

Center for Information Services and High Performance Computing (ZIH)

Introduction to HPC at ZIH

Chemnitz, July 10, 2014

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HPC wiki has the answer

DRESDEN

Please check our HPC wiki at https://doc.zih.tu-dresden.de

	HPC Compendium	ZiH
Startseite »» Zentral	e Einrichtungen » ZIH » Wiki	
	Ulf Markwardt Help	Logout Print Edit Attach Move Diffs
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		HPC SUPPORT
Create New Topic Index	FOREWORD	Operation Status
Changes		Ulf Markwardt: 33640
Notifications	This compendium is work in progress, since we try to incorporate more information with	Claudia Schmidt: 39833 hpcsupport@zih.tu-dresden.de
Statistics	increasing experience and with every question you ask us. We invite you to take part in	
	the improvement of these pages by correcting or adding useful information or commenting	LOGIN AND PROJECT APPLICATION
TWIKIHELP	the pages.	Phone: 40000
First TWiki Steps	Ulf Markwardt	Fax: 42328
TWiki Guide		servicedesk@tu-dresden.de
TWiki Tutorial	CONTENTS	
TWiki FAQ		
	Introduction	
	Access and Login	
	Our HPC Systems	
	 Taurus: general purpose HPC cluster (HRSK-II) 	
	Atlas: general purpose HPC cluster	
	Venus: SGI Ultraviolet Mars & Co: SGI Altix	
	Mars & Co: SGI Altix Hardware	
	File Systems and Data Management	
	Batch Systems	
	Runtime Environment	
	Software Development	

Center for Information Services & High Performance Computing

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Agenda

Infrastructure

- Compute hardware
- HPC file systems
- HPC environment at ZIH

2 Access

Overview

- Terms of Use
- Application for HPC projects
- Management of HPC projects
- Channels of communication
- Kinds of support





1 Infrastructure

• Compute hardware

- HPC file systems
- HPC environment at ZIH







Taurus

General purpose cluster from Bull for highly parallel HPC applications (2013)

- 137 TFlop/s total peak performance
 - Island 1: 270 nodes Intel Sandy Bridge (2 × 16 cores, AVX), RAM: 2,4,8 GB/core
 - <u>Island 2:</u> 44 nodes Intel Sandy Bridge (2 × 16 cores) + 2 NVIDIA Tesla K20x GPUs
 - <u>Island 3:</u> 180 nodes Intel Westmere, (2 × 12 cores), RAM: 4 GB/core
 - 2 SMP nodes with 1 TB RAM, Sandy Bridge (4 × 16 cores)
- Bullx Linux 6.3 (CentOS / RH)
- batch system Slurm







Taurus, phase II

Q1/2015: second phase with > 1 PFlop/s and 5 PB scratch



New building: Lehmann-Zentrum





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Venus

Large shared-memory System (SGI Ultraviolet) for memory-intensive computing (2013)

- 8 TB shared memory
- 10,6 TFlop/s peak performance
- 512 cores Intel E5-4650L (Sandy Bridge) 2,6 GHz
- 79 TB SAN disk storage
- SuSE Linux Enterprise Server 11
- batch system LSF







Atlas

General purpose cluster from Megware for capacity computing (2012)

- 51,8 TFlop/s peak performance
- 5888 cores AMD Opteron 6274 (4 × 16 cores) 2,2 GHz
- 92 nodes with 64 to 512 GB memory
- 13 TB memory
- 79 TB SAN disk storage
- SuSE Linux Enterprise Server 11
- batch system LSF

out of production: end 2014 (now only 78 no-des)









Infrastructure

- Compute hardware
- HPC file systems
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Overview

Hierarchy of file systems: speed vs. size vs. duration:

- RAM disk,
- local SSD,
- machine global /scratch,
- HPC global /projects, /home
- TUD global intermediate archive,
- TUD global long term storage.





