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CCP-WSI
a Collaborative Computational Project
in Wave Structure Interaction

Introduction to running OpenFOAM on Archer 2

Dr. Raynold Tan

Machine Learning for WSI

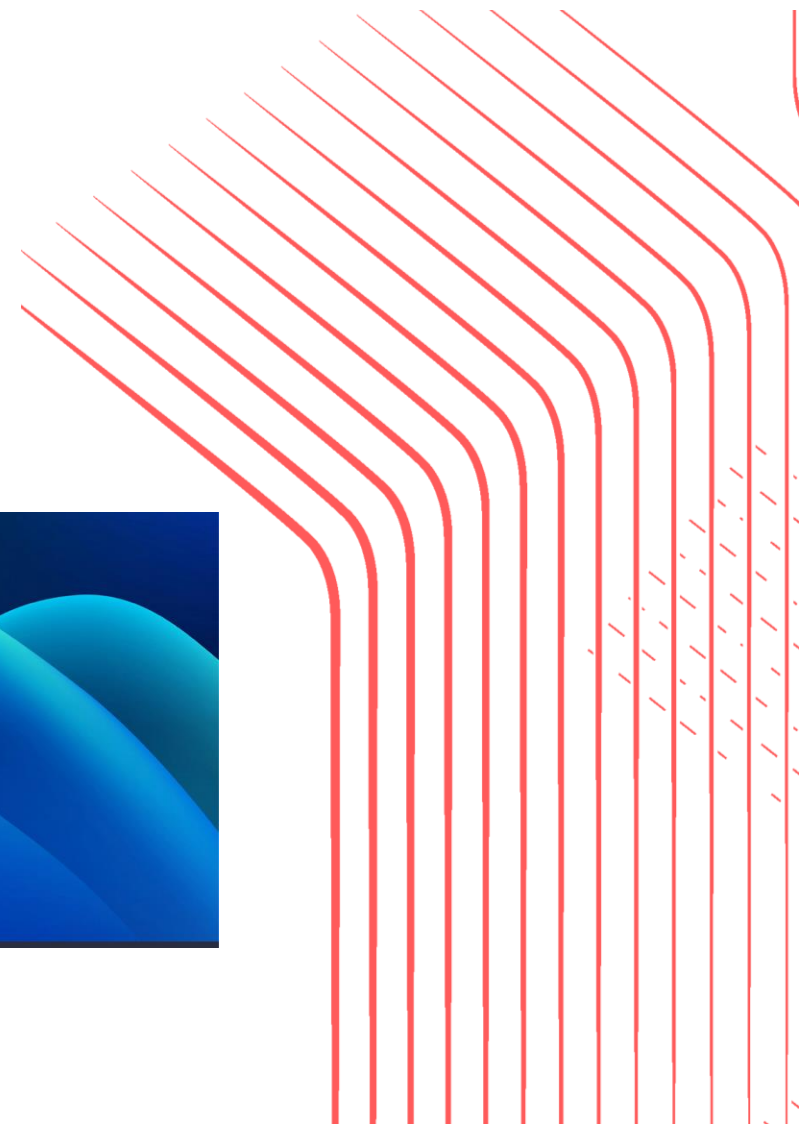
Register

Agenda

📅 4 - 5 Nov 2024

🕒 From 12 on 4th Nov

📍 Hybrid: Brunner-Mond Training Suite, Daresbury Laboratory, Keckwick Lane, WA4 4AD or Online



Archer 2 Hardware



Compute nodes

Nodes	5,860 nodes: 5,276 standard memory, 584 high memory
Processor	2× AMD EPYC™ 7742, 2.25 GHz, 64-core
Cores per node	128 (2× 64-core processors)
NUMA structure	8 NUMA regions per node (16 cores per NUMA region)
Memory per node	256 GiB (standard memory), 512 GiB (high memory)
Memory per core	2 GiB (standard memory), 4 GiB (high memory)
Interconnect	HPE Cray Slingshot, 2× 100 Gbps bi-directional per node

Login and data analysis nodes

Processor	2× AMD EPYC™ 7742, 2.25 GHz, 64-core
Cores per node	128 (2× 64-core processors)
NUMA structure	8 NUMA regions per node (16 cores per NUMA region)
Memory per node	512 GiB
Memory per core	4 GiB

