

Report about the collaboration between UITS/Research Technologies at Indiana University and the Center for Information Services and High Performance Computing at Technische Universität Dresden, Germany

Reporting Period: July 2010 to June 2011

*Robert Henschel
Craig A. Stewart
Thomas William
Matthias Müller
Wolfgang Nagel*

Indiana University

PTI Technical Report PTI-TR12-008

22 Mar 2012

Citation:

Henschel, R., C.A. Stewart, T. William, M. Müller, and W. Nagel. "Report about the collaboration between UITS/Research Technologies at Indiana University and the Center for Information Services and High Performance Computing at Technische Universität Dresden, Germany," Indiana University, Bloomington, IN. PTI Technical Report PTI-TR12-008, Mar 2012. Available from: <http://hdl.handle.net/2022/14295>



**PERVASIVE TECHNOLOGY
INSTITUTE**

INDIANA UNIVERSITY



**RESEARCH
TECHNOLOGIES**

INDIANA UNIVERSITY

University Information Technology Services
Pervasive Technology Institute

This material is based upon work supported in part by the National Science Foundation under Grant No. 0910812 to Indiana University for "FutureGrid: An Experimental, High-Performance Grid Test-bed." Partners in the FutureGrid project include San Diego Supercomputer Center at UC San Diego, University of Chicago, University of Florida, University of Southern California, University of Tennessee at Knoxville, University of Texas at Austin, Purdue University, University of Virginia, and T-U Dresden. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the NSF.

More information is available at: <http://futuregrid.org/>

Table of Contents

1. Summary	1
2. A Brief History	1
3. Success Stories	2
3.1. Application Performance Analysis	2
3.1.1. Performance Comparison of Windows HPC Server and Red Hat Linux using High Performance Computing Benchmarks.....	2
3.1.2. Participation in SPEC.....	2
3.1.3. Performance Analysis of a Molecular Dynamics Code	3
3.1.4. Supercomputing Conference 2011 poster submission	4
3.1.5. Hands on Support with Application Tracing	5
3.2. FutureGrid Related Activities	5
3.2.1. Vampir presentation within FutureGrid at SC10	5
3.2.2. FutureGrid poster at SC10	5
3.2.3. Hauptseminar topic on virtual machine performance analysis.....	6
3.2.4. Setup HPC partition within FutureGrid	7
3.3. 100Gbps Network Testbed	7
3.3.1. 100Gbps Testbed Workshop in January 2011	7
3.3.2. 100Gbps DFN Forum June 2011	8
3.3.3. 100Gbps poster at SC10 and ISC11 at ZIH booth.....	8
3.3.4. 100Gbps at the Lustre User Group	9
3.3.5. 100Gbps IU press release in November 2010.....	10
4. Short Term Projects	10
4.1. Enhancing Application Performance Analysis in Virtual Machine Environments 10	
4.2. Maintaining Vampir Installation at Indiana University	11
4.3. Craig Stewart presentation in Dresden in June 2011	11
4.4. Data Capacitor and ODI presentation in Dresden in October 2010	11
5. Ongoing Activities	11
6. Outlook	11

1. Summary

This report lists the activities and outcomes of the collaboration between Research Technologies, a division of University Information Technology Services at Indiana University (IU), and the Center for Information Services and High Performance Computing (ZIH) at Technische Universität Dresden.

Craig Stewart initiated this collaboration in 2003 when he was invited by ZIH to present as part of a colloquium series. It was formalized in 2008 by the signing of a memorandum of understanding (MOU), providing the framework for a tighter collaboration. The collaboration has already produced a number of results, including awards at international conferences, peer reviewed papers, successful grant proposals, and the exchange of researchers in order to foster information exchange between the two institutions. After National Science Foundation (NSF) awarded IU the FutureGrid grant in 2009, the collaboration entered a new phase, by directly funding an FTE at ZIH through the grant.

During this reporting period, three major projects are going on. First, IU and ZIH have intensified their collaboration in the area of performance analysis of parallel scientific applications and benchmarking. IU is using the Vampir toolchain developed at ZIH, a framework for detailed analysis of highly parallel scientific applications. For example, experts from both institutions are working together to analyze and optimize a molecular dynamics code that is developed at IU, and used on IU and nationally funded cyberinfrastructure. This work will benefit researchers at IU by improving the efficiency of the molecular dynamics application. A poster highlighting this work was submitted to (and accepted for) the Supercomputing 2011 Conference.

Second, ZIH has continued to be a valuable partner in the FutureGrid NSF grant. ZIH is responsible for providing expertise in the area of performance analysis and in particular using the Vampir toolchain in the grant. In addition, ZIH helps with setup and maintenance of the software stack on FutureGrid systems. Third, ZIH has partnered with IU for a 100Gbps network test bed that was installed in Germany. IU experts contributed knowledge of wide area file systems in order to optimize long-range file transfers in the testbed. This activity resulted in workshops, talks at conferences and the submission of papers. IU will be using this success for a similar, but more ambitious, 100Gbps network demonstration at this year's Supercomputing Conference. For this demonstration, IU has in turn partnered with ZIH.

