Responding to a Challenge: Remote Access and Digital Twins at MLZ

Georg Brandl, **Christian Felder**, Christian Franz, Peter Link

MLZ is a cooperation between
JÜLICH Forschungszentrum
Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung
Technical University of Munich

SARS-CoV-2

The COVID-19 crisis has created new challenges worldwide.

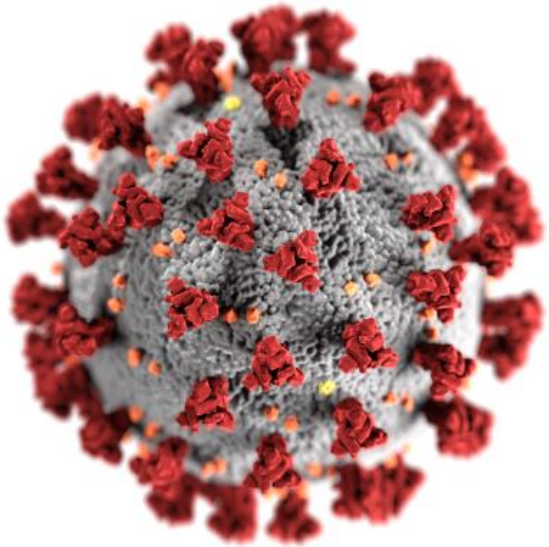
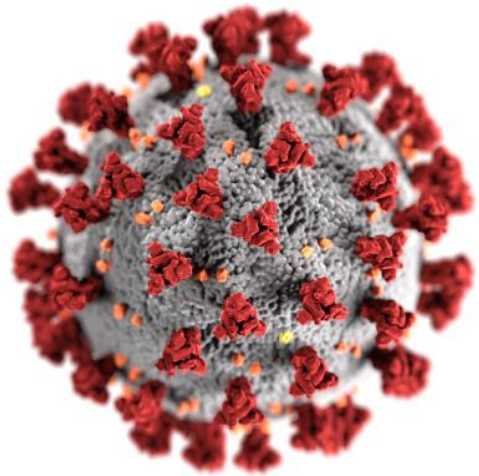


Figure 1: CDC / Alissa Eckert, MSMI, Dan Higgins, MAMS

SARS-CoV-2

Measures

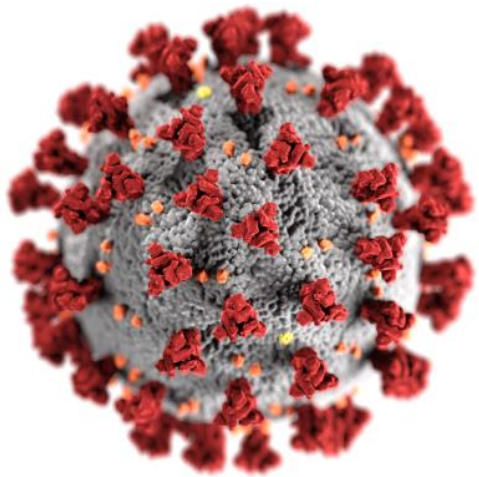
- Reduction of physical contacts
- Mobile working increasingly used
- Limited staff on site
- No experiments w/ users on site, including ILL and MLZ
  $\rightarrow$ But Mail-In Experiments



SARS-CoV-2

On the plus side

- **Catalyst** for digitalization
- Remote access to instrument control and data analysis systems
- Remote data access
- **Di**gital **T**wins



Remote Access

Differentiate between staff and users

Staff

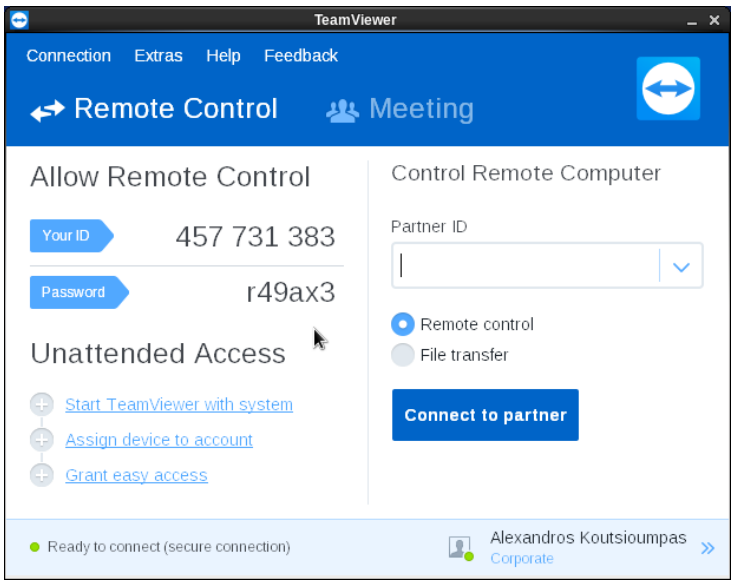
- Web-based remote desktop access for instrument control and data analysis systems
- `ssh` access using bastion hosts
- Direct access using vpn

