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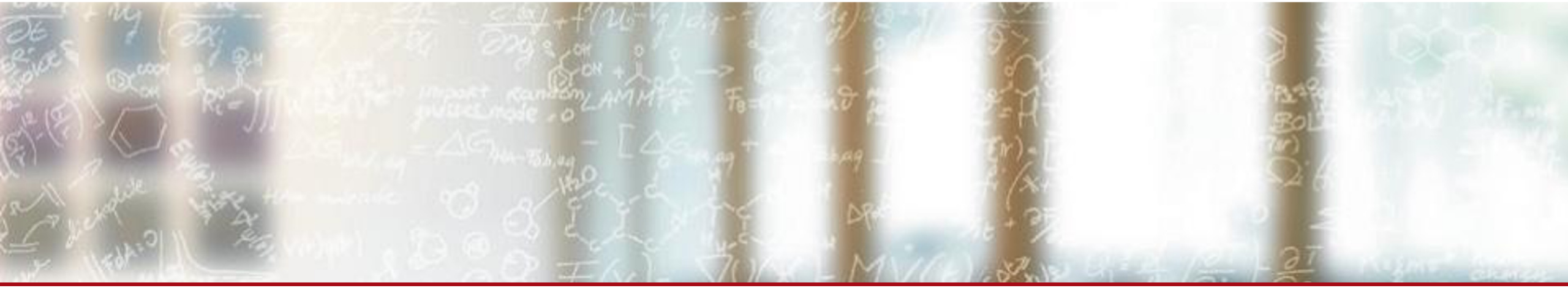

Automate your workflows on HPC with FirecREST API

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CSCS UserLab Day
Luzern, Switzerland

Motivation

Motivation

- As cloud technology and HPC evolve there is an increasing need from the user community to enable sophisticated services on the cloud to interface HPC resources
- Use cases such as CI/CD Pipelines, Workflow Orchestrators, Web Portals, are just few examples of what users can easily setup on a cloud provider but that present issues when interfacing HPC
- This shows the need of a programmatic layer on the HPC facility that abstracts and standardizes access to HPC resources

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Introducing FirecREST

FirecREST in a nutshell

- **FirecREST is an open-source web-enabled API to HPC resources developed by CSCS**

FirecREST in a nutshell

- **FirecREST is an open-source web-enabled API to HPC resources developed by CSCS**

- Presents standard programming interface
  - Based on RESTAPI concept
  - Independent of programming language (HTTP)
  - Translates web requests into HPC business logic
  - Parses back HPC results into web-friendly format

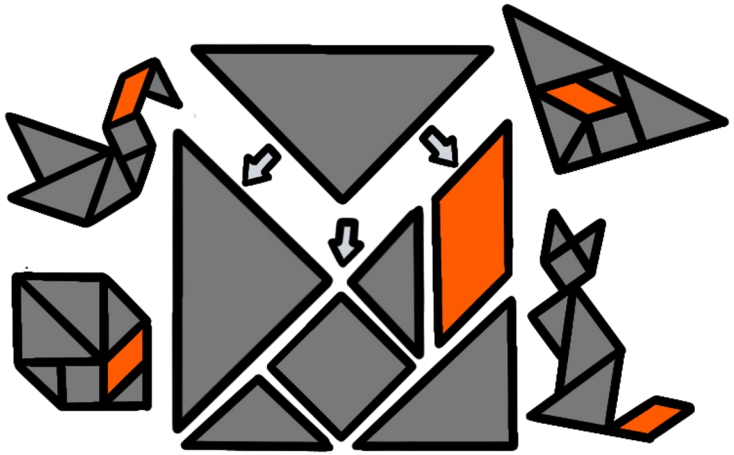
FIRECREST

FirecREST in a nutshell

- **FirecREST is an open-source web-enabled API to HPC resources developed by CSCS**
- Presents standard programming interface
- Provides web interface for classic HPC
  - Creation of web applications over HPC
  - Enables support for multiple devices

FirecREST in a nutshell

- **FirecREST is an open-source web-enabled API to HPC resources developed by CSCS**
- Presents standard programming interface
- Provides web interface for classic HPC
- Allows modular design to support different workflows and HPC systems
  - Abstracts HPC resources into components and objects



FirecREST in a nutshell

- **FirecREST is an open-source web-enabled API to HPC resources developed by CSCS**
- Presents standard programming interface
- Provides web interface for classic HPC
- Allows modular design to support different workflows and HPC systems
- Integrates with authentication and authorization layers
  - Relies on standard IAM solutions for authentication

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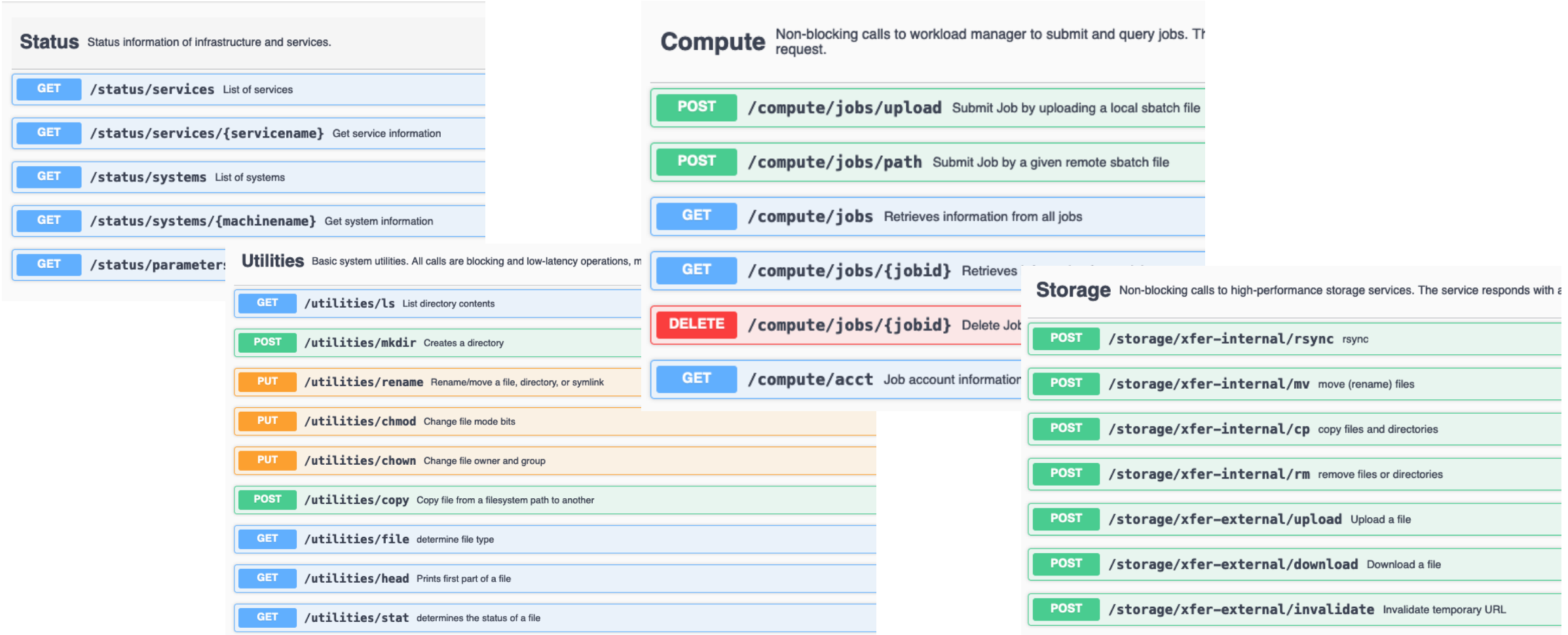
FirecREST at CSCS

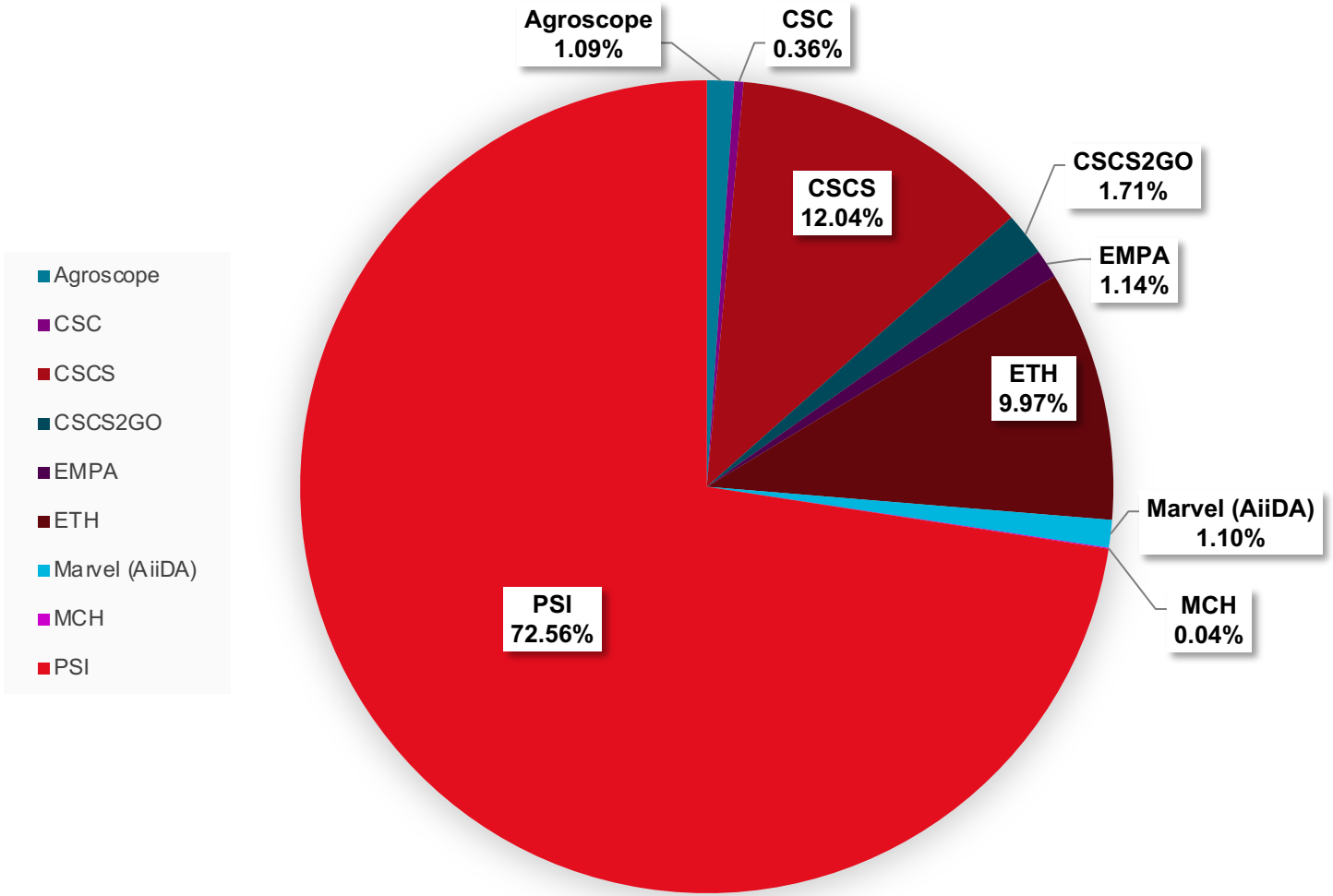
The FirecREST API

- FirecREST API specification: https://firecrest-api.cscs.ch



FirecREST usage per Project

- Data from last 2 years (systems: `daint` and `eiger`)