The report is structured as follows. In the beginning, the history of the collaboration between IU and ZIH is outlined, covering notable activities before this reporting period. In the following section, detailed information about the three major projects of this reporting period is presented. The next section briefly outlines smaller projects. The report concludes with a section about ongoing activities and an outlook into the next reporting period.

2. A Brief History

The collaboration between Research Technologies (RT) at Indiana University (IU) and the Center for Information Services and High Performance Computing (ZIH) at Technische Universität Dresden grew out of a visit from Craig Stewart as a Fulbright Senior Scholar to Dresden in 2006. RT and ZIH have a long history of collaboration, including winning together three major computing challenge awards at the Supercomputing Conference sponsored by the Association of Computing Machinery. The most recent victory was in 2008, when a team made up of informatics students from the Pervasive Technology Institute (PTI) Open Systems Lab and students from ZIH won a competition to most effectively run a set of scientific applications on a small supercomputer cluster. In addition, ZIH has participated in IU-led grant proposals, including the FutureGrid grant proposal the National Science Foundation (NSF) awarded to IU in August 2009.

The memorandum of understanding (MOU) for this collaboration was signed in November 2008 at the Supercomputing Conference in Austin, Texas. Major points of the collaboration include:

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

URL: <http://homepages.indiana.edu/web/page/normal/11187.html>

Two notable activities prior to this reporting period, but after signing the MOU in 2008, shall be highlighted. Robert Henschel provided detailed feedback on the usage of the Vampir toolchain at IU to ZIH in June 2009. This presentation summarized the usage of the tool at IU over one year, highlighting successful applications and pointing out items that could be improved.

The second activity is a Vampir tutorial that was held at IU in April 2010. The workshop was jointly organized by RT and ZIH, as part of FutureGrid. Thomas William, working for ZIH in Dresden, is currently funded through the grant. During a four-week stay in Bloomington, Thomas William and Robert Henschel prepared and presented a tutorial to give detailed insights into the Vampir toolchain, tailored to the needs of IU scientists. This talk was broadly advertised and visited by many performance group members of the FutureGrid project as well as RT and PTI staff members. The workshop also included a hands-on session. The talks as well as the materials from the hands-on session are available at the following website: <http://iu-pti.org/hpa/vampir-workshop-2010>.

3. Success Stories

This section briefly describes projects that have been completed successfully during this reporting period.

3.1. Application Performance Analysis

This section outlines all projects that are related to performance analysis of scientific applications.

3.1.1. *Performance Comparison of Windows HPC Server and Red Hat Linux using High Performance Computing Benchmarks*

To compare the performance of different High Performance Computing (HPC) platforms, benchmark suites consisting of different applications testing the various components of such large installations are commonly used. One de facto standard suite in HPC is the High Performance Computing Challenge (HPCC) benchmark and the SPEC MPI2007 benchmark. Although these applications are in theory able to run on Linux as well as on Microsoft Windows this has not been done before. As we had two systems available (one at IU and one at ZIH) that were able to run both operating systems, we studied which system would perform better at which task/application. After a substantial amount of work to port the benchmark suite and its several HPC applications from Linux to Windows we were able to run all the benchmarks on both OS installations (always using the same hardware). The results were unexpected as some applications were measurably better on Windows than on Linux (and vice versa). Although this work was done prior to this reporting period, it was presented at the SPEC Workshop in Paderborn in October 2010. As of the date of this report this submission to SPEC is still the only one performed on Windows.

