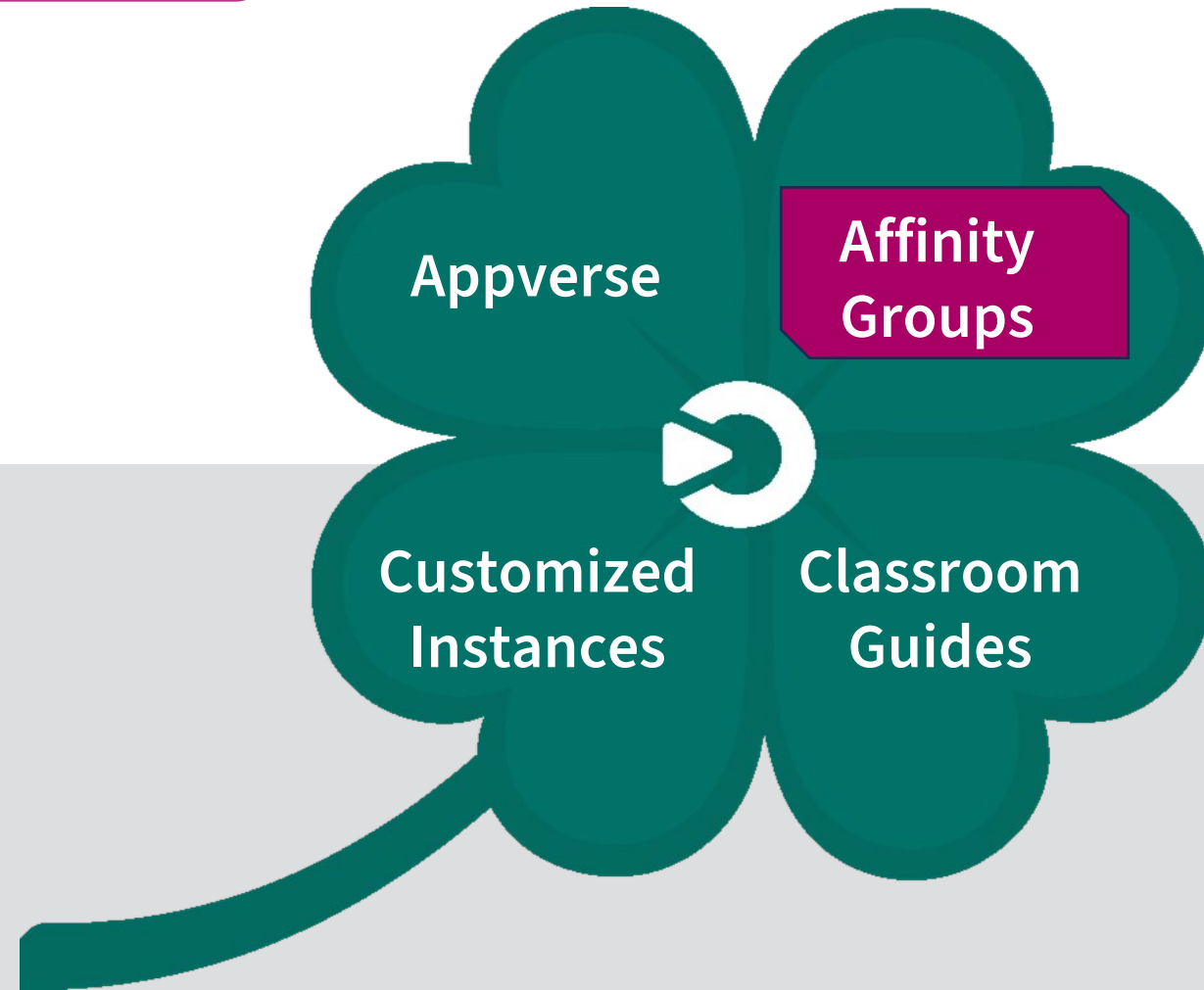
Long term area goals

- Integrated sets of tools, documentation, and training materials that researchers and educators can select from and use as templates to create an OOD environment tailored to their needs

