



Cyberinfrastructure Services from A to Z

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SGX3 Center of Excellence
HUBzero Platform
San Diego Supercomputer Center*

(software) Cyberinfrastructure

?

(software) Cyberinfrastructure

Software
Development

(software) Cyberinfrastructure

?

Software
Development

(software) Cyberinfrastructure

Technology
Planning

Software
Development

(software) Cyberinfrastructure

Technology
Planning

Software
Development

?

(software) Cyberinfrastructure

Technology
Planning

Software
Development

Dissemination
(at scale)

(software) Cyberinfrastructure

Technology
Planning

Software
Development

Dissemination
(at scale)

?

(software) Cyberinfrastructure

Technology
Planning

Software
Development

Dissemination
(at scale)

Sustainability

(software) Cyberinfrastructure

?

Technology
Planning

Software
Development

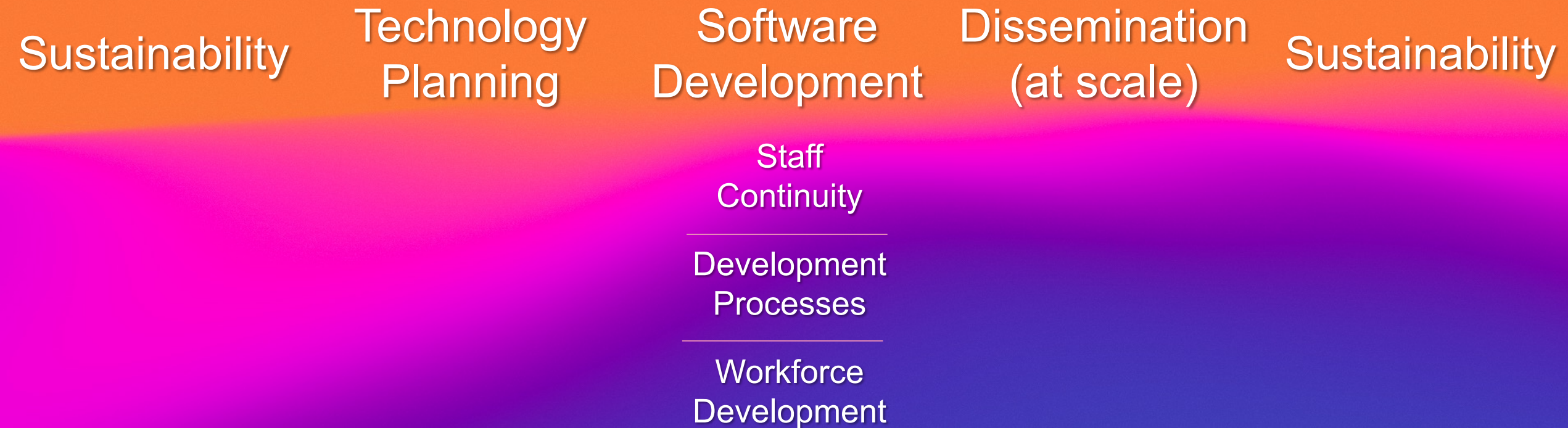
Dissemination
(at scale)

Sustainability

(software) Cyberinfrastructure



(software) Cyberinfrastructure



(software) Cyberinfrastructure



(software) Cyberinfrastructure



(software) Cyberinfrastructure



(software) Cyberinfrastructure



(software) Cyberinfrastructure



(software) Cyberinfrastructure Achieved through Pooled Service Organizations

Rev-Up

SGX3

hubzero

SDX

SGCI

Sustainability

Technology
Planning

Software
Development

Dissemination
(at scale)

Sustainability

Market Gap
Analysis

Software
Architecture

Staff
Continuity

Solution
Packaging

Marketing

User Pain
Point Analysis

User Experience
Design

Development
Processes

Community
Building

Selling

Financial
Viability

Technology Gap
Analysis

Workforce
Development

Mechanism of
Deployment

Maintaining &
Updating

SGX3



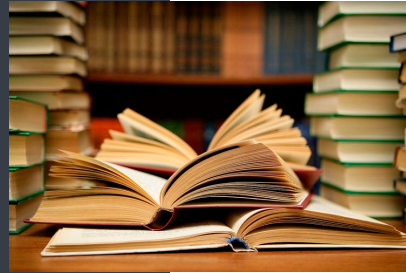
Rev-Up

revup@sdsc.edu

A programmatic approach to increase
non-commercialization based revenue
potential of software projects

Program Components

revup@sdsc.edu



Stage 1: Education

Teach fundamentals of project sustainability (like startups).

Stage 2: Consulting

Assist projects working through planning for sustainability (1-1 with experts).

Stage 3: Analysis

In depth analysis on revenue model and scaling issues.

Program Components

revup@sdsc.edu



Stage 1: Education

Teach fundamentals of project sustainability (like startups).

Stage 2: Consulting

Assist projects working through planning for sustainability (1-1 with experts).

Stage 3: Analysis

In depth analysis on revenue model and scaling issues.

Stage 4: Productionization

Development services by non-research team to make ready for production.

Stage 5a: Operation

Production operations support (infrastructure, customer service, etc.).

