GWDG
Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen

GWDG

www.gwdg.de

Cluster Introduction

VI-HPS Tuning Workshop

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Table of Contents

Login Nodes and Systems

- Main Login Nodes:
  - glogin[9-13].hpc.gwdg.de
  - glogin[9-10] = glogin.hpc.gwdg.de
  - glogin[11-13] = glogin-p3.hpc.gwdg.de
- Legacy and Special Login Nodes
  - Legacy Emmy-P2: glogin[4-8] = glogin-p2.hpc.gwdg.de
  - Legacy SCC: gwdu[101-102] = login-mdc.hpc.gwdg.de
  - Legacy HLRN: glogin.hlrn.de
  - Storage/Transfer: gwdu[107-108] = gwdg-storage.hpc.gwdg.de
- Documentation and SSH Key Fingerprint
  - SSH Key Fingerprint: SHA256:PPK0aO2QZ/k4duUx18Pp5AOKG/gFEBHgw/bl8vg9oJk
  - https://docs.hpc.gwdg.de/start_here/connecting/login_nodes_and_example_commands

Partitions

Three types of clusters: NHR, KISSKI, SCC

- NHR: Main Tier 2 Cluster
  - standard96 (CPU, Emmy) $\sim$ 1000 nodes (legacy, offline)
  - medium96s (CPU, Emmy) $\sim$ 400 nodes
  - grete (GPU) $\sim$ 35 A100 and $\sim$ 5 H100
- KISSKI: AI focused GPU only cluster
  - kisski $\sim$ 25 A100
  - kisski-h100 $\sim$ 10
- SCC: Tier 3 Cluster for University of Göttingen and Max Planck Society
  - scc-cpu (CPU, shared) $\sim$ 50
  - scc-gpu (GPU, shared) $\sim$ 25 (A100 and 1 H100)
- `https://docs.hpc.gwdg.de/how_to_use/compute_partitions`

Outline

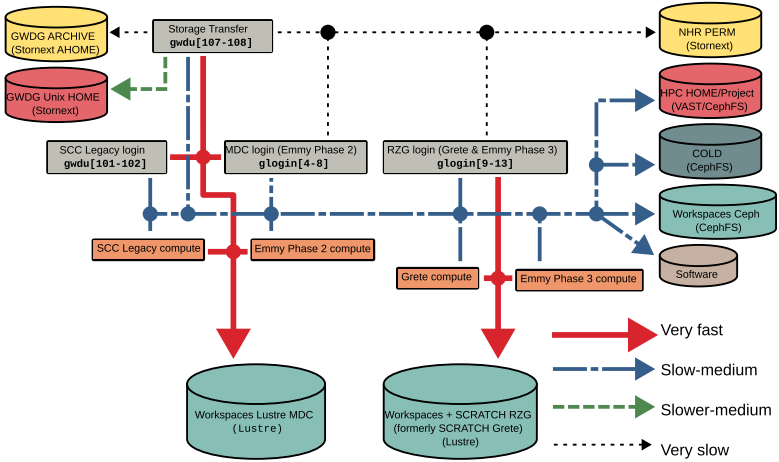
Storage systems

- $HOME: Home storage (VAST Data store) 60 GiB and 7 M files
- $PROJECT: Shared project storage
  - NHR+KISSKI: Vast Data store 3 TiB and 7 M files
  - SCC: Ceph-HDD storage 3 TiB and 3 M files
- Workspaces (temporary) $10 - 40$ TiB and 2 M files
  - NHR: lustre 30 days $\times$ 2 extensions (90 days)
  - SCC + NHR: Ceph-SSD 30 days $\times$ 2 extensions (90 days)
  - SCC + NHR: Ceph-HDD 60 days $\times$ 5 extensions (360 days)
  - Use the ws commands to manage:
    `https://docs.hpc.gwdg.de/how_to_use/storage_systems/workspaces`

Storage systems

- Tape Storage: NHR only (not for 10 years)
- Node local storage
  - Local SSD via $LOCAL_TMPDIR
  - RAM disk via $SHM_TMPDIR
  - https://docs.hpc.gwdg.de/how_to_use/storage_systems/temporary_storage
- Full overview: show-quota command
  - Soft limit as advertised
  - Hard limit equals 2 times soft limit

Storage Map


GWDG ARCHIVE (Stornext AHOME)
Storage Transfer gwdu[107-108]
NHR PERM (Stornext)
GWDG Unix HOME (Stornext)
HPC HOME/Project (VAST/CephFS)
SCC Legacy login gwdu[101-102]
MDC login (Emmy Phase 2) glogin[4-8]
RZG login (Grete & Emmy Phase 3) glogin[9-13]
COLD (CephFS)
Workspaces Ceph (CephFS)
SCC Legacy compute
Emmy Phase 2 compute
Grete compute
Emmy Phase 3 compute
Software
Workspaces Lustre MDC (Lustre)
Workspaces + SCRATCH RZG (formerly SCRATCH Grete) (Lustre)
Very fast
Slow-medium
Slower-medium
Very slow

Outline

Software stacks

- Current stack:
  - GWDG Lmod revision 25.04
  - Update in progress for revision 26.07
  - Emmy stack (CPU based)
  - Grete stack (GPU based)
- Legacy stacks:
  - NHR Lmod revision 24.05
  - SCC Lmod
  - HLRN Tmod
- Yes, we unified the software stack
- `https://docs.hpc.gwdg.de/software_stacks/list_of_modules`
- Or just ask Niklas

Module system

- Regular module commands: "module load", "module list", "module avail", and more
- "module spider" is your friend
- GPU modules only on GPU login node
- Use Spack if you need other modules
  - module load spack
  - source $SPACK_ROOT/share/spack/setup-env.sh
  - spack load, spack install, and friends
  - https://docs.hpc.gwdg.de/how_to_use/spack
- Apptainer
  - module load apptainer
  - https://docs.hpc.gwdg.de/software_stacks/list_of_modules/apptainer
- https://docs.hpc.gwdg.de/software_stacks/compilers_interpreters

Important Details

- Reservation: vi-hps-tuning
- Partitions:
  - Shared partition: standard96s:shared
  - Exclusive partition: medium96s
  - GPU partition (A100): grete:shared
- module spider if you cannot find something
- Shared storage space is in $PROJECT

Summary

- Please find all details here: `https://docs.hpc.gwdg.de`