UCIS4EQ installation + execution

-= A users' primer and hands-on quickstart tutorial =-

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List of abbreviations

API: Application Programming Interface
AWP: Anelastic Wave Propagation (open-source numerical engine)
DC: Docker container
EQ: Earthquake
ETHZ: Eidgenössischer Technische Hochschule in Zürich
HPC: High Performance Computing
IO, i/o: Input & Output
MN4/5: Marenostrum 4 / 5
PSHA: Probabilistic Seismic Hazard Analysis
Repo: Repository
RTE: Runtime Execution
RW: Read & Write
UCIS4EQ: Urgent Computing Integrated Services for EarthQuakes

1. Objectives of this document

This document was written with those intent upon learning how to install and run UCIS4EQ in mind.

First objective: to get you started quickly

This tiny tutorial is meant to get you (the unwary and still happy users) started fast. It will also explain (however rudimentarily) where some of the important moving parts of UCIS4EQ are located and roughly what they do. When putting this document together, I thought that the best way to keep computationally challenged or, if you prefer, non-HPC-oriented users happy might be to help them start executing UCIS4EQ fast so that results could be forthcoming without undue delay.

Second objective: to provide you with some background

Simultaneously the emphasis was also to prevent you (the now wary but still happy users) from either getting lost or becoming stranded at low tide while handling UCIS4EQ. Here "lost" mean uncomprehending when staring at error messages, whereas "low tide" is for instance when you are still launching that really important job at 20:54 on a Friday, everybody has left and you experience an issue. For that reason this tutorial will sometimes include small didactic notes, that the regular user can easily ignore. They are only meant to give new-comers some background and in the end impart them with a sense of what is happening.

Third objective: to collect options/perspectives to improve the user-friendliness and usability of the UCIS4EQ workflow.

This is a longer term goal and consists in improving and/or extending UCIS4EQ to the point that it becomes a turn-key package accessible to seismologists and others, whose main aspiration is to get their work done, not to read dry technical tutorials.

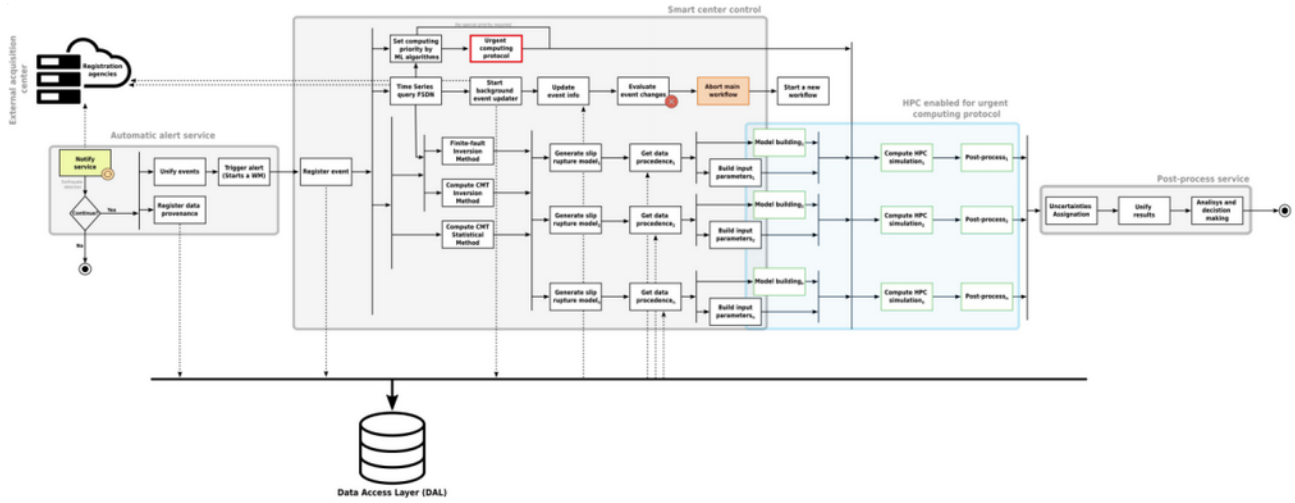
As it stands this tutorial should be considered work-in-progress. For that reason suggestions and critiques, isolated or by drove, are highly welcome and should be sent to the current document's maintainer.

