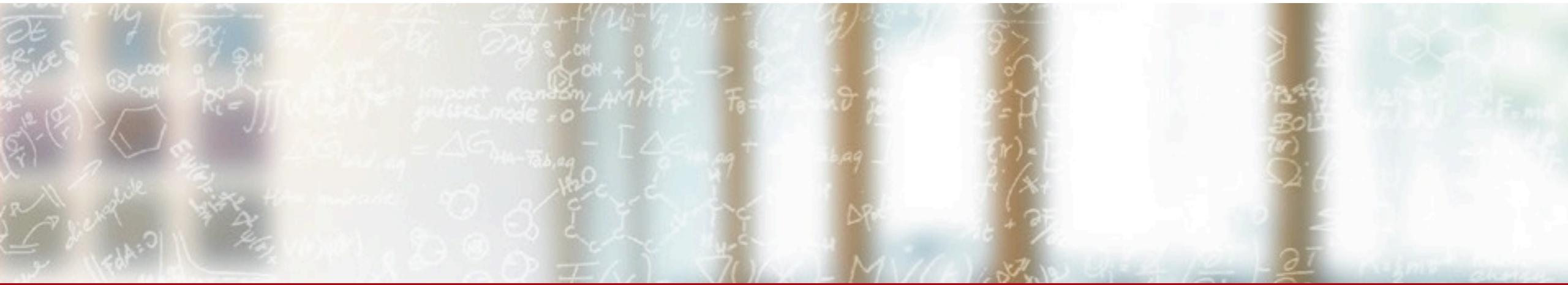




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General Information for Users on Alps

User Lab Day 2024

Luca Marsella and Tim Robinson, Service Managers at CSCS

Outline of the Presentation

- Introduction of Platforms
- Policies and Service Catalogue
- Documentation and Troubleshooting
- Community Slack Space and Status Page



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



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Introduction of Platforms

Glossary

Platform A subset of Alps on top of the infrastructure that enables the deployment of one or multiple vClusters

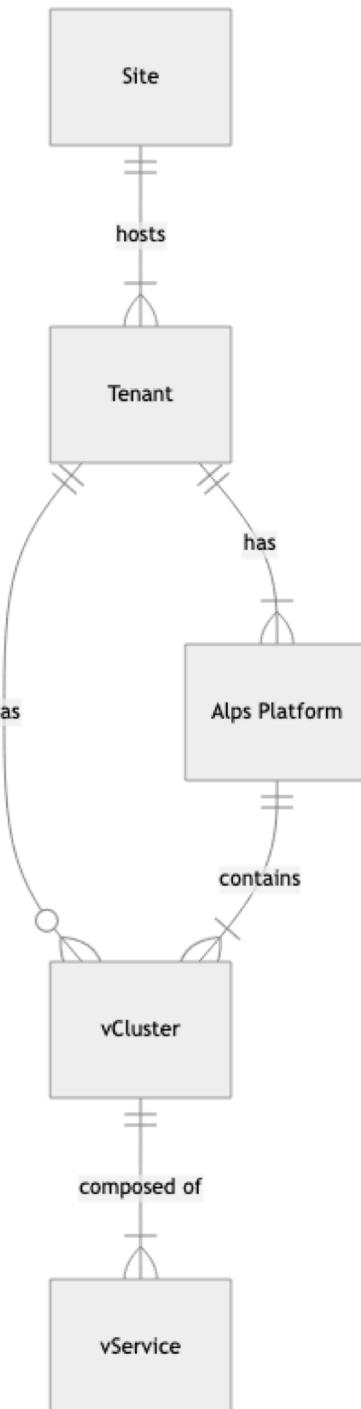
Site A physical place with the facilities to operate the infrastructure (CSCS in Lugano, EPFL in Lausanne, PSI in Villingen, ECMWF in Bologna)

Tenant Organization holding the underlying platform (CSCS, MCH, PSI,...)

vCluster (versatile cluster) Fusion of HPC and cloud technologies providing software-defined clusters on a supercomputing ecosystem

vService (versatile cluster microservice)

Small, independent, and loosely-coupled service hosted on a vCluster



HPC Platform

The HPC Platform targets general purpose HPC computing on Alps

Resources

- **GPU** nodes on **Piz Daint** (quad-socket Grace-Hopper superchip nodes)
- **Multicore** nodes on **Eiger** (dual-socket AMD CPU-only nodes)

