High Performance Computing

Infrastructure at DESY

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High Performance Computing Infrastructures at DESY
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Compute Infrastructures at DESY - Outline

- BIRD
  - Quick overview
- GRID, NAF, PAL
- HPC resources in Zeuthen
- HPC cluster
  - Hardware & Layout
  - Setup & Numa
  - Getting started
  - Monitoring & Operational model
  - Storage
  - Examples: Mathematica & Matlab

Compute Infrastructures at DESY - BIRD

> BIRD - Batch Infrastructure Resource at DESY

- See http://bird.desy.de/info (being updated)
- General purpose batch farm
- Getting access: via registry batch resource → UCO@desy.de
- Problems: UCO@desy.de; Bird.Service@desy.de

OS	# Hosts	Cores/Host	Total cores	RAM/Core	Total RAM
SLD6-64	17	4-12	168	8-48GB	0.5TB
SLD5-64	157	8-48	1520	8-126GB	4.1TB
Total	174	4-48	1688	8-126GB	4.6TB

- Environments for mpi or GPU jobs
  - High latency 1GE backbone
  - Jobs with heavy inter-process communication will suffer

Compute Infrastructures at DESY - BIRD

- GPUs are embedded into the BIRD farm

Host	OS	Hardware	GPUs	Drv / Cuda	Bird Resource	
It-gpu01	SL5-64	Intel Xeon 2.5GHz 16 cores 24GB ram	Fermi 2*M2050 448 cores, 3GB	Nvidia 260.24 Cuda 3.2	-l h=it-gpu01 -l gput=nvidiaM2050	Needs upgrade
It-gpu02	SL5-64	AMD Opteron 870 2GHz 8 cores 16GB ram	Tesla 1*C870	Nvidia 270.41.19 Cuda 4.0	-l h=it-gpu02 -l gput=nvidiaC870	Will retire soon
It-gpu03	SL5-64	AMD Opteron 6128 2GHz 16 Cores 24GB ram	Fermi 2*C2070 448 cores, 6GB	Nvidia 270.41.19 Cuda 4.0.17	-l h=it-gpu03 -l gput=nvidiaC2070	Accelereys Jacket
It-gpu04	SL6-64	Intel Xeon 2.4GHz 24 cores 24GB ram	Fermi 2*M2070 448 cores, 6GB	Nvidia 304.51 Cuda 5.0.35	-l h=it-gpu04 -l gput=nvidiaC2070	
It-gpu05	Coming soon		Kepler K20 2496 cores, 5GB			

- Interactive login via qrsh
  - ssh -XY pal; ini bird; qrsh -l h=it-gpu03 -l gput=nvidiaC2070 ...
  - Graphical apps like matlab possible (xhost; DISPLAY)

HPC cluster - History

- Zeuthen has a long HPC history
  - APE1 in 1987 → APEnext in 2005 (array processor experiment)
  - QPACE for lattice QCD simulations based on IBM PowerXCell 8i processors
  - GPE - GPU Processing Experiment (HadronPhysics2 project).
  - NIC – John von Neumann Institute for Computing (DESY, GSI, FZJ)

- DESY Hamburg
  - Started in 2011 with retired hardware. Initiated by Ilya Agapov
  - 64*8 cores and distributed Fraunhofer filesystem (fhgfs)
  - 20GE Infiniband backbone (on an old switch)
  - Proofed to be rather useful, just the old hardware was dying rapidly.
  - Retired the old test-cluster last year and migrated to a new system → it-hpc cluster

HPC Cluster – Hardware

> Compute Nodes:

- **16 Dell PowerEdge R815**
  - 4 CPU AMD Opteron(TM) Processor 6276 2.3GHz
    - Per CPU 16 Bulldozer Cores with 64 GB RAM
  - 256 GB RAM
  - Numa Architecture
  - 10GE Ethernet
  - QDR Infiniband (40GB/s)

- **2 PowerEdge C6145**
  - 4 CPU AMD Opteron(TM) Processor 6276 2.3GHz
    - Per CPU 16 Bulldozer Cores with 48 GB RAM
  - 192 GB RAM
  - Numa Architecture
  - 10GE Ethernet
  - QDR Infiniband (40GB/s)

DESY

HPC Cluster – Hardware

> Storage Nodes:

- **4 Dell PowerEdge R510**
  - 2 CPU Intel(R) Xeon(R) CPU E5503 @ 2.00GI
    - Per CPU 2 Cores with 6 GB RAM
  - 12 GB RAM
  - QDR Infiniband (40GB/s)
  - 20 TB / 12 Disc / Raid 6
- **1 PowerEdge 2950**
  - 2 CPU Intel(R) Xeon(R) CPU E5345 @ 2.33GHz
    - Per CPU 4 Cores with 4 GB RAM
  - 8 GB RAM
  - Numa Architecture
  - 1 GE Ethernet
  - QDR Infiniband (40GB/s)

HPC Cluster – Hardware

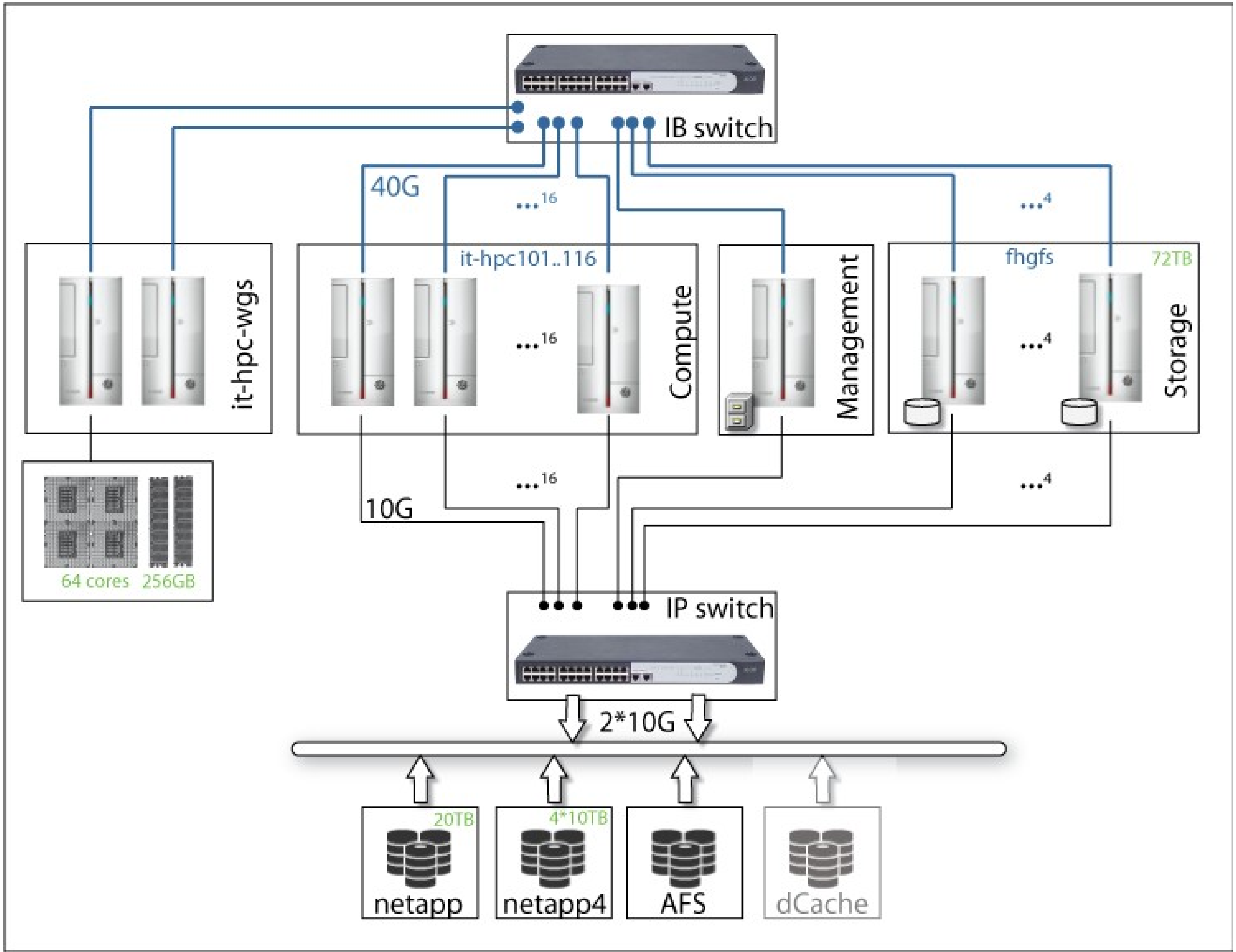
InfiniBand is a switched fabric communications link used in high-performance computing and enterprise data centers.
Its features include high throughput, low latency, quality of service and failover, and it is designed to be scalable. The InfiniBand architecture specification defines a connection between processor nodes and high performance I/O nodes such as storage devices. (wikipedia)

> Infiniband Infrastructure:

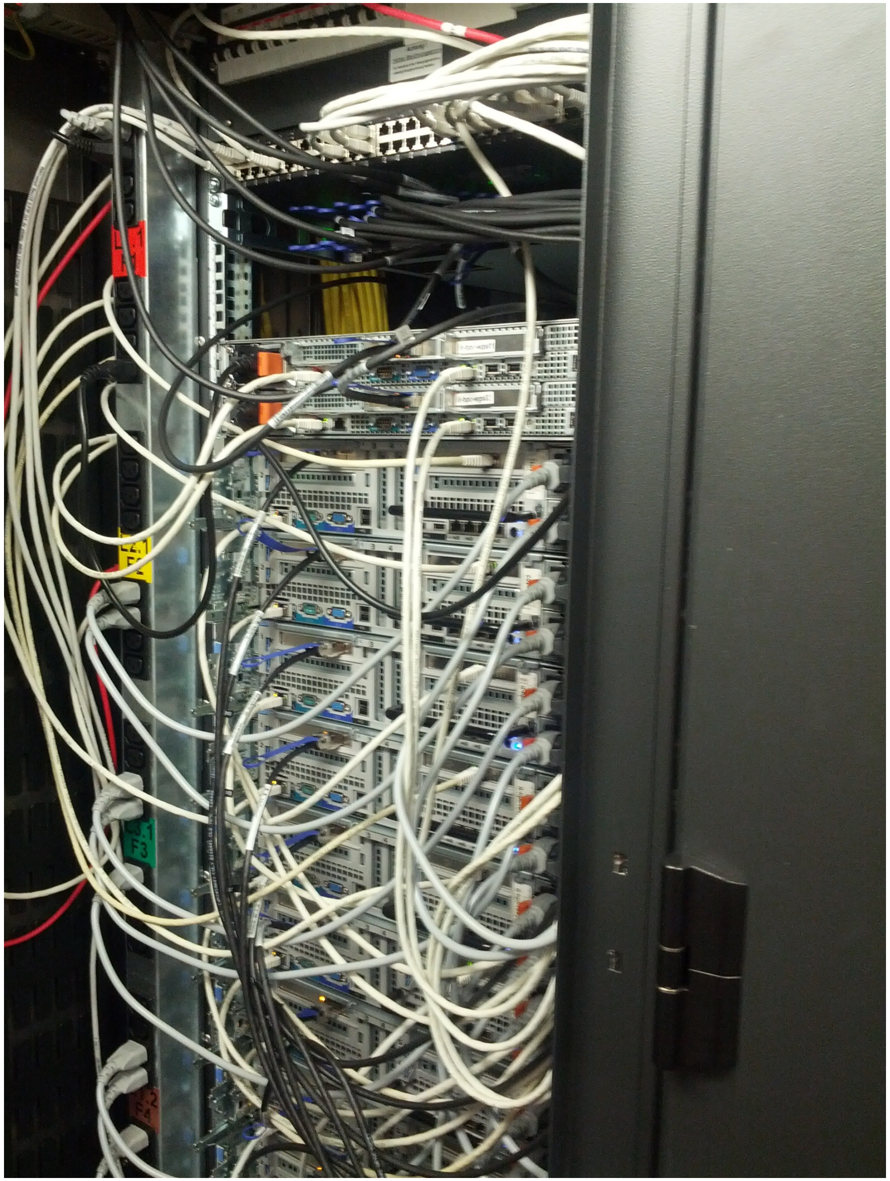
- Mellanox SX6036 InfiniBand/VPI Switch Systems
  - 36 Ports
  - 56 GBIT/s FDR
  - Managed
- Mellanox Connect-X3 QDR Cards

HPC Cluster – Layout

1024 (+128) cores – 4TB (+0.38TB) memory – >100TB temporary storage
56G infiniband backbone – interlagos PCI-E2



HPC Cluster – Pictures



HPC Cluster – Setup/Optimization

- Setup
  - Scientific Linux 6.3 (always updated)
    - No automatic updates → maintenance
    - No salad/yum/cron jobs
    - Xymon monitoring
  - AFS/Kerberos
  - IPoIB configuration

- Optimizations
  - Bound infiniband card to core
  - Switch of timer interrupt
  - Unlimited locked-in-memory address space

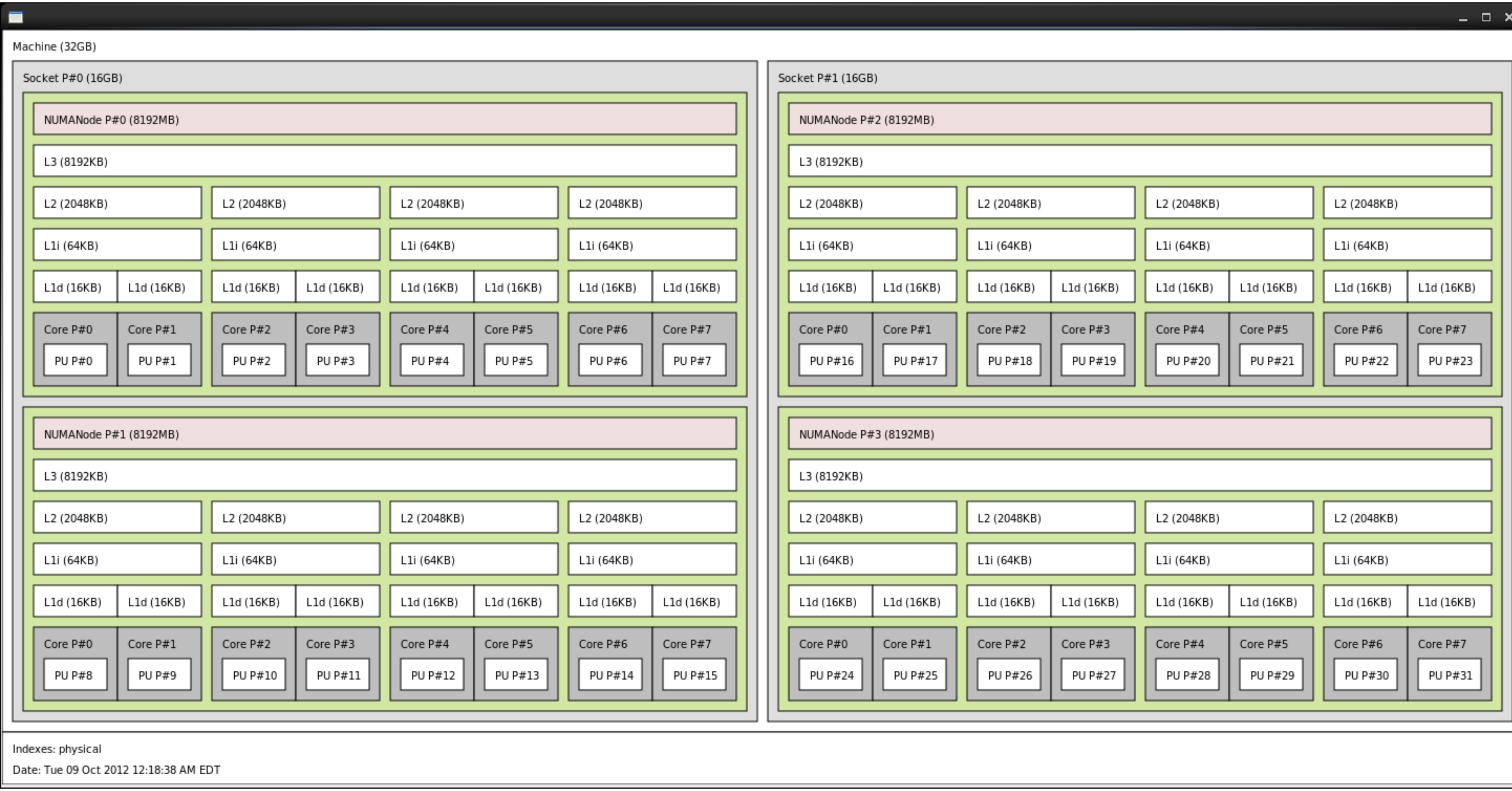
HPC Cluster – Numa Hardware

Non-Uniform Memory Access (NUMA) is a computer memory design used in multiprocessing, where the memory access time depends on the memory location relative to a processor. Under NUMA, a processor can access its own local memory faster than non-local memory (memory local to another processor or memory shared between processors). (wikipedia)

