CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

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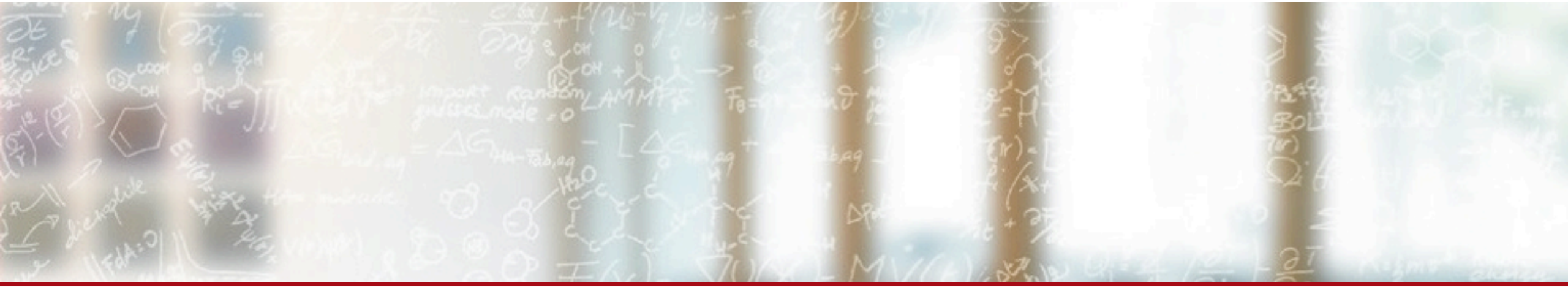


User Lab Policies & Service Catalog on Alps

User Lab Day 2023

Luca Marsella, CSCS

Outline of the Presentation

- Service Catalog
- User Lab Policies
- Troubleshooting
- Useful Links

Alps infrastructure in the CSCS machine room
Source: https://www.cscs.ch/computers/alps

Service Catalog

Computing Resources

GPU/hybrid nodes and **multicore nodes** (14:15 - 14:45 Alps Infrastructure)

Computing time on Cray systems is accounted in **node hours**

- Resources are assigned over **three-months windows**
  - **Quotas reset** on April 1st, July 1st, October 1st and January 1st
- Use thoroughly the quarterly compute budget within the time frame
- Unused resources in the allocation periods **cannot be recovered**

Check your budget in the **current allocation window**

- Overview of resources on https://account.cscs.ch

More information: https://user.cscs.ch/access/accounting

Storage Resources (14:45 - 15:15 Storage & Data Strategy)

/users and **/project**

- Access **r+w** from login nodes (UAN), storage for datasets, code and scripts
- Better performance with larger files (archive small files with **tar**)

Users are NOT supposed to run jobs here

- **Reliability** over **performance**: **/project** read-only on compute nodes (CN)
- Folders **backed up**: data retention until 3-months after the end of the project

Environment variables for quick access

- **$HOME** pointing to personal folder (per cluster)
- **$PROJECT** pointing to group folder

More information: https://user.cscs.ch/storage/file_systems

Data Transfer

Data transfer service to get files from/to CSCS file systems (External Transfer)

- Service implemented using the Globus Online Endpoint
- The CSCS endpoint requires authentication with CSCS credentials

Data mover service with a dedicated Slurm queue (Internal Transfer)

- The service submits jobs on the **datamover** cluster at no charge
- Direct access via ssh to the nodes of this cluster is not allowed

More information: https://user.cscs.ch/storage/transfer

Long Term Storage

Storage repository with long term retention capabilities

- Provide persistent identifiers (PID) and set public access if needed
- Data easily accessible from a web browser (HTTPS protocol)
- RESTful API to integrate with third party applications
- Scalable service that can cope with large volumes of data
- Resiliency due to data protection measures against failures

User Lab: up to 2 TB of LTS storage quota (for 10 years) free of charge per project

More information: https://user.cscs.ch/storage/lts

Multi-factor authentication

Users are required to authenticate using multi-factor authentication (MFA)

- MFA implemented at CSCS as two-factor authentication
- Users receive an email with the details about the procedure
  - One factor is the user login and password pair ("thing you know")
  - The other factor is the one-time password (OTP, "thing you have")

MFA applies to web-based services and SSH connections

- CSCS supports authenticators that follow the TOTP open standard
- Certified SSH keys are created with a **validity limited in time**

More information: https://user.cscs.ch/access/auth/mfa

Container runtime environment: Sarus

Sarus runs Linux containers on HPC environments:

- Developed following the specific requirements of HPC systems
- Spawns isolated containers built by users for a specific application
- Extensible runtime by means of OCI hooks for custom hardware

Compatible with the Open Container Initiative (OCI) standards:

- Pulls from registries with OCI Distribution Specification or Docker
- Imports and convert images with the OCI Image Format (e.g. Docker)
- Uses an OCI-compliant runtime to spawn the container process

More information: https://user.cscs.ch/tools/containers/sarus

FirecREST

FirecREST is a RESTful API for managing HPC resources at CSCS

- integrate FirecREST into web-enabled portals and applications
- securely access CSCS services (job submissions, data transfer,…)
- hands-on introduction with PyFirecREST
  - Python wrappers for the FirecREST API to showcase its functionality

Users can make HTTP requests to perform the following operations:

- Basic system utilities like ls, mkdir, mv, chmod, chown,…
- Actions with the Slurm workload manager (submit, query, cancel jobs)
- Data transfer: internal (between CSCS systems) and external

More information: https://user.cscs.ch/tools/firecrest

Interactive computing with JupyterLab

JupyterLab is the web-based user interface for Project Jupyter

- Create and share documents with live code, equations, visualization, …
- Same notebook document format as the classic Jupyter Notebook
- Ability to work with multiple documents using tabs or splitters side by side

CSCS JupyterLab powered by JupyterHub with a ready-made Python kernel

- You can add your own kernels based on your own virtual environments
- Multi-user hub spawning multiple instances of single-user Jupyter server
- Interactive execution of JupyterLab over single and multiple nodes

More information: https://user.cscs.ch/tools/interactive/jupyterlab

Regression testing with ReFrame

ReFrame is a framework for regression tests on HPC systems

- Abstract away the complexity of the interactions with the system
- Separate the logic of a regression test from the low-level details
- Users can write portable regression tests, focusing on functionality

CSCS provides ReFrame pre-configured for its systems:

- ReFrame can be accessed with **module load reframe-cscs-tests**
- The module provides the configuration as well as regression tests
- Users can run the tests already provided by CSCS staff

More information: https://user.cscs.ch/tools/reframe

User Environment (11:45 - 12:30 Alps User Environment)

Alps User Environment (uenv mount with compiler, MPI library,...)

- AI/ML : PyTorch, TensorFlow,…
- Materials Science: CP2K, QuantumESPRESSO, VASP,…
- MD Simulations: GROMACS, LAMMPS, NAMD,…
- Visualization: Paraview, Visit, VMD,...

Cray Programming Environment:

- programming environment on Cray systems with performance tools

More information:
https://confluence.cscs.ch/display/KB/User+Environments+on+Alps

User Lab Policies

General Policies

The code of conduct outlines proper practices

- **Access to Source Codes:** you agree to make codes available for support
- **Scientific Advisory Committee:** committee members must not be contacted
- **Acknowledgements:** you must acknowledge the use of CSCS resources in all publications related to your production with reference to the "*project ID ###*"

User Regulations define basic guidelines

- **Accounts are personal** and sharing them is forbidden
- **Data ownership**: access to and use of data of other accounts without prior consent from the principal investigator is strictly prohibited
- **ETH Zurich Acceptable Use Policy for Telematics Resources ("BOT")**

Access to CSCS resources **may be revoked to users violating the policies**

Data Retention Policies

Data backup for **active projects**:

- Data in **/users** and **/project** folders is backed up (past 90 days)
- Data in **/project** folders removed **3 months** after the **end of the project**

As soon as a the project **expires**:

- Data backup is **disabled** immediately
- **No data recovery** after the final data removal

No backup for data in **scratch**:

- No recovery in case of **accidental data loss**
- No recovery of data deleted due to the cleaning policy

More information: https://user.cscs.ch/storage/recovery

Policies on the /scratch filesystem

Fast workspace for running jobs

- Designed for **performance** rather than reliability
- **Cleaning policy**: files **older than 30 days deleted** daily
- **No backup:** users should transfer data after job completion

Soft quotas to prevent performance degradation

- On **inodes** (files and folders) to avoid large numbers of small files
- On **disk occupancy** with a **grace time** to allow data transfer

More information: https://user.cscs.ch/storage/file_systems/scratch

Fair Usage Policies

Slurm workload manager

- The job scheduler is a shared resource among users submitting jobs
- **Do not submit large numbers of jobs** and commands at the same time
- We will be forced to kill jobs and limit new submissions