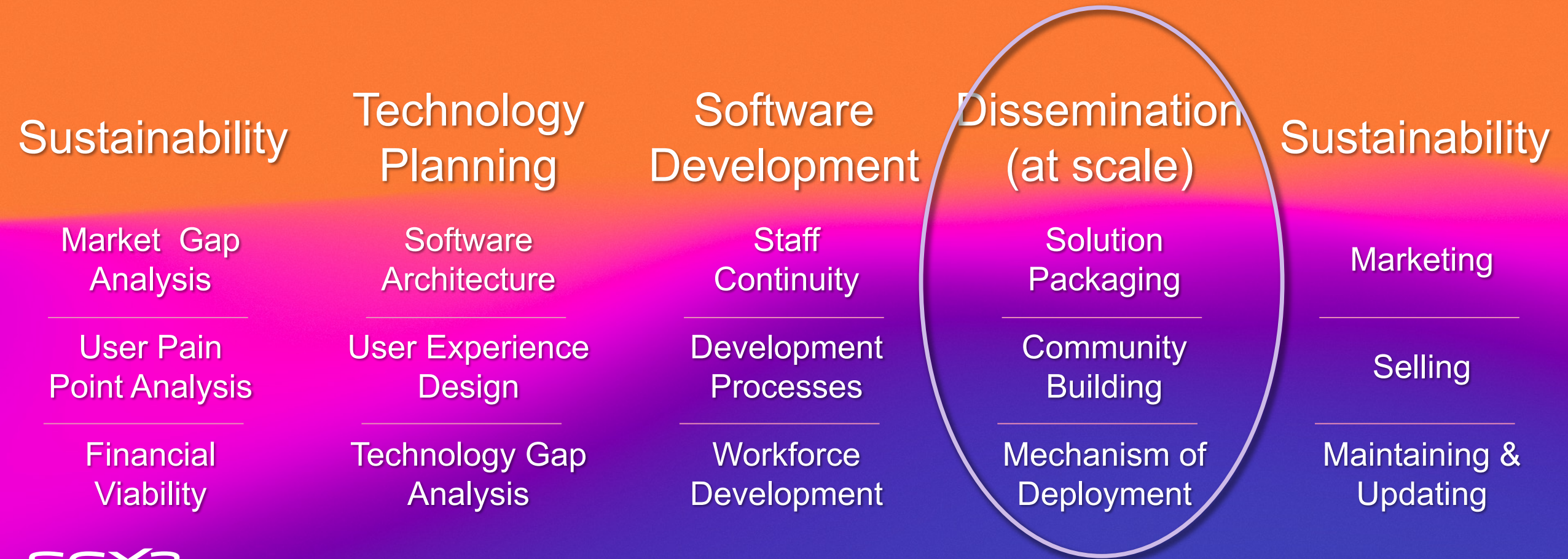
Stage 5b: Sales

Creation and operation of sales pipeline (prospect generation to deal closing).

Upfront

Afterward

(software) Cyberinfrastructure



Put it on a Science Gateway



1

You need users to become sustainable

2

Science Gateways are simple interfaces to gain more users and increase impact

3

Science Gateways can “share the load” among many investigators with many software packages

An abstract, colorful sketch of two hands reaching towards each other. The hands are rendered with thick, expressive lines and filled with vibrant colors like orange, red, green, and blue. The background is white with faint, sketchy outlines of the hands and fingers. The overall style is artistic and dynamic, suggesting a connection or interaction.

Science Gateways...

...are about web-based
platforms for scientific
connections.


```
document.getElementById(div).innerHTML = errMess;
else if (i==2)
{
    var atpos=inputs[i].indexOf("@");
    var dotpos=inputs[i].lastIndexOf(".");
    if (atpos<1 || dotpos<atpos+2 || dotpos>inputs[i].length-1)
    document.getElementById('errEmail').innerHTML = "Error";
    else
    document.getElementById(div).innerHTML = "OK";
}
```



Scientific Software to Supercomputers...


```
document.getElementById(div).innerHTML = errormsg;
else if (i==2)
{
    var atpos=inputs[i].indexOf("@");
    var dotpos=inputs[i].lastIndexOf(".");
    if (atpos<1 || dotpos<atpos+2 || dotpos>inputs[i].length-1)
    document.getElementById('errMsg').innerHTML = "Invalid email address";
    else
    document.getElementById(div).innerHTML = "Valid email address";
}
```



...to massive audiences of
researchers and students




```
document.getElementById(div).innerHTML += errormsg;
else if (i==2)
{
    div = divs[i];
    var atpos=inputs[i].indexOf("@");
    var dotpos=inputs[i].lastIndexOf(".");
    if (atpos<1 || dotpos<atpos+2 || dotpos>inputs[i].length-1)
    document.getElementById('errEmail').innerHTML += "Invalid email address  

else
    document.getElementById(div).innerHTML += "Valid email address";
}
```



