More Sustainable HTC Computing

How to better utilize compute resources.

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DESY IT

Two sessions

The NAF: Introduction to the NAF

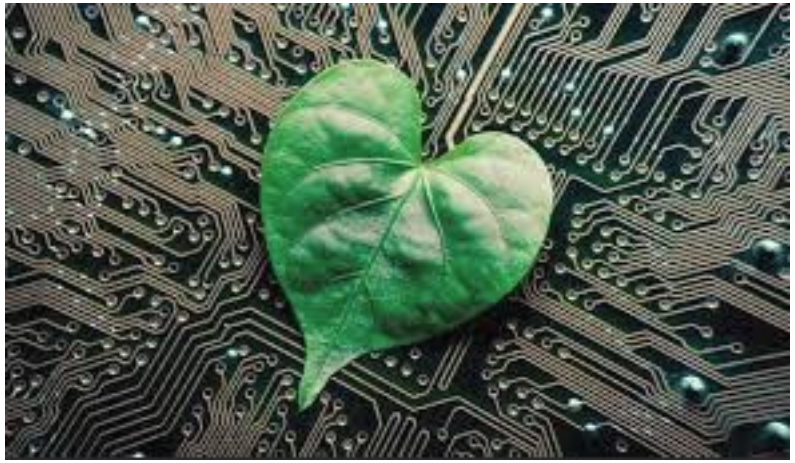
- General sustainability considerations
- What is the NAF? A (short) introduction
- The different building blocks
- Software on the NAF
- Storage on the NAF
- Remote storage
- Getting support

The NAF: Introduction to the NAF II (batch computing)

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

… but first some toughts about sustainability

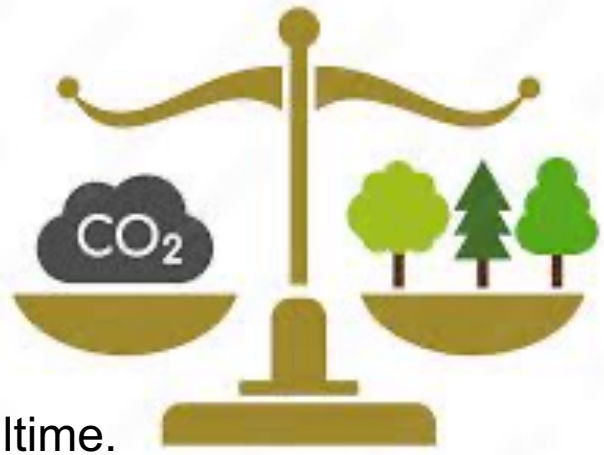
- IT is a major energy consumer
- IT equipment has a footprint beyond energy



- 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.:
  - 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

Projektingenieurin/Wissenschaftlerin (w/m/d) für energie-effiziente wissenschaftliche IT-Infrastrukturen

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Das Deutsche Elektronen-Synchrotron DESY mit mehr als 3000 Mitarbeiter:innen an den Standorten Hamburg und Zeuthen zählt zu den weltweit führenden Forschungszentren. Im Mittelpunkt der Forschung steht die Entschlüsselung der Struktur und Funktion von Materie, von den kleinsten Teilchen des Universums bis hin zu den Bausteinen des Lebens. Damit trägt DESY zur Lösung der großen Fragen und drängenden Herausforderungen von Wissenschaft, Gesellschaft und Wirtschaft bei. Mit hochmoderner Forschungsinfrastruktur, interdisziplinär angelegten Forschungs-Plattformen und internationalen Vernetzungen verfügt DESY über ein hochattraktives Arbeitsumfeld im wissenschaftlichen, technischen und administrativen Bereich sowie für die Ausbildung von hochqualifiziertem Nachwuchs.

