

## Hands-on: how to use EESSI

EESSI Community Meeting @ Amsterdam 14 Sept 2022 Kenneth Hoste (HPC-UGent)

# Let's get our hands dirty with EESSI!

- From end user's perspective
- Assumption is that CernVM-FS + EESSI configuration is in place
  - See hands-on session this afternoon on how to install EESSI from scratch
- Practical setup
  - We will use the EESSI Cluster-in-the-Cloud @ AWS
  - Virtual Slurm cluster where workernodes are auto-started when jobs appear
  - EESSI is installed natively on cluster workernodes (not on login node!)
  - If you want to join the hands-on session, let us know your GitHub account name
  - We will use the SSH public key(s) attached to your GitHub account to give you access



# Step 1: Get logged in to CitC cluster

- If you don't have an account on the CitC cluster yet, contact Kenneth, Thomas, or Alan (either live or via Slack)
- If you have an account, log in with your GitHub handle:

ssh example@3.250.220.9



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anna an	
Activate the web console with: systemctl enablenow cockpit.socket	
Last login: Mon Sep 12 15:34:31 2022 from 157.193.5.72	

More info on the cluster at <u>github.com/EESSI/hackathons/tree/main/2022-01/citc</u>

#### Step 2: Prepare some science...

Clone the EESSI demo repository in your account,

so you have some supported scientific workloads to play with.



\$ git clone https://github.com/EESSI/eessi-demo

\$ ls eessi-demo

Bioconductor CitC GROMACS LICENSE Magic\_Castle OpenFOAM README.md TensorFlow scripts

### Step 3: Start an interactive job

- Start an interactive Slurm job, so you get a shell on a workernode
- A workernode may need to be booted first for you (takes ~3min)
- You will need to specify a node type via -C shape=... (see list nodes command)
- Optional: start a screen or tmux session first

. . .

• Example (feel free to pick a different node shape!):

\$ srun -N1 -n8 -C shape=c6g.2xlarge --time=1:0:0 --pty /bin/bash

[boegel@fair-mastodon-c6g-2xlarge-0001 ~]\$



# Step 4: Initialize the EESSI environment

- The EESSI pilot CernVM-FS repository is now available:
  - \$ ls /cvmfs/pilot.eessi-hpc.org
  - 2021.06 host\_injections latest versions
  - Note: "ls /cvmfs" may not show anything, you need to address the repo itself!
- Source our init script to set up your environment:
  - \$ source /cvmfs/pilot.eessi-hpc.org/latest/init/bash
- Keep an eye out for the auto-detection of the host CPU!
  - Using aarch64/graviton2 as software subdirectory



### Step 5: Science!

- A (small) wealth of scientific software is now available, optimized for the host CPU of the system
- See output produced by "module avail"
- Now get some science done using one of our demo scripts:

```
cd ~/eessi-demo/TensorFlow/
./run.sh
```

• Startup may take a while the first time (CernVM-FS is downloading files in background)





EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS Paper (open access): https://doi.org/10.1002/spe.3075

Website: https://www.eessi-hpc.org

Join our mailing list & Slack channel https://www.eessi-hpc.org/join

Documentation: https://eessi.github.io/docs

GitHub: https://github.com/eessi

Twitter: @eessi\_hpc

YouTube channel (brand new!)

Monthly online meetings (first Thursday, 2pm CEST)