Connecting people and resources to accelerate discovery by empowering the science gateway community

SGCI

Science Gateways Community Institute: Subsidized Services and Consultancy to Facilitate Research on Your Campus

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Award Number
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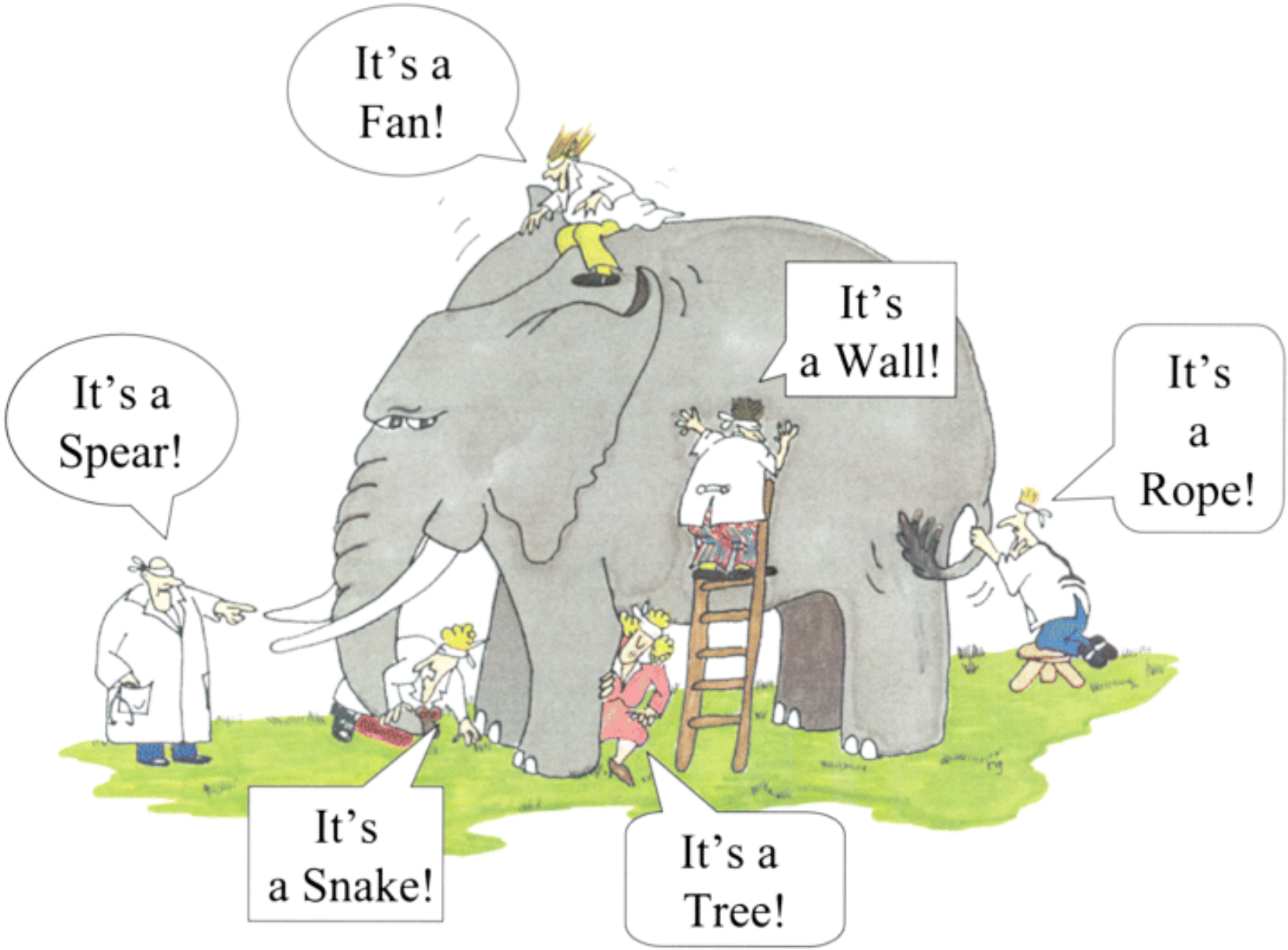
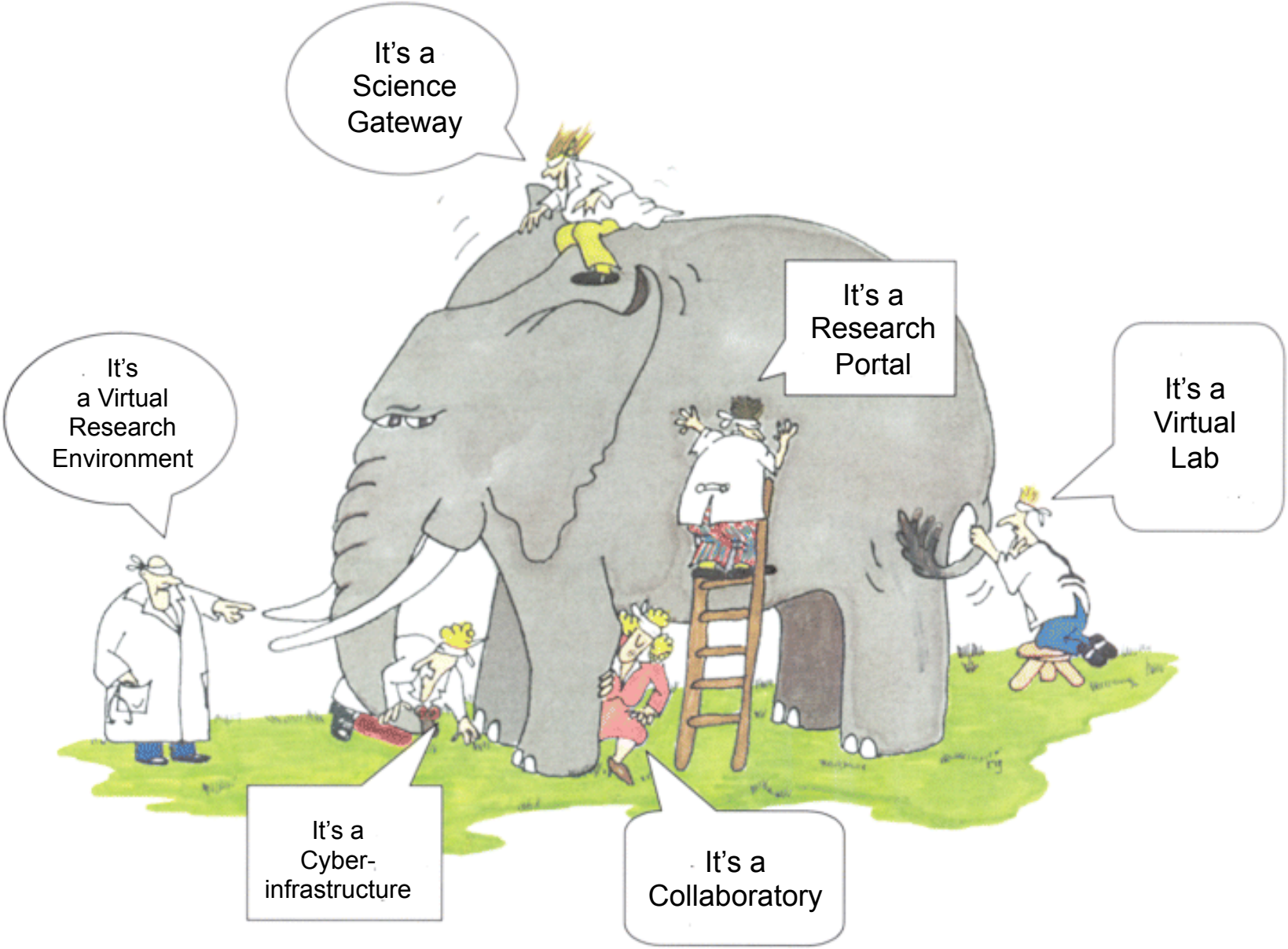
Science Gateways

- Increased complexity of
  - today's research questions
  - hardware and software
  - skills required
- Greater need for openness and reproducibility
  - Science increasingly driving policy questions
- Opportunity to integrate research with teaching
  - Better workforce preparation

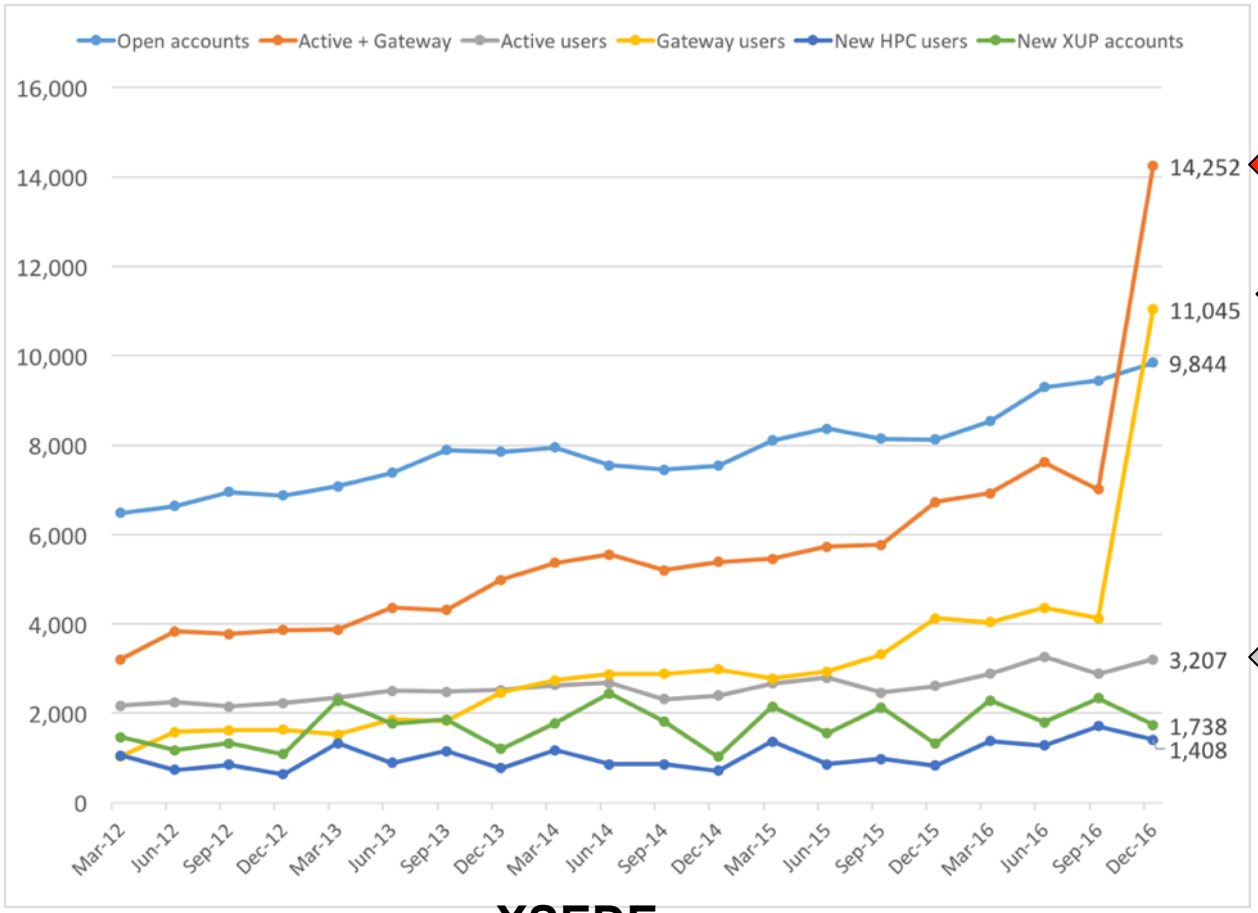
We need end-to-end solutions that provide ***broad access*** *to advanced resources and allow* ***all*** *to tackle today's challenging science questions.*

SGCI


It's a Fan!
It's a Spear!
It's a Wall!
It's a Rope!
It's a Snake!
It's a Tree!