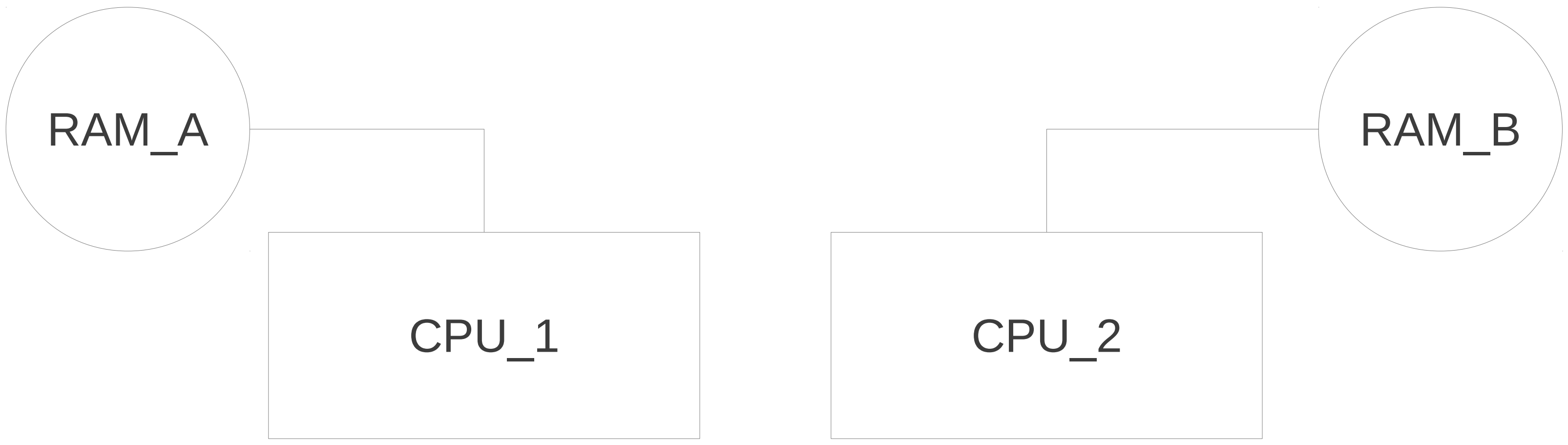
- All compute nodes are numa machines
- To gain the full potential of the nodes you should consider the architecture
- Tools like likwid are helpful (necessary?)
  - Examine Numa topology
  - Profile software on Numaarchitecture
  - Bind proccesses to cores
- Multicore CPU make it even more complicated
  - Shared caches
  - Shared FPU
  - Different Levels of aggregation
- Commercial software is not always numa aware