What's coming: FirecREST on Alps

- HPC Platform
  - `https://api.cscs.ch/hpc/firecrest/v1 -H "X-Machine-Name: daint"`
  - `https://api.cscs.ch/hpc/firecrest/v1 -H "X-Machine-Name: eiger"`

- Machine Learning Platform
  - `https://api.cscs.ch/ml/firecrest/v1 -H "X-Machine-Name: bristen"`
  - `https://api.cscs.ch/ml/firecrest/v1 -H "X-Machine-Name: clariden"`

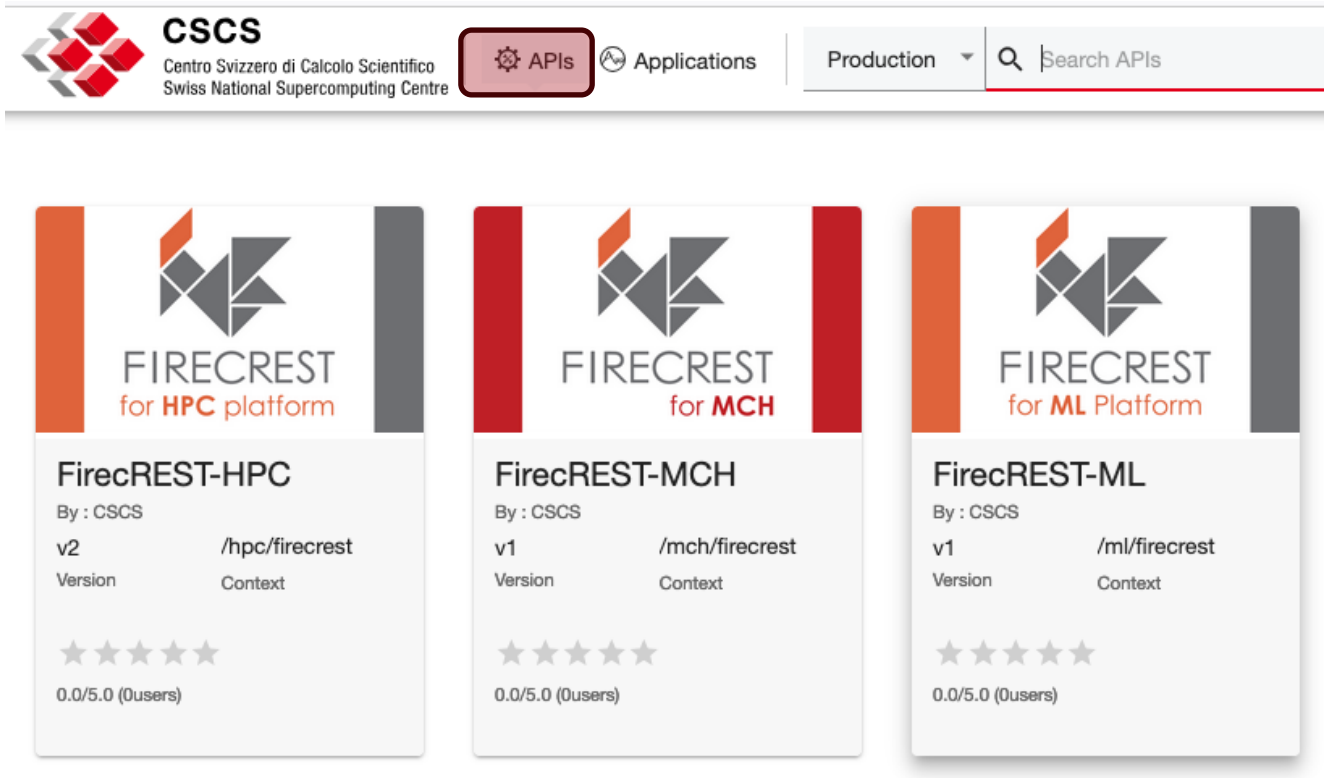
- Weather & Climate Platform
  - `https://api.cscs.ch/wc/firecrest/v1 -H "X-Machine-Name: santis"`

- MeteoSwiss Platform (only accessible from MCH newtork)
  - `https://api.cscs.ch/mch/firecrest/v1 -H "X-Machine-Name: balfrin"`

CSCS Developer Portal

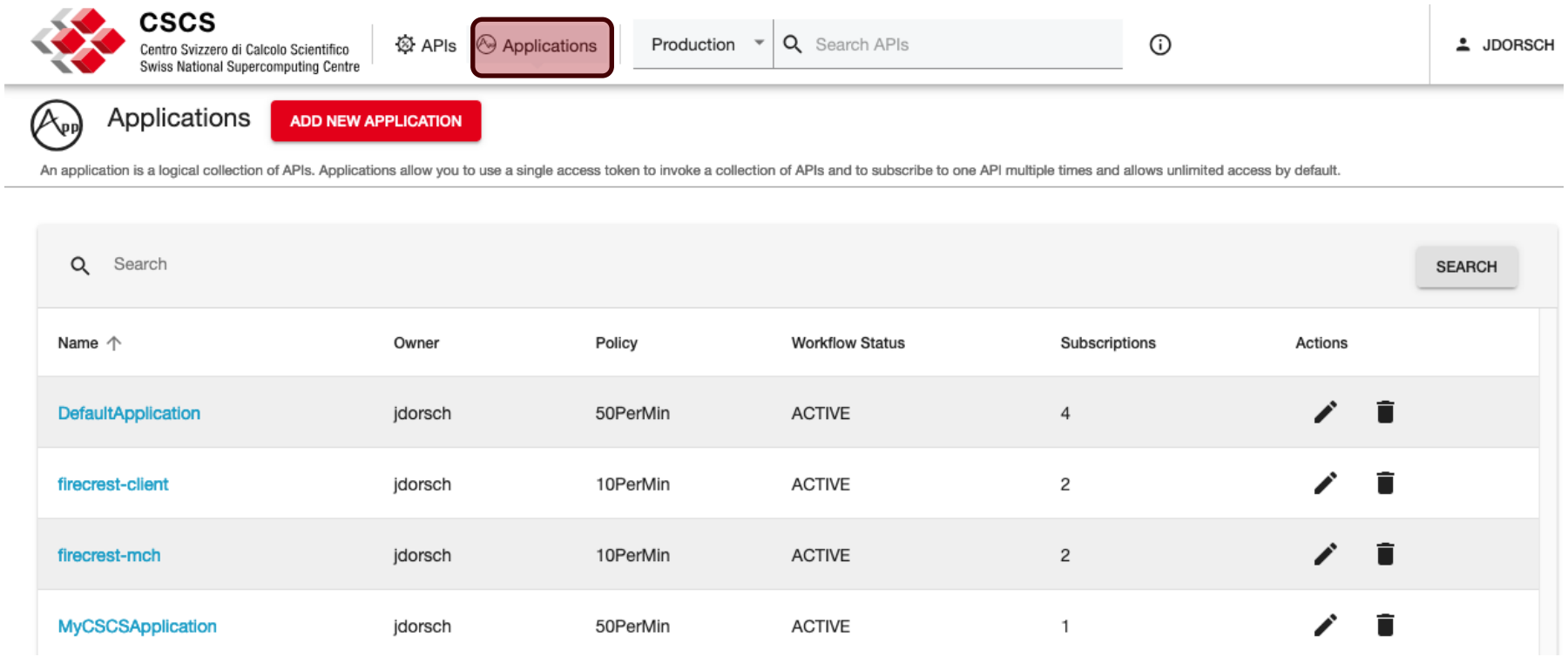
- Used for subscribing to FirecREST Platform APIs

