

PRACE Winter School, 8th December 2021

HPC workshop Joining Instructions

Pre-requisites

- Good knowledge of Linux and command line commands from a user perspective is required.
- An up-to-date web browser (e.g. Firefox, Chrome)
 - What browsers does the Management Console support? See FAQ:
 - <https://aws.amazon.com/console/faq-console/>
- An up-to-date version of the Zoom client

What to expect on the day

All times in UTC+2

08:30 → 09:00 Welcome & Tech Check 30m

- Welcome message by organisers
- You will receive a login hash number and other required information to sign in to Event Engine via Zoom chat
 - this will be available throughout the day for those who cannot make it to this session.
- The AWS team will be available to help with clarifying instructions and address any issues

09:00 → 10:30 Hands-on Session 1: Scientific Computing with EC2 and S3 on AWS, hands-on practice

Speaker: Austin Cherian (Sr. HPC/Batch Developer Advocate, AWS),

- The main presentation will take place in the main room
- Participants will be placed in break-out rooms to follow the hands-on guide assisted by AWS instructors

10:30 → 10:45 Coffee Break

10:45 → 12:15 Hands-on Session 2: HPC on AWS: set up and configuration, hands-on practice

Speakers: Austin Cherian (Sr. HPC/Batch Developer Advocate, AWS), Bruno Silva (Academic Research Solutions, AWS)

- The main presentation will take place in the main room
- Participants will be placed in break-out rooms to follow the hands-on guide assisted by AWS instructors

12:15 → 13:00 Lunch Break

13:00 → 14:00 Hands-on Session 3: Heterogeneous HPC with LAMMPS and remote visualisation on AWS, hands-on practice.

Speaker: Fabio Baruffa (Sr. HPC Solutions Architect, AWS)

- **Note:** Participants that don't attend **Hands-on Session 2** will not meet the pre-requisites for hands-on work on **Hands-on Session 3** but will still be able to follow the presentation and understand the concepts.

14:00 → 15:00 Talk: Running large-scale OpenFOAM simulations on AWS

- no hands-on - questions answered in the main room.

15:00 → 15:15 Coffee Break

15:15 → 16:15 Talk: Large-scale GROMACS biomolecular simulations using AWS Batch

- no hands-on - questions answered in the main room.

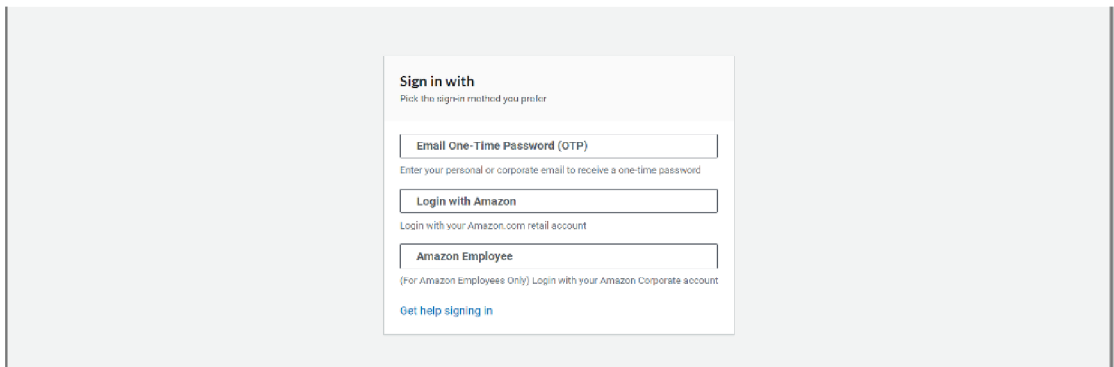
16:15 → 17:15 Talk: Event-driven Simulation at scale using EFISPEC3D on AWS

- no hands-on - questions answered in the main room.

Joining Instructions

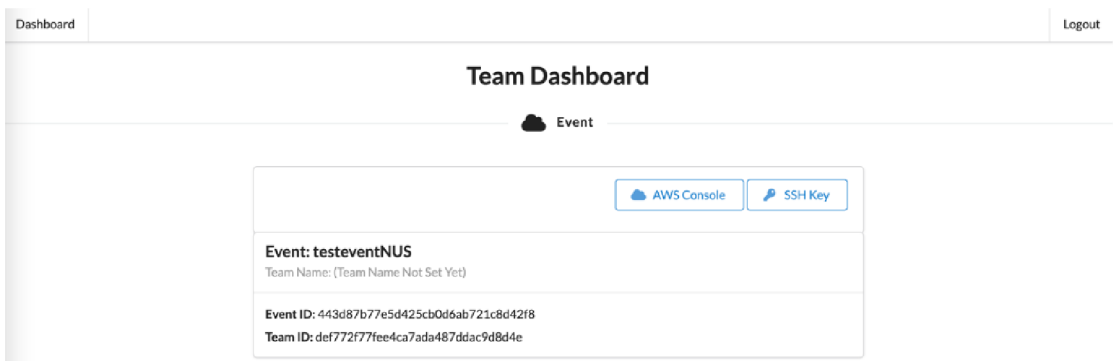
1. Join the Workshop via the Zoom link:
 - a. <https://us02web.zoom.us/j/86839894827?pwd=bnR1UXQ0NDJRS3JnV3g1TURxc1FIQT09>
2. Access to your individual AWS account will be done using AWS Event Engine - <https://dashboard.eventengine.run/>
 - a. You will be asked for a Hash number - **this number will be provided to the entire cohort via Zoom on the day.**
 - b. Once you provide the Hash, you should see a page that looks like this:

c.



- d. click **“Email One-Time Password (OTP)”**.
- e. Provide the **email you used to register for the event**
- f. After a few minutes you will receive a message with your (OTP) - check your spam box if more than 5 minute have passed without seeing the message in your inbox.
- g. Once you insert the number you will be taken to a page that should looks like this:

h.



- i. Click on **“AWS Console”** - you should then be taken to a page containing the following section:

j.

Login Link

[Open AWS Console](#) [Copy Login Link](#)

Credentials / CLI Snippets

Mac / Linux Windows

Mac or Linux

```
export AWS_DEFAULT_REGION=ap-southeast-1
export AWS_ACCESS_KEY_ID=
export AWS_SECRET_ACCESS_KEY=
export AWS_SESSION_TOKEN=
```

How do I use the AWS CLI?

Checkout the AWS CLI documentation here: <https://docs.aws.amazon.com/cli/latest/userguide/cli-chap-welcome.html>

k. Click on “Open AWS Console”. And you should see a page similar to this one:

l.

m. Congratulations! You have arrived!

3. Command line work will be done using **AWS Cloud9 IDE**. We will walk you through the setup steps at the start of **Hands-on Session 1** and **Hands-on Session 2**

4. **Note:**

- We highly recommend that you join the 8:30 (UTC+2) Welcome & Tech Setup session** to check that your environment is working correctly. You will be able to re-join later with the same event hash, repeating the steps above.
- Participants that don't attend **Hands-on Session 2** will not meet the pre-requisites for hands-on work on **Hands-on Session 3** but will still be able to follow the presentation and understand the concepts.
- For any clarification regarding instructions, please email Dr. Bruno Silva - bcsilva@amazon.co.uk.