HPC Cluster – Numa Hardware

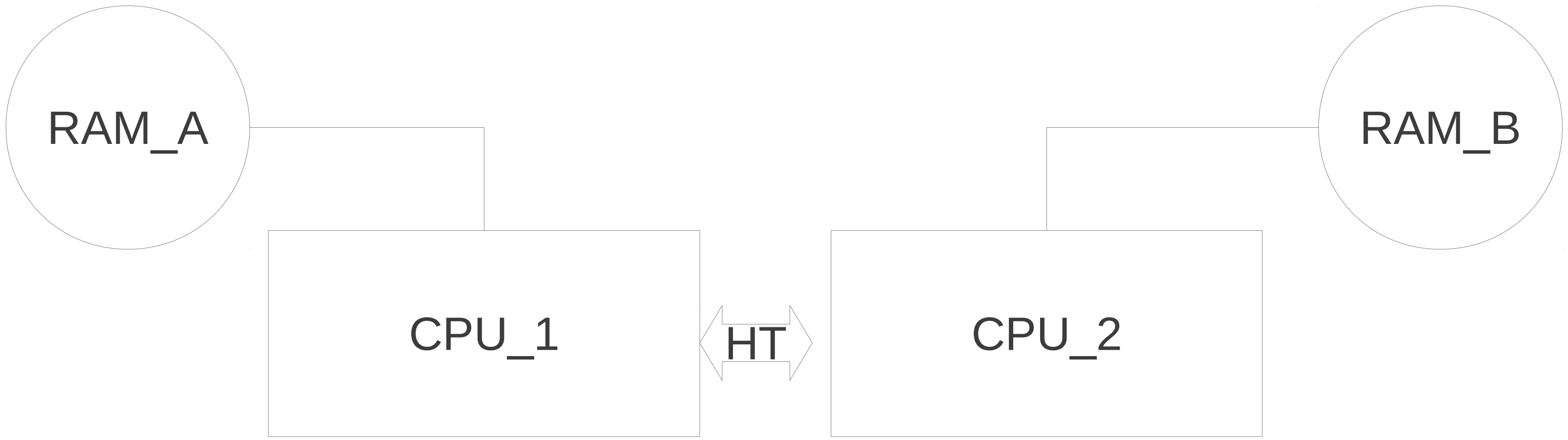
Example: 2 Socket Bulldozer System



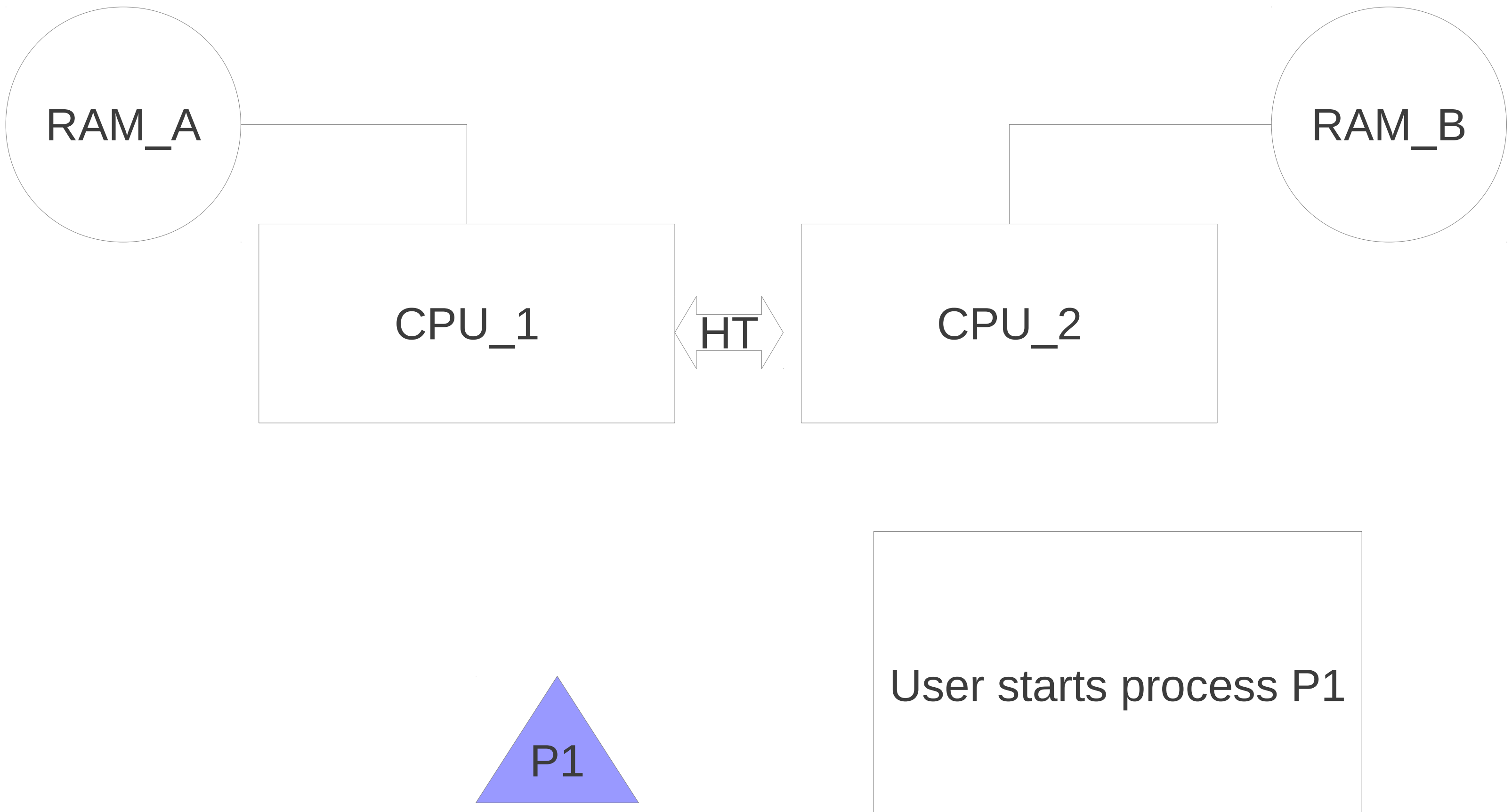
HPC Cluster – Numa Hardware



HPC Cluster – Numa Hardware

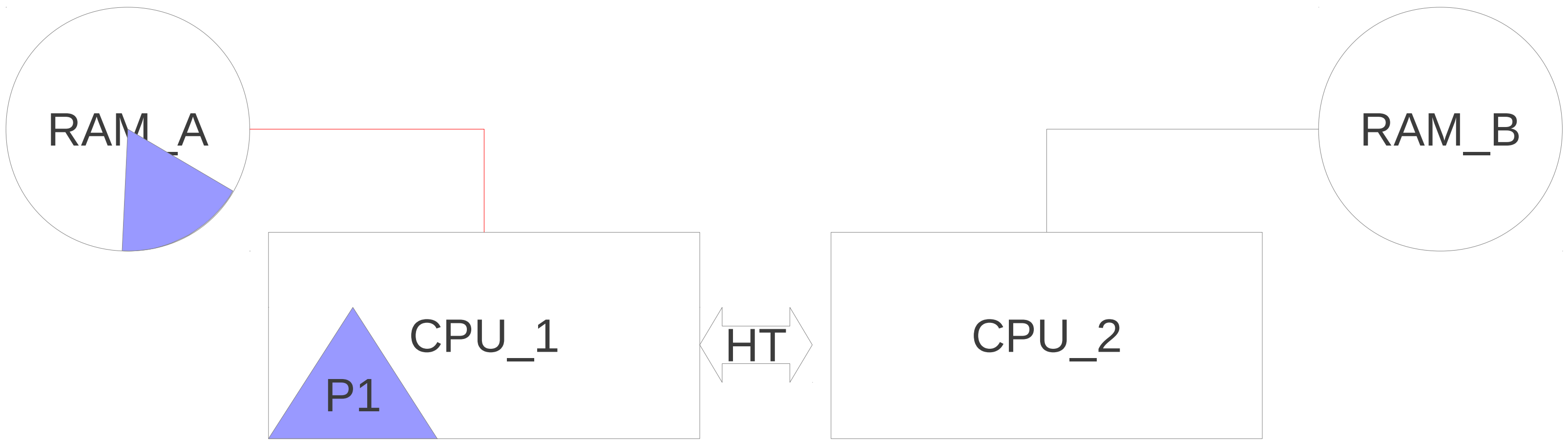


HPC Cluster – Numa Hardware



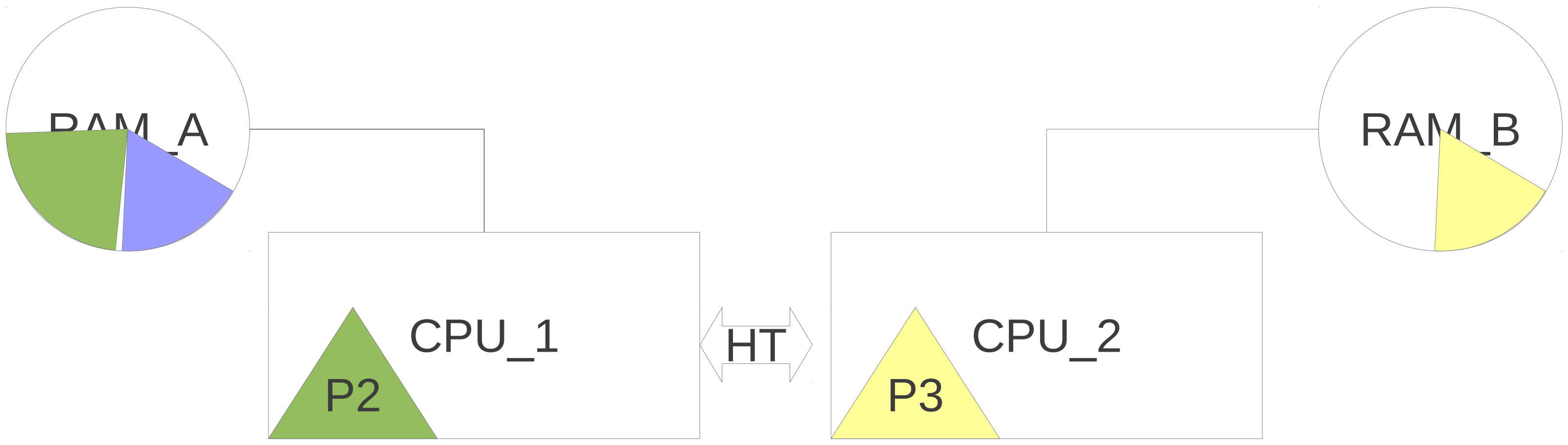
User starts process P1

HPC Cluster – Numa Hardware



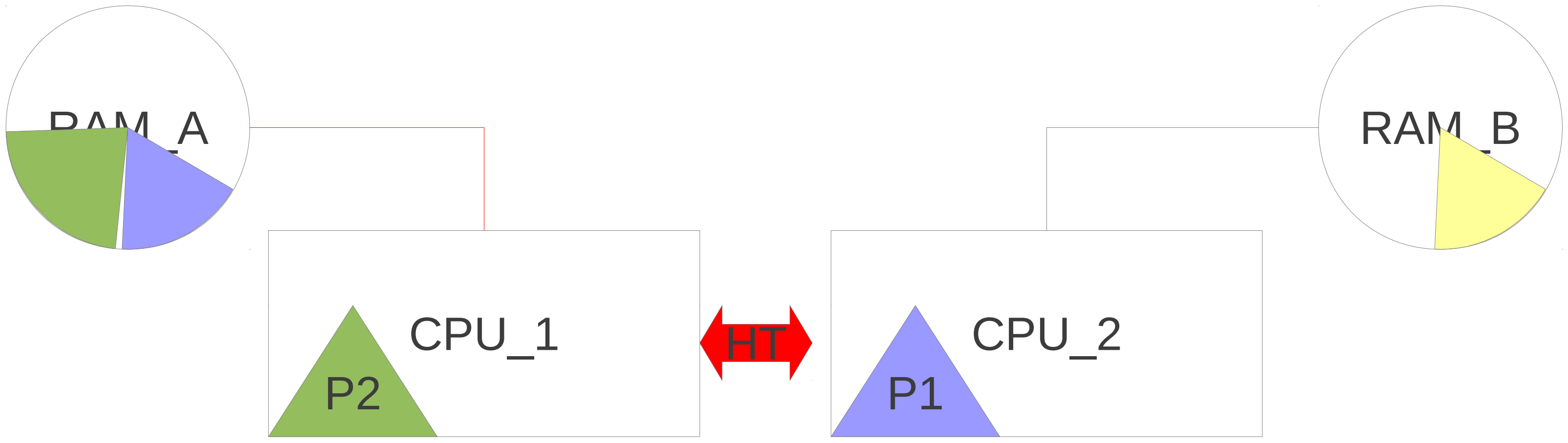
process P1 runs on CPU_1 and allocate Memory on RAM_A

HPC Cluster – Numa Hardware



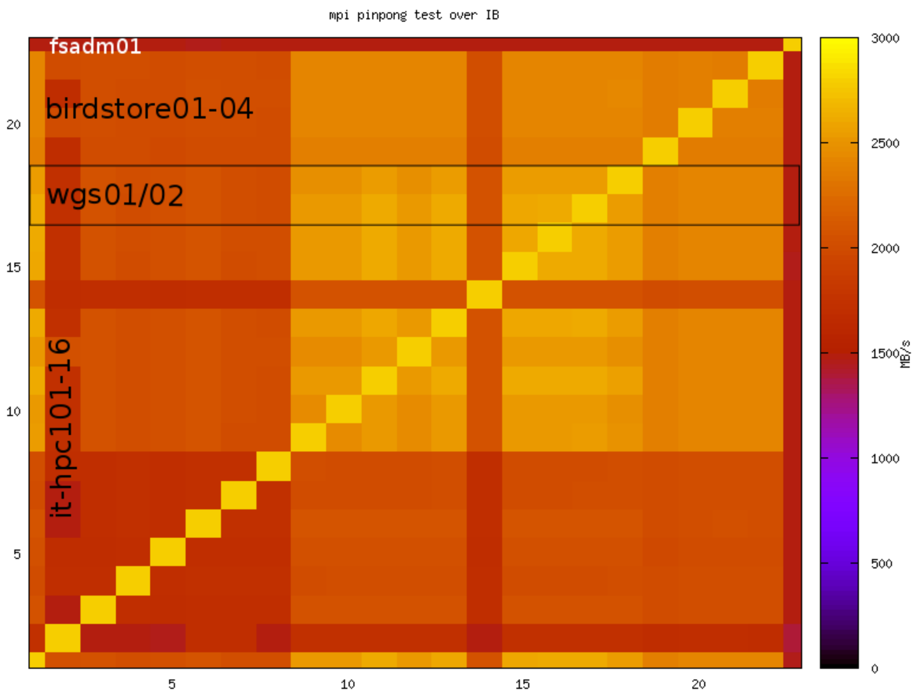
process P1 is
suspended and
still allocate
Memory on RAM_A