Die DESY Gruppe IT betreibt neben allgemeinen Diensten für alle DESY Bereiche auch große Rechnerinfrastrukturen für wissenschaftliche Datenhaltung und Datenanalyse für alle Forschungsbereiche von DESY und des European-XFEL. Ziel des EU-Projekts "Research Facilities 2.0" ist es, große wissenschaftliche Infrastrukturen und Institute nachhaltiger zu gestalten. Die dabei verwendeten und entwickelten Methoden sollen auch nutzbar sein für andere Bereiche, und somit eine breite Auswirkung auf die Gesellschaft haben. Fokus des Projektes ist ein besseres Verständnis der Scope-2 Emissionen und Verfahren für deren massive, langfristige Reduktion zu entwickeln. Auch die Reduktion von Scope-3 Emissionen durch geeignete Betriebsmodelle soll untersucht werden. Gesucht werden zwei Kolleg:innen die federführend nachhaltigere Infrastrukturen für die wissenschaftliche Datenhaltung und Datenanalyse am DESY konzipieren und implementieren. Sie arbeiten dazu mit anderen Teams innerhalb der IT, aber auch innerhalb von DESY und mit anderen internationalen Forschungseinrichtungen zusammen.

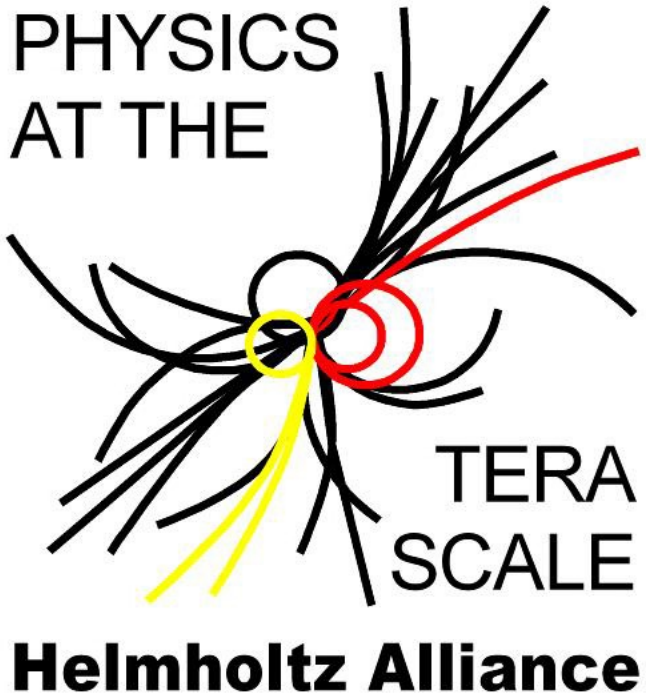
Who are you?

What do you expect from this workshop?

First part:
Introduction to the NAF

What is the NAF?