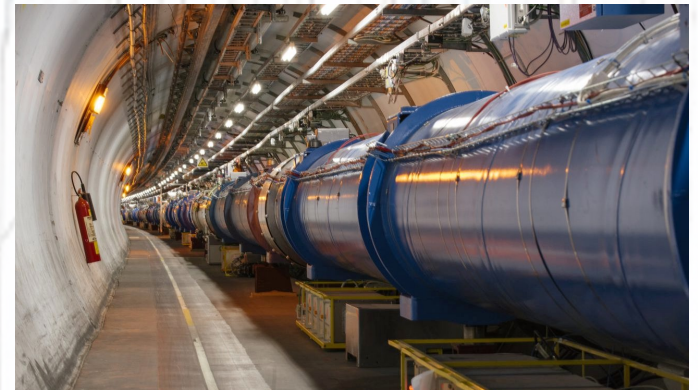
...to expensive instruments

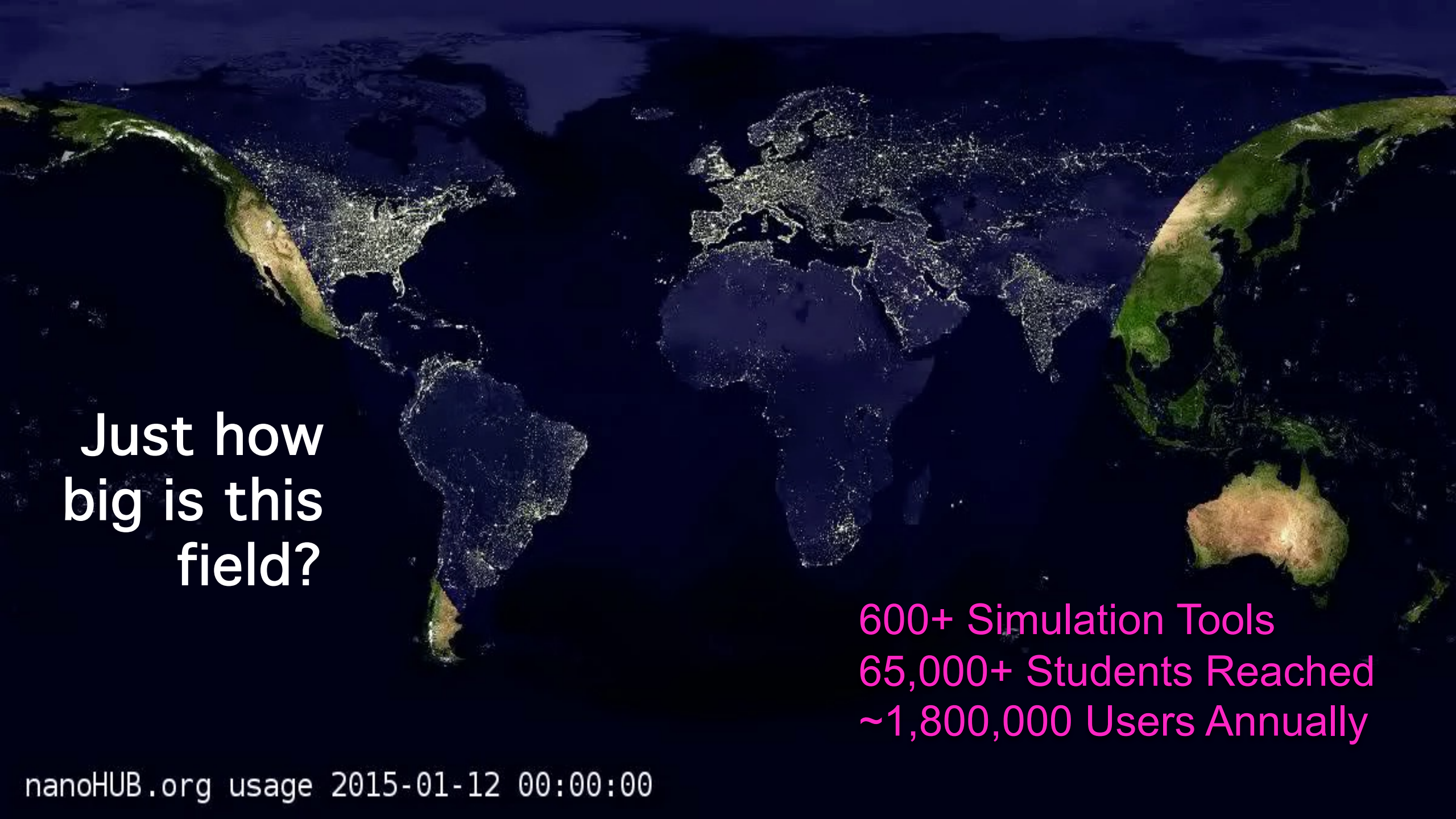



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}
```



...to data





Just how
big is this
field?

600+ Simulation Tools
65,000+ Students Reached
~1,800,000 Users Annually

Does it
matter?

Gateways
have direct
science
impact

CIPRES Science Gateway Usage Statistics 12

- 1.36 million TeraGrid/XSEDE jobs submitted by 39,831 unique users.
- Average of 506 new XSEDE users registered in each of the last 12 months.
- 130 million core hours of TeraGrid/XSEDE time distributed to scientists.
- Used for curriculum delivery by at least 114 instructors.
- Supported at least 6,000 publications.



- **Supported at least 6,000 publications.**

Does it
matter?

Gateways
have science
collaboration
impact

2431 vetted
citations

nanoHUB Citation Network (2000-2020)



Three distinct dot sizes indicate the level of influence on h-index
• Papers with relatively low secondary citations • Papers with potential to influence h-index ● Papers affecting the h-index

Does it matter?

Gateways have financial impact

PDB Archive contains >1 TB of Structure Data for Proteins, DNA, and RNA

The PDB Archive

- Grows at the rate of nearly 10% per year
- Used to download >2 million structure data files per day
- Managed by International collaboration US-Asia-Europe
- Manages "Big Data" as global Public Good

PDB Data

- Enable research in subject areas from Agriculture to Zoology (Analysis)
- Contributed data to nearly >1 million published research papers
- Used by >400 biological data resources