RAM disk

Available at Venus (at the moment):

- only allowed from within an LSF job, can only use a part of the memory assigned to the LSF job;
- module load ramdisk make-ramdisk <size of the ramdisk in GB>
- path to the ramdisk is fixed to /ramdisks/<JOBID>
- accessible from the whole machine,
- for fast copy:

parallel-copy.sh <source directory or file> <target directory>

• ramdisk will automatically be deleted at the end of the job

More info at https://doc.zih.tu-dresden.de





Local disk

Recommended at Taurus (Atlas):

- SSD: best option for lots of small I/O operations, limited size (\sim 50 GB),
- ephemeral: data will be deleted automatically after 7 days,
- each node has its own local disk. Attention: Multiple processes on the same node share their local disk,
- path to the local disk is /tmp





Scratch file system

Fastest parallel file systems at each HPC machine:

- large parallel file system for high bandwidth,
- data may be deleted after 100 days,
- paths to scratch file system are /scratch/<login> and /scratch/<project> with access rights for the whole HPC project, resp.
- All nodes of the machine share this file system.





Common file system for all ZIH's HPC machines:

- Very slow and small, but with multiple backups.
- Deleted files are accessible via the logical .snapshot directory. This directory contains weekly, daily, and hourly snapshots. Copy your file to where you need it.
- Paths to permanent storage are
 - /home/<login> (20 GB !) and
 - o /projects/<projectname>

with different access rights (cf. Terms of Use).

• All HPC systems of ZIH share these file systems.

Do not use the permanent file system for production! Frequent changes slow down or even disable the backup.





Archive

Common tape based file system:

- really slow and large,
- expected storage time of data: about 3 years,
- access under user's control.





Data transfer

Special data transfer nodes are running in batch mode to comfortably transfer large data between different file systems:

- Commands for data transfer are available on all HPC systems with prefix **dt**: dtcp, dtcp, dtls, dtmv, dtrm, dtrsync, dttar.
- The transfer job is then created, queued, and processed automatically.
- User gets an email after completion of the job.
- Aditional commands: dtinfo, dtqueue.

Very simple usage like

dttar -czf /archiv/jurenz/taurus_results_20140523.tgz \
 /taurus_scratch/jurenz/results





Infrastructure

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Installed software is organized in modules.

A module is a user interface, that:

- allows you to easly switch between different versions of software
- dynamically sets up user's environment (PATH, LD_LIBRARY_PATH, ...) and loads dependencies.

Private modules files are possible (e.g. group-wide installed software).





Module groups

Modules are ordered into groups (just 2 examples, each):

- compilers
 - gcc/4.7.1
 - intel/2013(default)
- libraries
 - boost/1.49
 - python/2.7.5-scipy
- tools
 - cmake/2.8.11
 - nedit/5.5
- applications
 - lammps/2013aug-gpu
 - paraview/4.0.1





Current modules

Abinit, ADOL-C. AllpathsLG, Amber, Ansys, Beast, BLACS, Boost, Bowtie, clang, CLUSTALW, cmake, COMSOL, CP2K, CTool, DDT, DFTB+, Dune, Dvninst. EMBOSS. FDTD Solutions, Feep, FreeSurfer, FFTW, FSL, Gamess, Gaussian, GCC, GDB, git, GnuPlot, GrADS, Gromacs, GSL, HMMER, HPCToolkit, Hypre, Infernal, Intel Suite, ITPP, Lammps, LibNBC, L-BFGS-B, Liggghts, Ilvm Is-dyna, Lynx, Mathematica, Matlab, Meep, METIS, MKL, MUST, NAMD, NCBI ToolKit, Numeca, NWChem, OCaml, Octave, Open Babel, Open MPI, Open64, Oprofile, OpenFOAM, OpenProspect, PAPI, ParMetis, Paraview, pcre - library, PDToolkit, Perl, PETSc, PGI, PHYLIP, PhyML, PLINK, PyCUDA, PyMOL, PyMPI, Python/SciPy, QT libraries, QuantumEspresso, R-Project, Samtools, SAPT, Scalapack, Scalasca, ScaFES, Score-P, Siesta, Silo-Library, svn, TBB, Tecplot, TIFF, TINKER, Totalview, TrinityRNASeq, Turbomole, VASP, VampirTrace, Visit, VTK, Yade DEM, Wannier90





Modules - How to

module avail - lists all available modules (on the current system)
module list - lists all currently loaded modules
module show <modname> - display informations about <modname>
module load <modname> - loads module modname
module switch <mod1> <mod2> - unloads mod1; loads mod2
module rm <modname> - unloads module modname
module purge - unloads all modules

```
~> module load boost
boost version 1.49 for x86_64 architecture loaded.
openmpi version 1.6.4 for x86_64 architecture loaded.
gcc version 4.6.2 for x86_64 architecture loaded.
~> module switch gcc gcc/4.7.1 && gcc --version
gcc (GCC) 4.7.1
~> module rm gcc
gcc version 4.7.1 for x86_64 architecture unloaded.
~> module purge
boost version 1.49 for x86_64 architecture unloaded.
openmpi version 1.6.4 for x86_64 architecture unloaded.
```





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Modules for HPC applications

- MPI library from BULL (OpenMPI): module load bullxmpi
- Compiler: module load intel/2013-sp1







Infrastructure

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Overview

Who can use the HPC systems at ZIH?

