

More Sustainable HTC Computing

How to better utilize compute resources.

NAF Admin Team

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DESY IT

Two sessions

Introduction to the NAF



🕒 9:15 AM - 10:45 AM

- General sustainability considerations
- What is the NAF? A (short) introduction
- The different building blocks
- Software on the NAF
- Storage on the NAF
- Remote storage
- Getting support

The NAF and Batch Computing



🕒 1:45 PM - 3:15 PM

- Basic concepts of batch clusters
- basic usage: Hello-world jobs
- more advanced jobs, multiple jobs, DAG
- interactive jobs
- information on running/past jobs, debugging
- Sustainability in batch

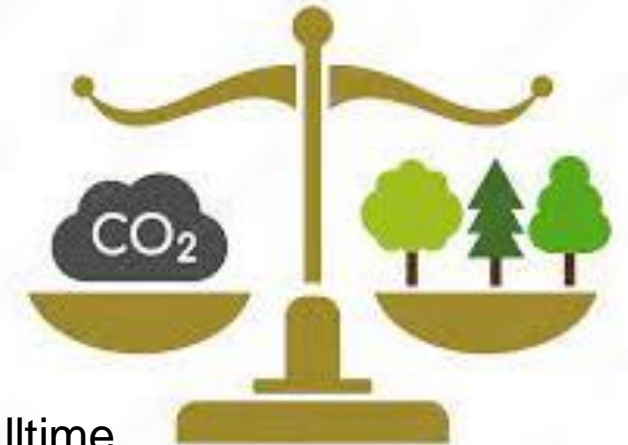
... but first some thoughts about sustainability

- IT is a major energy consumer
- IT equipment has a footprint beyond energy
- Users:
 - Most efficient usage of resources
 - → Optimize workflows, optimize algorithms, optimize code
- Resource providers:
 - Chose efficient hardware, optimize setup
 - Well think about lifecycle of systems
 - Reduce non-IT energy consumption, reuse waste heat
- Research infrastructures, energy providers, society
 - Provide more renewable energy, use more renewable energy, use renewable energy when it is available



Some more qualitative aspects

- Computers consume energy
 - We estimate that in average, computing one hour on one CPU core (with access to data store)
 - consumes 0.28 kWh of energy
 - produces 0.014 kg of CO₂ (according to the German power mix)
 - which is equivalent to that produces on 0.095 km on a VW Golf
- ... the NAF batch system has ~9000 CPU cores and operates 24x7x365
- e.g. jobs are getting killed by the batch system because they exceeded their walltime.
 - e.g. in the 7 days before 29.8.2023:
 - equivalent to ~20.000 core-h of walltime
 - 5600 kWh of energy ... or 33 kW of average power
 - 280 kg of CO₂ ... would need 1200 large trees to capture that (large tree captures around 12 kg CO₂/year)
 - 1900 km on a VW Golf



Who are you?

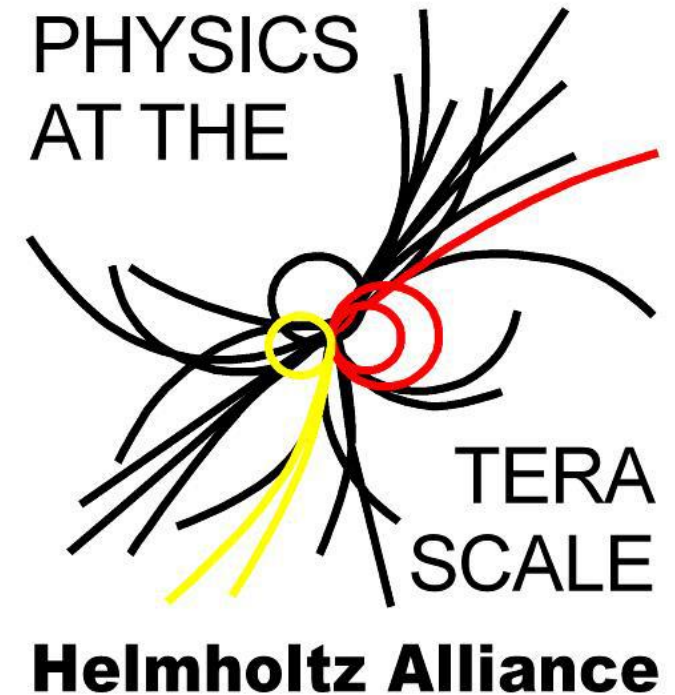
What do you expect from this workshop?

