The IU/ZIH Collaboration An Overview

Robert Henschel, Thomas William

Matthias Müller, Craig Stewart, Matthias Lieber, Michael Kluge, Stephen Simms, Ralph Müller-Pfefferkorn, Ulf Markwardt, Andreas Knüpfer, Guido Juckeland, Wolfgang Nagel, Scott Michael, Matt Link

PERVASIVE TECHNOLOGY
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Thanks!

- Everyone at IU and ZIH for keeping this collaboration alive for almost 10 years!

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The IU/ZIH Collaboration?!

Merriam-Webster: **collaboration** *noun*
1. the state of having shared interests or efforts
2. the work and activity of a number of persons who individually contribute toward the efficiency of the whole

Wikipedia: *For other uses, see* **Collaboration (disambiguation)**

- Collaboration is working together to achieve a goal. It is a recursive process where two or more people or organizations work together to realize shared goals, (this is more than the intersection of common goals seen in co-operative ventures, but a deep, collective, determination to reach an identical objective)… by sharing knowledge, learning and building consensus.

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The IU/ZIH Collaboration?!

Working together, benefitting from different perspectives and strengths.

- Sharing knowledge
- Working on interesting projects

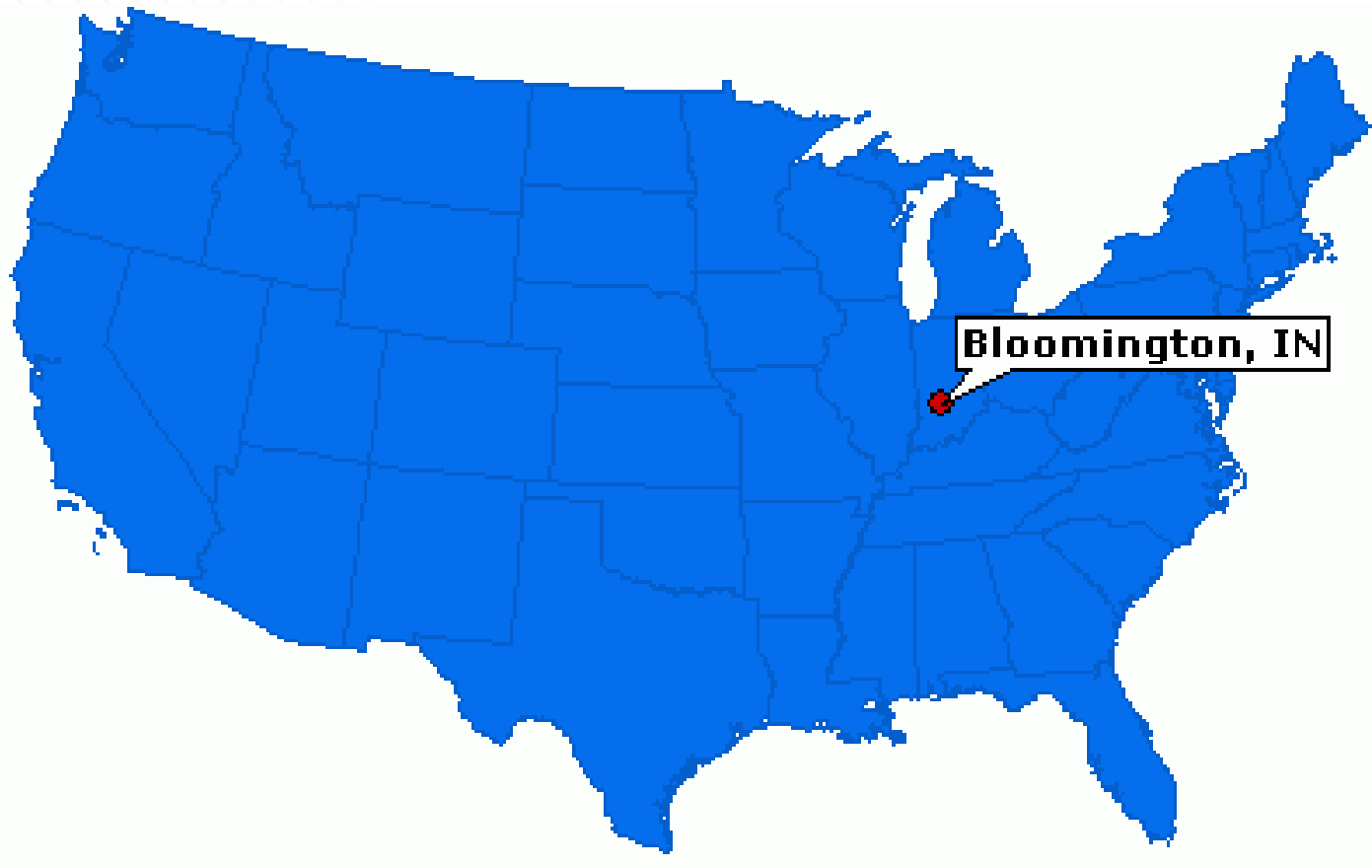- Joint papers, activities
- Joint proposals for funding

