

Cyberinfrastructure for Research: From campus growth to national trends (Parts I & III of III)

Craig A. Stewart

ORCID ID 0000-0003-2423-9019

Jetstream Principal Investigator

Executive Director, Indiana University Pervasive Technology
Institute

Associate Dean, Research Technologies

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Introduction and outline

- Goal of this talk: Provide information that will help the effort to “propel MSU higher up the Research Computing landscape” (from Sharan Kalwani’s morning talk) & help MSU turn those advances in computing into advances in discovery
- What is cyberinfrastructure, anyway?
 - First used in security briefing by Richard Clark in 1998
 - Cyberinfrastructure consists of systems, advanced instruments and data repositories, visualization environments, and people, all linked together by software and high-performance networks to improve research productivity and enable breakthroughs not otherwise possible.
- Outline
 - A bit of IU history
 - Some thoughts about the current technology environment
 - Nationally accessible resources (effort, but no \$\$ needed)
 - Cyberinfrastructure as an ecosystem problem
- Note: slides will be posted online within a day or two



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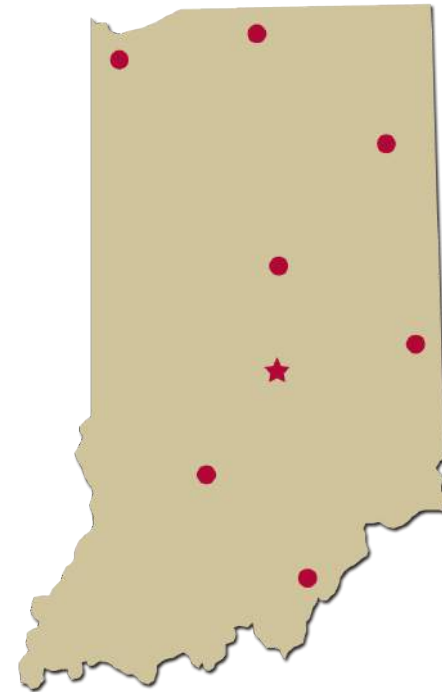


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IU – Founded in 1820

| Campus | Academic appointees | Nonacademic Staff | Undergrad Students | Grad. & Prof. Students |
|---------------|---------------------|-------------------|--------------------|------------------------|
| IUB | 2,942 | 5,379 | 32,371 | 9,762 |
| IUPUI | 3,895 | 4,449 | 22,271 | 8,180 |
| IU Northwest | 425 | 243 | 5,636 | 548 |
| IU South Bend | 542 | 305 | 7,860 | 630 |
| IU East | 267 | 159 | 4,052 | 134 |
| IP Fort Wayne | N/A | N/A | N/A | N/A |
| IU Kokomo | 191 | 138 | 3,581 | 138 |
| IU Southeast | 498 | 243 | 6,203 | 701 |
| Totals | 8,760 | 10,916 | 81,974 | 20,093 |



IU Health Patient Metrics – 2012/2013

| | |
|-------------------|-----------|
| Admissions | 143,219 |
| Outpatient visits | 2,244,320 |
| Staffed beds | 3,326 |



Indiana University Health



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Strategy Matters

- IU Goals
 - To be a leader, “in absolute terms for uses and applications of IT.” (1996, Myles Brand, IU’s 16th President)
 - To be one of the great public universities of the 21st Century. (2008, Michael A. McRobbie, IU’s 18th President)
- Achieving these goals requires changes in infrastructure, funding, technology, and culture.
- “Culture eats strategy for breakfast” – but only if you are not careful about pace, timing, and tactics. With the right tactics and enough time strategy can change culture.



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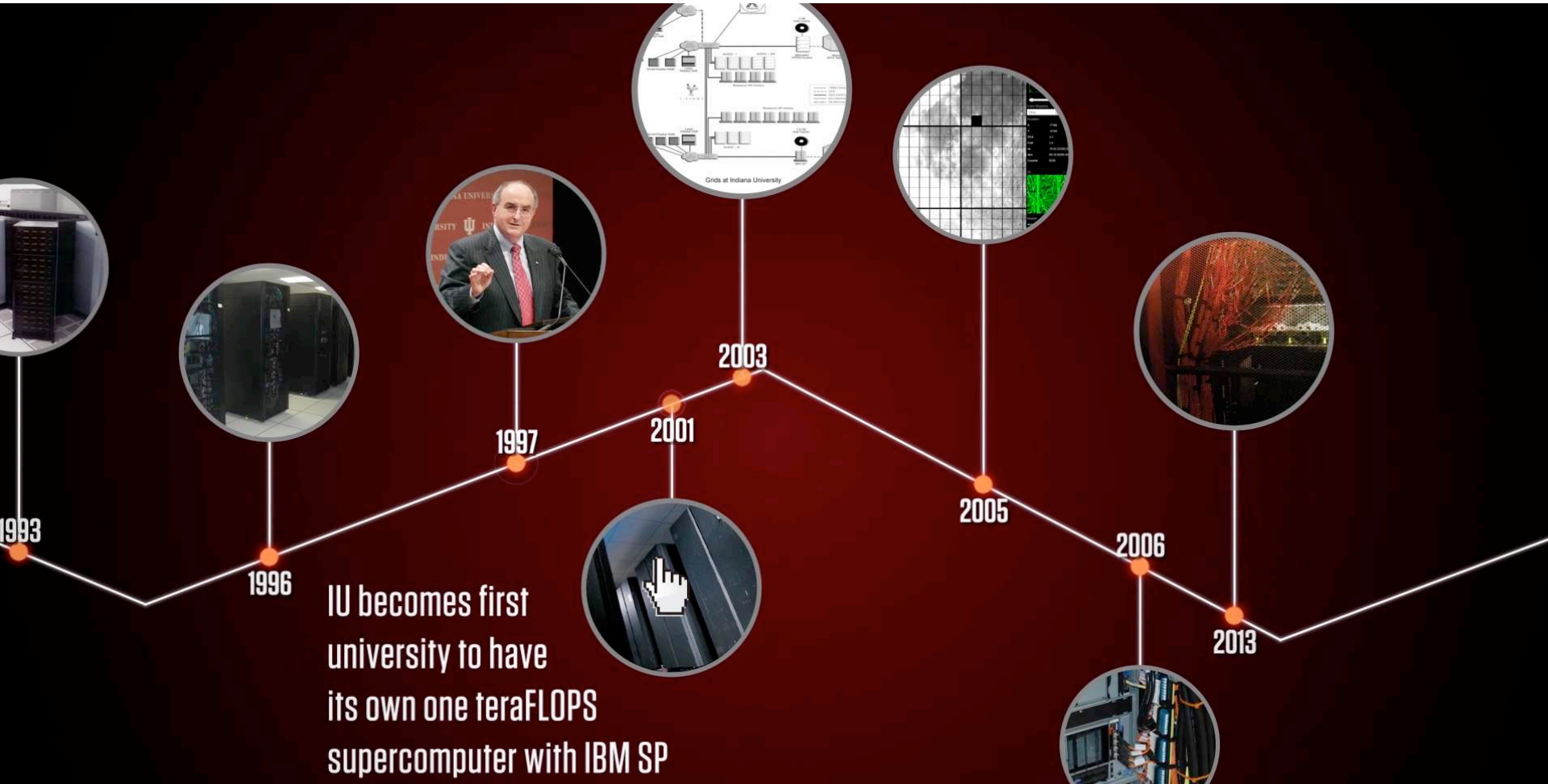
- Goals (draft)
- Enhance quality and quantity of research done at IU by providing an excellent research computing environment which both responds to needs and creates new possibilities for IU's researchers. [Partnering making new types of research possible]
 - ? Achieve national prominence in research computing, enabling this to be an area of competitive advantage for IU
 3. Provide ~~rese~~ leadership in ~~use~~ deployment + use of new computing technologies