First part:

Introduction to the NAF

What is the NAF?

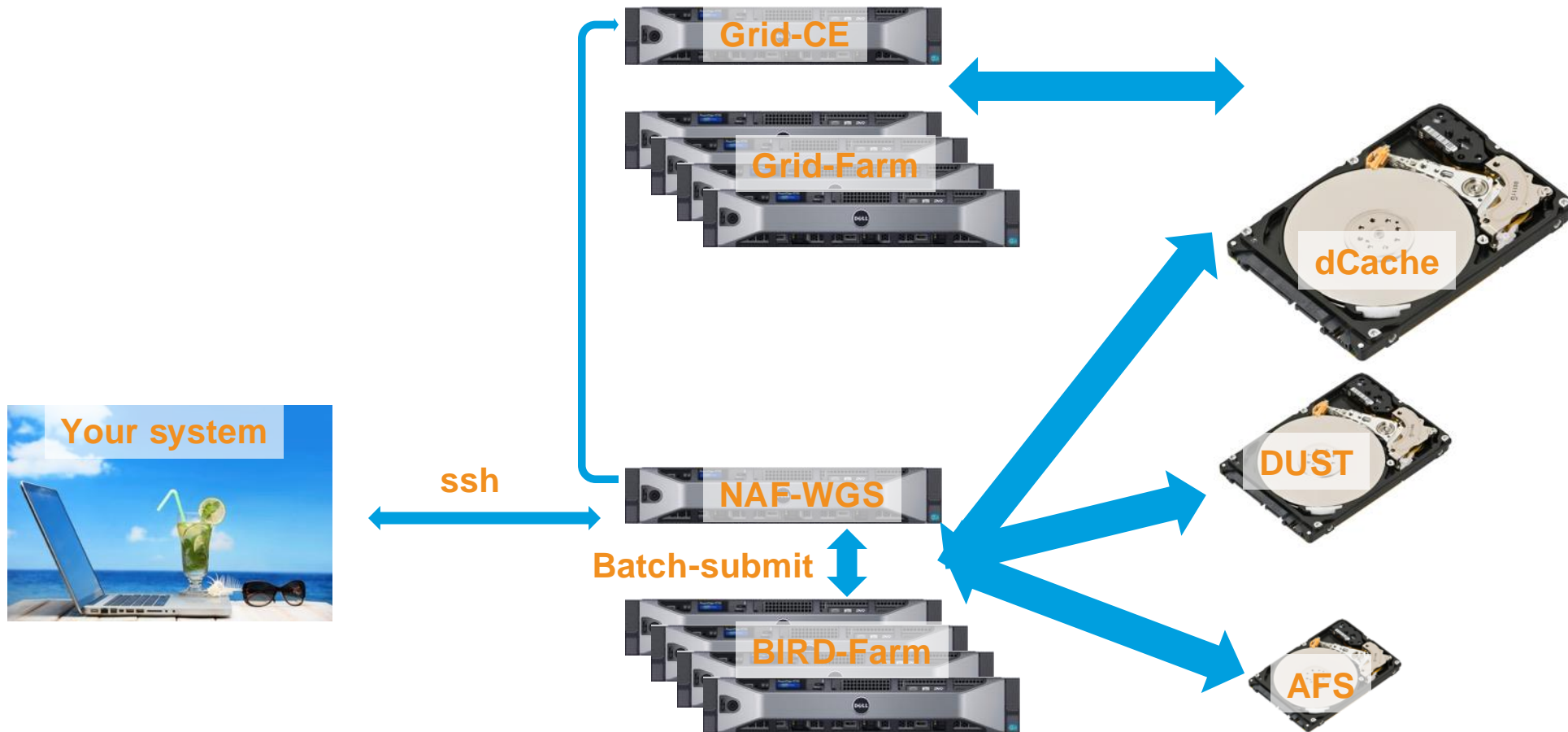
- NAF stands for „National Analysis Facility“
 - *National* means: For people working in institutes in the Terascale Alliance
 - *Analysis* means: Analysing data taken in the Terascale Alliance
 - *Facility* means: Something where you can do real work
- Basically: The NAF is a facility where **YOU** can do your analysis (and stuff around your analysis)



Who can use the NAF?