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Indiana University

Bloomington, IN

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Indiana University

3D Computer Rendering by Indiana University Architect's Office
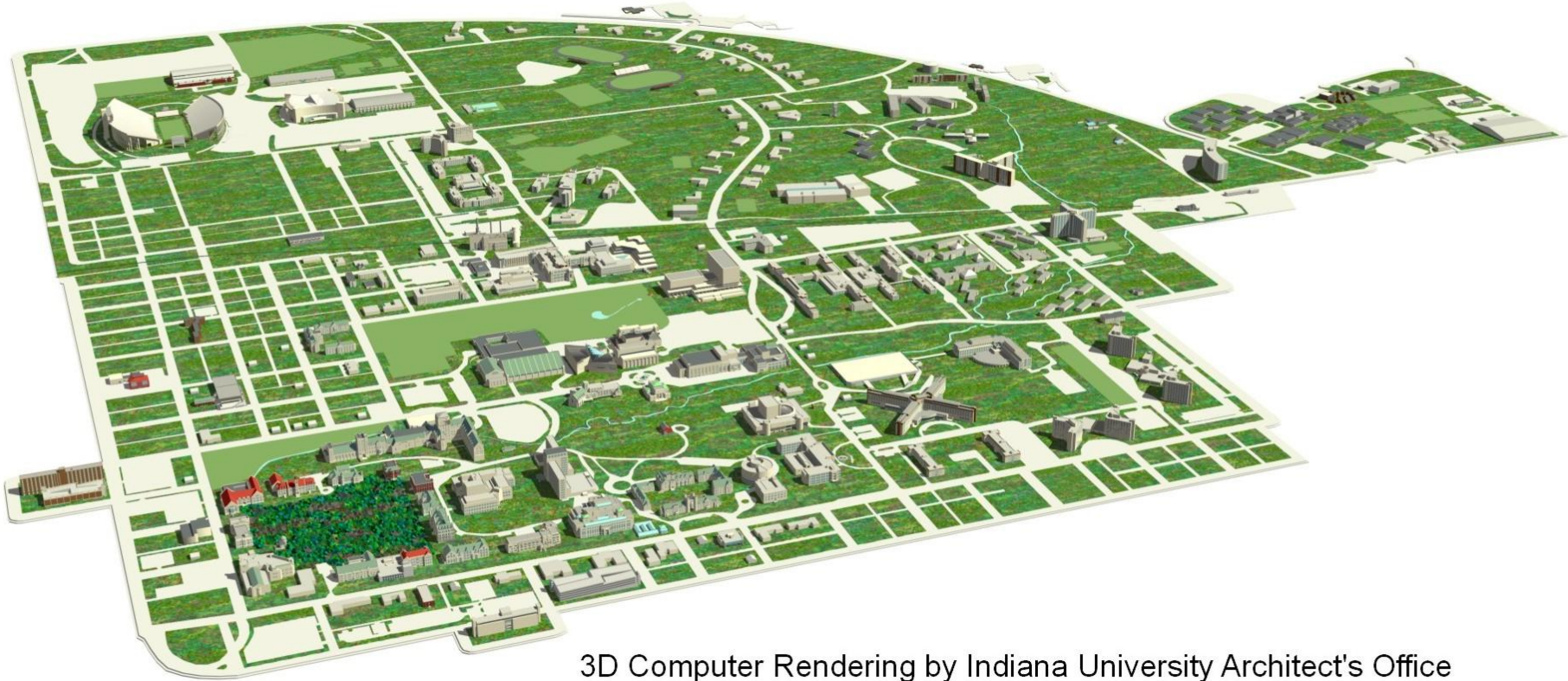
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Indiana University

