SGCI

Science Gateways
Community Institute

S2I2 HEP

S2I2: Science Gateways Community Institute

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http://sciencegateways.org/
7 December 2016

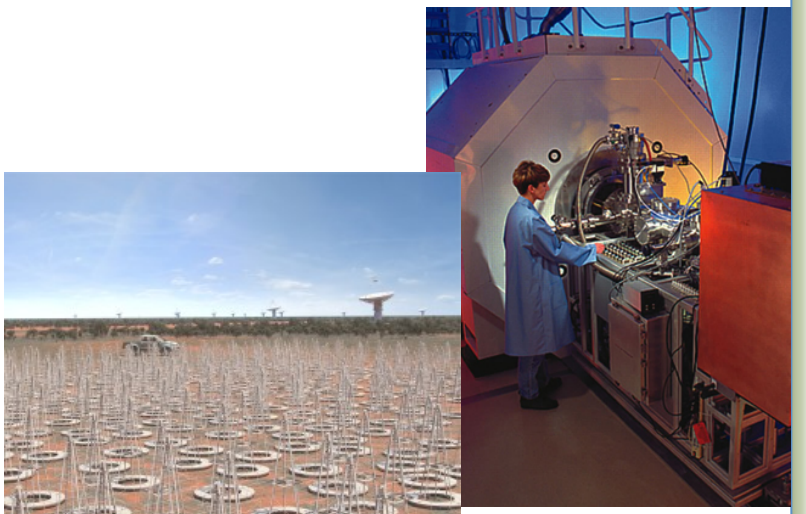
What are science gateways? Why are they important?

- 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.*

What are science gateways? Why are they important?

- Explosion in the quantity, variety and complexity of data (e.g., NGS, SKA)
- Questions can be answered impossible to even ask about 10 years ago
- Costs far reduced (e.g., Human Genome project, 15 years, ~$2 billion; today ~3 days, $1000)

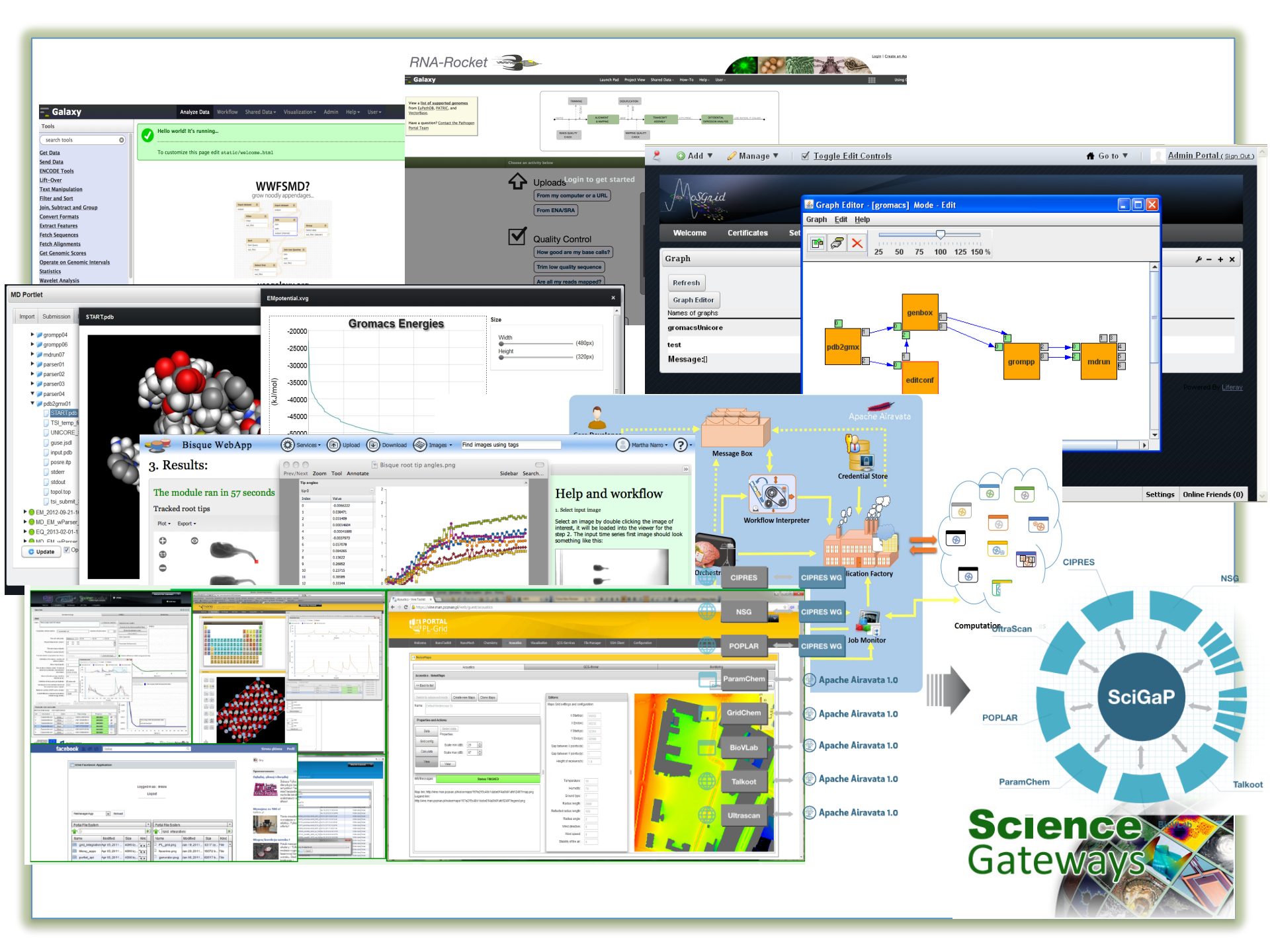


Science Gateways – NSF Definition

Science Gateways (also known as portals and hubs) are themselves synergistic focal points where scientists form growing communities; where digital resources, expensive equipment, and collaboration resources are available to those who would otherwise not have access to them; and where the public can participate in the scientific process, spanning science and engineering research and education. Gateways assemble and integrate some of the most complex components of today's cyberinfrastructure (CI), making them accessible to a wider spectrum of users through easy-to-use interfaces. They provide researchers with unified human and programmable access to facilities:

- computing resources (e.g., supercomputers, clouds),
- instruments (e.g., telescopes, sensor networks),
- data (e.g., data collections, collaborative spaces),
- software (e.g., simulation, modeling, and analysis capabilities, workflow systems),
- and more,

thus increasing the value of these facilities. They make the interdisciplinary collaborations needed to solve the most complex problems more feasible. They support CI abstractions that allow scalable, dynamic use of diverse CI without demanding detailed and complex technical understanding of CI components, and provide scalable solutions for solving classes of problems, eliminating the need for thousands of individual infrastructure installations.