From Research and Academic Computing retreat in 1997 – in midst of UITS formation

Goals (Draft)

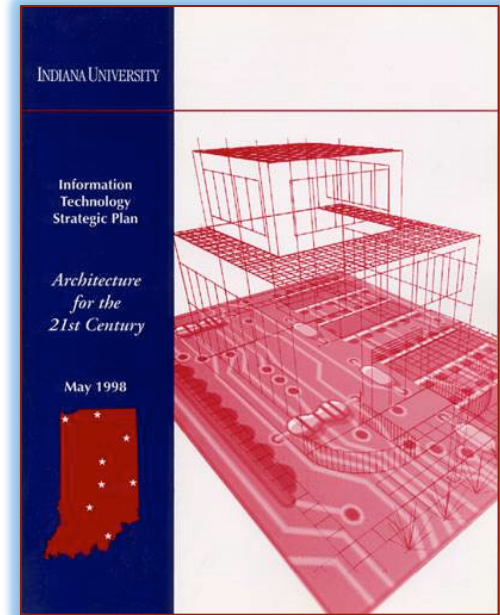
1. Enhance quality and quantity of research done at IU by providing an excellent research computing environment which both responds to needs and creates new possibilities for IU's researchers. [Partnering making new types of research possible]
2. ?Achieve national prominence in research computing, enabling this to be an area of competitive advantage for IU?
3. Provide leadership in deployment and use of new computing technologies

- 1996: Everyone at IU who knows how to use a supercomputer fits in a small conference room.
- 1997: *“Why does IU have a display at the Supercomputing Conference?”*
- 1998: Start involvement in grid activities that would lead to IU managing OSG operations
- 2001: Wins largest MRI grant award given by NSF that year.
- 2003: Part of TeraGrid
- 2005: Data Capacitor (MRI)
- 2008: FutureGrid
- 2014: Jetstream



1998 – Indiana University Information Technology Strategic Plan: Architecture for the 21st Century

- A University IT strategic plan – *not a strategic plan for the university IT organization*
- 10 Recommendations, 68 Actions
- Theme: Get the technology stacks right (We did not have them right in 1997)



Financing

Network access *"In the language of today's technology, No busy signals!"*

Incentivize use of IT

Teaching and learning IT

Research

Student systems

Telecomm convergence

Learning IT

Digital libraries

Policies



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Organizational structure – largely established in 1997

- CIO
 - UITs
 - Learning Technologies
 - Client Services and Support
 - Enterprise Software
 - Networks
 - Research Technologies
 - GlobalNOC
 - Pervasive Technology Institute - Collaborative organization:
 - UITs Research Technologies
 - National Center for Genome Analysis Support
 - Center for Applied Cyberinfrastructure Research
 - Data to Insight Center
 - Digital Science Center
 - ***PTI is not a technology-driven organization. It is a mission- and values-driven organization. We drive technology to support IU's mission.***
 - University Security & Policy Offices
- Other important roles at IU: President, VPR, Associate Vice Provost for Research, IU School of Medicine Executive Associate Dean



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2008: 2nd IU IT Strategic Plan, *Empowering People*

- The hard part: role-centric view: 15 Recommendations, 72 Actions.
- <http://ep.iu.edu>