Audience includes

- **User Lab** (Peer reviewed allocation programs)
- **Partners** (EMPA, ETH Zurich, Marvel, UZH, USI,...)
- [cscs2go](#) (targeting primarily Swiss researchers from Academia and SMEs)

ML Platform

The Machine Learning Platform targets AI/ML computing on Alps

Resources

- **GPU nodes on Clariden** (quad-socket Grace-Hopper superchip nodes)
- Additional vClusters with NVIDIA A100, AMD Mi250 and Mi300 GPUs

Audience is primarily the **Swiss AI** Initiative

- Build capacities for advanced, large-scale AI systems for the benefit of society
- Over 70 professors from Swiss universities and research centres
- Co-led by ETH Zurich and EPFL

CW Platform

The Climate and Weather Platform targets climate science computing on Alps

Resources

- **GPU nodes on Säntis** (quad-socket Grace-Hopper superchip nodes)

Audience includes

- **EXCLAIM**
Project for ICON-based km-scale climate simulations (ETH Zurich)
- **C2SM** Center for Climate Systems Modelling
Eawag, EMPA, ETH Zurich, MeteoSwiss, WSL
- User Lab projects in climate and weather domains



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Policies

General Policies

The [code of conduct](#) outlines some responsibilities of the user community

- **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 allocation with reference to the “*project ID ####*”

[User Regulations](#) define guidelines for the usage of CSCS resources

- **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 Information and Communications Technology](#)

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

Data Retention Policies

Data backup for **active projects**:

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

As soon as a project **expires**:

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

No backup for data on **scratch file system(s)**:

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

More information on **Data Recovery** at <https://confluence.csccs.ch/x/kYBOLw>

Policies of the scratch file system

The capacity storage (capstor) features 100 PB in a Lustre file system

Cleaning policy: files **older than 30 days deleted** daily

No backup: you should transfer data after batch job completion

Soft quotas to prevent performance degradation

- Quota on **total number of files and folders** (inodes)
- Quota on **amount of data** with a **grace time** to allow data transfer

More information on **scratch** at <https://confluence.csccs.ch/display/KB/scratch>

Fair Usage Policies

Slurm workload manager

- The batch scheduler is a shared resource
- **Do not continuously poll the scheduler** to determine job states
- **Do not submit hundreds of jobs** in a short space of time
- We may be forced to kill jobs and limit new submissions

Login (User Access) nodes

- **Compute- or memory-intensive processes are not permitted**
- Heavy processes will be terminated **without warning**
- **Submit Slurm batch jobs** to run application codes on compute nodes

Support Policies

We offer timely response with **direct assistance** or **escalation processes**

- Support is **limited to the scope** of your project proposal
- We cannot guarantee the resolution of all issues

Supported community codes and user applications

- We are committed to help you run up-to-date supported community codes
CSCS staff cannot fix application-specific issues
- Best-effort support deploying and optimizing user applications

Prioritization case impact, complexity, knowledge transfer, time to solution

Collaborative support consult online docs and provide detailed information

Resource Allocation Policies

Computing time on vClusters is allocated and accounted in **node hours**

- Resources are assigned in **three-month windows**
 - **Quotas are reset** on April 1st, July 1st, October 1st and January 1st
 - Try to use your compute budget evenly and consistently across the windows
 - Unused resources in a given window **cannot be transferred to the next**

More information on **Policies** at <https://confluence.csccs.ch/x/UQBYLw>



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Service Catalogue

Multi-factor authentication and SSH connections

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 MFA authenticators that follow the TOTP open standard
- SSH is only possible with keys generated by the CSCS SSHSERVICE
- **Keys are valid for 24 hours**, after which a new key must be generated

More on MFA at <https://confluence.cscs.ch/x/VwBYLw>

Programming Environment

We provide several ways to build software for running on vClusters

- **uenv** developed and fully supported at CSCS
- Cray Programming Environment (CPE) supported via HPE/Cray
- Containers (often a good choice for machine learning workloads)

No modules are loaded by default at login!