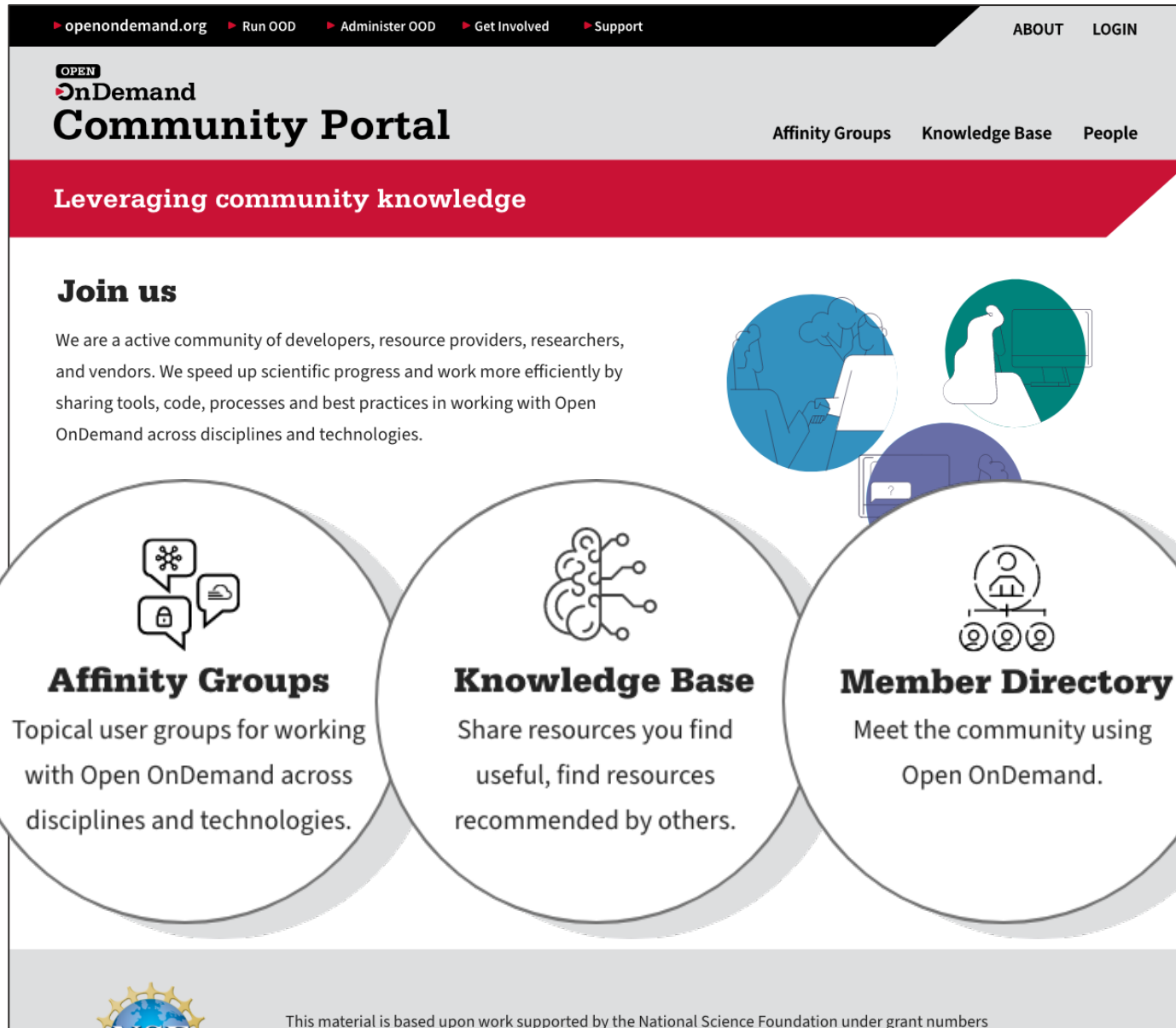
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Community Portal



The screenshot shows the Open OnDemand Community Portal homepage. At the top, there's a navigation bar with links: openondemand.org, Run OOD, Administer OOD, Get Involved, Support, ABOUT, and LOGIN. Below this is the 'OPEN OnDemand Community Portal' header. A red banner reads 'Leveraging community knowledge'. The main content area features a 'Join us' section with a paragraph about the community. Below this are three large circular icons representing 'Affinity Groups', 'Knowledge Base', and 'Member Directory', each with a brief description. The footer includes a small globe icon and a disclaimer about NSF funding.

openondemand.org Run OOD Administer OOD Get Involved Support ABOUT LOGIN

OPEN
OnDemand
Community Portal

Affinity Groups Knowledge Base People

Leveraging community knowledge

Join us

We are a active community of developers, resource providers, researchers, and vendors. We speed up scientific progress and work more efficiently by sharing tools, code, processes and best practices in working with Open OnDemand across disciplines and technologies.