IT Foundations

1. Infrastructure
2. Networks
3. Collaboration
4. Financials
5. Security
6. Environment
7. IT Staff

Human-centric IT

8. IT Development
9. Institutional Data
10. Student Success
11. Engagement Beyond

Grand Challenges

12. Scholarly Record
13. Health Care
14. Teaching & Learning
15. Research & Scholarship



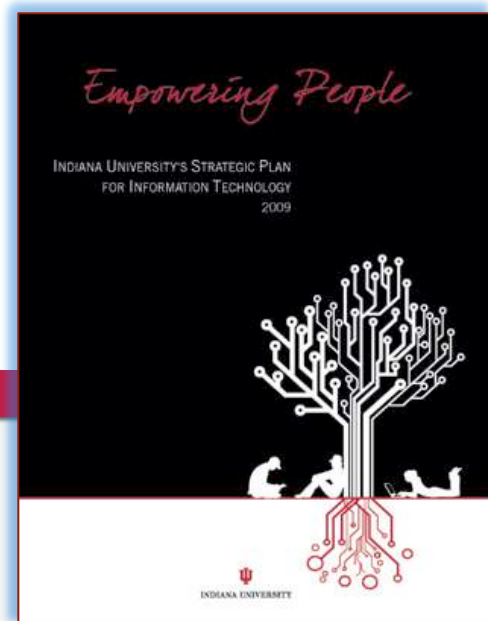
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RT Goals for 2020 (apply to all staff)

- **Each researcher's amplifier will go to 11**
- **IU researchers, scholars, students, and artists will:**
 - Use information technology within a policy and security framework that serves as a model for academia and the US in general.
 - Be able to pursue their academic and creative activities with no limitations created by access to data, and few limitations caused by access to computational power.
 - Be able to examine and present research results or artistic creations in ways that are intuitive and enhance effectiveness through:
 - 2- and 3-D display and interface resources generally available in offices, labs and meeting rooms.
 - State-of-the-art. large-scale facilities located conveniently throughout IU.
 - Have access to resources that:
 - Grow in capability and capacity predictably, steadily, and in ways that keep IU researchers at the leading edge of discovery.
 - Are available resiliently by design (24 x 365 at never less than 75% aggregate capacity).
 - Are available immediately when immediacy is essential.
 - Are accessible through interfaces that are intuitively usable by the large majority of IU researchers.



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RT Goals for 2020 (2) (apply to all staff)

Indiana residents will:

- Benefit from new, high-quality jobs created by IU's advanced IT environment (at rates exceeding the present job-creation rate and contributing to the Indiana economy). Such jobs will be created in three ways:
 - Bring federal money into the state to create new jobs.
 - Attract existing companies to locate major business operations in Indiana.
 - Create new companies through commercialization of IU innovations.
 - We will measure accomplishment by job creation (direct and indirect), and by IU rankings in major economic assessments – rising at least five places in one of the major rankings from 2008 to 2020.
- Have access to education and training so anyone growing up in Indiana can strive for and obtain one of these high-quality jobs. The School of Informatics and Computing and other IU schools produce well-educated graduates, many of whom stay in Indiana.
- Have an improved quality of life stemming from these achievements:
 - We will help IU biomedical research and health services communities improve state rankings in such major health indicators as obesity and tobacco use.
 - US and world residents will benefit through access to information technology services and IT-related information made available by IU and benefit from IT-related outcomes of IU discoveries and innovations.



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We've supported some REALLY cool and important research and creative activity along the way.

- Higgs boson
- One-Degree Imager
- Operation Ice Bridge
- Just doin' the neutron dance
- *Daphnia* genome
- Fetal alcohol spectrum disorder
- Indiana CTSI
- Cell-surface function
- History of philosophy and science
- Variations
- Ethnography
- Music composition
- Fine arts
- Performing arts



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Fine Arts



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Light Totem by Rob Shakespeare;
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Performing Arts



IUPUI Percussionist / Composer Scott Deal

IU Cinema – e.g., DCP for Herzog films

Image: <http://en.wikipedia.org/wiki/File:Fitzcarraldo.jpg>



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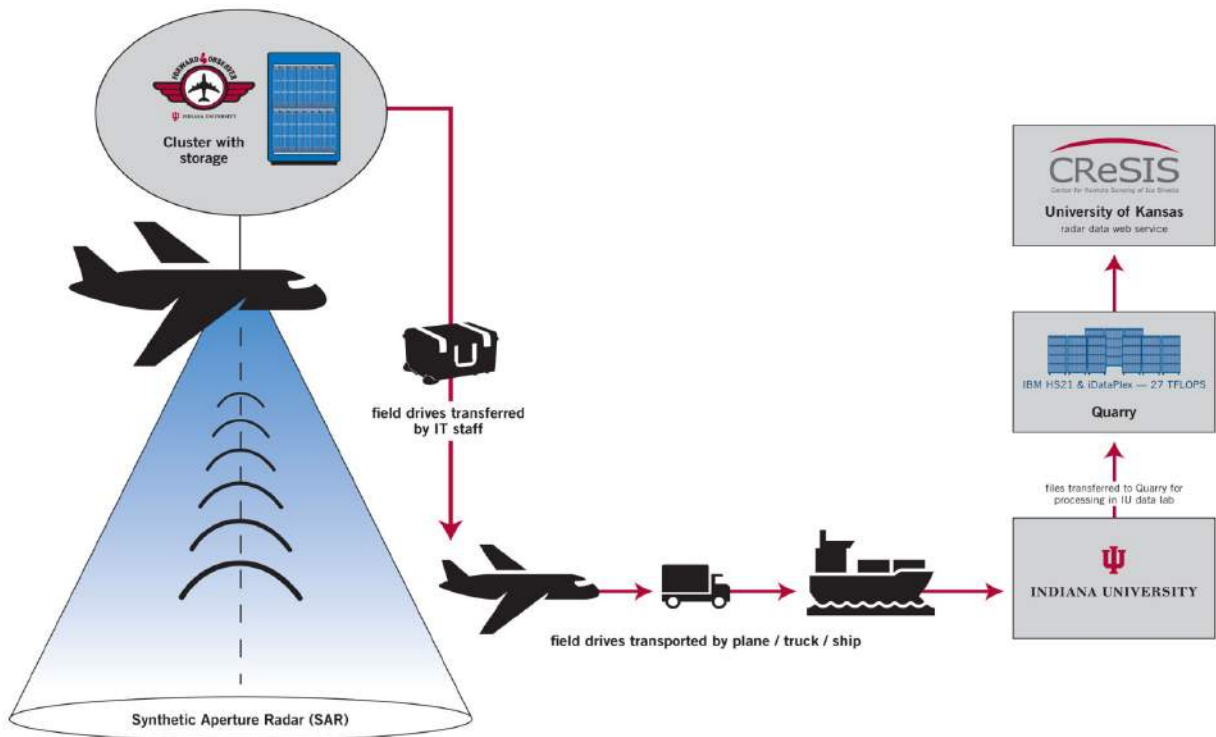
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Grand Challenges – Global Warming