URL: <http://www.spec.org/workshops/2010/paderborn/program.html>

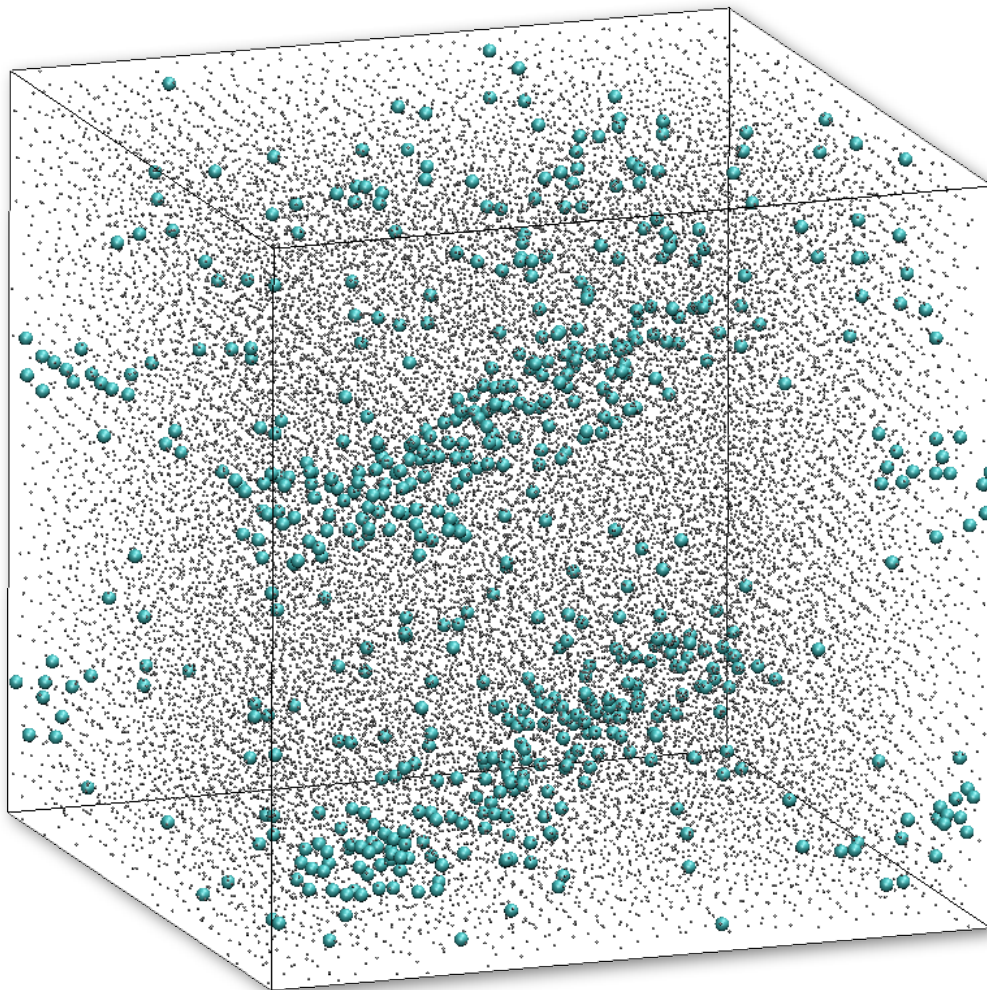
IU ScholarWorks: <http://hdl.handle.net/2022/9919>

3.1.2. *Participation in SPEC*

IU and ZIH are both members of the High Performance Group (HPG) of the Standard Performance Evaluation Corporation (SPEC). This group develops and maintains standard benchmarks for High Performance Computing systems. During the development of the SPEC OpenMP2012 benchmark suite,

IU contributed a molecular dynamics application to the benchmark. This application was developed at IU, and integrating it into the benchmark will allow IU to gather performance data on a wide variety of HPC systems in the future. IU and ZIH are also working closely together within HPG to push forward the creation of a power metric for HPC benchmarks.

3.1.3. *Performance Analysis of a Molecular Dynamics Code*

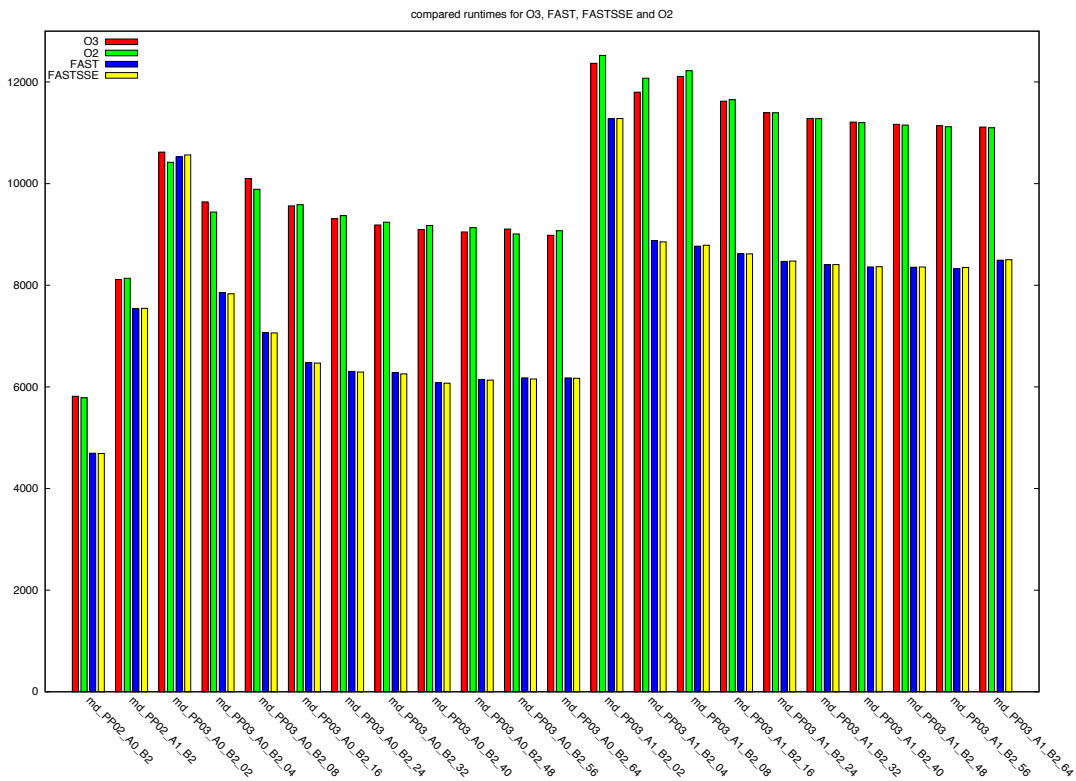


A molecular dynamics code developed at IU for simulating the diffusion in dense nuclear matter in white dwarf stars was analyzed. The code is highly configurable, allowing for exploiting different parallelization paradigms and additional fine tuning with a range of parameters.