The cost to replicate the contents of the PDB archive is estimated at
\$16 billion (USD) (Analysis)

PDB Data Impact

- Basic and applied research
- Patent applications
- Discovery of lifesaving drugs
- Innovations that can lead to new product development and company formation
- STEAM education: PDB-101 provides curricula and online tools for teachers and students

>1,000,000 Data Consumers worldwide served every year

Researchers, scientists, educators, students, curious public, medical professionals, patients, and patient advocates

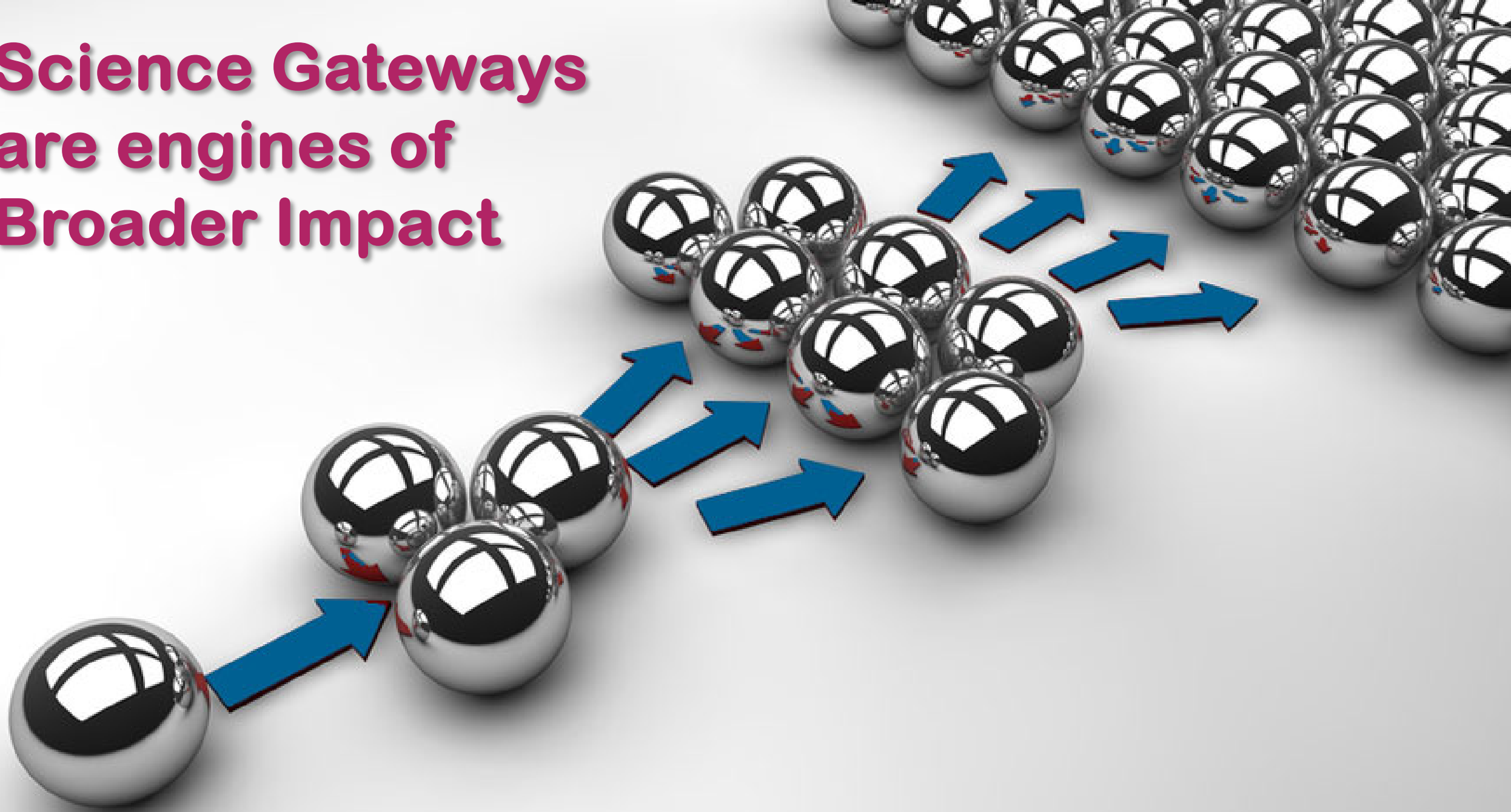
Public and Private sectors, including pharmaceutical and biotechnology companies

Generates return on investment of
~1,500 times federal funding
(Analysis)

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Generates return on investment of
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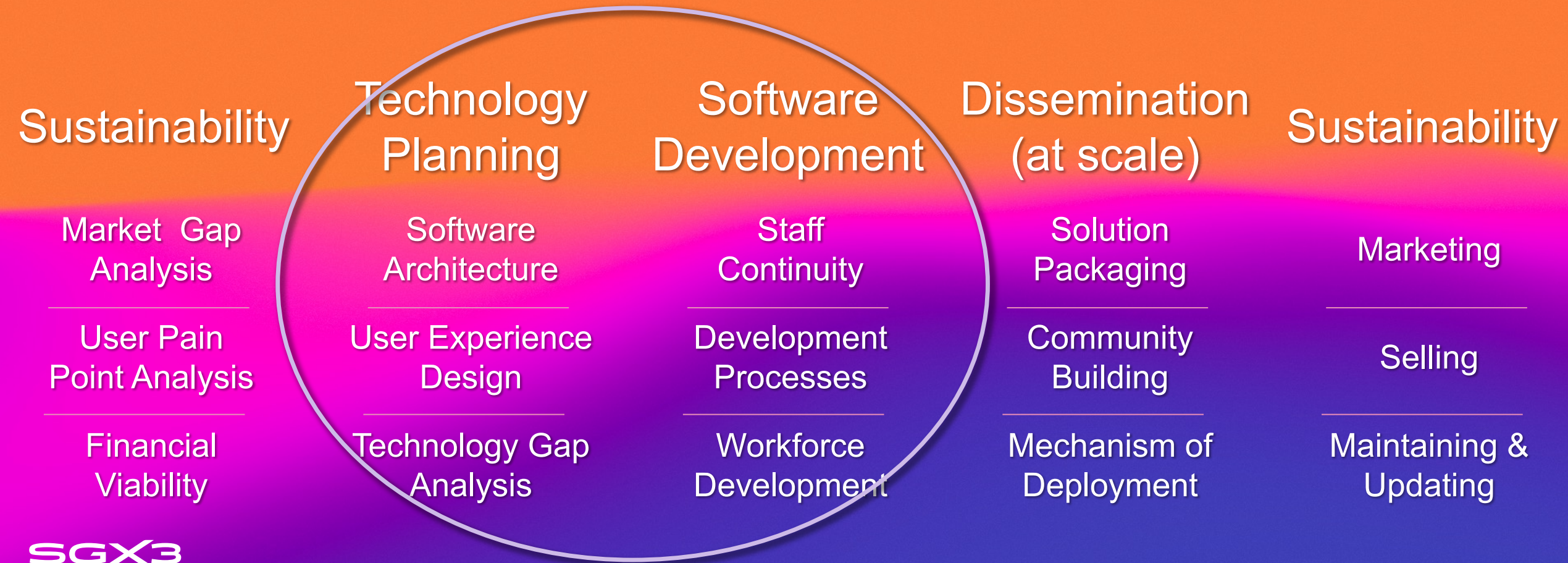
**Science Gateways
are engines of
Broader Impact**





**Science Gateways are
sustainability habitats
for scientific
applications, their
creators,
their users.**

(software) Cyberinfrastructure



hubzero

Building Gateways Since 2002

Functional Capabilities of the HUBzero Science Gateway Platform

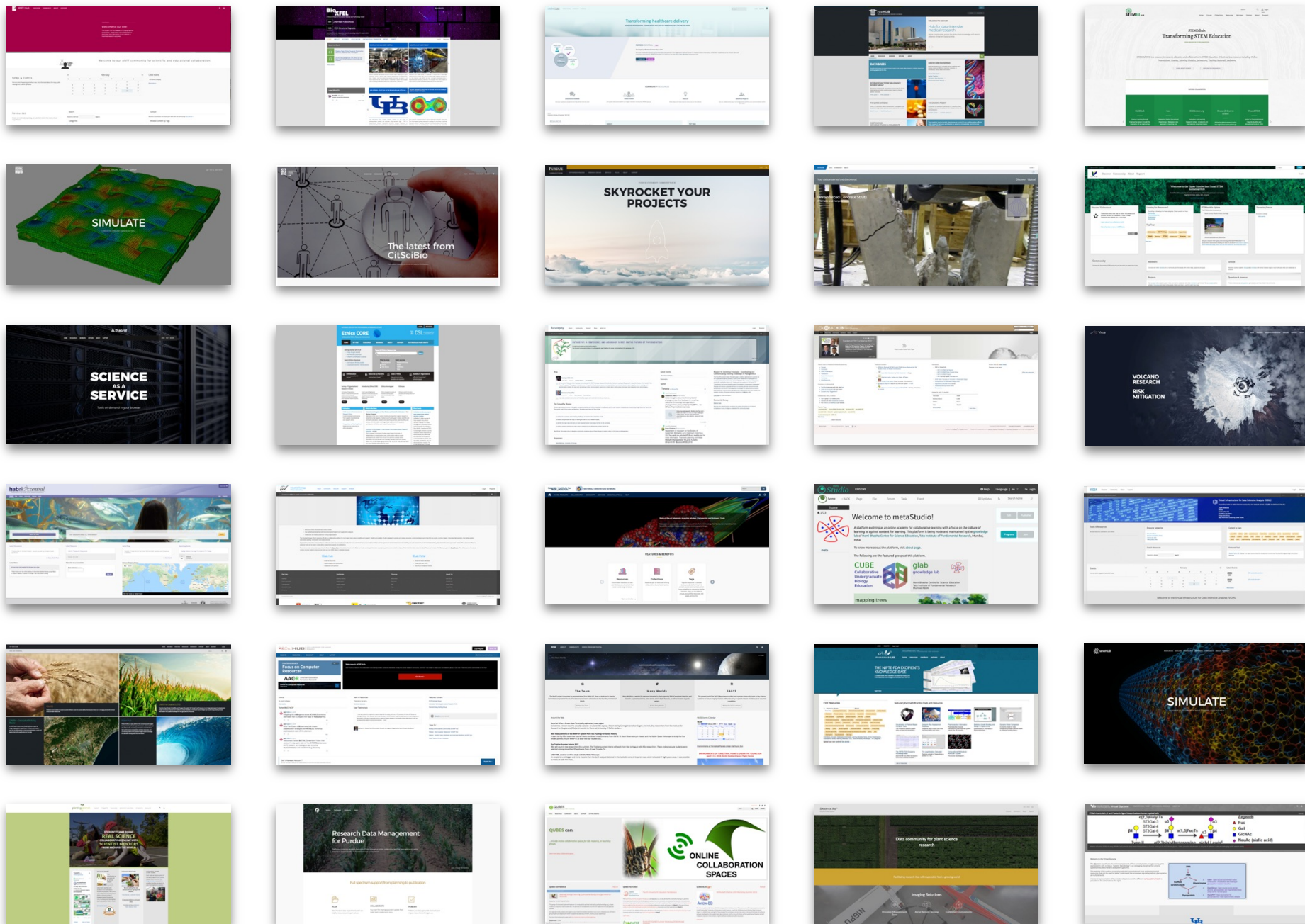
Community
Interaction / Collaboration

Knowledge
Dissemination /
Publication

hubzero

Resource, Data, Analytics &
Application Sharing

Many hubs
operated
20+
Disciplines
18
Organizations
+ others in
opensource
environments
hubzero



Customized Application Development

hubzero

hubzero

— [ABOUT](#) [ENGAGE](#) [SERVICES](#) [NEED HELP?](#)

Bring your software
to the web

Sponsored Research Projects