It's a Science Gateway
It's a Research Portal
It's a Virtual Lab
It's a Virtual Research Environment
It's a Cyber-infrastructure
It's a Collaboratory

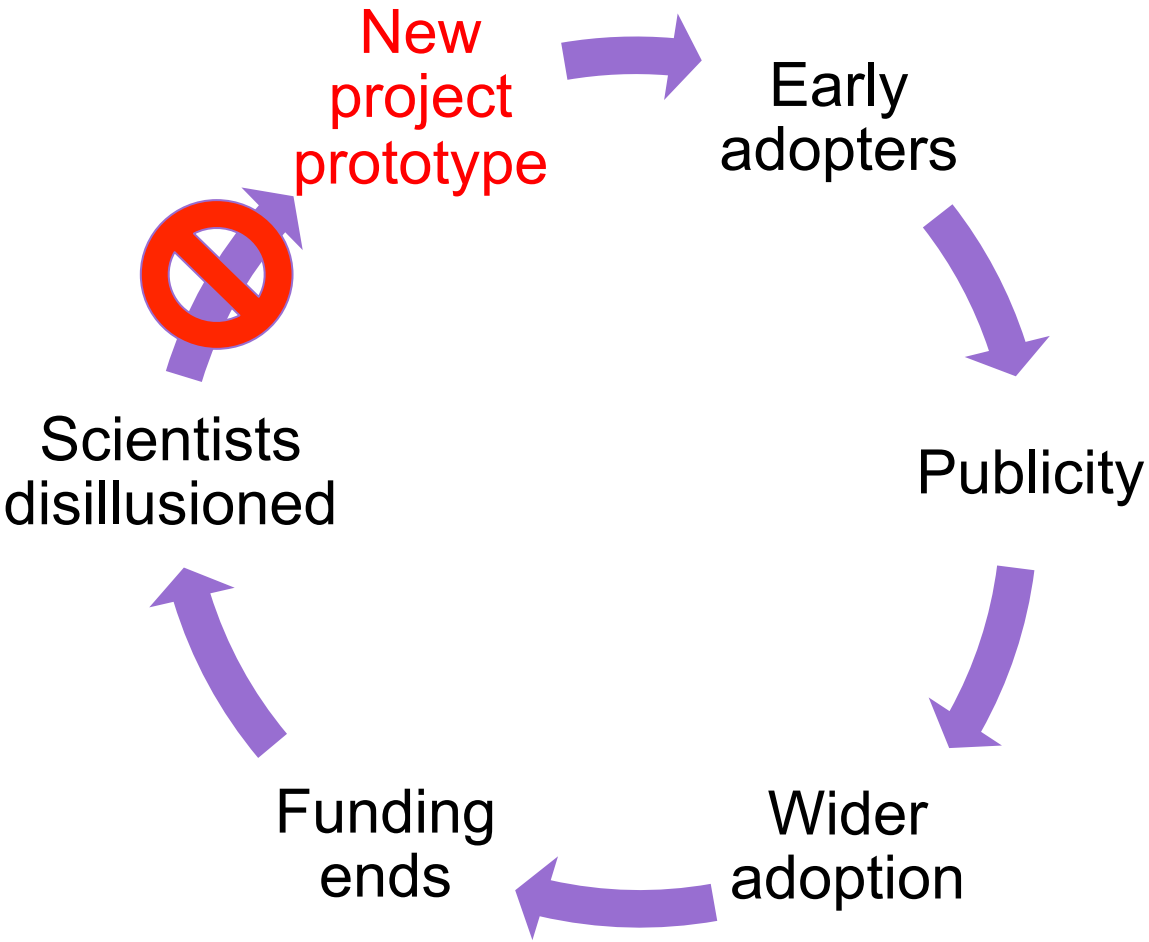
Gateway users are 77% of active XSEDE users in Q4 2016



XSEDE users

This is largely due to the CIPRES and I-TASSER gateways, but others are gaining

Typical Lifecycle of a Science Gateway



Science Gateways Survey 2014

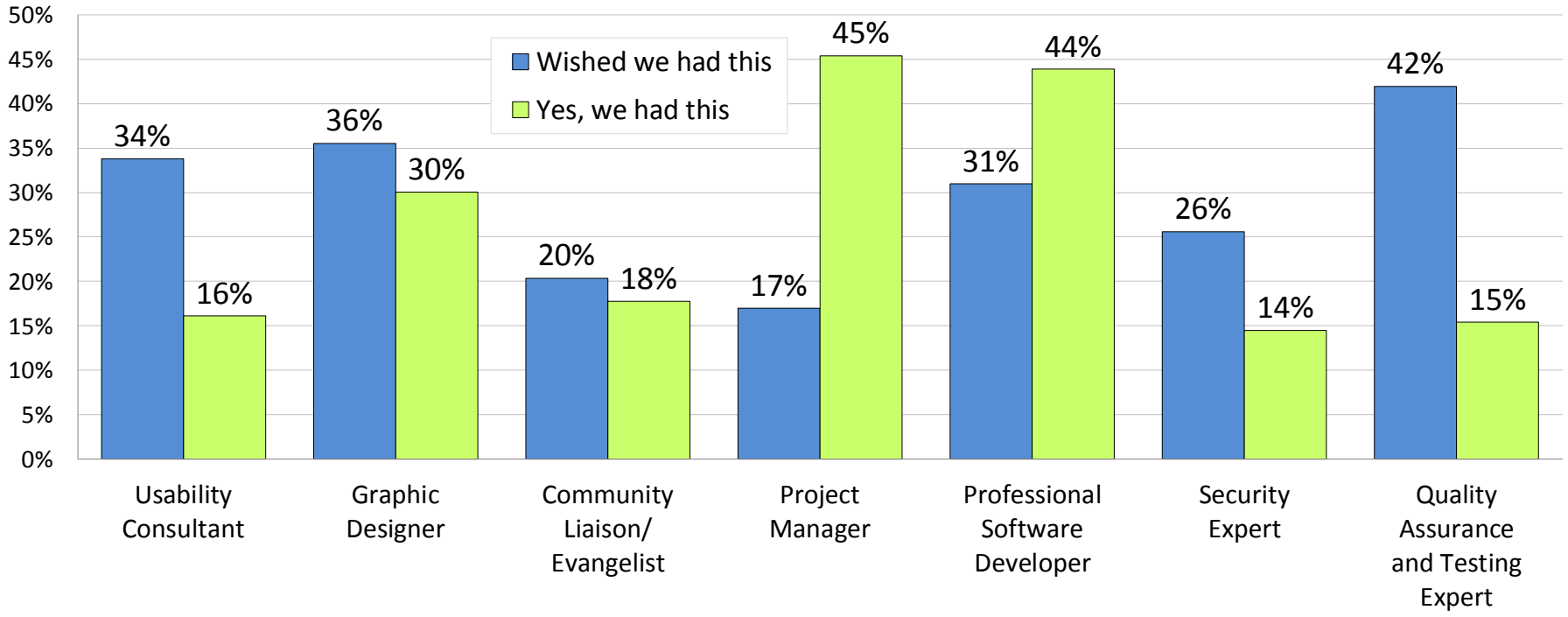
- sent out to 29,000 persons
- 4,957 responses from across domains
- 52% from life, physical or mathematical sciences
- 32% from computer and information sciences or engineering
- 45% develop data collections
- 44% develop data analysis tools

What services would be helpful?

