To technical/billing owners

- Manage accounts and quotas
- Billing, cost allocation and reports
- Integrate your own workflow with job automation APIs

Manage accounts and quotas

Account hierarchy

If you are on behalf of an institute or an enterprise, most likely, you will have a billing account. Then you may have consumer accounts to consume resources with jobs or sub-billing accounts to grant departments autonomy power.

Each sub-account has its team members, quota, alert settings, and scratch folder.

There are two types of members: regular members and coordinators. Coordinators will have almost the same power as you within that sub-account unless you don't want them to modify their quota.

You don't have to become a coordinator to change sub-account settings. Instead, you may get access by using the account "**Child accounts**."

When viewing usage and jobs on a billing account, the system will show you the status of the entire account hierarchy. Therefore, you don't need to enter a sub-account.

You may manage quotas of individual sub-account. Please see this article to understand how quotas work.

Follow this guide to check jobs that are submitted from your account hierarchy.

To manage team members of each sub-account, please follow this guide.

Billing, cost allocation and reports

You may download your monthly bill anytime under the "**Billing**" tab on your account page.

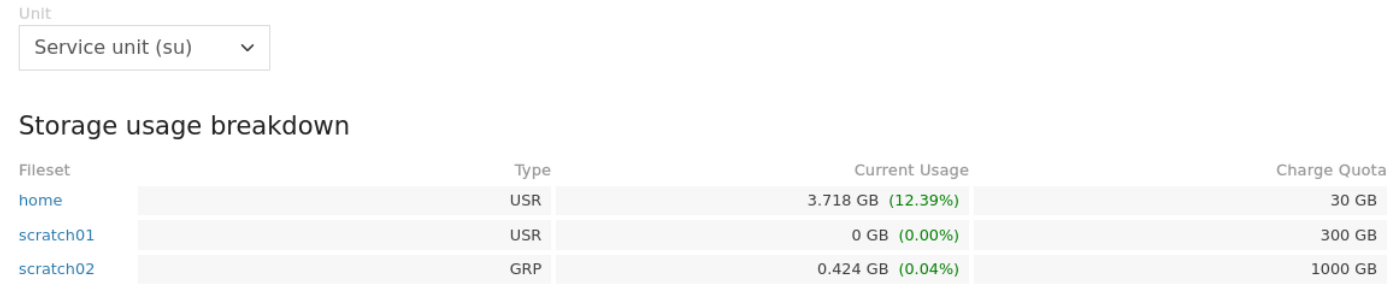
This article covers how OAsis HPC charges. There are three components, and we will discuss them one by one.

1. Monthly storage charge
2. Resource usage charge
3. Fixed additional charge

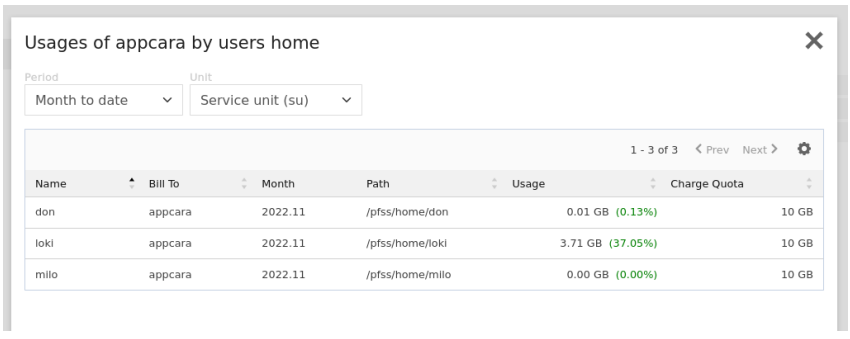
Storage

We charge storage every month by the maximum reserved space in gigabytes. All three types of file sets will be counted.

You may check the current reserved space and actual consumption anytime on the account page under "**Usage: Storage**".