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Aiding global environment and Indiana economy



- Working with Cummins to explore combustion of new biofuels
- How are soot particles created during and after combustion?
- Collaborating with Convergent Sciences, maker of the popular Converge CFD application, and Lawrence Livermore National Lab



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Switch to XSEDE mode



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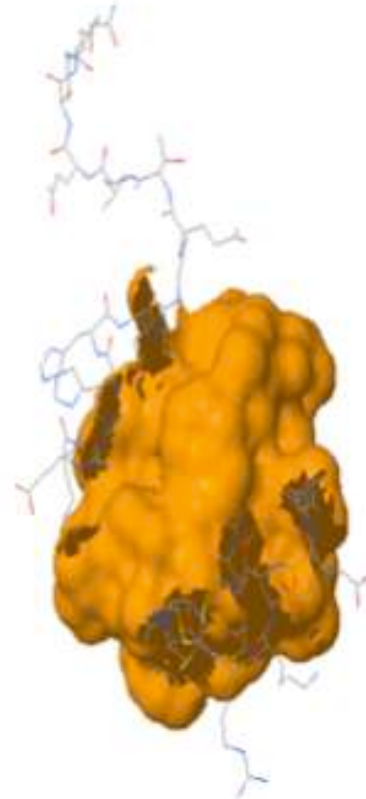
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OSG example - SPLInter - Structural Protein-Ligand Interactome

- Utilizes Autodock Vina for simulated structure model and scoring
- Input data from the Protein Data Bank and ZINC compound database along with other publically available sources
- Web-based search interface returns docked structure jmol visualization.
- Nearly limitless work – 35k proteins and 35M chemical compounds – 1.2T possible docked pairs from PDB and ZINC
- Each individual job takes about 3 minutes
- **From early 2013 to present almost 61M CPU hours on OSG approaching 1B docked pairs**



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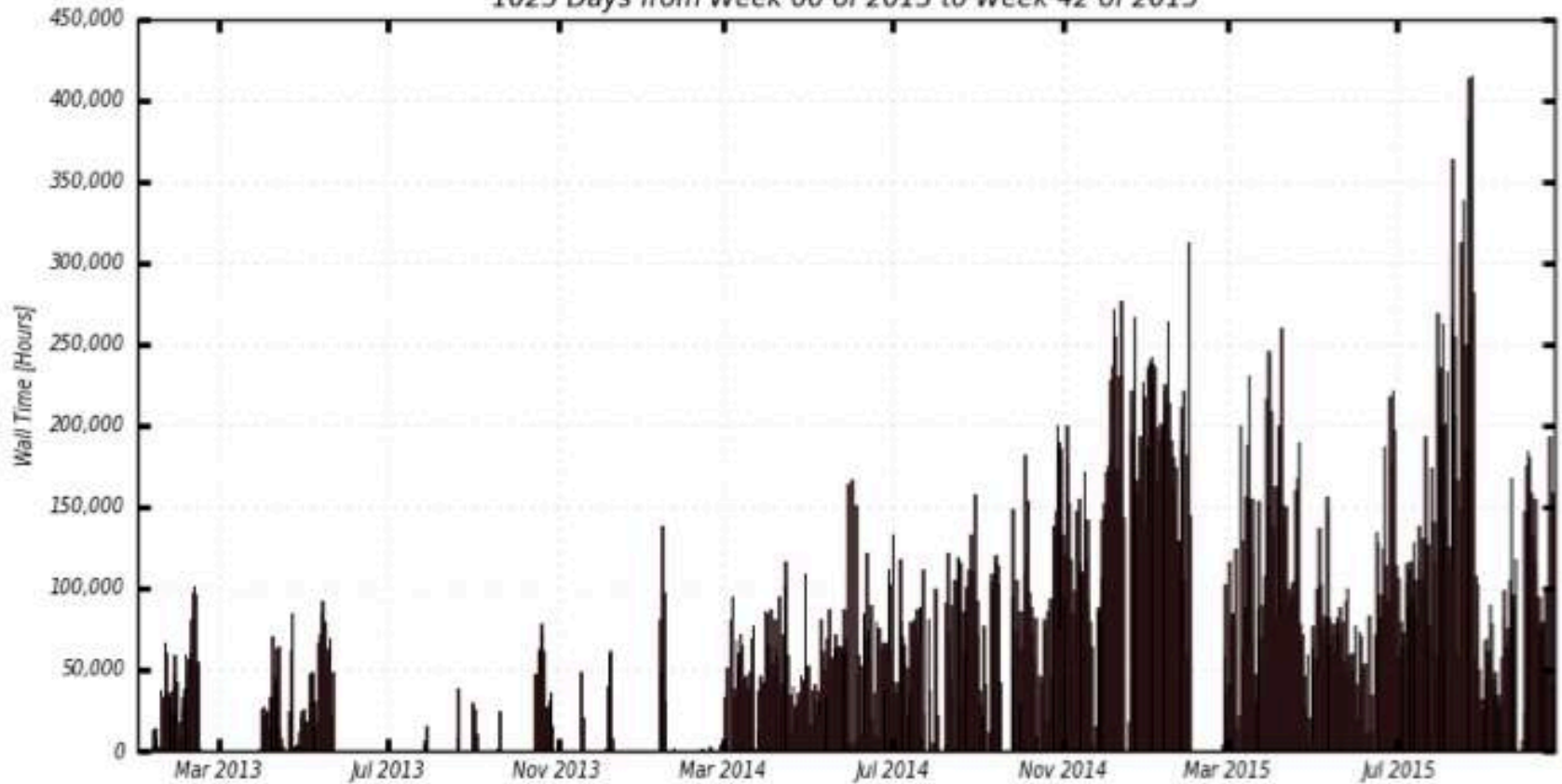
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Daily Hours By Project