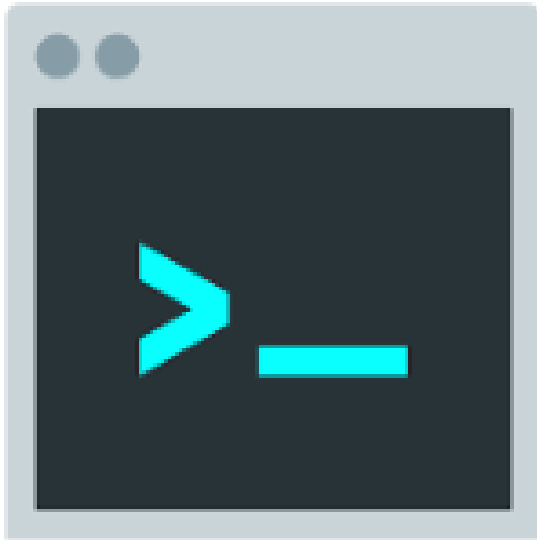
- The political answer:
 - You are from a Terascale Alliance institute
 - You are in LHC, doing analysis (ATLAS, CMS, LHCb)
 - You are in Belle, ILC, legacy HERA
- The technical answer:
 - You need a DESY account from
 - Each user group has (a set of) login machines, e.g.: `naf-atlas.desy.de`
 - Access to this login machines (→ your group admin)
 - You need the “batch” resource to be able to submit jobs (→ your group admin / UCO)

You – and the LHC compute & storage at DESY



Workgroupserver to login to

- try logging into a WGS:
- open a terminal on your laptop
- `ssh USERNAME@naf-NNN.desy.de`