2. UCIS4EQ: a high level view

UCIS4EQ is a workflow for the deterministic modelling of seismic waves in an urgent computing context. It consists of containerized microservices written in Python. One of those microservices is a wrapper that launches **Salvus**, a high-performance solver edited by Mondaic AG, on BSC's compute/storage infrastructure MN4/5. A high level view (shown below) was presented by Marta Pienkoska as early as 2021[1].

TODO

1 M. Pienkowska, J. E. Rodríguez, J. de la Puente, and A. Fichtner, “Deterministic modelling of seismic waves in the Urgent Computing context: progress towards a short-term assessment of seismic hazard,” presented at the EGU21, Harvard, Mar. 03, 2021. doi: 10.5194/egusphere-egu21-15516.



3. Key individuals

3.1- Author(s) of the code

Juan Esteban Rodríguez <jrodriguez@frontwave.io>, FrontWave imaging, SL (ex CASE Dept, BSC)

- The UCIS4EQ code was developped at BSC as part of the ChEESE project, funded from the European Union's Horizon 2020 research and innovation program, under the Grant Agreeme'nt No 823844.

3.2- Contributor(s) to the code

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Sergio Mendoza <sergio.mendoza@bsc.es>, BSC
Josep de la Puente <josep.delapuente@bsc.es>, BSC

- The UCIS4EQ code and Docker image registry are currently located at https://gitlab.bsc.es/wavephenomenagroup/ucis4eq.

3.4- Advanced user(s)

Marisol Monterrubio <marisol.monterrubio@bsc.es>, BSC
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4. Licenses

5. Solvers

5.1- Salvus

Salvus is a high-performance solver for spectral-element wave propagation (forward compute), full waveform modeling and inversion (backward compute). Salvus is published by Mondaic. Its executable binary is currently located (in MN4) at:

`/gpfs/projects/bsc44/earthquake/UCIS4EQ/Salvus/bin/salvus`

Salvus covers meshing, model building, data management and full waveform inversions in a scalable manner, taking advantage of NVIDIA GPU support using CUDA. It runs on ARM and POWER PC architectures as well as on CPU based on the x86-64 instruction set.

Marenostrum 4 (MN4) users can run Salvus in two ways:

- as part of a microservice with deported execution, e.g. as part of the UCIS4EQ workflow,
- as a standalone binary.

To execute the stand-alone binary of Salvus, the Marenostrum user places the job in a queue, using Slurm, the BSC queue manager used for batch processing:

```
> sbatch /gpfs/projects/bsc44/earthquake/UCIS4EQ/runs/.../<my_job>.slurm
```

The `<my_job>.slurm` executable is a custom file with a specific structure and syntax:

```
> cat /gpfs/projects/bsc44/earthquake/UCIS4EQ/runs/.../<my_job>.slurm
#!/bin/bash
#SBATCH --jobname=<my_jobname>
#SBATCH --time=12:00:00
#SBATCH --nodes=50
#SBATCH --tasks-per-node=48
#SBATCH --ntasks=2400
#SBATCH --error=<my_jobname_SalvusRun.e>
#SBATCH --output=<my_jobname_SalvusRun.o>
#SBATCH --qos=<my_picked_queue>
#SBATCH --mail-type=start|end|all|none
#SBATCH --mail-user=<my_email_address>

cd $SLURM_SUBMIT_DIR
module load fabric
export I_MPI_EXTRA_FILESYSTEM_LIST=gpfs
export I_MPI_EXTRA_FILESYSTEM=on

/usr/bin/srun --overlap --ntasks=$SLURM_NTASKS --ntasks-pernode=\
$SLURM_NTASKS_PER_NODE /gpfs/projects/bsc44/earthquake/UCIS4EQ/Salvus/bin/salvus \
compute /gpfs/projects/bsc44/earthquake/UCIS4EQ/runs/.../salvus_wrapper/\
salvus_input_rupture.toml
```

where:
`/gpfs/projects/bsc44/earthquake/UCIS4EQ/runs/.../salvus_wrapper/salvus_input_rupture.toml` is a required `toml` file. It describes a specific event's compute grid geometry, domain meshing, rupture model and as well as the ground velocities along Z (vertical), N and E (horizontal plane), at each recording station location.