- You need to load the module **cray** first with the following command
module load cray
- Then the modules available in the default CPE can be listed with
module avail

More on **CPE** at https://confluence.cscs.ch/x/_gD0E

uenv: User Environments

uenv provide programming environments and application software

Typically application-specific, domain-specific or tool-specific

- **uenv** contains only what is required for the application or tool to run
- CSCS provides some ready-made and supported user environments
- Advanced users can create their own **uenv** with the tools provided

Packaged in a single **squashfs** file

- Can be shared in an artifactory or stored on a file system
- Independent of each other and of CPE
- Built on top of the base image, not the CPE

uenv: Tools

Command Line Interface (CLI)

- **squashfs-mount**: low-level tool for mounting environments
- **uenv**: command line tool for interacting with environments

Slurm plugin at <https://github.com/eth-cscs/slurm-uenv-mount>

- Manages the loading of images on compute nodes

Stackinator at <https://eth-cscs.github.io/stackinator>

- Tool for generating images from a declarative recipe

Github with CSCS images at <https://github.com/eth-cscs/alps-spack-stacks>

- CI/CD pipeline to build, test and deploy images

uenv: Mount Points

/user-environment

- **Programming environments**
 - Compilers, libraries, profilers (e.g.: HDF5, FFTW, MPI, OpenBLAS...)
 - Can be application specific (e.g.: supporting ICON builds)
- **Application environments**
 - CP2K, GROMACS, LAMMPS, NAMD, QuantumEspresso, VASP...

/user-tools

- **Supporting tools**
 - Debuggers (DDT)
 - Text editors
 - Visualization (ParaView, Visit, ...)

uenv: Benefits for You

Single image in a SquashFS file

- Managed in a registry/artifactory
- Performance decoupled from file system

Defined by a **simple declarative recipe**

- The same environment can be easily rebuilt
- Useful after system upgrades

Small set of system dependencies

- Only need to rebuild if **libfabric** or **Slurm** are changed

More on **uenv** at <https://confluence.csccs.ch/x/bYDTKQ>

Container Engine

Container Engine **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 on [Container Engine](#) at <https://confluence.cscs.ch/x/B4BFLg>

Continuous Integration / Continuous Deployment (CI/CD)

CI/CD to **build containers** and run them at CSCS

- Dockerfile with build instructions
- Name for the container in the registry
- The build will be taken care by the CI implementation

Pipelines: git providers with [webhooks](#) (GitHub, GitLab, Bitbucket)

- A typical pipeline consists of at least one build job and one test job
- Build job: a new container with your most recent code changes is built
- Test job: the new container is run within an MPI job

More on [CI/CD](#) at <https://confluence.cscs.ch/x/UAXJMw>

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

HTTP requests to perform various 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 on [FirecREST](#) at <https://confluence.cscs.ch/x/ewBWM>

Interactive Computing with JupyterLab

[JupyterLab](#) is the web-based user interface for [Project Jupyter](#)

- Create and share **documents with live code**, equations, visualization, ...
- Ability to work with multiple documents using tabs or splitters side by side

We provide [JupyterHub](#) deployments on most vClusters

- Notebook servers are launched on compute nodes
- Some **ready-made kernels** are provided: Python, Julia, etc
- You can **add your own kernels** based on your own virtual environments
- Can **execute kernels on multiple nodes** with IPyParallel

More on [JupyterLab](#) at <https://confluence.csccs.ch/x/fQBWM>

Storage Resources: Capacity Storage

Most vClusters on Alps mount the capacity storage (**capstor**) as scratch file system

- 100 PB Lustre built on spinning disks
- **Best I/O performance on large files**
- Raw performance
1 TB/s I/O bandwidth
300K write IOPS and 1.5M read IOPS



Storage Resources: Flash File System

The ML Platform also mounts the flash file system iopstor

- 3 PB Lustre filesystem built on Flash memory
- High **Input/Output operations per second (IOPS)**
- Raw performance
240 GB/s write and 600 GB/s read bandwidth
13 M write IOPS and 18.4 M read IOPS



Storage Resources: /users and /store

Storage for datasets, code and scripts

- Access **r+w** from the User Access Nodes (UAN)
- Better performance with larger files (archive small files with **tar**)

Permissions and data retention

- Folders **backed up**: data retention until 3-months after projects end

Environment variables for quick access

- **\$HOME** pointing to personal folder **/users/\$USER**
- **\$STORE** pointing to group folder under **/store**

More on [**File Systems**](#) at <https://confluence.cscs.ch/x/w4DOLg>

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

More information on [Data Transfer](#) at <https://confluence.cscs.ch/x/IIBOLw>

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 on [**Long Term Storage**](https://confluence.cscs.ch/x/p4BOLw) at <https://confluence.cscs.ch/x/p4BOLw>