Affinity Groups
Topical user groups for working with Open OnDemand across disciplines and technologies.

Knowledge Base
Share resources you find useful, find resources recommended by others.

Member Directory
Meet the community using Open OnDemand.

This material is based upon work supported by the National Science Foundation under grant numbers

Newly launched—features will be rolling out:

- New Affinity Groups
- Events, Announcements, & Community Badges
- Integrating the Appverse, Customized Instances, and Classroom content

ondemand.connectci.org

Affinity Groups

Affinity Groups are a place to connect with the community on topics related to Open OnDemand.

KEY FEATURES

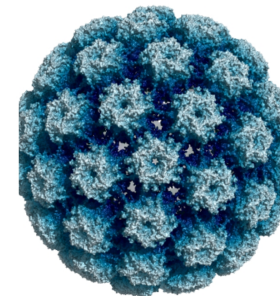
- Links to Communication channels (Discourse, GitHub, etc.)
- Central repository for documentation, code samples, tutorials, and other resources
- Optional member email lists and place for recommended infrastructure
- Announcements, events, and trainings

Flexible usage: Groups can be short or long term, and they can be primarily repositories or include active discussion.

Remote Instrumentation

This affinity group serves as a central hub for those using OnDemand with Remote Instrumentation. Joining this group will keep you updated with news, announcements, and events related to Remote Instrumentation with Open OnDemand.

Cryo-electron microscopy (cryo-EM) is rapidly becoming a key tool for studying the molecular architecture of cells, viruses, and protein assemblies. Advances in microscope design, image processing, and automation are making cryo-EM faster, more precise, and capable of resolving a wider range of biological structures. Combined with techniques like X-ray crystallography and NMR, cryo-EM is now enabling atomic-resolution models of complex molecular assemblies.



[Join](#) [Slack](#) [Q & A](#) [GitHub](#)

Collapse All

Knowledge Base Resources

NAME	TAGS	TYPE
CryoSPARC Guide	ERN PEARC	Documentation
The ERN Cryo-EM Federated Instrument Pilot Project	ERN PEARC	Publication
Ecosystem for Research Networking develops platform for remote scientific instrument control	ERN OnDemand federated-instrument	Article


See ALL


Discourse Recent Topics

QUESTION	LAST UPDATE
CryoSparc OOD Application	2/25/25
Reverse proxy response body substitution?	1/19/25

See All

Community

 **Shania France**
UMass Amherst

 **Tamara Smiths**
Lawrence Livermore

Member Email List

cryoem@lists.connectci.org 

No emails

Upcoming Events

3/18/25 - 3/20/25
GOOD 2025: Global Open OnDemand Conference
04/03/25 1:00 PM EST
Open OnDemand Tips and Tricks Call

ALL EVENTS

Announcements

01/10/25
Ecosystem for Research Networking develops platform for remote scientific instrument control with Open OnDemand

01/10/25
Ecosystem for Research Networking develops platform for remote scientific instrument control with Open OnDemand

ALL ANNOUNCEMENTS

Affinity Group Coordinators

Each Affinity Group needs two or more Coordinators.

Time commitment is minimal and includes:

- Moderating knowledge base content
- Communication via slack, email, discourse, or zoom
- Attending best practices meetings during office hours, initially monthly, and then quarterly.