The aim of the parallel analysis is to measure the scalability limits of the different parallel code implementations and to detect bottlenecks possibly preventing further parallel efficiency. This work has been done using the Vampir toolchain.

The IU “md” code is used almost on a daily basis by IU researchers, both on IU systems and on nationally funded cyberinfrastructure. The “md” code can be built as a pure OpenMP, a pure MPI, or a hybrid application. In addition, the code can use MDGRAPE-2 boards to accelerate parts of the computation, and a CUDA accelerated version is under development.

In addition to IU resources, this project also uses FutureGrid machines India (iDataPlex) and Xray (Cray XT5m). Xray is right now the main development platform. Below is an example of different code-combinations that were run on Xray using different compiler flags to determine the optimal serial version, which will then be used in subsequent experiments with the OpenMP/MPI parallel versions.



3.1.4. Supercomputing Conference 2011 poster submission

The first result of the MD performance analysis presented above was an electronic poster that was submitted to the 2011 Supercomputing Conference. In this poster we presented the collaboration between RT and ZIH, the internals of the code, the tools we applied and the results gathered doing a serial and parallel analysis. This is an electronic poster that will also be shown at the IU booth at the conference. Below is a screenshot of the overview slide:

PERFORMANCE-STUDIES OF A MOLECULAR DYNAMICS CODE

Evaluating Serial, Thread and Process-Parallel Performance

Molecular Dynamics

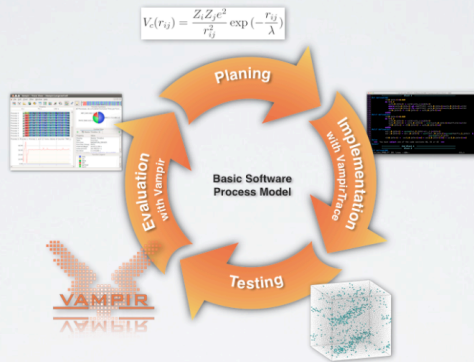
A molecular dynamics code simulating the diffusion in dense nuclear matter in white dwarf stars is analyzed in this collaboration. The code is highly configurable allowing MPI, OpenMP, or hybrid runs and additional fine tuning with a range of parameters.

Serial Analysis

The first step in the code analysis is to identify the best performing parameter set. This configuration represents the most promising candidate for further parallel analysis.

Parallel Analysis

Aim of the parallel analysis is to measure the scalability limits of the different parallel code implementations and to detect bottlenecks possibly preventing further parallel efficiency. This work has been done with the parallel analysis framework Vampir.



Authors

T. William, M. Weber, D. Röhrig - ZIH, TU Dresden
 D. K. Berry, R. Henschel - UIITS, IU Bloomington
 J. Hugtto, A. S. Schneider, C. J. Horowitz - Physics, IU Bloomington

Collaboration between PTI and ZIH

In 2008 a collaboration between the Technische Universität Dresden, Center for Information Services and High Performance Computing (ZIH), in Germany and the Indiana University, Pervasive Technology Institute (PTI), was founded to mutually benefit from common research areas.

These research topics include:

- ▶ Data-centric computing
- ▶ Computing for biological and life sciences
- ▶ Wide area distributed file systems
- ▶ Parallel computing performance

This collaboration involves ZIH maintaining a stack of performance evaluation tools inside the NSF FutureGrid project. For the analysis an HPC system called Xray, a Cray XT5m which is part of the FutureGrid hardware, was used. Xray consists of Quad-core 64-bit AMD Opteron series 2000 processors. PGI compilers version 9.0.4 and the optimized xtp-barcelona module provided by Cray have been used.

This document was developed with support from the National Science Foundation (NSF) under Grant No. 0910812 to Indiana University for "FutureGrid An Experimental, High-Performance Grid Testbed". Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the NSF.

TECHNISCHE UNIVERSITÄT DRESDEN

ZIH

IU Bloomington
Pervasive Technology Institute

INDIANA UNIVERSITY

3.1.5. Hands-on Support with Application Tracing

Thomas William provides hands-on support with tracing parallel scientific applications, both to members of RT and to researchers at IU. This includes the maintenance of the various Vampir toolchain installations at IU as well as user support in tracing applications. Projects that have benefited from his involvement are the initial analysis of the GPU performance of the NBODY6 code, an n-body code used in the astrophysics community and I/O optimizations of the IU developed hydro code.

3.2. FutureGrid Related Activities

This section outlines activities that are related to ZIH's participation in the IU-led FutureGrid NSF grant.