The `toml` file is obtained based on the contents of `/gpfs/projects/bsc44/earthquake/UCIS4EQ/runs/[…]/salvus_wrapper/salvus_input.yaml` which contains descriptive parameters for:

- the seismic event of interest,

- the receiving stations' locations,
- the precomputed mesh's file paths if the mesh is not computed on the fly

The mesh, whether pre-computed or computed on-the-fly, depends on the wave's highest resolved frequency of interest. Accordingly Salvus's treatment of frequency largely governs mesh and memory requiremens at time of execution. "*The highest resolvable frequency - or the shortest period, respectively - is the main external driver governing the mesh generation. It influences the wavelengths of the wavefield (or "polynomial_degree"), the effective medium which results in a homogenized model, as well as the resolution of topography and bathymetry which yield the effective domain. The computational costs are proportional to the number of elements and the number of time steps.*" (cit. Mondaic's documentation pages). Resolving higher frequencies will obviously increase the overall computational cost users will incur.

- the bathymetry and topography (if applicable),
- the kinematic rupture model's Standard Rupture Format (`*.srf`) file's fully qualified path.

In the latter `*.srf` file, the general fault surface is represented by a distribution of point sources (subfaults). Each sub-fault's point-source description contains the kinematic (displacement) information necessary to compute the contribution of that subfault to the total response to the fault rupture.

5.2- AWP

The Anelastic Wave Propagation (AWP) numerical engine is an open-source solver based on finite differences. It powers the CyberShake HPC workflow with planar topography (squashed mesh model), and was developed to perform PSHA studies for Southern California by SCEC (the Southern California Earthquake Center). It is instrumental in providing Physics-Based Probabilistic Seismic Hazard Analysis (PB-PSHA) by computing a large set of earthquake synthetic ground-motion time histories from kinematic rupture scenarios on 3D finite faults.

...Versión CPU (versión de Juane) corre en Power9
Versión CPU (versión de Edu) corre en MN4

With non-planar topography on GPU (Power9) -- TODO

6. Installing UCIS4EQ

- Install the following resources on your host:

- `docker` (Community Edition), `docker-compose`
  If you are unfamiliar with that technology, follow this tutorial to get started. Supplement it with those official docs if necessary.

- `git`
  If you are unfamiliar with that technology, and its GitHub or GitLab incarnation, follow this tutorial to get started.

- Secure at least read-access permissions to the current repo https://gitlab.bsc.es/wavephenomenagroup/ucis4eq/

- Pick `<basedir>` as your working directory on your local host's filesystem to clone the above git repository. This will bring the complete code suite onto your local host.

```
> cd <basedir>
> git clone https://gitlab.bsc.es/wavephenomenagroup/ucis4eq.git
```

- To run UCIS4EQ on your host while running Salvus on MN4 successfully, a number of preliminary steps are necessary. Those steps are described in the following sections.

6.1- Secure an account on Marenostrum

That should include zero-login access to the supercomputing resources:

- Marenostrum (x86_64 CPU CPU cluster),
- Minotauro (Bull CUDA cluster),
- `/gpfs/` (MN4 distributed storage system).

Create your SSH asymmetric key pair (e.g. 4096 bit RSA) to access the four nodes `{dt01,mn1,mn2,mn3}.bsc.es`. This key should include a passphrase for security.

```
> cd ~/.ssh
> ssh-keygen -t rsa -b 4096 -C "<your_bsc_email>" -f ~/.ssh/bsc_id_rsa \
      -P "<your_passphrase>"
> chmod go-r ~/.ssh/bsc_id_rsa.pub
> ssh-copy-id <your_hpc_username>@dt01.bsc.es
```

By default ssh-copy-id should add the last created public key to your remote hosts `~/.ssh/authorized_keys` file. If successful you should now be able to log in onto any of the above four MN4 nodes without the need to provide a password. Try it for instance with:

```
> ssh -l <your_hpc_username> dt01.bsc.es
> cat ~/.ssh/authorized_keys
```

6.2- Set up your HPC user to run Salvus and to access events' static data

Salvus requires a quick access to event-related static data to avoid solver execution delays induced by lengthy data transfer to compute nodes. For this reason the weightier part of that data needs to be stored where accessing it will not incur delays, i.e. on the dedicated MN4 file system `/gpfs/projects/bsc44/...`.

To meet those requirements, the HPC user should be a member of the `bsc44` Unix group on MN4, with the following permissions:

```
/gpfs/projects/bsc44       drwxrws---
```

The above is enough to give you access to the Salvus binary and to the bulk of static data needed to run the solver for specific faults and fault geometries related to events. There are additional static data access requirements as detailed in the following sub-section .