RNA-Rocket
Galaxy
Analyze Data
Workflow
Shared Data
Visualization
Admin
Help
User
Tools
search tools
Get Data
Send Data
ENCODE Tools
Lift-Over
Text Manipulation
Filter and Sort
Join, Subtract and Group
Convert Formats
Extract Features
Fetch Sequences
Fetch Alignments
Get Genomic Scores
Operate on Genomic Intervals
Statistics
Wavelet Analysis
Hello world! It's running...
To customize this page edit static/welcome.html
WWFSMD?
grow noodly appendages...
Uploads
From my computer or a URL
From ENA/SRA
Quality Control
How good are my base calls?
Trim low quality sequence
Are all my reads mapped?
Login to get started
Add
Manage
Toggle Edit Controls
Go to
Admin Portal
Sign Out
MoSGrid
Welcome
Certificates
Graph
Refresh
Graph Editor
Names of graphs
gromacsUnicore
test
Message:[]
Graph Editor - [gromacs] Mode - Edit
Graph Edit Help
25 50 75 100 125 150 %
genbox
pdb2gmx
editconf
grompp
mdrun
Powered By Liferay
Settings
Online Friends (0)
MD Portlet
Import
Submission
START.pdb
grompp04
grompp06
mdrun07
parser01
parser02
parser03
parser04
pdb2gmx01
START.pdb
TSI_temp_f
UNICORE_
guse.jsdl
input.pdb
posre.itp
stderr
stdout
topol.top
tsi_submit_
EM_2012-09-21-1
MD_EM_wParser
EQ_2013-02-01-1
MD_EM_wParser
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Gromacs Energies
(kJ/mol)
-20000
-25000
-30000
-35000
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-45000
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Size
Width
(480px)
Height
(320px)
Bisque WebApp
Services
Upload
Download
Images
Find images using tags
Martha Narro
3. Results:
The module ran in 57 seconds
Tracked root tips
Plot
Export
Bisque root tip angles.png
Prev/Next
Zoom
Tool
Annotate
Sidebar
Search...
Tip angles
tip-0
Index
Value
Help and workflow
1. Select input image
Select an image by double clicking the image of interest, it will be loaded into the viewer for the step 2. The input time series first image should look something like this:
Apache Airavata
Message Box
Credential Store
Workflow Interpreter
Orchestr
lication Factory
CIPRES
CIPRES WG
CIPRES WG
CIPRES WG
Job Monitor
Computation
CIPRES
NSG
UltraScan
POPLAR
ParamChem
Talkoot
SciGaP
PORTAL PL-Grid
NSG
POPLAR
ParamChem
GridChem
BioVLab
Talkoot
Ultrascan
Apache Airavata 1.0
Apache Airavata 1.0
Apache Airavata 1.0
Apache Airavata 1.0
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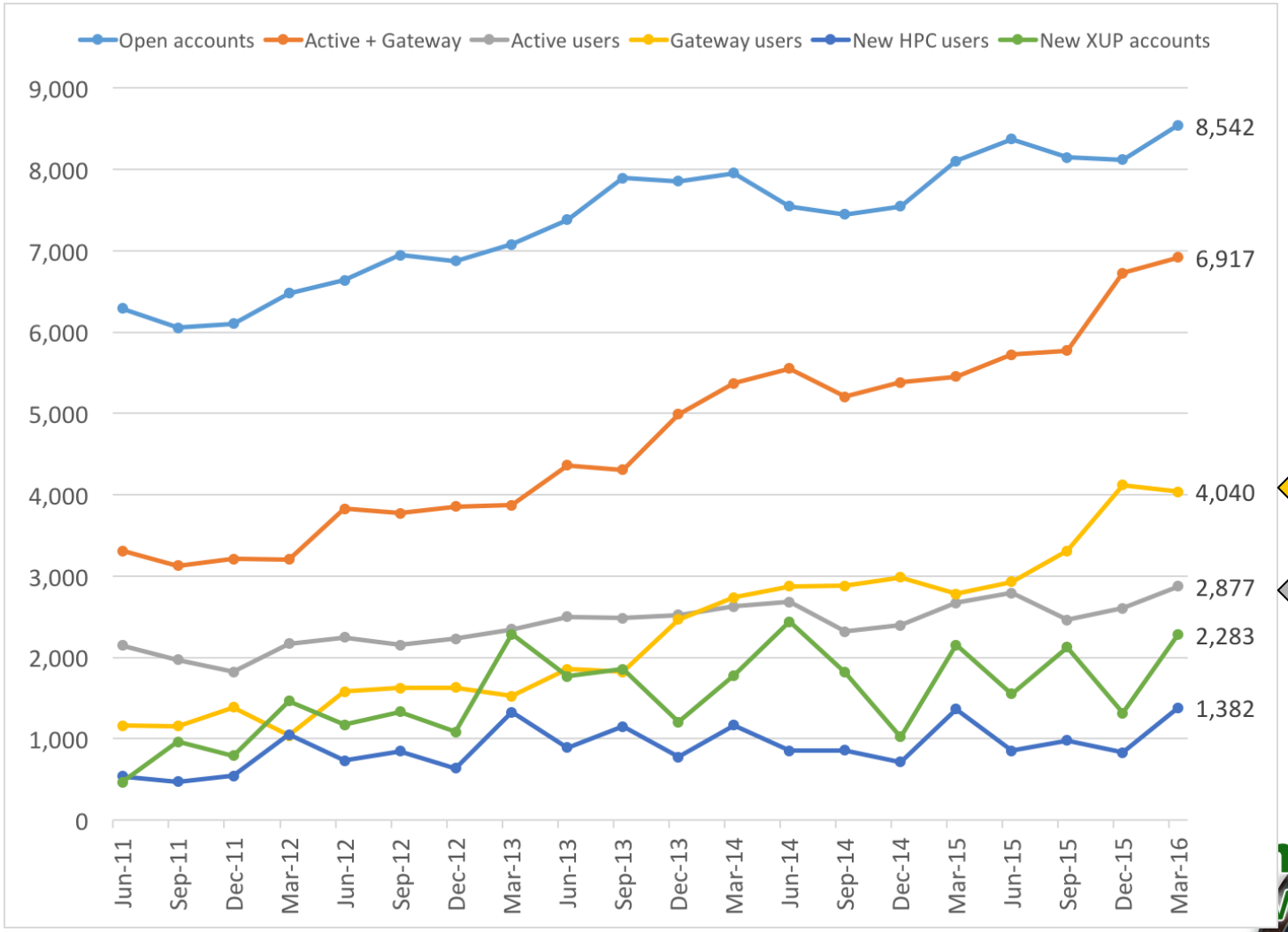
facebook
Science Gateways

