Quick start using a CNCA supercomputer

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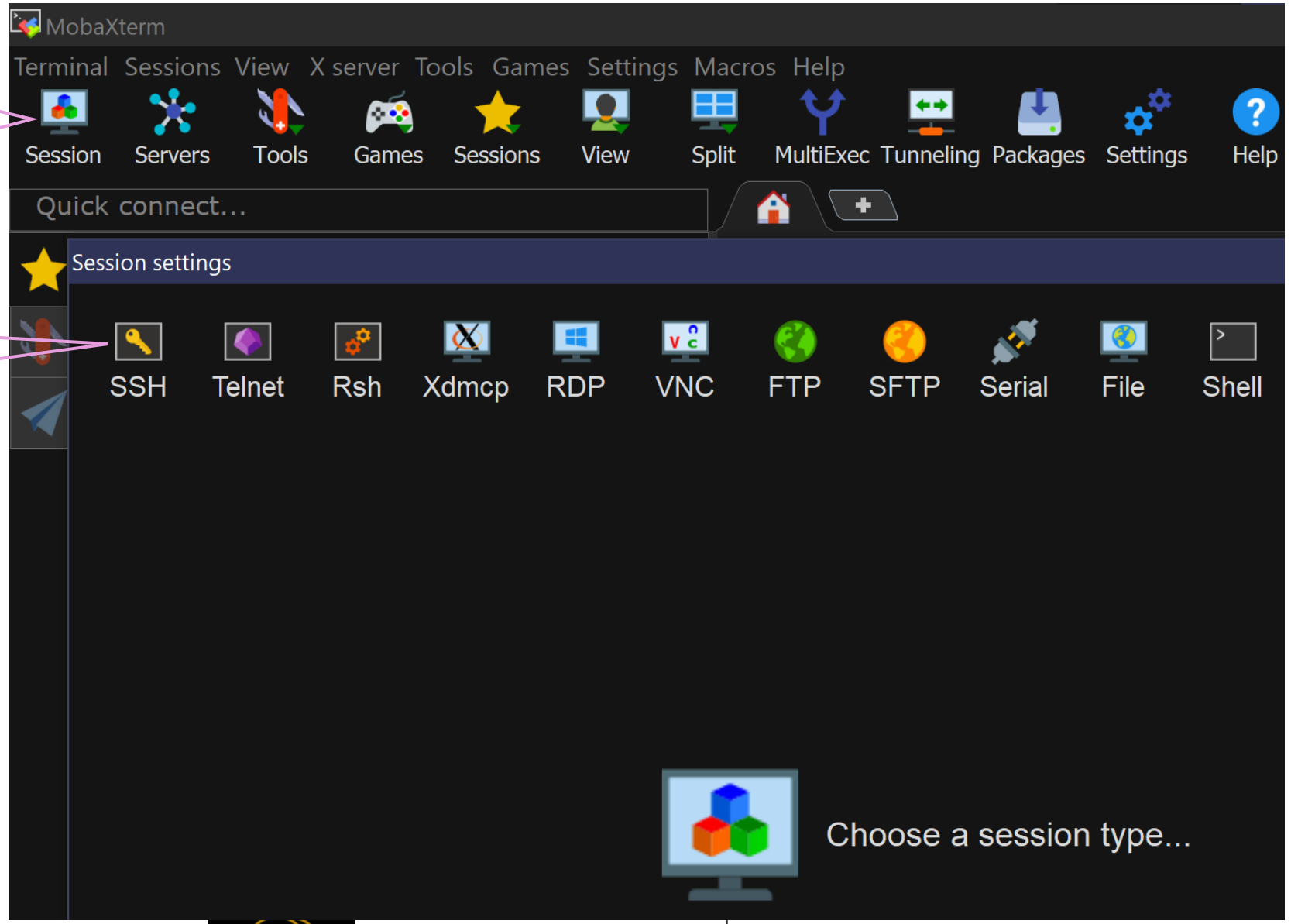
Tools

If using a Microsoft Windows OS:

- MobaXTerm Home Edition (available from https://mobaxterm.mobatek.net/)



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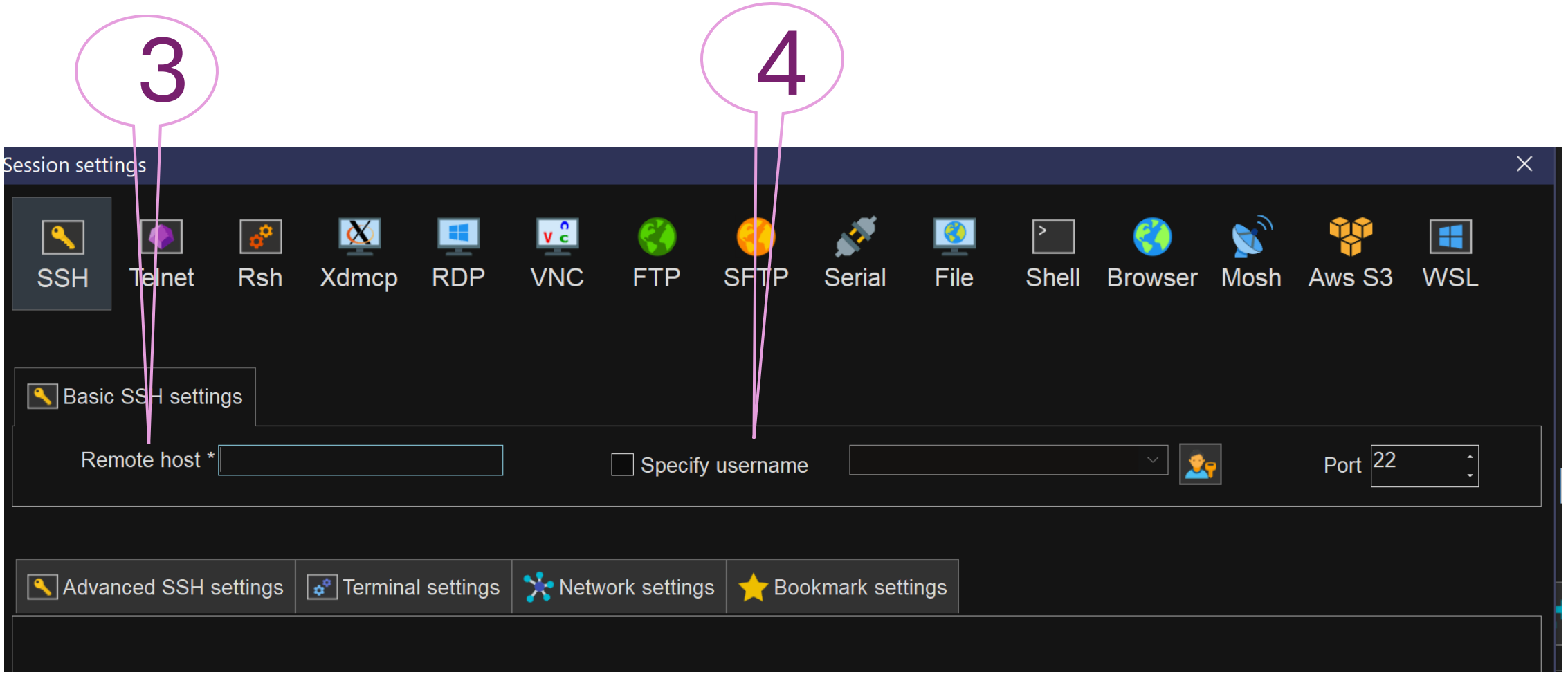

