

# Maxwell for XFEL

The XFEL partitions serve for operation and simulations for the XFEL accelerator at DESY. Not to be confused with the European XFEL!° Talk to the M admins or XFEL team if you believe you should have access but don't.

For details about the setup of these partitions please have a look at the pages on [hardware](#), [limits](#) and [constraints](#) .

## Partitions

The XFEL resources are "divided" into three partitions:

- The **xfel-op** partition. It's a highest priority partition. Jobs in this partition will immediately **cancel any jobs in the all, xfel-sim or xfel-guest partition** using the same nodes!
- The **xfel-sim** partition. It's a high priority partition. Jobs in this partition will immediately **cancel any jobs in the all or xfel-guest partition** using the same nodes!
- The **xfel-guest** partition. It's a regular priority partition combining all XFEL and PETRA4 resources. Jobs in this partition will terminate jobs in the all partition (like on any other partition). Jobs in the xfel-guest partition will be terminated by any jobs in the xfel-op, xfel-sim or petra4 partition using the same nodes.

## Interactive Login Nodes

There are no login nodes associated with the XFEL resources in Maxwell.

- **ssh max-display.desy.de**: will connect you to one of the display nodes. FastX might your better choice. Please have a look at the [Remote Login](#) and the [FastX documentation](#).
- **ssh max-wgs**: will connect you to the generic login node.
- **Please note**: max-display.desy.de is directly accessible from outside. All other login nodes can only be reached by first connecting to bastion.desy.de.

Login nodes are always shared resources sometimes used by a large number of concurrent users. Don't run compute or memory intense jobs on the login nodes, use a batch job instead!

## The XFEL Batch resource in Maxwell

As a first step login to one of the login nodes and check which Maxwell resources are available for your account using the my-partitions command:

## my-partitions

```
[@max-wgs ~]$ my-partitions
```

```
Partition Access Allowed
groups
```

```
-----
----
      all      yes   all          <----- will be available if any of the
resources below is "yes!"
      cfel      no    cfel-wgs-users
      cms       no    max-cms-uhh-users,max-cms-desy-users
      cms-desy  no    max-cms-desy-users
      cms-uhh   no    max-cms-uhh-users
      cssb     no    max-cssb-users
      epyc-eval no    all
      exfel     yes   exfel-wgs-users
      exfel-spb no    exfel-theory-users,school-users
      exfel-th  no    exfel-theory-users
      exfel-theory no    exfel-theory-users
      exfel-wp72 no    exfel-theory-users
      fspetra  no    max-fspetra-users
      grid     no    max-grid-users
      jhub     no    all
      maxwell  yes   maxwell-users,school-users          <----- might be granted if you have
suitable applications
      p06      no    max-p06-users
      petra4   no    p4_sim
      ps       no    max-ps2-users
      psx     no    max-psx2-users
      uke      no    max-uke-users
      upex     yes   upex-users,school-users
      xfel-guest no    max-xfel-guest-users,p4_sim          <----- look for this one as a member of
XFEL guest or PETRA4
      xfel-op  no    max-xfel-op-users                    <----- look for this one as a member of
XFEL OP
      xfel-sim no    max-xfel-sim-users                    <----- look for this one as a member of
XFEL SIM
```

If it says "yes" for partition "xfel" you are ready to go. If so you will also see a "yes" at least for partition "all". If not: get in touch with M admins! Let's assume that you've got the xfel-guest-resource. Same rules apply to the other xfel partitions/resources.

If you have an application, which is started by a script called my-application, and doesn't require a GUI, you can simply submit the script as a batch-job:

## sbatch

```
[@max-wgs ~]$ sbatch --partition=xfel-guest --time=12:00:00 --nodes=1 my-application
Submitted batch job 1613895
```

```
# the job might already be running
```

```
[@max-wgs ~]$ squeue -u $USER
```

```
      JOBID PARTITION   NAME     USER ST       TIME  NODES NODELIST(REASON)
      1614464 xfel-gues  my-app   user  R         0:06     1 max-p4-001
# Status of the job                R: running. PD: pending
```

This works for any application smart enough not to strictly require an X-environment, matlab, comsol, ansys, mathematica, idl and many others can be executed as batch jobs. To make it more convenient you can add the SLURM directives directly into the script:

### SBATCH script

```
[@max-wgs ~]$ cat my-application
#!/bin/bash
#SBATCH --partition=xfel-guest
#SBATCH --time=1-12:00:00 # request 1 day and 12 hours
#SBATCH --mail-type=END,FAIL # send mail when the job has finished or failed
#SBATCH --nodes=1 # number of nodes
#SBATCH --output=%x-%N-%j.out # per default slurm writes output to slurm-<jobid>.out. There are a number
of options to customize the job
[...] # the actual script.
```

The email-notification will be sent to <user-id>@[mail.desy.de](mailto:mail.desy.de). That should always work, so you don't actually need to specify an email-address. If you do, please make sure it's a valid address. For further examples and instructions please read [Running Jobs on Maxwell](#).

If you think that it's much to complicated to write job-scripts or if you can't afford to invest the time to look into it: we are happy to assist. Please drop a message to [maxwell.service@desy.de](mailto:maxwell.service@desy.de), we'll try our best.

## Running interactive batch jobs

If you absolutely need an interactive environment, X-windows features like a GUI, there are options to do that in the batch environment. For example:

### salloc

```
# request one node for 8 hours:
[@max-wgs ~]$ salloc --nodes=1 --time=08:00:00 --partition=xfel-guest
salloc: Pending job allocation 1618422
salloc: job 1618422 queued and waiting for resources
salloc: job 1618422 has been allocated resources
salloc: Granted job allocation 1618422
salloc: Waiting for resource configuration
salloc: Nodes max-p4-012 are ready for job

# now you got a node allocated. So you can ssh into the node
[@max-wgs ~]$ ssh max-p4-012
[@max-p4-012 ~]$ # run your application!
[@max-p4-012 ~]$ exit # this terminates the ssh session, it does NOT terminate the allocation
logout
Connection to max-p4-012 closed.
[@max-wgs ~]$ exit
exit
salloc: Relinquishing job allocation 1618422
# now your allocation is finished. If in doubt use squeue -u $USER or svview to check for running sessions!
```

There are a few things to consider:

- Interactive jobs with salloc easily get forgotten, leaving precious resources idle. We do accounting and monitoring!
- Keep the time short: there is hardly a good reason to run an interactive jobs for more than the working hours. Use a batch job instead.
- Terminate allocations as soon as the job is done!

## Other Maxwell Resources

Being member of XFEL-OP and maybe having access to the xfel-guest partition doesn't need to be the end of the story. If you have parallelized applications suitable for the Maxwell cluster you can apply for the Maxwell resource like everyone else on campus. Please send a message to [maxwell.service@desy.de](mailto:maxwell.service@desy.de) briefly explaining your use case. You can easily distribute your job over the partitions:

### multiple partitions

```
[@max-wgs ~]$ cat my-application
#!/bin/bash
#SBATCH --partition=xfel-op,maxwell,xfel-guest,all
#SBATCH --time=1-12:00:00 # request 1 day and 12 hours
#SBATCH --mail-type=END,FAIL # send mail when the job has finished or failed
#SBATCH --nodes=1 # number of nodes
#SBATCH --output=%x-%N-%j.out # per default slurm writes output to slurm-<jobid>.out. There are a number
of options to customize the job
[...] # the actual script.
```

The partition will be selected from xfel-op OR maxwell OR xfel-guest OR all starting with the highest priority partition. So your job will run on the xfel-op partition if nodes are available, on the maxwell partition if nodes are available and finally on the all partition if none of the other partitions specified have free nodes. Keep in mind that you should however select the partition according to the type of work you are doing. And a job can never combine nodes from different partitions, so check the [limits applying to partitions](#).

To check availability of nodes and characteristics use sinfo (<https://slurm.schedmd.com/sinfo.html>)

#### sinfo

```
[@max-wgs ~]$ sinfo -p xfel-guest -o "%10P %.6D %8c %8L %12l %8m %30f %N"
PARTITION  NODES CPUS      DEFAULTT TIMELIMIT    MEMORY  AVAIL_FEATURES          NODELIST
xfel-guest   38 40        1:00:00  14-00:00:00  256000  INTEL,V4,E5-2640,256G  max-ferrari[001-024],max-p4-[001-014]
```

```
[@max-wgs ~]$ sinfo -p xfel-guest -o "%10P %.6D %10s"
PARTITION  NODES JOB_SIZE
xfel-guest   38 1-24
```