developer.cscs.ch



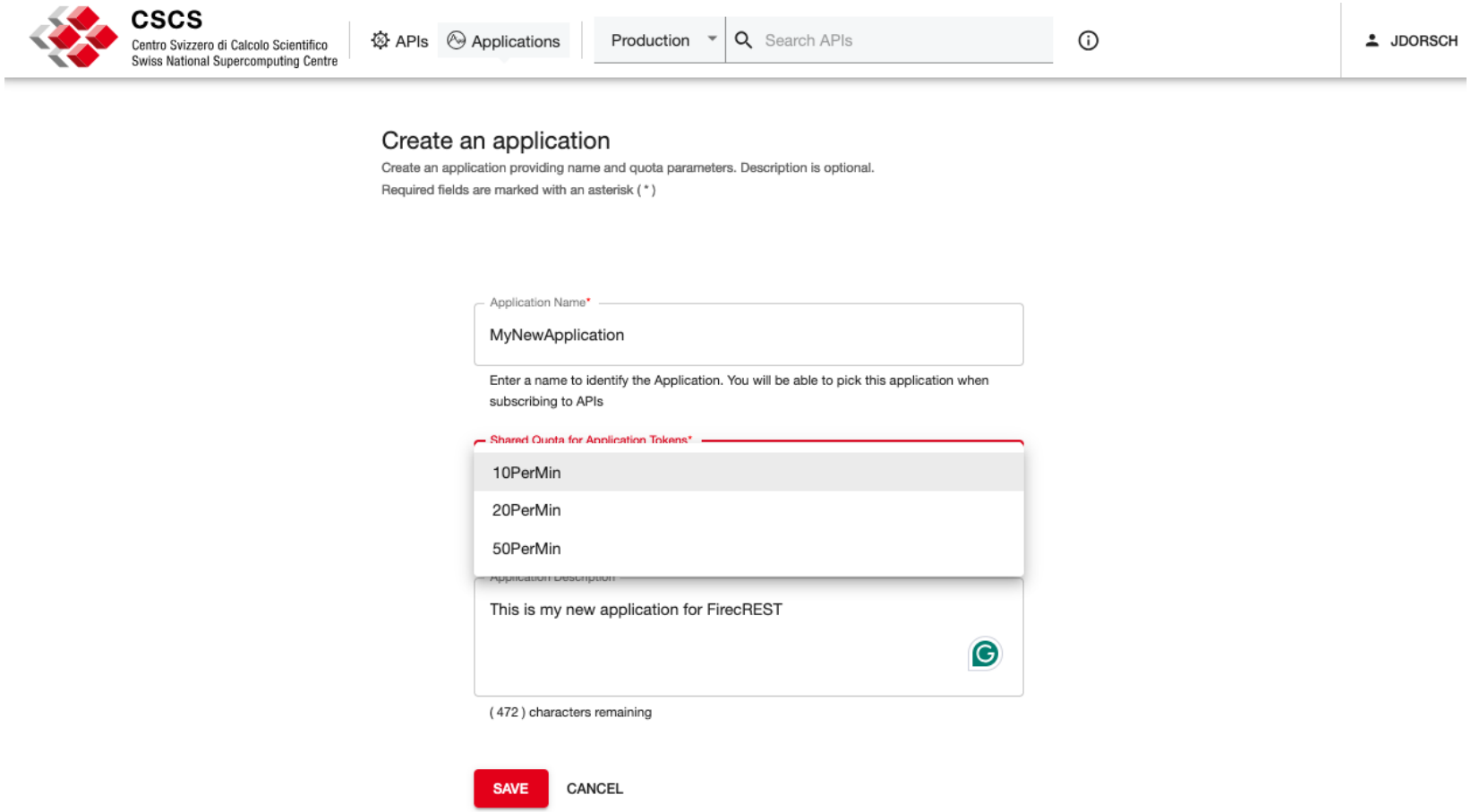
CSCS Developer Portal

- List of your applications



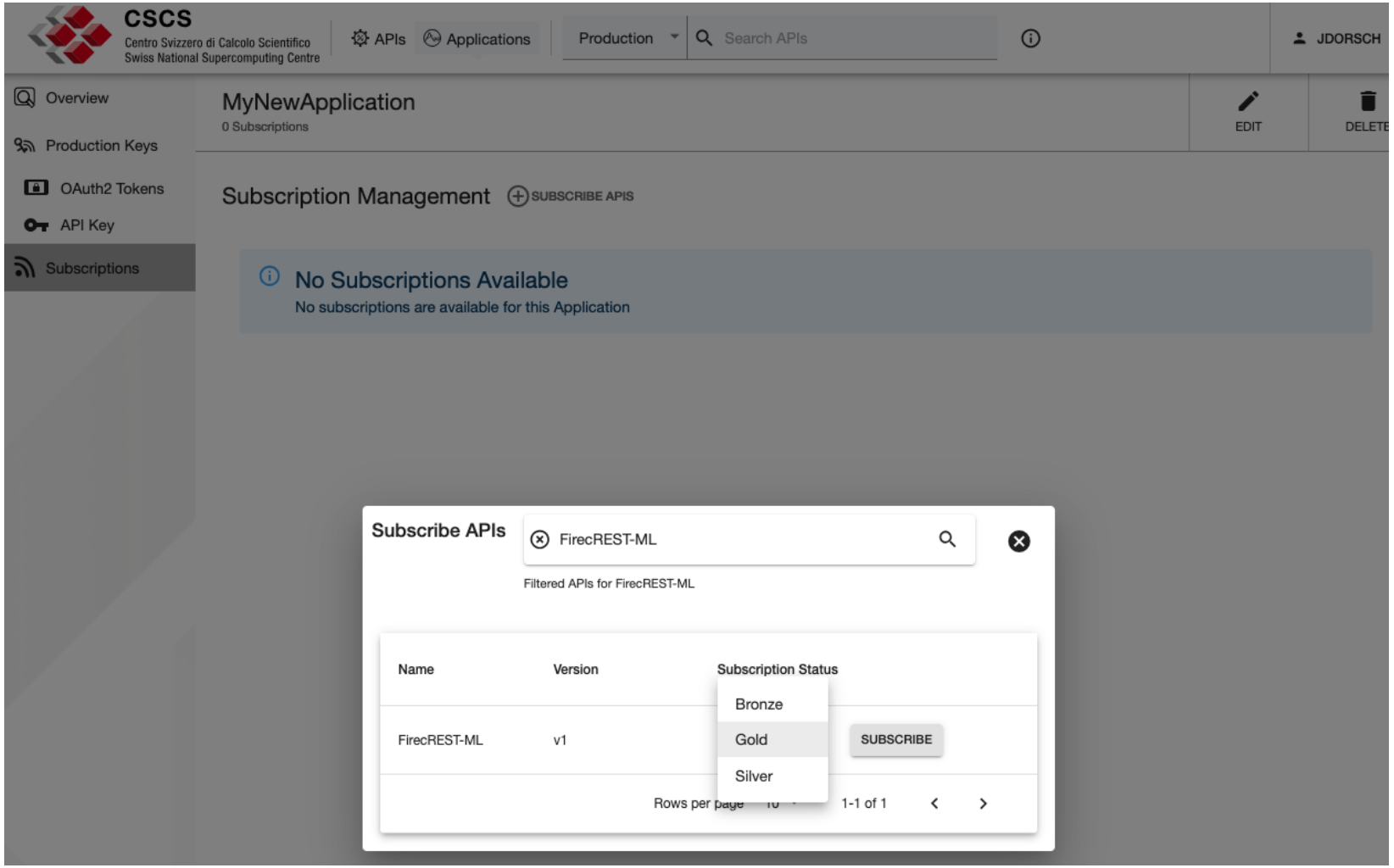
CSCS Developer Portal

- Create a new application



CSCS Developer Portal

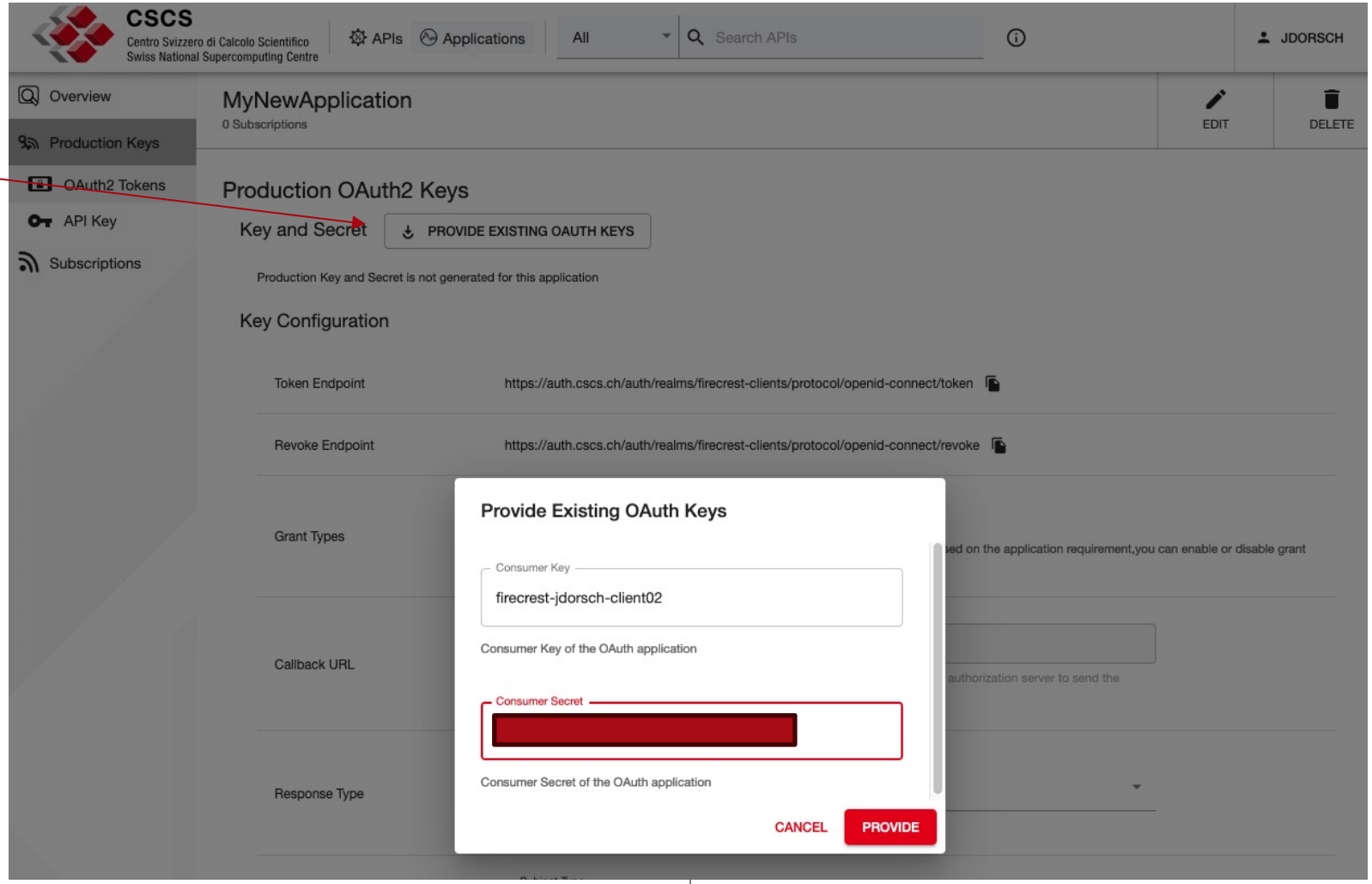
- Subscribe your new application to one of FirecREST APIs