Archer 2 Hardware

Component	Details
Processor	2x AMD Zen2 (Rome) EPYC 7742, 64-core, 2.25 Ghz
Cores per node	128
NUMA structure	8 NUMA regions per node (16 cores per NUMA region)
Memory per node	256 GB (standard), 512 GB (high memory)
Memory per core	2 GB (standard), 4 GB (high memory)
L1 cache	32 kB/core
L2 cache	512 kB/core
L3 cache	16 MB/4-cores
Vector support	AVX2
Network connection	2x 100 Gb/s injection ports per node

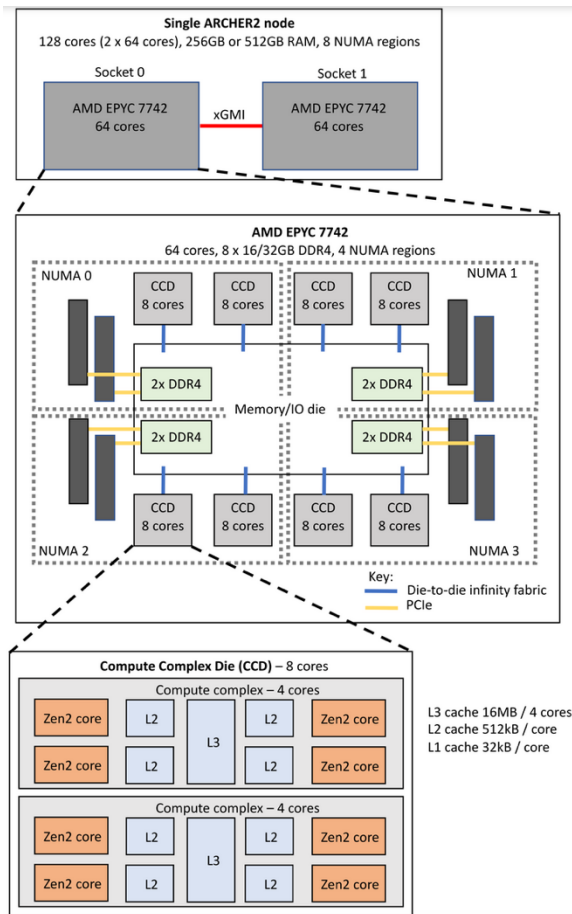


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Getting an Account



Getting an Account

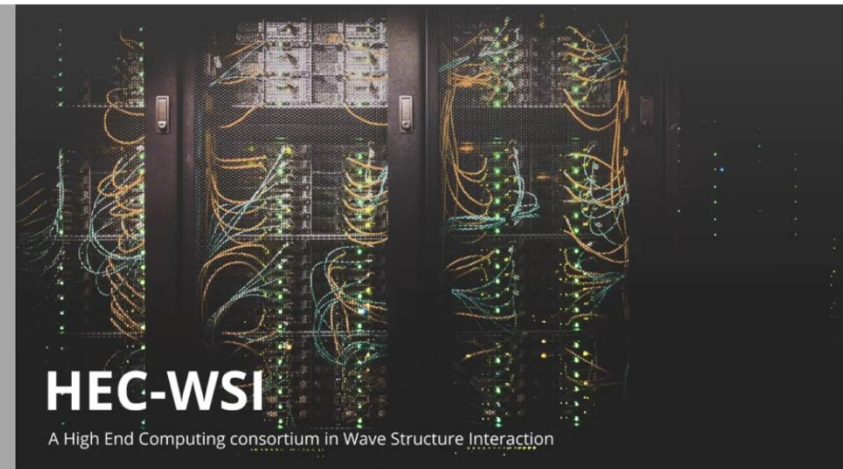


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HEC-WSI aims to facilitate world-class wave structure interaction (WSI) research using national High-End Computing (HEC) resources. If you are interested in applying for time on ARCHER2 for your WSI research you've come to the right place!



For the Collaborative Computational Project in Wave Structure Interaction (CCP-WSI) please visit our [partner site](#).



