

# CASINO installation instructions

## for single- and multi-processor PCs

The CASINO package is designed to be installed in the user's home directory and compiled from the source. This guarantees portability and flexibility, but clearly it also requires a bit of initial setup. This is a quick installation guide for single- and multi-processor PCs without a batch-queue system.

Notice that you need a UNIX environment to use CASINO. It is possible to install CASINO under Windows using Cygwin. Some people have reported success under Mac OS X with the g95 compiler, but we haven't checked this personally. Here we will assume that you have a Linux PC. For other cases, see the CASINO manual.

## 1 Single processor machines

For single processor machines you have to follow three steps.

### 1.1 Install a Fortran 90 compiler

In terms of performance, the Intel Fortran compiler (as of version 9.1) is the best choice. However you have to pay for it (unless you are a self-funded student, basically). The free alternatives are the g95 compiler and the GCC's gfortran compiler. Here we will assume you want the latter, which we recommend. If your Linux distribution is one of:

- Fedora Core, version  $\geq 3$
- OpenSuSE, version  $\geq 10$
- Ubuntu, version  $\geq 7$

then you can fetch the relevant package from your installation sources and install it automatically with the provided system tools. Otherwise, google for "gfortran" and follow the links. Do not use any gfortran version prior to 4.1, they're buggy. Version 4.3 (latest) is faster than older versions, but you'll need to install it by hand (NB, the installation process is very simple, so do consider the option).

### 1.2 Set up the environment

CASINO needs to know what your architecture and compiler are, so you will need to edit your shell's *runtime configuration* (rc) file in order to set new environment variables. If you use the `bash` shell, edit the file `~/.bashrc`, add the lines

```
export QMC_ARCH=linuxpc-gcc
export QMC_TMPDIR=$HOME/temp
export PATH=$PATH:$HOME/CASINO/bin_qmc/utils/$QMC_ARCH
```

at the end of the file, save it, and type `source ~/.bashrc`. If you use the `tcsh` shell<sup>1</sup>, edit the file `~/.cshrc`, add the lines

```
setenv QMC_ARCH linuxpc-gcc
setenv QMC_TMPDIR $HOME/temp
setenv path=($path $HOME/CASINO/bin_qmc/utils/$QMC_ARCH)
```

at the end of the file, save it, and type `source ~/.cshrc`.

### 1.3 Compile CASINO

Extract the CASINO distribution in your home directory by issuing `cd ~ ; tar xzvf CASINO_v2.1_beta.tar.gz`. Then type `cd ~/CASINO/src ; make`. Finally type `cd ~/CASINO/utils ; make`.

---

<sup>1</sup>Changing shells is as easy as typing `chsh` on the prompt and entering `/bin/bash` as your new shell. This doesn't affect CASINO, of course, but it will increase your happiness level by 50% or more.

## 2 Multi-processor machines

Most new computers come with more than one processor (usually two, sometimes four). If you want to take full advantage of your SMP machine, follow these instructions instead (the single-processor installation is possible, but it will only allow one-node runs).

### 2.1 Install a Fortran 90 compiler

Proceed as for the single-processor case.

### 2.2 Install an MPI library

Let's install OpenMPI (we'd be interested in hearing how other MPI packages work, as we haven't tried installing them on PCs).

- Download OpenMPI from [www.open-mpi.org](http://www.open-mpi.org)
- Extract from the archive and change into the newly created directory
- Type

```
./configure CC=gcc FC=gfortran F77=gfortran --prefix=/opt/openmpi/gfortran
make all
sudo make install
make clean
```

- Edit your `.bashrc` file, and add `/opt/openmpi/gfortran/bin` to your `PATH`, and `/opt/openmpi/gfortran/lib` to your `LD_LIBRARY_PATH`.

### 2.3 Set up the environment

Proceed as in the single-processor case, except that you have to choose `linuxpc-gcc-parallel` as your `QMC_ARCH`.

### 2.4 Compile CASINO

Proceed as in the single-processor case.

## 3 Other stuff

CASINO has a bunch of useful utilities (redundantly enough) to perform a variety of tasks, and some of these may require additional packages on your computer. To get the best out of CASINO, install the following packages:

- Grace - a plotting tool
- Gnuplot - another plotting tool (NB, need version  $\geq 4$ )
- BC - a command-line calculator which is used by the `ve` utility

Enjoy!