- Founded in 1820
- 8 campuses
- 110,000 students, 9,000 faculty

- HPC systems are operated by Research Technologies (RT), a division of University Information Technology Services (UITS)
- Application software support is done by Scientific Applications And Performance Tuning (SciAPT)
- Open access to graduate students, faculty and staff

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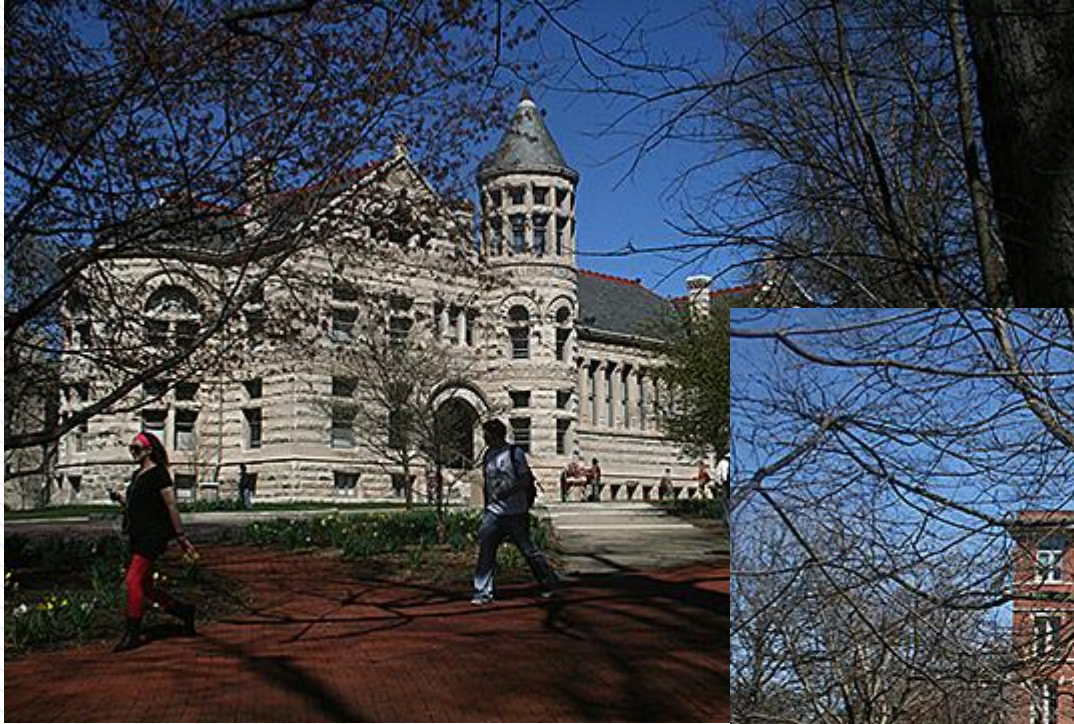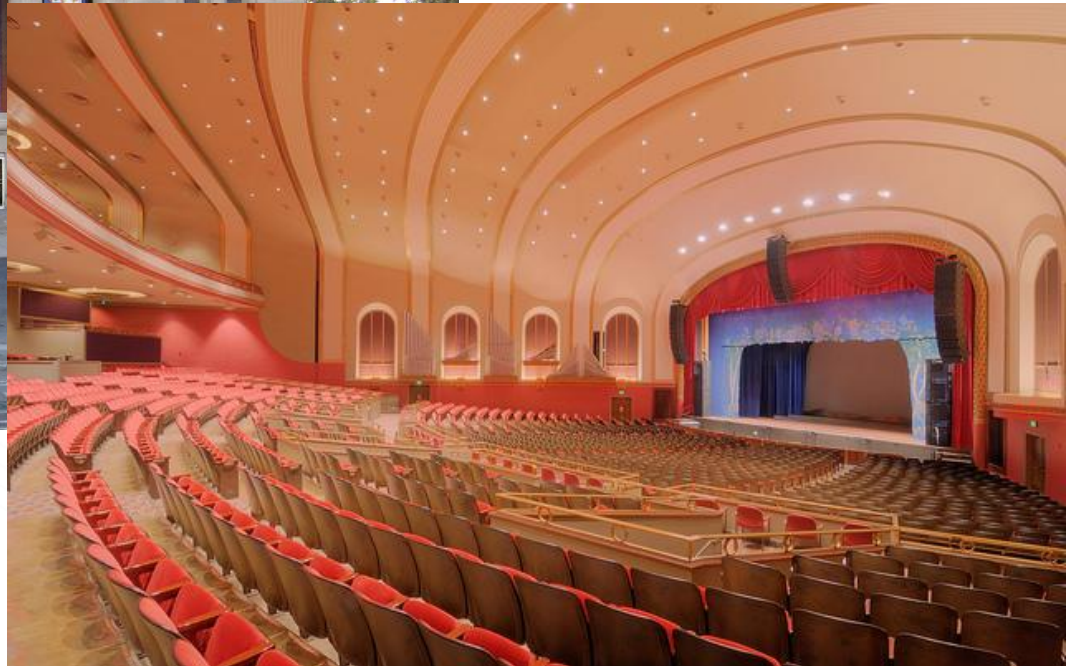ZIH Colloquium
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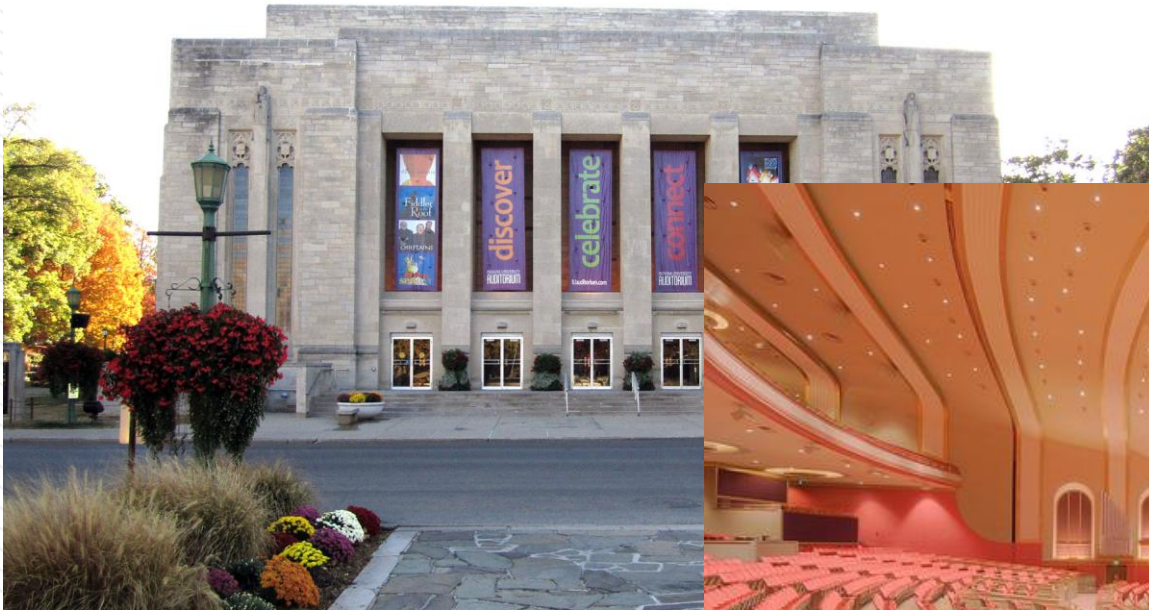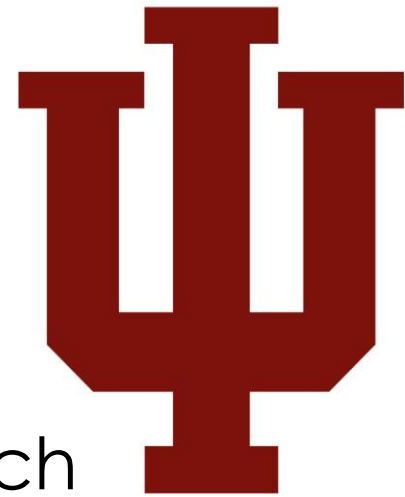
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History