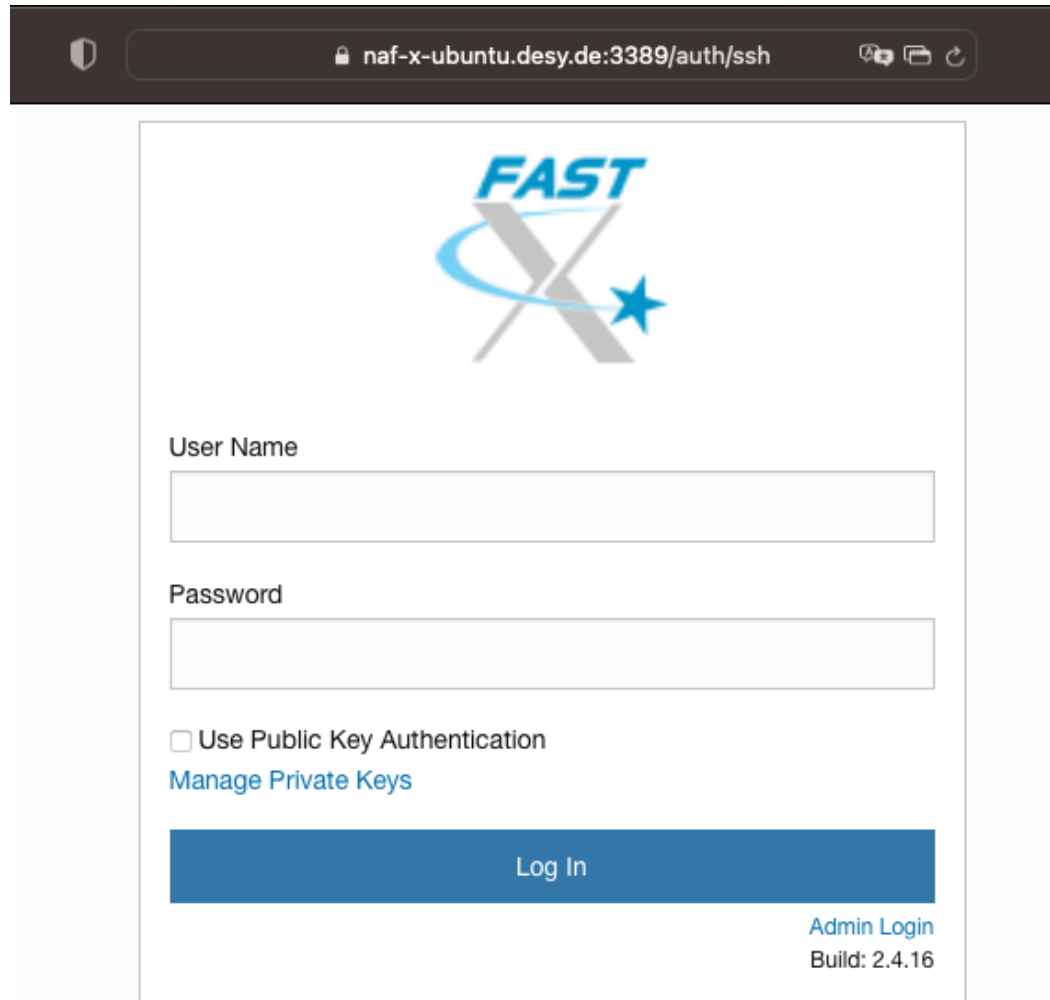


The WGS: Login Node, WorkGroupServer, Interactive Node, ...

- Each group has a set of own WGS
- Why own?
- How many?
- How many resources?
- **Usage of WGS (from the NAF docu)**
- **Be reasonable** when you use the WGS as you are **sharing the resources** with your colleagues and any (mis)use will affect them. So, please be careful and nice to your colleagues. As a rule of thumb, use the WGS for development, **short (<10min) test jobs, graphical things**, ... Do not use the WGS for **longer lasting processes**, or processes that do not require interactive return. Such processes are best placed onto the batch system - which has much more resources and resource control mechanisms.
- We check WGS on a daily basis, and if we find long running jobs or jobs consuming huge amounts of memory, we write an automated email.
- We have to reboot systems to activate new kernels. Using load balancing and alias mechanisms, we try hard to keep logins alive for at least one week. Sometimes we must act faster, though.

