

InstitutsClusterII: Brief Information for new Users

Steinbuch Centre for Computing (SCC), KIT

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This publication shall facilitate the beginning of work with InstitutsClusterII (IC2) at Steinbuch Centre for Computing (SCC) of KIT. InstitutsClusterII is a distributed memory parallel computer with 480 16-way so-called thin compute nodes where each node has two Intel Xeon Octa-Core sockets with 2.6 GHz frequency and 64 GB local memory, 5 16-way so-called fat compute nodes where each node has four Intel Xeon Octa-Core sockets with 2.67 GHz frequency and 512 GB local memory and 2 16-way login nodes where each node has two Intel Xeon Octa-Core sockets with 2.6 GHz frequency and 64 GB local memory. All nodes comprise local disks and network adapters and are connected by an InfiniBand 4X QDR interconnect. The fast and scalable parallel file system Lustre is supported via an independent InfiniBand interconnect.

If you run into troubles when working on IC2 please contact the ic-hotline (see chapter 9) or responsible staff members of SCC.

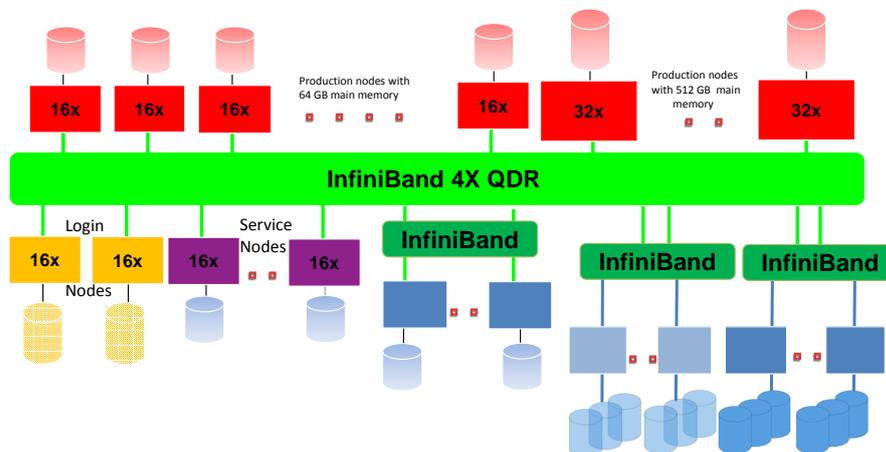


Figure 1: Configuration of InstitutsClusterII (IC2)

1 Configuration

InstitutsClusterII (IC2) is a distributed memory parallel computer with 480 so-called thin compute nodes and 5 so-called fat compute nodes. The thin nodes are equipped with 16 cores, 64 GB main memory, local disks and network adapters, whereas the fat nodes are equipped with 32 cores, 512 GB main memory, bigger local disks and network adapters. The operating system is the same as on the login nodes.

The parallel file system Lustre is used for globally visible user data like the home- and a work-directory. The environment variable `$HOME` points to the home-directory and `$WORK` points to the work-directory. The home-directories of InstitutsClusterII and HC3 are the same.

2 Login

IC2 has 2 dedicated login nodes. Both login nodes are equipped with 16 cores, 64 GB main memory, local disks and network adapters. The operating system Linux (SLES 11) runs on the login nodes (and all other nodes), so that working on a single node of IC2 is comparable with working on a workstation.

2.1 Login on a Login Node

There are 2 login nodes on IC2 each with 16 cores. The selection of the login node is done automatically. If you are connecting another time to a login node, the sessions might run on the other (login) node of IC2. Only the secure shell `ssh` is allowed to login. Other commands like `telnet` or `rlogin` are not allowed for security reasons.

A connection to IC2 can be established by the command

```
ssh kit-account@ic2.scc.kit.edu
```

Be aware that the password can not be changed directly on IC2! Please change it on the web site:

<https://intra.kit.edu> (Link: Meine Daten)

If you are using OpenSSH (usually installed on Linux based systems) and you want to use a GUI-based application on IC2 like e.g. the debugger DDT, you should use the command

```
ssh -X kit-account@ic2.scc.kit.edu
```

with the option `-X`.