- ZIH is the state computig center for HPC.
- Available for universities and research institutes in Saxony.
- Free of charge.

Life cicle of a project (* outside TU Dresden)

- Project admin (leader) fills in an online application form
- Sech user fills out an HPC login form, stamp, fax (*)
- An account is generated (20.000 CPUh) to evaluate the computational needs.
- Prepare full project application
- Scientific board (Wissenschaftlicher Beirat) decides, resources are granted
- O Data removal at the end of the project where to?





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Overview

"Nutzungsbedingungen für die HPC-Systeme am ZIH" cover

- data security of personal meta data
- rights and duties of project leaders and project administrators
- data handling





Data handling

We assume that only project related files are in the HPC file systems. (Support team has root access.)

- Access to data after closing a login:
 - in /projects: user and project administrator
 - in /home: only the user
- For seamless work over multiple years: store project data only in /projects.
- Data can be erased by ZIH (e.g. automatically):
 - after 7 days in /tmp,
 - after 100 days in /scratch,
 - 15 months after the closing of the project or login in /projects and /home





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Persöhnliche Angaben.

see https://doc.zih.tu-dresden.de

TU Dresden - HPC-Projektsystem

Startseite » ... » Zentrale Einrichtungen » ZIH » Hochleistungsrechnen (HPC) » Zugang

PROJEKTANTRAG

Um auf den Hochleistungsrechnem großere Projekte bearbeiten zu können, ist es notwendig, vorab einen Projektantrag zu stellen. Diese werden durch den Wissenschaftlichen Beirat des ZIH begutachtet. Die Bewilligung erfolgt maximal für ein Jahr. Die Projektaufzeit nurs notwendigenewise ein Jahr umfassen; sie kann vanieren, gegebenerfalls unterliegt das Projekt mehreren Bewilligungszeiträumen.

Es besteht die Möglichkeit, zu jedem Zeitpunkt neue bzw. weitere Projektanträge zu stellen, die je nach Verfügbarkeit von Reszuren bewiligt werden können. Ummittebar nach Eingang der Online-Antrage können Sie eine Svalukerungsprässe von 10.000 CPU hnutzen, um Recherzeit-Abschätzungen für den ausführlichen Projektantrag durchzuführen. Loter von HPC-Projekten ist grundstitzlich der Lehrstuhlinhaber der jeweiligen Arbeitsgrupen. In dessen Auftrag fauren aber auch Mittebert die Antragestellung übernehmen.

Geben sie hier ihre Daten als Antragssteller an. Nicht die Daten des Projektleiters. Wenn sie als Antragsteller auch der Projektleiter sind, können sie dies in Schritt III angeben.





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PROJEKTANTRAG

Persöhnliche Angaben.







Projektbeschreib

Überprüfen d Angaben.



Um auf den Hochleistungsrechnem größere Projekte bearbeiten zu können, sit es notwendig, vorab einen Projektantrag zu stellen. Diese werden durch den Vissenschäftlichen Beitra die Sith Beydrachterb. Die Bewilligung erfolgt maximal für ein jahr: Die Projektandzeit muss nich notwendigerweise ein jahr umfassen; sie kann vanieren, gegebenenfalls unterliegt das Projekt mehreren Bewilligungszeitariumer. Es beateltu die Mohjekteit, zu jedem ze Einpunkt neue bewierer Brojektandrage zu stellun, die janch verfügsbeart von Ressourcen bewilligt werden konnen. Umrittelbar nach Eingang der Online Antrage konnen Sie eine Evoluerungsphass von 10.000 CPU houtzen, um Recherzielt-Abschatzungen dur den ausdährlichen Prosikantrage durchzufturten. Inter Ver-Perciekten ist understäuft durchschatungen der Leinstuhlichhaber der inweiligen

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Arbeitsgruppe. In dessen Auftrag können aber auch Mitarbeiter die Antragsstellung übernehmen.



