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Institute of Computing CI

Access to the Cluster

Preparing the environment

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ICS cluster - icsmaster

- 1 login node
  - `icslogin01`
- 42 compute nodes
  - `icsnode[01-42]`
  - 32 nodes only with CPU
    - 2 x Intel E5-2650 v3, 20 (2 x 10) cores
    - 24x64 GB, 8x128 GB RAM
  - 8 nodes with GPU
    - 2 x Intel E5-2650 v3, 20 (2 x 10) cores
    - 1 x NVIDIA GeForce GTX 1080, 2560 CUDA cores
    - 128 GB RAM
  - 2 multi GPU nodes
    - 2 x Intel Xeon Silver 4114, 20 (2 x 10) cores
    - 2 x NVIDIA GeForce GTX 1080 Ti or GTX 2080 Ti
    - 100 GB RAM

Accessing icsmaster

- You will receive your login credentials by email
- Connect to the cluster using ssh

```
$ ssh studXX@hpc.ics.usi.ch
```

- To avoid typing the password you can generate a ssh-key and copy it to the cluster. Execute this **on your laptop**!

```
$ ssh-keygen
$ ssh-copy-id -i ~/.ssh/id_rsa.pub studXX@hpc.ics.usi.ch
```

Note: Copying the command from the pdf slide might not work due to the '~' character!

Accessing icsmaster

- Add host configuration to `~/.ssh/config`

```
Host icsmaster
    Hostname hpc.ics.usi.ch
    Port 22
    User studXX
    IdentityFile ~/.ssh/id_rsa
```

- Now you can connect to icsmaster without password

```
$ ssh icsmaster
```

Moving data

- laptop → icsmaster

```
$ scp file.c icsmaster:~/remote_dir/
$ scp -r local_dir icsmaster:~/remote_dir/
```

- icsmaster → laptop

```
$ scp icsmaster:~/remote_dir/file.c local_dir/
$ scp -r icsmaster:~/remote_dir/ local_dir/
```

Modules

- Software on the cluster is organized into modules
- Before using some program, you have to load a module

```
$ module load gcc
```

- You can load a specific version of a module

```
$ module load gcc/10.1.0
```

- You can unload modules you don't want anymore

```
$ module unload gcc
```

- List currently loaded modules

```
$ module list
```

- List all available modules

```
$ module avail
```

Editing code

- To edit files on the cluster you can use vim

```
$ vim main.c
```

- For easier moving / editing, you can mount home directory from cluster to your local machine, then you can work with files on the cluster as if it would be on your laptop
  - First install FUSE and SSHFS from `https://osxfuse.github.io`
  - Then you can mount remote directory

```
$ sshfs icsmaster: <mountpoint>
```

  - And unmount

```
$ umount <mountpoint>
```

Compiling code

- Load modules before compiling the code

```
$ module load gcc
```

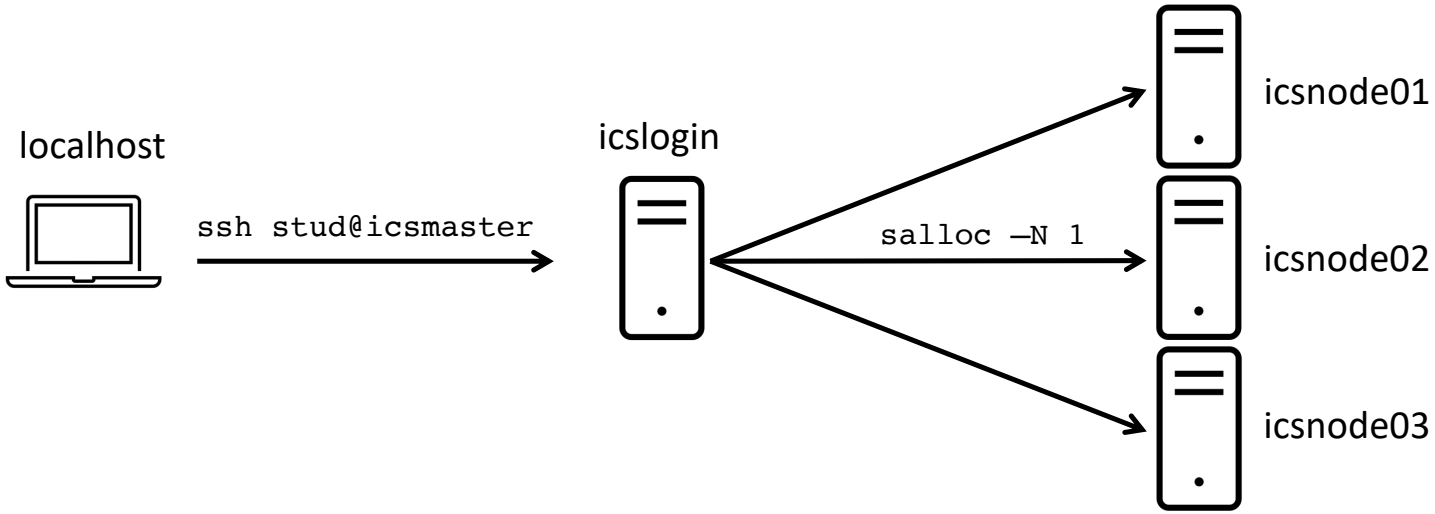
- Then you can compile the code

```
$ gcc main.c -o main
```