3 Copying Data onto IC2

You will see the home-directory of HC3 and InstitutsClusterII if you have an account on one of them. There is additional file space that can be accessed by using the environment variable `$WORK`.

To achieve a high security level the files must be transferred by the secure copy command `scp` or the command `rsync` that again uses the command `scp`.

The command `rsync` is used similar to the command `scp`. In the following recommendation the specified directory and all subdirectories of the computer you are logged in are copied recursively to the user typed instead of `user-id` on IC2 into the directory `Copy_of_dir`.

```
rsync -av local_computer_directory/ user-id@ic2.scc.kit.edu:Copy_of_dir
```

To guarantee consistent data neither batch jobs on your workstation nor batch jobs on IC2 should run while the data are copied.

Further informations on the command `rsync` are available by manual pages (`man rsync`).

4 Choosing your User Environment

IC2 supports the use of Modules software to make it easier to configure and modify the user environment. Modules software enables dynamic modification of your environment by the use of modulefiles. A modulefile contains information to configure the shell for an application.

We provide modules for all supported compilers, debuggers, tools and libraries. Modulefiles that are available on IC2 can be viewed by the command `module avail[able]`. To view the modulefiles that are currently loaded in your environment, issue the command `module list`. By default the following modulefiles are available:

- `dot` adding the current directory to your environment variable `PATH`,
- `intel` loading the Intel C/C++ and Fortran compiler in a stable version and
- `openmpi` loading OpenMPI in the latest stable version.

You can load a modulefile in to your environment to enable easy access to software that you want to use by executing the command `module add <modulefile>`. To unload a modulefile that is currently loaded the command `module rm <modulefile>` must be executed.

If e.g. you want to use the GNU compiler instead of the Intel compiler (this is the default compiler), you just have to type `module add gcc`. The command `module rm intel` can be omitted because unloading of an arbitrary loaded compiler will be done automatically within our Module environment when loading another compiler.

5 Compiler and Parallelization Environment

On IC2 different compilers are available for the programming languages Fortran90/95, C, C++ and Java. The most important parallelization environments are the Message Passing Interface MPI for jobs running on many nodes and OpenMP for jobs running within one node.

The default compiler is the Intel compiler called by `ifort` for Fortran programs, `icc` for C programs and `icpc` for C++ programs. The GNU compiler suite can also be chosen for both Fortran and C/C++; exchanging of the compiler can simply be done by the command `module add gcc`.

For the compilation of message passing applications with MPI there are special compiler scripts like `mpif77` for Fortran77 programs, `mpif90` for Fortran95 programs, `mpicc` for C programs and `mpiCC` for C++ programs.

Further information on compilers and the parallelization environment can be found in *InstitutsClusterII User Guide*.

6 Batch System JMS

A few nodes are provided for interactive operations. All other nodes can only be accessed by the batch system JMS using SLURM. Batch jobs are submitted by the command `job_submit`. A required parameter is the name of the executable for jobs running on a single core or rather `"mpirun name_of_executable"` for jobs running on more than one core or a shellscript; required options are the required resources like number of cores, CPU-time and main memory. Information on `job_submit` can be displayed by the command `job_submit -H` and actual limitations of the job queues by the command `job_info`.

7 User Guide

All manuals on InstitutsClusterII are available online in PDF-format. The substantial local adjustments on usage of IC2 are outlined in InstitutsClusterII User Guide.

8 Important Addresses for Online Informations

- **InstitutsClusterII Website at Steinbuch Centre for Computing**
<http://www.scc.kit.edu/dienste/ic2.php>
- **InstitutsClusterII User Guide**
<http://www.scc.kit.edu/scc/docs/IC/ug/ugic2.pdf>
- **Homepage of HPC and Clustercomputing**
<http://www.scc.kit.edu/dienste/hpc.php>
- **Homepage of Steinbuch Centre for Computing (SCC)**
<http://www.scc.kit.edu/>
- **Maintenance and Repair Information**
<http://www.scc.kit.edu/dienste/stoerungen.php>

9 Contact

- **IC2 Hotline**
ic2-hotline@lists.kit.edu
Phone: +49 721 608-48011