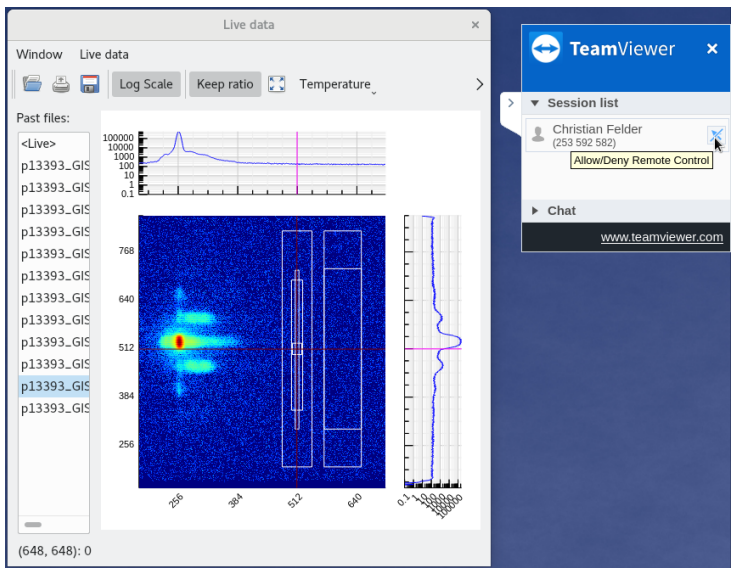
Guests/User

- **Supervised** remote desktop access to instrument control and data analysis systems

Remote Access for Users

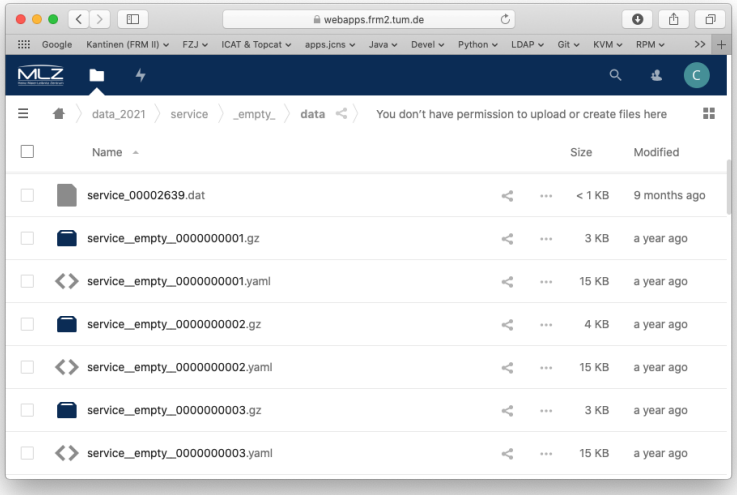
- MLZ wide solution: TeamViewer
- Well known remote desktop client
- Allows fine grained access controls
- Instrument scientists at all times responsible for keeping the experiment safe and running





Remote Data Access

- Instrument control stores data in proposal directory
- Web-based access to proposal directory based on Nextcloud
- One instance for each instrument
- Login w/ useroffice (GhOST) account