Have HUBzero be part of your team

New capability development

Intellectual contribution

Broader impact

CHECK IT OUT

No Hassle Hub

Cost effective
Continuous upgrades
Continuous security monitoring
Continuous patching
Dedicated community manager representative

CHECK IT OUT

Open Source

No cost
Modify the code yourselves
Host on your machine

CHECK IT OUT

CHECK IT OUT

CHECK IT OUT

No Hassle
Hub Service

Can be HIPAA
Aligned
Where
Needed

Bring your software
to the web

No Hassle Hub

- Cost effective
- Continuous upgrades
- Continuous security monitoring
- Continuous patching
- Dedicated community manager representative

CHECK IT OUT

No Hassle Hub

- Cost effective
- Continuous upgrades
- Continuous security monitoring
- Continuous patching
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CHECK IT OUT

Open Source

- No cost
- Modify the code yourselves
- Host on your machine

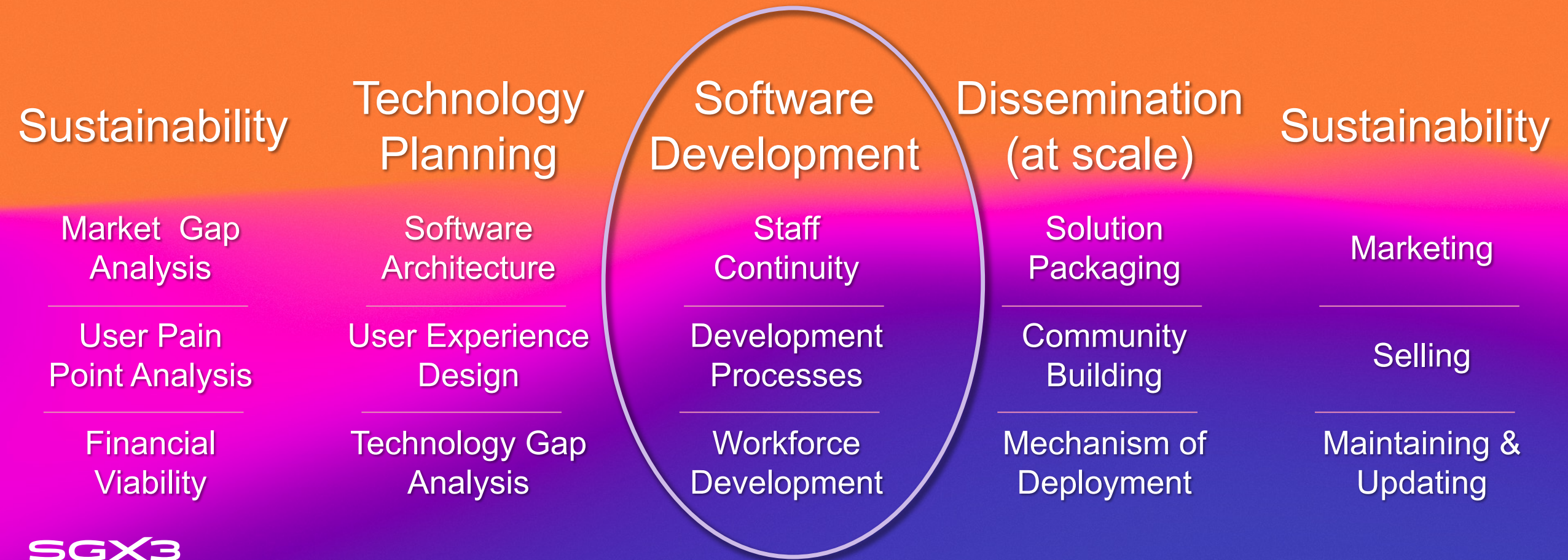
CHECK IT OUT

CHECK IT OUT

CHECK IT OUT

Less than 1/3 the cost of an FTE

(software) Cyberinfrastructure



hubzero

Building Gateways Since 2002

hubzero

Building Gateways Since 2002

Supporting (some) Code Since
2002

The Hubzero logo, featuring the word "hubzero" in a green, lowercase, sans-serif font. The letter 'b' is stylized with a circular arrow around it.

Responsible for the
product ownership of
the Hubzero® Platform



Responsible for
professional
development and
operations of Hubzero
based science
gateways AND other
software CI efforts

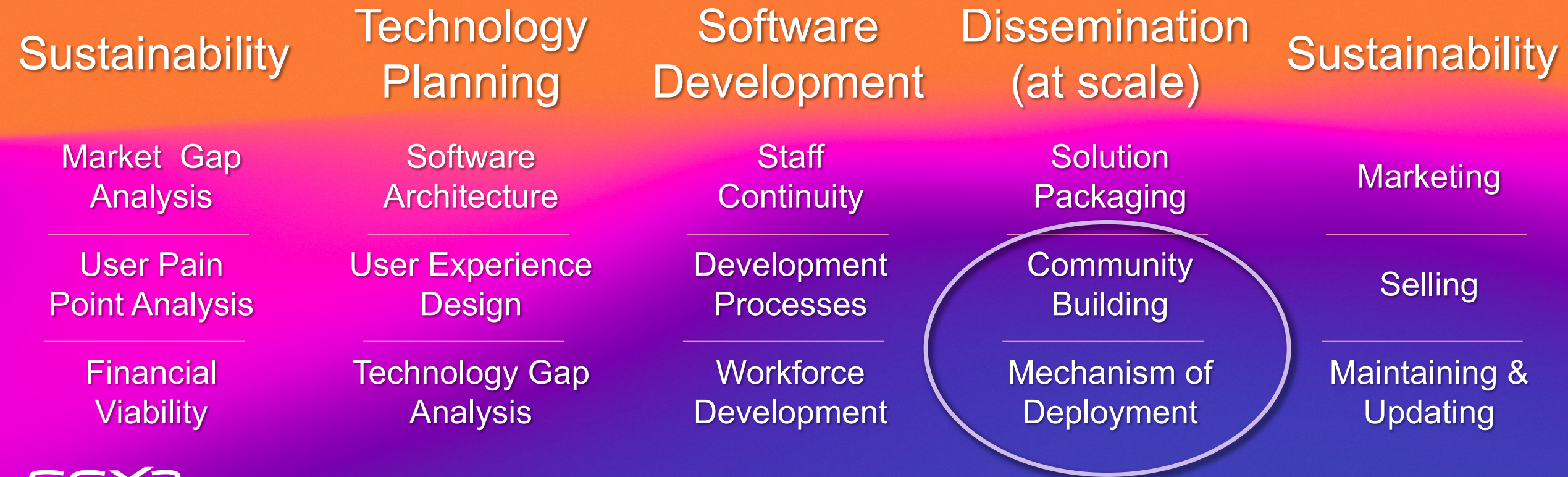
The logo for hubzero, with 'hub' in a bold, rounded green font and 'zero' in a thinner, rounded green font.