3 – cirrus.a.incd.pt 4 – the username

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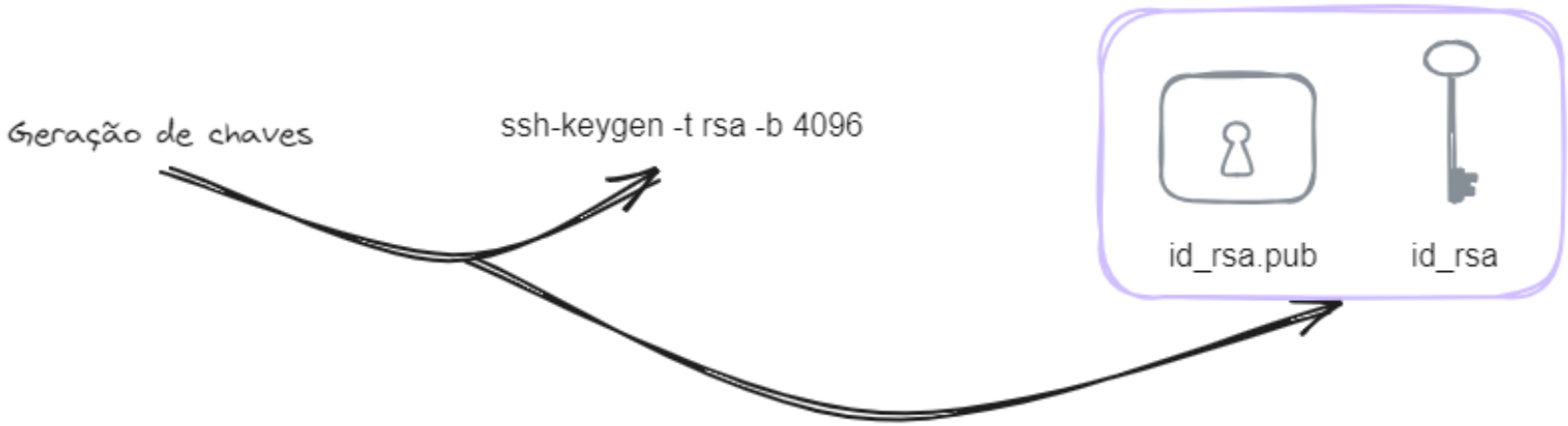
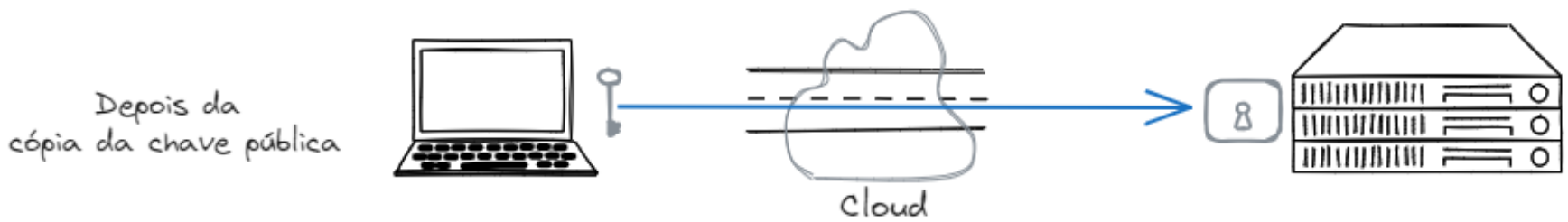
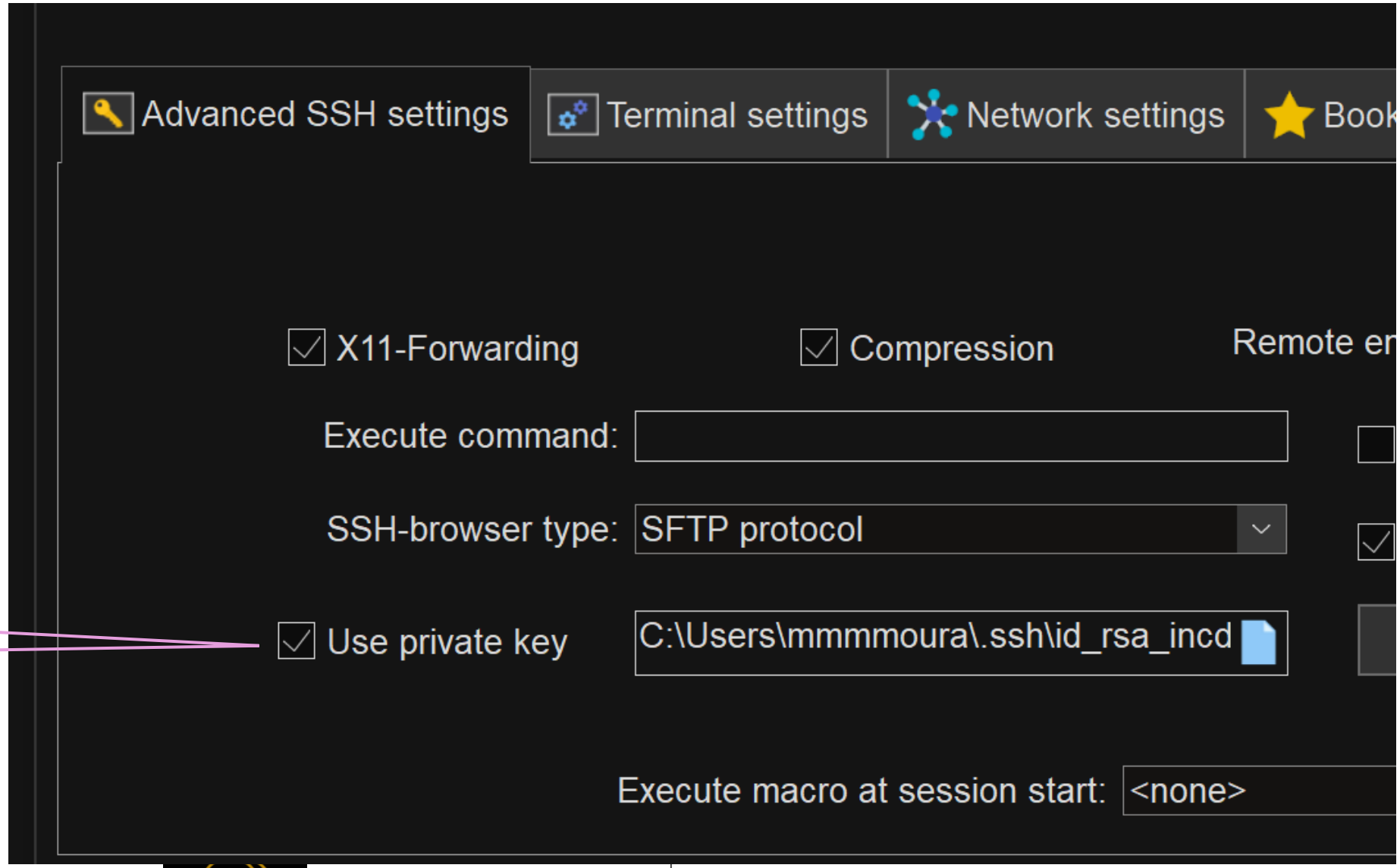
Cloud