Login nodes:

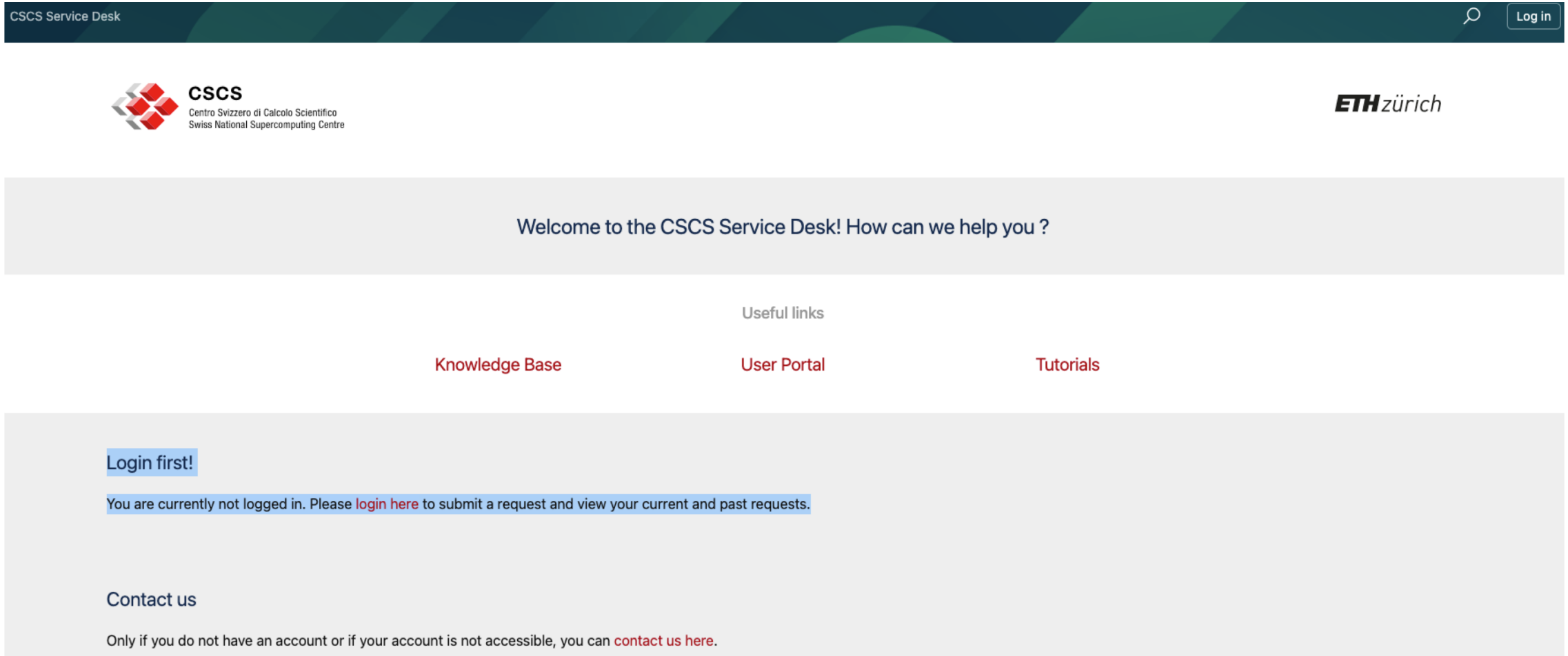
- **Running applications on login nodes is not allowed**
- Submit your simulations with the Slurm scheduler on compute nodes
- **Heavy processes** running on login nodes will be **terminated**

More information: https://user.cscs.ch/access/accounting/#policies

Troubleshooting

What to do in case of trouble?

Access the CSCS Service Desk at https://support.cscs.ch



How to submit a support request

Useful links to the documentation available online

- Knowledge Base (KB) at https://confluence.cscs.ch/display/KB
- User Portal at https://user.cscs.ch
- Tutorials at https://www.cscs.ch/publications/tutorials