3.2.1. Vampir presentation within FutureGrid at SC10

A talk was given at the booth of IU at the Supercomputing 2010 Conference. This was done during a group meeting of the performance group of FutureGrid. The topic of the talk was instrumenting programs inside virtual machines and the possibility of using hardware performance counters inside the virtual environment. As one of the design goals of virtualization is to prohibit virtual machines (VMs) from accessing hardware directly and hardware performance counters are all about direct low-level hardware access this poses a real challenge. Right now the PAPI developers are working on a design document describing how this information could be made available inside the VMs.

3.2.2. FutureGrid poster at SC10

To showcase our efforts in FutureGrid the ZIH booth featured a poster about the IU-led FutureGrid:

Center for Information Services and HPC (ZIH)

Future Grid

Performance Analysis Committee

- Evaluate the FutureGrid infrastructure as it is developed and deployed
- Help users to leverage the FutureGrid infrastructure for their experiments

Instrumentation

- Help developers to instrument their software
- Set up alerts to detect problems

Benchmarking

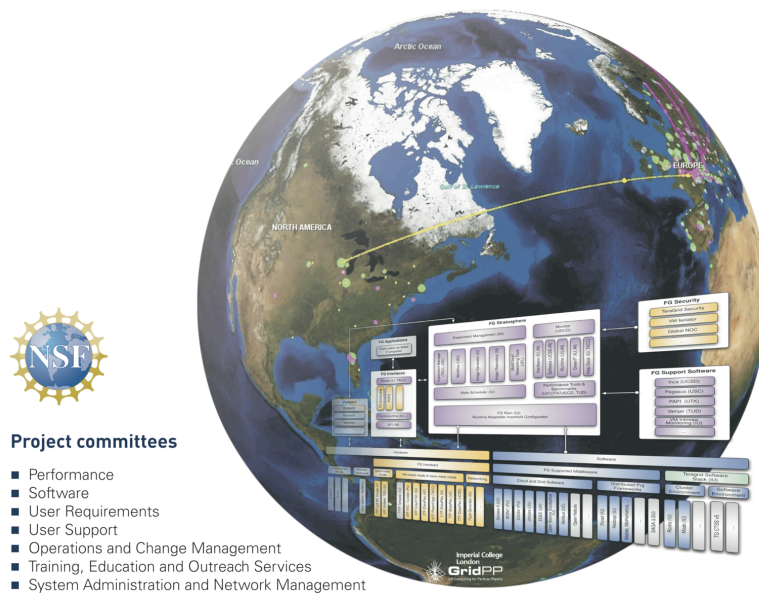
- Determine set of benchmarks
- Establish baseline for performance
- Validate infrastructure improvements
- Detect degradations

Performance Portal

- Provide a web portal to publish results
- Inspired by the EGEE Grid Observatory web pages

Performance Tools

- Provide users with tools
- Extend virtual machines with PAPI and Vampir
- Extend Vampir to incorporate load and monitoring data



Contact: Thomas William
Phone: +49 351 463-38474
Email: thomas.william@zih.tu-dresden.de
WWW: www.tu-dresden.de/zih



3.2.3. Hauptseminar topic on virtual machine performance analysis

A student from Technische Universität Dresden evaluated KVM and Xen – two virtualization technologies – comparing usability and performance. The work included benchmarks to measure the performance as well as a comparison from the user point of view, trying to find out which one is easier to use on a daily basis. Two different benchmark suites were used:

- Tapper (AMD testing suite)
- BenchIT (ZIH – application-kernel based benchmark suite)

Starting from a 30,000-foot view of how the systems are working and have to be set up, different configurations and their I/O performance were tested. This topic was assigned based on current work in FutureGrid. The Hauptseminar was presented in Dresden in June 2011. The work will be released as a ZIH report.

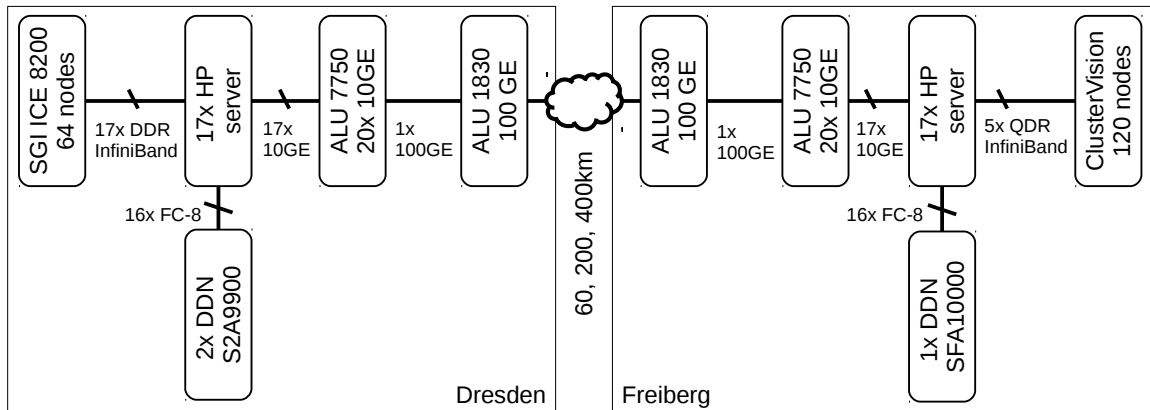
3.2.4. Set up HPC partition within FutureGrid

The RT High Performance Applications group together with ZIH helped set up the HPC partition of the x86 clusters in FutureGrid. This involved installation of libraries and applications as well as setting up guidelines of how to structure the software environment. We developed and defined the structure and naming scheme of the modules in order to provide a consistent view of all FutureGrid systems. Vampir and VampirTrace were documented extensively in the FutureGrid portal.