Geração de chaves
ssh-keygen -t rsa -b 4096
id_rsa.pub
id_rsa


Depois da
cópia da chave pública
Cloud



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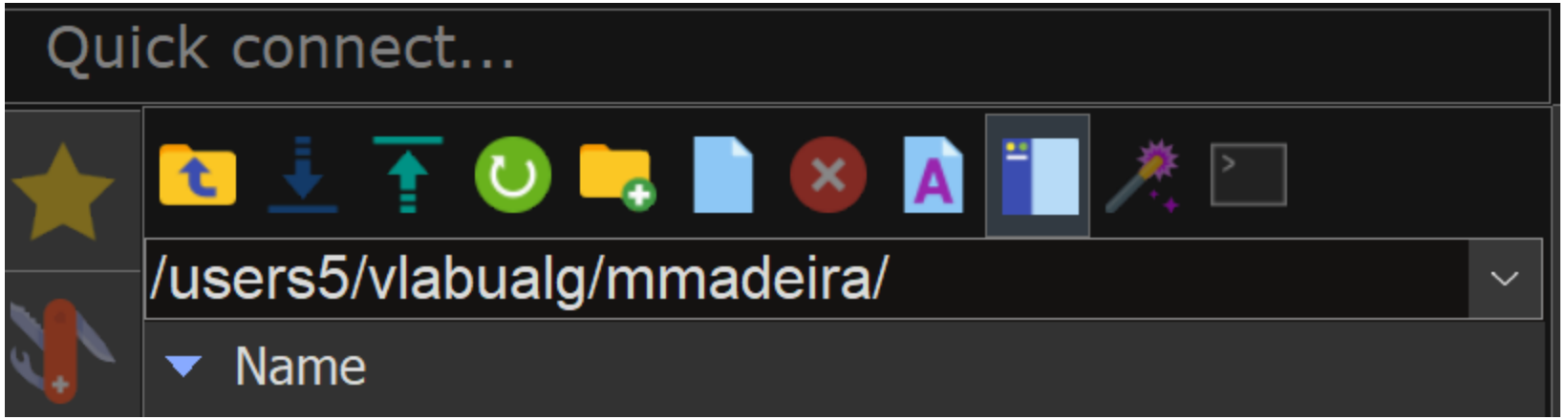
MobaXterm buttons



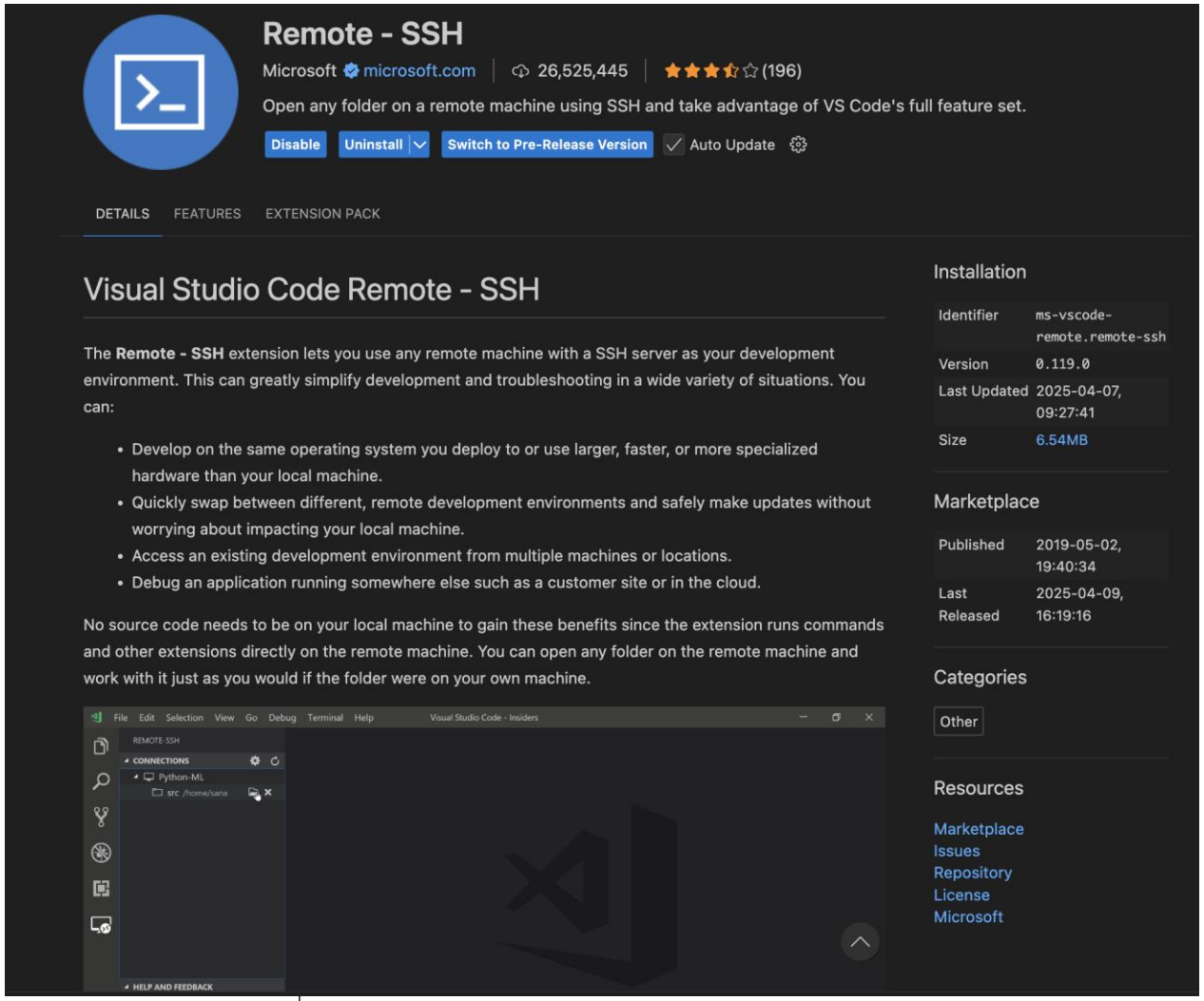
Tools

If using a Microsoft Windows OS:
- MobaXTerm Home Edition (available from https://mobaxterm.mobatek.net/)