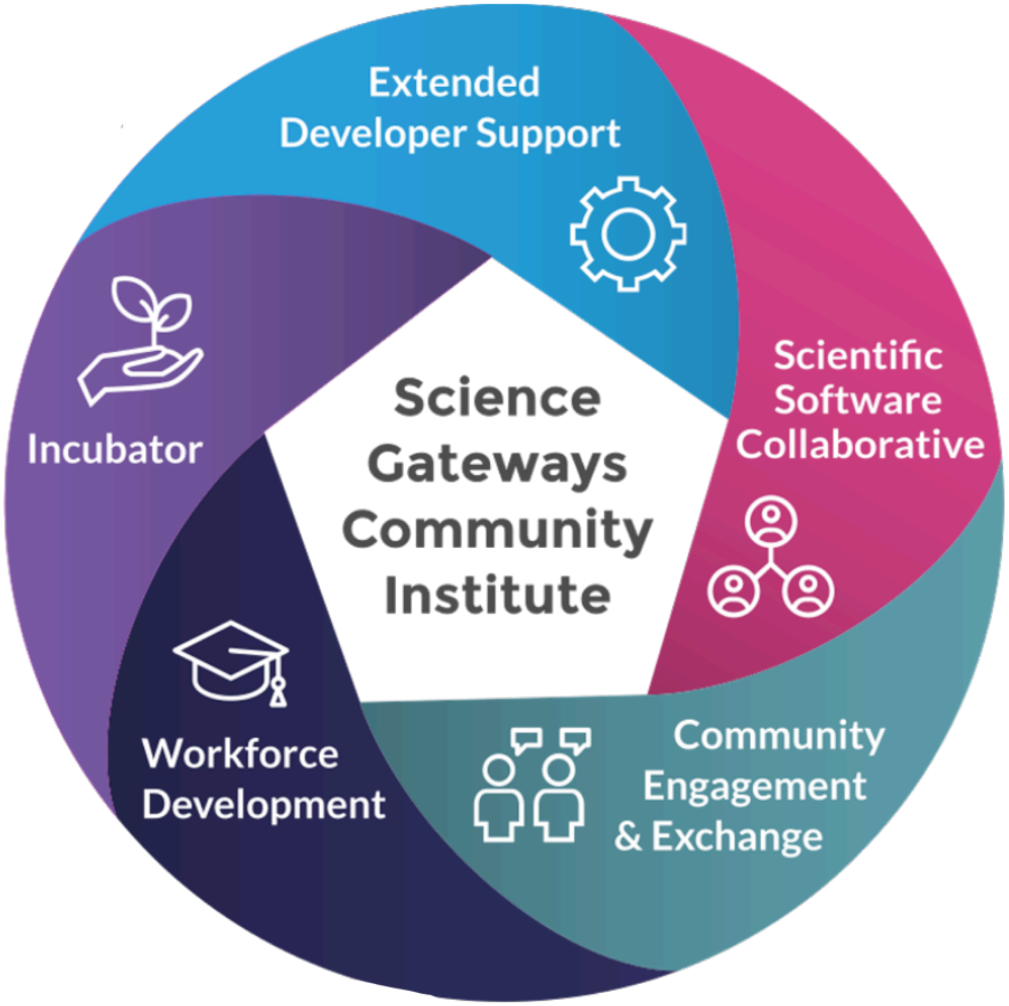
Proposed Service	% Interest
Evaluation, impact analysis, website analytics	72%
Adapting technologies	67%
Web/visual/graphic design	67%
Choosing technologies	66%
Usability Services	66%
Visualization	65%
Developing open-source software	64%
Support for education	64%
Community engagement mechanisms	62%
Keeping your project running	62%
Legal perspectives	61%
Managing data	60%
Computational resources	59%
Mobile technology	59%
Database structure, optimization, and query expertise	59%
Data mining and analysis	58%
Cybersecurity consultation	57%
Website construction	57%
Software engineering process consultation	53%
Source code review and/or audit	51%
High-bandwidth networks	45%
Scientific instruments or data streams	44%
Management aspects of a project	38%

Science Gateways Survey 2014

Well-designed gateways require a variety of expertise



Science Gateways Community Institute



- Diverse expertise on demand
- Longer term support engagements
- Software and visibility for gateways
- Information exchange in a community environment
- Student opportunities and more stable career paths

Incubator Service

A Framework for Decision Making

Technology Planning
- Choosing technologies
- Cybersecurity
- Software engineering
- Interfaces to compute and data

Business Planning
- Business model development
- Financial planning
- Project management
- Software licensing
- Staff and sustainability planning

Client Interaction Planning
- Usability studies
- Web/visual/graphic design
- Impact measurement
- Community engagement
- Support for education

Specialized Expertise

Security
- Center for Trustworthy Scientific Cyberinfrastructure

Sustainability
- Nancy Maron, creator of the ITHAKA S+R course on Sustaining Digital Resources

Evaluation & Impact Measurement
- Ann Zimmerman Consulting

Campus Resource Development

Network / Cohort Formation

Common Experiences
- Training sessions
- Group interactions

Continuing Engagement
- Customized structure, content, goals
- Mentoring
- Pay It Forward

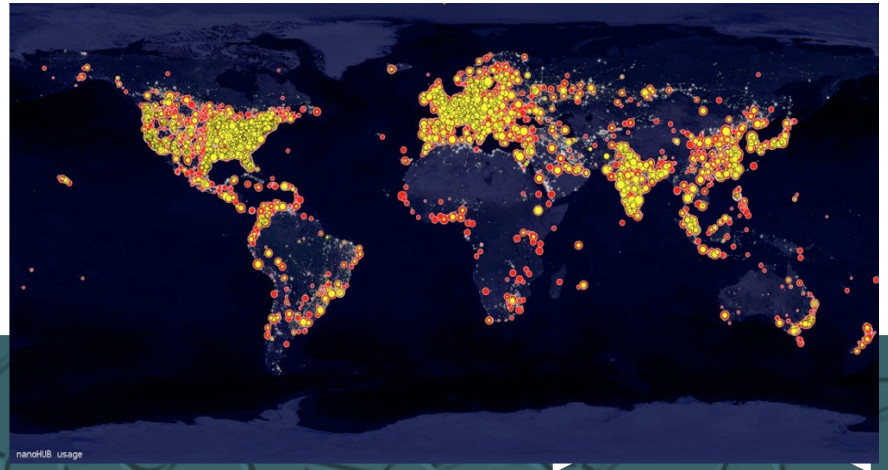
An Ongoing Dispassionate Ear

Technologies

- Widely used complete frameworks (Galaxy, HubZero, Open Science Framework, Globus Data Portal etc.)
- RESTful APIs and support of multiple programming languages in widely used frameworks (Apache Airavata, the Agave platform, etc.)
- Reused interface implementations such as the one of CIPRES with its RESTful API (CIPRES has served more than 20,000 users to date)
- Science gateways as a service with provision of hardware in the background such as SciGap (Science Gateway Platform as a Service)

Lessons learned: approaches should be technology agnostic, using APIs and standard web technologies OR deliver a complete solution

Community Engagement is key

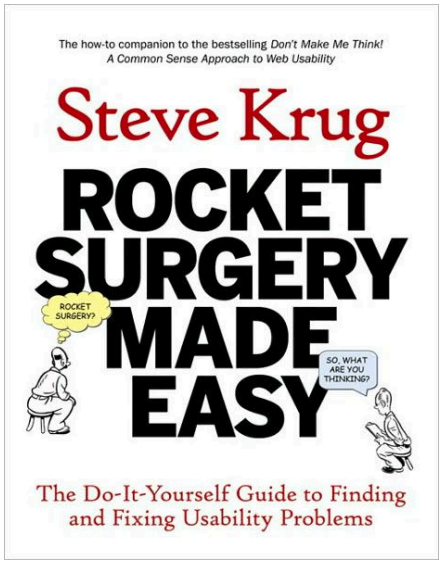


HubZero instances world wide

Usability

“After all, usability really just means that making sure that something works well: that a person … can use the thing - whether it's a Web site, a fighter jet, or a revolving door - for its intended purpose without getting hopelessly frustrated.”

(Steve Krug in “Don't make me think!: A Common Sense Approach to Web Usability”, 2005)



User-Centered Design

Goal?

- Ease of use
- Ease of learning
- Satisfaction

user-friendly usability

User-Centered Design

What?

What are the types of artifacts we design?

~~interfaces~~ entire systems

User-Centered Design

Who?

Who are the users?

What are their goals? needs? mental models? expectations?

User-Centered Design

Goal: enable users to accomplish **their** goals with…

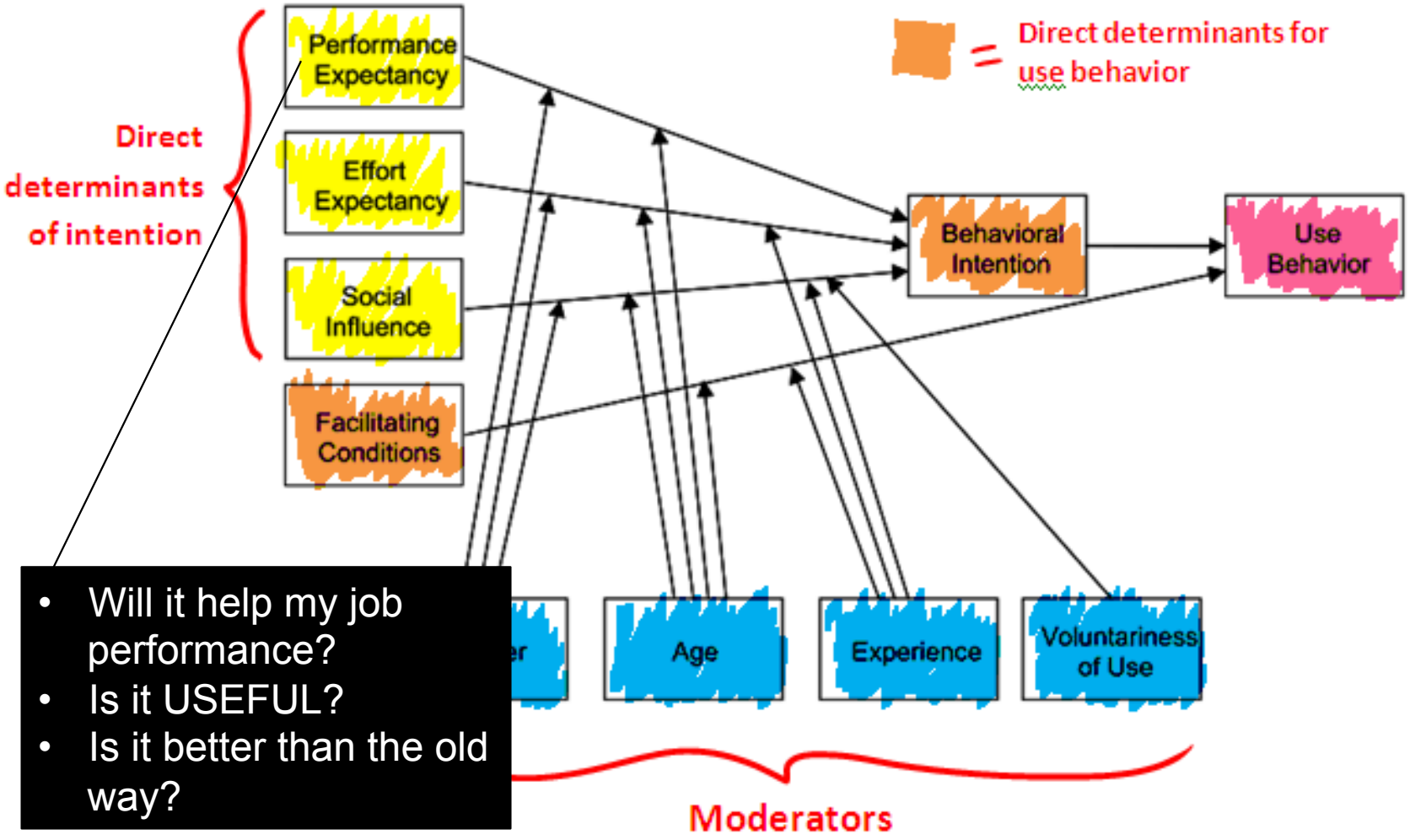
- Ease of use
- Ease of learning
- Satisfaction

User-Centered Design

Why?