6.3- Gain access to https://b2drop.bsc.es

That should include in particular the B2DROP folder `UCIS4EQ/` owned by Marisol Monterrubio <marisol.monterrubio@bsc.es>, which contains:

- `UCIS4EQ/Data/Events/SlipDistributions/`
- `UCIS4EQ/Data/Regions/`
- `UCIS4EQ/Setup/AAS/config_{stations,events,dataselect}.json`
- `UCIS4EQ/Setup/DALv2/`
- `UCIS4EQ/Setup/SCC/indexPriority/PGA_database` **** in disuse**
- `UCIS4EQ/Runs/`

To secure access to `b2drop.bsc.es`, send an email from BSC to <datamanagement@bsc.es> with your request. After receiving a username and setting up your credentials, ask any known user of directory UCIS4EQ to share its contents with you.

At time of writing, users of the UCIS4EQ folder are: Claudia Abril, Cedric Bhihe, Eduardo Cabrera, Jorge Ejarque, Sergio Mendoza, Marisol Monterrubio, Nihad Mammadli, Natalia Zamora at BSC, and Marta Pienkowska at ETH.

The contents of directory UCIS4EQ en `https://b2drop.bsc.es` include static data needed to specify events to be submitted to Salvus for execution. The UCIS4EQ filetree, i.e. the organization of its contents in a tree made of

sub-folders and individual files, must correspond to the output of:

```
> cd <basedir>
> find . -type f -exec grep -A2 -i B2DROP {} \;
```

- At time of writing an exception to the previous comment is the `UCIS4EQ/Setup/SCC/indexPriority/` path pattern currently in disuse. Paths identifying with that pattern and referenced in the code can be disregarded.

6.4- Create the following path

The solver, Salvus, persists some of its output files. For that reason you need to create:

```
/gpfs/scratch/<your_hpc_group>/<your_hpc_username>/Eflows4hpc/Ucis4eq/
```

in MN4's GPFS scratch storage volume.

6.5- Modify setup files in `<basedir>/data/`

File: **DAL.json**

```
{
  "BSC_B2DROP": {
    "user": "<your_b2drop_username>",
    "pass": "<your_b2drop_passwd>",
    "url": "https://b2drop.bsc.es/remote.php/webdav/",
    "datamapping": "UCIS4EQ/StaticDataMappingV2.json",
    "output": "UCIS4EQ/Runs"
  },
  "local": {
    "path": "/workspace/"
  },

  "BSC_DT":{
    "user": "<your_hpc_username>",
    "url": "dt01.bsc.es",
    "path": "/gpfs/scratch/<your_hpc_group>/<your_hpc_username>/Eflows4hpc/Ucis4eq"
  }
}
```

File: **Sites.json**

```
{
  "MN4": {
    "user": "<your_hpc_username>",
    "url": "mn1.bsc.es",
    "path": "/gpfs/scratch/<your_hpc_group>/<your_hpc_username>/Eflows4hpc/Ucis4eq/",
    "resources": {
      ....
```

- The rest of the `Sites.json` file requires modification to conform to the resources you can commandeer on the computing infrastructure. Your resource privileges are partially controlled by Slurm, and can be visualized with:

```
> ssh -l <your_hpc_username> dt01.bsc.es
> bsc_queues
QUEUE NAME          MAX TIME     MAX PROC
bsc_case            2-00:00:00   2400       <- maximum duration: 48h, and 50 nodes
```

```
debug               02:00:00     768        <- maximum duration: 2h, and 16 nodes
interactive         02:00:00     4          <- maximum duration: 2h, and 2 nodes
```

In debugging mode or when beginning as a UCIS4EQ user, choosing "debug" will afford you maximum run-times of 7200s and a maximum of 16 nodes for 768 processes. You can modify the rest of the `Sites.json` file accorrdingly, leaving "`1`" for the number of nodes to be used whenever the associated task is sequential (not parallelized).

6.6- Create a second SSH asymmetric 4096 bit RSA key pair w/ a blank passphrase on your local host

```
> cd ~/.ssh
> ssh-keygen -t rsa -b 4096 -C <your_bsc_email> -f ~/.ssh/docker_mn_id_rsa -P ""
> chmod go-r ~/.ssh/docker_mn_id_rsa.pub
> ssh-copy-id <your_hpc_username>@dt01.bsc.es
```

The last command will actually copy your public key to the remote user's `~/.ssh/authorized_keys` (creating the file, and directory, if necessary).

This second key pair is needed for the local containers executing microservices locally to execute and monitor Salvus on MN4. The key pair's private key is embedded in secondary Docker images built from the primary Ubuntu 20.4 Docker image used by UCIS4EQ. In a second step, as `docker-compose` prepares to launch services, docker containers are built and run from the secondary images.