Alternatives for Windows OS/MacOS:
- Visual Studio Code

Starting a remote session using VS Code

- Install the following extension if not already installed



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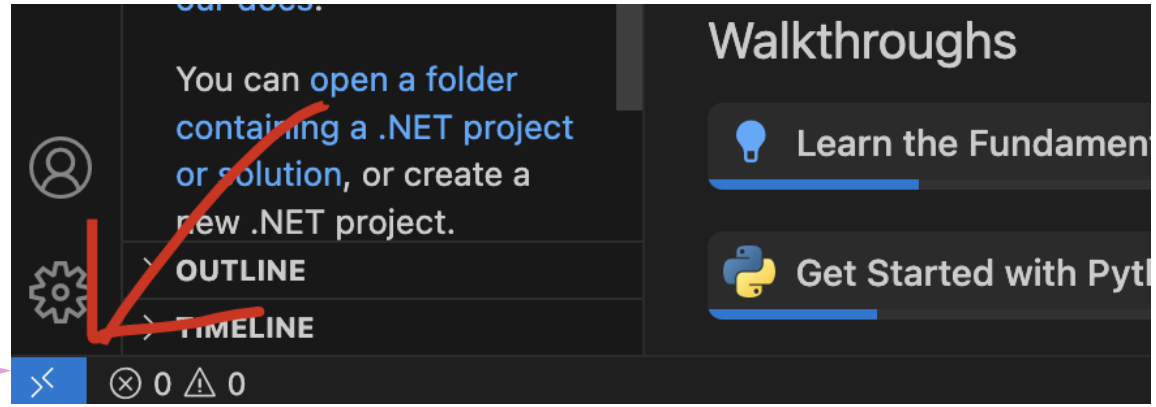
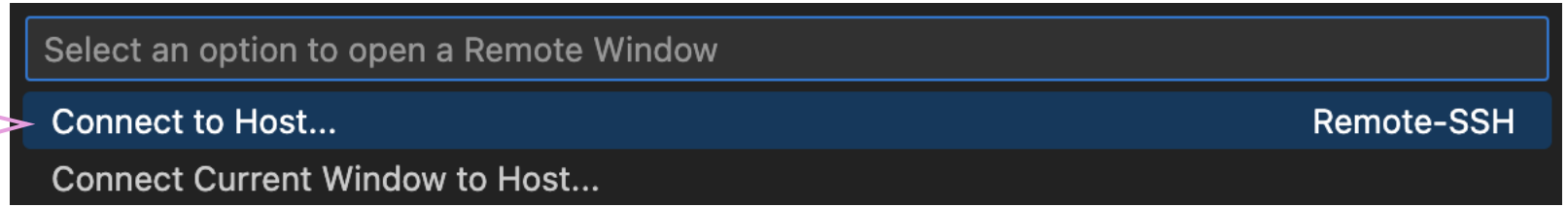
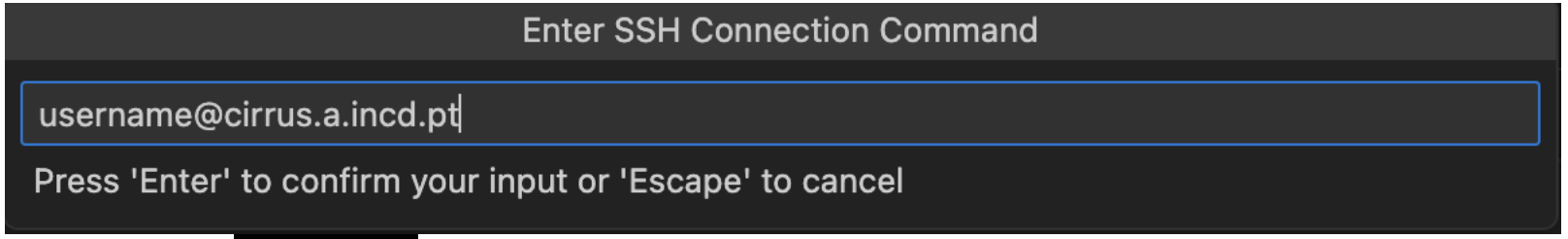


1



2



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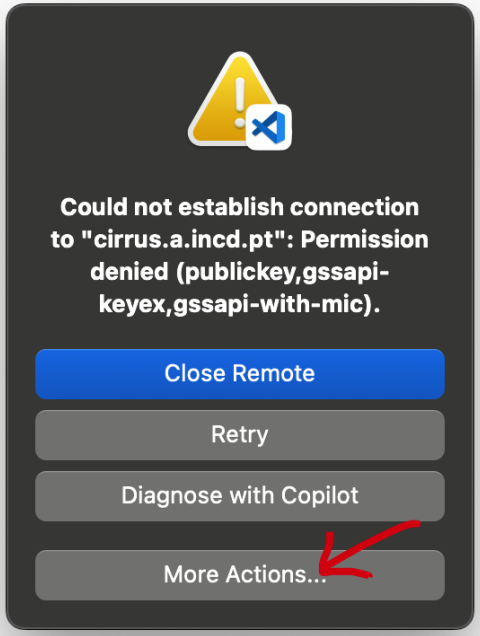
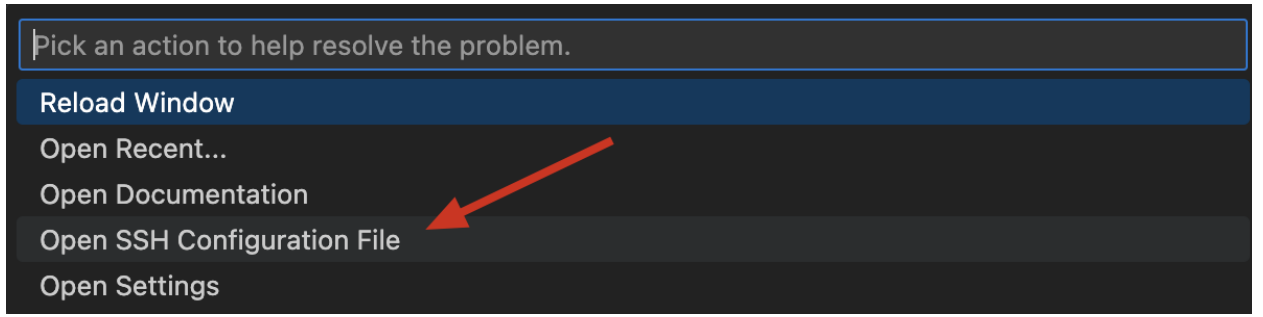
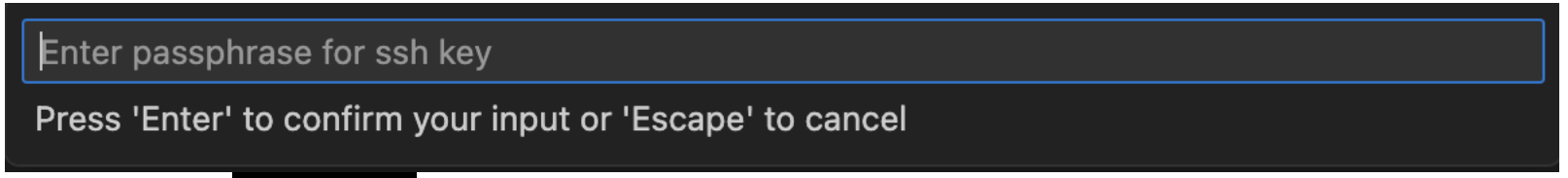
When encountering this error follow these steps:





Make sure your config includes:
IdentifyFile ~/Path/To/Private_Key

```
Host cirrus.a.incd.pt
  HostName cirrus.a.incd.pt
  User username
  IdentityFile ~/.ssh/id_rsa_incd
```



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Tools

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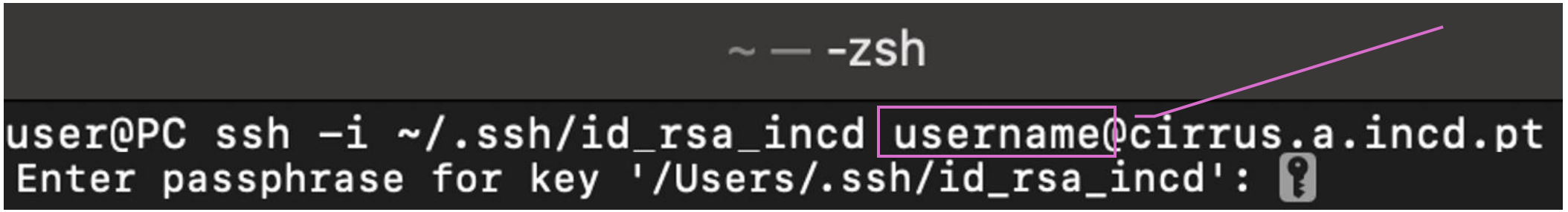
Alternatives for Windows OS/MacOS:
- Visual Studio Code

If using the terminal:

Define the username if different from your current user



After log in

```
##############################################################################
#                                                                            #
#      NCG INGRID Public Login Service                                       #
#      ingrid.helpdesk@lip.pt                                                #
#                                                                            #
# Auto logout after 12 hours with no activity                                #
#                                                                            #
# https://wiki.incd.pt/books/manage-jobs/chapter/manage-slurm-jobs           #
#                                                                            #
#                Max                                                         #
# PARTIT. NODES CORES NODETYPE                                               #
# hpc*       13 1728  AMD   EPYC 7643                          (default )    #
# fct        13 1728  AMD   EPYC 7643                          (reserved)    #
# short      18   36  AMD   EPYC 7643                    (30 min. max.)      #
# gpu         2  192  AMD   EPYC 7643  + NVidia A100                        #
# gpu         2  192  AMD   EPYC 7552  + NVidia Tesla V100s + Tesla T4      #
# gpu         2  192  AMD   EPYC 7552  + NVidia Tesla T4    + Tesla T4      #
#                                                                            #
# 01-04-2024: AlmaLinux 8 is now the official cluster                        #
#             old cluster user interface based on CentOS 7 available on:     #
#             cirrus7.a.incd.pt                                              #
#                                                                            #
##############################################################################
```

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Environment Management

Cirrus uses **environment modules** to manage compilers (GCC, Intel), MPI versions, Python, etc.

module avail	**# show available modules**
module spider	**# search for a module**
module load [module]	**# load a module**
module list	**# list all loaded modules**
module unload [module]	**# unload a module**
module purge	**# unload all modules**

Environment Management

module avail

```
------------------------------------------------------------------------ /cvmfs/sw.el8/modules/hpc/intel ------------------------------------------------------------------------
   gmxMMPBSA/1.6.3          intel/libs/gsl/2.7              intel/libs/libpng/1.6.39    intel/netcdf-cxx4/4.3.1       intel/openmpi/4.1.4
   intel/castep/24.1        intel/libs/hdf5/1.14.0          intel/libs/nlopt/2.7.1      intel/netcdf-fortran/4.6.1    intel/openmpi/4.1.6 (D)
   intel/gamess/2023-R2     intel/libs/hdf5/1.14.3    (D)   intel/mvapich2/2.3.7        intel/nwchem/nwchem-7.2.2
   intel/libs/blas/3.11.0   intel/libs/jemalloc/5.3.0       intel/netcdf-c/4.9.2        intel/openfoam-org/11
   intel/libs/fftw/3.3.10   intel/libs/lapack/3.11.0        intel/netcdf-cxx/4.2        intel/openfoam/2306

------------------------------------------------------------------------ /cvmfs/sw.el8/modules/gpu ------------------------------------------------------------------------
   cuda/10.2    cuda/11.8    cuda/12.6              (D)    nvhpc-nompi/23.1    tensorflow/2.14.0
   cuda/11.2    cuda/12.1    nvhpc-byo-compiler/23.1       nvhpc/23.1          tensorflow/2.18.0 (D)

------------------------------------------------------------------------ /cvmfs/sw.el8/modules/bio ------------------------------------------------------------------------
   R/4.2.2                          blast-plus/2.12.0         fastqc/0.12.1       (D)    htslib/1.17       (D)    picard/3.1.1             star/2.7.6a
   R/4.4.3                          blast-plus/2.14.1   (D)   figtree/0.12.1             igv/2.12.3               plink/1.07               star/2.7.10b       (D)
   admixture/1.3.0                  bowtie2/2.4.2             figtree/1.4.3       (D)    iqtree2/2.1.2            plink2/2.00a4.3          stringtie/3.0.0
   alphafold/2.3.2                  bowtie2/2.5.1       (D)   finestructure/4.1.1        iqtree2/2.2.2     (D)    popoolation2/1.201       suitesparse/7.8.2
   alphapulldown/2.0.1              bwa/0.7.17                freebayes/1.3.6            jellyfish/2.3.1          raxml/8.2.12             transdecoder/5.5.0
   autodock-gpu-develop/11.3.0      chimera/1.18              gatk/4.5.0.0               kallisto/0.50.1          salmon/1.10.3            transdecoder/5.7.1 (D)
   autodock-vina/1.2.3              chromopainter/0.0.4       grenepipe/0.14.0           mrbayes/3.2.7a           samtools/1.8             trimgalore/0.6.10
   bcftools/1.8                     cutadapt/4.4              hisat2/2.2.1               openbabel/3.0.0          samtools/1.17       (D)  trinity/2.14.0
   beagle/5.4                       eigensoft/8.0.0           hmmer/3.3.2                orca/6.0.1               sickle/1.33              vcftools/0.1.14
   bismark/0.23.0                   evigene/23.7.15           hmmer/3.4           (D)    orca/shared/5.0.4        sratoolkit/3.0.0         vcftools/0.1.16    (D)
   bismark/0.24.1             (D)   fastqc/0.11.9             htslib/1.8                 orca/static/5.0.4        stAIcalc                 vina-gpu/2.1

  Where:
   D:  Default Module

If the avail list is too long consider trying:

"module --default avail" or "ml -d av" to just list the default modules.
"module overview" or "ml ov" to display the number of modules for each name.
```

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Environment Management

module avail	# show available modules
module spider	# search for a module
module load [module]	# load a module
module list	# list all loaded modules
module unload [module]	# unload a module
module purge	# unload all modules

Environment Management

module spider

```
username@cirrus $ module spider python

----------------------------------------------------------------------------
  python:
----------------------------------------------------------------------------
     Versions:
        python/3.7
        python/3.8
        python/3.10
        python/3.11

----------------------------------------------------------------------------
  For detailed information about a specific "python" package (including how to load the modules)
use the module's full name.
  Note that names that have a trailing (E) are extensions provided by other modules.
  For example:

     $ module spider python/3.11
----------------------------------------------------------------------------
```