Significant developments in XSEDE as well
Gateway users surpass login users in 2013
Increase in 2015 due to automated user-counting

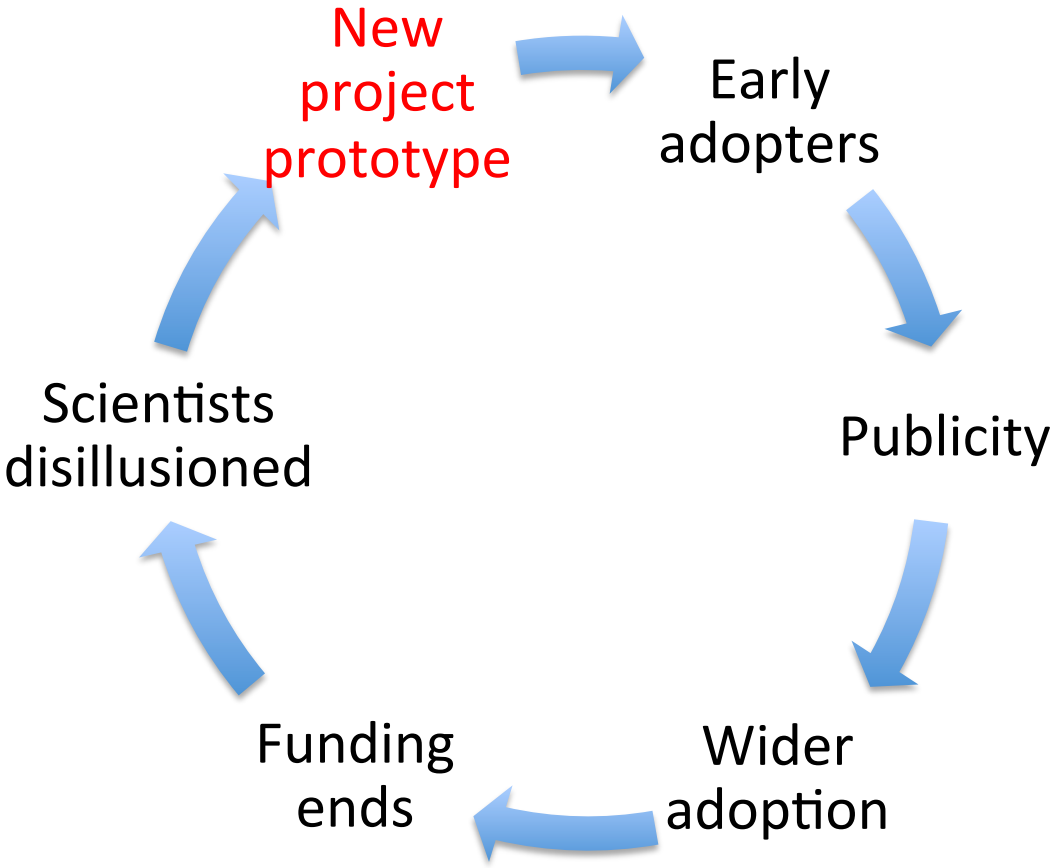


Gateways

Login

Source: David Hart

A Typical Life Cycle of a Science Gateway

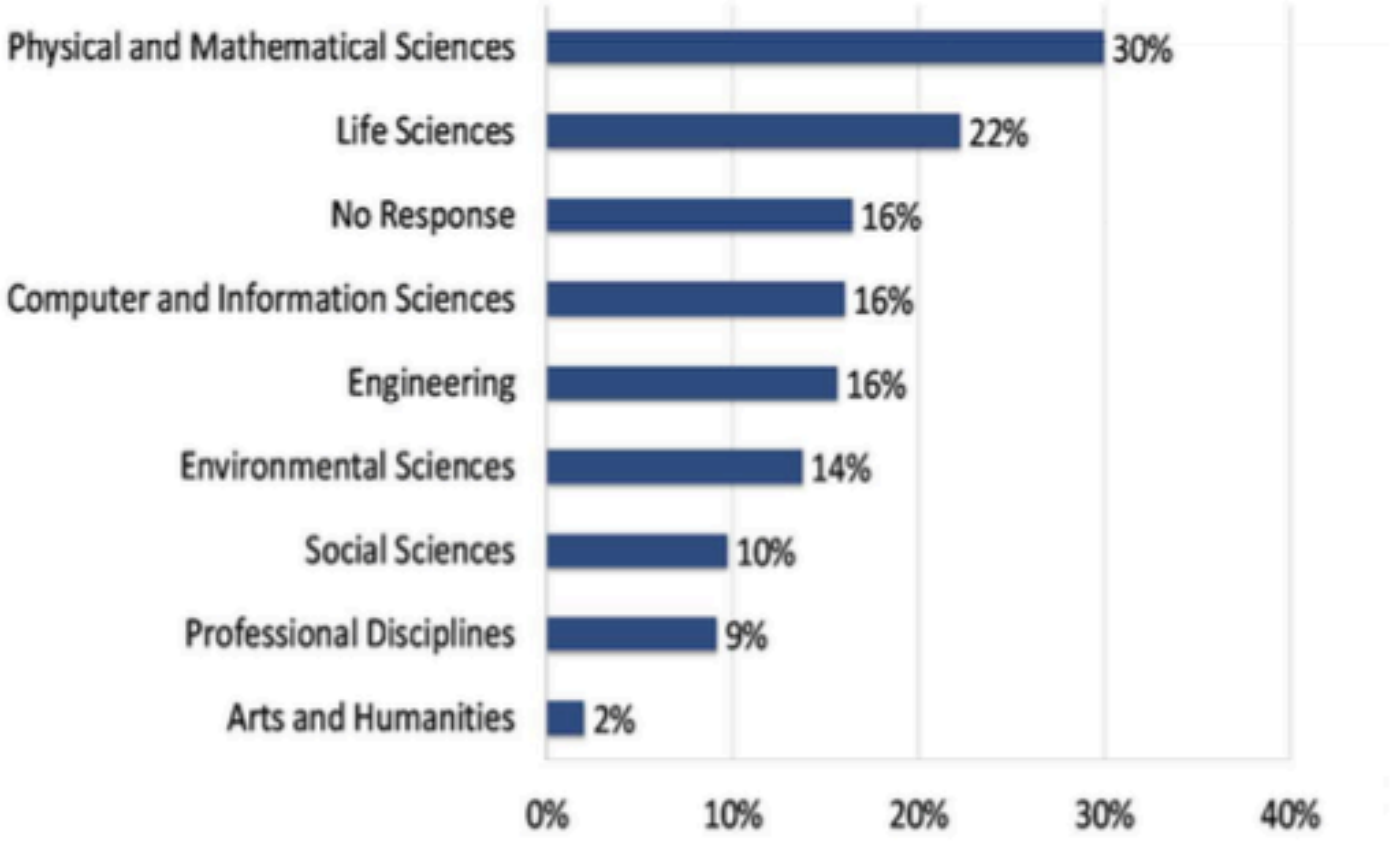


Gateways enable research, but are not research projects themselves

