

Introduction for MPI for Marine Microbiology

Services, High Performance Computing, Bioinformatics

Eric Helmvoigt
eric.helmvoigt@gwdg.de

Christian Köhler
christian.koehler@gwdg.de

Hans-Georg Sommer
hans-georg.sommer@gwdg.de

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hpc@gwdg.de

Basic services

High Performance Computing

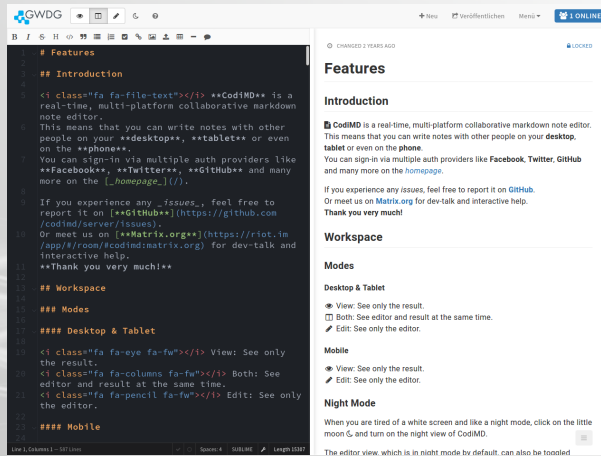
Applications/Bioinformatics

Further resources

Basic services

<https://pad.gwdg.de>

- collaborative editing in really real-time
- supports Markdown syntax
- live preview
- customizable privacy



The screenshot displays the CodiMD web interface. The top navigation bar includes the GWDG logo, a search icon, a document icon, a pencil icon, a share icon, and a user icon. On the right, there are buttons for '+ Neu', 'Veröffentlichen', 'Menü', and 'ONLINE'. The main editor area is split into two panes. The left pane shows a markdown document with the following content:

```
1 # Features
2
3 ## Introduction
4
5 <i class="fa fa-file-text"></i> **CodiMD** is a
6 real-time, multi-platform collaborative markdown
7 note editor.
8 This means that you can write notes with other
9 people on your **desktop**, **tablet** or even
10 on the **phone**.
11 You can sign-in via multiple auth providers like
12 **Facebook**, **Twitter**, **GitHub** and many
13 more on the [_homepage_]().
14
15 If you experience any _issues_, feel free to
16 report it on [**GitHub**](https://github.com
17 /codimd/server/issues).
18 Or meet us on [**Matrix.org**](https://riot.im
19 /app/#/room/#codimd:matrix.org) for dev-talk and
20 interactive help.
21 **Thank you very much!**
22
23 ## Workspace
24
25 ### Modes
26
27 #### Desktop & Tablet
28
29 <i class="fa fa-eye fa-fw"></i> View: See only
30 the result.
31 <i class="fa fa-columns fa-fw"></i> Both: See
32 editor and result at the same time.
33 <i class="fa fa-pencil fa-fw"></i> Edit: See only
34 the editor.
35
36
37 #### Mobile
```

The right pane shows a live preview of the markdown content. It includes a header 'Features', a sub-header 'Introduction', and the corresponding text from the markdown. It also includes a section 'Workspace' with a sub-header 'Modes' and three modes: 'Desktop & Tablet', 'Mobile', and 'Night Mode'. The 'Desktop & Tablet' section shows three icons: a single eye for 'View: See only the result.', a double eye for 'Both: See editor and result at the same time.', and a pencil for 'Edit: See only the editor.' The 'Mobile' section shows a single eye for 'View: See only the result.' and a pencil for 'Edit: See only the editor.' The 'Night Mode' section shows a moon icon and text: 'When you are tired of a white screen and like a night mode, click on the little moon ☾ and turn on the night view of CodiMD.' At the bottom of the right pane, it says: 'The editor view, which is in night mode by default, can also be toggled.'