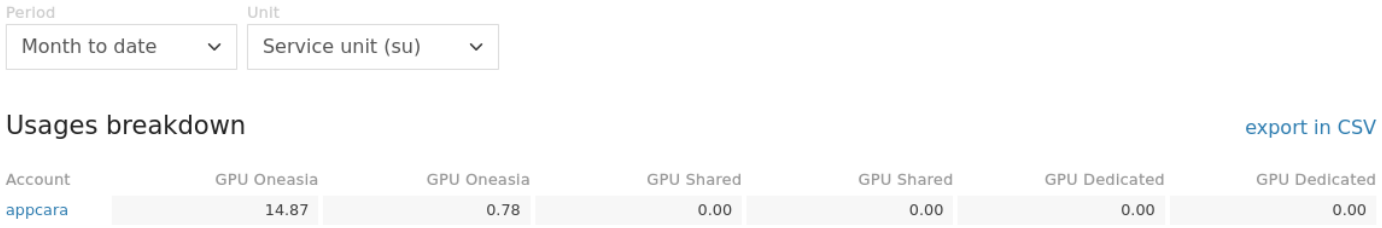
The above report aggregated status among your entire account hierarchy. You may click an individual file set to inspect the breakdown status on the following screen:



Depending on individual contracts, discounts, free-of-charge credit, and tiered pricing may apply.

Resource usage

Similar to the quotas mechanism we discussed, our resource charge consists of 6 meters. Go to the account page and click "**Usage: Job**"; you should see the following page displaying usages for each sub-account.



You may click an individual account name to break down users' usage further.

Besides using the web portal, you may also check the current usage with the CLI client. For example, to check output the above chart in the console in JSON format:

```
$ hc charges -a appcara -o
json                                                    15:39:58
# {
#  "account": "appcara",
#  "charges": {
#    "shared_csu": 0.0,
#    "oneasia_csu": 14.866667,
#    "oneasia_gsu": 0.7766,
#    "dedicated_csu": 0.0,
#    "shared_gsu": 0.0,
#    "dedicated_gsu": 0.0
#  },
#  "key_mapping": {
#    "oneasia_gsu": "GPU charge (Oneasia)",
#    "oneasia_csu": "CPU/Mem charge (Oneasia)",
#    "dedicated_gsu": "GPU charge (Dedicated)",
#    "dedicated_csu": "CPU/Mem charge (Dedicated)",
#    "shared_csu": "CPU/Mem charge (Shared)",
#    "shared_gsu": "GPU charge (Shared)"
#  }
# }
```

Depending on individual contracts, discounts, free-of-charge credit, and tiered pricing may apply.

Additional charge

Depending on individual contracts, additional charges may appear on your bill. It can be a proportional discount or a fixed amount for support and maintenance.