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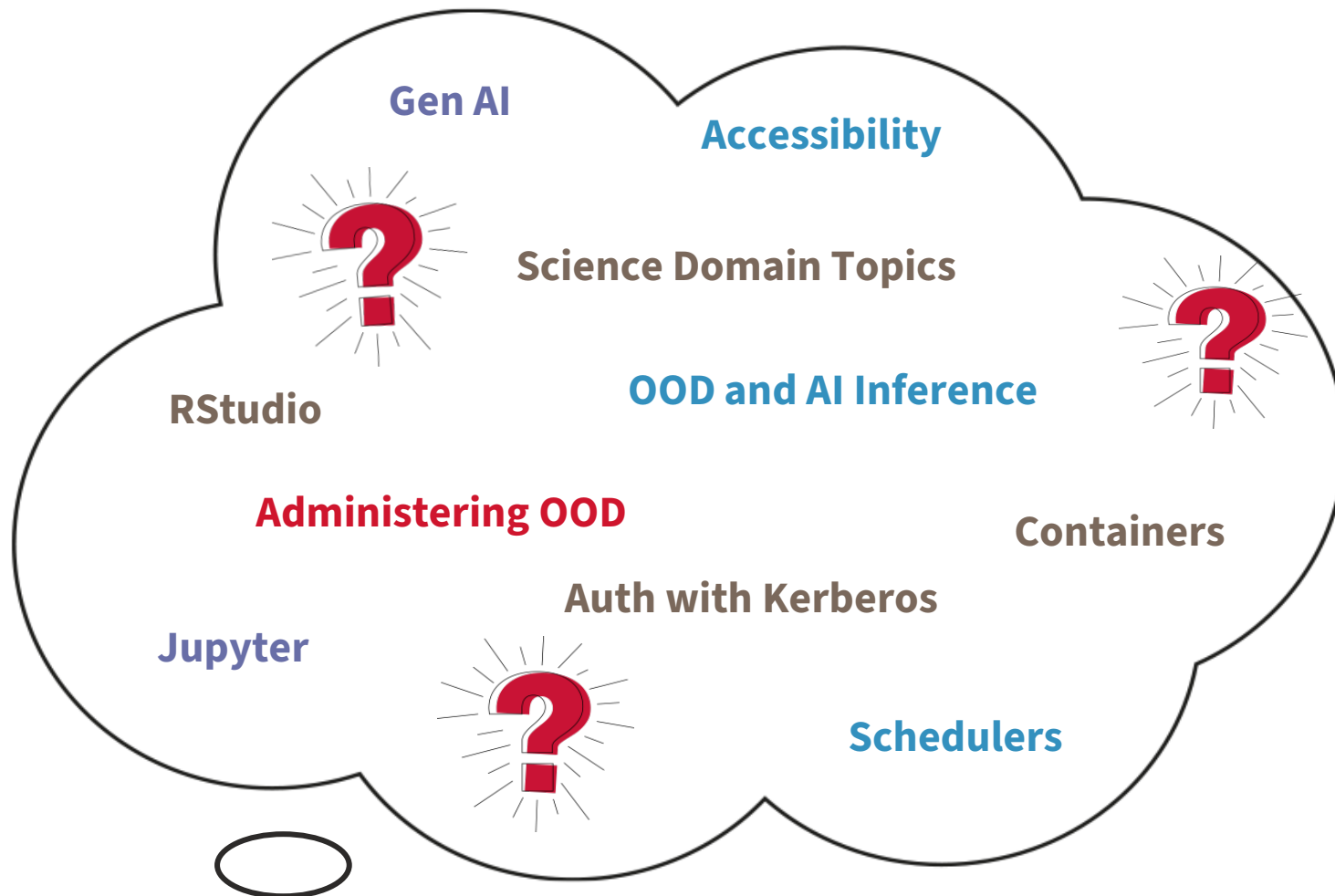
Get the Cap!



While supplies last—
coordinators of active
Affinity Group will get the
Open OnDemand Cap at
PEARC25

Affinity Groups Topics

Add your ideas for groups to Menti



Affinity Group Next Steps

Goal: Choose the first set of affinity groups to ensure a GOOD start!

1. Poll Interest

Tomorrow morning we will release a google doc with the affinity group ideas from Menti. People can indicate interest in membership or being a coordinator. (this will NOT be a firm commitment)

2. Create New Groups

We will create affinity groups for ideas that have at least two coordinators and five interested people.

Login to the Portal

Login

Create an account or use a Campus Champions, CCMNet, or ACCESS-CI account



Create your Profile

Add your skills and interests

Set your Password

For new accounts, use the **Edit Community Persona** button to set your password

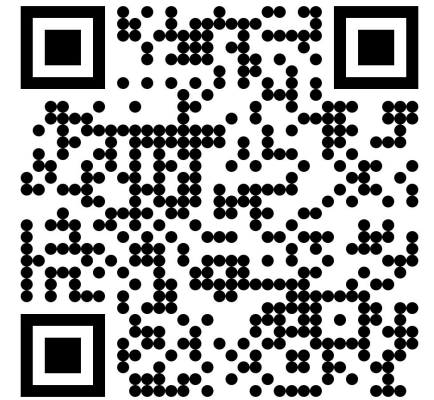
Vote for Affinity Groups



Lots of great ideas, but we need your input to go forward.

Go to the Google Sheet with Affinity Group ideas and mark which ones you are interested in. Add your name if you could be a coordinator.