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PROJEKTANTRAG

u.ä	Zeitraum, den Projektleiter
	Angabe über die benötigten Resourcen (Machinen, CPU-Zeit, Speicher).
IV	Angaben über die verwendete Software
V	Projektbeschreibung
VI	Überprüfen der Angaben.

FCHNISCHE

DRESDEN

	Allgemein	
Name des Projektes	Luftqualität	
Projektbeginn	August • 2014 • 2	
Projektende	Juli • 2015 •	
Wissenschaft	Philosophie Kategorizierungen nach der DFG	•
Förderung	BMBF	-
Antragsart	Erstantrag O Folgeantrag	_
Fails S	Projektleiter ie selost der Projektleiter sind, lassen sie diese Felder b	itte frei.
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PROJEKTANTRAG



Machine	Rechenzeit	CPU-Anzahl pro Job	Arbeitsspeicher pro Kern (GByte)	Scratch-temporär (GByte)
□ SGI UV 2000 (venus) ²²				
🗆 IBM iDataPlex dx360M2 (triton) ²²				200
♥Megware-Cluster (atlas)	10000	64	8	
🗆 HPC-Microsoft Cluster (titan)				
✓Bull-Cluster (taurus) ²	10000	128	8	200
Projekt-Home (GByte) max. 30068 möglich	300			
		bestätigen		





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PROJEKTANTRAG

Die folgenden Angaben helfen uns ihren Projektaccount schon von Beginn an an ihre Bedürfnisse anzupassen

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PROJEKTANTRAG

Spätestens bei einer CPU Zeit von über 10000h ist eine ausführliche Projektbeschreibung notwendig. Ein Template dafür bzw. für einen Statusbericht bei Polgeanträgen finden Sie unter: https://tu-dresden.de/die_tu_dresden/zentrale_einrichtungen/zih/hpc/zuggan/projektantrag.

Image: Section of the bendlighten Resource and Resour	Projektbeschreibung 2 deutsche Kurfassung		
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bestätigen			





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PROJEKTANTRAG

Überprüfen sie Ihre Angaben. Wenn alles richtig ist, schicken sie den Antrag ab.

Deutschland		Deutschland		
e Matil E mag/aux orytage/prig/ta/pri/	544		Statistical States	dan -
		Projekt (Erstantrag)		
Titel	Luftqualität			
Zeitraum	Aug 2014 bis Jul	2015		
Förderung	Bundesministeri	um für Bildung und Forschung		
Beschreibung	labore et dolore ea rebum. Stet c ipsum dolor sit a dolore magna ali rebum. Stet clita	or sit amet, consetetur sadipscing e magna aliquyam erat, sed diam volu lita kasd gubergren, no sea takimat met, consetetur sadipscing elitr, se quyam erat, sed diam voluptua. At v kasd gubergren, no sea takimata si	iptua. At vero eos i a sanctus est Lore d diam nonumy eir iero eos et accusai	et accusam et justo duo dolores m ipsum dolor sit amet. Lorem mod tempor invidunt ut labore et m et justo duo dolores et ea
Kommerzielle Softwarepakete	MATLAB			
Bevorzugte Compiler	GCC			
Programmiersprachen	C++			
Arten der verwendendeten Software		Public Domain		
Programmiermodelle	Hybrid, MPI			
		beantragte Resourcen		
Projekt-Home	300 GB			
	CPU-time	CPU-count per job	Memory (GByte)	Scratch-temporär (GByte)
Machine	(hours)			
	(hours) 10000	64	8	200

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IV V

VI

Überprüfen der Angaben.

Full proposal

The test period should be used to determine the further needs and document this in an an extended proposal for the scientific board ("Wissenschaftlicher Beirat"). The extended proposal should include:

- presentation of the problem and description of project content (with references of publications),
- achieved preliminary work, pre-studies with results, experiences,
- target objectives and target cognitions,
- physical and mathematical methods or solutions,
- computational aspects: algorithms, software, for parallel codes: parallel efficiency,
- needed resources: CPU time, memory per core, storage iterms of capacity and frequency.
- A few figures might be helpful to understand the description.





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Who...