CSCS Developer Portal

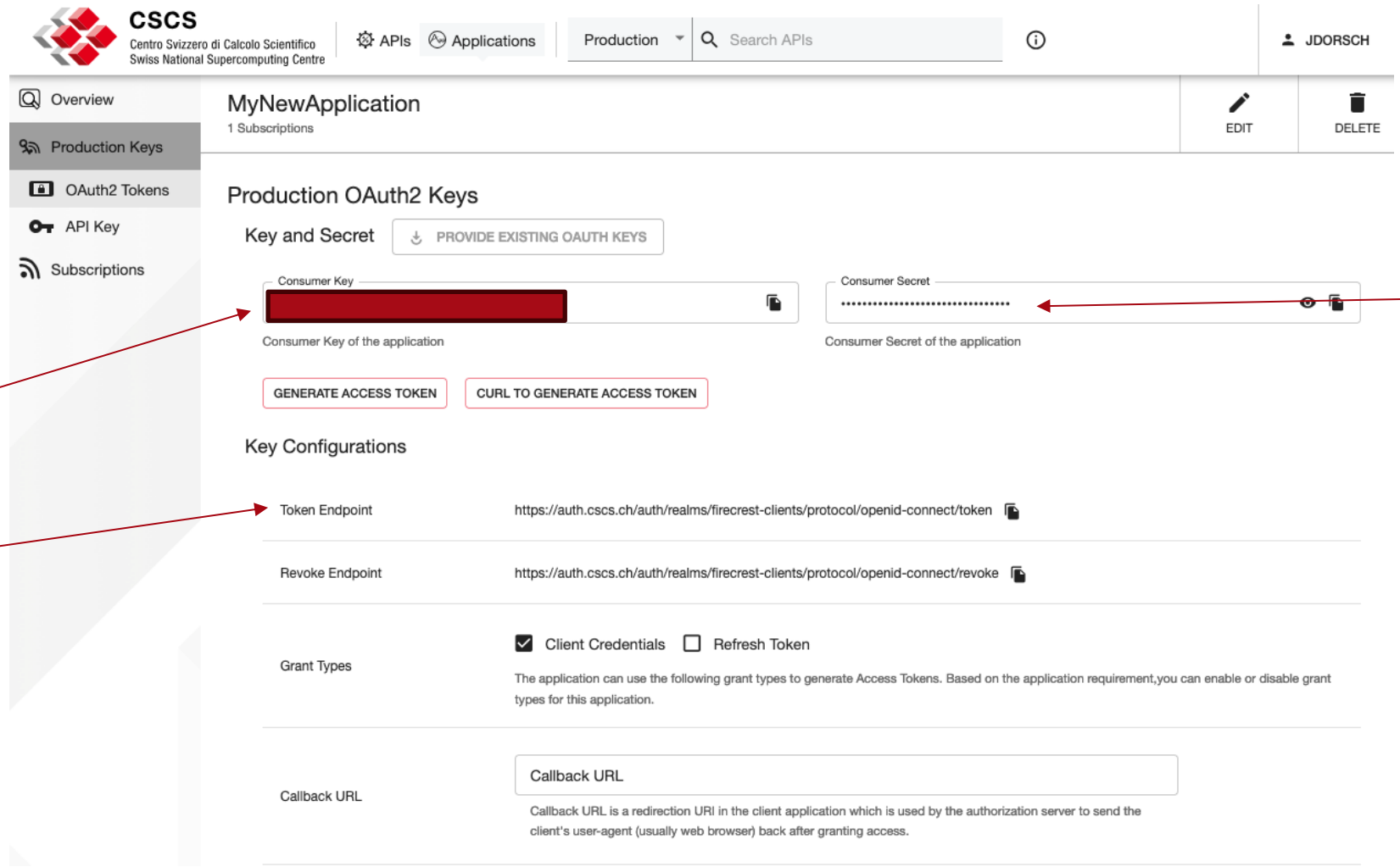
- You can migrate your client created on `oidc-dashboard-prod.cscs.ch`

Important: if you don't migrate your existing client, it won't work on Alps!!!



CSCS Developer Portal

- If you want to create new credentials for your application to interface FirecREST API



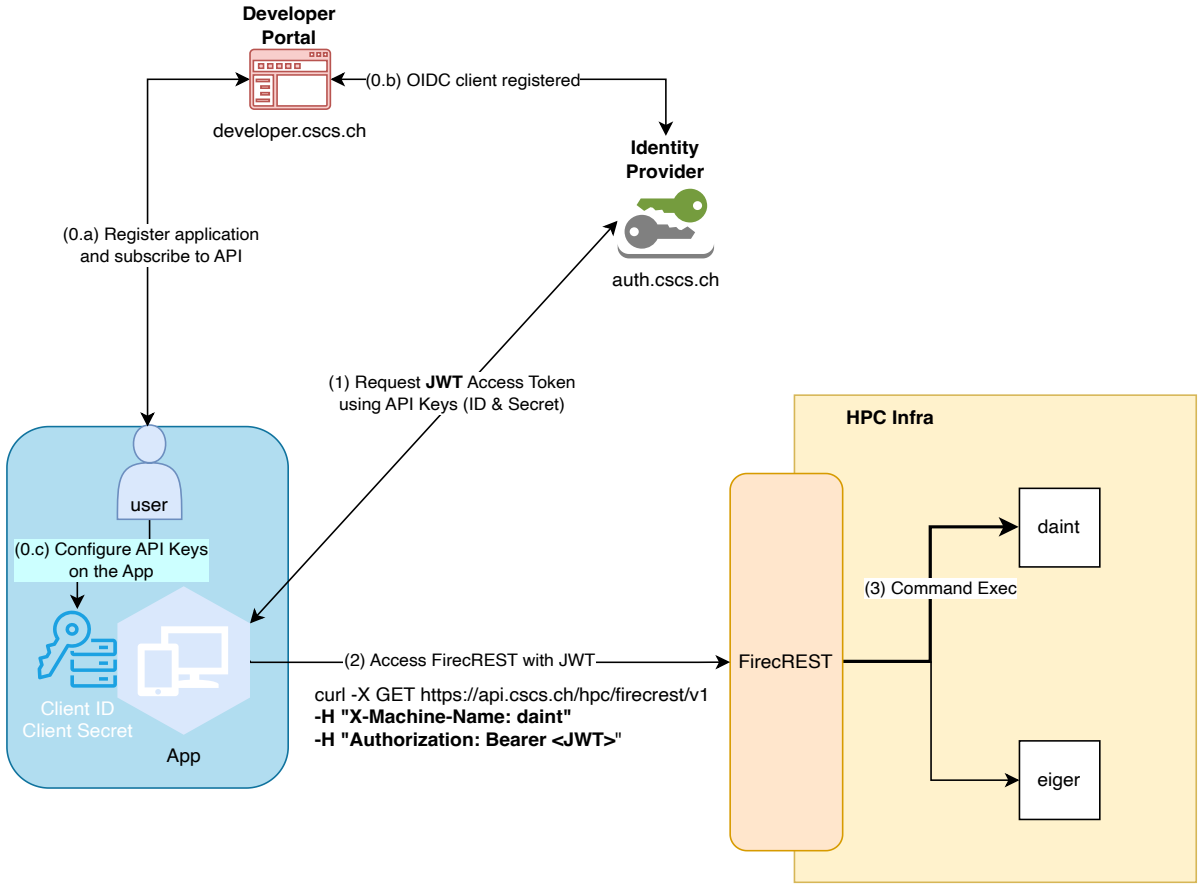
Consumer Key = FIRECREST_CLIENT_ID

Token Endpoint = AUTH_TOKEN_URL

Consumer Secret = FIRECREST_CLIENT_SECRET

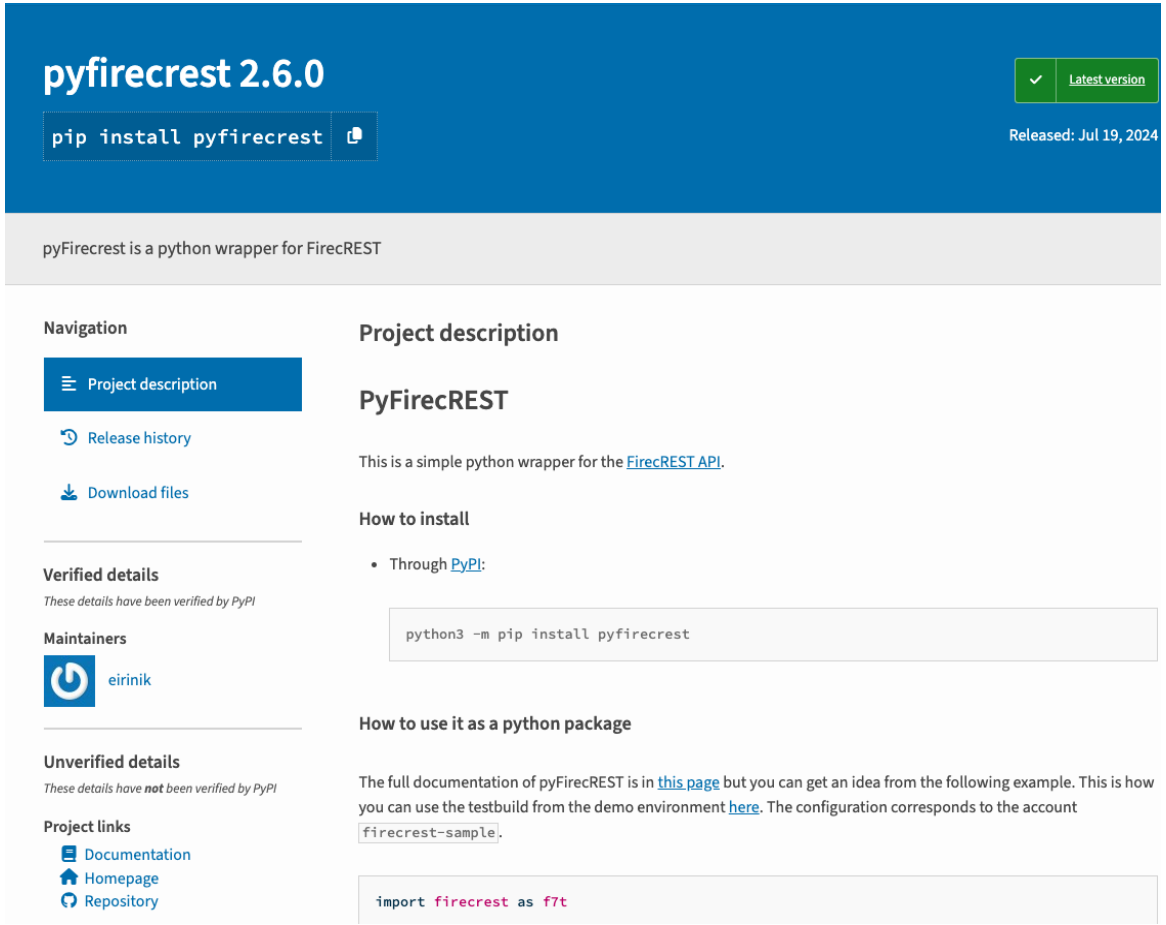
FirecREST IAM layer

- IAM relies on JWT from an IdP supporting Open ID Connect (OIDC)/OAuth2 standard
- The key pair obtained on Developer Portal is used to obtain JWT to access FirecREST
- Client ID and Secret can be used as secrets in an application for fetching JWT access token automatically, enabling robot-to-API communication