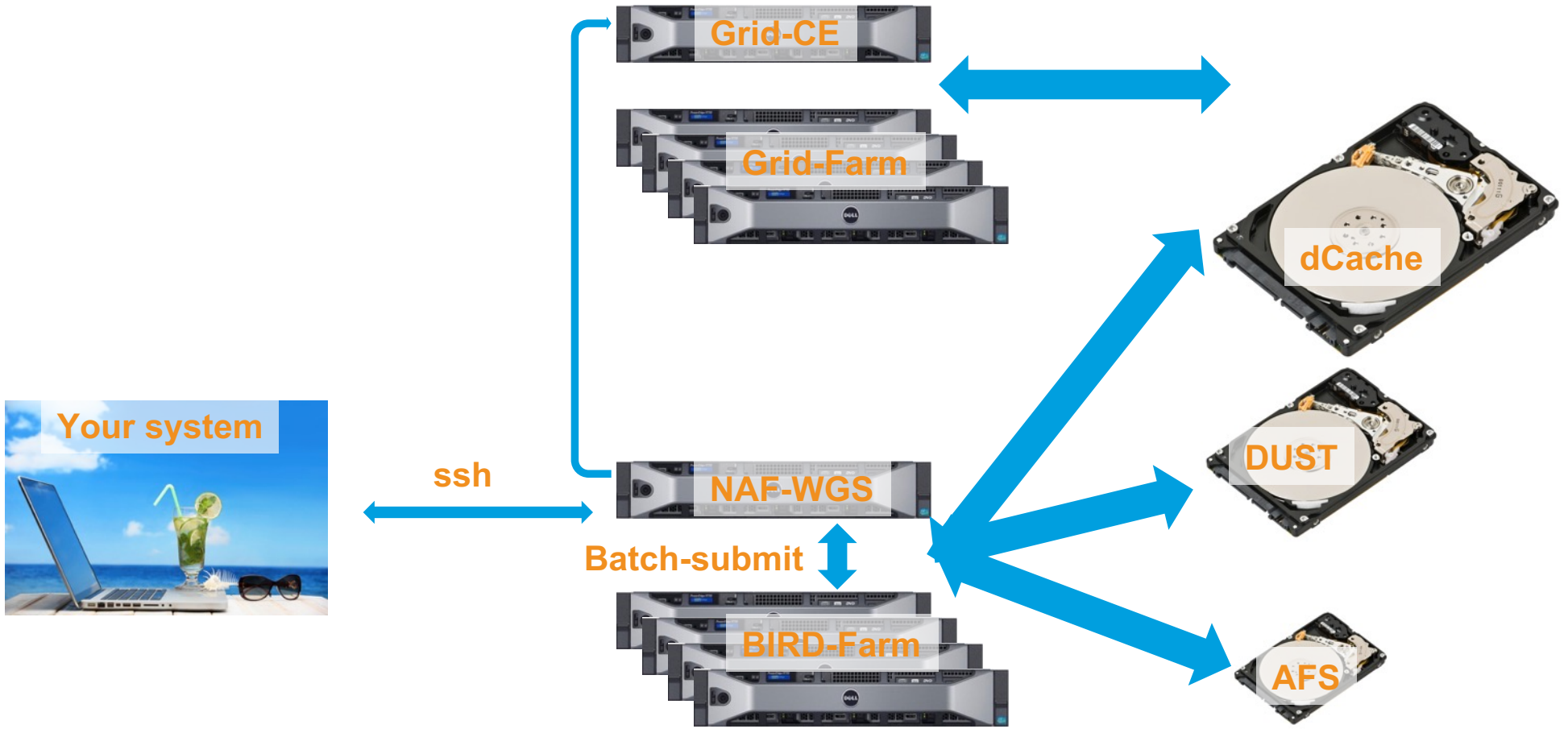
- NAF stands for „National Analysis Facility“
  - *National* means: For people working in institutes in the Terascale Alliance
  - *Analysis* means: Analysing data taken in the Terascale Alliance
  - *Facility* means: Something where you can do real work
- Basically: The NAF is a facility where **YOU**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

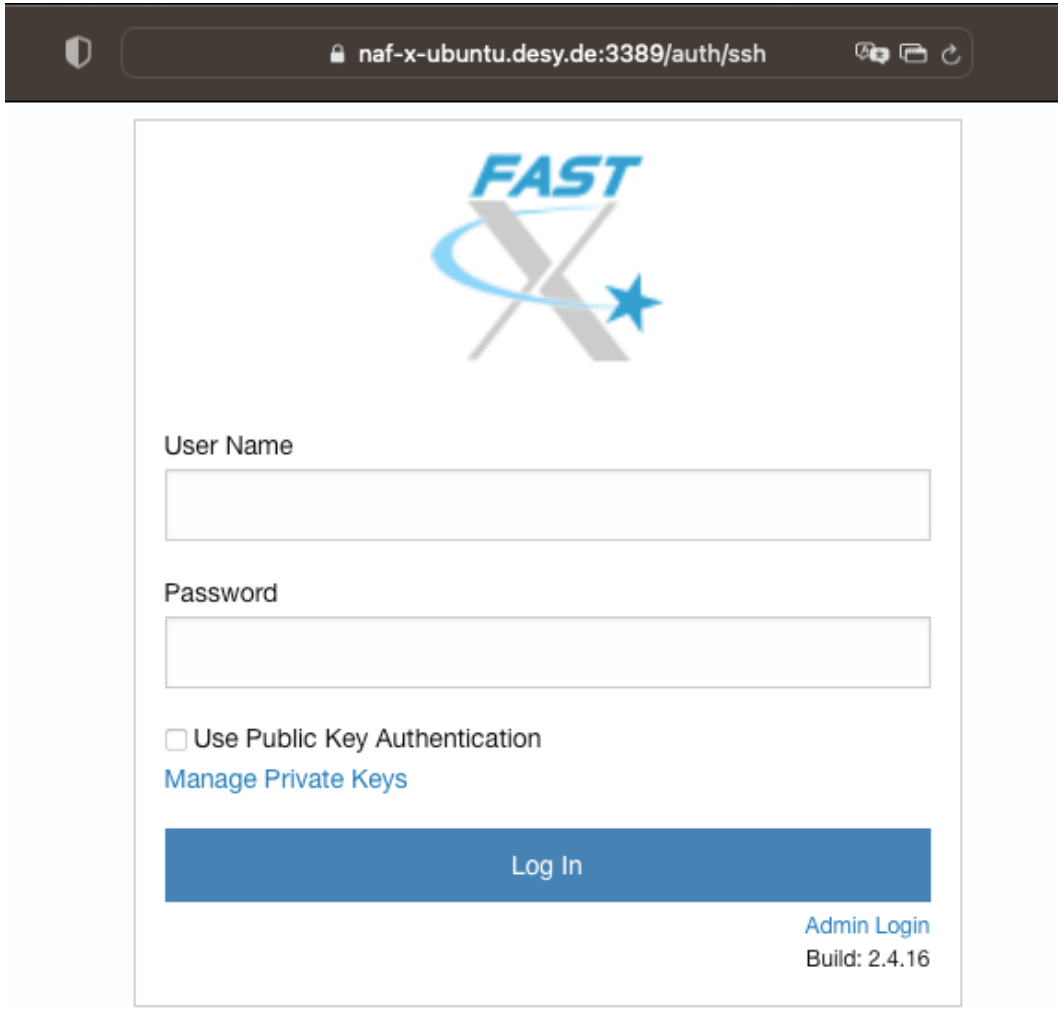
The WGS: Login Node, WorkGroupServer, Interactive Node, …