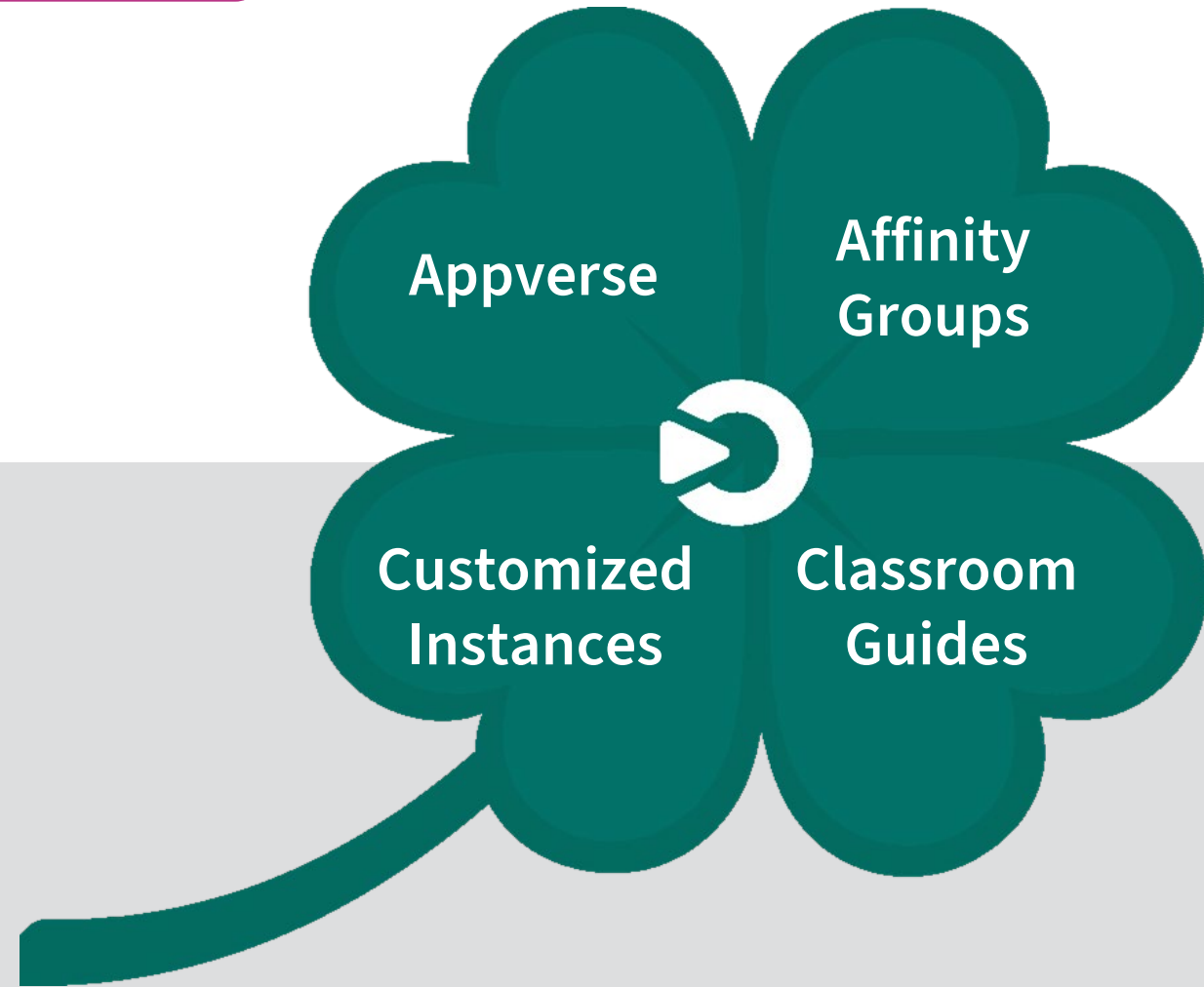
**New Community Portal
where Affinity Groups
will live**



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Domain solutions for the sciences,
engineering & education



GOODLUCK Year 1 Goals

- Project Management Framework
 - Community Meeting
 - Community Management Portal Pilot
-
- Appverse Pilot
 - Classroom Guide Framework
 - Affinity Groups Pilot
 - Customized Instance Pilot



Questions

Your input and feedback is requested!

Appverse (Dhruva)

- What should the app verification process consider?
- How will apps on the Appverse be supported?
- What mechanisms will support different fields of science?

Customized Instances (Alan)

- What are your pain points in deploying applications through OOD?
- What types of applications would you like to share with other users?

Questions

Classroom (Karen)

- What are your pain points with respect to supporting classroom use?
- Have you created any custom apps for classroom use?
- What are the emerging needs in classroom support?