pyFirecREST Library

- pyFirecREST is a Python library that simplifies the usage of the FirecREST for scripting
- Includes transparent integration with OIDC/OAuth2 for JWT Access Token
- Enhances response time using AsyncIO interface (Async pyFirecREST)
- **Facilitates integration with several tools that exposes APIs or SDK via Python or scripting languages**



pyFirecREST Library

- From pyFirecREST version 1.3.0 also support a CLI for FirecREST

```
jdorsch@laptop ~$ export FIRECREST_URL=https://api.cscs.ch/hpc/firecrest/v1
jdorsch@laptop ~$ export FIRECREST_CLIENT_ID=<CONSUMER_KEY>
jdorsch@laptop ~$ export FIRECREST_CLIENT_SECRET=<CONSUMER_SECRET>
jdorsch@laptop ~$ export AUTH_TOKEN_URL=https://auth.cscs.ch/auth/realms/firecrest-clients/protocol/openid-connect/token
jdorsch@laptop ~$
jdorsch@laptop ~$ firecrest filesystems

                      Status of filesystems for `daint`
+-------------------------------------------------------------------------------+
| Name    | Path                  | Status code | Status    | Description        |
|---------+-----------------------+-------------+-----------+--------------------|
| HOME    | /users                | 200         | available | Home filesystem    |
| SCRATCH | /capstor/scratch/cscs | 200         | available | Scratch filesystem |
+-------------------------------------------------------------------------------+
```

pyFirecREST Library

- From pyFirecREST version 1.3.0 also support a CLI for FirecREST

```
jdorsch@laptop ~$ firecrest ls /capstor/scratch/cscs/jdorsch/newdir --system=daint
                    Files in system `daint` and path `/capstor/scratch/cscs/jdorsch/newdir`
+-----------------------------------------------------------------------------------------------------------------+
| Filename             | Type | Group   | Permissions | Size      | User    | Last modified       | Link target |
|----------------------+------+---------+-------------+-----------+---------+---------------------+-------------|
| demo.ini             | -    | csstaff | rw-r-----+  | 782       | jdorsch | 2023-12-19T10:02:29 |             |
| demo.yaml            | -    | csstaff | rw-r-----+  | 1666      | jdorsch | 2023-12-20T13:56:01 |             |
| README.md            | -    | csstaff | rw-r-----+  | 2564      | jdorsch | 2023-12-20T09:27:08 |             |
| testsbatch_todi.sh   | -    | csstaff | rw-r-----+  | 668       | jdorsch | 2023-12-19T17:44:17 |             |
| testsbatch_todi2.sh  | -    | csstaff | rw-r-----+  | 582       | jdorsch | 2023-12-19T09:39:24 |             |
| uploaded_file1.tar   | -    | csstaff | rw-r-----+  | 180788580 | jdorsch | 2023-12-18T16:36:39 |             |
| uploaded_file2.tar   | -    | csstaff | rw-r-----+  | 180788580 | jdorsch | 2023-12-13T14:35:41 |             |
+-----------------------------------------------------------------------------------------------------------------+
```

```
jdorsch@laptop ~$ firecrest submit /Users/jdorsch/tests/sbatch/testsbatch_daint.sh --system=daint
{
    'job_data_err': '',
    'job_data_out': '',
    'job_file': '/capstor/scratch/cscs/jdorsch/firecrest/5d73fec9d0a03596caff2c153f5b3931/testsbatch_daint.sh',
    'job_file_err': '/capstor/scratch/cscs/jdorsch/firecrest/5d73fec9d0a03596caff2c153f5b3931/slurm-358188.out',
    'job_file_out': '/capstor/scratch/cscs/jdorsch/firecrest/5d73fec9d0a03596caff2c153f5b3931/slurm-358188.out',
    'job_info_extra': 'Job info returned successfully',
    'jobid': 358188,
    'result': 'Job submitted',
    'firecrest_taskid': '5d73fec9d0a03596caff2c153f5b3931'
}

jdorsch@laptop ~$ firecrest poll --system=daint
                                        Accounting data for jobs
+-----------------------------------------------------------------------------------------------------------------+
| Job ID | Name     | Nodelist  | Nodes | Partition | Start time          | State   | Time     | Time left | User    |
|--------+----------+-----------+-------+-----------+---------------------+---------+----------+-----------+---------|
| 358188 | f7t_test | nid006592 | 1     | normal    | 2024-08-28T09:34:41 | RUNNING | 00:38:24 | Unknown   | jdorsch |
+-----------------------------------------------------------------------------------------------------------------+
```

Use Cases

Use Cases

- Continuous Integration (CI) Pipelines
  - CI pipelines are used to facilitate testing and integration of scientific software releases across programming environments and hardware systems
  - Challenges to setup a CI Pipeline in HPC are mostly related to SSH connection
    - Access with valid credentials
    - Cloning source code repository in target machine's node
    - Keep alive the connection during pipeline execution
    - Providing constant output from commands
  - With the help of FirecREST users can
    - Use the same approach for different technologies (GitLab CI, GitHub Actions, Jenkins CI, etc)
    - Thanks to the abstraction layer, test the software for different architectures and software stacks
    - Solve authentication and connectivity issues

Use Cases

- Continuous Integration (CI) Pipelines
  - `ci/ci_script.py`

Importing pyFirecREST

FirecREST credentials from environment

Creating FirecREST object

System check and job submission

Printing job output

Job polling and result check

```python
# importing PyFirecREST
import firecrest as f7t

# Setup variables of the client
CLIENT_ID = os.environ.get("FIRECREST_CLIENT_ID")
CLIENT_SECRET = os.environ.get("FIRECREST_CLIENT_SECRET")
FIRECREST_URL = os.environ.get("FIRECREST_URL")
AUTH_TOKEN_URL = os.environ.get("AUTH_TOKEN_URL")

# Auth Object definition
idp = f7t.ClientCredentialsAuth(CLIENT_ID, CLIENT_SECRET, AUTH_TOKEN_URL)

# FirecREST client defintion
client = f7t.Firecrest(firecrest_url=FIRECREST_URL, authorization=idp)

# Check System Status via pyFirecREST
system_state = client.system(system_name)

if system_state["status"] == "available":
    # Submit job via pyFirecREST
    job = client.submit(system_name, "submission_script.sh")

    print(f"Submitted job: {job['jobid']}")

    print(f"\nSTDOUT in {job['job_file_out']}")
    stdout_content = client.head(system_name, job['job_file_out'], lines=100)
    print(stdout_content)

    print(f"\nSTDERR in {job['job_file_err']}")
    stderr_content = client.head(system_name, job['job_file_err'], lines=100)
    print(stderr_content)

    # Poll job status via pyFirecREST
    poll_result = client.poll(system_name, jobs=[job["jobid"]])
    if poll_result[0]["state"] != "COMPLETED":
        print(f"Job was not successful, status: {poll_result[0]['state']}")
        exit(1)

else:
    print("System {system_name} is not available")
    exit(1)
```

Use Cases

- Continuous Integration (CI) Pipelines
  - `.github/workflows/ci.yml`

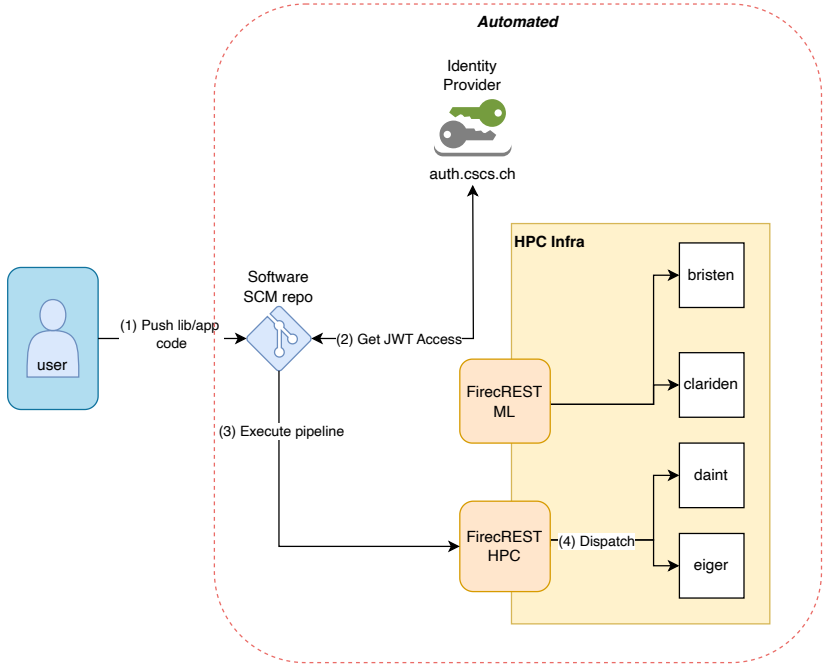
```yaml
name: CI
on:
  push:
    branches: [ "main" ]
  pull_request:
    branches: [ "main" ]

jobs:
  test_mycluster:
    runs-on: ubuntu-latest
    strategy:
      matrix:
        system_name: ["daint"]

    steps:
      - uses: actions/checkout@v3

      - name: setup python
        uses: actions/setup-python@v4
        with:
          python-version: '3.7'

      - name: install python packages
        run: |
          python -m pip install --upgrade pip
          pip install pyfirecrest==2.1.0

      - name: Run testing script
        env:
          FIRECREST_CLIENT_ID: ${{ secrets.F7T_CLIENT_ID }}
          FIRECREST_CLIENT_SECRET: ${{ secrets.F7T_CLIENT_SECRET }}
          FIRECREST_URL: ${{ secrets.F7T_URL }}
          AUTH_TOKEN_URL: ${{ secrets.F7T_TOKEN_URL }}
        run: ci/ci_script.py --system=${{ matrix.system_name }} --branch=${{ github.ref_name }}
                --repo=${{ github.server_url }}/${{ github.repository }}.git --account=ci_user
```