7. Running UCIS4EQ

7.1- Create your runtime execution (RTE) landscape

Simply issue:

```
> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" LOCATION="<location>" \
      PD_USER="<username>" docker-compose up
```

or its simplified version:

```
> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" docker-compose up
```

The command above leaves two RTE variables LOCATION and PD_USER undefined.

- the former specifies the cluster on which Salvus is run.
- the latter is required to launch Salvus on the ETH cluster named "Piz Daint".

When not executing on the Piz Daint cluster ignore those two variables, provided you also edit the file <basedir>`/Ucis4eq/deployment/dockers/Dockerfile-credentials`, commenting out the following line:

```
#RUN ssh $PD_USER@ela.cscs.ch ssh-keyscan daint.cscs.ch >>
/root/.ssh/known_hosts;\ exit 0
```

When run the code creates a Docker network (*`Network ucis4eq_default`*) and launches 7 Docker containers (DCs) as decribed in Table 1 below. Those constitutes your RTE landscape, where runtime and execution(s) are asynchronous.

	Containers	Images at registry.gitlab.bsc.es/wavephenomenagroup/ucis4eq/	Services	Deployment
1	ucis4eq-DAL-1	mongo:4.2	DAL	Auto
2	ucis4eq-workflowmanager-1	workflowmanager	workflowmanager	Auto/Manual
3	ucis4eq-dashboard-1	dashboard	dashboard	Auto/Manual
4	ucis4eq-salvus-1	salvus	salvus	Auto/Manual
5	ucis4eq-microservices-1	microservices	microservices	Auto/Manual
6	ucis4eq-slipgen-1	slipgen	slipgen	Auto/Manual
7	ucis4eq-listener-1	listener	listener	Auto/Manual

***Table 1**:From their respective images, respectively containers and services can be run and deployed automatically (Auto) and/or manually (Manual).*

Irrespectively of whether services are launched automatically or manually, as soon as all them are deployed you will need to feed your idling services data for them to run an actual job. This is done in two ways (with and without a listener service) as described in the next section (Section 7.2).

7.2- Create a job ID and feed a seismic event to UCIS4EQ

7.2.1 Active "*listener*" service

When the "*listener*" service is active, UCIS4EQ sends periodic pull request every 60s to one or more of the major seismological agencies and FDSN data centers online, e.g.:

"IRIS": "http://service.iris.edu/fdsnws/"
"INGV": "http://webservices.ingv.it/fdsnws/"
"IMO": "http://www.orfeus-eu.org/fdsnws/"
"GEOFON": "https://geofon.gfz-potsdam.de/fdsnws/"
"SCEDC": "http://service.scedc.caltech.edu/fdsnws/"
"NCEDC": "http://service.ncedc.org/fdsnws/"
"NOA": "http://eida.gein.noa.gr/fdsnws/"
etc...

The "*Listener*" service pulls new events, whose specifications format complies with the FDSN RESTful web service characteristics. Those selected for urgent computing following specific criteria (including Moment magnitude, etc.) are automatically included in the UCIS4EQ computing workflow.

7.2.2 Inactive "*listener*" service

When the "*listener*" microservice is not used:
- compute jobs are not automatically meted a unique job id (UUID),
- seismic events are not automatically pulled from various seismological agencies across the world and fed to the UCIS4EQ flowmanager.

In that latter case, UCIS4EQ users need first to specify a job ID value for the key "`uuid`", in a specific JSON file. This can be done manually with any text editor, or via CLI like so:

```
> jq '.uuid = "<new_job_id>"' <my_data.json> >| <my_data.json>
```

Followed by:

```
> curl -X POST -H 'Content-Type: application/json' -d \
      @<my_data.json> http://127.0.0.1:5001/PyCOMPSsWM
```

The latter command, `curl -X ...`, specifies a custom request method (`POST`) to use when communicating with the UCIS4EQ Workflow Manager (WM) service based on PyCOMPSs, and reachable via the HTTP server client

at `127.0.0.1:5001` on port 5001. As an example the instruction may submit the file content of <basedir>/data/SAMOS_EQ_Event_DEMO.json to the WM. The set of complete instructions becomes:

```
> cd <basedir>/Ucis4eq
> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" docker-compose up
> jq '.uuid = "<new_job_id>"' data/SAMOS_EQ_Event_DEMO.json >| \
      data/SAMOS_EQ_Event_DEMO.json
> curl -X POST -H 'Content-Type: application/json' -d \
      @data/SAMOS_EQ_Event_DEMO.json http://127.0.0.1:5001/PyCOMPSsWM
```