Science Gateways

Science Gateway Survey 2014

- 29,000-person survey
- 4957 responses from across domains

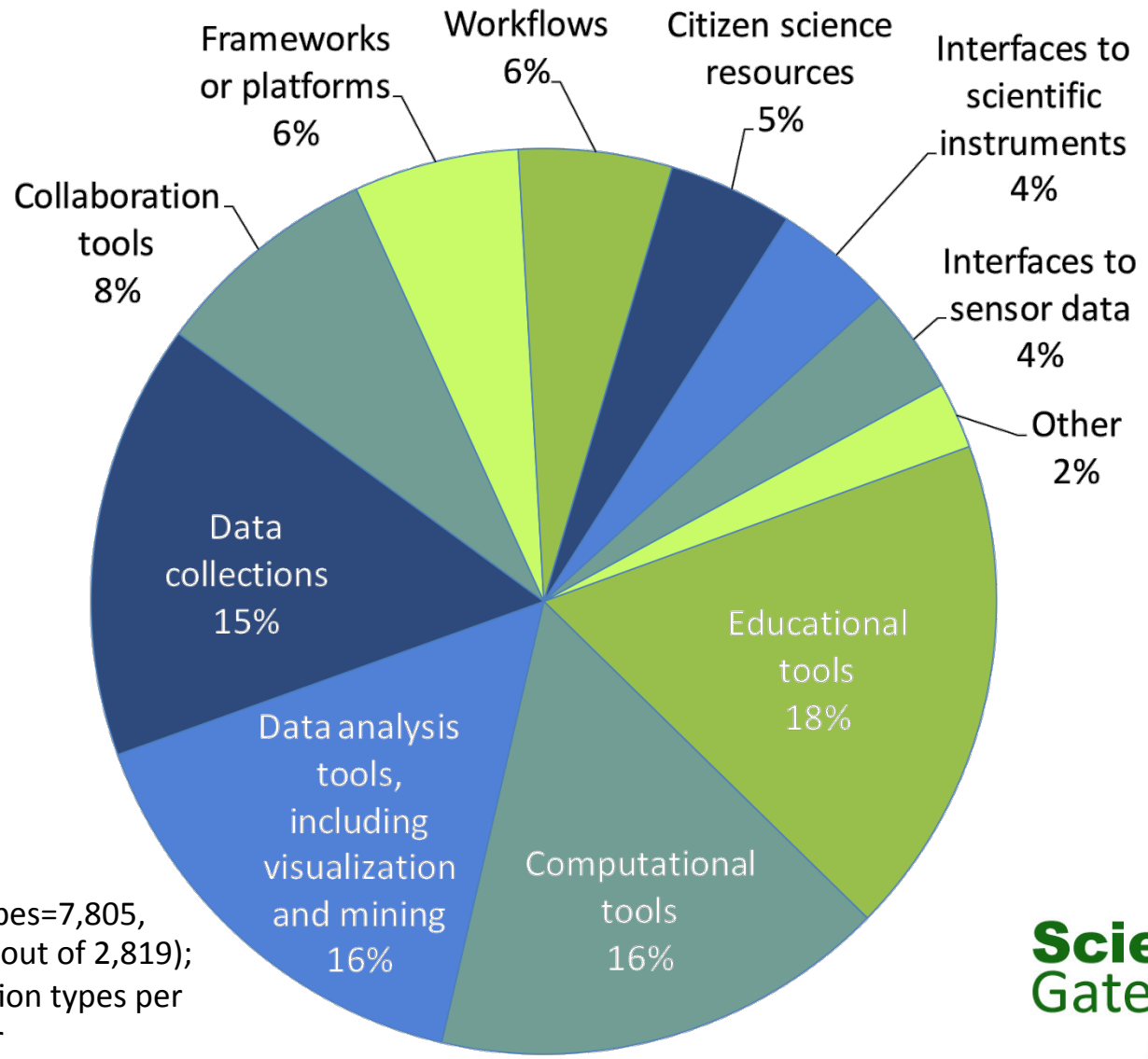


Science Gateway Survey 2014

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%

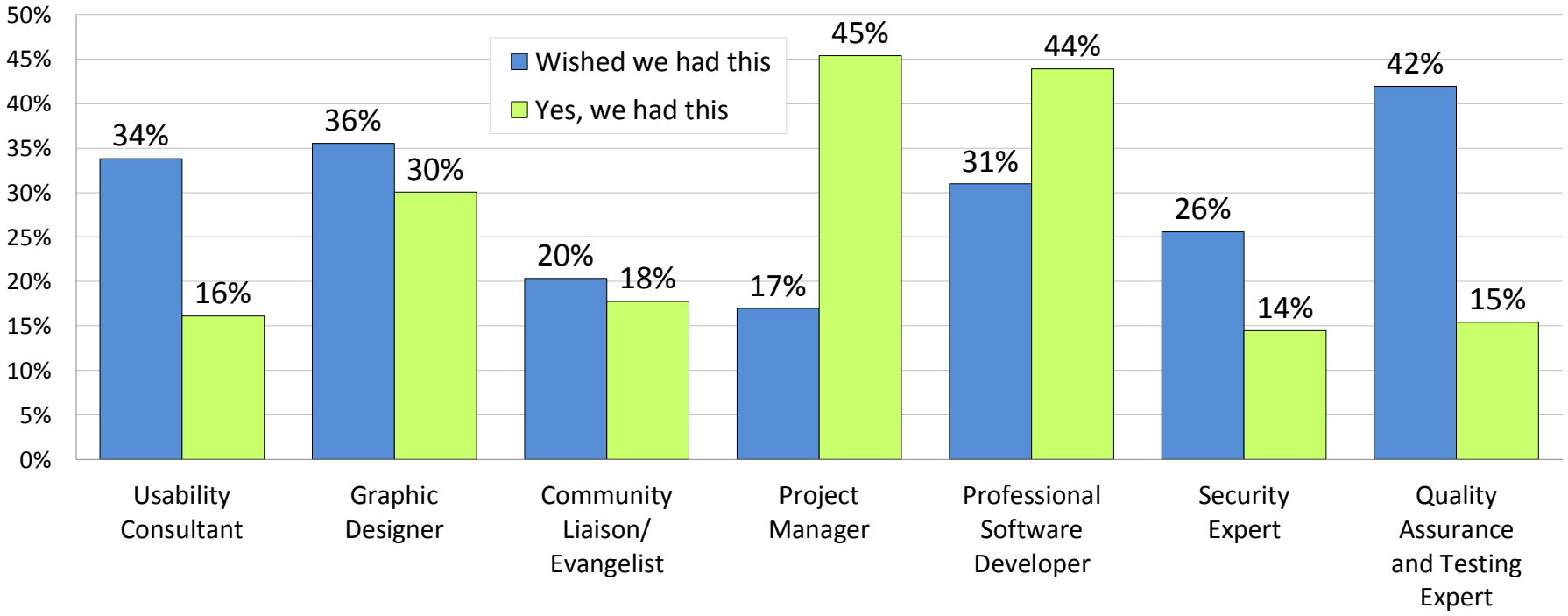
57% played some role in gateway creation
and these gateways were used for a variety of purposes