- Each group has a set of own WGS
- Why own?
- How many?
- How many resources?

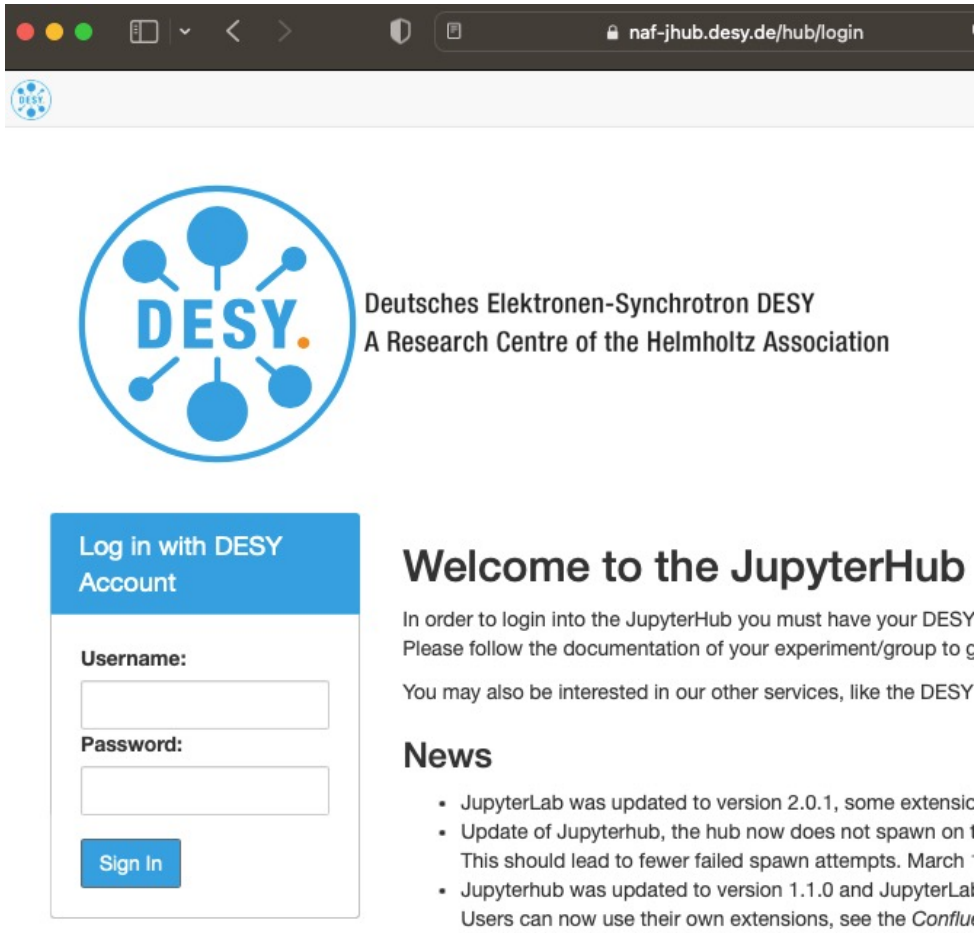
- **Usage of WGS (from the NAF docu)**
- **Be reasonable** when you use the WGS as you are **sharing the resources** with your colleagues and any (mis)use will affect them. So, please be careful and nice to your colleagues. As a rule of thumb, use the WGS for development**, short (<10min) test jobs, 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

