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