- 2003 ZIH Colloquium of Craig Stewart and HPC Challenge award at SC03
- 2006 Craig and Matthias Müller research visit
- 2007 Bandwidth Challenge at SC07
- 2008 Cluster Challenge at SC08 MOU signed
- 2009 FutureGrid award
- 2010 100Gbps test bed in Dresden
- 2011 SCinet Research Sandbox at SC11
- 2012 Trinity and NCGAS

Einladung

zum

ZHR-Kolloquium

Titel: **Computational biology: strategies and challenges**

Referent: **Dr. Craig Stewart**
Director of Research of Academic Computing, Indiana University

Abstract:

The sequencing of the human genome was hailed as a tremendous achievement for science, and rightly so. Yet it was more a beginning than an end, as it provided only a piece of the raw materials needed to understand biological systems in a thorough and predictive fashion. In this talk I will describe some of the challenges we have faced at IU in working with biomedical researchers to employ high performance computing and data storage systems. In particular, some of the successes in large scale computation and large scale data management problems will be described. As well, an overview of some of the grand challenge problems facing computational biology and bioinformatics will be described, including opportunities in systems biology and the role grids may play in the application of computational techniques to biological and biomedical problems.

Dr. Craig Stewart is Director of Research and Academic Computing at Indiana University, and Director of the Information Technology Core of the Indiana Genomics Initiative. Dr. Stewart is a biologist by training, and has worked in scientific and high performance computing for more than a decade and a half. His personal research interests include HPC architectures and computational phylogenetics.

Ort: **Willers-Bau C207**
Zeit: **Freitag, den 20. Juni 2003, 10.00 Uhr**

gez. Prof. Dr. W.E. Nagel

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Date: August 2, 2012

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COUNTRY: **Germany**

PARTNER INSTITUTION: *Technische Universitat, Dresden*

IU CAMPUS: **Bloomington and Indianapolis**

IU UNIT/DEPT: Office of the Vice President for Information Technology

Contact: Craig Stewart

Address: 601 E. Kirkwood Avenue

Franklin Hall 116

Bloomington, IN 47405

Phone: (812) 855-4240

E-Mail: stewart@iu.edu

Description: Indiana University Office of the Vice President for Information Technology and School of Informatics and Technische Universitat Dresden - Center for Information Services and High Performance Computing establish an Agreement of Friendship and Cooperation to formalize their long standing relationship. Both parties agree to establish a joint research and development partnership, with initial themes including data-centric computing, computing for the biological and life sciences, wide area distributed file systems, and parallel computing

History cont'd

- Data Capacitor (Lustre, networks), Vampir (performance analysis) and computational biology (fastDNAml, Trinity) as main drivers of the collaboration

- MOU topics:
  - Data-centric computing
  - Computing for the biological and life sciences
  - Wide area distributed file systems
  - Parallel computing performance

People

- 2003 Craig Stewart presents at ZHR colloquium and organizes Minisymposium – Bioinformatics at PARCO in Dresden
- 2006 Holger Brunst gives a Vampir tutorial at IU
- 2006 Craig and Stephen Simms visit Dresden and Matthias Müller visits IU
- 2007 Michael Kluge, Guido Juckeland, Andreas Knüpfer, Robert Henschel, participate in Bandwidth Challenge
- 2008 Robert moves to IU, Guido visits IU
- 2008 3 Students from Dresden participate in Cluster Challenge
- 2009 Robert gives Vampir Feedback talk in Dresden
- 2009 Thomas William starts work in FutureGrid grant
- 2010 Stephen and Robert visit Dresden for 100Gbps test bed work
- 2010 Thomas gives Vampir workshop at IU
- 2011 Thomas visits IU for 100Gbps SCinet Research Sandbox work
- 2012 Matthias Lieber visits IU for Trinity project
- 2012 Robert visits Dresden for Trinity, Vampir Feeback and this presentation