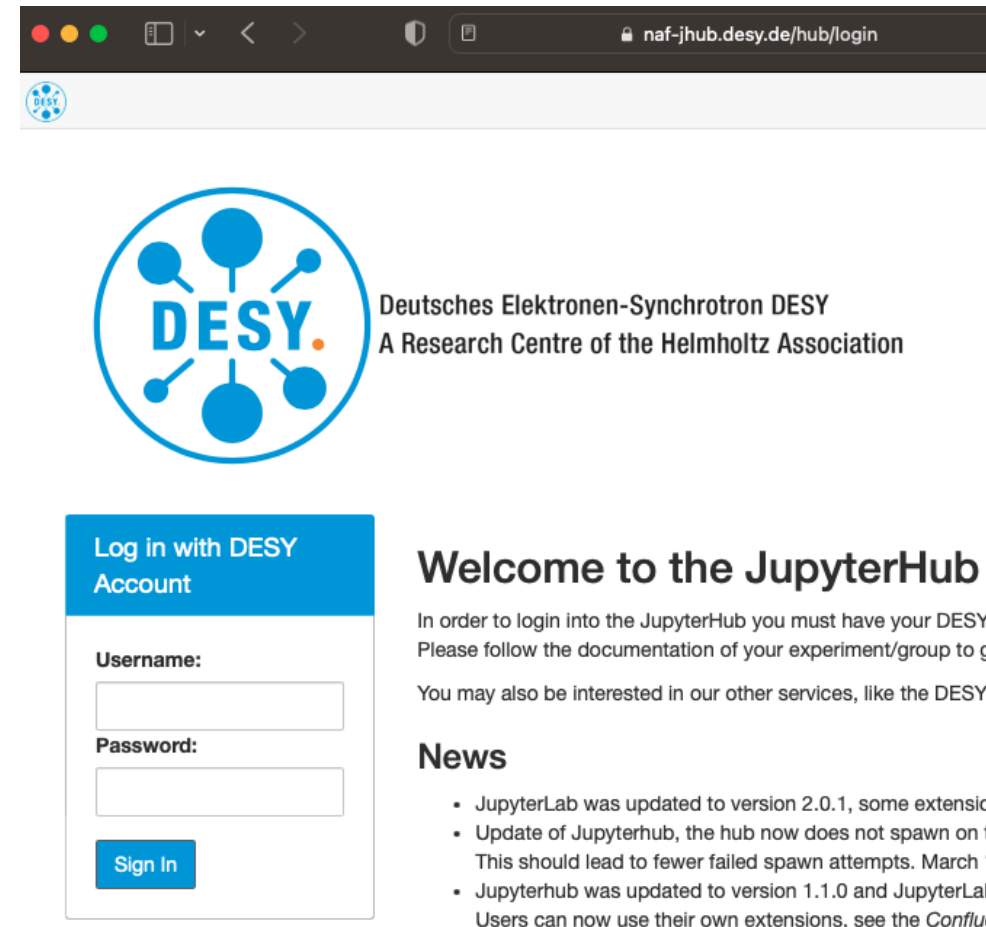
Other access means

- Graphical access: FastX to the NAF remote desktop



The screenshot shows a web browser window with the address bar displaying `naf-x-ubuntu.desy.de:3389/auth/ssh`. The main content area features the FAST logo at the top. Below it, there are input fields for 'User Name' and 'Password'. A checkbox labeled 'Use Public Key Authentication' is present, with a link 'Manage Private Keys' below it. A large blue 'Log In' button is at the bottom. In the bottom right corner, there is a link for 'Admin Login' and the text 'Build: 2.4.16'.

- JupyterHub



The screenshot shows a web browser window with the address bar displaying `naf-jhub.desy.de/hub/login`. The page features the DESY logo, which consists of a blue circle with several smaller circles connected by lines, and the text 'Deutsches Elektronen-Synchrotron DESY' and 'A Research Centre of the Helmholtz Association' to its right. Below the logo, there is a blue box with the text 'Log in with DESY Account'. Underneath this, there are input fields for 'Username:' and 'Password:', followed by a blue 'Sign In' button. To the right of the login box, there is a section titled 'Welcome to the JupyterHub' with a paragraph of text and a link. Below this, there is a 'News' section with a list of updates.

Welcome to the JupyterHub

In order to login into the JupyterHub you must have your DESY Account. Please follow the documentation of your experiment/group to get access.

You may also be interested in our other services, like the DESY Wiki.

News

- JupyterLab was updated to version 2.0.1, some extensions are not compatible with this version.
- Update of Jupyterhub, the hub now does not spawn on 1.1.0. This should lead to fewer failed spawn attempts. March 2020.
- Jupyterhub was updated to version 1.1.0 and JupyterLab 2.0.1. Users can now use their own extensions, see the Confluence page.

What is this?



Why is the WGS slow? What is the footprint of my job? ...

- What goes on on a server?
 - top or (nicer) htop (htop -u kemp)
- NFS traffic:
 - nfsiostat 1
 - nfsiostat 1 /nfs/dust/atlas
- general, including some IO:
 - sar 1
 - vmstat 1
- Discussion 1: Interpretation:
 - Is 10% IO wait a lot? acceptable? negligible?
- Discussion 2:
 - What is *my* job doing? Am I responsible for a slow system?