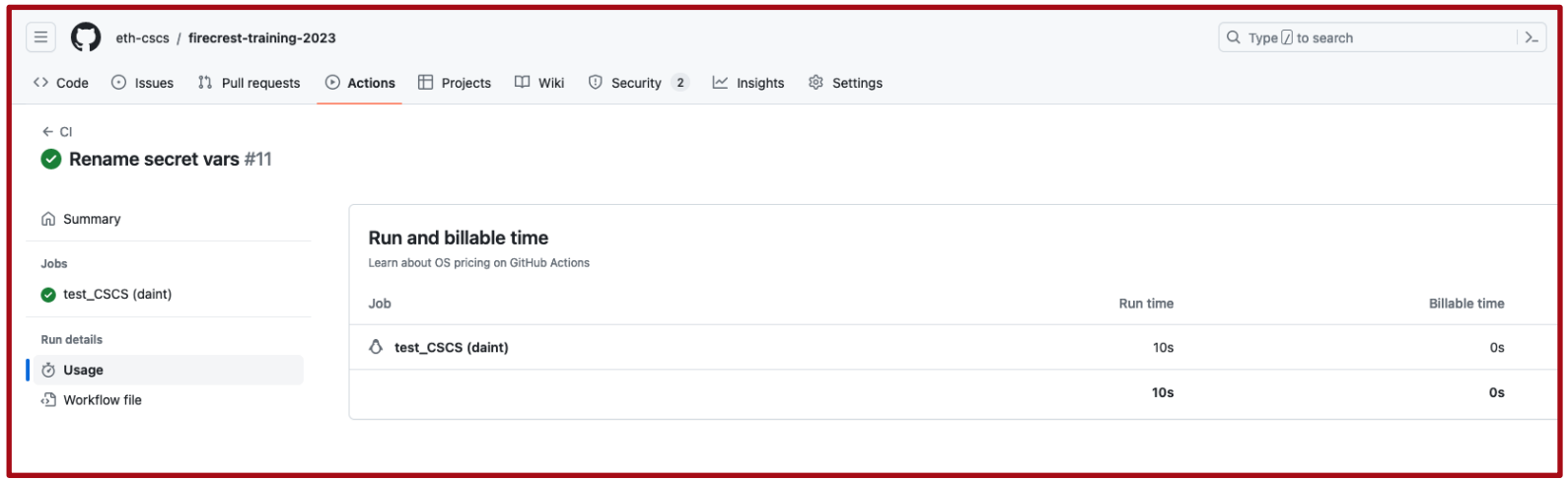
pyFirecREST installation

Environment setup

Use Cases

- Continuous Integration (CI) Pipelines





Use Cases

- Regression Testing
  - ReFrame is a framework for regression testing on HPC system
  - It allows periodic testing of scientific software ensuring performance and integrity
  - The pipeline of ReFrame for each test presents the following stages: (1) setup, (2) compile, (3) run, (4) sanity, (5) performance, and (6) cleanup
  - ReFrame needs to be installed and executed in the HPC system in which the software is being tested
  - With FirecREST it is possible to run a ReFrame test from a laptop or any public cloud provider, thus detaching the operation of the service from the HPC provider

Use Cases

- Regression Testing
  - ReFrame provides a Python class for schedulers. We can use pyFirecREST to adapt a `"firecrest-scheduler"` scheduler by extending the `SlurmJobScheduler` class

```python
from reframe.core.schedulers.slurm import SlurmJobScheduler
import firecrest as f7t

@register_scheduler('firecrest-scheduler')
class FirecrestJobScheduler(SlurmJobScheduler):

    def __init__(self, *args, **kwargs):
      (...)
      # Setup the FirecREST Client
      self.client = f7t.Firecrest(firecrest_url=firecrest_url,
                                  authorization=f7t.ClientCredentialsAuth(CLIENT_ID, CLIENT_SECRET, TOKEN_URL))

    def submit(self, job):
        # Job Submission
        submission_result = self.client.submit(self._system_name, os.path.join(job._remotedir, job.script_filename) )

    def poll(self, *jobs):
        # Update the status of the jobs
        poll_results = self.client.poll(
            self._system_name, [job.jobid for job in jobs]
        )

    def cancel(self, job):
        # Cancel a job
        self.client.cancel(job.system_name, job.jobid)
        job._is_cancelling = True
```

Use Cases

- Regression Testing
  - ReFrame requires of a configuration file, where the `"firecrest-scheduler"` among other settings, must be set

```
site_configuration = {
    'systems': [
        {
            'name': 'daint',
            'descr': 'Daint-Alps vCluster',
            'modules_system': 'lmod',
            'partitions': [
                {
                    'name': 'nvgpu',
                    'scheduler': 'firecrest-scheduler', ### <-- registered scheduler
                    'environs': [
                        'builtin',
                        'PrgEnv-cray',
                        'PrgEnv-gnu',
                        'PrgEnv-nvhpc',
                        'PrgEnv-nvidia'
                    ],
                },
                {
                    'name': 'amdgpu',
                    'scheduler': 'firecrest-scheduler', ### <-- registered scheduler
                    'time_limit': '10m',
                    'environs': [
                        'builtin',
                        'PrgEnv-cray',
                        'PrgEnv-gnu'
                    ],
                },
            ]
        },
    ],
    ...
}
```

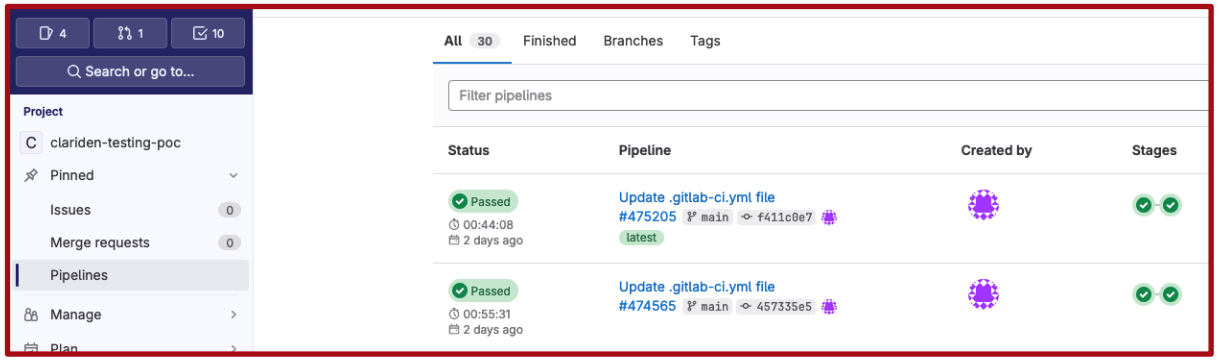
Use Cases

- Regression Testing
  - Finally, this is set on a CI Pipeline and it can be executed by a Runner from any server

```yaml
image: python:3.9
stages:
  - setup
  - run

clone_repos:
  stage: setup
  script:
    - git clone -b develop https://github.com/reframe-hpc/reframe.git       ## reframe suite
    - git clone -b alps https://github.com/eth-cscs/cscs-reframe-tests.git. ## test repository
  artifacts:
    paths:
      - reframe/
      - cscs-reframe-tests/
    expire_in: 5 days

bootstrap_and_run:
  image: python:3.12
  stage: run
  variables:
    FIRECREST_URL: "https://api.cscs.ch/hpc/firecrest/v1"  ## <-- configuring FirecREST-scheduler
    AUTH_TOKEN_URL: "https://auth.cscs.ch/auth/realms/firecrest-clients/protocol/openid-connect/token" ## IdP Token URI
    FIRECREST_SYSTEM: "mycluster" ## <-- HPC system to test
  script:
    - pip install pyfirecrest==2.2.1 ## <-- installing pyFirecREST
    - ./bin/reframe --version
    - ./bin/reframe -C ../cscs-reframe-tests/config/cscs.py -c ../cscs-reframe-tests/checks/ -r -Sbuild_locally=0 --
mode=production -vvv --max-retries=2
  artifacts:
    paths:
      - /builds/ci-user/reframe-firecrest-scheduler-test/reframe/reframe.log
     - ~/.reframe/reports/run-report-{sessionid}.json
```

Use Cases

- Regression Testing




```
518 [     FAIL ] (134/137) MemoryOverconsumptionMpiCheck /6a7583af @clariden:nvgpu+PrgEnv-gnu
519 P: cn_avail_memory_from_sysconf: 482 GB (r:0, l:None, u:None)
520 P: cn_max_allocated_memory: 472 GB (r:497, l:-0.05, u:None)
521 ==> test failed during 'performance': test staged in '/builds/ekoutsaniti/clariden-testing-poc/reframe/st
    age/2024-03-05_04-06-05/clariden/nvgpu/PrgEnv-gnu/MemoryOverconsumptionMpiCheck'
522 [     FAIL ] (135/137) MemoryOverconsumptionMpiCheck /6a7583af @clariden:nvgpu+PrgEnv-nvidia
523 P: cn_avail_memory_from_sysconf: 482 GB (r:0, l:None, u:None)
524 P: cn_max_allocated_memory: 471 GB (r:497, l:-0.05, u:None)
525 ==> test failed during 'performance': test staged in '/builds/ekoutsaniti/clariden-testing-poc/reframe/st
    age/2024-03-05_04-06-05/clariden/nvgpu/PrgEnv-nvidia/MemoryOverconsumptionMpiCheck'
526 [       OK ] (136/137) MemoryOverconsumptionMpiCheck /6a7583af @clariden:amdgpu+PrgEnv-cray
527 P: cn_avail_memory_from_sysconf: 457 GB (r:0, l:None, u:None)
528 P: cn_max_allocated_memory: 484 GB (r:497, l:-0.05, u:None)
529 [       OK ] (137/137) MemoryOverconsumptionMpiCheck /6a7583af @clariden:amdgpu+PrgEnv-gnu
530 P: cn_avail_memory_from_sysconf: 465 GB (r:0, l:None, u:None)
531 P: cn_max_allocated_memory: 484 GB (r:497, l:-0.05, u:None)
532 [----------] all spawned checks have finished
533 [==========] Retrying 1 failed check(s) (retry 1/2)
534 [----------] start processing checks
535 [ RUN      ] MemoryOverconsumptionMpiCheck /6a7583af @clariden:nvgpu+PrgEnv-gnu
536 [ RUN      ] MemoryOverconsumptionMpiCheck /6a7583af @clariden:nvgpu+PrgEnv-nvidia
537 [       OK ] (1/2) MemoryOverconsumptionMpiCheck /6a7583af @clariden:nvgpu+PrgEnv-gnu
538 P: cn_avail_memory_from_sysconf: 480 GB (r:0, l:None, u:None)
539 P: cn_max_allocated_memory: 473 GB (r:497, l:-0.05, u:None)
```