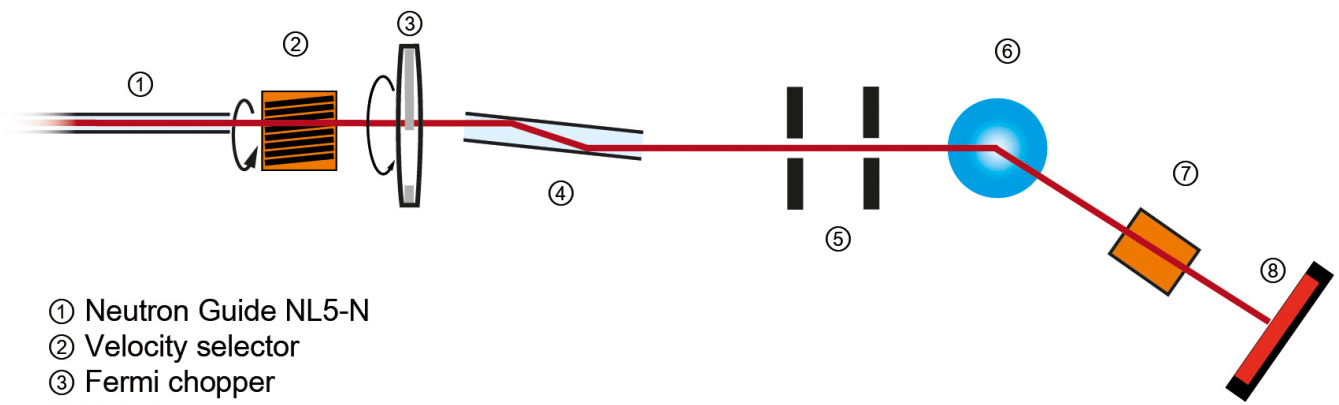


Nextcloud

→ https://webapps.frm2.tum.de/intranet/{instrument}-data

Digital Twins

- **Di**gital **T**win: virtual representation of an instrument
- Simulation of neutron scattering at the sample w/ varying input parameters
- Coupled w/ the **i**nstrument **c**ontrol **s**ystem of the physical/virtual experiment



① Neutron Guide NL5-N
② Velocity selector
③ Fermi chopper
④ Polariser
⑤ Slit pair
⑥ Hexapod sample table
⑦ Polarisation analyser (^{3}He)
⑧ Detector

Digital Twins

For existing- and new communities

- Reduce entry threshold for new users
  $\rightarrow$ first experience w/ performing an experiment at LSF
- Preparation before the experiment
  - Estimate neutron flux at the sample,
    e.g. different settings and different resolutions
  - Expected results w/ standard samples
  - Time consumption (including timing for movement)

$\Rightarrow$ Higher efficiency during beamtime and higher success rates

Digital Twins

Virtual experiments using NICOS

- Instrument definition w/ virtual devices, in parallel to the real setup
  $\Rightarrow$ **Operation identical** to the real instrument
- **Virtual device positions** used as **input parameters** for the simulation
- Usually **virtual detector** devices as **glue code** to simulation backends, e.g.:
  - McStas
  - Vitess
- Results processed as if from real experiments
  $\Rightarrow$ **Identical file formats**

Digital Twins

Lab course

- Web-based online training system based on Apache Guacamole and containers
- Login w/ useroffice (GhOST) account or autogenerated account for trainees
- Configureable teams of mentors and trainees
- Different access levels
  - Trainee: Individual session
  - Mentor: Individual- and trainee sessions

Digital Twins

Fully automated and configurable using ansible playbooks

```
teams:
  - name: usermeeting2021-kws
    instrument: nicos_virt_mlz.kws2
    mentors_dn:
      - "uid=c.felder@fz-juelich.de,{{ ldap_user_base_dn }}
    mentors:
      - c.felder@fz-juelich.de
    trainees:
      - kws-peter.link@frm2.tum.de
      - kws-cfranz@frm2.tum.de
      - kws-g.brandl@fz-juelich.de
```