HPC Cluster – Numa Hardware

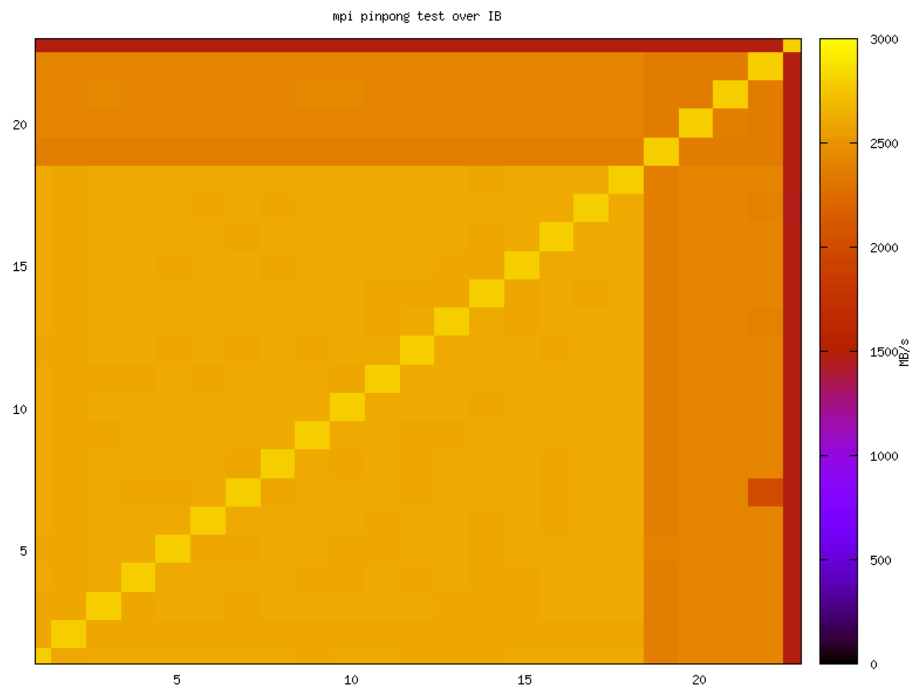


process P1 is rescheduled on CPU_2 and allocate Memory on RAM_A

Simple example - binding sockets and IB adapter



host-host ib bandwidth without socket binding



host-host ib bandwidth with socket binding

Using the HPC cluster

HPC Cluster – First steps

> Pre-requisites:

- Multi-core capable applications
- embarrassingly parallel problems Bird or Grid (if an option)
- 32/64 cores per node with 8/4GB per core prefer <= 8GB/core
    - Single core performance of AMD interlagos not so great
    - If you need lots of memory/core different architectures might be favorable
    - Could be added to it-hpc if that‘s a common requirement

> Uncertain your application is suitable?

- Get in touch!
- Run tests on it-hpc-wgs!
    - it-hpc-wgs are freely accessible.
    - Identical configuration like it-hpc(xxx), but slightly less memory (192GB)

HPC Cluster – First steps

> Gaining access:

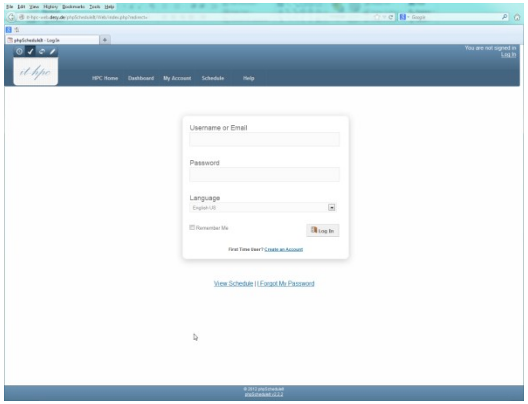
- Access is restricted to „registered“ users
  - No restrictions on it-hpc-wgs!

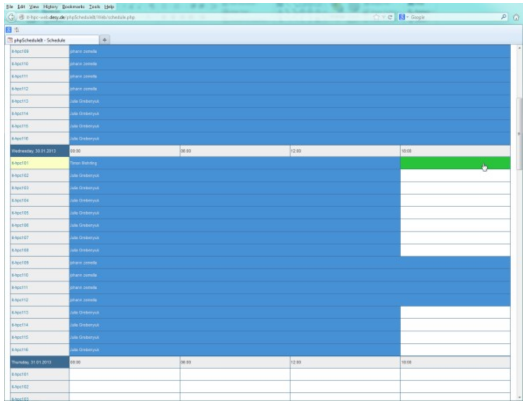
- Send mail to unix@desy.de or uco@desy.de asking for it-hpc „resource“
  - Let us know what kind of application you intend to run
  - Helps us providing essential dependencies
  - Helps us to plan future expansions

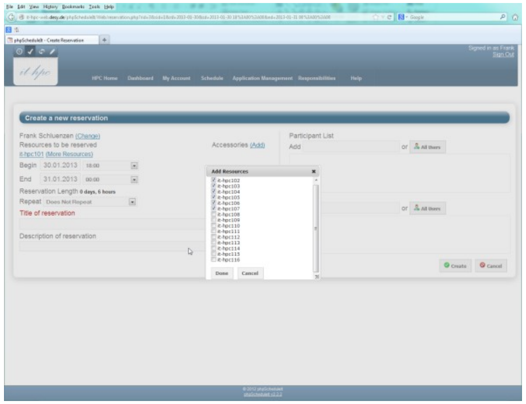
HPC Cluster – First steps

> Scheduling:

- Create an account on the it-hpc web-calendar:
  - Use your DESY account name (not the password!)
  - Currently not kerberized.
- Reserve resources
  - Co-operative model, no fair-share
  - Reservation for full nodes – no sharing of hosts
  - Currently fixed 6h time slots (can be adjusted if needed).
  - Don‘t reserve all nodes for a long time!
  - We do some accounting, if it gets too much out of balance, the model might be adjusted.



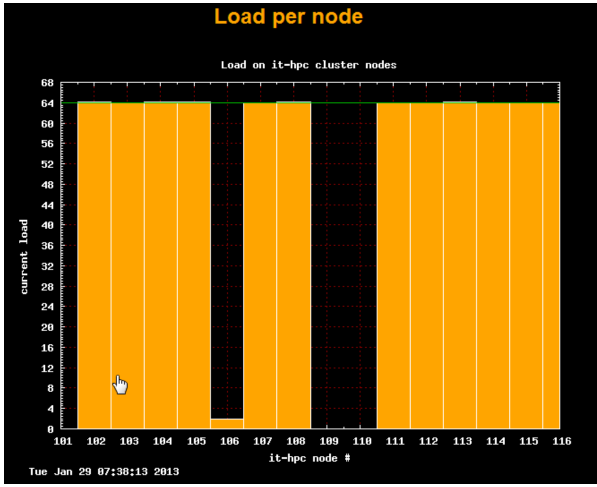




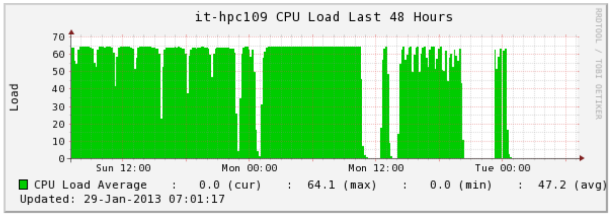
HPC Cluster – Monitoring

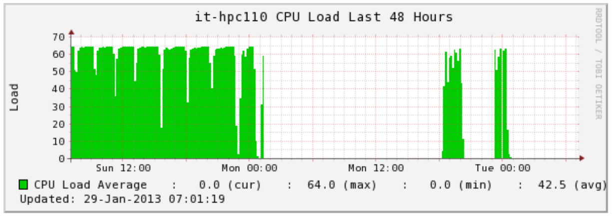
> Reservations:

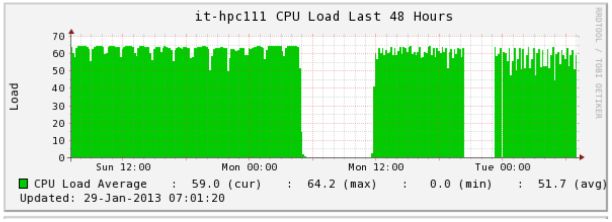
- Currently don‘t enforce reservations
  - That will change soon!
  - Jobs without reservation have low chance of survival
- Jobs conflicting with a reservation will be terminated
  - Jobs exceeding the reservation will be terminated as well.
- Over-subscription creates an alert
  - Load > 64 will slow everything down
  - No termination of jobs.

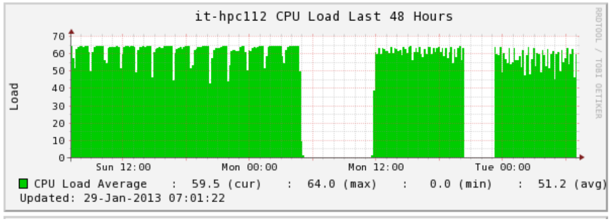


5’ update cycle from xymon









HPC Cluster – Running jobs

- Scientific SW & Compiler usually installed in /opt/<app>/<version>
  - idl, intel, maple, mathematica, matlab, pgi
  - AFS-hosted; but no token required
  - Can be changed to local installations if needed
  - Own software: best on /data/netapp or /afs

- OpenMPI in 2 variants
  - openMPI-1.5.x and openMPI-intel-1.5.x
    - +mpich2-1.2.x

- Compiler
  - gnu 4.4.x, pgi-2012/13, intel-2012/13
  - gnu 4.7.x in /data/netapp/it/tools permits interlagos optimization (`-march=dbver1`)
  - Be careful with intels optimization
    - Floating point model defaults to „*value unsafe optimization*"
    - Intel recommends `–fp-model precise –fp-model source` to be on the safe side
    - Other apps (e.g. matlab) have similar "issues"

HPC Cluster – Running jobs

> Initialize

- `ini` deprecated on SL6, use `module` instead
    - `module avail` to display
    - `module load intel.2011`
    - `module load mathematica`
    - `module load openmpi-x86_64` etc

- For openmpi propagate the prefix
    - `mpirun --prefix /usr/lib64/openmpi …`
    - or: `module load openmpi-x86_64` (in e.g. .zshrc)

Running

- `/usr/lib64/openmpi/bin/mpirun --prefix /usr/lib64/openmpi –mca orte_base_help_aggregate 0 –mca btl_openib_warn_default_gid_prefix 0 –np 1024 –hostfile mpi.hosts <app>`

- Remember to assemble the hostfile corresponding to your reservation (addon to booking?)
- Start the jobs preferably on it-hpc-wgs
- Where to store data?