1025 Days from Week 00 of 2013 to Week 42 of 2015



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So... what does success look like for IU right now?



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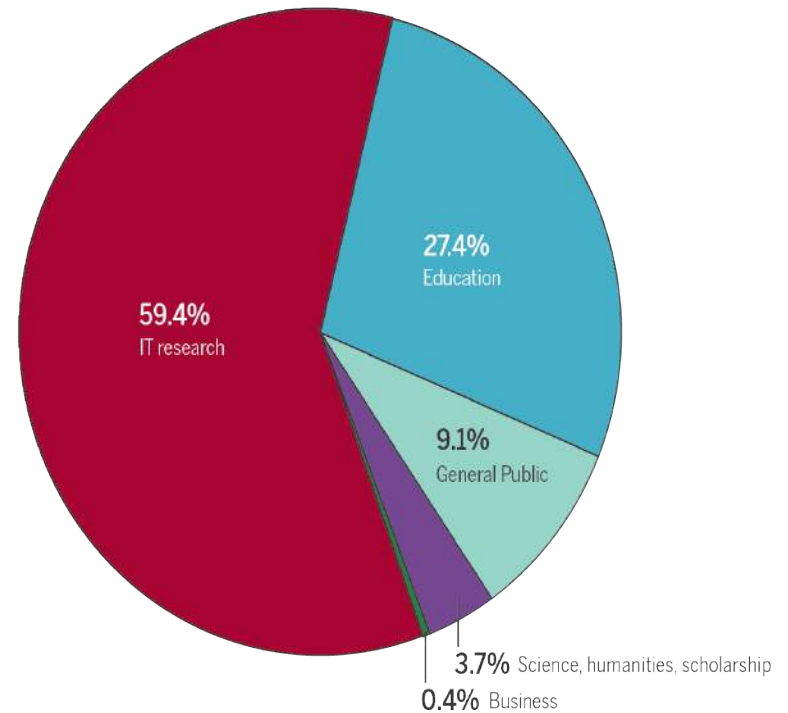


How the State and US sees us: Education and Outreach



PTI EOT Events by Attendance Numbers

Overall audience reached during reporting period: 7706



Graphic by Ryan Cobine and Beth Plale



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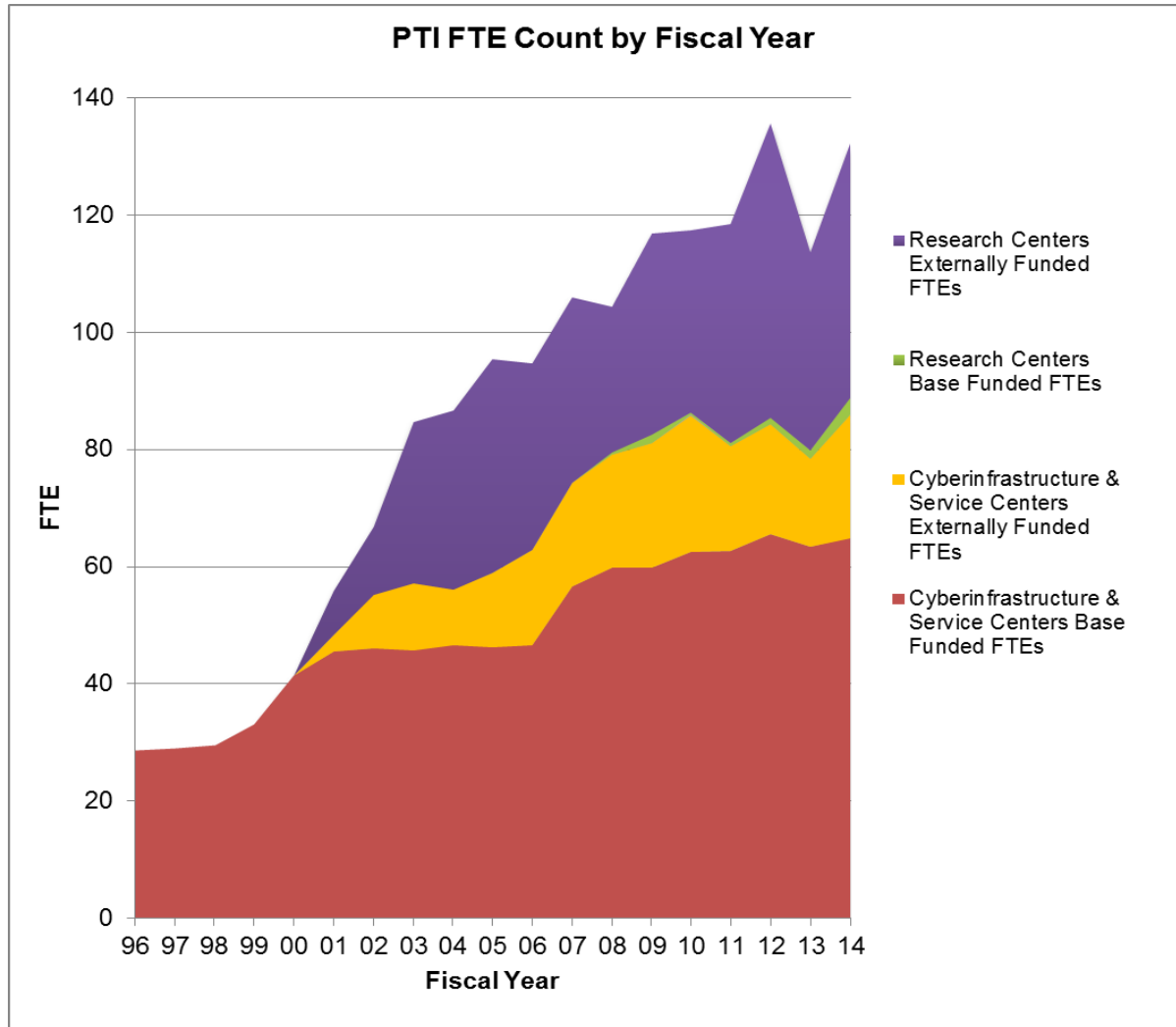
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Promises, promises: Continued job growth...