Recurring work will be done in maintaining software packages for the various FutureGrid systems as well as documentation and online tutorials.

3.3. 100Gbps Network Testbed

This section outlines activities that are related to IU's participation in the ZIH led 100Gbps network testbed.

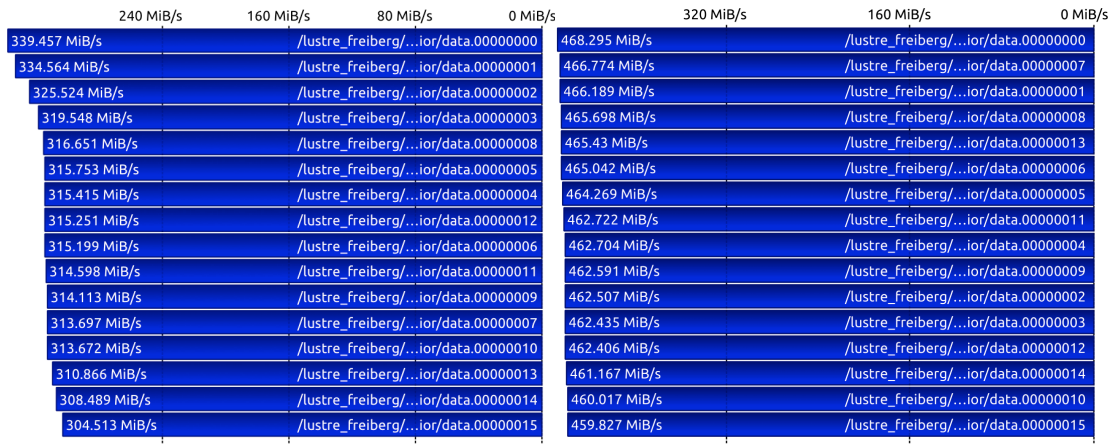


In collaboration with Alcatel Lucent, DDN and T-Systems the first single wavelength 100Gbps link build of commercially available components was set up between the two German universities in Dresden and Freiberg. Geographically, the distance between both locations is about 37km, and the length of the fiber dedicated to the project is about 60 km. We also used Fibre Channel (FC) cable boxes to expand the testbed to 200 km and 400 km. Alcatel-Lucent provides the service switch that connects both sides and can transmit 100Gbps on a single wavelength.

IU's expertise in HPC wide area network (WAN) file systems was essential to exploit the full duplex capability of the 100Gbps link and led to a press release described further down in the text. Data Capacitor project lead Stephen Simms visited Dresden to help set up and tune the parallel file system Lustre that was used for the application benchmarks.

3.3.1. 100Gbps Testbed Workshop in January 2011

The first of the 100Gbps testbed workshops was held in Dresden. It consisted of presentations of each subproject that showed results gathered so far as well as an outlook to the next steps we wanted to take at that point in time. This is when our ideas for having a switchable configuration of the line-length 60-200-400km were finalized. These different configurations will enable us to measure the impact of latency in detail. The IU/ZIH collaboration showed first results of I/O-burst experiments on the 100Gbps link. From our set of results, we showed performance properties of the TCP layer first, as they provided the baseline for all other tests. We then described the setup and results gathered using the parallel file system Lustre, one of three parallel file systems used in the testbed. The first target was to saturate the 100Gbps link using Lustre. In addition, bursts of read and write requests allowed us to investigate performance properties related to irregular traffic patterns as these are more common in "real-world" networks than streams (which are used to achieve peak bandwidth).



The above chart shows the data rate throughout the whole experiment timeframe. On the left are the averages per file (using 16 HP nodes each writing one file); on the right are maximum transfer rates of single bursts. We were using at least 5GB/s and 7.2GB/s at maximum using only the 16 HP servers and no additional cluster-nodes (which were used to achieve peak throughput).