ShareLaTeX

<https://sharelatex.gwdg.de>



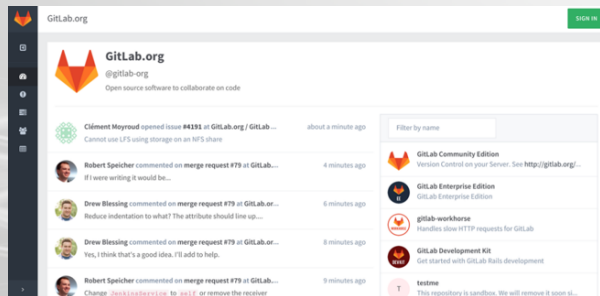
- Online collaborative LaTeX editor
- Documentation
<https://www.sharelatex.com/learn>

A screenshot of the ShareLaTeX web interface. The top header bar is dark blue with the text "MPIMM GWDG Services, HPC and Bioinfo 21.01.2021" and several icons. Below this is a toolbar with "Source" and "Rich Text" tabs, a "Recompile" button, and a download icon. The left sidebar shows a file explorer with folders "resources", "fonts", and "images", and files "macros.tex" and "slides.tex" (selected). The main editor area shows LaTeX code with line numbers 138 to 147. The code includes a frame containing a URL to sharelatex.gwdg.de and a list of services: "Online collaborative LaTeX editor" and "Documentation". The right sidebar shows a list of "Basic services" including "High Performance Computing" and "Applications/Bioinformatics", along with "Further resources". The GWDG logo is visible in the top right of the right sidebar.



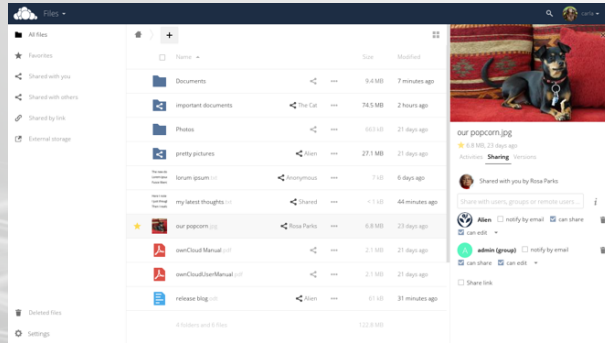
`https://gitlab.gwdg.de`
(login with short email address)

- Just like GitHub but:
 - Open Source
 - Hosted at GWDG
 - More private projects
 - ... (other cool things)



<https://owncloud.gwdg.de>

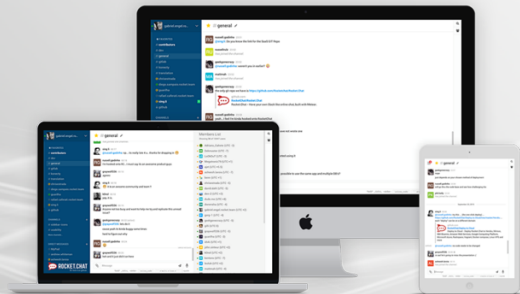
- Just like Dropbox but:
 - Open Source
 - Hosted at GWDG
 - 10 Gb space!
 - Amazing network speed when accessing from the university network.
- ... (other cool things)



<https://chat.gwdg.de>



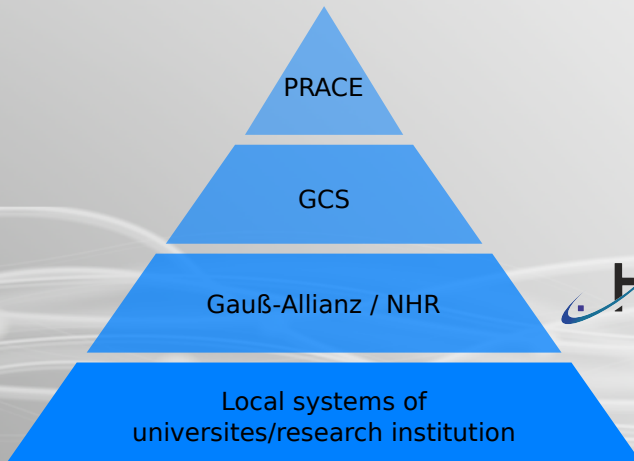
- Chat service
- Similar to Slack
- Access through web portal
- Clients for all Android and iOS also available