	PID	USER	PRI	NI	VIRT	RES	SHR	S	CPU%	MEM%	TIME+	Command
c	31856	kemp	20	0	182M	2476	1080	S	0.0	0.0	0:00.24	sshd: kemp@pts/29
c	31857	kemp	20	0	124M	3720	1852	S	0.0	0.0	0:00.22	-bash
c	31971	kemp	20	0	182M	2476	1084	S	0.0	0.0	0:00.05	sshd: kemp@pts/30
c	31972	kemp	20	0	124M	3708	1860	S	0.0	0.0	0:00.18	-bash
c	40867	kemp	20	0	106M	1412	532	D	17.9	0.0	0:10.92	dd if=/dev/zero of=/tmp/local.img bs=1M count=10k
c	40901	kemp	20	0	130M	3076	1624	R	1.4	0.0	0:00.14	htop -u kemp

- State “D” : Waiting for Disk (or network disk)
 - Might indicate a problem if observed for a longer time
 - e.g. NFS server problem
 - e.g. close to 100% quota
- State “Z” : Zombie
 - Is definitely a problem ... if consuming lots of CPU or RAM → write to helpdesk, only reboot can fix
- IT informs per email if cpu > or RAM > ...
 - sometimes a simple “kill \$PID” does not help
 - difference SIGTERM and SIGKILL

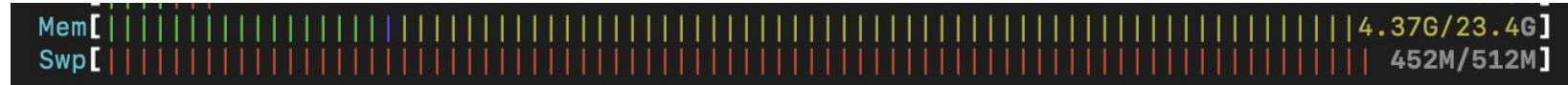
Can't login to the WGS? ... and some other WGS problems

- `ssh naf-atlas13.desy.de`
 - Connection refused ... or the like
 - Have you tried `naf-atlas.desy.de` (without the 13 ?)
 - → We have many WGS, and might be doing maintenance on this special one. Preferably use the generic one.

```
Could not chdir to home directory /afs/desy.de/user/x/xxx: Connection timed out
/usr/bin/xauth:  error in locking authority file /afs/desy.de/user/x/xxx/.Xauthority
-bash: /afs/desy.de/user/x/xxx/.bash_profile: Connection timed out
[xxx@naf-cms14 /]$ pwd
/
```

- Problem with your AFS – home
 - Drop naf-helpdesk a message, with your account, and the WGS in question (naf-cms14 in this case)
- WGS freezing randomly:
 - Sometimes, AFS/NFS is slow to react when many files are in a directory
 - If no clue: inform naf-helpdesk with [user,time,WGS,path] ... we might or might not find a reason, but good for us to know anyhow

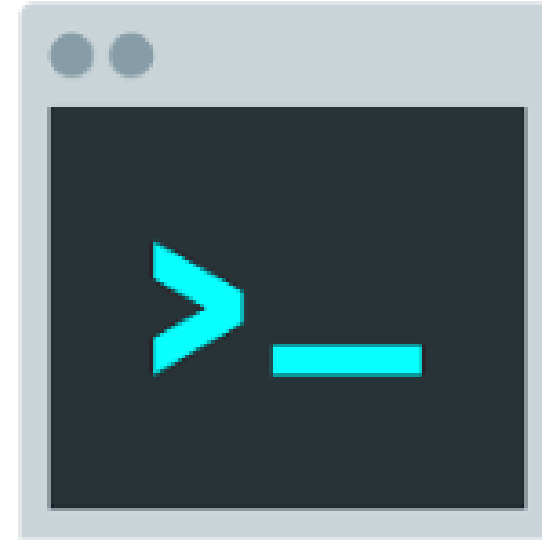
RAM story



- RAM is used as file system cache
 - high RAM occupancy is not necessarily a problem
- High Swap is OK: unused MEM pages are stored on disk
 - ... unless the swapd has lots of CPU time (or vmstat swap-in/swap-out is increased)
- The Kernel kills processes when RAM is getting too tight
 - over the years, it has gotten better at spotting the right culprit