7.2.3 Manual service deployment

Each microservice detailed in Table 1 can be deployed manually and run independently from others. This is useful in debug mode to isolate outputs from each service, i.e. to avoid stdout being flooded by mixed outputs coming from all microservices. The best display configuration to adopt for that purpose is to open as many terminal windows or PTSs as you have services. In each PTS window or tile, issue one of the following commands taken from the sequence hereafter:

```
> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" docker-compose \
      -f docker-compose-debug.yml up workflowmanager

> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" docker-compose \
      -f docker-compose-debug.yml up dashboard

> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" docker-compose \
      -f docker-compose-debug.yml up microservices

> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" docker-compose \
      -f docker-compose-debug.yml up slipgen

> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" docker-compose \
      -f docker-compose-debug.yml up salvus

> SSH_PRV="$(\cat ~/.ssh/docker_mn_id_rsa)" docker-compose \
      -f docker-compose-debug.yml up listener
```

As the MongoDB service is alway automatically launched, no command is needed to launch it. When the "*listener*" or "*dashboard*" services are not required, simply do not issue the corresponding "`docker-compose up`" command. Once issued the above commands will trigger the deployments of each corresponding service. Observe the outputs in each terminal to ensure that the corresponding service is satisfactorily deployed . Finally, in yet another terminal window, issue:

```
> jq '.uuid = "<new_job_id>"' <my_data.json> >| <my_data.json>
> curl -X POST -H 'Content-Type: application/json' -d \
      @<my_data.json> http://127.0.0.1:5001/PyCOMPSsWM
```

where, as noted previously, `<my_data.json>` is the relative path to the static input file identifying a seismic event. So Salvus may perform its magic, recall that paths when relative are based on <basedir>/ as defined earlier.

7.3- Test UCIS4EQ with a dry run

You may decide to launch dry runs. They are essentially attempts at real execution launches, without executing the compute-job. This is generally done to ensure that all input files and the general compute setup is correct without committing jobs to the infrastructure. To do so simply comment out job submission instructions:

```
submission.run ...
```

in `salvus.py` and `SlipGen.py`.

7.4- Monitor the current UCIS4EQ job

You can carry out routine checks on your current jobs' executions.

7.4.1 Monitoring with Docker

`> docker ps [-a|-l]` # lists container(s) on the local HOST

`-a` = `all` (active and inactive)

`-l` = `latest` (latest created container)

7.4.2 Monitoring via Flask server

Visit the web page: http://127.0.0.1:8050 to visualize bottlenecks and errors on compute jobs.

7.4.4 Monitoring via CLI on MN4

`MN4> watch squeue` # type `CTRL-C` to quit.

7.5- Stop/quit a UCIS4EQ job

Issue `CTRL-C` twice on your local host tty for each microservice launched independently in order to end their respective container execution, followed by:

```
> docker compose down
```

The latter command will erase all current UCIS4EQ docker containers from your local host.

Additionally you can verify that your Marenostrum file tree was correctly populated with result files. This however does not guarantee a correct job completion as no error control is performed on the correct execution of Salvus from UCIS4EQ. The file tree lookup command is:

```
> tree -L 4 /gpfs/scratch/<your_hpc_group>/<your_hpc_username>/Eflows4hpc/Ucis4eq/
```

Take note of the `<code_name>` given to the execution of interest and as shown in the JSON file:

`<basedir>/data/<event_ref>.json`

at key `"uuid"`. This `<code_name>` is used by UCIS4EQ to generate a new tar ball that contains all result plots:

`/gpfs/scratch/<your_hpc_group>/<your_hpc_username>/Eflows4hpc/Ucis4eq/event_<code_name>/salvus_plots/event_<code_name>.tar.gz`

8. Miscellanea

8.1- Garbage collection (keep your slate clean)

To remove all Docker containers (including those currently running):

```
> docker rm -f $(docker ps -a -q)
```

To list locally available Docker images:

```
> docker images
```

`To remove selected Docker images, find a pattern common to all of them and place it in the pattern matching condition in the `awk' cmd below:`

```
> docker rmi -f < <(docker images | awk '/.../ {print $3}')
```

8.2- Spawn new Docker images upon changing the UCIS4EQ code