A platform as leverage
for science gateway
creation

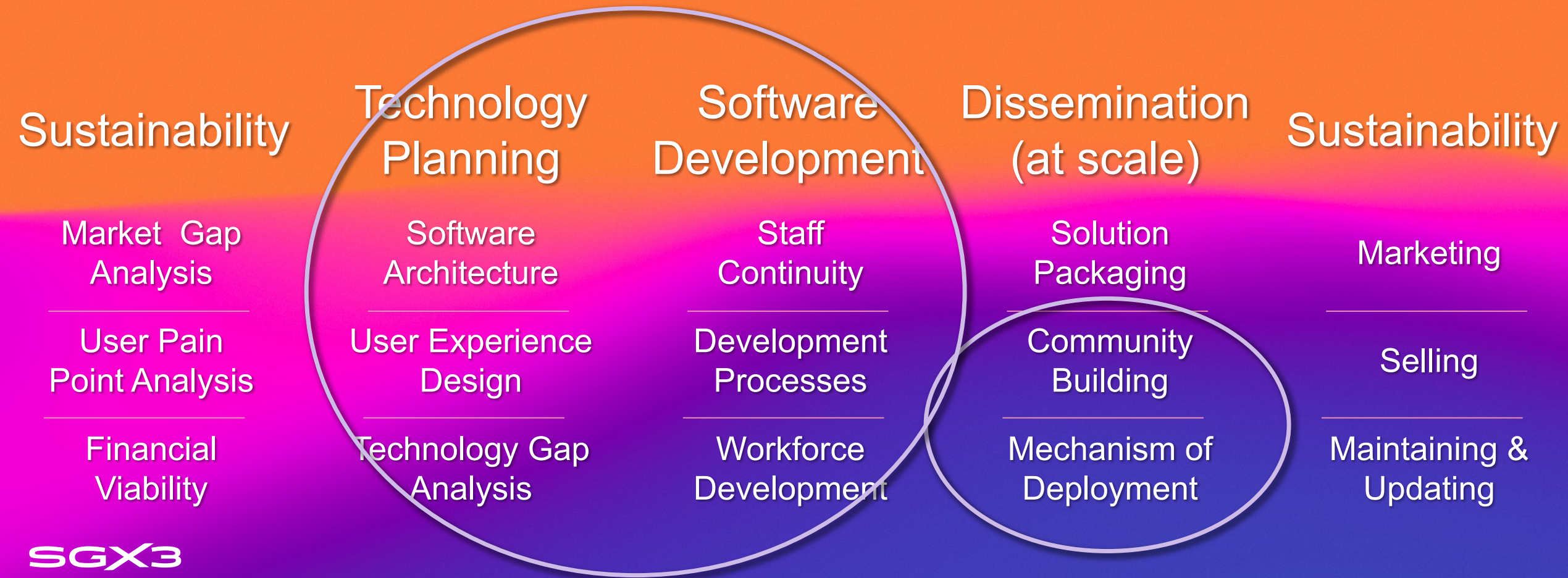


A team with
sustainable
development practices
and team continuity
for software CI
projects

(software) Cyberinfrastructure



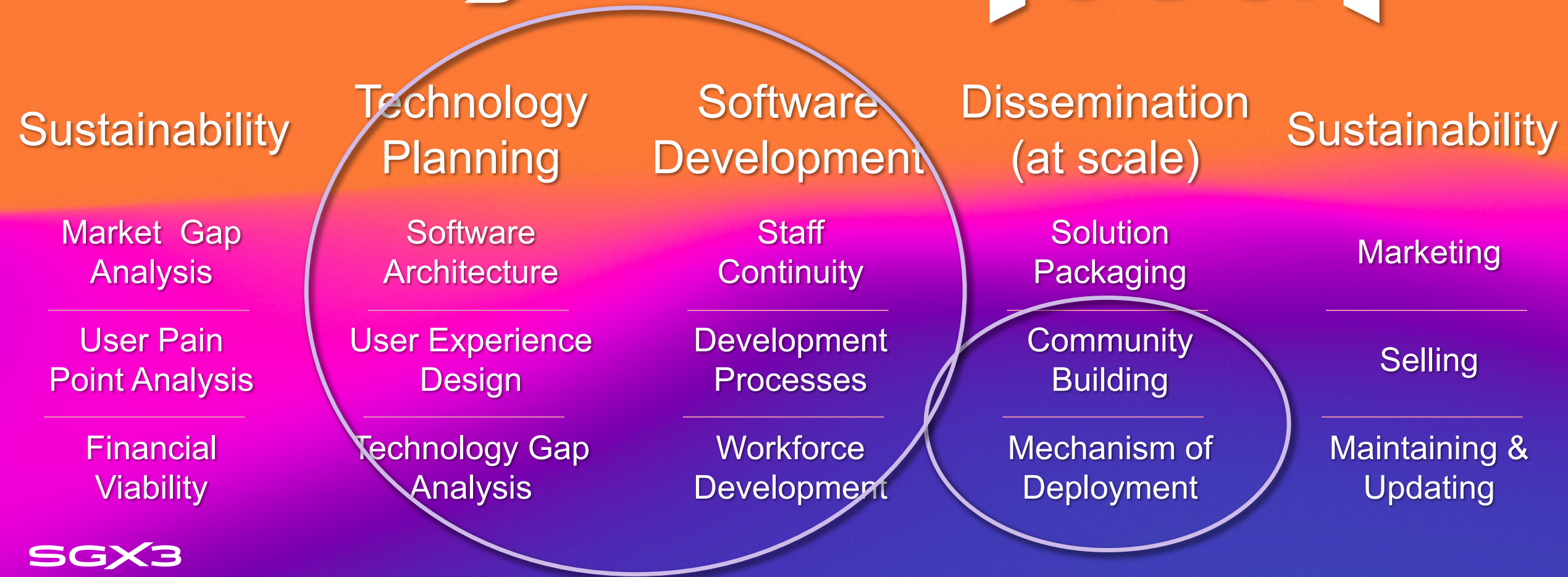
(software) Cyberinfrastructure



(software) Cyberinfrastructure

SGX3

SGCI





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



Science Gateways Community Institute

sciencegateways.org

Award Number
ACI-1547611





Fortunately
you are not
alone.

A banner for the Science Gateways Catalog. The background features a collage of scientific images: a colorful, swirling pattern on the left, a satellite map of a coastal area on the right, and a deep-space image of a galaxy at the bottom left. The SGCi logo is prominently displayed in the upper center, with the text 'Science Gateways Community Institute' to its right.

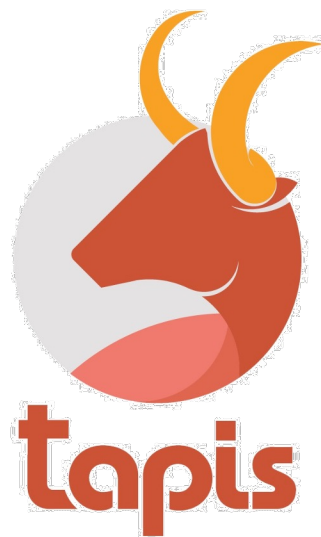
Science Gateways Catalog

Total Entries: 600





Fortunately
you are not
alone.



hubzero





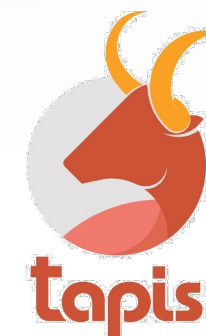
UNfortunately
you are not
alone.



hubzero

Science Gateways Catalog

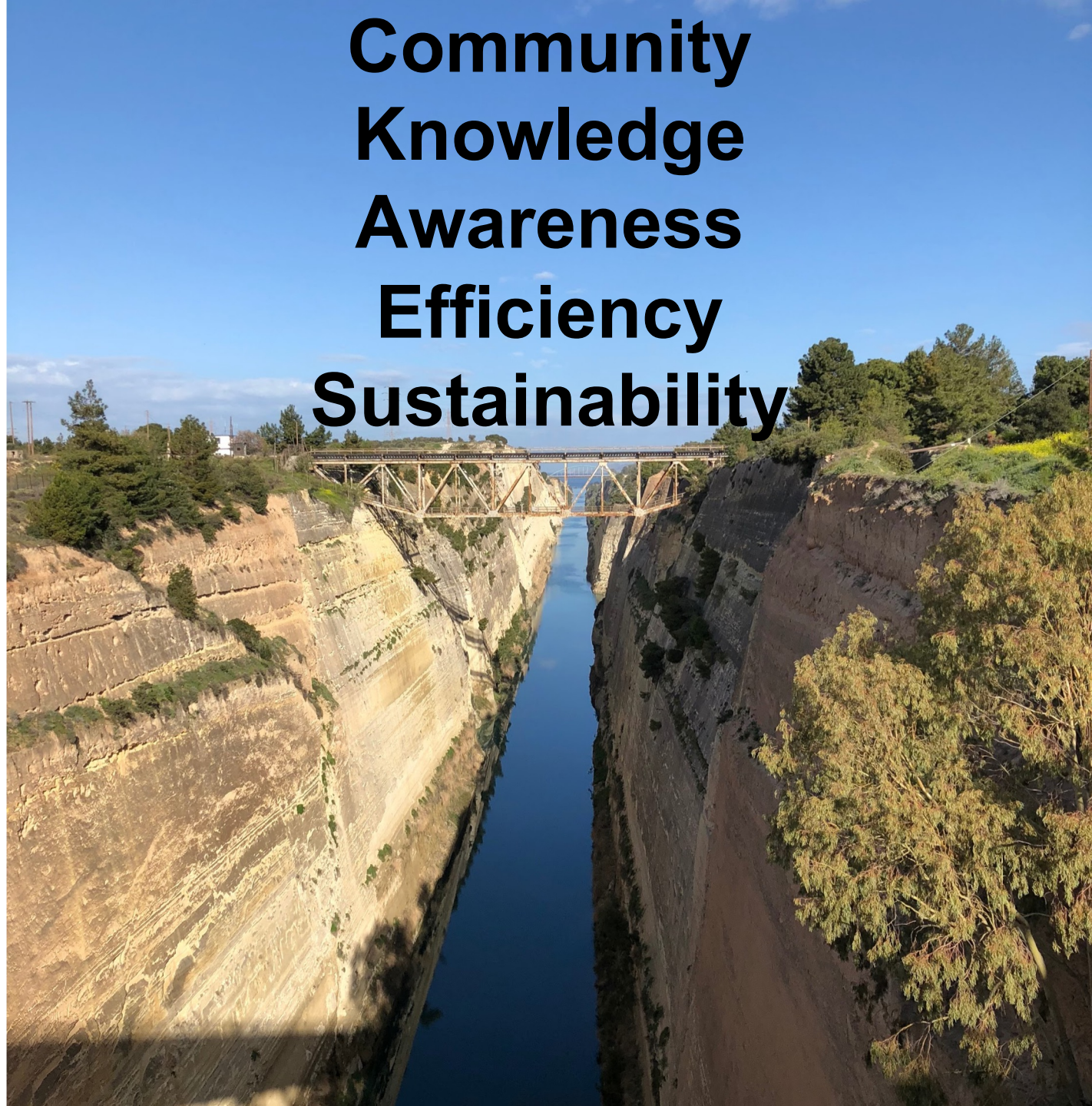
Total Entries: 600



“How hard can it be? It’s just a web site.”



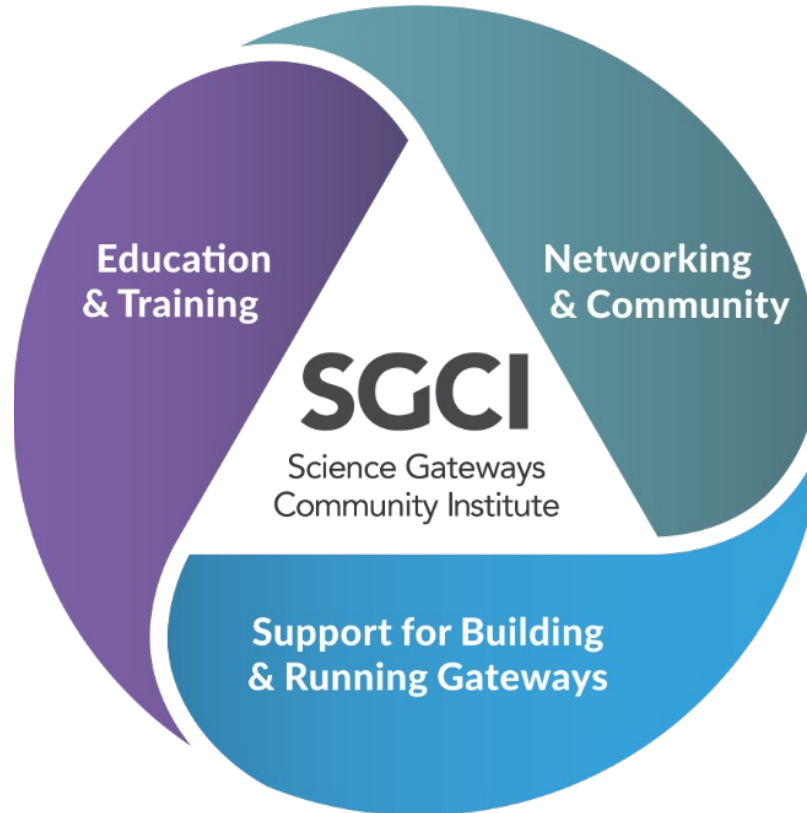
The formation of
an institute...
to bridge gaps and
institutionalize
best practices



An Overview of the Science Gateways Community Institute



- Website Resources & Materials
- Webinar Series
- Gateway Focus Week
- Student-focused Internship and Hackathon Programs
- Certificate / Educational Programs



- Partner Program