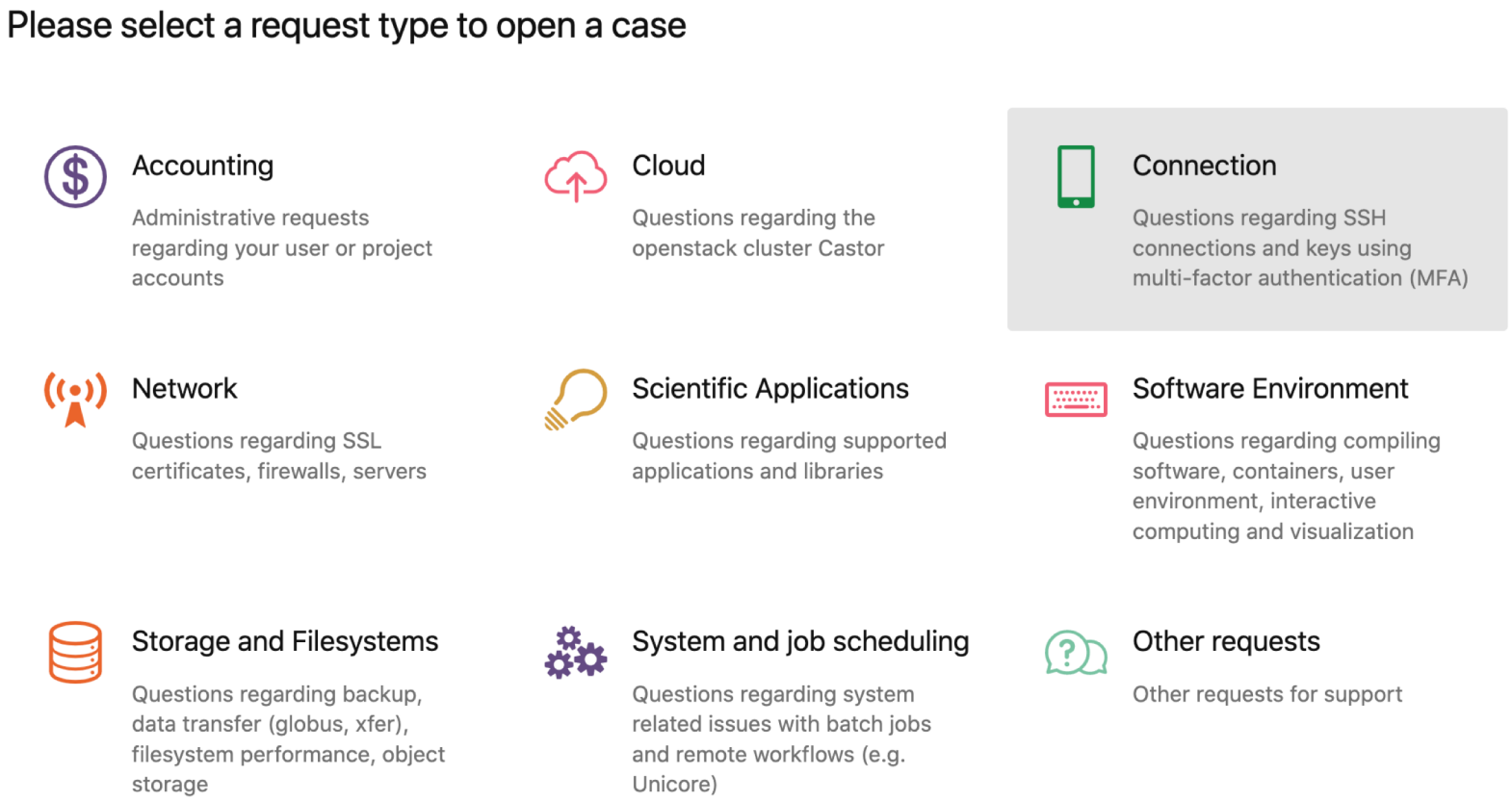
Submit a support request **if you can't find a solution** in the documentation

- **Login first** using your CSCS credentials
- The contact form should only be used if you cannot login

Request types in the CSCS Service Desk

Requests types are only available after logging in

- Choose the best matching **request type**
- Use the type **Other requests** only if you can't find a match
- A better match will help us react faster