- \bullet project leader (normally chair of institute) \rightarrow accountable
- \bullet project administrator (needs HPC login) \rightarrow responsible What...
 - manage members of the project (add + remove),
 - check storage consumption within the project,
 - retrieve data of leaving members
 - contact for ZIH





Online project management

TECHNISCHE

DRESDEN

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Detailansich	nt	Mitarbeiter		Statistik			
Allgemein							
Titel	They are they	internet in the Processon of	stemmin Permiting)				
unix-group	r menerication						
Projektdauer	01. August 2009	9 - 31. August 2014					
Förderung							
Antragsart	Erstantrag						
Hardware							
Maschine		CPU-Zeit (Stunden)	CPU-Anzahl pro Job	Speicher (GByte)			
Megware-Cluster (atl	as)	700.000	128	100			
SGI UV 2000 (venus	;)	500.000	128	100			
Bull-Cluster (taurus)		700.000	128	100			
Spezifikatione	n						
Programmiermodell	e	OpenMP, MPI					
Bevorzugte Compiler		PGI, Intel, GCC	PGI, Intel, GCC				
Programmiersprachen		Fortran 95, Fortra	Fortran 95, Fortran 90, Fortran 77, C++, C				
Arten der verwendendeten Software		Kommerztelle Sof	Kommerzielle Software, Public Domain, Eigenentwicklung				



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Online project management

lame	Mail	Login	
	Addar Addr. Add	ndigingit.	Als Administrator festlegen deaktivieren
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wy//Toyles/v/	and and a strength of the state	17/744	Als Administrator festlegen
ende			
r Nutzer darf rechr			
	ügen und aktivieren Projekte hinzugefügt werden kann, benötig o	dieser ein gült	iges ZIH-Login.
einem gültigen ZIH- ktivieren.	Login, kann sich der Nutzer dann über folger	nden Link für	das Projekt aktiveren und
	n.tu-dresden.de/managers/Members/addToF		



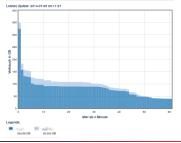


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 $\mathsf{ZIH} \to \mathsf{users}:$

- next training course "Introduction to HPC at ZIH" November 6, 2014
- HPC wiki: https://doc.zih.tu-dresden.de
 - link to the operation status,
 - knowledge base for all our systems, howtos, tutorials, examples...
- mass notifications per signed email from the sender "[ZIH] HPC Support" to your address ...@mailbox.tu-dresden.de or
 - ...@tu-dresden.de for:
 - problems with the HPC systems,
 - new features interesting for all HPC users,
 - training courses
- email, phone in case of requests or emergencies (e.g. uses stops the file system).





Channels of communication

$\mathsf{User} \to \mathsf{ZIH}$

- Trouble ticket system:
 - advantages
 - reach group of supporters (independent of personal availability),
 - issues are handled according to our internal processes,
 - entry points
 - email: hpcsupport@zih.tu-dresden.de
 - phone: service desk (40000)
 - planned: self service portal
- personal contact
 - phone call, email, talk at the Mensa
 - socializing is fine... but: risk of forgetting





Channels of communication

$\mathsf{User} \to \mathsf{ZIH}$

- Trouble ticket system:
 - advantages
 - reach group of supporters (independent of personal availability),
 - issues are handled according to our internal processes,
 - entry points
 - email: hpcsupport@zih.tu-dresden.de
 - phone: service desk (40000)
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Infrastructure

2 Access

Overview

- Terms of Use
- Application for HPC projects
- Management of HPC projects
- Channels of communication
- Kinds of support





HPC management topics:

- HPC project proposal,
- login,
- quota, accounting etc.





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- HPC project proposal,
- login,
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HPC usage requests:

- Why does my job not start? and other questions concerning the batch system
- Why does my job crash?
- How can I ...





HPC Software questions:

- help with the compiling of a new software
- installation of new applications, libraries, tools
- update to a newer / different version





HPC Software questions:

- help with the compiling of a new software
- installation of new applications, libraries, tools
- update to a newer / different version
- \rightarrow restrictions of this support:
 - only if several user groups need this
 - no support for a particular software
 - allow for some time





Performance issues

- joint analysis of a piece of SW
- discussion of performance problems
- detailed inspection of self-developed code
- in the long run: help users to help themselves





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Storage capacity issues

- joint analysis of storage capacity needs
- joint development of a storage strategy