3.3.2. 100Gbps DFN Forum June 2011

In June we presented the results gathered using the different configurations (60km, 200km, 400km) in Bonn at the 4th DFN-Forum (<http://www.dfn2011.uni-bonn.de>). The talk included burst tests on TCP level done using a framework called BenchIT that was developed at ZIH. Additionally I/O bursts using software called IOR were done comparing latencies of bursts over 60km, 200km, and 400km on the file system level. The slides from the talk are available on the web:

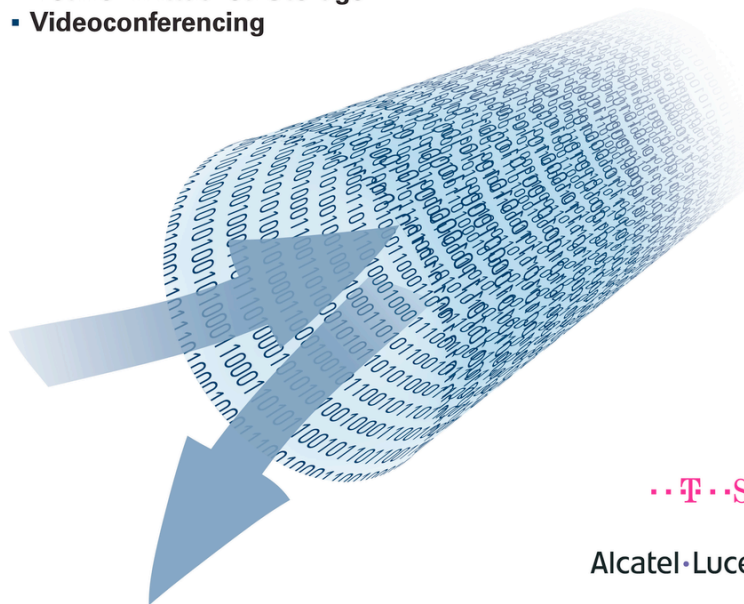
<http://www.dfn.de/veranstaltungen/technologieforum/forum4/>

3.3.3. 100Gbps poster at SC10 and ISC11 at ZIH booth

The poster showcasing the 100Gbit/s testbed gathered huge attention at the Supercomputing Conference 2010 in New Orleans – particularly the members of Internet2 were very interested in our experiences setting up the initial configuration. The poster was also shown at the ZIH booth at the International Supercomputing Conference in June 2011 in Hamburg.

100 GBIT/S TESTBED

- Synthetic Stress Tests
- 10 GByte/s Wide Area Lustre[®], GPFS and FhGFS File Systems
- Distributed Cluster of Virtual Servers
- Network Attached Storage
- Videoconferencing



Contact: Wolfgang Wunsch
Phone: +49 351 463-32593
Email: wolfgang.wuensch@tu-dresden.de
WWW: www.tu-dresden.de/zih

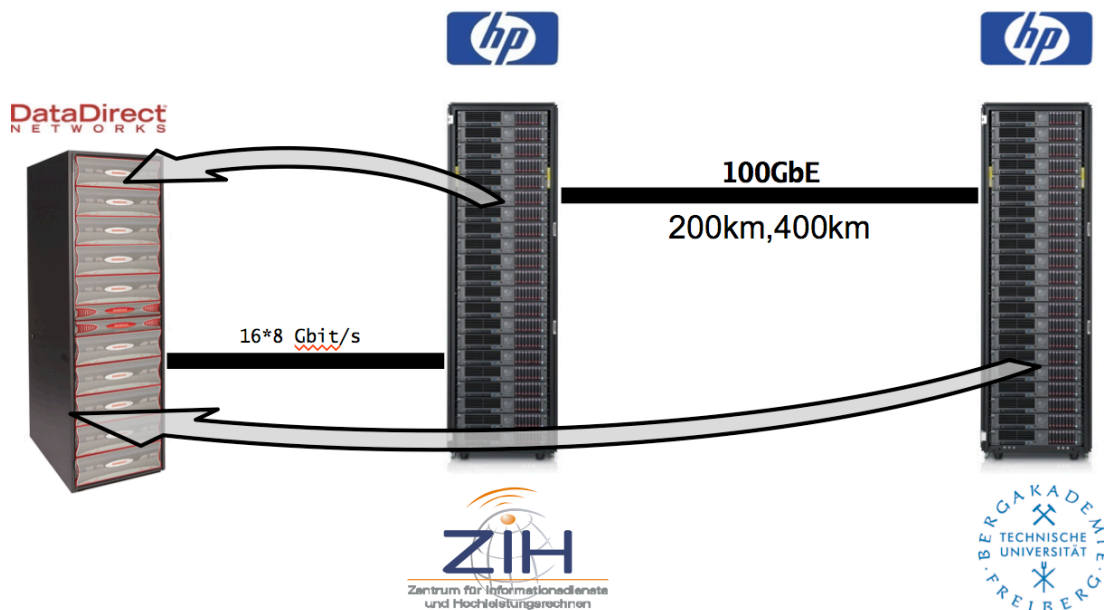


3.3.4. 100Gbps at the Lustre User Group

IU and ZIH attended the Lustre user group meeting in Orlando, Florida from April 12th, 2011, through April 14th, 2011, and gave talks about wide area network (WAN) usage of the Lustre file system.

IU presented a talk on “Empowering Multi-site Heterogeneous Workflows with Lustre-WAN” and especially on enabling distributed workflows.