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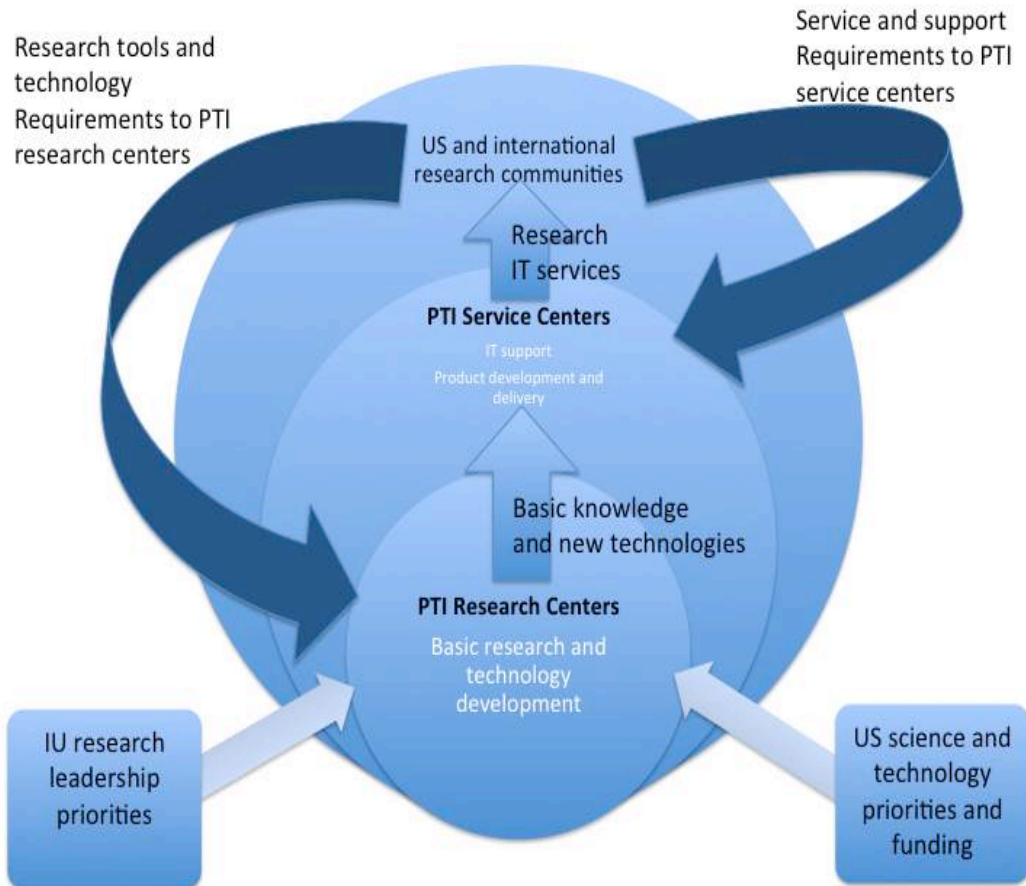
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IUPTI in the world



Based on original graphic by Beth Plale and D.F. "Rick" McMullen



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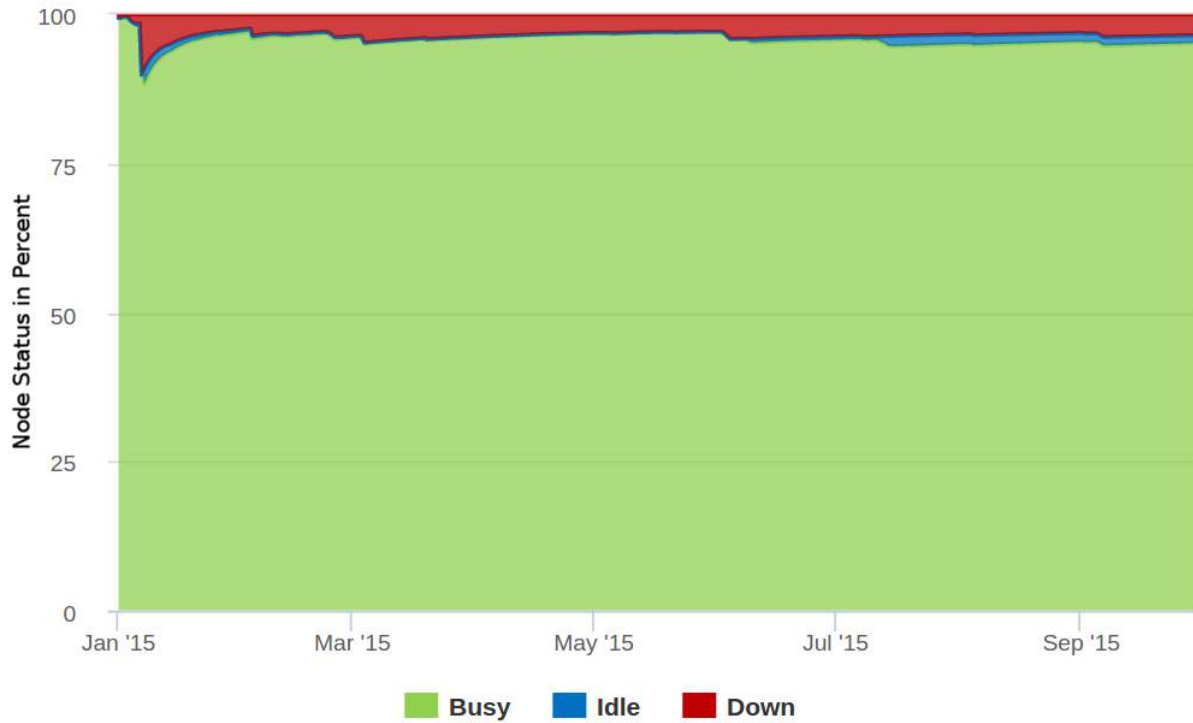
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Big Red II Utilization