Integrate your own workflow with job automation APIs

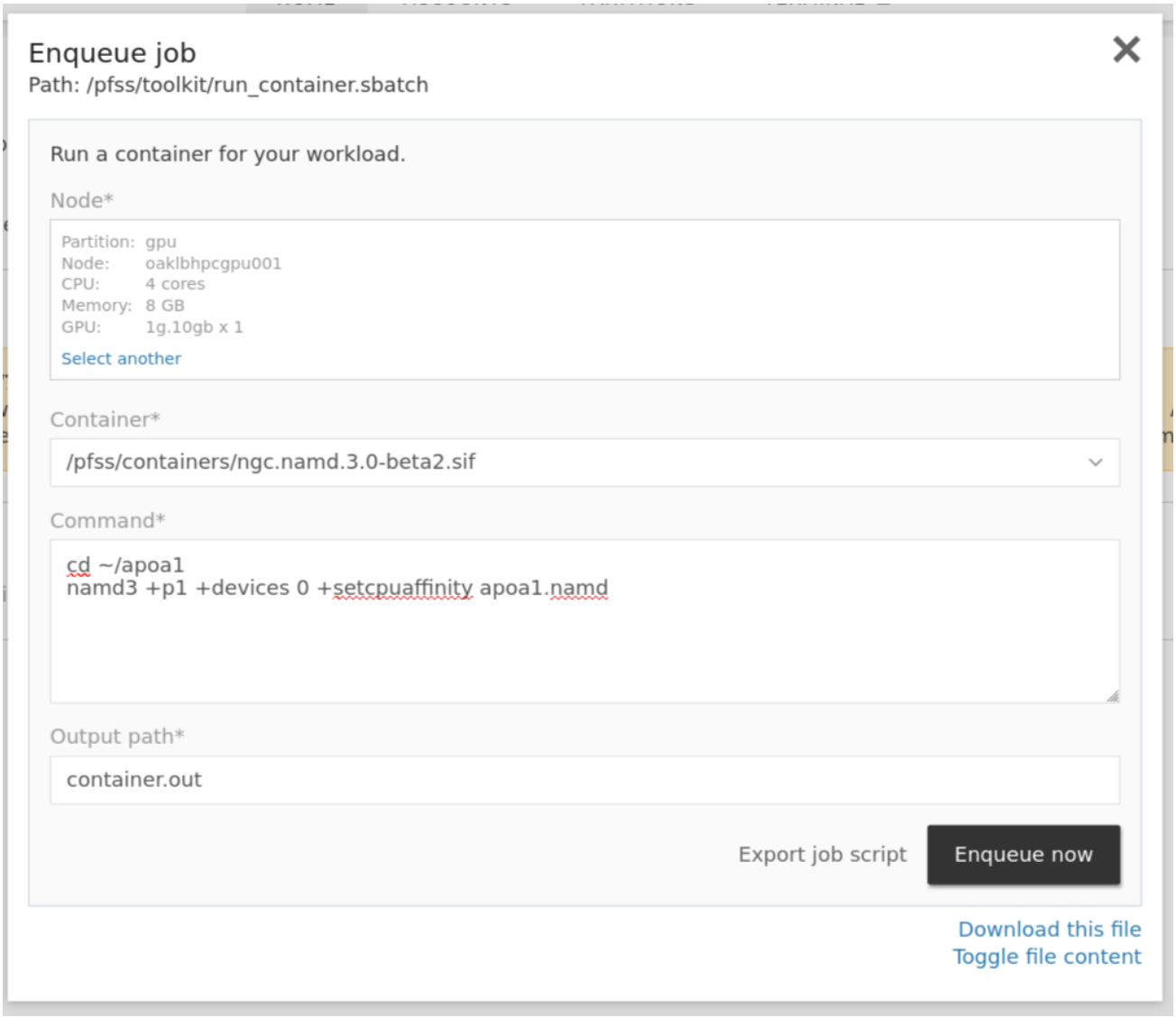
OAsis offers job automation APIs that allow you to enqueue and inspect jobs easily. This means you can seamlessly integrate HPC into your workflow engine as a component. For example, you can use it to finetune machine learning models with new data or set up simulation jobs using your own tooling.

This article will use the Molecular Dynamics Simulation case as an example, but the concept should generally apply to all types of workloads.

For the simulation of the ApoA1 protein in a water box and the study of energy changes, we will be using NAMD. NAMD is available in various distributions, with OAsis offering it as both the Lmod system and the container version packaged by NVIDIA NGC. We will use the container version in this article.

Run the simulation using quick job

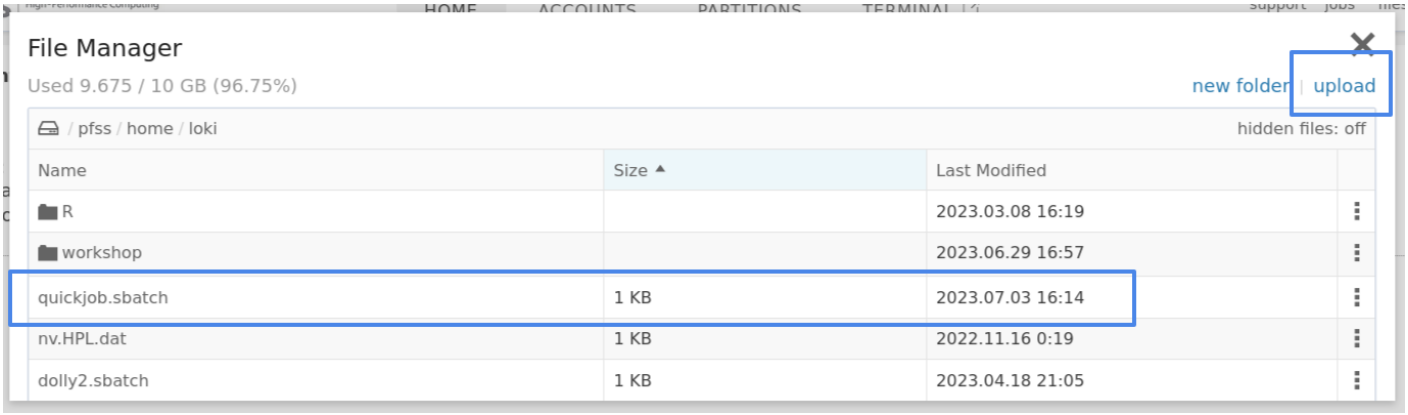
We can run container-based jobs easily in the web portal. Access Jobs > Run container and fill in the following:



Enqueue the job, and you should see the job output (log file) on the following screen:

Please wait until the job is completed. Once that's done, repeat step 1, but click on the "Export job script" button this time. This will allow you to download a **quickjob.sbatch** file. This file is a standard SLURM job script that can be enqueued using the **sbatch** command.