Use Cases

- Workflow Orchestrator
  - Apache AirFlow (AF) offers a framework for defining workflows, particularly in the Machine Learning (ML) domain
  - AF doesn’t provide a native HPC integration for WLM
  - The workaround on integration with HPC systems is to use custom commands for job submission and monitoring.
  - FirecREST can be integrated in AF using the Operator API
  - The integration with FirecREST allows writing Directed Acyclic Graphs (DAGs) that could include tasks that run on HPC facilities

Use Cases

- Workflow Orchestrator

```python
import firecrest as f7t
from airflow.models.baseoperator import BaseOperator
from airflow import AirflowException

# setting up the FirecREST Base Operator for AirFlow

class FirecRESTBaseOperator(BaseOperator):
    (...)
    #  FirecREST client object
    client = f7t.Firecrest(firecrest_url=firecrest_url,
                           authorization = f7t.ClientCredentialsAuth(CLIENT_ID, CLIENT_SECRET, TOKEN_URL))

class FirecRESTSubmitOperator(FirecRESTBaseOperator):
    """Airflow Operator to submit a job via FirecREST"""

    def __init__(self, system: str, script: str, **kwargs) -> None:
        super().__init__(**kwargs)
        self.system = system
        self.script = script

    def execute(self, context):
        (...)
        while True:
            if self.client.poll_active(self.system, [job['jobid']]) == []:
                break
            time.sleep(10)
        job_info = self.client.poll(self.system, [job['jobid']])
        if job_info[0]['state'] != 'COMPLETED':
            raise AirflowException(f"Job state: {job_info[0]['state']}")
        return job
```

Use Cases

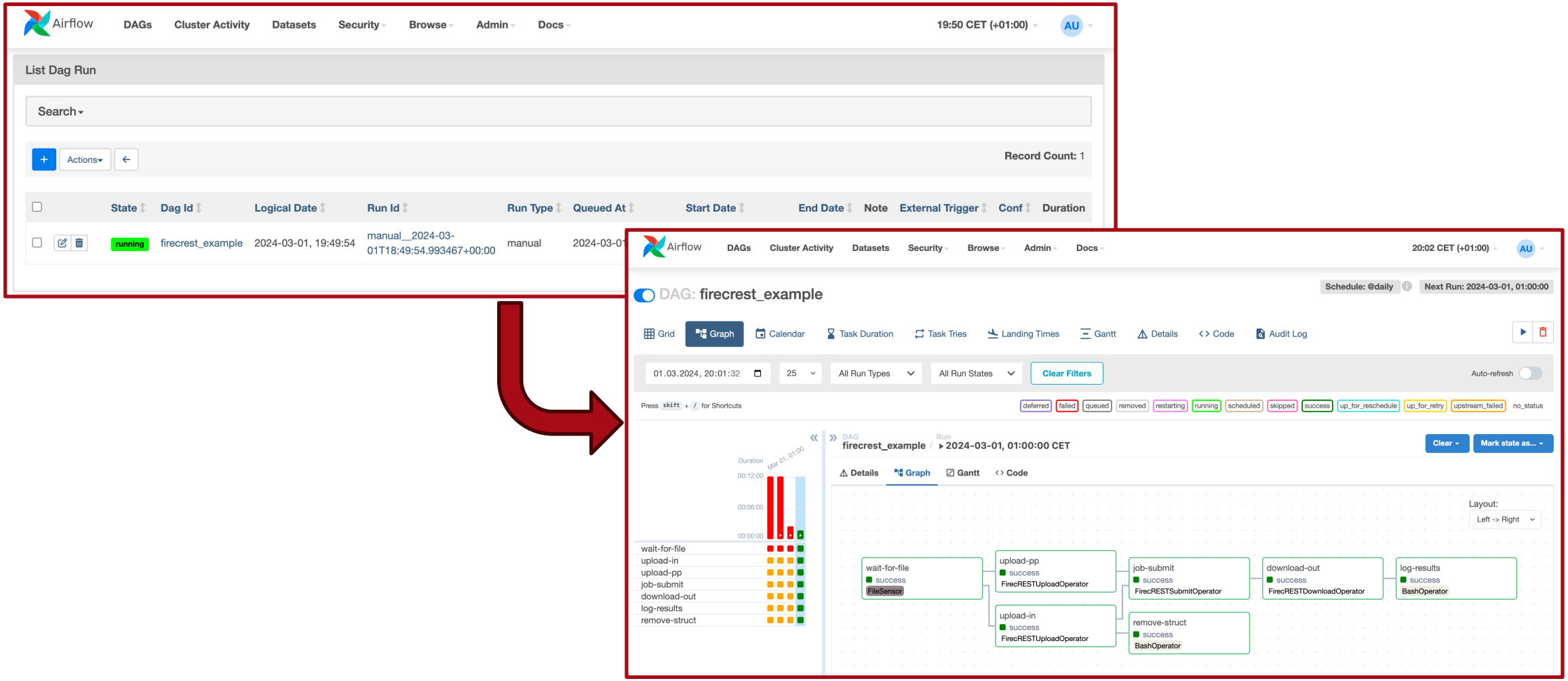
- Workflow Orchestrator
  - DAG example (`firecrest-airflow-dag.py`)

1. Detect that a new structure has been produced
2. Upload the structure and its pseudopotential to the HPC Cluster
3. Submit a job to the HPC Cluster to compute the properties
4. Download the output of the calculation
5. Log the relevant values
6. Delete the file with the structure

```python
from airflow import DAG

from airflow.operators.bash import BashOperator
from airflow.sensors.filesystem import FileSensor

from firecrest_airflow_operators import (FirecRESTSubmitOperator,
                                         FirecRESTUploadOperator,
                                         FirecRESTDownloadOperator)

with DAG( dag_id="firecrest_example", tags=["firecrest-executor"]) as dag:

    wait_for_file = FileSensor( task_id="wait-for-file", ... )

    upload_in = FirecRESTUploadOperator(task_id="upload-in", ... )

    upload_pp = FirecRESTUploadOperator(task_id="upload-pp", ... )

    submit_task = FirecRESTSubmitOperator(task_id="job-submit", ... )

    download_task = FirecRESTDownloadOperator(task_id="download-out", ... )

    log_results = BashOperator(task_id="log-results", ... )

    remove_struct = BashOperator(task_id="remove-struct", ... )
```

Use Cases

- Workflow Orchestrator



Use Cases

- Interactive Computing
  - JupyterHub (JH) it's a multi-user hub that enables launching Jupyter Notebooks from a web browser to compute nodes
  - JH is usually used for interactive computing for PoC of code, dataset exploration, and educational/training purposes
  - In HPC Clusters, JH is commonly paired with the `batchspawner` package to submit jobs to compute nodes.
  - The `batchspawner` configuration requires sysadmins to install and configure the WLM daemon in JH host and configure the key sharing between daemon and controller
  - This complicates the deployment of JH and restrict the systems that can operate with this tool

Use Cases

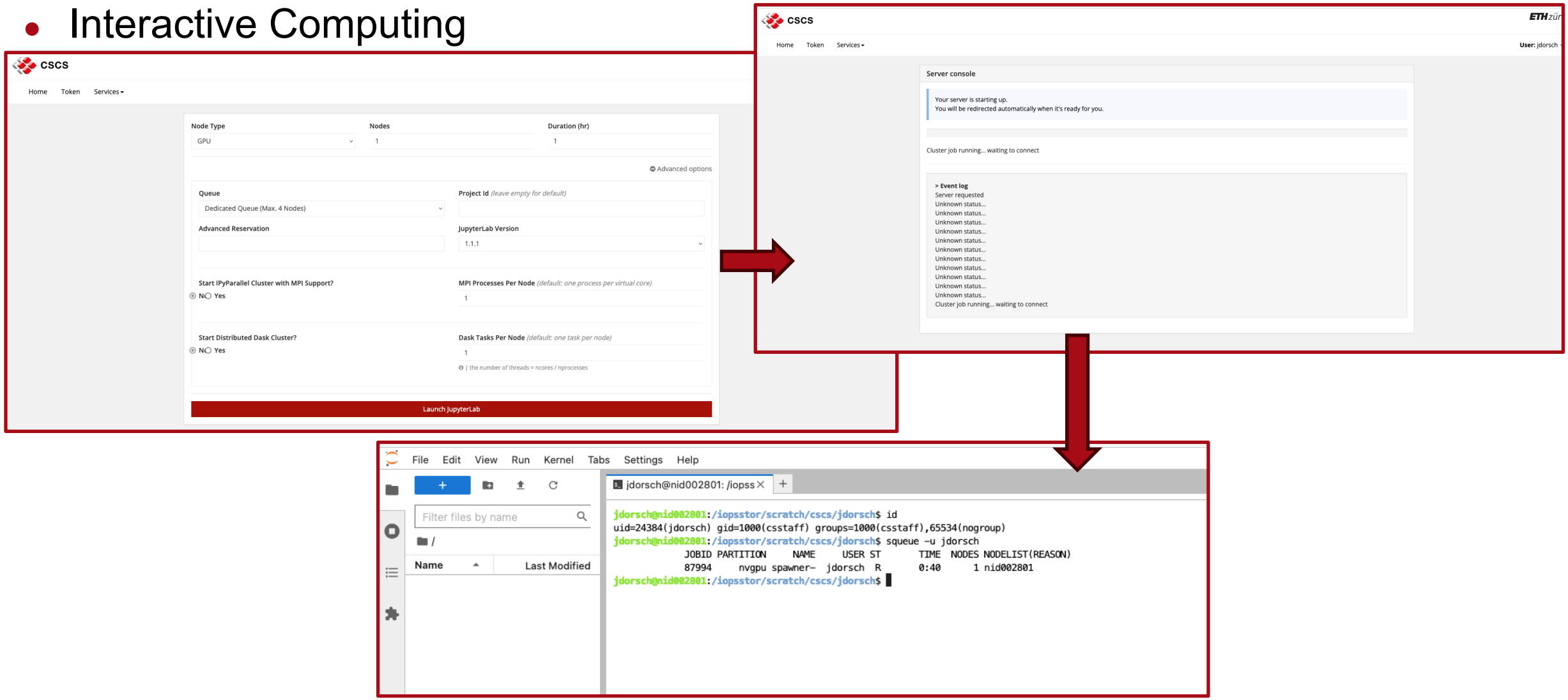
- Interactive Computing
  - With pyFirecREST, and taking advantage of the JupyterHub `Spawner` base class, a customized FirecREST Spawner (`FirecRESTSpawnerBase`) has been created and configured in a JupyterHub image