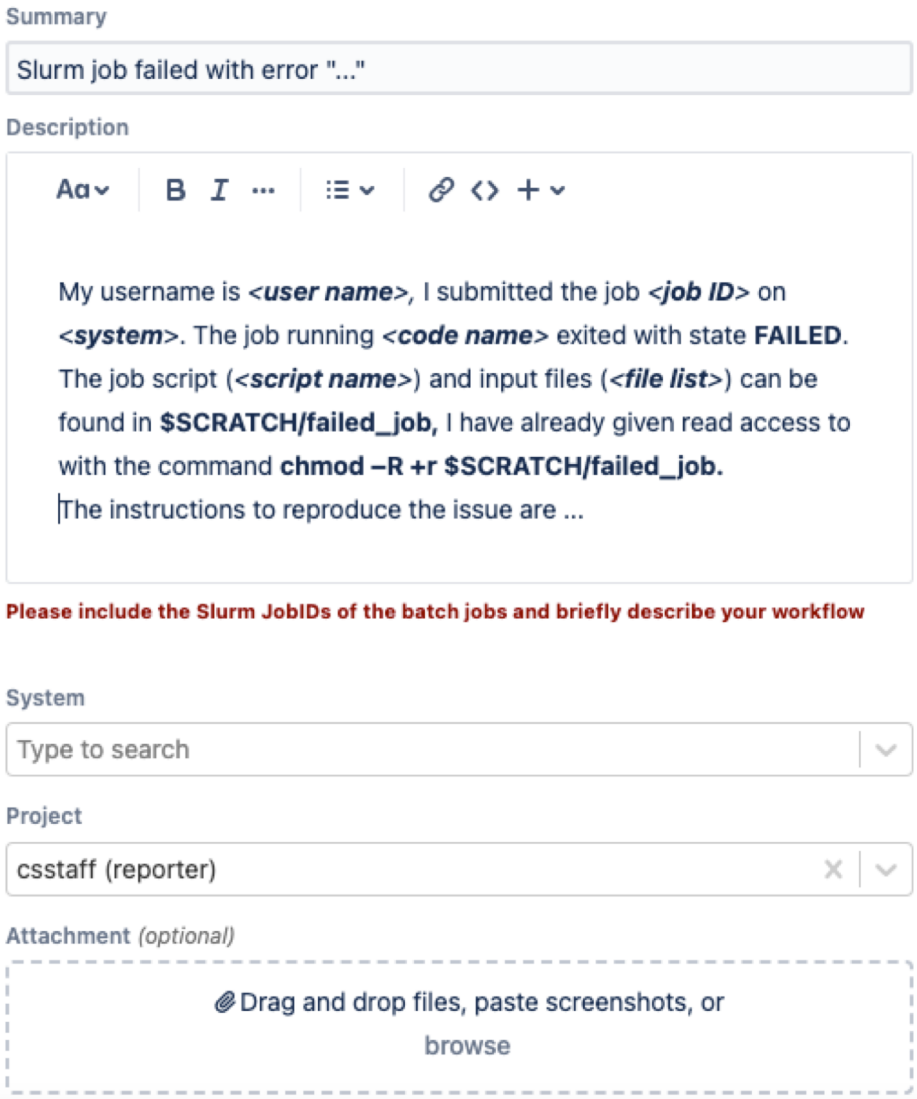
Example of a support request

Summary

- Matching articles that might help will pop-up from the KB as you type

Description

- Please provide the information needed to reproduce the issue
- Include the **Slurm jobid** and the path to the **Slurm job script**
- Copy scripts and source files to **$SCRATCH** and give us access