- Pro tip: add `module load ...` to your `~/.bashrc`
  - It will load modules automatically when you log in

Running code

- When you log in to the cluster, you are on login node `icslogin01`
  - You can use login node to edit and compile your code
  - **But you should never run the code on login node**
- For running your code, there are 42 compute nodes
  - `icsnode[01-42]`
- There are two ways how you can work on compute node
  - Interactive session
  - Batch job



Interactive session

- In interactive session you have direct access to compute node from your terminal
- Interactive session is useful especially for debugging
- When you allocate a node, nobody else can use it at the same time
- But it can take a long time to get access to the node

- First you have to allocate the node
- Let's say you want 1 node for 1 hour

```
$ salloc --nodes=1 --time=01:00:00
```

- Then you can run your app on the compute node

```
$ ./your_app
```

- Or you can use srun that does the allocation automatically

```
$ srun --nodes=1 ./your_app
```

Batch job

- When running batch job, you don't have direct access to the compute node
- You write a script with commands you want execute on the node
- The script is added to a queue and executed later
- Output of the script is written to a file. You can look at is when the job is finished
- Batch job is useful when you have working code and you want to run your app on large data

Batch job

- Job script template

```
#!/bin/bash -l

#SBATCH --job-name=my_job
#SBATCH --time=01:00:00
#SBATCH --nodes=1
#SBATCH --output=%j.out
#SBATCH --error=%j.err

# load modules

# your commands
```

- Add job to a queue

```
$ sbatch job.sh
```

- Show your running and queued jobs

```
$ squeue -u studXX
```

- Cancel job

```
$ scancel <job_id>
```

Reservation

- During the HPC lectures there are several nodes reserved only for you
- Use argument `--reservation=HPC_tuesday` or `--reservation=HPC_wednesday`

```
$ salloc --reservation=HPC_tuesday
$ srun --reservation=HPC_tuesday ./your_app
```

- Use the reservation only in the class
- When the reservation is not active, your job will stay in queue until the next class

- In class (with reservation)

```
$ srun --reservation=HPC_tuesday ./your_app
```

- At home (no reservation)

```
$ salloc --nodes=1 --time=01:00:00
$ ./your_app
```

Specifying resources

- You can call `salloc`, `sbatch` or `srun` with the following parameters

`-N` or `--nodes`	set number of nodes
`-n` or `--ntasks`	set number of tasks
`--mem=MB`	Specify the real memory required per node
`--exclusive`	Only your job is allowed on the nodes allocated to this job

- For debugging use `--mem=10GB`
  - You can share node with other users
  - It's easier to get node for you and for others
- For running benchmarks use `--exclusive`
  - To make sure only your job is running on the node
  - Other jobs can't influence your measurements

Git repository with source codes

- We prepared for you a git repository with source codes for this class
  - `https://github.com/oschenk/hpc2021`
- Clone the repository on both icsmaster and your laptop

```
$ git clone https://github.com/oschenk/hpc2021.git
```

- Later we will update the repository with source codes for other lectures and assignments
- To download the latest version use

```
$ git pull
```