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Documentation

Decommissioning of the CSCS User Portal at <https://user.cscs.ch>

Documentation migrated
CSCS Knowledge Base
<http://docs.cscs.ch>

Announcements on
CSCS Status Page
<https://status.cscs.ch>



cscs

The screenshot shows the CSCS User Portal homepage. At the top right is the ETH Zürich logo. The main navigation bar includes links for "CSCS User Portal", "Getting Started", "Scientific Computing", "Storage", "Tools", and "My Projects". On the left, there's a sidebar with "HOME" and links to "Getting Started", "Scientific Computing", "Storage", and "Tools". Another sidebar below it lists "USEFUL LINKS" such as "Account and Resources Tool", "CSCS Website", "Events", "Tutorials", "Production Repository", and "CSCS Service Desk". The main content area features a section titled "Latest News" with the following entries:

- 31.07.2024 Decommissioning of Piz Daint**
As announced to the CSCS HPC users mailing list on 31 July 2024, Piz Daint Cray XC50/40 is at the end of its life, therefore CSCS engineering teams will focus on Alps. Consequently, we will not provide new versions of scientific applications and support on the old Piz Daint will be on a best-effort basis.
- 31.01.2024 FirecREST back in service**
The FirecREST maintenance has been completed: the FirecREST version has been updated to the latest release 1.14.0, backward compatible with older workflows, that therefore should not be affected. Please have a look at the latest features provided by the new release [here](#).
- 24.01.2024 FirecREST maintenance on January 31st 2024**
A maintenance of the [FirecREST service](#) is scheduled on Wednesday January 31st 2024 from 09:00 to 12:00 CET. We apologize for any inconvenience this may cause: please feel free to [contact us](#) if you have any concerns.

At the bottom, a note says: "For a collection of all news and updates, please access the [News Archive](#) and the [Piz Daint Updates](#)".

CSCS Knowledge Base (KB) at <https://docs.cscs.ch>

The KB replaces the User Portal

- Online Documentation can be **searched** easily with Confluence
- **Articles** displayed in panels following User Portal names
- New sections **How-to-articles** and **Troubleshooting articles**

The screenshot displays the CSCS Knowledge Base (KB) interface. At the top left is a "Live Search" bar with a placeholder "Please search the Knowledge Base here". Below it is a detailed search syntax explanation. To the right is a "Q & A" section containing links to "Frequently Asked Questions (FAQ)", "How-to articles", "Troubleshooting articles", and a link to "Submit a request on the CSCS Service Desk". The main content area is organized into several panels:

- Online Documentation**:
 - Getting Started**: Links to "Access", "Access to CSCS Systems (New)", and "Account and Resources Management Tool". A "More articles in Getting started" link is also present.
 - Programming Environment**: Links to "Containers" and "UENV user environments". A "More articles in Programming Environment" link is also present.
 - Storage**: Links to "Data Recovery", "Data Transfer", and "File Systems". A "More articles in Storage" link is also present.
- User Guides**:
 - Links to "Alps (Clariden) User Guide", "Alps (Eiger) User Guide", and "Santis Early Access". A "More articles in User Guides" link is also present.
- Scientific Computing**:
 - Links to "Data Science", "Scientific Applications", and "Visualisation and I/O". A "More articles in Scientific Computing" link is also present.
- Tools**:
 - Links to "FirecREST", "Interactive supercomputing", and "Kubernetes Clusters". A "More articles in Tools" link is also present.



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Troubleshooting

What to do in case of trouble?

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



Welcome to the CSCS Service Desk! How can we help you ?

Useful links

[Knowledge Base](#)

[User Portal](#)

[Tutorials](#)

[Login first!](#)

You are currently not logged in. Please [login here](#) to submit a request and view your current and past requests.

Contact us

Only if you do not have an account or if your account is not accessible, you can [contact us here](#).

How to submit a support request

Useful links to documentation and status available online

- Knowledge Base (KB) at <https://docs.cscs.ch>
- Status Page at <https://status.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

More on [**How to submit a support request**](#) at <https://confluence.cscs.ch/x/LYH8LQ>

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

Please select a request type to open a case



Accounting

Administrative requests regarding your user or project accounts



Cloud

Questions regarding the openstack cluster Castor



Connection

Questions regarding SSH connections and keys using multi-factor authentication (MFA)



Network

Questions regarding SSL certificates, firewalls, servers



Scientific Applications

Questions regarding supported applications and libraries



Software Environment

Questions regarding compiling software, containers, user environment, interactive computing and visualization



Storage and Filesystems

Questions regarding backup, data transfer (globus, xfer), filesystem performance, object storage



System and job scheduling

Questions regarding system related issues with batch jobs and remote workflows (e.g. Unicore)



Other requests

Other requests for support

Example of a good 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 the necessary permissions to access

Summary

Slurm job failed with error "..."