This figure shows BRII CPU utilization from January 2015 through September 2015. Nodes are represented as a percent.



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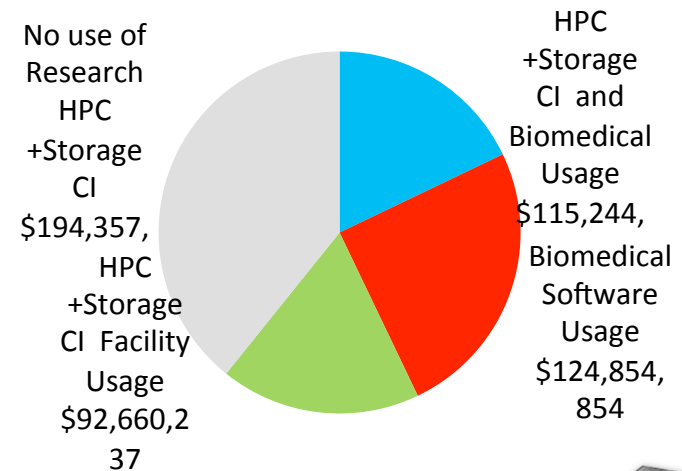


Current Status – October 2015

- Success in *breadth* of disciplines using IU HPC systems
- Success in promoting mid-level parallel jobs and use of Cray in *extreme scaling mode*
- Karst Condo model well accepted:
 - 32 of 288 nodes are owned by researchers
 - 700 of 1,000 total TB on RFS II
- Strong evidence supporting good ROI on HPC investments.
 - Proposal pending with NSF to expand and distribute our work as part of “XDMoD Value Analytics”
- Jetstream M&O supplements for \$7.5M submitted, planned production mid-spring 2016

| System | Disciplines @ IUPUI | Disciplines @ IUB | Total (Unique) |
|---------------|---------------------|-------------------|----------------|
| Big Red II | 72 | 144 | 164 |
| Karst | 123 | 161 | 216 |
| Totals | 141 | 200 | 244 |

IU C&G with Accounts on IU HPC Systems (association)



*Research File System



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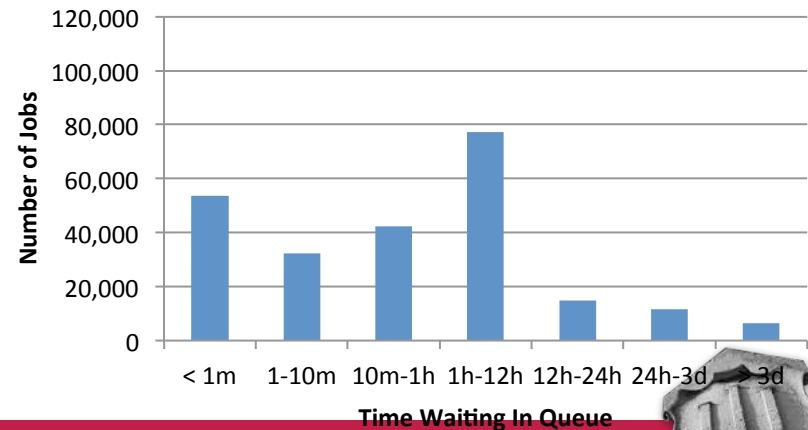
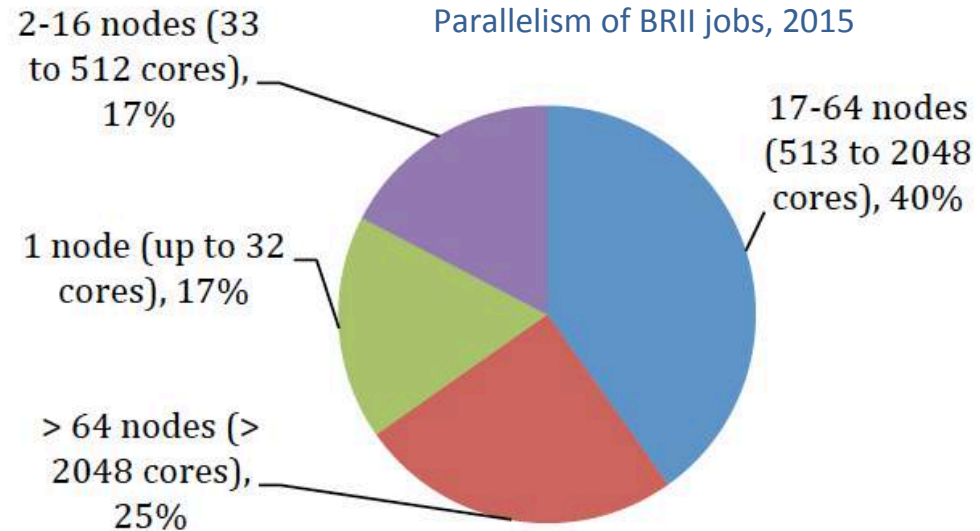
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Current Challenges

- Need more resources for very large scale jobs on Big Red II
- Queue wait time on Big Red II
- BRII operating at 95.2%, Karst at 95% capacity
- Monthly downtime (1st Tuesday) top complaint on recent survey
- New technology inflection points have left Karst processors and RFS storage behind (Xeon processors, old version of GPFS).