n of application types=7,805, by 2,756 creators (out of 2,819); mean=2.8 application types per application creator

Science Gateways

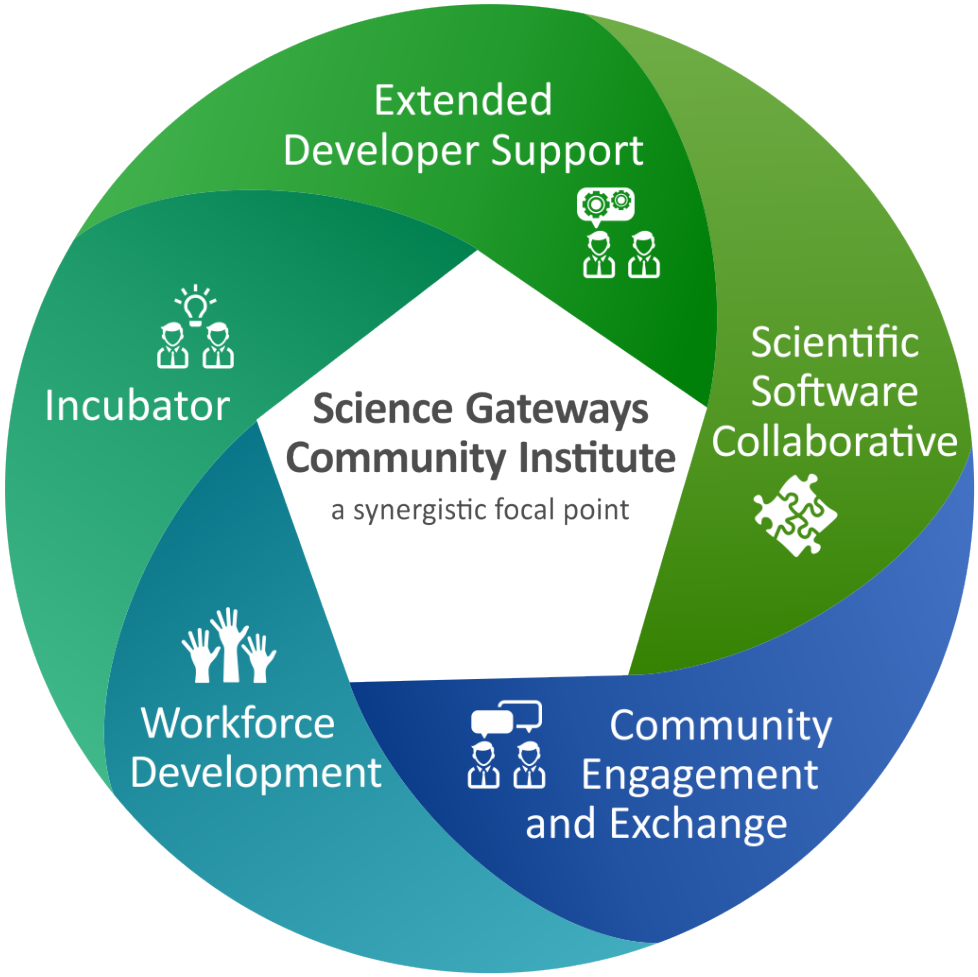
Well-designed gateways require a variety of expertise



n=2,756 respondents or 98% of application creators

Science Gateways

The 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

Science Gateways

Incubator Service

Expertise for the gateway lifecycle

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

Science Gateways

Extended Developer Support

Dedicated SGCI staff work directly with clients to build and enhance gateways

Focus

- Front-end development
- Gateways using all types of CI
- 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
Sensors

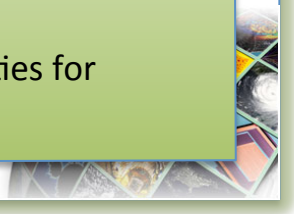
Airavata
HUBzero
AGAVE
Jupyter
Galaxy
And more…

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



Scientific Software Collaborative

Leveraging existing investments in gateway technologies

Give developers a *single destination for gateway software,* services and resources to easily build, maintain and manage science gateways.

- Create **more gateways** to advance scientific discovery, by making them easier to build
- Create **more researchers using gateways** by increasing awareness and number of gateways
- Enable NSF projects to **integrate** into the software institute and promote their products

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"

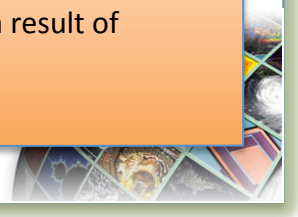
- API integration
- Variety of services
  - Information
  - Security
  - Execution
  - Data
  - Event
  - Accounting
- Hosting opportunity

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



Community Engagement and Exchange

Key to a successful institute

Gathering place for scientific web developers across NSF directorates, federal agencies, and international boundaries

- Community members are eager to connect

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

Gateways 2016 – a success with about 120 participants

Gateways 2016

Help make Gateways 2017 even better! Answer our conference evaluation now.

Did you attend a tutorial? Please evaluate it!