Description

Aa **B** I ... ≡ ⌂ ⌂ +

My username is <user name>, I submitted the job <job ID> on <system>. The job running <code name> exited with state FAILED. The job script (<script name>) and input files (<file list>) can be found in \$SCRATCH/failed_job, I have already given read access to with the command chmod -R +r \$SCRATCH/failed_job.
The instructions to reproduce the issue are ...

Please include the Slurm JobIDs of the batch jobs and briefly describe your workflow

System

Type to search

Project

csstaff (reporter)

Attachment (optional)

Drag and drop files, paste screenshots, or
browse

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

My cases

Open requests Created by anyone

Type	Reference	Created	Summary
[dom]	[dom] Error using CDT 22.09 with PrgEnv-nvidia (SD-57760)	03/Mar/23 11:41 AM	IN PROGRESS

Comment on this request...

ACTIVITY

Luca Marsella (CSCS) 03/Mar/23 11:41 AM LATEST
Thanks Vincenzo Annaloro (CSCS)!

Vincenzo Annaloro (CSCS) 03/Mar/23 11:37 AM
Hi Luca,
I'm investigating the problem on DOM about the missing cdt/22.09 on ELOGIN and CNS.
Cheers,
Vincenzo

Your request status changed to: In Progress 03/Mar/23 9:59 AM

DETAILS

Description
Hi,
I have re-triggered the regression tests of the non default Cray PE 22.09 loading the module cdt/22.09 after the last intervention on Dom, as I have described in [VCMSA-88](#).

IN PROGRESS

Don't notify me
Share
Resolve
Cancel Request

SHARED WITH

Luca Marsella (CSCS) Creator



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Community Slack Space

Community Slack Space

CSCS Users Slack <https://cscs-users.slack.com>

A new space for you **to interact with fellow CSCS users**

- **Community** driven approach
- Get **rapid responses** to quick questions
- **Share experiences** and best practices

Recommendations

- Encourage your team members to join!
- Please always **be kind and considerate** to others
- Misbehaviour could result in a ban from the Slack space



Channels

The space includes the following channels

- **#daint**
Early access phase of vCluster Daint on Alps
- **#general**
Default Slack channel for general purpose posts
- **#introductions**
Learn more about your fellow users and their science
- Discover **more channels** on the Slack space