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Environment Management

module avail	# show available modules
module spider	# search for a module
module load [module]	**# load a module**
module list	**# list all loaded modules**
module unload [module]	**# unload a module**
module purge	**# unload all modules**

Environment Management

module load + **module list**

```
[username@cirrus $ module load python/3.10
[username@cirrus $ module list

Currently Loaded Modules:
  1) gcc-11.3   2) gcc11/openmpi/4.1.4   3) python/3.10
```

Environment Management

module avail	# show available modules
module spider	# search for a module
module load [module]	# load a module
module list	# list all loaded modules
module unload [module]	**# unload a module**
module purge	**# unload all modules**

Environment Management

module unload

```
[username@cirrus $ module unload python/3.10
[username@cirrus $ module list

Currently Loaded Modules:
  1) gcc-11.3   2) gcc11/openmpi/4.1.4
```

Environment Management

module avail	# show available modules
module spider	# search for a module
module load [module]	# load a module
module list	# list all loaded modules
module unload [module]	# unload a module
module purge	**# unload all modules**

Environment Management

module purge

```
[username@cirrus $ module purge
[username@cirrus $ module list
 No modules loaded
 username@cirrus $
```

Examples

Example 1 – distinguishing output from the job script and from the job load
Example 2 – what if something goes wrong: %j.err
Example 3 – MPI in C
Example 4 – OpenMP in C
Example 5 – MPI + OpenMP in C
Example 6 – GPU in C

Example 1 – Hello HPC World

hello.sh

```
#!/bin/bash

## If you want to be updated by mail
#SBATCH --mail-user=your_user_name@your_mailserver
#SBATCH --mail-type=ALL

#SBATCH --job-name=hello
#SBATCH --partition=hpc
#SBATCH --qos=cpuvlabualg
#SBATCH --ntasks=1

## The result of the job,
## respectively stdout e stderr
#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err

module load python
echo "Hello HPC World, from bash script!"
python3 hello.py
```

hello.py

```
#!/usr/bin/python3
# -*- coding: utf-8 -*-

"""
(c) Margarida Madeira e Moura, 2024
Demo just_hello

"""
print("Hello HPC World, from Python!")
```

Submit your job:

$ sbatch hello.sh

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Example 1 – Hello HPC World.out

```
username@cirrus $ cat hello.21772859.out
* ------------------------------------------------------------
* Running PROLOG for hello on Tue May 6 15:07:06 WEST 2025
*    JOB_NAME                : hello
*    JOB_ID                  : 21772859
*    JOB_PARTITION           : hpc
*    JOB_USER                : username
*    JOB_ACCOUNT             : vlabualg
*    JOB_QOS                 : normal
*    NODE_LIST               : hpc071
*    SLURM_NNODES            : 1
*    SLURM_NPROCS            : 1
*    SLURM_NTASKS            : 1
*    SLURM_CPUS_ON_NODE      : 1
*    SLURM_TASKS_PER_NODE    : 1
*    SLURM_JOB_CPUS_PER_NODE : 1
*    SLURM_MEM_PER_CPU       : 5000
*    SUBMIT_HOST             : cirrus.a.incd.pt
*    WORK_DIR                : /users5/vlabualg/examples/just_hello
*    JOB_SCRIPT              : /users5/vlabualg/examples/just_hello/hello.sh
* ------------------------------------------------------------
Hello HPC World, from bash script!
Hello HPC World, from Python!
username@cirrus $
```

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Example 2 – Hello HPC World.err

```
username@cirrus $ cat hello.21772948.out
* ------------------------------------------------------------
* Running PROLOG for hello on Tue May 13 05:47:13 WEST 2025
*    JOB_NAME                : hello
*    JOB_ID                  : 21772948
*    JOB_PARTITION           : hpc
*    JOB_USER                : username
*    JOB_ACCOUNT             : vlabualg
*    JOB_QOS                 : normal
*    NODE_LIST               : hpc071
*    SLURM_NNODES            : 1
*    SLURM_NPROCS            : 1
*    SLURM_NTASKS            : 1
*    SLURM_CPUS_ON_NODE      : 1
*    SLURM_TASKS_PER_NODE    : 1
*    SLURM_JOB_CPUS_PER_NODE : 1
*    SLURM_MEM_PER_CPU       : 5000
*    SUBMIT_HOST             : cirrus09.a.incd.pt
*    WORK_DIR                : /users5/vlabualg/username/examples/just_hello
*    JOB_SCRIPT              : /users5/vlabualg/username/examples/just_hello/hello.sh
* ------------------------------------------------------------
Hello HPC World, from bash script!
username@cirrus $
```

hello.id.out

```
username@cirrus $ cat hello.21772948.err
  File "/users5/vlabualg/examples/just_hello/hello.py", line 9
    print("Hello HPC World, from Python!)
          ^
SyntaxError: unterminated string literal (detected at line 9)
username@cirrus $
```

hello.id.err

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sacct

```
username@cirrus $ sacct
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
21772859           hello        hpc   vlabualg          1  COMPLETED      0:0
21772859.ba+       batch              vlabualg          1  COMPLETED      0:0
21772859.ex+      extern              vlabualg          1  COMPLETED      0:0
```

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sacct

```
username@cirrus08 just_hello]$ sacct --format=User,JobID,Jobname,partition,state,time,start,end,elapsed,MaxRss,MaxVMSize,nnodes,ncpus,nodelist -u username --start 2024-12-10
     User JobID           JobName  Partition      State  Timelimit               Start                 End    Elapsed     MaxRSS  MaxVMSize   NNodes      NCPUS        NodeList
--------- ------------ ---------- ---------- ---------- ---------- ------------------- ------------------- ---------- ---------- ---------- -------- ---------- ---------------
username 19093687          hello        hpc  COMPLETED 4-00:00:00 2024-12-10T16:13:15 2024-12-10T16:13:16   00:00:01                               1          1          hpc067
         19093687.ba+      batch             COMPLETED            2024-12-10T16:13:15 2024-12-10T16:13:16   00:00:01          0       956K        1          1          hpc067
         19093687.ex+     extern             COMPLETED            2024-12-10T16:13:15 2024-12-10T16:13:16   00:00:01          0          0        1          1          hpc067
         19093687.0      python3             COMPLETED            2024-12-10T16:13:16 2024-12-10T16:13:16   00:00:00          0         4K        1          1          hpc067
username 19093704          hello        hpc  COMPLETED 4-00:00:00 2024-12-10T16:22:57 2024-12-10T16:22:58   00:00:01                               1          1          hpc067
         19093704.ba+      batch             COMPLETED            2024-12-10T16:22:57 2024-12-10T16:22:58   00:00:01          0         4K        1          1          hpc067
         19093704.ex+     extern             COMPLETED            2024-12-10T16:22:57 2024-12-10T16:22:58   00:00:01          0          0        1          1          hpc067
username 19093715     brute_for+        hpc  COMPLETED 4-00:00:00 2024-12-10T16:31:07 2024-12-10T16:31:10   00:00:03                               1          1          hpc067
         19093715.ba+      batch             COMPLETED            2024-12-10T16:31:07 2024-12-10T16:31:10   00:00:03          0        20K        1          1          hpc067
         19093715.ex+     extern             COMPLETED            2024-12-10T16:31:07 2024-12-10T16:31:10   00:00:03          0          0        1          1          hpc067
username@cirrus08 just_hello]$
```