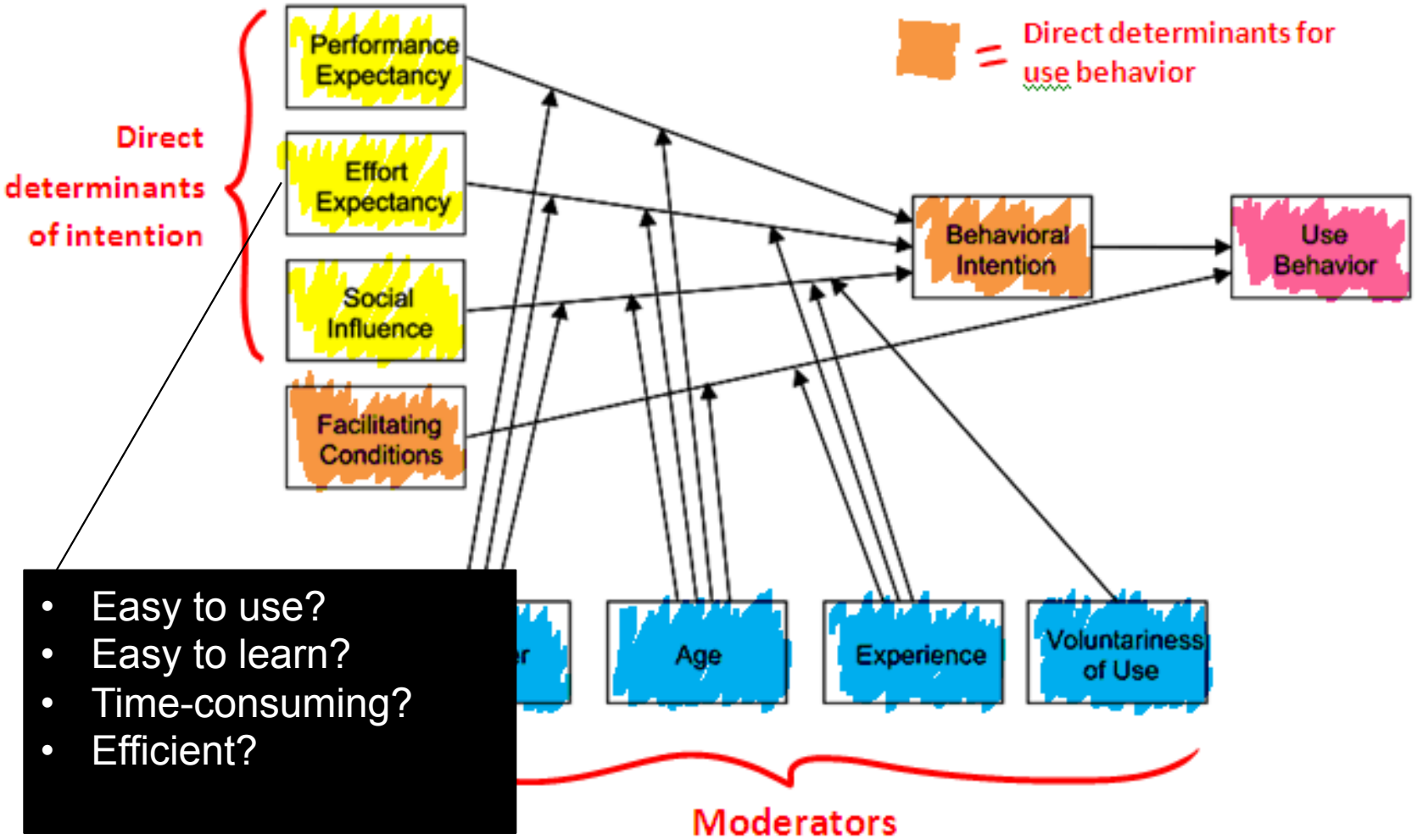
- Ease of use
- Ease of learning
- Satisfaction

Unified Theory of Acceptance and Use of Technology (UTAUT)
Venkatesh et al, 2003



- Will it help my job performance?
- Is it USEFUL?
- Is it better than the old way?

Unified Theory of Acceptance and Use of Technology (UTAUT)
Venkatesh et al, 2003



- Easy to use?
- Easy to learn?
- Time-consuming?
- Efficient?

Unified Theory of Acceptance and Use of Technology (UTAUT)
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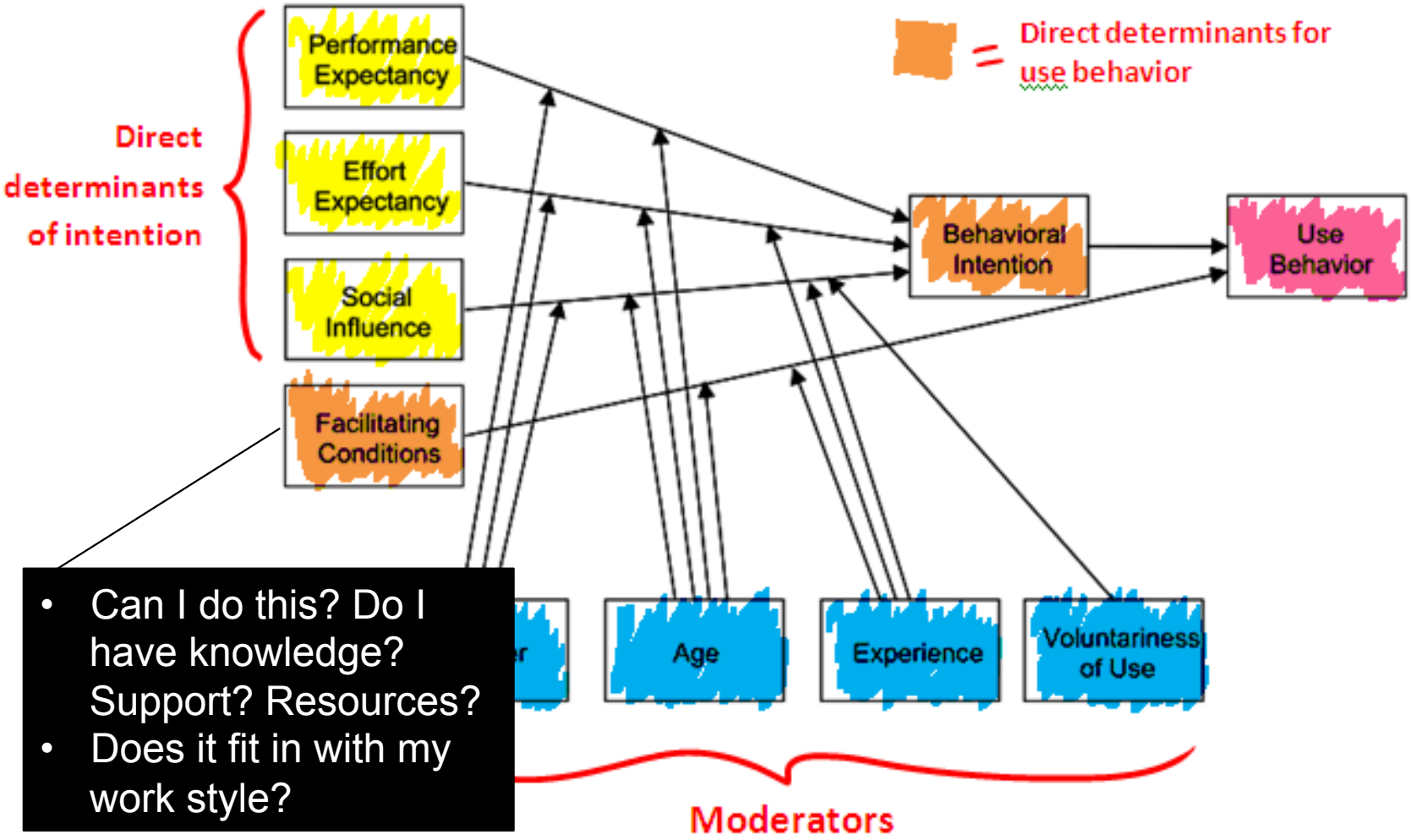
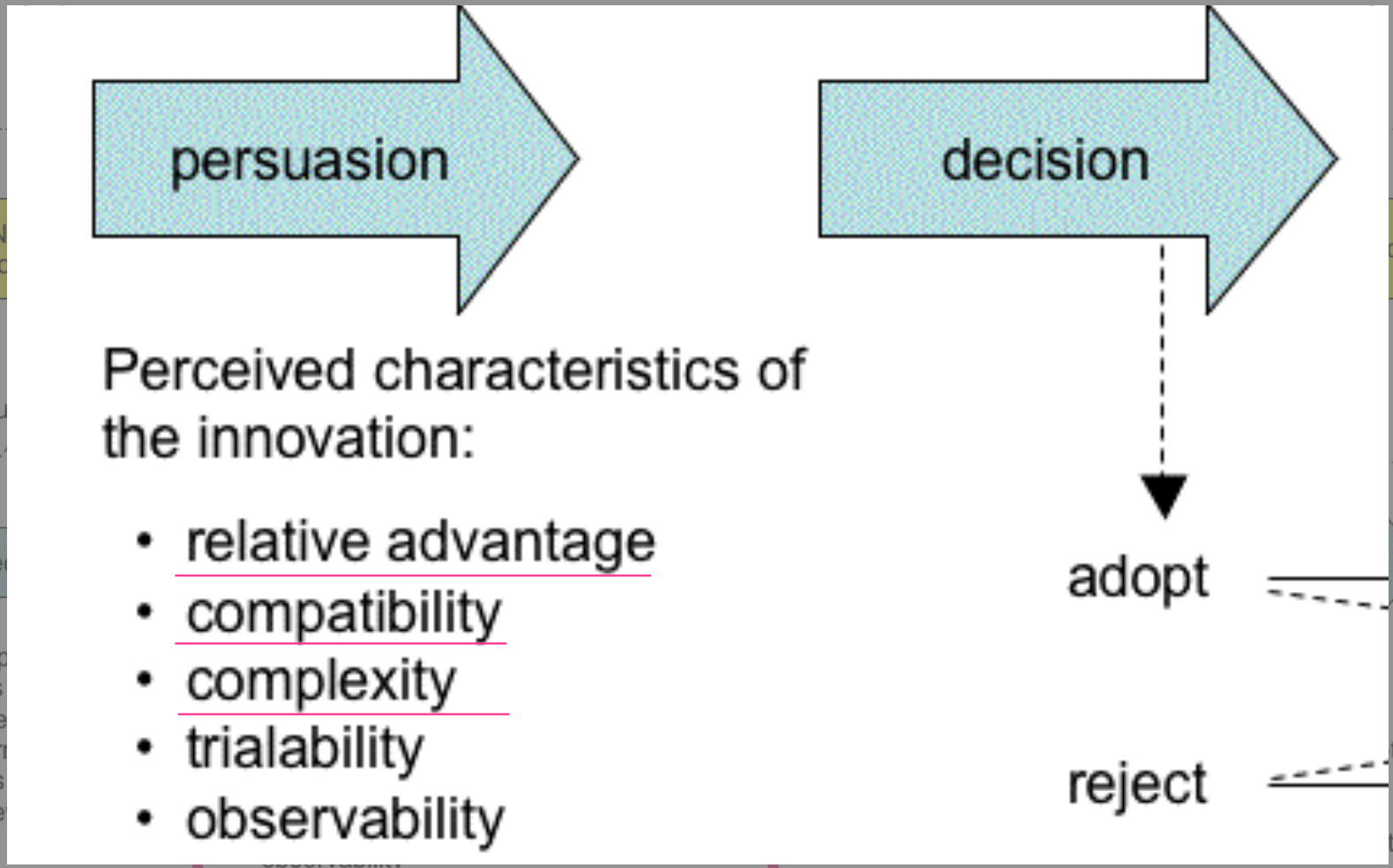