HPC Cluster – Using storage

> AFS

- Secure, low volume storage.
- TSM Backup possible
- Global File System. Accessible from everywhere
- Good for final results.
- ACL for fine grade right management
- Keep in mind: no token extension, difficult in long running jobs (> 24h)
- Read and Write speed problems

HPC Cluster – Using storage

> NFS (ver. 3/4)

- /data/netapp and /data/netapp4
- 20 TB at the moment without quota
- Secure storage
- Good for long term storage
    - larger volumes of final results
    - Store group specific software
    - Fast user/group home directories
- Per default not accessible from outside it-hpc
- Backup possible
- Cooperative storage

HPC Cluster – Using storage

> dCache

- High performance distributed storage
- Possible connection to tertiary Storage Systems (Tape robot)
- Currently not mounted, but could be mounted via NFS4.1
- Let us know if that‘s a requirement

HPC Cluster – Using storage

> FHGFS

- /data/fhgfs
- 72TB without quota
- Low latency, fast read and write
- Data transfer via Infiniband
- Good for short term temporary storage.
  - Interprocess communication
  - Staging data files
- No export outside the it-hpc cluster
- No backups, no protection
- Cooperative storage (otherwise we would delete chronology)

HPC Cluster – Using storage

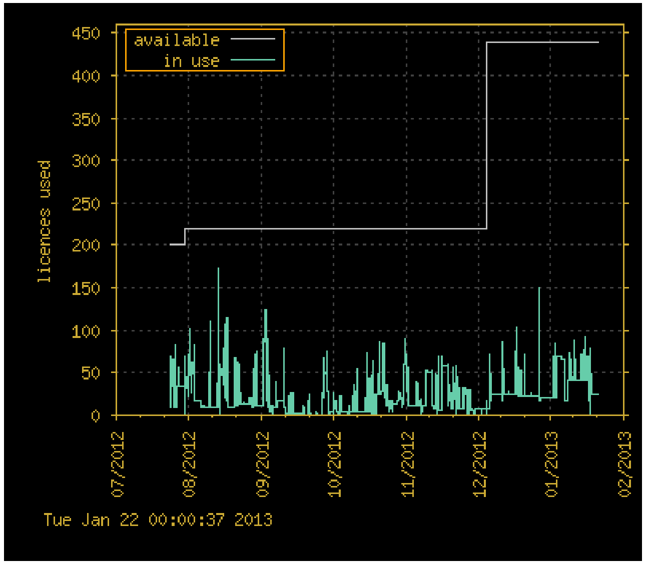
> FHGFS Key benefits

- **Distributed File Contents and Metadata**
  - strict avoidance of architectural bottle necks.
  - distribution of file system metadata (e.g. directory information)
- **HPC Technologies**
  - scalable multithreaded core components
  - native Infiniband support
- **Easy to use**
  - FhGFS requires no kernel patches
  - graphical cluster installation and management tools
- **Increased Coherency** (compared to simple remote file systems like NFS)
  - changes to a file are always immediately visible to all clients.

HPC Cluster – Running mathematica

> Licenses available

- 440 SubKernel licenses occupying a single main-license
- Usually a substantial number of licenses available



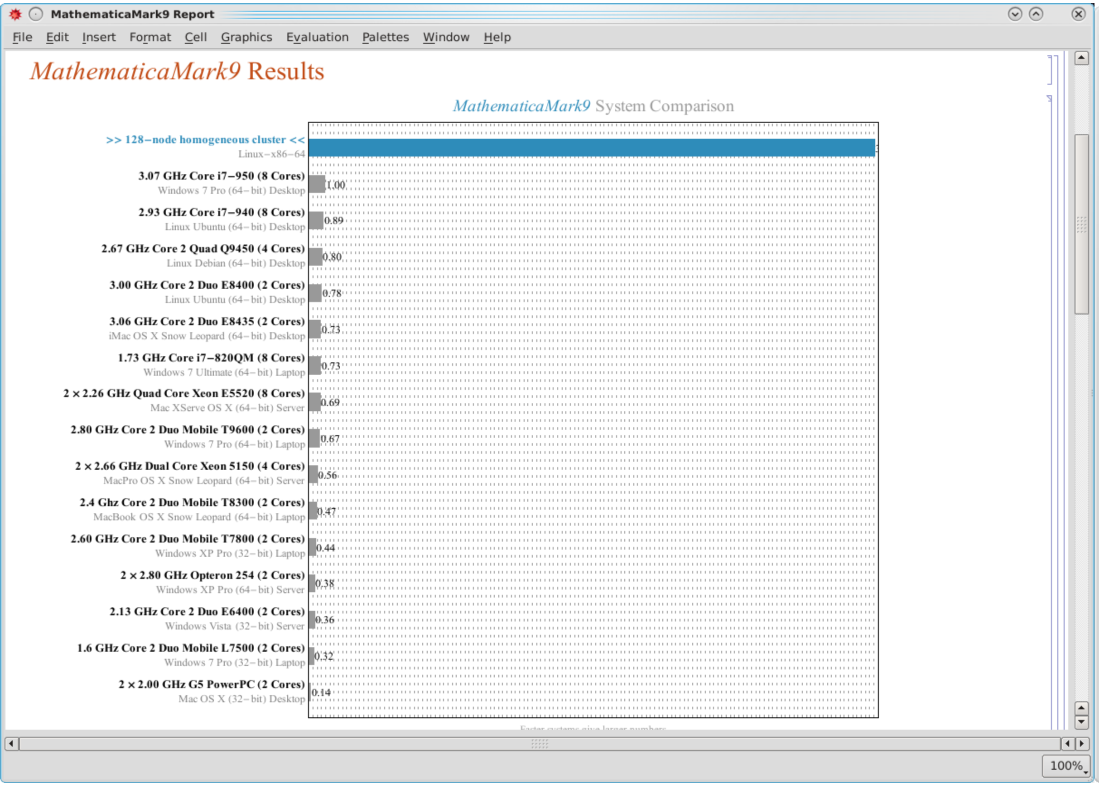
> Mathematica lightweight-grid

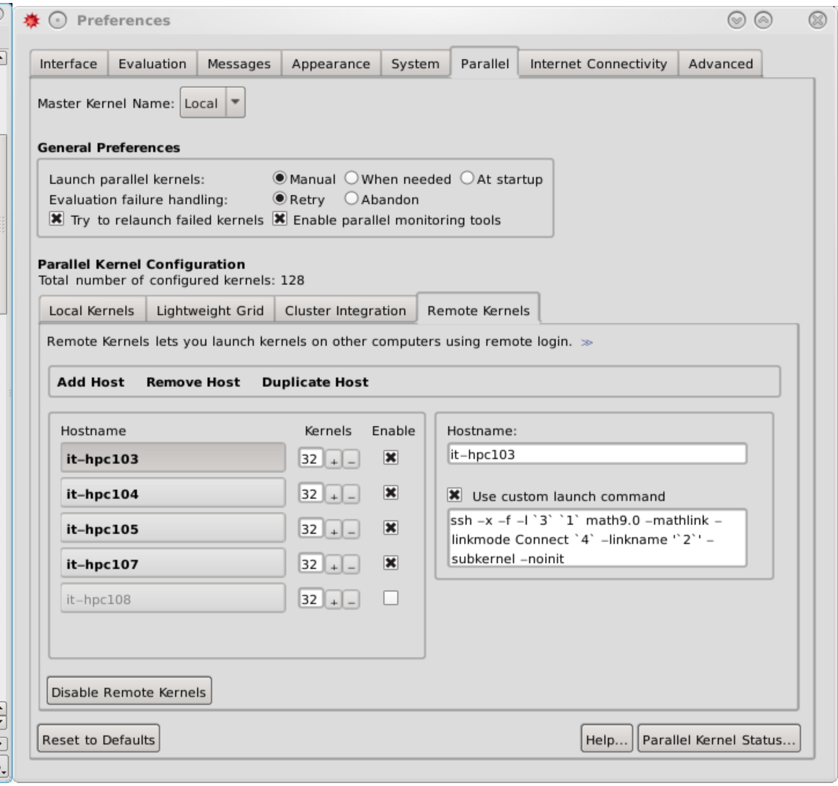
- Requires startup of tomcat server
- Currently not an option on the cluster

> Parallel kernel configuration

- Easily done from within the application
- Unmanaged
- Requires some care selecting the number of kernels per host.