To list the waiting queue, use:
squeue

To cancel a job, use:
scancel <JOBID>

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```
username@cirrus08 just_hello]$ sacct --format=User,JobID,Jobname,partition,state,time,start,end,elapsed,MaxRss,MaxVMSize,nnodes,ncpus,nodelist -u username --start 2024-12-10
     User JobID           JobName  Partition      State  Timelimit               Start                 End    Elapsed     MaxRSS  MaxVMSize   NNodes      NCPUS        NodeList
--------- ------------ ---------- ---------- ---------- ---------- ------------------- ------------------- ---------- ---------- ---------- ------- ---------- ---------------
username 19093687          hello        hpc  COMPLETED 4-00:00:00 2024-12-10T16:13:15 2024-12-10T16:13:16   00:00:01                              1          1          hpc067
         19093687.ba+      batch             COMPLETED            2024-12-10T16:13:15 2024-12-10T16:13:16   00:00:01          0       956K       1          1          hpc067
         19093687.ex+     extern             COMPLETED            2024-12-10T16:13:15 2024-12-10T16:13:16   00:00:01          0          0       1          1          hpc067
         19093687.0      python3             COMPLETED            2024-12-10T16:13:16 2024-12-10T16:13:16   00:00:00          0         4K       1          1          hpc067
username 19093704          hello        hpc  COMPLETED 4-00:00:00 2024-12-10T16:22:57 2024-12-10T16:22:58   00:00:01                              1          1          hpc067
         19093704.ba+      batch             COMPLETED            2024-12-10T16:22:57 2024-12-10T16:22:58   00:00:01          0         4K       1          1          hpc067
         19093704.ex+     extern             COMPLETED            2024-12-10T16:22:57 2024-12-10T16:22:58   00:00:01          0          0       1          1          hpc067
username 19093715     brute_for+        hpc  COMPLETED 4-00:00:00 2024-12-10T16:31:07 2024-12-10T16:31:10   00:00:03                              1          1          hpc067
         19093715.ba+      batch             COMPLETED            2024-12-10T16:31:07 2024-12-10T16:31:10   00:00:03          0        20K       1          1          hpc067
         19093715.ex+     extern             COMPLETED            2024-12-10T16:31:07 2024-12-10T16:31:10   00:00:03          0          0       1          1          hpc067
username@cirrus08 just_hello]$
```

To list the waiting queue, use:
squeue

```
username@cirrus $ squeue
JOBID    PARTITION NAME       USER        ST TIME       NODES CPUS TRES_PER_NODE  NODELIST

21772922 hpc       hello      username    PD 0:00       1     4    N/A
```

To cancel a job, use:
scancel <JOBID>

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Parallel Programming Models: MPI vs OpenMP

Feature	OpenMP	MPI
Memory Model	Shared memory (same node)	Distributed memory (multi-node)
Typical Use	Multithreading	Multiprocessing
Syntax	Pragmas / directives	Function calls
Communication	Implicit (via memory)	Explicit (via messages)
Cirrus Usage Example	--cpus-per-task=4	--ntasks=4

Example 3 – Hello_MPI

```c
#include <mpi.h>
#include <stdio.h>

int main(int argc, char** argv) {
    MPI_Init(NULL, NULL);

    int world_size;
    MPI_Comm_size(MPI_COMM_WORLD, &world_size);

    int world_rank;
    MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);

    printf("Hello from process %d of %d\n", world_rank, world_size);

    MPI_Finalize();
}
```

```
#!/bin/bash
## If you want to be updated by mail
#SBATCH --mail-user=youremail@example.com
#SBATCH --mail-type=ALL

#SBATCH --job-name=hello
#SBATCH --partition=hpc     # Partition to submit to
#SBATCH --nodes=1           # Number of nodes
#SBATCH --ntasks=4          # Total number of MPI tasks
#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err

module load gcc11/openmpi/4.1.4

mpicc -o hello_mpi hello_mpi.c

mpirun ./hello_mpi
```

Submit your job:

$ sbatch hello_mpi.sh

Example 3 – Hello_MPI

```
* ------------------------------------------------------------
* Running PROLOG for hello on Thu Apr 10 07:48:02 WEST 2025
*    JOB_NAME                : hello
*    JOB_ID                  : 21003264
*    JOB_PARTITION           : hpc
*    JOB_USER                : username
*    JOB_ACCOUNT             : vlabualg
*    JOB_QOS                 : normal
*    NODE_LIST               : hpc080
*    SLURM_NNODES            : 1
*    SLURM_NPROCS            : 4
*    SLURM_NTASKS            : 4
*    SLURM_CPUS_ON_NODE      : 4
*    SLURM_TASKS_PER_NODE    : 4
*    SLURM_JOB_CPUS_PER_NODE : 4
*    SLURM_MEM_PER_CPU       : 5000
*    SUBMIT_HOST             : cirrus.a.incd.pt
*    WORK_DIR                : /users5/vlabualg/username/examples
*    JOB_SCRIPT              : /users5/vlabualg/username/examples/hello_mpi.sh
* ------------------------------------------------------------
Hello from process 3 of 4
Hello from process 0 of 4
Hello from process 1 of 4
Hello from process 2 of 4
```

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Example 4 – Hello_OpenMP

```bash
#!/bin/bash
## If you want to be updated by mail
#SBATCH --mail-user=youremail@example.com
#SBATCH --mail-type=ALL

#SBATCH --job-name=omp_hello          # Job name
#SBATCH --partition=hpc               # Partition to submit to
#SBATCH --qos=normal                     # Adjust to a valid QoS for your project
#SBATCH --nodes=1                     # Run on a single node
#SBATCH --ntasks=1                    # Only one task (OpenMP uses threads, not tasks)
#SBATCH --cpus-per-task=4             # Number of OpenMP threads
#SBATCH --output=%x.%j.out            # Standard output
#SBATCH --error=%x.%j.err             # Standard error

module load gcc-11.3                      # Load GCC with OpenMP support

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

gcc -fopenmp -o omp_hello omp_hello.c

# Run the program
./omp_hello
```

Submit your job:
$ sbatch omp_hello.sh

```c
#include <omp.h>
#include <stdio.h>
#include <stdlib.h>

int main (int argc, char *argv[])
{
int nthreads, tid;

/* Fork a team of threads giving them their own copies of variables */
#pragma omp parallel private(nthreads, tid)
  {

  /* Obtain thread number */
  tid = omp_get_thread_num();
  printf("Hello World from thread = %d\n", tid);

  /* Only master thread does this */
  if (tid == 0)
    {
    nthreads = omp_get_num_threads();
    printf("Number of threads = %d\n", nthreads);
    }

  }  /* All threads join master thread and disband */
}
```

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Example 4 – Hello_OpenMP