- Can I do this? Do I have knowledge? Support? Resources?
- Does it fit in with my work style?

Diffusion of Innovations - Rogers, 1962



User-Centered Design

Why?

Because usability and user experience are predictors of technology adoption.

User-Centered Design

What can I do?

research

test

iterate

Usability Test

Spend one hour a week on a usability test and the increase of usability is overproportional!

Usability Test

Go to http://sciencegateways.org/

Find:

- How can you partner with us?
- How can you apply for developer services?
- How can you sign up for the email list?

Bootcamp at a Glance

- 5 full days
- Knowledge dissemination
- Interactivity
- Community formation
- Putting away the normal daily routine
- Homework

Incubator Bootcamp – Magic Moments

The lightbulb effect, who I can unify community request for support to create a funding request to campus leadership. I'm planning to organize the gateway community on our campus, including humanities, libraries, engineering and science and create a strategic budget request to our campus leadership.

I was really impressed by the common challenges faced by such diverse projects. They were diverse in their maturity, goals, and disciplinary contexts and yet we all could learn from each other by addressing the shared challenges.

For me, it was the realization of our team after the second day that we weren't in a black box of "where do we go from here", but could see a path to making our gateway sustainable in the next 5 years (50% nsf funding) and 10 years (0% nsf funding).

Extended Developer Support

Focus

- Front-end development
- Gateways using all types of C
- Both sides give 2-month to 1-year commitment
- Well-defined engagements with work plans
- Technology agnostic

Data
Education
Analysis Tools
Instruments
Computation
Workflows
Collaboration
Sensor

Airavata
HUBzero
AGAVE
Galaxy
Jupyter
And more…

Mission

- Bring new gateways into existence
- Adapt existing gateways to new resources and technologies
- Provide "burst" support to help gateways with smaller issues

Benefits

- Reinforce Incubator lessons
- Develop deep understanding of community needs that feed into other Institute areas
- Capture and document support efforts for scalability
- Hands-on opportunities for student participants

SGCI

Scientific Software Collaborative

End-to-End Solutions

- Serve a diverse set of scientific domains
- Out-of-the-box gateway solution that can be customized
- Based on Docker – executable images that are the skeleton for a secure and functioning gateway
- Portable and reproducible
- Community-contributed

Software Integration & Community Contribution

- Docking mechanisms for community-contributed software, including NSF SI2
- Incorporate community standards

Software Marketplace for Science Gateways

"Use-what-you-need"

- API integration
- Variety of services
  - Information
  - Security
  - Execution
  - Data
  - Event
  - Accounting
- Hosting opportunity

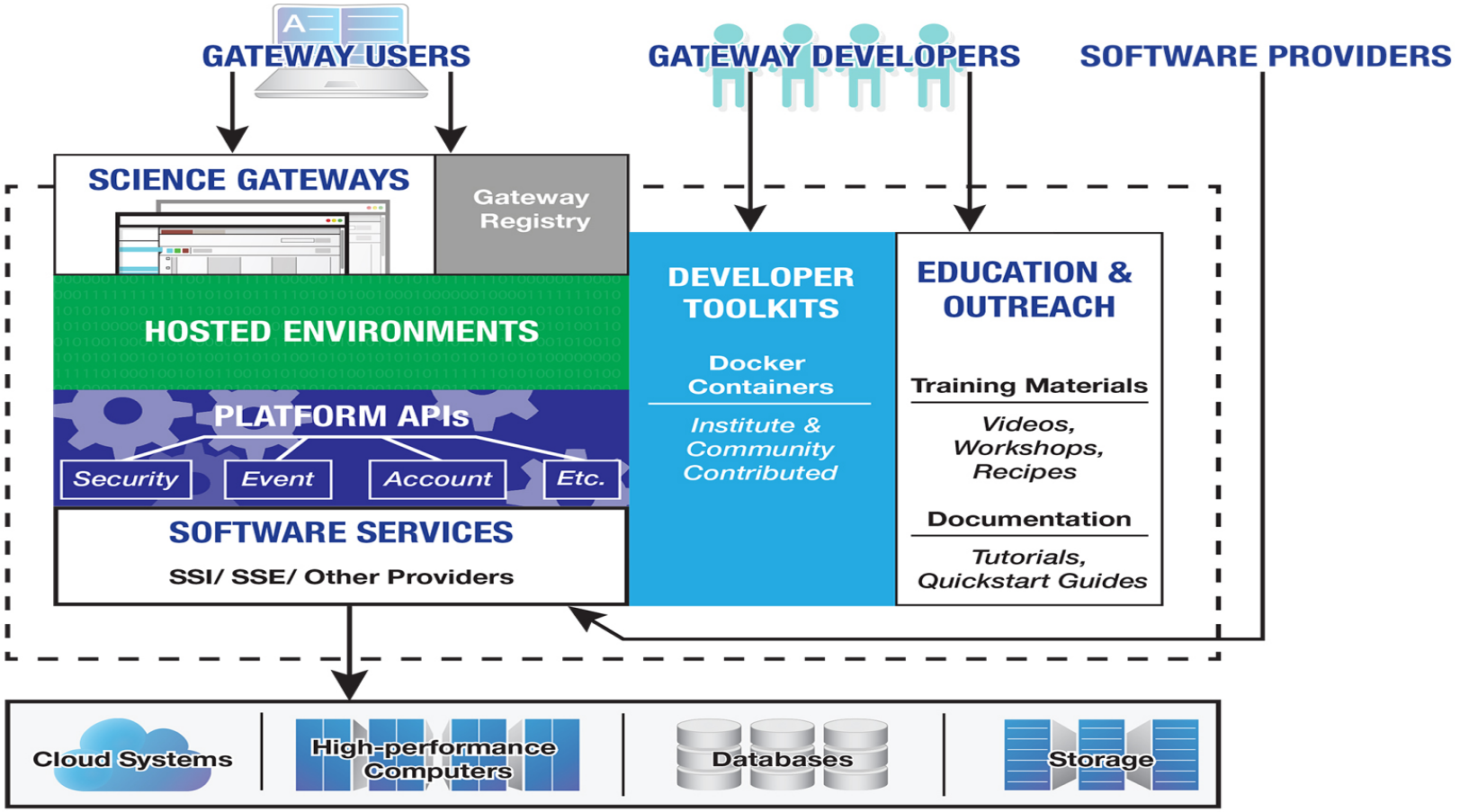
Gateway Discovery

- Open registry
- Promotes use of existing science gateways
- Community-contributed
- Admin approval
- Automated cleanup

Engage Other Areas of Institute

- Support projects leverage Collaborative components
- Framework evolves as a result of gateway engagements
- Community outreach

Scientific Software Collaborative



Community Engagement and Exchange

Website Activities

- Discussion forums
- Gateway showcase with case studies
- Symposium series
- News: media coverage, related happenings, academic publications, job openings, events calendar
- Curated blog with guest authors,
- Professional development: synchronous and asynchronous training
- Capture client/user feedback on web and through other areas

Annual Conference

- Tutorials and workshops
- Paper presentations
- Invited keynotes and panels
- Interactive elements: Open Space, poster session
- Travel support for students and campus IT staff

Builds on 10 years of experience with GCE and IWSG series

Outreach to Complementary NSF Initiatives

- NSF SI2 projects
- Large NSF projects
- Science and Technology Centers
- Engineering Research Centers
- MolSSI software institute collaboration