The 11th Gateway Computing Environments Conference (formerly GCE)
Wednesday and Thursday, November 2 & 3, 2016
Hosted at the San Diego Supercomputer Center in San Diego, California

Science gateways serve as connection points, assembling various components of advanced cyberinfrastructure—data collections, instruments, supercomputers, clouds, collaboration capabilities, and analytical tools—behind streamlined, user-friendly interfaces. They are typically a community-developed web portal or a suite of desktop applications. By providing access to top-tier resources, gateways enable researchers with a common goal as well as students and members of the broader community.

Gateway developers and users — regardless of their domain area — have a lot in common but have had few venues for exchanging experiences. The newly expanded Gateways annual conference (formerly the Gateway Computing Environments workshop series) will be an opportunity for gateway creators and enthusiasts to learn, share,

Watch the recorded keynotes and panel from Gateways 2016! Posted on our YouTube Channel.

Search

Search

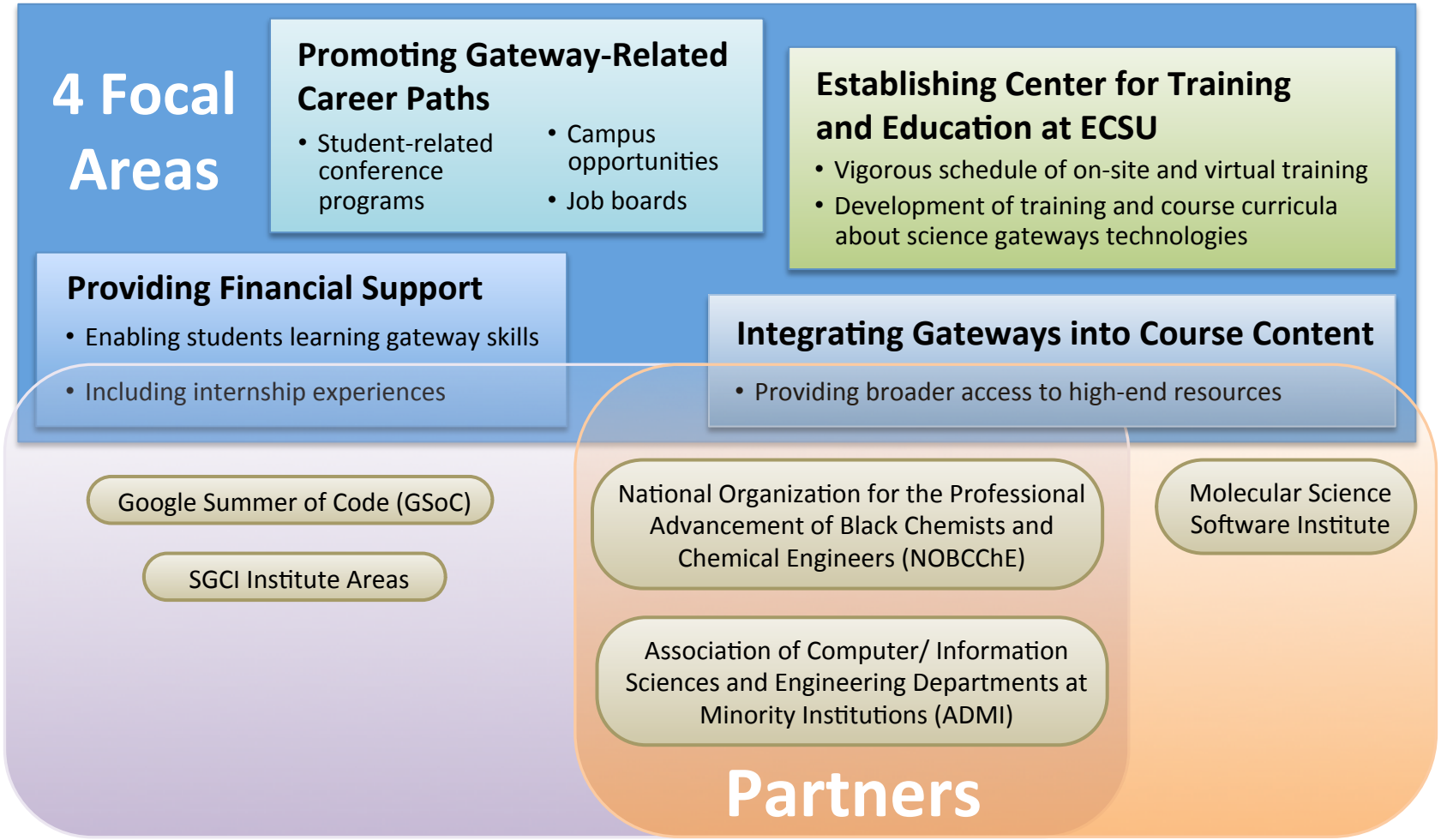
Related Pages

- Gateways 2016
  - Program
  - Presentation Abstracts
  - Registration, Lodging and Travel
  - Call for Participation
  - Resource Expo
  - Sponsorship
  - Presenter Information

Follow Us!