Affinity Groups (Lissie)

- How can Affinity Groups help your work?
- What Affinity Group features will be helpful for you?
- Are there Affinity Groups you would coordinate?

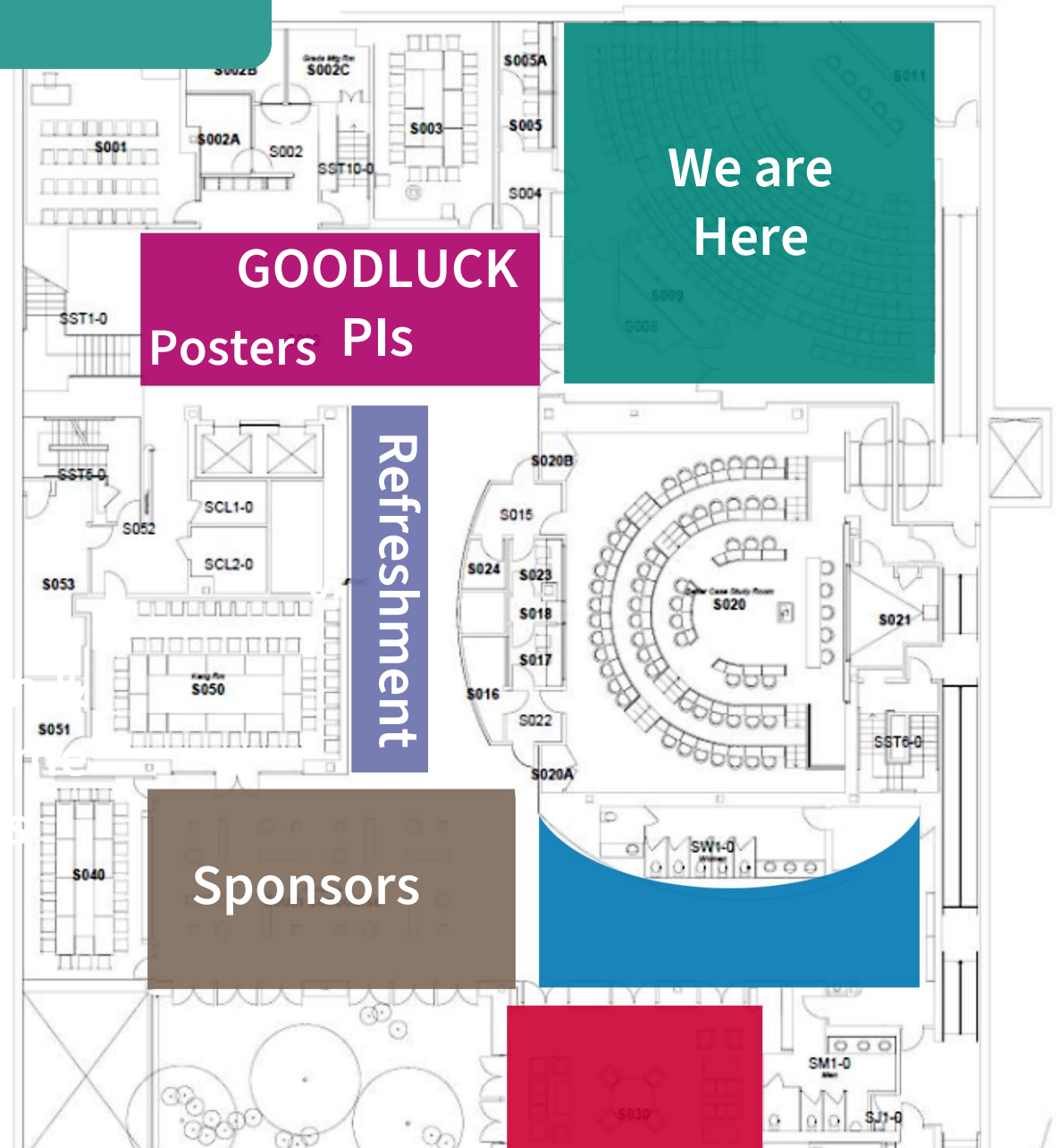
Idea Marketplace

Enjoy Refreshments

Discuss ideas with the
GOODLUCK Team

Visit the Poster Gallery

Meet our Sponsors



Reminder



Wednesday - Fenway Social

6-9:30 pm

Backstage tour

Ballpark-themed food and beverages

Buses leave from CGIS (here) at 6pm sharp and return starting at 8:45pm

Thank You!

See you out there!