<https://hec-wsi.ac.uk/>



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Getting an Account

HEC-WSI Access Modes

The resources allocated to the HEC-WSI are awarded as 'ARCHER2 time only', i.e. the following access modes only provide access to ARCHER2 resources and not funding for other items (such as staff time). ARCHER2 costs are notional rather than real costs.

The HEC-WSI currently offers three access modes (plus a dedicated allocation for early career researchers (ECRs) incl. training and support):

- Porting and Benchmarking (PB);
- Code Development (CD), and;
- Project Access (PA).

Call	Closing date	Notes	Application form link
Porting & Benchmarking (PB)	Always open	a short project of 3 months duration with a small number of allocation units for testing scalability	<u>PB Form</u>
Code Development (CD)	Always open	a 6-month project with a small allocation for improving software performance	<u>CD Form</u>
Project Access (PA)	No call currently open	a 12-month project with a large allocation for project runs	Available soon
ECR	Always open	Dedicated allocation for early career researchers (ECRs) including training and support	Available soon

Application advice

Scientific case

Coming soon

Technical case

Coming soon

Assessment timetable

The HEC-WSI Management Team will review and approve applications through the PA and CD modes on a monthly basis. A panel will assess applications to Project Access (PA) calls. The Project Access Panel will comprise members of the HEC-WSI management team and at least one invited external observer who will give independent feedback on the HEC-WSI processes.



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<https://hec-wsi.ac.uk/access-resource/access-modes/>

Getting an Account

Following a successful application for ARCHER2 resource, via the HEC-WSI, the first thing you must do, before you can access the resource, is to join the HEC-WSI project on the SAFE system

Step 1 Create a **SAFE** account (if you have not already) and log on to SAFE

Step 2 Go to the 'Projects' tab and select 'Request access'

Step 3 On the 'Apply for project membership' page, select the project for which you wish to request access (all HEC-WSI-supported projects are under the HEC-WSI project, e773)

Step 4 On the following 'Apply for project membership' page, check the project is correct (i.e. e773 for the HEC-WSI project). NOTE: the 'access route' defaults to 'Request machine account'. Select 'Apply'

Step 5 On the SAFE Login account Request' page check the project is correct (i.e. e773 – HEC WSI). Select the 'Machine' you wish to access. NOTE: the HEC-WSI project is restricted to the archer2 machine so ensure that the 'archer2' machine is selected and click 'Next'

Step 6 You'll then need to complete the 'SAFE Login account Request'.

- Add a username
- Confirm that you accept the Terms and Conditions of Access
- You'll then need to add an 'SSH public key'

<https://hec-wsi.ac.uk/access-resource/using-archer2/applying-for-project-membership/>

Step 7 Await approval. Once the HEC-WSI Support Team have received your request, and ensured your details are consistent and correct, your application will be approved. This will give you access to the HEC-WSI project (e773) on SAFE (which has zero CUs allocated to it).

Step 8 The HEC-WSI Support Team will create a sub-group for your specific allocation, e.g. e773-PB-0101, and allocate the awarded resource. You, and additional members (specified in your application for HEC-WSI resources), will be added to this sub-group.

Step 9 If you wish to add additional members (not declared on your original application) to your sub-group you must contact the HEC-WSI Support Team, with details of the additional members and confirmation of their nationalities, before their project membership can be approved.



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Logging into Archer 2

Logging into Archer 2

Step 1 If this is the first time you have logged onto ARCHER2 (with this particular login account) you will need to acquire your 'initial password' from the SAFE system. The SAFE web interface is used to provide your automatically generated initial password for logging onto ARCHER2 (see the [SAFE Documentation](#) for more details). The password can be found by logging into your SAFE account, selecting your HEC-WSI-related login account from the 'Login Accounts' tab and clicking on 'View Login Account Password'.