The Slack space **is not** meant for submitting support requests

- Use the CSCS Service Desk at <https://support.cscs.ch>





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Status Page

Status Page at <https://status.cscs.ch>

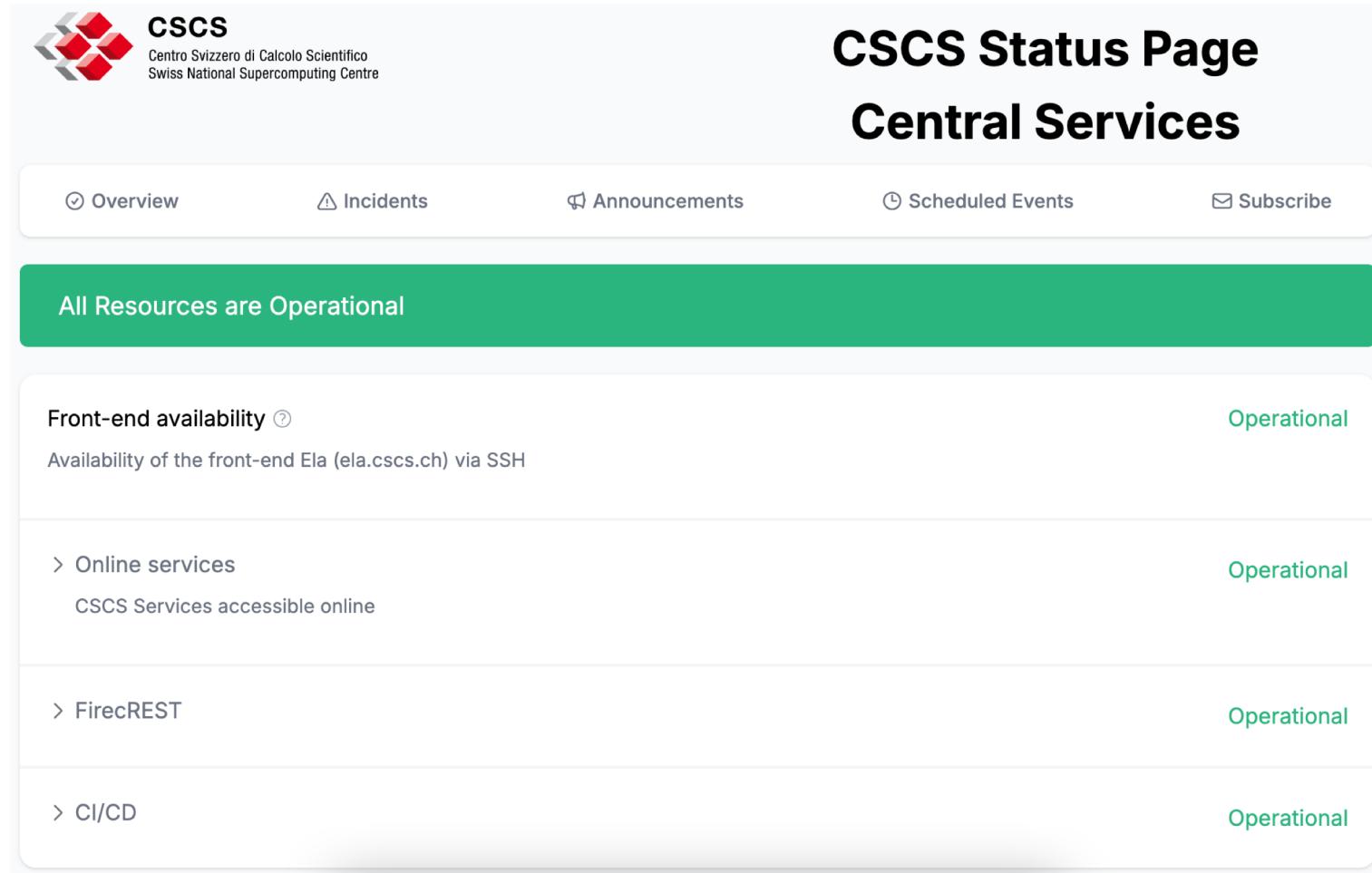
The Status Page reports

- Incidents
- Announcements
- Scheduled Events

Status of resources

- Online services
- Front end system

Subscribe to get notifications



The screenshot shows the CSCS Status Page interface. At the top, there is the CSCS logo and name. Below the logo, a navigation bar includes links for Overview, Incidents, Announcements, Scheduled Events, and Subscribe. A prominent green banner states "All Resources are Operational". The main content area displays four service status entries: "Front-end availability" (Operational), "Online services" (Operational), "FirecREST" (Operational), and "CI/CD" (Operational). Each entry includes a brief description and an "Operational" status indicator.

Service	Status
Front-end availability	Operational
Online services	Operational
FirecREST	Operational
CI/CD	Operational

Useful Links

- CSCS Service Desk
 - <https://support.cscs.ch>
- CSCS User Slack
 - <https://cscs-users.slack.com>
- Knowledge Base
 - <https://docs.cscs.ch>
- Status Page
 - <https://status.cscs.ch>

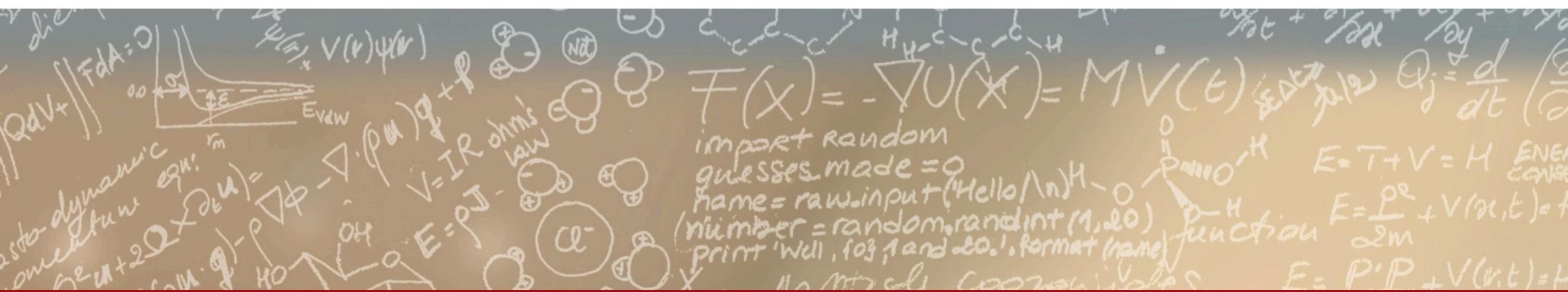




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Thank you for your kind attention