High Performance Computing

HPC landscape in Germany

T0: Europe, T1/2: Germany, T3: local





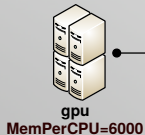
- Bernhard Bandow (CIDBN)
- Marcus Boden (Batch systems, monitoring)
- Christian Boehme (Coordination, Third-party consulting)
- Tim Ehlers (Admin coordination, security)
- Nils Kanning (DLR)
- Christian Köhler (Applications & Development, HLRN committees)
- Sebastian Krey (Storage & I/O, Statistics applications)
- Azat Khuziyakhmetov (DLR, research)
- Rosemarie Meuer (DLR)
- Hendrik Nolte (Research, MRI software)
- Jack Ogaja (Applications & Development)

- compute partition: 255 systems with 5416 cores
- fat partition (high mem): 36 systems with 256 GB - 2TB mem
- GPU partition: 20 Tesla K40, 32 GeForce GTX 980, 14 GeForce GTX 1080
- Storage: StorNext connection (HOME), 2.15 PB HPC FS (BeeGFS)
- 3x login nodes (reachable from GöNET)
- integration of systems from various institutes

Scientific Compute Cluster (SCC)



agqxxx
cores: 32, mem: 192 GB



scratch

agtxxx
cores: 48, mem: 384 GB



gpu
MemPerCPU=8000

ampxxx
cores: 96, mem: 384 GB



medium
MemPerCPU=4000

Modular Data Center (MDC)

dfaxxx
cores: 24, mem: 512 GB



fat
MemPerCPU=21333

fat+
fat

sbatch -p
srun -p

medium
gpu

dmpxxx
cores: 24, mem: 128 GB



medium
MemPerCPU=5300

Faßberg

dsuxxx
cores: 40, mem: 1536 GB



fat+
MemPerCPU=37500



scratch2

dgexxx, dtexxx
cores: 24, mem: 128 GB



gpu
MemPerCPU=5300

- your HOME is available on all nodes
- /scratch high performance BeeGFS for parallel IO (site-local!)
- \$AHOME points to your tape archive directory

- about 230 active users, ca. 181,000 jobs/month
- Application domains & software
 - Quantum chemistry, Molecular dynamics
 - Bioinformatics, Genomics, Evolutionary Biology
 - Astrophysics, Cosmology, Numerical Fluid Dynamics
 - Computer Algebra
 - Machine Learning
 - Medical Imaging (e.g. MRI)
 - Data Analytics: Python, R, Spark, ...

- about every five years: energy cost doesn't justify continuing operation of old systems
- most recent procurement from 2020/11
- expansion of the HLRN system on the technical level
- Intel OmniPath fabric, direct water cooling (CPU/mem)
- additional GPU partition

- 96 standard nodes (2 Xeon Platinum 9242, 2x48 cores, 384 GB memory)
- 2 GPU nodes with 8 Tesla V100/32
 - 2 Xeon Gold 6252, 2x24 cores, 384 GB memory
- 12 GPU nodes with 4 Quadro RTX5000
 - 2 Xeon Gold 6242, 2x16 cores, 192 GB memory
- 100 GBit/s Intel Omni-Path interconnect
- 1.7 PB /scratch storage (of which 100TB are flash based)

HLRN (prev.) at FMZ: compute nodes



HLRN (prev.) at FMZ: storage system



SCC Installation at MDC



New Data Center



(=primary installation site for new cluster procurements)

Applications/Bioinformatics

- Interactive **Jupyter** notebooks can use HPC as a backend
- **TensorFlow** is a popular AI tool that can use CPU and GPU dynamically
- **Apache Spark** clusters can be spawned as multi-node HPC jobs



- dedicated high mem (1T) system `gwd100.gwdg.de`
- also hosts RStudio server (web-based IDE)
- more information: <https://bioinfo.gwdg.de/>

Further resources

Where to begin?



1. get a GWDG account
2. contact us: `hpc@gwdg.de`
 - account activation
 - mailing list `hpc-announce` for latest system news
3. outside GöNET? connect with VPN or use `ssh login.gwdg.de` (worldwide access)
4. SSH to frontend nodes

Where to get more information?



- **Info wiki** <https://info.gwdg.de> shows you information about
 - Basic access
 - Hardware overview
 - How to submit jobs
 - Advice on most common applications
- We offer **courses** on SCC usage, programming with MPI, OpenMP, CUDA, Python, Research Data Management and more
→ **GWDG Academy**
- **Support** mail address: hpc@gwdg.de
- Rocket.Chat channel [#hpc-users](#)

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- **Thanks for your attention! Questions?**