HPC Cluster – Running mathematica





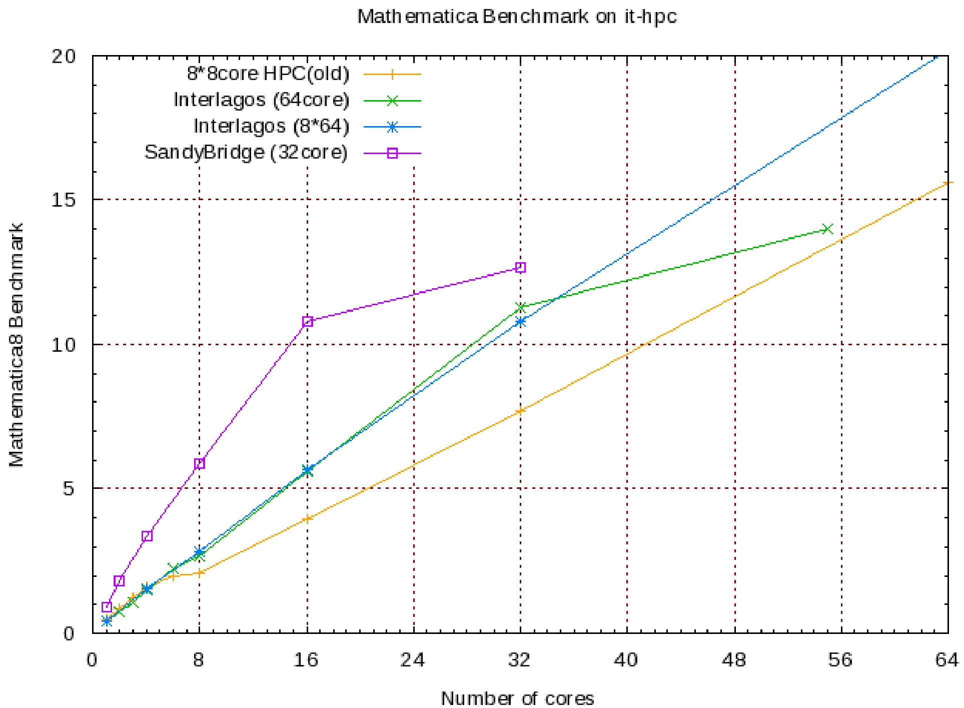
Mathematica benchmark with 128 cores …

HPC Cluster – Running mathematica

> Mathematica benchmarks

- Scales well up to 32-bit cores, gets worse beyond that
  - But true for other architectures as well

- Mathematica has troubles acquiring much more than 50 cores
- Using up to 32-48 cores per node should be fine.



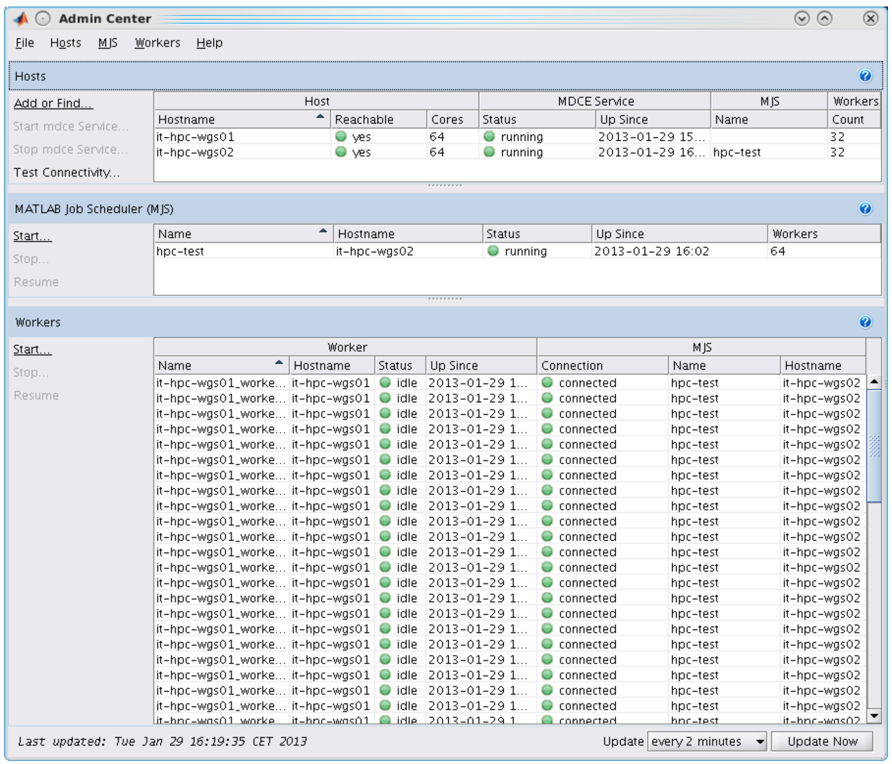
HPC Cluster – Running matlab

> New: Matlab Distributed Computing Server

- 128 kernel licenses 128 core job with a single matlab / distributed computing toolbox

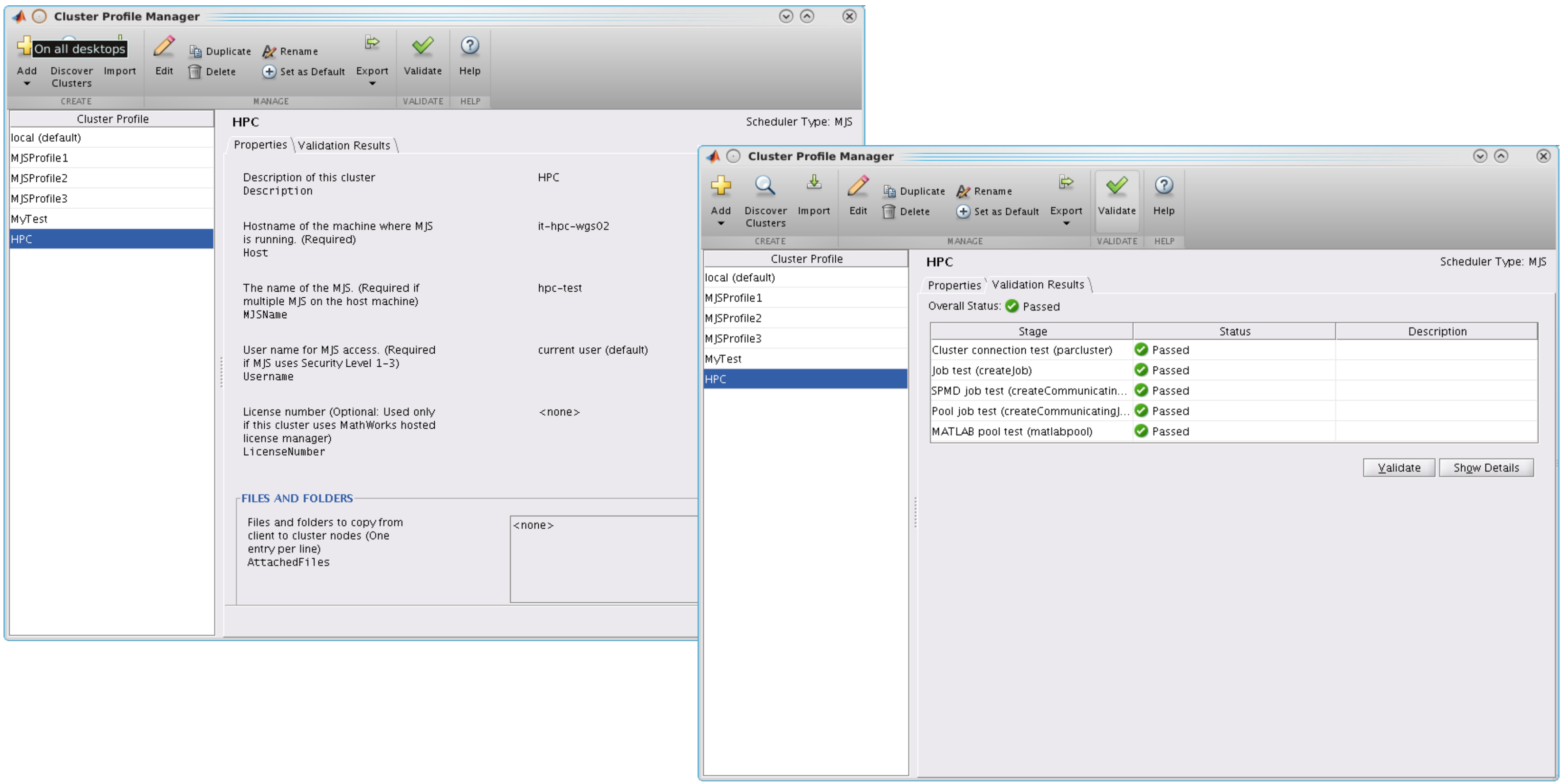
> Currently need to start the matlab scheduler as root

- No automatic startup yet. If frequently used, we could add that to the web-calendar.