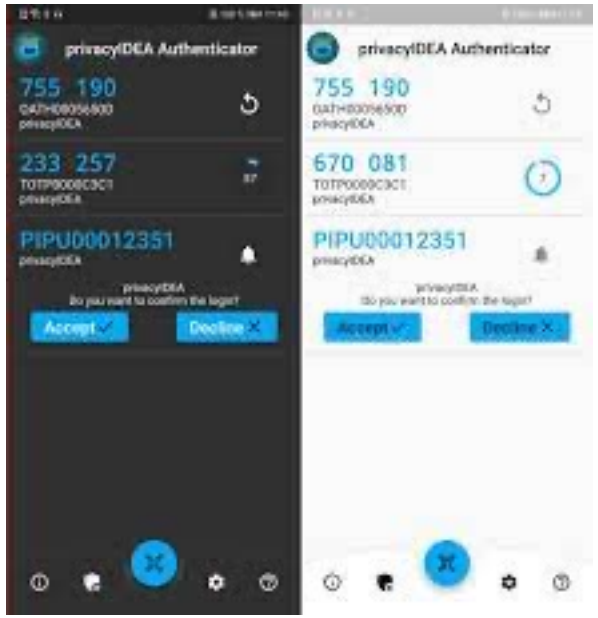
- Graphical access: FastX to the NAF remote desktop



- JupyterHub



What is this?


privacyIDEA Authenticator
755 190
233 257
PIPU00012351
privacyIDEA
Accept
Decline
privacyIDEA Authenticator
755 190
670 081
PIPU00012351
privacyIDEA
Accept
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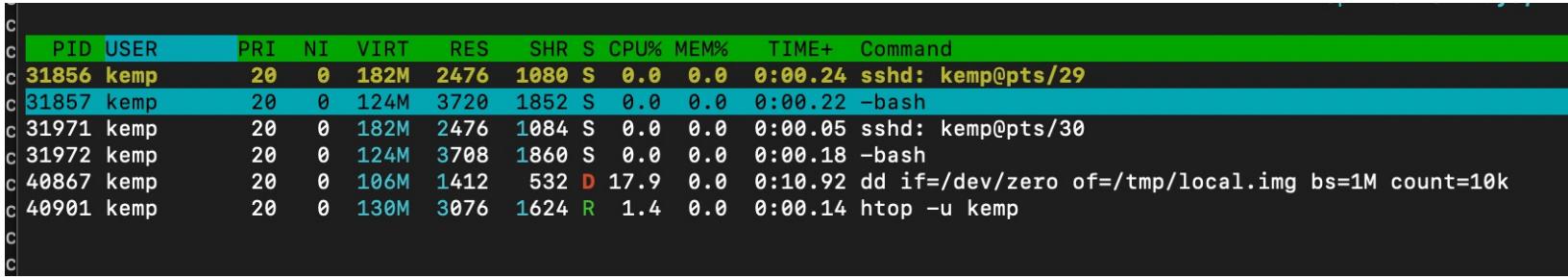
Why is the WGS slow? What is the footprint of my job? …



- 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?