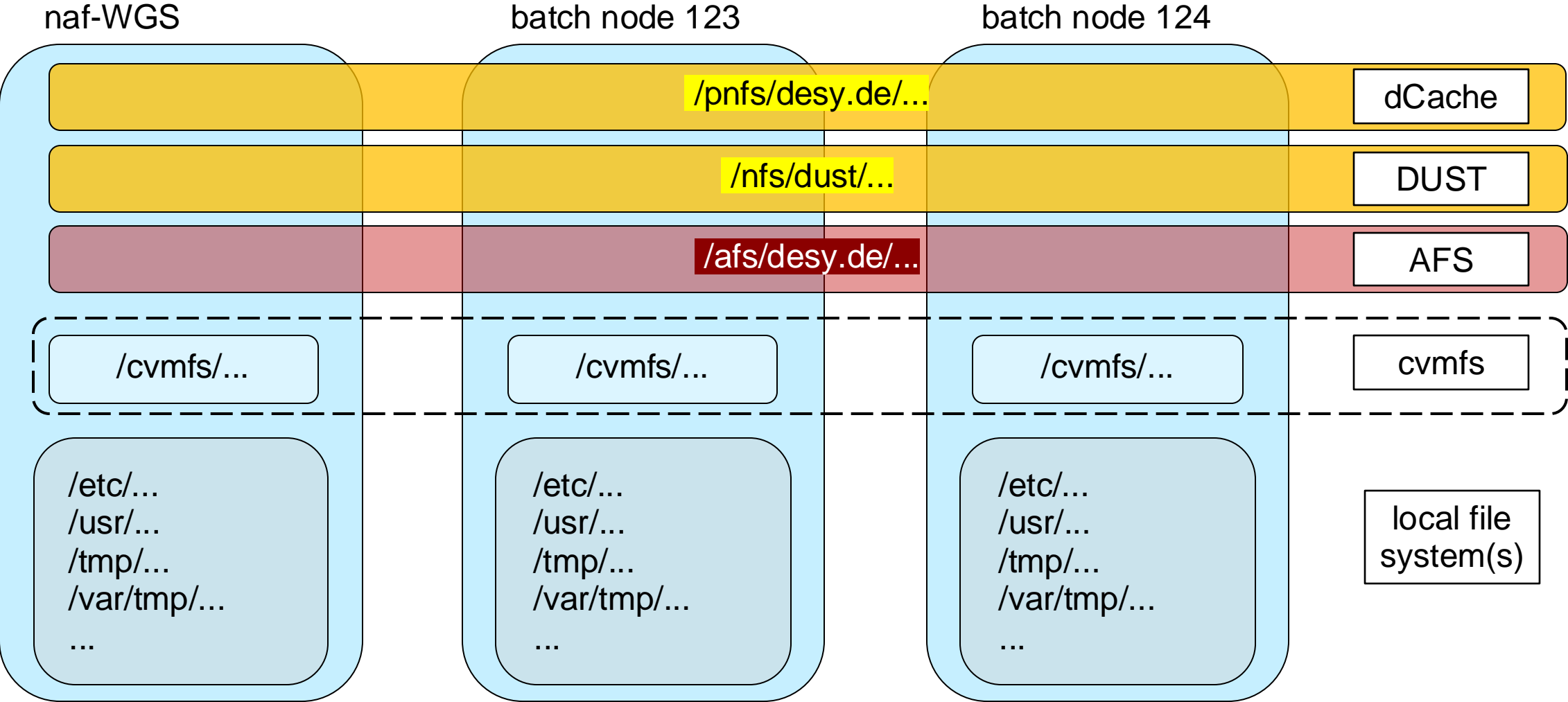
Software on the NAF

- Local system installed
- module (and AFS)
- cvmfs
- group software (if any)



Storage in the NAF

Local and Shared Mount Namespaces



Why so many of them?

