First steps on the clusters

This page explains what to do after having successfully connected to one of the clusters.

Step-by-step guide

1. What is installed on the clusters

   To see the list of installed software (modules), load the compiler and the MPI implementation you intend to use and do
   module spider

   Open Source or proprietary?

   On our systems, we have compiled and installed software modules either with Intel Compiler and Intel MPI or GCC and MVAPICH2 and those are the only supported compiler/MPI combinations.

2. Getting the examples

   Once you have logged in to the machine, we suggest you download the examples with the command:

   git clone https://c4science.ch/diffusion/SCEXAMPLES/scitas-examples.git

   Here is a list of our examples:
Advanced
- FakeJobArray
- JobArray
- JobArray2
- OccupyOneNode

Basic
- hello.run
- MPI
- one_GPU.run
- Pi_integral
- Pi_mc

Modules
- Abaqus
- adf
- Ansys
- Comsol
- cp2k
- cpmd
- fluent
- gaussian
- GPU_amber
- GPU_gromacs
- maple
- Mathematica
- Matlab
- molpro
- oommf
- ParaView
- R
- spark
- tensorflow
- vasp

3. Running the examples

Enter the directory scitas-examples and choose the example to run by navigating the folders. We have three categories of examples: Basic (examples to get you started), Advanced (including hybrid jobs and job arrays) and Modules (specific examples of installed software).

To run an example, e.g. HPL-mpi of the Advanced category, do:

```
sbatch --partition=debug hpl.run
```

or, if you do not wish to run on the debug partition,

```
sbatch hpl.run
```

4. Running interactive jobs

An interactive job allows you to connect directly to a compute node and type commands that run on the compute node. Simply type the command `Sinteract` from the login node to start an interactive session with 1 core and 4GB of memory for 30 minutes.

You can use the parameters to `Sinteract` (for help type: `interact -h`) to request more resources or more time.

options:
-c cores cores per task (default: 1)
-n tasks number of tasks (default: 1)
-t time as hh:mm:ss (default: 00:30:00)
-m memory as #[K|M|G] (default: 4G)
-p partition (default: parallel)
-a account (default: phpc2017)
-q qos as [normal|gpu|gpu_free|mic|...] (default: )
-g resource as [gpu|mic][:count] (default is empty)
-r reservation reservation name (default is empty)

e.g. to run an mpi job with 16 processes for one hour using 32 GB of memory on a debug node:

Sinteract -n 16 -t 01:00:00 -m 32G -p debug

On the Izar cluster, the -g option is necessary to request the desired number of GPUs. For example:
Sinteract -g gpu:1

Related articles

- Connecting to the clusters
- First steps on the clusters
- Ask for help
- Using software on the SCITAS clusters