

Parallel and High Performance Computing

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Solution Series 1

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Development and execution in an HPC environment

2 Remote access and file transfer

Exercise 1: Simple connection

To connect to the front node of a cluster if it is your first time.

- ssh <username>@<machine>
- ssh -l <username> <machine>

Front nodes:

- helvetios.hpc.epfl.ch
- izar.hpc.epfl.ch
- Connect to helvetios front node.
- Check the different folders /home, /scratch.

Exercise 2: Using scp

How to use scp / pscp.exe

- Send data to remote machine:
 - scp [-r] <local path> <username>@<remote>:<remote path>
- Retrieve data from remote machine:
 - scp [-r] <username>@<remote>:<remote path> <local path>
- Copy a file from your machine to the cluster.
- Retrieve a file from the cluster to your machine.

Exercise 3: Connection using keys

- Generate a pair of public/private key using ssh-keygen.
- Copy the public key ssh/id_rsa.pub using scp in a file called ssh/authorized_keys on the remote machine.
- Try to connect (it should not ask your password).

3 Compiling code on clusters

Exercise 4: Compilation

```
GCC: g++ -o <executable> <sources>
Intel: icpc -o <executable> <sources>
```

- Compile the code hello.c.
- Note: remember to load either gcc or intel modules, respectively, before invoking the compilations above.

Exercise 5: Separated compilation

```
g++ -c <source>
g++ -o <executable> <object 1> ... <object n>
```

- Enter the folder hello-separated-files
- Generate hello.o
- Generate greetings.o
- Generate hello from hello.o greetings.o

Exercise 6: Module command

- List all available modules
- Try g++ --version
- Load the module gcc
- Try again g++ --version
- Try icpc --version
- Load the intel module
- Try again icpc --version
- List the currently loaded modules

Exercise 7: Makefiles

- Enter the folder hello-makefile
- Read the Makefile
- Add the -Wall -Werror option to the compilation options
- Compile the code
- Introduce an error or a warning in the code (e.g., declare a non used variable).
- Compile the code

4 Submitting a job

Exercise 8: SLURM: first commands

- Check the queue state
- Use salloc to allocate one node with --qos=math-454 --account=math-454
- Try srun hostname, we will see this command more in detail in later exercise sessions
- Exit the allocation to note block resources: exit or Ctrl-d

Exercise 9: SLURM: command sbatch

- Write a script that runs the hello world code
- Try your script.

 note: in general you should not try your codes on the front node there is a debug partition for that
- Submit your script with sbatch using the QOS
- Try squeue -u <username> or Squeue
- A file named slurm-<jobid>.out should have been created, check its content Add the QOS as an option directly in the script
- Submit it again

5 Basics on GIT

Exercise 10: First step with Git

- If you do not have git installed, get it from https://git-scm.com/downloads or from your package manager
- Go on https://gitlab.epfl.ch and login with your EPFL credentials.
- Once connected go to the preferences page (left bar, user icon on top)
- In the **User settings** > **SSH Keys** menu add your public ssh key. This key will be used to connect to the git server through **ssh**.

Exercise 11: First steps with Git

- git clone <repo url> [local name]: Clone a repository
 git add <files...>: Stage modified/new files
 git commit -m "comment": Commit staged files
 git pull: Pull and merge remote modifications
 git push: Push the local modifications to the remote server
- git status: Check the local state
- Now you should be able to clone a repository

 Either create a repository or git clone git@gitlab.epfl.ch:math454-phpc/test-repo.git
- Create a file, use a filename that will not clash with the others
- Check the state of your working copy
- Add the file to the repository
- Commit your modifications
- Clone the same repository in a different folder
- Pull the potential modifications from the server
- Push your changes to the server

Exercise 12: Generate and solve conflicts

- Modify the file created in the previous exercise in both clones
- Commit this both modifications

- Pull and push in one of the clone
- Pull in the second clone, You should get a conflict

```
<<<<<<<<
One version
=======
Other version
>>>>>>>
```

- Check the local status
- Correct the conflict and commit using git commit -a
- Push the modifications

Exercise 13: Branches / merges

- git branch <name>: Create a new branch from the current HEAD
 git checkout <name>: Switch to the specified branch
- git merge <name>: Merge the branch specified in the current one
- git branch -d: Delete a branch
- git branch -a: List all branches
- git log: List the different commits of the current branch
- git log --graph --all: Show also the branches
- Create a branch with the name of your choice
- Modify a file and commit the changes
- Checkout the master branch
- Modify a file and commit the changes
- Merge the branch previously created in the master branch
- List all branches
- Print the logs of the different modifications
- Delete the merged branch

Exercise 14: Handle remotes

- git init --bare: Create a new server
- git remote add server <url>: Add a remote server
- git remote -v: Show the remotes configured
- git push <remote name>: Push to a given remote
- Connect on the front node of your favorite cluster
- Create a new folder that will contain your server
- In this folder initialize a new git server
- In one of the former clone of scitas-test add the new remote URL <cluster name>:<path to repo>
- List the remotes to see if everything looks correct
- Push the local content to the new server
- On the cluster clone this new server URL <path to repo>
- Note: The access permission on this new server are based on the file system permissions