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Nationally we are at a point of particularly rapid change

- Opportunities
 - Vast majority of data created today are born digital.
- Diversity of analysis frameworks
 - Traditional MPI & OpenMP parallel programming
 - MapReduce
 - Cloud computing in general
 - New interfaces such as gateways
- HPC Exascale and “Big Data” have a lot in common.
 - Node level performance
 - Mostly a difference in data access patterns diversity of processors
- Industry
 - Stability of AMD – Intel – Nvidia détente is gone
 - What about ARM, Open Power?
- National ecosystem issues
 - XSEDE – NSCI – OSG – InCite - Campuses



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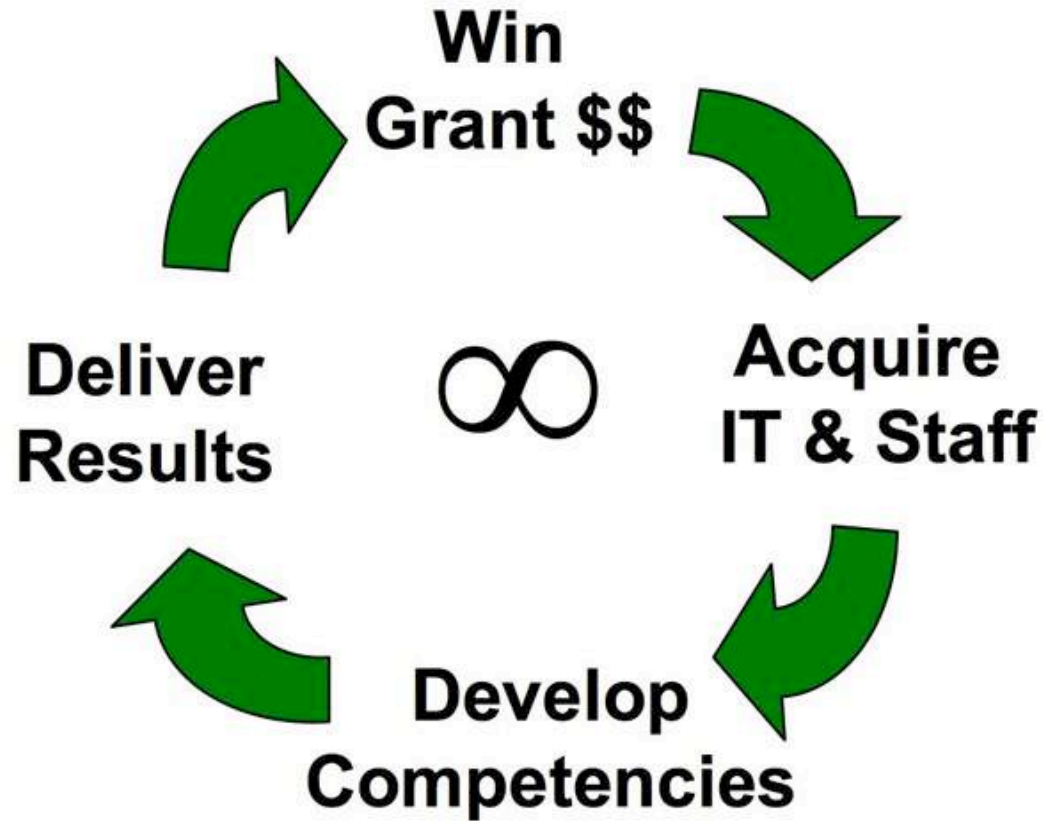
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Some thoughts for MSU - Positive Feedback Loop



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Some thoughts for MSU, cont. – Money and mission

- Some of the 7 Laws of Money (*Michael Phillips, Shambala Sun)
 - 1. Do it! Money will come when you are doing the right thing.
 - 3. Money is a dream.
 - 4. Money is a nightmare.
 - 6. You can never really receive money as a gift.
- Why do we (OVPIT/PTI/RT) pursue grant awards?
 - In the sincere belief that we are better suited to doing specific tasks than anyone else in the world, and that the world will benefit from our doing those tasks
 - In the belief that pursuing a grant award will provide local as well as national benefits
- Campus issues
 - Local strategy and consistency are essential. (You need today's Publius Cornelius Scipio, not today's Hannibal.)
 - Work like #\$\$%#\$\$% to get federal monies.
 - To be successful as a university, faculty and staff who believe in the common goal of the university must demonstrate that in the form of intellectually meaningful, ongoing collaboration.
- Similarities and differences with F1 (thanks & apologies to Sharan Kalwani)
 - Speed matters
 - Overtaking in CI/HPC is much more like trail running than F1. It is doable – with persistence, Keep plodding, and try to minimize faceplants.



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It will never be perfect - We Live the Myth of Sisyphus (thank heavens)



"The struggle itself...is enough to fill a [person's] heart. One must imagine Sisyphus happy."

—Albert Camus

Sisyphus (1548-1549) by Titian, Prado Museum, Madrid, Spain
http://en.wikipedia.org/wiki/File:Punishment_sisyph.jpg
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