Online Training

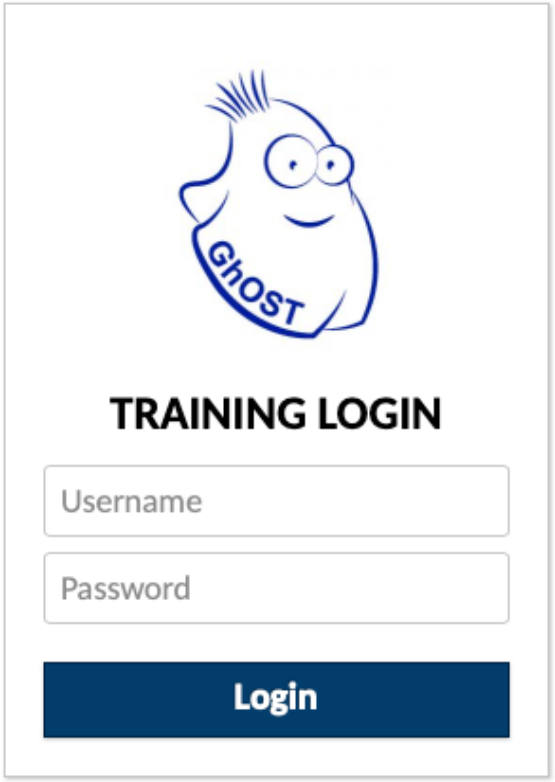


Figure 2: https://training.mlz-garching.de/jcns

Digital Twins

GA for virtual experiments

- Create virtual experiments on demand
- Need to scale
  - vertically: memory + cpu cores
  - horizontally: across multiple nodes
- Orchestrate containers automatically

$\Rightarrow$ Cloud infrastructure / Kubernetes (K8s)

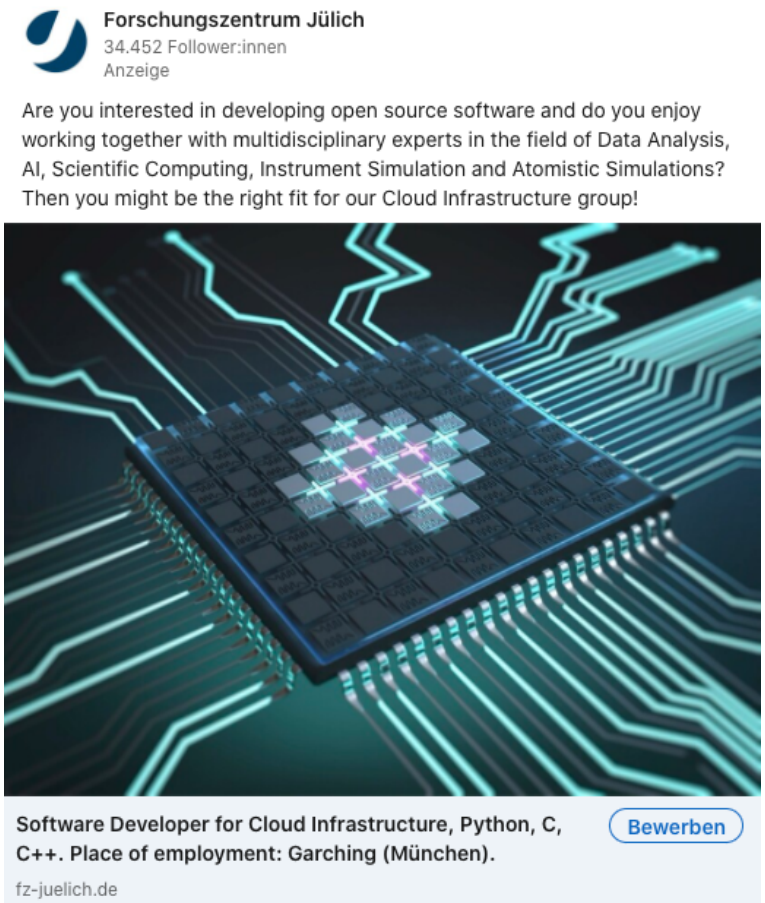
- Also useful for **D**ata **A**nalysis **a**s **a** **S**ervice

Digital Twins

In the future

- Domain specific simulation backends
- Bring your own virtual sample
  $\rightarrow$ Domain specific interfaces for sample modelling
- Coupled w/ the **i**nstrument **c**ontrol **s**ystem of the **physical experiment**
- Swift comparison of measured- and simulated data using AI & ML
  $\Rightarrow$ Increased understanding of the results in real-time
  $\Rightarrow$ Beamtime optimization
- Standardized interface for connecting **ICS** w/ **DiT**s
  $\rightarrow$ **Di**gital **T**win Platform for **A**nalytical **R**esearch **I**nfrastructure Experiments

Thanks for your attention



Get invovled! We're hiring!

Reference number: 2021-455

Software Developer for Cloud Infrastructure, Python, C, C++

Reaching out

Christian Felder M. Sc.

c.felder@fz-juelich.de

+49 - 89 158 860 773