- State “D” : Waiting for Disk (or network disk)
  - Might indicate a problem if observerd 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

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)

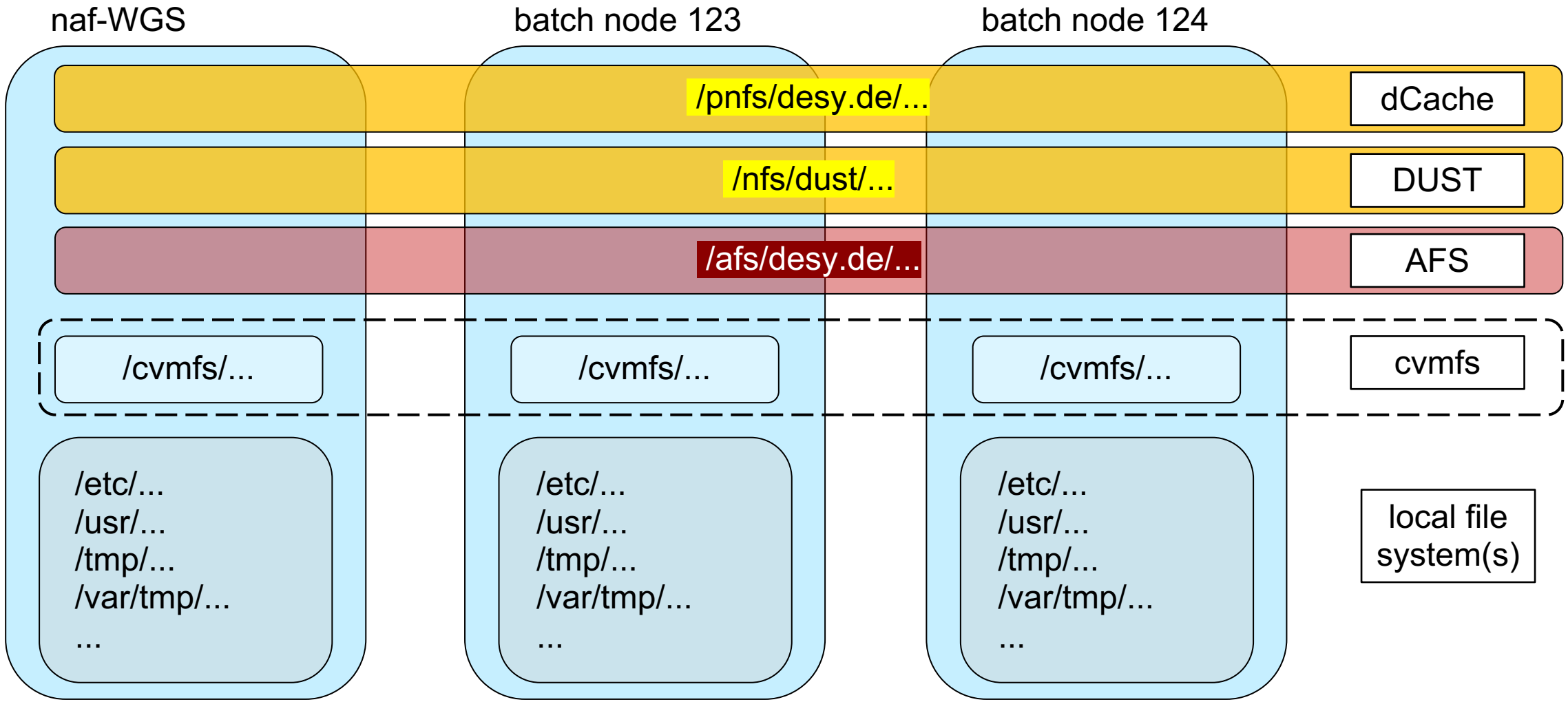
- The Kernel kills processes when RAM is getting too tight
  - over the years, it has gotten better at spotting the right culprit

Software on the NAF

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

Storage in the NAF

Local and Shared Mount Namespaces



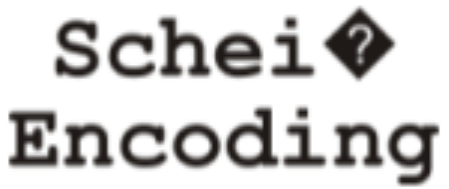
Why so many of them?

- 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



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
```

dCache network storage

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 experimt-own documentation