http://sciencegateways.org/gateways2016/

Workforce Development: Keep the best and the brightest in the sciences

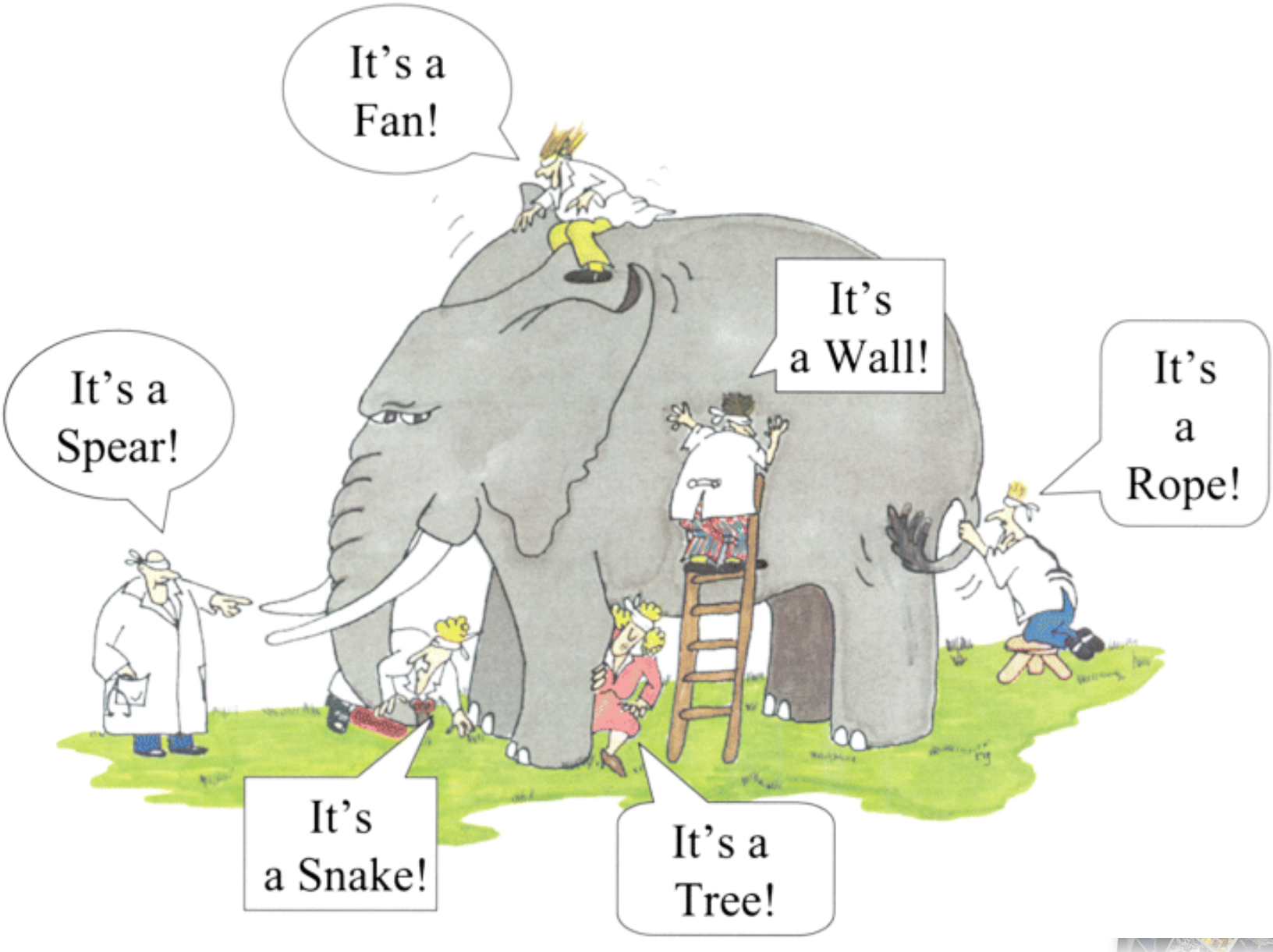


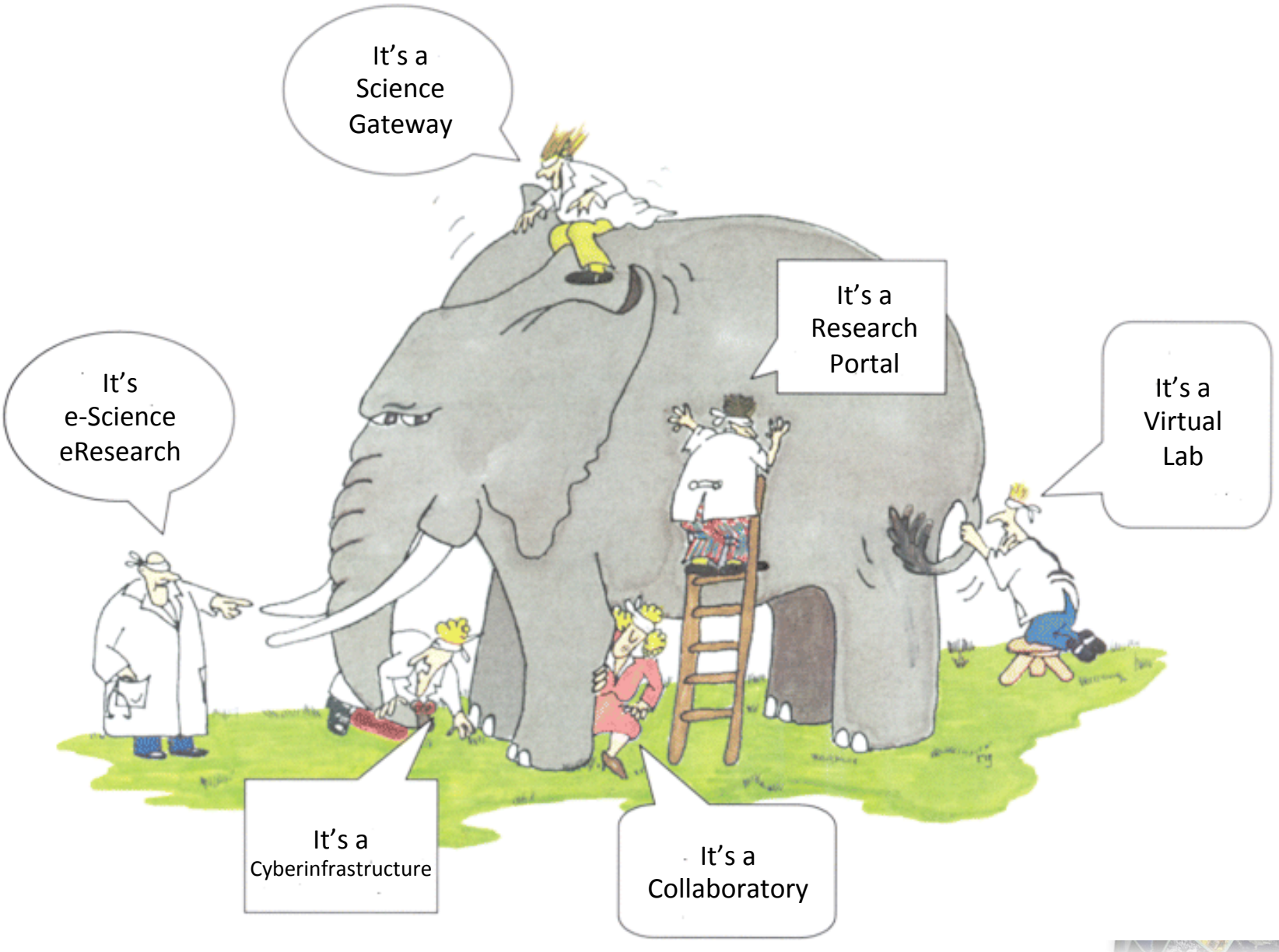
Opportunities

- 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

Challenges for SGCI

- Many researchers/developers are not aware that they need/create “Science Gateways”


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 e-Science eResearch
It's a Cyberinfrastructure
It's a Collaboratory

Challenges for SGCI

- Many researchers/developers are not aware that they need/create “Science Gateways”
- Sustainability beyond funding