  - `Spawner` base class needs **`start()`**, **`poll()`**, and **`stop()`** methods to be implemented

```python
import firecrest as f7t
from jupyterhub.spawner import Spawner

class FirecRESTSpawnerBase(Spawner):
  # Start Jupyter notebook
  def start(self):
    self.job = client.submit(self.host, script_str=script)

  # Polling Jupyter notebook status
  def poll(self, jobid):
    self.job = client.poll(self.host,jobid)

  # Stop Jupyter notebook
  def stop(self, jobid):
    client.cancel(self.host, self.job_id)
```

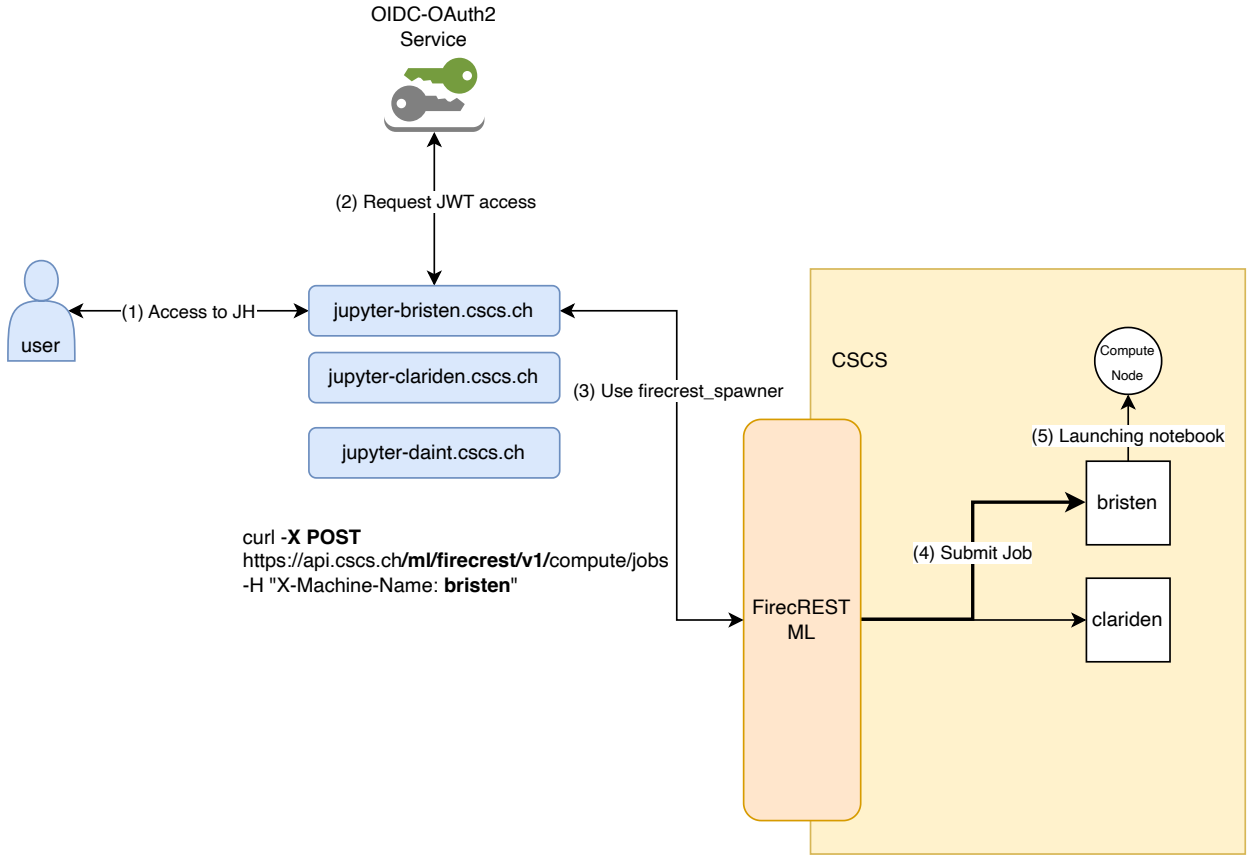
Use Cases

- Interactive Computing



Use Cases

- Interactive Computing
  - Reduces the requirements on the HPC infrastructure side in terms of administration, machine provisioning, networking, etc.
  - The “recipe” can be replicated for several HPC systems by changing the configuration to a different system
  - Integration with IAM allows the same OIDC client for JH and FirecREST



Use Cases

- Scientific Portals
  - Another example of the use of FirecREST is to create Graphical User Interface applications that allow users to interface filesystems, workload managers, and data transfer operations in a visual interface
  - At CSCS we've developed the FirecREST UI for the HPC Platform

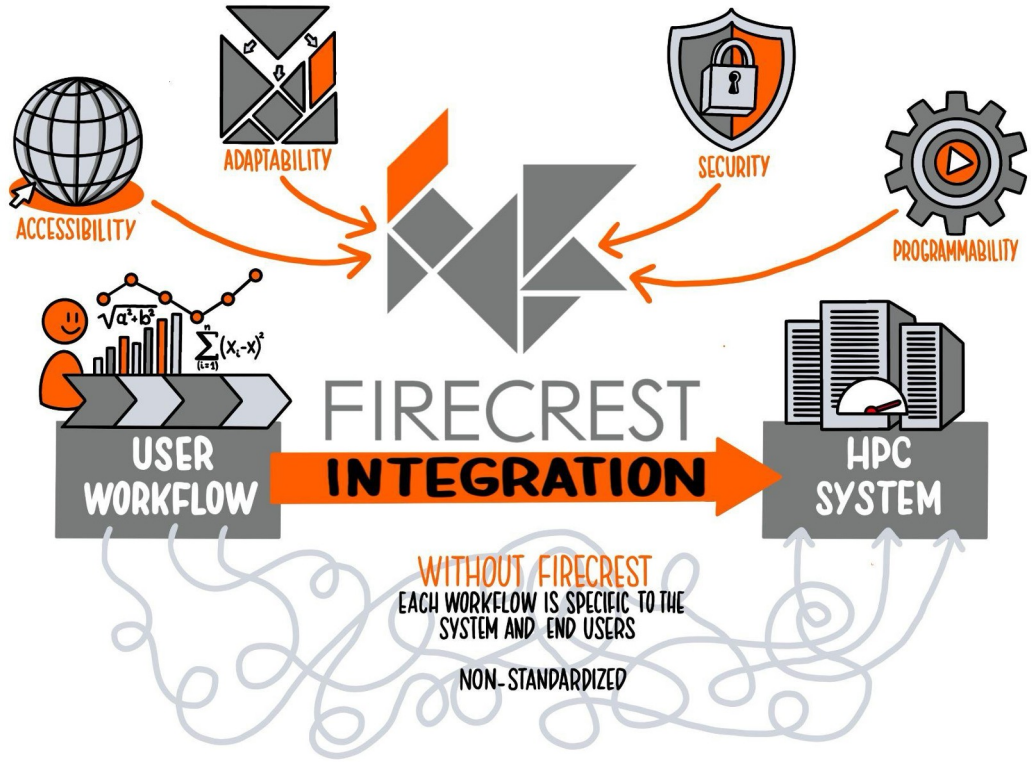
firecrest-ui-hpc.cscs.ch

Conclusions

Conclusions

- FirecREST provides a uniform and standard interface for workflows, which empowers you to create applications on the top of HPC

- Facilitates the integration of complex services for HPC, which allows scientific and academic communities to deploy their own services



Links and references

- More on FirecREST
  - API Reference: firecrest-api.cscs.ch
  - FirecREST product page at CSCS: products.cscs.ch/firecrest
  - FirecREST public repository: github.com/eth-cscs/firecrest
  - FirecREST Docs (use cases): firecrest.readthedocs.io
  - pyFirecREST and CLI Docs: pyfirecrest.readthedocs.io
  - Join our community on Slack: firecrest-community.slack.com
  - Contact us: firecrest@cscs.ch

This the team that will support you

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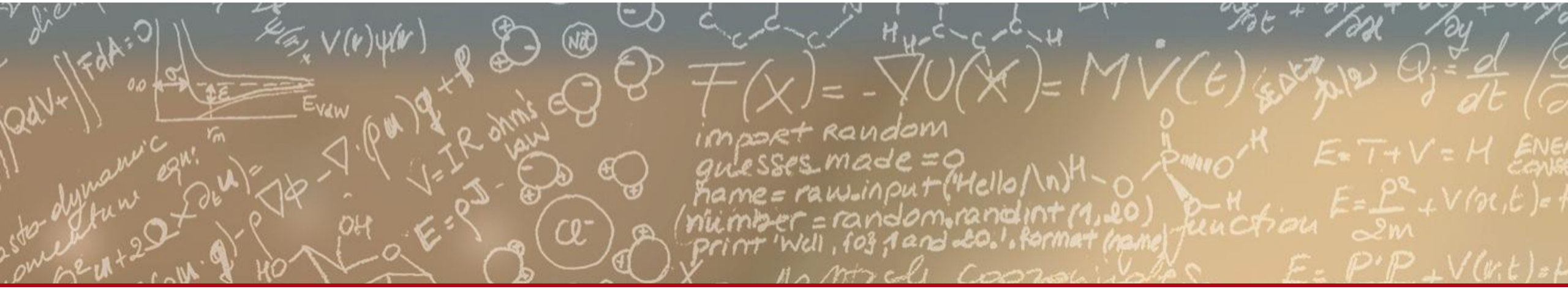

Thank you for your attention.