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Projects

Bandwidth Challenge, Cluster Challenge, SCinet Research Sandbox 100Gbps test bed, Trinity performance tuning, NBody6 GPU tracing, IUMD performance analysis, Vampir tutorial, SPEC benchmarks, SPEC MPI2007 on Windows HPC, SC and ISC conference submissions, Workshop and conference presentations and posters, ScaleMP proof of concept instrumentation, CellBE tracing, FutureGrid, module logging, benchmarking, Bloomington/Dresden network tuning and dynamic circuits, mlRho performance analysis

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Example: 100Gbps

- 100 Gbps from Dresden to Freiberg
  - Stephen Simms from IU contributed Lustre experise
  - Future Generation Computer Systems journal article
- 100 Gbps from Bloomington to Seattle
  - Thomas William contributed 100 Gbps and Vampir expertise
  - SC12 paper

Example: Trinity

- Collaborative effort of
  - TU Dresden / ZIH   (M. Lieber)
  - NCGAS   (R. LeDuc, L.-S. Wu, P. Nista)
  - BROAD Institute   (B. Haas)
  - SciAPT   (R. Henschel, T. William)

- ~ 3 PM effort during March/April/May 2012
- ~ 1 PM effort during July/August 2012

Goal
Speed-up RNA-Seq analysis with Trinity

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Example: Trinity

- Significantly reduced runtime, while maintaining correctness of results

- XSEDE12 paper

- Source code committed to official SourceForge repository

- Working on establishing a continued collaboration between IU/ZIH/Broad, to further optimize Trinity

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Ongoing Activities

- Weekly meetings for specific projects
- Monthly IU/ZIH video conference
- Yearly IU/ZIH report

- Promoting the collaboration
  - ZIH Info
  - PTI major project review
- Ongoing projects
  - Trinity performance analysis and tuning
  - Vampir support and feedback

Keeping the Collaboration Alive

- Subcontract through FutureGrid
- Monthly IU/ZIH video conference and dedicated meetings
- Integration into weekly group meetings
- New and interesting topics
- Broadening participation – anyone?!
- Video conferences and in person meetings
- IU/ZIH dinner at ISC
- SC logistics support for ZIH

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Recent IU/ZIH Joint Publications

- Windows/Linux comparison using SPEC benchmarks
  - SPEC Workshop presentation and paper: **A Performance Comparison using HPC Benchmarks: Windows HPC Server 2008 and Red Hat Enterprise Linux 5**
- 100Gbps Dresden / Freiberg
  - Future Generations Computer Systems Journal: **Performance and quality of service of data and video movement over a 100 Gbps testbed**
  - IU/ZIH press release
- 100Gbps Indianapolis / Seattle
  - SC12 paper: **Demonstrating Lustre over a 100Gbps Wide Area Network of 3,500km**
  - SC11 press release about 100Gbps WAN
- IUMD Code
  - E-Poster SC11: **Performance Studies Of A Molecular Dynamics Code**
  - CUG12 paper: **Analysis and Optimization of a Molecular Dynamics Code using PAPI and the Vampir Toolchain**
  - IWOMP paper about SPEC OMP2012: **SPEC OMP2012 - An Application Benchmark Suite for Parallel Systems using OpenMP**
- Trinity
  - XSEDE12 paper: **Trinity RNA-Seq Assembler Performance Optimization**
  - IU/ZIH/Broad press release

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Conclusion

- Overall, the IU/ZIH collaboration is very productive (and a lot of fun)
- Highly interesting and educational to see cultural and institutional differences between IU/ZIH and USA/Germany

Future:

- More synergistic and more strategic
- Broader and more result oriented participation

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Thank you for your attention!

Questions?

Robert Henschel
Indiana University
henschel@iu.edu

Thomas William
GWT-TUD GmbH
thomas.william@gwtonline-fb.de