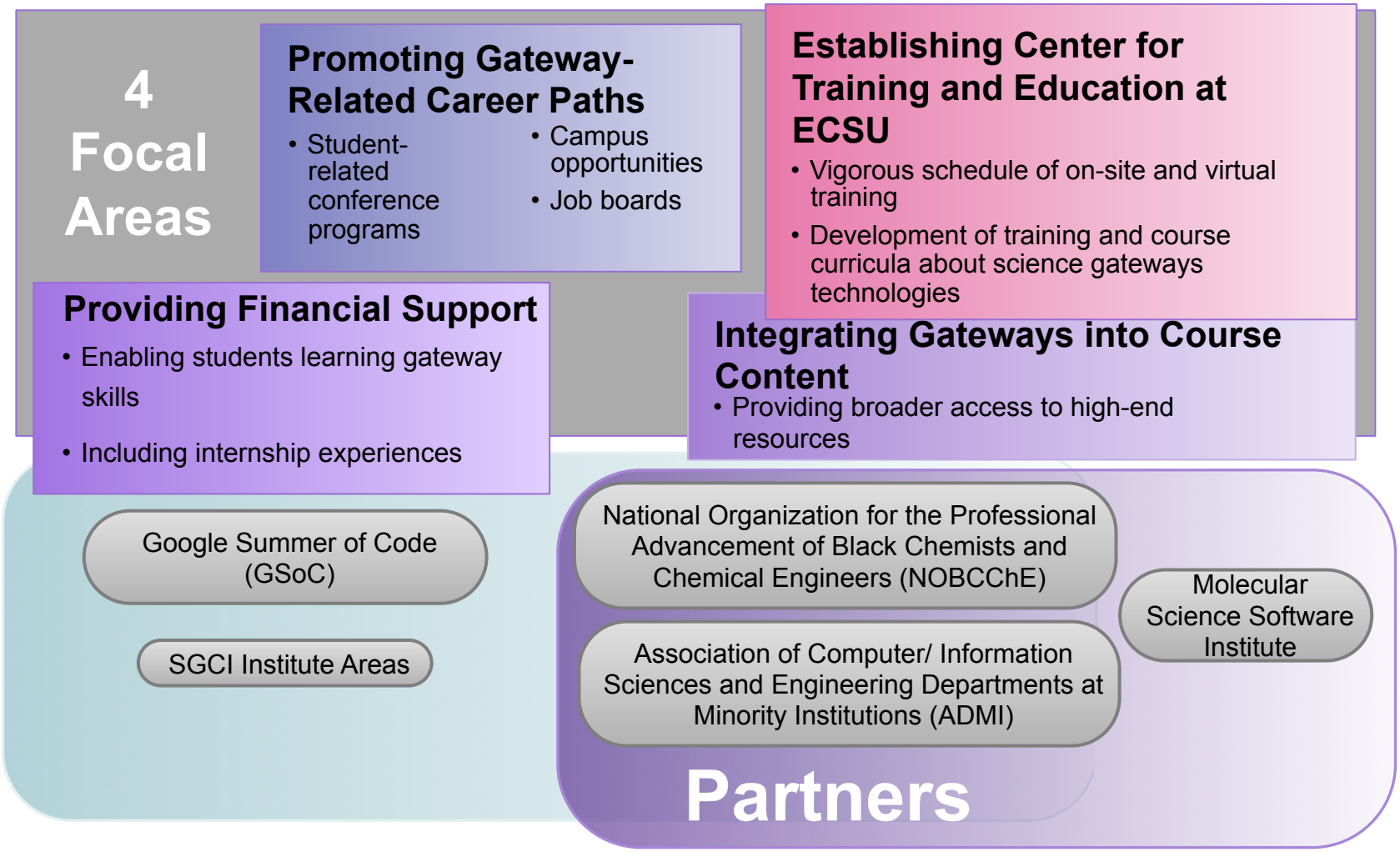
Campus Gateway Groups

- Task force builds campus-based expertise
- Channel for scaling institute services

Conferences and Workshops

- 2006: GCE (Gateway Computing Environment) workshop series started – successful 10th anniversary in 2015
- 2009: IWSG (International Workshop on Science Gateways) workshop series started – successful 9th anniversary in 2017
- since 2013: GCE partners with IWSG on yearly special issue
  9th IWSG took place 19-21 June 2017 in Poznań, Poland – next year in Edinburgh, Scotland
- since 2015: GCE and IWSG partnering with Australian IWSG-A (International Workshop on Science Gateways – Australia) on yearly special issue
  3rd IWSG-A will take place 16-17 October in Brisbane, Australia
- 2016: GCE extended to Gateways conference with 120 participants at the first event
  Gateways 2017 will take place 23–25 October 2017 in Ann Arbor, Michigan,USA

Workforce Development



Opportunities

- Get advice (sustainability, usability, cybersecurity, other) on your existing gateway
- Work with SGCI to build a gateway for you
- Find a working gateway or gateway development software in our catalog
- Learn how to set up a gateway group on your campus
- Keep up to date on gateway developments
  - webinar series, gateways in the news, google scholar feed, case studies, annual conference, blog posts
- Enroll a student in an internship program to learn gateway development
- Partner with SGCI on your own projects, technologies and events

Opportunities

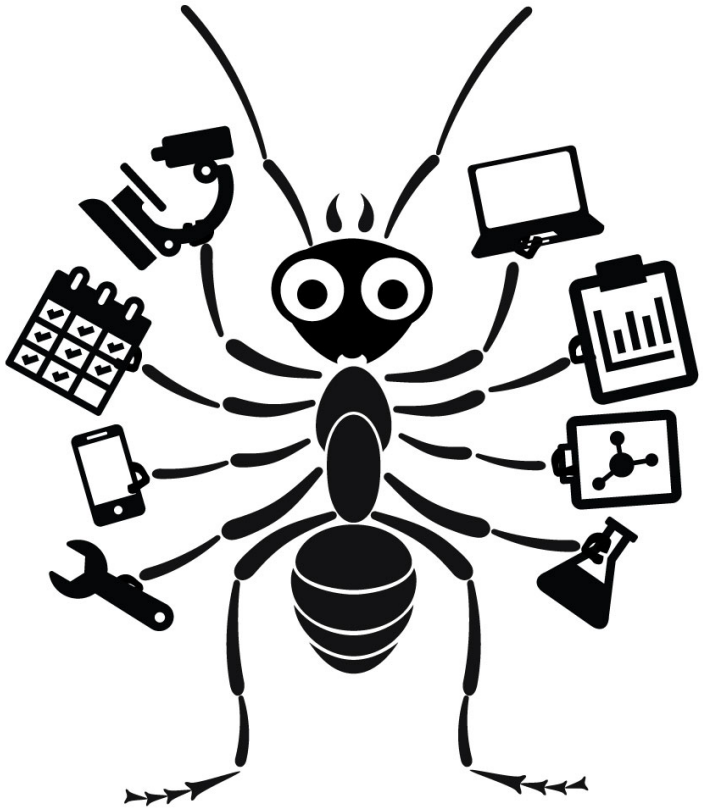
- A breadth of interesting topics in the science gateway creation process
  - Novel frameworks and web applications
  - Inter- and multidisciplinary work
  - Contributing to grand challenges, e.g., Malaria eradication
  - HPC usage…
- A breadth of interesting roles
  - HPC programmers, designers, statisticians, librarians, machine learning experts, usability experts,…

Challenges

- Some topics and roles are only needed for part of the project

⇒ Not fully funded positions via one project

⇒ For diverse expertise, several different people are needed



Your Campus

Is your campus seeing an increasing number of research projects that include web-based applications using HPC? Does each group have to hire developers independently?

This can be time consuming and inefficient, but there is a solution.

YOU ARE NOT ALONE!

Addressing Software Sustainability on Your Campus

SGCI
Science Gateways Community Institute

Is your campus seeing an increasing number of research projects that include web-based applications? Does each group have to hire developers independently? This can be time consuming and inefficient.

You are not alone.

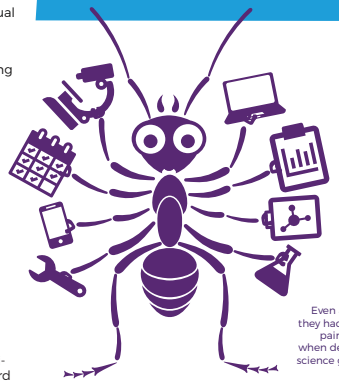
THERE IS A SOLUTION

Creating a central pool of expertise on your campus offers many benefits including:

- Great visibility for the institution's research activities
- Synergy between projects
- Shared resources, costs and expertise across departments
- Expertise that is otherwise difficult for individual projects to obtain
- Lower learning curves
- Ability to retain top-quality research computing support by providing interesting projects

Science gateways are online, end-to-end solutions that provide broad access to advanced resources. They provide a community space for science and engineering research and education, allowing all to tackle today's challenging science questions.

Gateways are an **increasingly common component of funded activities** by many agencies. Individual PIs find it challenging to recruit and sustain teams that offer the diversity of expertise necessary for developing gateways.



Even ants wish they had an extra pair of hands when developing science gateways!

NOW IS THE RIGHT TIME!

WE CAN HELP YOU!

- We can provide supplemental expertise where you don't have it.
- We can provide support for your journey to creating a campus-based group.
- We can provide ongoing advice based on campuses who have successfully created their own groups.

HOW TO START?

Contact us to request a free consultation, webinar, or on-campus visit to start your path toward sustainable gateway development.

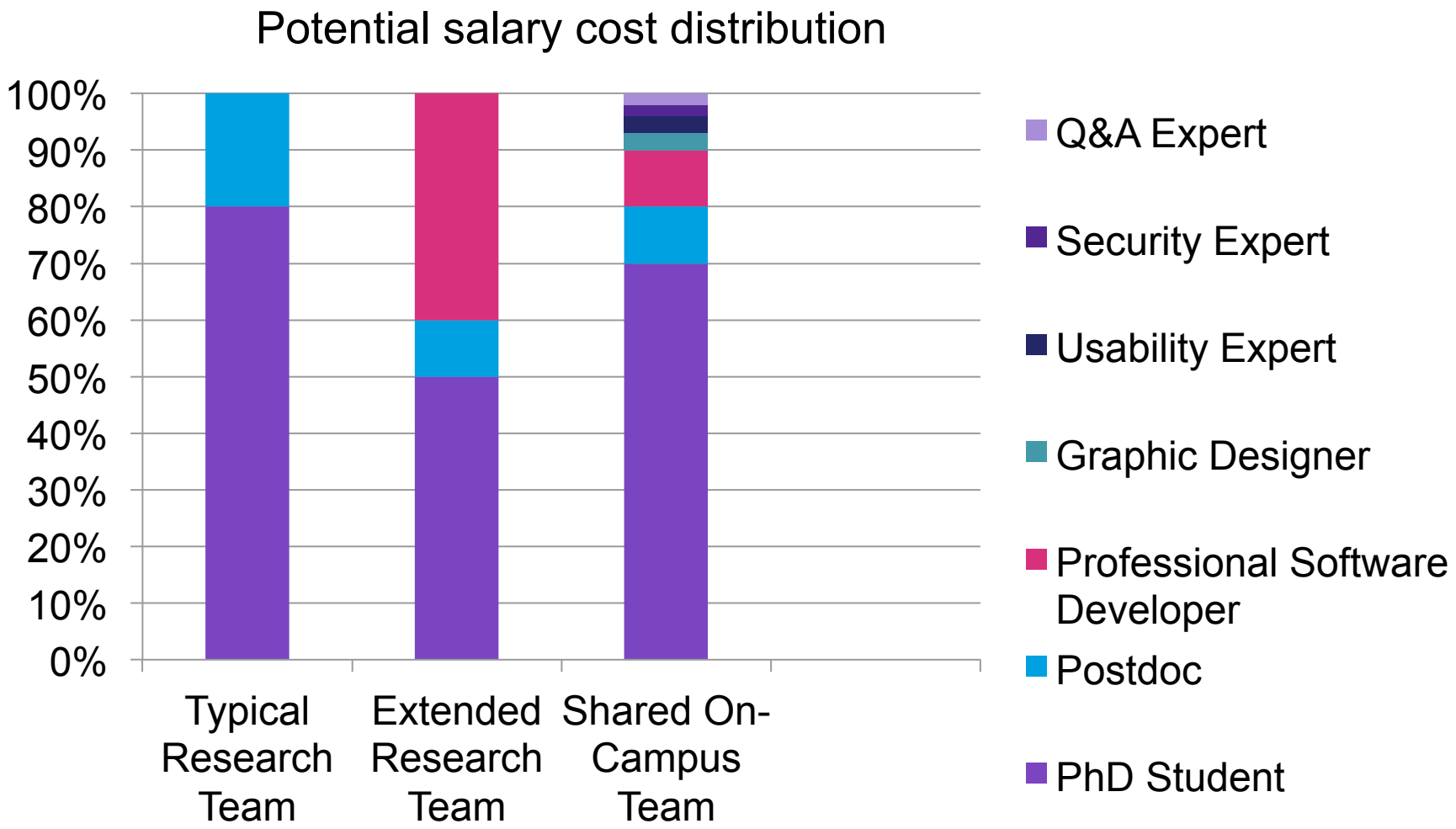
INTERESTED? CONTACT US!