- Affiliates Program
- Blog, News & Job Postings
- Community Forum
- Annual Conference
- Community Consensus Tech Forum

- Hands-on Development Support
- Usability Design / Analysis
- Operations & Sustainability Advice from Consultants
- Cybersecurity Consulting
- Catalog of Gateways & Software

sciencegateways.org





An Overview of the Science Gateways Community Institute

- Website Resources & Materials
- Webinar Series
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Final Year of NSF Funding

- Partner Program
- Affiliates Program
- Blog, News & Job Postings
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sciencegateways.org



SGX3

Extend. Expand. Exemplify.

A Center of Excellence to Extend Access, Expand the Community,
and Exemplify Good Practices for CI through Science Gateways.

Award
#2231406



SGX3

So SGCI got more funding then huh?

SGX3

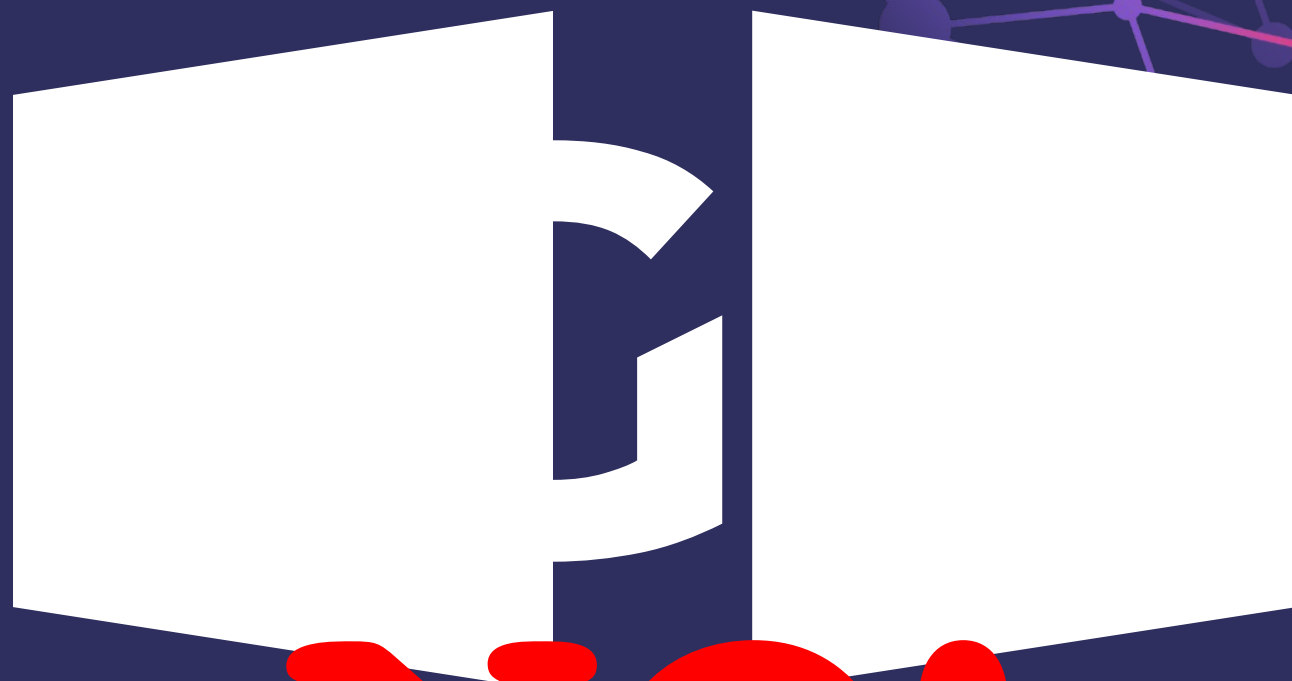
So SGCI got more funding then huh?

NO!

An abstract network graphic in the top right corner, featuring a complex web of interconnected nodes and lines. The nodes are colored in shades of purple, blue, and pink, and the lines are thin and light blue.

ISGCI





NO!





Science Gateways
Community Institute

Connecting People
Creating Solutions
Accelerating Discovery

A network diagram consisting of a complex web of interconnected nodes and lines. The nodes are represented by circles in various shades of blue, purple, and pink, and the lines connecting them are thin, colored lines. The overall effect is a dense, interconnected mesh.

SGCI has facilitated some great impact stories and has shown an on average 7x acceleration in gateway development.