Step 2 On the ARCHER2 system, interactive access is achieved using SSH, either directly from a command-line terminal or using an SSH client. Assuming you have followed the HEC-WSI's [applying for project membership](#) instructions, and have already generated an SSH Key pair associated with your login account, you can log onto ARCHER2 using the following command, (remembering to replace <username> with your username):

```
ssh <username>@login.archer2.ac.uk
```

Alternatively, if you wish to allow remote programs, especially graphical applications, to control your local display, such as for a debugger, use

```
ssh -X <username>@login.archer2.ac.uk
```

NOTE: If your SSH key pair is not stored in the default location (usually ~/.ssh/) on your local system, you may need to specify the path to the private part of the key with the -i option to ssh. For example, if your key is in a file called ~/keys/SSHKey_ARCHER2 you would use the following command to log in:

```
ssh -i ~/keys/SSHKey_ARCHER2 <username>@login.archer2.ac.uk
```

Step 3 If you have set one, you will also have to enter the passphrase associated with your SSH key pair. If this is your first time logging onto ARCHER2 (with this particular login account), when prompted, you will have to enter your initial password (obtained from SAFE as per Step 1 above). You will then be prompted to set a new password. NOTE: after your initial login, and password reset, you will only need to enter your new password (and SSH key pair passphrase, if set).

TIP: Your new password must have both capital and lowercase letters, numbers and special characters.



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Overview of Archer 2 Environment

Overview of Archer 2 Environment

- Logging into Archer 2: `ssh <username>@login.archer2.ac.uk`
- You will be at your home directory, type `pwd`, `/home/e773/e773/<username>/`
- Go to your work directory, `cd /work/e773/e773/<username>/`
- This will be the **main directory**, where you should compile custom code and run cases.

File Transfer

`scp [options] <path_to_source> <username>@login.archer2.ac.uk:<path_to_destination>`

`rsync [options] <path_to_source> <username>@login.archer2.ac.uk:<path_to_destination>` (rsync is better!)

`rsync [options] -e ssh <path_to_source> <username>@login.archer2.ac.uk:<path_to_destination>`

Basic Slurm Command

`sinfo` – Get information on the partition and resources available

`sbatch jobscript.sh` – submit a job submission script named jobscript.sh

`squeue -u <username>` - get the current status of jobs submitted to the scheduler for the specified user

`scancel <jobID>` - cancel a specific job for the given jobID, get jobID from squeue command.

Overview of Archer 2 Environment

Using the module command

`module list [name]` - List modules currently loaded in your environment, optionally filtered by [name]

`module avail [name]` - List modules available, optionally filtered by [name]

`module spider [name]/[version]` - Search available modules (including hidden modules) and provide information on modules, Unlike `module avail`, this includes modules that are not currently able to be loaded due to the fact you have not yet loaded dependencies to make them directly available

`module load [name]` - Load the module called name into your environment

`module remove [name]` - Remove the module called name

`module swap [old] [new]` - Swap module new for module old

`module help [name]` - Show help information on module name

`module show [name]` - List what module name actually does to your environment

Shell environment

`export OMP_NUM_THREADS = 4` – define an example environment variable

`echo $OMP_NUM_THREADS` – show the value of a specific environment variable

`unset OMP_NUM_THREADS` – remove an environment variable



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Submitting Jobs



Hands On Session

Running OpenFOAM on Archer 2

<https://docs.archer2.ac.uk/research-software/openfoam/>

```
auser@ln01> module avail openfoam
----- /work/y07/shared/archer2-lmod/apps/core -----
openfoam/com/v2106                openfoam/org/v9.20210903 (D)
openfoam/org/v8.20200901
```

```
user@ln01:> module load PrgEnv-gnu
user@ln01:> module load openfoam/com/v2106
```

The module defines only the base installation directory via the environment variable `FOAM_INSTALL_DIR`. After loading the module you need to source the `etc/bashrc` file provided by OpenFOAM, e.g.

```
user@ln01:> source ${FOAM_INSTALL_DIR}/etc/bashrc
```

Hands On Session

Job submission on Archer 2 for Serial Run using sbatch scripts

Submit job: [sbatch file_name.sh](#),

Check status of job: [squeue -u username](#)

```
#!/bin/bash
```

```
#SBATCH --job-name=SerialRun
```

```
#SBATCH --nodes=1
```

```
#SBATCH --ntasks-per-node=1
```

```
#SBATCH --cpus-per-task=1
```

```
#SBATCH --time=12:00:00
```

```
#SBATCH --account=acct\_name
```

```
#SBATCH --partition=standard
```

```
#SBATCH --qos=standard
```

```
#SBATCH --export=none
```

partition = <standard/highmem/serial>

qos = <standard/highmem/taskfarm/short/long/largescale/lowpriority/serial/reservation>