http://sciencegateways.org/campusgroups
help@sciencegateways.org

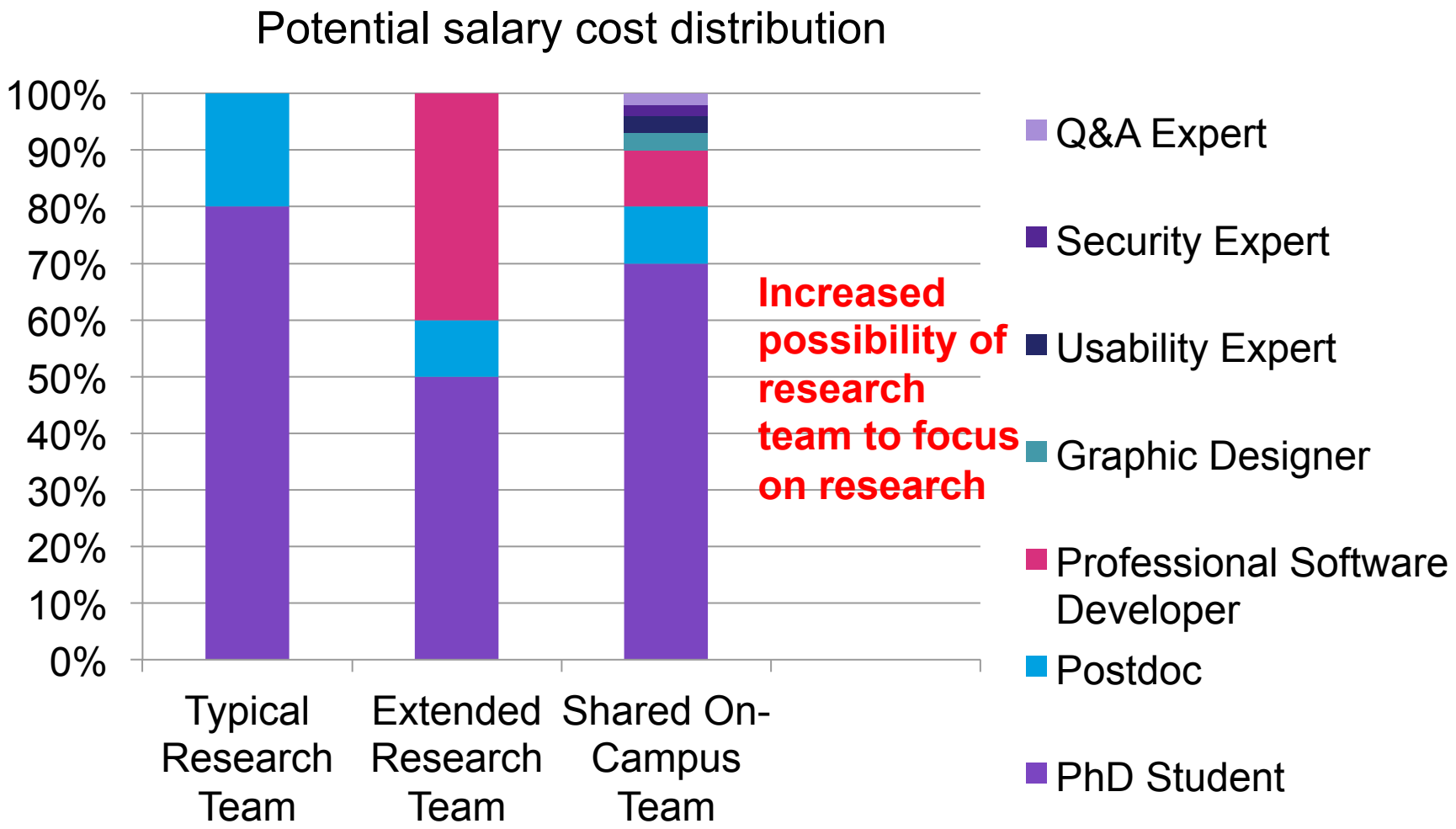
The **Science Gateways Community Institute (SGCI)** is an online and physical resource that supports science gateways with free services, including community building, consulting, and opportunities for sharing expertise, technologies, and practices.

SGCI

Sustainability via On-Campus Teams



Sustainability via On-Campus Teams



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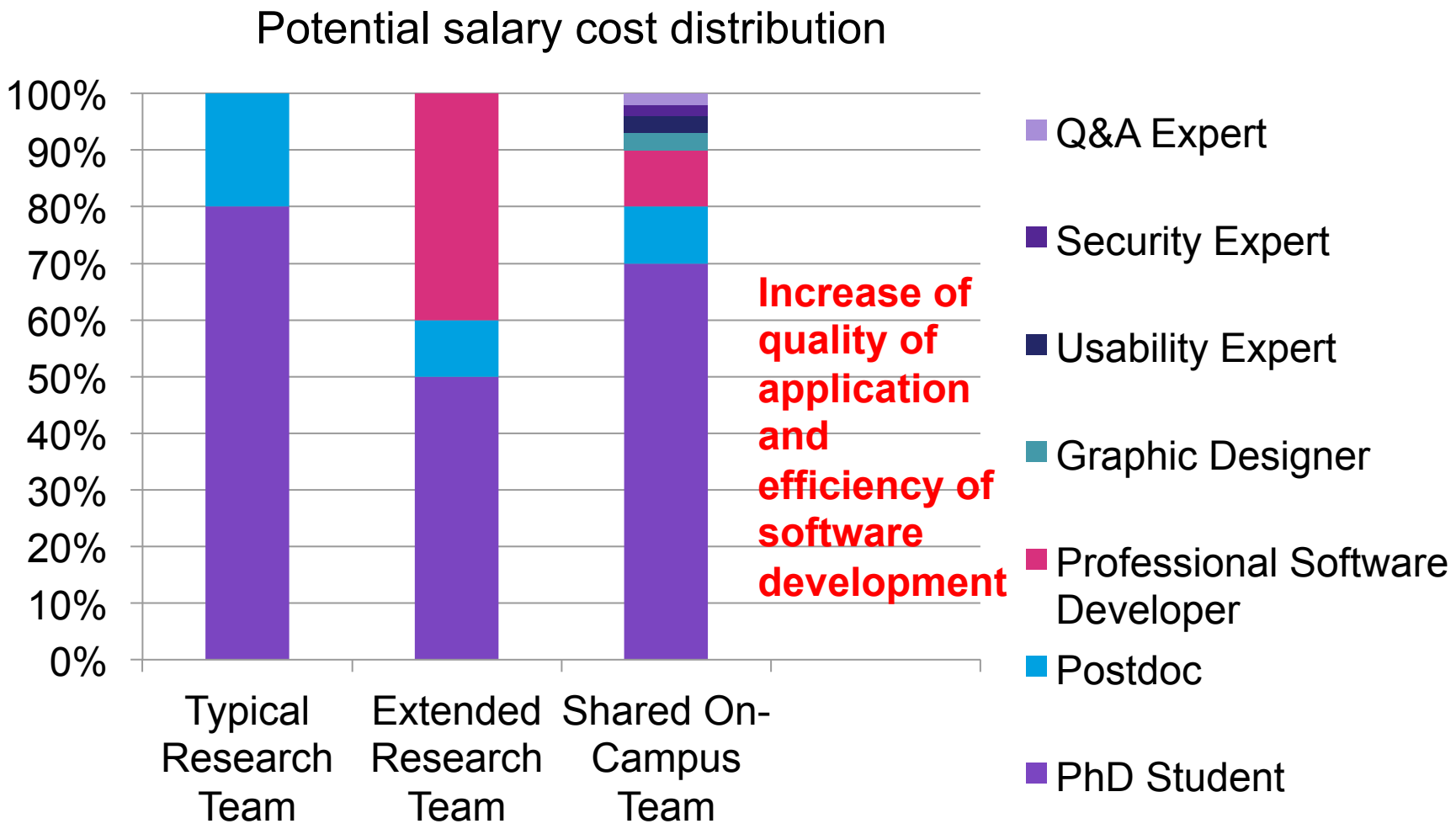

Sustainability via On-Campus Teams

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Success Stories

Some universities have successful centers/groups with centralized services for science gateways

- Center for Research Computing at University of Notre Dame
- HUBzero® Team at Purdue University
- Science Gateways Research Center at Indiana University
- Science Gateway Group at TACC at the University of Texas, Austin
- …

ND CRC in 2006-2008

- Effort with 7 FTEs centrally funded
- HTC and HPC Computing and basic user support
  - One centrally funded cluster plus multiple faculty funded clusters in various cabinets on campus
  - Around 300 active users
  - 80% centrally funded hardware
- No other kinds of research computing services
- Underserved social sciences and humanities for their need on science gateways
- ~1000 faculty, ~12000 students

ND CRC Mission

CRC engages in computational science, fosters multidisciplinary research and provides advanced computational tools and services. The CRC works to facilitate discoveries across science, engineering, the arts and humanities, social sciences, business and other disciplines.

ND CRC Vision

To become an internationally recognized multidisciplinary research computing center based upon our reputation for facilitating and accelerating discovery through effective and novel applications of cyberinfrastructure.