The second talk by ZIH presented our experiences and lessons learned while setting up and tuning Lustre on the 100Gbps testbed. We were especially interested in how small file transfers are affected by latency. We therefore did tests writing to the same disk system in Dresden directly from Dresden and from Freiberg over the 100G line:



3.3.5. 100Gbps IU press release in November 2010

Following the setup of Lustre on the test bed, peak performance studies were made with the help of IU (Steven Simms, Robert Henschel) and Whamcloud (Eric Barton). The achieved goals were presented in a press release: http://www.hpcwire.com/hpcwire/2010-11-15/indiana_university_announces_saturation_of_first_commercial_100_gigabit_link.html

4. Short-term Projects

This section lists short-term activities that have been performed in this reporting period.

4.1. Enhancing Application Performance Analysis in Virtual Machine Environments

As part of FutureGrid, we looked into extending the VampirTrace performance gathering framework to collect data from virtual machines on top of operating system and application data. The first virtual machine solution that we analyzed was the vSMP hypervisor from ScaleMP. This technology is in use in FutureGrid to aggregate compute nodes into one shared memory system to accommodate large memory jobs. We had several talks with representatives from ScaleMP about starting a collaboration. We intended to investigate how well certain IU codes performed using vSMP and keep using a familiar performance tool for this work. vSMP has a lot of command line tools that provide insight into what the vSMP layer is doing “behind the scenes” during an application run. This additional data could be merged into a trace to help figure out whether a bad computational performance of a code is due to the code itself, vSMP or the combination thereof. ZIH gave a presentation showing the possibilities Vampir offers and ScaleMP made a few suggestions which data to incorporate first. An instrumented version of HPL was chosen as the experiment example and vSMP statistics were collected in parallel during the trace run to be added to the trace post mortem.

In parallel, the Hauptseminar topic was assigned to a student in Dresden to get a better understanding of how performance monitoring could be done in other hypervisors, i.e. KVM or XEN.

4.2. Maintaining Vampir Installation at Indiana University

ZIH has helped keep the Vampir installation current at Indiana University. This has allowed us to exploit more complex features of the tracing environment, such as CUDA/GPU tracing and external library tracing. The Vampir toolchain is currently available on Big Red, Quarry and Mason.

4.3. Craig Stewart presentation in Dresden in June 2011

Craig Stewart presented a colloquium talk at ZIH in Dresden about campus bridging and cloud technology development within US cyberinfrastructure, with emphasis on new innovations at IU.

4.4. Data Capacitor and ODI presentation in Dresden in October 2010

Stephen Simms and Robert Henschel jointly presented two successful IU-led projects as part of the ZIH colloquium series in October 2010. The talk has renewed our work with ZIH in the area of wide area file systems.

5. Ongoing Activities

To foster active participation in this collaboration we have created various recurring activities. The purpose of those meetings is sharing information on new opportunities for collaboration as well as reporting on the status of existing projects.

Thomas William from ZIH participates in the weekly group meetings of the High Performance Applications (HPA) group of RT. This ensures that he is kept in the loop about all activities here at IU and allows everyone in HPA to engage Thomas in application performance analysis related activities. This has sparked a number of smaller projects and has led to a wider adoption of the Vampir toolchain, which IU is licensing from ZIH for eight years. This has also led to IU becoming more active in providing feedback about the Vampir tool to ZIH, allowing us to positively influence the development roadmap.

On top of the regular weekly group meetings, Thomas and members of HPA get together as needed to talk about specific projects. The widespread availability of video conferencing technology at IU and ZIH dramatically improves the quality and outcomes of such meetings, allowing us to not only see and hear each other but at the same time also share computer screens for analyzing data.

We have organized a monthly meeting that is dedicated to this collaboration. Here we discuss longer-term goals and activities. Invitations to participate are distributed widely on both sides.

An important part of this collaboration is personal interaction. Representatives from both institutions get a chance to meet each other in person at least twice a year, at the International Supercomputing Conference in Germany in summer and at the Supercomputing Conference in the United States in the fall. However, due to the large number of activities that are going on at these conferences, those interactions are usually very short. To further build personal ties, it is our goal to have at least one visit per year to the respective other institution. In the period of this report, members from IU have visited ZIH two times to work on the 100Gbps networking project (October 2010 and February 2011) and once in June 2011 to work on general projects related to this collaboration.

6. Outlook

For the year ahead, the following activities have already been planned.

As the 100Gbps tested draws to a close, two final activities are scheduled. IU will send a representative to the final workshop in Mannheim in September 2011 and IU and ZIH will work on a journal paper that will also be submitted in October 2011.

IU is planning a 100Gbps demonstration at this year's Supercomputing 2011 Conference. ZIH will participate in this demonstration by running a performance analysis workflow. Thomas William will be at IU for the month of October to prepare this work.

IU will continue to help ZIH with their presence at the Supercomputing Conference, mainly improving logistics for ZIH.

We are planning to organize a session about parallel file system performance for the International Supercomputing Conference in 2012. IU and ZIH will jointly organize this track, soliciting input from the broader HPC community.