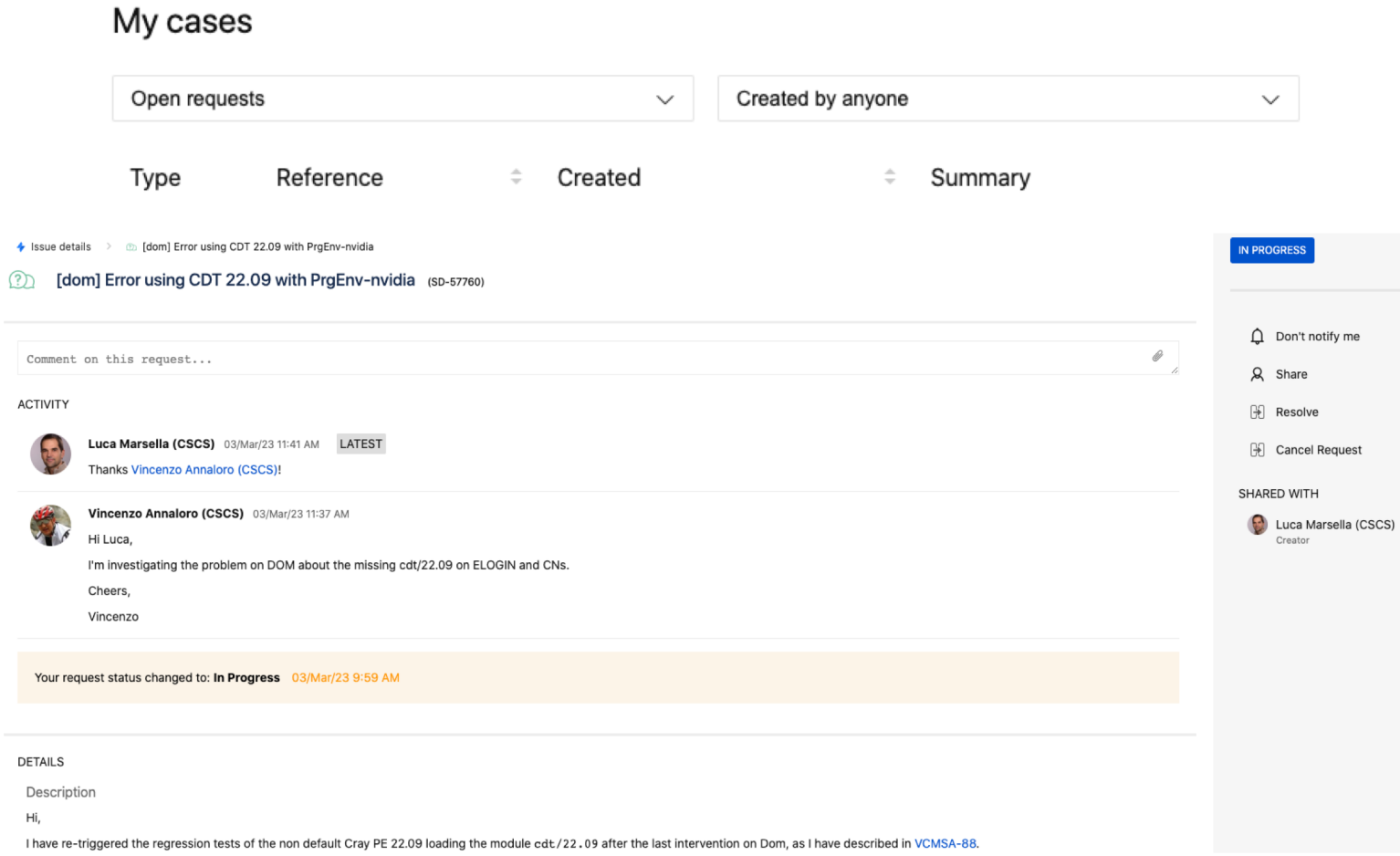
Monitoring your requests

Cases on the Service Desk:

- **Filter** the list of cases
- Check case **status**
- **Review** the messages

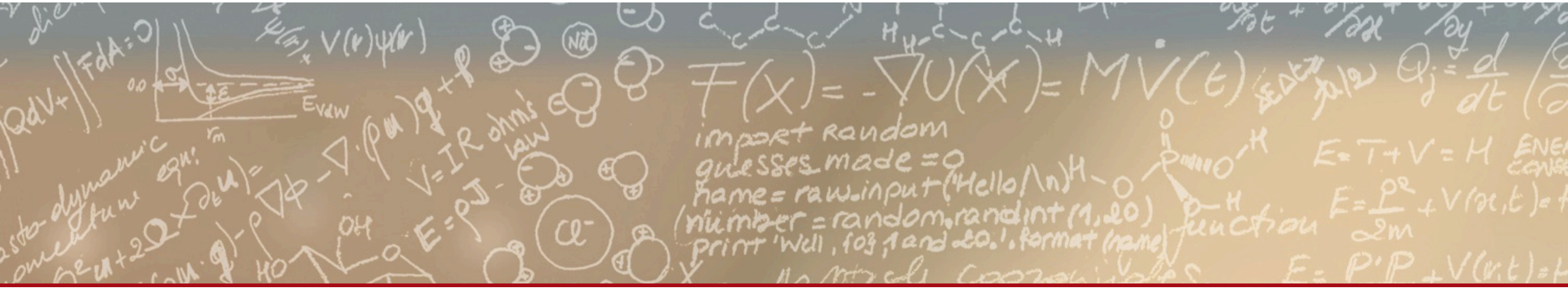
Select a specific case:

- **Share** with other users
- **Resolve** the case if solved
- **Cancel** if sent by mistake



Useful Links

- User Portal
  - http://user.cscs.ch
- Knowledge Base
  - https://confluence.cscs.ch/display/KB/CSCS+Knowledge+Base
- CSCS Service Desk
  - https://support.cscs.ch



Thank you for your kind attention