Module PrgEnv-gnu is necessary for openfoam installation, default environment used, gnu compiler

```
module load PrgEnv-gnu
```

```
export FOAM_INSTALL_PATH="/work/c01/c01/yiyuntan/OpenFOAM/OpenFOAM-v2212"
```

```
# source OpenFOAM bash
```

```
source ${FOAM_INSTALL_PATH}/etc/bashrc
```

```
export FOAM_USER_APPBIN=/work/c01/c01/yiyuntan/OpenFOAM/yiyuntan-v2212/platforms/linux64CrayDPInt32Opt/bin
```

```
export FOAM_USER_LIBBIN=/work/c01/c01/yiyuntan/OpenFOAM/yiyuntan-v2212/platforms/linux64CrayDPInt32Opt/lib
```

```
blockMesh
```

```
setFields
```

```
interFoam > log.interFoam
```

It is possible to load installed version of openfoam on archer 2 from module load.

Hands On Session

Job submission on Archer 2 for Parallel Run using sbatch scripts

Submit job: `sbatch file_name.sh`,

Check status of job: `squeue -u username`

```
#!/bin/bash
```

```
#SBATCH --job-name=MultiParallelOnCompute
```

```
#SBATCH --nodes=1
```

```
#SBATCH --ntasks-per-node=128
```

```
#SBATCH --cpus-per-task=1
```

```
#SBATCH --time=12:00:00
```

```
#SBATCH --account=acct_name
```

```
#SBATCH --partition=standard
```

```
#SBATCH --qos=standard
```

```
#SBATCH --export=none
```

partition = <standard/highmem/serial>

qos = <standard/highmem/taskfarm/short/long/largescale/lowpriority/serial/reservation>

Module PrgEnv-gnu is necessary for openfoam installation, default environment used, gnu compiler
Module gsl is only needed when one want to use waveFoam solver from waves2Foam

```
module load PrgEnv-gnu
```

```
module load gsl
```

```
export FOAM_INSTALL_PATH="/work/c01/c01/yiyuntan/OpenFOAM/OpenFOAM-v2212"
```

```
# source OpenFOAM bash
```

```
source ${FOAM_INSTALL_PATH}/etc/bashrc
```

Necessary step to source the OpenFOAM environment to use commands. Alternatively, It is possible to load installed version of openfoam on archer 2 from module load.

```
export FOAM_USER_APPBIN=/work/c01/c01/yiyuntan/OpenFOAM/yiyuntan-v2212/platforms/linux64CrayDPInt32Opt/bin
```

```
export FOAM_USER_LIBBIN=/work/c01/c01/yiyuntan/OpenFOAM/yiyuntan-v2212/platforms/linux64CrayDPInt32Opt/lib
```

```
blockMesh
```

```
setFields
```

```
decomposePar
```

```
srun --nodes=1 --ntasks=128 --tasks-per-node=128 --exact --mem=80000M --cpu_bind=cores interFoam -parallel > log.interFoam
```



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<https://docs.archer2.ac.uk/user-guide/scheduler/>

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Hands On Session

Other possible job submission options

- <https://docs.archer2.ac.uk/user-guide/scheduler/>
- Running multiple, full-node subjobs within a larger job – multi-nodes, multiple srun commands
- Running multiple subjobs that each use a fraction of a node – single node, multiple srun commands
- Interactive Jobs – apply srun command on the login terminal directly.

Full system

```
auser@ln01:> salloc --nodes=8 --ntasks-per-node=128 --cpus-per-task=1 \  
--time=00:20:00 --partition=standard --qos=short \  
--account=[budget code]
```

When you submit this job your terminal will display something like:

Full system

```
salloc: Granted job allocation 24236  
salloc: Waiting for resource configuration  
salloc: Nodes nid000002 are ready for job  
auser@ln01:>
```

Useful in the context of running coupled simulations with multiple solvers.



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Questions?

References

OpenFOAM: User Guide v2112

<https://www.openfoam.com/documentation/guides/v2112/doc/openfoam-guide-parallel.html>

Archer 2 User Guide, <https://docs.archer2.ac.uk/user-guide/scheduler/>

Archer 2 Hardware, <https://docs.archer2.ac.uk/user-guide/hardware/>



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