```
* ------------------------------------------------------------------
* Running PROLOG for omp_hello on Fri Apr 11 05:02:46 WEST 2025
*    JOB_NAME                : omp_hello
*    JOB_ID                  : 21013153
*    JOB_PARTITION           : hpc
*    JOB_USER                : username
*    JOB_ACCOUNT             : vlabualg
*    JOB_QOS                 : normal
*    NODE_LIST               : hpc070
*    SLURM_NNODES            : 1
*    SLURM_NPROCS            : 1
*    SLURM_NTASKS            : 1
*    SLURM_CPUS_ON_NODE      : 4
*    SLURM_TASKS_PER_NODE    : 1
*    SLURM_JOB_CPUS_PER_NODE : 4
*    SLURM_MEM_PER_CPU       : 5000
*    SUBMIT_HOST             : cirrus08.a.incd.pt
*    WORK_DIR                : /users/vlabualg/username/examples/OpenMP
*    JOB_SCRIPT              : /users/vlabualg/username/examples/OpenMP/omp_hello.sh
* ------------------------------------------------------------------
Hello World from thread = 0
Number of threads = 4
Hello World from thread = 2
Hello World from thread = 3
Hello World from thread = 1
```

Example 5 – Hello_Hybrid

```c
#include <mpi.h>
#include <omp.h>
#include <stdio.h>

int main(int argc, char *argv[]) {
    int rank, size;

    // Initialize MPI
    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank); // process ID
    MPI_Comm_size(MPI_COMM_WORLD, &size); // total number of processes

    // Parallel OpenMP region inside each MPI process
    #pragma omp parallel
    {
        int tid = omp_get_thread_num();              // thread ID
        int nthreads = omp_get_num_threads();        // threads in this process

        printf("Hello from thread %d out of %d in MPI process %d out of %d\n",
               tid, nthreads, rank, size);
    }

    MPI_Finalize(); // Finalize MPI
    return 0;
}
```

Example 5 – Hello_Hybrid

```
#!/bin/bash
## If you want email notifications
#SBATCH --mail-user=youremail@example.com
#SBATCH --mail-type=ALL

#SBATCH --job-name=hybrid_hello         # Job name
#SBATCH --partition=hpc                 # Partition
#SBATCH --qos=normal                    # Adjust to valid QoS for your project
#SBATCH --nodes=1                       # Number of nodes
#SBATCH --ntasks=2                      # Number of MPI processes
#SBATCH --cpus-per-task=4               # Threads per MPI process (OpenMP)
#SBATCH --output=%x.%j.out              # Standard output
#SBATCH --error=%x.%j.err               # Standard error

module load gcc11/openmpi/4.1.4         # Load MPI + OpenMP-capable compiler

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo "Compiling hybrid hello with mpicc and OpenMP support..."
mpicc -fopenmp -o hello_hybrid hello_hybrid.c

echo "Running hybrid hello..."
mpirun ./hello_hybrid
```

Submit your job:

$ sbatch hello_hybrid.sh

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Example 5 – Hello_Hybrid

```
* ------------------------------------------------------------
* Running PROLOG for hybrid_hello on Fri Apr 11 05:20:30 WEST 2025
*    JOB_NAME               : hybrid_hello
*    JOB_ID                 : 21013306
*    JOB_PARTITION          : hpc
*    JOB_USER               : username
*    JOB_ACCOUNT            : vlabualg
*    JOB_QOS                : normal
*    NODE_LIST              : hpc070
*    SLURM_NNODES           : 1
*    SLURM_NPROCS           : 2
*    SLURM_NTASKS           : 2
*    SLURM_CPUS_ON_NODE     : 8
*    SLURM_TASKS_PER_NODE   : 2
*    SLURM_JOB_CPUS_PER_NODE : 8
*    SLURM_MEM_PER_CPU      : 5000
*    SUBMIT_HOST            : cirrus08.a.incd.pt
*    WORK_DIR               : /users/vlabualg/username/examples/hybrid
*    JOB_SCRIPT             : /users/vlabualg/username/examples/hybrid/hello_hybrid.sh
* ------------------------------------------------------------
Compiling hybrid hello with mpicc and OpenMP support...
Running hybrid hello...
Hello from thread 0 out of 4 in MPI process 0 out of 2
Hello from thread 2 out of 4 in MPI process 0 out of 2
Hello from thread 0 out of 4 in MPI process 1 out of 2
Hello from thread 2 out of 4 in MPI process 1 out of 2
Hello from thread 3 out of 4 in MPI process 1 out of 2
Hello from thread 1 out of 4 in MPI process 1 out of 2
Hello from thread 3 out of 4 in MPI process 0 out of 2
Hello from thread 1 out of 4 in MPI process 0 out of 2
```

Example 6 – Hello_GPU

```c
#include <stdio.h>

__device__ const char *STR = "HELLO WORLD!";
const char STR_LENGTH = 12;

__global__ void hello()
{
    printf("%c\n", STR[threadIdx.x % STR_LENGTH]);
}

int main(void)
{
    int num_threads = STR_LENGTH;
    int num_blocks = 1;
    hello<<<num_blocks,num_threads>>>();
    cudaDeviceSynchronize();

    return 0;
}
```

```
#!/bin/bash

#SBATCH --mail-user=youremail@example.com
#SBATCH --mail-type=ALL

#SBATCH --job-name=hello00
#SBATCH --partition=gpu
#SBATCH --qos=gpuvlabualg

#SBATCH --gres=gpu

#SBATCH --output=%x.%j.out
#SBATCH --error=%x.%j.err

module purge
module load cuda/12.6
nvcc -o hello hello.cu

echo `hostname`
srun ./hello
```

Submit your job:
$ sbatch hello.sh

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Example 6 – Hello_GPU

```
* ------------------------------------------------------------
* Running PROLOG for hello00 on Mon Nov 25 19:41:43 WET 2024
*    JOB_NAME                : hello00
*    JOB_ID                  : 18969544
*    JOB_PARTITION           : gpu
*    JOB_USER                : ilyass
*    JOB_ACCOUNT             : vlabualg
*    JOB_QOS                 : gpuvlabualg
*    JOB_GPUS                : 0
*    NODE_LIST               : hpc060
*    SLURM_NNODES            : 1
*    SLURM_CPUS_ON_NODE      : 1
*    SLURM_TASKS_PER_NODE    : 1
*    SLURM_JOB_CPUS_PER_NODE : 1
*    SLURM_GPUS_ON_NODE      : 1
*    SUBMIT_HOST             : cirrus09.a.incd.pt
*    WORK_DIR                : /users5/vlabualg/ilyass/GPU
*    JOB_SCRIPT              : /users5/vlabualg/ilyass/GPU/hello.sh
*
*    GPU 0                   : Name                Tesla V100S-PCIE-32GB
*                            : SN                  1421220029960
*                            : Driver              560.35.03
*                            : Memory              32494 MBytes
*                            : Multiprocessors     80
*                            : Cores/Multiprocessor 64
*                            : Cores               5120
* ------------------------------------------------------------
```

```
hpc060.a.incd.pt
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```

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References

Software used in the presentation:

- mobaxterm, vscode
- Environment software
- Python
- Mpi
- Openmp
- CUDA

Codes from:

- https://developer.nvidia.com/cuda-education
- https://hpc-tutorials.llnl.gov/

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Examples adapted from LLNL HPC Tutorials

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