Sustainability

- Sustainability plans should include securing expertise, manpower, talent, money
- Problems:
  - Universities/institutes would like to dictate the prices
  - PIs have their “day jobs” - maybe they don’t want to be entrepreneurs and they don’t want to start businesses
  - Research groups don’t have the money to pay or are not willing to pay
  - Software should be open access
- Distinguish between software and services
- Software is free and open access => Communities all over the world can set up their own instances but they also have to maintain it themselves for changes/adaptions and support for user communities
- Services should be chargeable: adaptions, support/maintaining community, usage of resources => a marketplace for services
- Services cannot handle discontinuity, this is bit different for software which is static and inherently has a longer shelf life

Sustainability

- Start as early as possible at the community to ask for money (small amounts) and have price tags from the beginning on services - even without charging - to make the community aware of the cost or show cost of comparable services sold in industry
- Incubator programs
- Achieve policy changes at universities/institutes to support sustainability via demands from funding bodies
- Technology transfer groups supported by state/funding bodies' individuals
- Using the ecosystem of companies writing STTR grants etc.
- Crowdfunding
- Career paths for developers
- on-campus developer groups
- Involving PhD students/postdocs

Challenges for SGCI

- Many researchers/developers are not aware that they need/create “Science Gateways”
- Sustainability beyond funding
- Attracting and selecting “right” customers

Customers of Training

Science Gateways

Challenges for SGCI

- Many researchers/developers are not aware that they need/create “Science Gateways”
- Sustainability beyond funding
- Attracting and selecting “right” customers
- Attracting partners to contribute to repository

Partners

- Often already existing open-access repository
- A larger audience probably means more customers, which might be too much for a support team

=> Solutions tailored to each partner!

Next Event

HICSS-50 Minitrack on Science Gateways and Portals (January 2017)

The Hawaii International Conference on System Sciences (HICSS-50) will be January 4-7, 2017, at Hilton Waikoloa Village on Hawaii's Big Island. We are organizing a Science Gateways and Portals minitrack at the conference. The conference provides a unique and highly interactive environment for researchers to exchange perspectives and ideas in various areas of information, computer, and system sciences.

Minitrack Details for ST: Science Gateways and Portals

January 5, 2016 from 4:00-5:30pm in Kohala 3

- "Science Gateways: The Long Road to the Birth of an Institute" by Sandra Gesing, Nancy Wilkins-Diehr, Maytal Dahan, Katherine Lawrence, Michael Zentner, Marlon Pierce, Linda Hayden, Suresh Marru
- "Maintaining a Science Gateway – Lessons Learned from MoSGrid" by Lukas Zimmermann, Richard Grunzke, Jens Krüger
- Panel on Science Gateways, including Maytal Dahan (SGCI), Jens Krüger (MoSGrid), Kelly Gaither (Texas Advanced Computing Center), and others

About the "Science Gateways and Portals" Minitrack

This Minitrack is part of the "Software Technology" track.

Science gateways are a community-specific set of tools, applications, and data collections that are integrated together via a web portal or a desktop application, providing access to resources and services for distributed data management and distributed computing infrastructures (DCIs). They offer easy and intuitive access to computing infrastructures and instruments irrespective of their location. The challenges in the area of gateways are manifold: from intuitive user interfaces and security features through efficient data and workflow management to parallelization of applications employing parallel and distributed architectures. In the last decade, quite a few

Team

Maytal Dahan

Maytal joined the Texas Advanced Computing Center (TACC) at The University of Texas at Austin in August 2002 as a Software Developer. She is involved in several software projects that develop middleware and web portal applications. Maytal is the project lead for the XSEDE User portal and managed the User Information and interfaces in XSEDE. Maytal was Co-PI […]

Sandra Gesing

Sandra Gesing is a research assistant professor and computational scientist at the University of Notre Dame. Previously, she worked as a research associate at the University of Edinburgh, UK, and at the University of Tübingen, Germany, where she also received her PhD. Additionally, she has extensive experience working as a project manager and developer in industry. Her […]

Linda Hayden

Dr. Hayden holds a PhD in Mathematics and Education. She is presently the Associate Dean of the School of Mathematics, Science and Technology at Elizabeth City State University, and the Director of the Center of Excellence in Remote Sensing Education and Research (CERSER). The CERSER program works in partnership with federal agencies, other universities and […]

Katherine Lawrence

Katherine Lawrence is an independent scholar affiliated with the University of Michigan School of Information. She collaborates with individuals and groups as a researcher, writer, educator, and facilitator. Her most recent research project was "Opening Science Gateways to Future Success," funded by the National Science Foundation's Office of Cyberinfrastructure. The goal of this project was […]

Suresh Marru

Marru leads the science gateway program in the XSEDE project. He is a Co-Principal Investigator on the NSF funded Open Gateway Computing Environments and leads the service oriented architectures and scientific workflow efforts. Marru is deeply involved in various Science Gateway efforts including GridChem, UltraScan, BioVLAB and OLAS projects. Earlier he was instrumental in success of the […]

Stephen Mock

Stephen Mock is director of Advanced Computing Interfaces (ACI) at the Texas Advanced Computing Center (TACC). Steve has been involved in developing web-based science gateways, portals, middleware, and web service APIs since 2000 for use in the high performance computing arena. He has worked on the iPlant Project, Agave, the XSEDE User Portal, the TACC […]

Marlon Pierce

I'm the assistant director at the Community Grids Lab at Indiana University. I lead projects in Grid Web Portal and Web Service application development to support Geographical Information Systems, earthquake modeling applications, and chemical informatics applications. And some other stuff. You may have noticed I got a promotion–maybe the blog helped. My full and short […]

Nancy Wilkins-Diehr

Nancy Wilkins-Diehr is Associate Director at SDSC and co-director of XSEDE's Extended Collaborative Support program. She has been involved in science gateways and their interfaces to high-performance computing since 2005. Nancy received her Bachelor's degree from Boston College in Mathematics and Philosophy and her Master's degree in Aerospace Engineering from San Diego State University. She has […]

Michael Zentner

Michael Zentner is a Senior Research Scientist at the Rosen Center for Advanced Computing (RCAC) at Purdue University working on visualization and data analysis. Prior to joining Purdue, he was founder/senior team member of several information technology companies, where he created innovative solutions for extracting patterns from data, collaboration, and constrained optimization. Dr. Zentner has […]

and more!

Acknowledgements

- The whole team of SGCI
- NSF award id 1547611

SGCI

Science Gateways
Community Institute

Thanks for your attention!

http://sciencegateways.org/

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