Minimum Requirements

Hardware

Abinit requires at least 1 CPU, 4Gb of RAM and 4Gb of disk space to perform the calculations of the tutorials and the test suite. The most complex calculations may require more than 10,000 CPUs, more than 1Tb of RAM, and a few Tb of disk space.

Any recent desktop or laptop computer is in principle able to perform calculations with Abinit.

Compilers

To be correctly built, Abinit requires a working development environment providing both a C and a Fortran compiler.

On desktop and laptop computers, we recommend:

- the GNU Compiler Collection;
- the Intel Parallel Studio XE Toolchain;

which we have extensively tested.

Since the choice is up to the system administrator on HPC environments, we also support the IBM and NAG compilers.

Parallelism

OpenMP and multithreading

If your computer has multiple cores, you might want to take benefit from all of them instead of running Abinit in serial mode. There are 2 ways of achieving it: OpenMP and Multithreading.

Various parts of Abinit have been optimized to work with OpenMP. In addition, the latter is usually directly provided by compilers and does not require the installation of additional libraries. The build system of Abinit is able to set the corresponding compile flags automatically for a dozen popular compilers if you ask for OpenMP at configure time. Should this not be the case for you, please consult the documentation of your compilers and contact us once you have found and successfully tried the flags to provide.

Abinit does not provide support for multithreading but can benefit from multithreaded versions of its external dependencies, as long as the multithreaded operations are entirely performed externally. Please note that Abinit is not developed with thread-safety in mind and use multithreading with a lot of care.
MPI

GPU

From: https://wiki.abinit.org/ - Tips for ABINIT users and developers


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