(if you don't want to take the storybook with you please leave at the front desk)

SGX3



ISGC

A Center of Excellence and a Software Institute to
serve the Science Gateways Community.

Helping...

- Community Focused
- Workforce Focused
- Future Focused
- Working Toward Preparing for the Future

Building...

- Development Service Focused
- Operations Service Focused
- Heavy Touch Consulting
- Working Toward Self-Sustainability



A new Cyberinfrastructure Center of Excellence for Science Gateways

SGX3 – NSF Funded

- ✓ Community building activities
- ✓ Workforce development activities
- ✓ Light-touch consulting / advisory services
- ✓ Envisioning the future through Blueprint Factories
 - ✓ ACCESS
 - ✓ PATH
 - ✓ Materials Genome Initiative
 - ✓ Sustainability practices
 - ✓ more to come...

SGCI – Client Funded

- ✓ Heavy-touch consulting / other services
- ✓ Software team augmentation / outsourcing
- ✓ Professional science gateway operations

(software) Cyberinfrastructure Achieved through Pooled Service Organizations

Rev-Up

SGX3

hubzero

SDX

SGCI

Sustainability

Technology Planning

Software Development

Dissemination (at scale)

Sustainability

Market Gap Analysis

Software Architecture

Staff Continuity

Solution Packaging

Marketing

User Pain Point Analysis

User Experience Design

Development Processes

Community Building

Selling

Financial Viability

Technology Gap Analysis

Workforce Development

Mechanism of Deployment

Maintaining & Updating

(software) Cyberinfrastructure Achieved
through Pooled Service Organizations

Rev-Up
SGX3

hubzero

SDX
SGCI

SGX3