Upload it back to the cluster via the file browser to finish the setup.



Run the job programmatically using the hc CLI client

> Ensure you are using the latest hc client before proceeding. This article is tested with hc version 0.0.196.

We are going to use two APIs: **enqueue-job** and **job-status**. You may inspect their usage using the **--help** argument.

```
> hc enqueue-job --help
hc-enqueue-job
Enqueue a job

USAGE:
    hc enqueue-job [OPTIONS] --path <PATH>

OPTIONS:
    -h, --help
            Print help information

    -o, --output-format <OUTPUT_FORMAT>
            set output format

    -p, --path <PATH>
            File path in the cluster. e.g., /pfss/toolkit/mpitest.sbatch
> hc job-status --help
hc-job-status
Show specific job status

USAGE:
    hc job-status [OPTIONS] --job-id <JOB_ID>

OPTIONS:
    -h, --help
            Print help information

    -j, --job-id <JOB_ID>
            ID of the job

    -o, --output-format <OUTPUT_FORMAT>
            set output format
```

Let's use the two sub-commands to enqueue a new job and then inspect it's status.

```
$ hc enqueue-job --path=/pfss/home/loki/quickjob.sbatch
Submitted batch job 164337

$ hc job-status -j 164337
JobState:completed
```

Run the job programmatically using Python

Below is a Python sample code demonstrating how to call the OAsis RESTful API, specifically the "me", "enqueue-job", and "job-status" API functions.

```
import requests
import time
import hashlib
import hmac
import json

# hide InsecureRequestWarning message, you may delete these two lines
import urllib3
urllib3.disable_warnings(urllib3.exceptions.InsecureRequestWarning)

api_key = "<API-KEY>" # replace your api key
api_key_secret = "<API-KEY-SECRET>" # replace your api key secret
baseUrl = "https://hpccenter.hk"

def getSignature(api_key_secret, path, ts):
    mac = hmac.new(api_key_secret.encode(), digestmod=hashlib.sha256)
    mac.update(f"{path}|{ts}".encode())
    return mac.hexdigest()

def getHeaders(api_key, api_key_secret, path):
    ts = int(time.time())
    headers = {
        "req-at": str(ts),
        "req-api-key": api_key,
        "req-signature": getSignature(api_key_secret, path, ts),
    }
    return headers

def getResult(baseUrl, path, method = "get", payload={}):
```

```
    url = baseUrl + path
    if method == "get":
        response = requests.get(url, headers=getHeaders(api_key, api_key_secret, path), verify=False)
    else:
        response = requests.post(url, json=payload, headers=getHeaders(api_key, api_key_secret, path),
verify=False)

    if response.status_code == requests.codes.ok:
        return response.json()
    else:
        print("Error:", response.status_code, response.text)
        raise Exception("api call error")

# get login user information
path = "/api/me"
result = getResult(baseUrl, path)
print(result)

# get job status
jobId = "<JOB-ID>" # replace your job id
path = "/api/job-status?job-id=" + str(jobId)
result = getResult(baseUrl, path)
print(result)

# enqueue job
jobFilePath = "<JOB-FILE-PATH>" # replace your job file location, e.g.
/pfss/home/<USERNAME>/<FILENAME>.sbatch
payload = {
    "path": jobFilePath
}
path = "/api/enqueue-job"
result = getResult(baseUrl, path, "post", payload)
print(result)
```

Make sure to replace `"<API-KEY>","<API-KEY-SECRET>"` with your actual API key obtained from the OAsis platform. Also replace `"<JOB-ID>","<JOB-FILE-PATH>"` with the actual data.

This code covers the basic functionality of retrieving user information, enqueueing a job with specified parameters, and checking the status of a job using the RESTful API endpoints provided by OAsis.