- Different in scope and availability
- Different in available size of installation
- Different in available user directory size
- Different in connection to backup
- Different in performance
- Different in protocols and access methods



Storage dos and don'ts

... or: <https://confluence.desy.de/display/IS/Storage+Resources+and+File+System+Layout>

- AFS
 - Backup ... IO limited, size limited, some restrictions w.r.t number of files and file names
- DUST:
 - No backup
 - Few, large files are nicer than many, small files: Files <128k contribute more to quota
 - Keep old and very old files:
 - <https://www.desy.de/~hannappj/dustUsage/> (only accessible from DESY Intranet)
 - Recommendation: Limit yourself to base ASCII (and best no space) ... no Emojis, UTF-8
- dCache (see next slide)
- CVMFS
 - ... very large files or container images might cause troubles

Schei? 
Encoding

<https://confluence.desy.de/display/IS/Storage+Resources+and+File+System+Layout>

Network filesystems are mounted EVERYWHERE on NAF: No need to scp/rsync/... between components!

Storage tips

- How much space do I have?
- DUST:
 - statistics collected once per hour
- AFS:
 - No such tool for dCache
 - Experiments might control usage
- Local file systems:
 - (Network filesystem gives unmeaningful information)
- Information on one directory (I have read permissions on)

```
[naf-atlas13::kemp>my-dust-quota
Fileset Name      Usage (TB)  Limit (TB)  Use (%)  File Usage
user.af-atlas.kemp 0.534      1.0         53.43    124899
[naf-atlas13::kemp>my-dust-quota -g
Fileset Name      Usage (TB)  Limit (TB)  Use (%)  File Usage
user.af-atlas.kemp 0.534      1.0         53.43    124899
group.af-atlas.atlas-d 0.369      1.0         36.95    218866
```

```
[naf-atlas13::~~>fs lq -hu
Volume Name      Quota      Used %Used  Partition
user.kemp        16.0G      10.0G      63%        47%
[naf-atlas13::~~>fs lq -hu xxl/
Volume Name      Quota      Used %Used  Partition
xxl.kemp         7.6G       7.3G      96%<<     76%    <<WARNING
```

```
[naf-atlas13::~~>df -h /tmp/
Filesystem      Size  Used Avail Use% Mounted on
/dev/xvda6      59G   3.8G   52G    7% /tmp
```

```
[naf-atlas13::kemp>du -sch gcc-11.4.0*
365M  gcc-11.4.0
937M  gcc-11.4.0-non
133M  gcc-11.4.0.tar.gz
1.5G  total
[naf-atlas13::kemp>du -sch --inodes gcc-11.4.0*
11K   gcc-11.4.0
28K   gcc-11.4.0-non
1     gcc-11.4.0.tar.gz
39K   total
```

Do's und Don'ts:

- Keep the numbers of jobs accessing the same files to a minimum. Don't have 1k jobs read the same file over and over again
- Storage does not scale linearly into infinity; 2 Jobs reading the same file might half the time to wait for results, 1k jobs do not reduce the runtime by a factor of 1k
- Be aware, that the storage is also a shared resource; excessively reading the same file again and again will have a negative impact on your colleagues reading data from the same storage node or blocking the worker nodes for your colleagues and other NAF communities
- Keep file sizes reasonable, merge output into few larger files; many small files can over the long run cost performance in file listings
- **Tape:** Some NAF groups (ILC, Belle and CMS/ATLAS in the future) have data only stored on tape. These file need to be staged in advance. If you get a permission denied error when reading files; check the locality of the file. In order to prevent issues on the NAF, reading a file that is only on tape is forbidden

Remote storage (outside of DESY)

- Through XrootD, Grid-FTP or WebDAV data can be read from remote sites, e.g. CERN, FNAL or BNL
- Keep in mind due to limited bandwidth accessing/transferring the data can waste CPU time
- Ideally, try to transfer the data first, then submit jobs; or keep in mind the lower performance when requesting job slots on NAF



support & documentation

- **Infrastructure support**
 - Multi-level support within IT
 - Dedicated Queues in our Ticket system
 - naf-helpdesk@desy.de
- **Experiment support**
 - Organized by experiments
 - Mailing lists
- Good communication between experts from IT and experiments needed
 - e.g. via the NUC (users committee)



- **Documentation:**
- Lots of stuff under:
 - <https://naf.desy.de/>
 - <https://bird.desy.de/>
 - and probably some experiment-own documentation