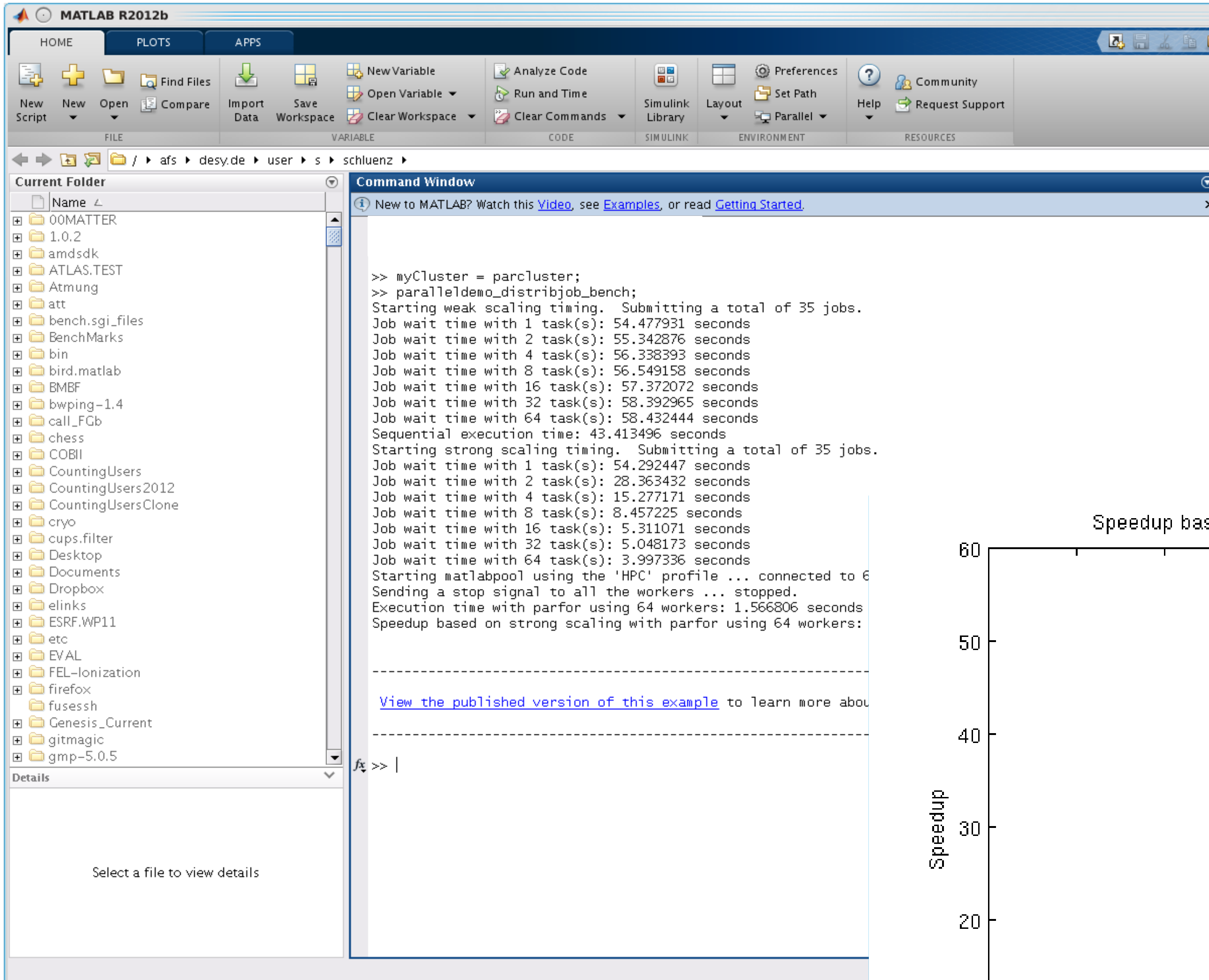
HPC Cluster – Running matlab

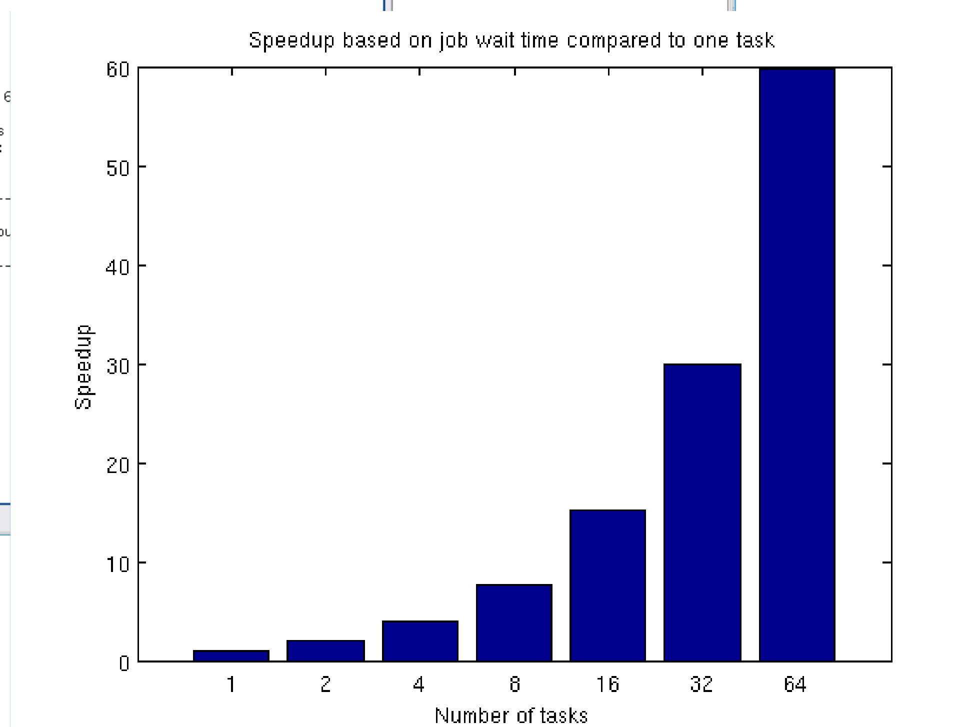
> Once the scheduler is running, job submission from a desktop is easy:




```
>> myCluster = parcluster; matlabpool(myCluster);
>> myrun = matlabpool('open','HPC','64','AttachedFiles',{nb1.m,nb2.m});
```

HPC Cluster – Running matlab





Matlab benchmark with 2*32 cores

GPU computing - workshops

> PNI-HDRI workshop on (parallel) Computing for Photons and Neutrons

- 04-05.03.2013
- See: https://indico.desy.de//event/7333

> Terascale Alliance Workshop on GPU computing

- 15-16.04.2013
- See: https://indico.desy.de//event/7143

> Matlab Advanced Tutorial

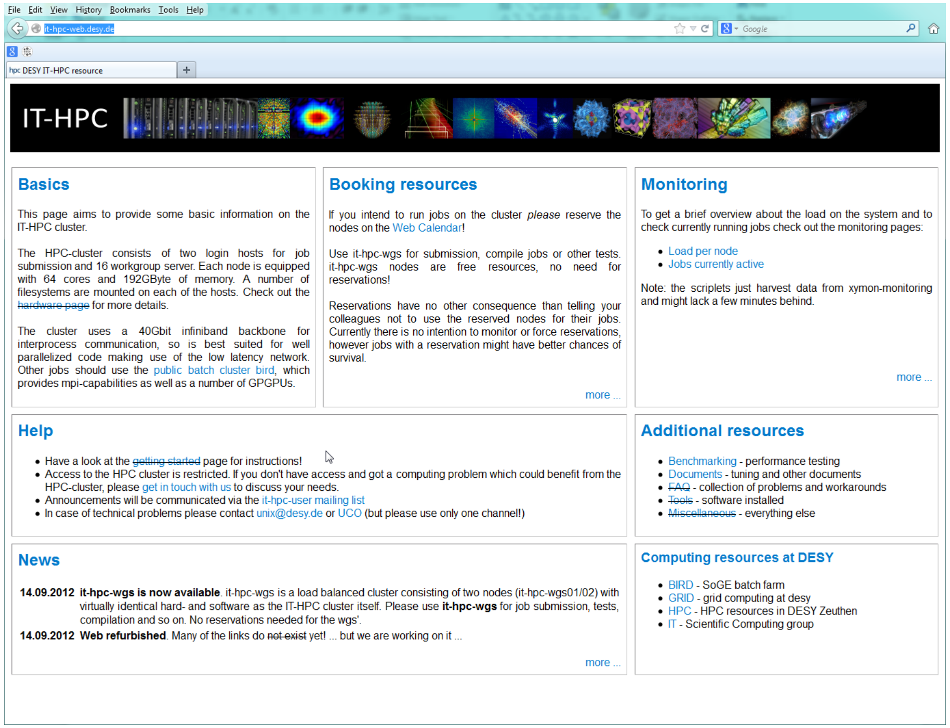
- In preparation

> Anything else (mpi, c++)?

- it-training@desy.de

HPC Cluster – Information

- Web:
  - http://it.desy.de/services/computing_infrastructure
  - http://it-hpc-web.desy.de (only DESY-internal)



- Contact:
  - uco@desy.de
  - unix@desy.de

- Announcements
  - Subscribe to it-hpc-user@desy.de

Questions? Comments?