ND CRC Director's thoughts on Vision

- "Nice vision, but how we get there?"
- "What should we do first?"
- "Users should tell us what they need…"
- "HPC works fine, so let's focus on CI Development…"
- "We need portals and other collaborative environments"
- "We need good user support, and good, straight resource usage policies"
- "We need CI and HPC teams working together"
- "How do we fund all these with very limited resources?"
- "What is available out there?
- And so on…

Implementation by Jarek Nabrzyski

Take the risk and hire people first

➔ train people

➔ generate / bring projects

➔ assign people to projects and focus on getting more projects and more people -> etc...

➔ if not successful then exit, i.e. quit ☺

Fortunately, we had many projects, mostly science gateway projects of various kinds and difficulty.

ND CRC in 2017

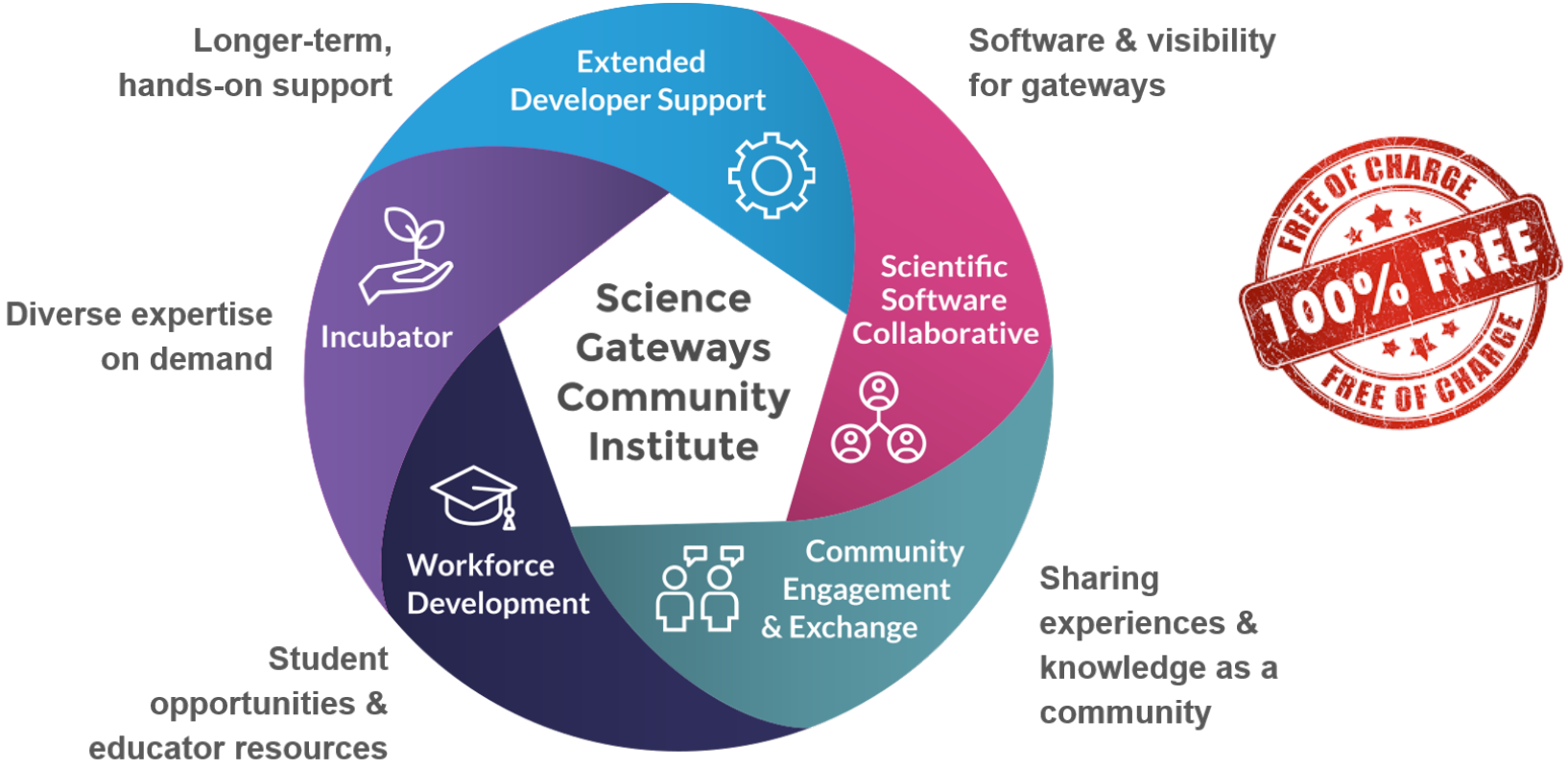
- 45 FTEs with 70% of the staff salaries supported through grants and services
- HTC and HPC Computing and user support
  - 26,000 cores
  - 1,800 active users
  - 10 HPC engineers and user support staff
  - 30% of compute nodes are centrally funded
- Cyberinfrastructure development
  - ~15-20 CI projects each year with ~35 faculty from various departments including social sciences and humanities
  - supported by ~15 research programmers, ~8 computational scientists, some FTE fractions of HPC engineers, and a few (7) grad students and undergraduate interns (4-6)
- ~1000 faculty, ~12000 students

Lessons Learned by the Four Teams

- You need an evangelist to build/sustain teams
- You are going to have staff turnover
- Plug into your talent reservoir
- Put effort into your onboarding process
  - Get people contributing to your software and projects as quickly as possible
- Keep alumni involved
  - Developer mailing lists for example
  - Potentially hire as consultants
- Use internal and external resources for creating/ maintaining science gateways

Funding Mechanisms – External Resources

Now is the right time – Get support from SGCI via diverse services!



Funding Mechanisms – External Resources

- Get support from SGCI via diverse services
- Contractors from mature science gateway frameworks

⇒ Means to create and/or maintain science gateway(s) successfully while working on building up internal resources

Funding Mechanisms – Internal Resources

- Funding via involvement of some person months in grants
- Funding on some hard money from universities
- Funding via re-charge
- Funding via NSF for building facilitators/ cyberpractitioner career-paths (under development - models like full funding the first year and increasing responsibility on the side of universities)

Using Existing Free On-Campus Resources

- Do you have people such as “digital librarians”? They are generally not only serving humanities and have great knowledge about data preservation, data lifecycle, programming skills, ..
- Do you have data scientists? They probably know about machine learning, meta-data, ontologies, statistics …
- Do you have an HPC center? They know how to access HPC resources, VMs, containerization, distributed data management …

Identify key contacts and evangelists on your campus

- Deans?
- Department chairs?
- HPC colleagues?
- Web developers?
- Gateway group?

"We like to bring together people from radically different fields and wait for the friction to produce heat, light and magic. Sometimes it takes a while."

Sharing resources

- Share human resources (librarians, data scientists, web developers, HPC specialists,…)?
- Share free resources such as office space?
- Which departments?
- Possibility between universities?
- Presentations at events (new faculty events, meetings within faculty, meetings between departments, …)?

Role Play

Devil's advocate

Ask for free resources!

Role Play

It will be painful…

but beneficial to put yourself in this role

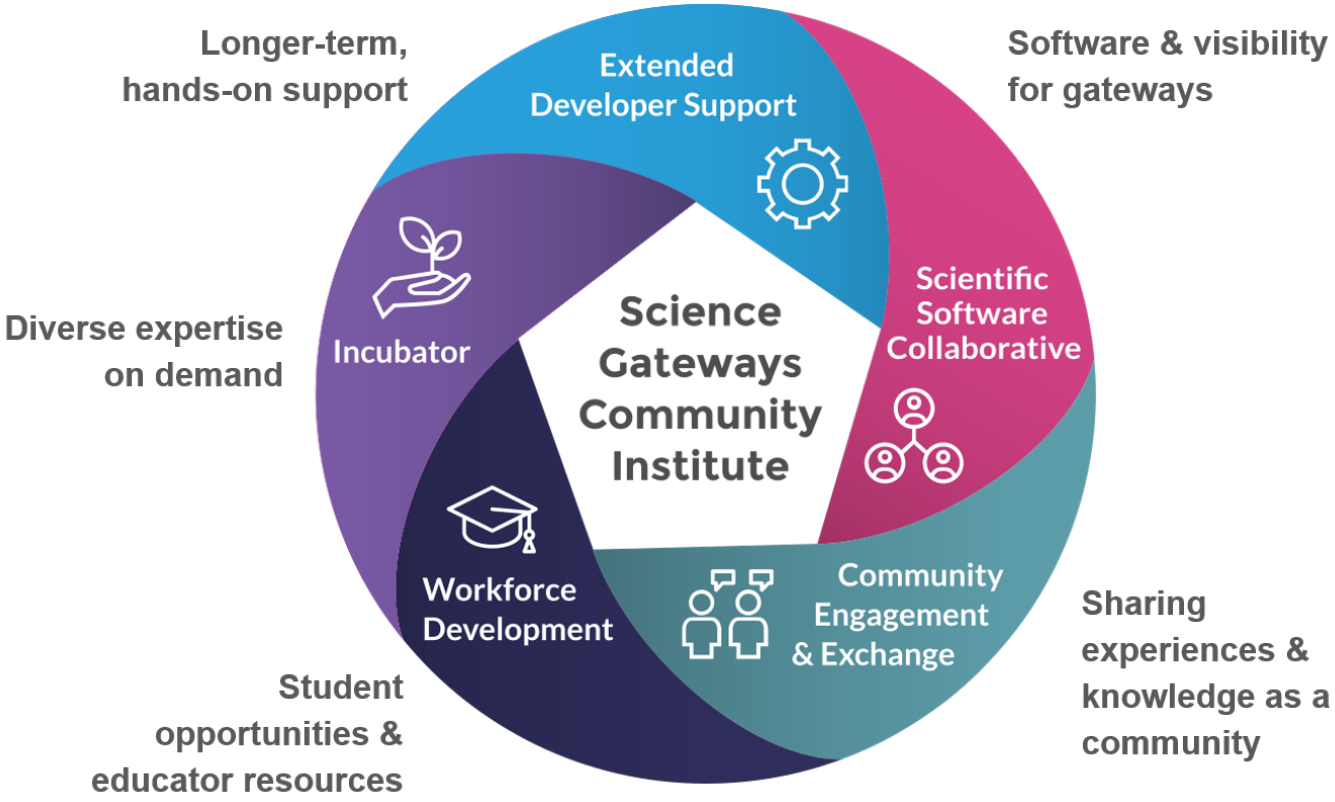
Scenario

NSF offers funding for three years for a "cyberpractitioner": first year 80%, second year 50%, third year 20%. You would like to use the funding for a usability specialist.

Ask the dean (Henry)!

Your own roadmap

YOU ARE NOT ALONE!



https://sciencegateways.org/
https://sciencegateways.org/engage/bootcamp