

# DelPhi Compilation Manual

DelPhi Development Team 2018

2018

## 1 Linux users

Current DelPhi C++ (Version 8.1) allows users to compile the DelPhi program into different versions by turning on and off appropriate flags from a single distribution. Ensure that the following software are installed before you compile DelPhi program:

- C++ compiler such as GCC 5.4.0 and above
- boost library installed in /usr/include and its path is recognized in the user environment
- OpenMPI (v 2.1.1 and above) or MPICH (v 3.1.4 and above) if OMP and MPI version of DelPhi, respectively, executable is desired.

To compile the DelPhi C++, after downloading the DelPhi source code from DelPhi website, type the following:

1. For the regular executable (simple single thread/CPU version), type:

```
$ tar -xf Delphicpp_v8.1_Linux.tar
$ cd Delphicpp_v8.1_Linux
$ cd Release
$ make all
```

An executable named **delphicpp\_release** will be generated when the compilation process is finished.

2. A multi-threading OpenMP executable (able to utilize the maximum computing power of a multi-core CPU to accelerate the calculations):

First open the folder 'src' located in the source code's folder and in the file of **src/interface/environment.h** uncomment the line `///#define PARALLEL_OMP`. Then type the following:

```
$ tar -xf Delphicpp_v8.1_Linux.tar
$ cd Delphicpp_v8.1_Linux
$ cd Release_omp
$ make all
```

An executable named **delphicpp\_omp\_release** will be generated when the compilation process is finished.

3. A multi-CPU MPI executable (able to utilize the computing power of CPUs across multiple computing nodes on one HPC cluster):

First open the folder 'src' located in the source code's folder and in the file of **src/interface/environment.h** uncomment the line `///#define PARALLEL_MPI`. Then type the following:

```
$ tar -xf Delphicpp_v8.1_Linux.tar
$ cd Delphicpp_v8.1_Linux
$ cd Release_mpi
$ make all
```

An executable named **delphicpp\_mpi\_release** will be generated when the compilation process is finished.

**To developers:** Compilation folders (Debug, Debug\_omp, and Debug\_mpi) are also provided to developers so that DelPhi can be compiled into corresponding "Debug" versions, which can be loaded into a debugger for finding the bugs, and studying how the program is executed, etc..

**Regular users are NOT suggested to compile the DelPhi program in these folders!**

**Running the MPI version of the DelPhi program on a HPC cluster:** Users who are interested in running the MPI version of DelPhi program are advised to contact your administrator first before compiling and running the MPI version of the DelPhi program on your HPC cluster. A sample PBS script to submit computing job on the Palmetto cluster ([www.palmetto.clemson.edu](http://www.palmetto.clemson.edu)) is provided in below for your easy reference but it is subject to necessary changes depending on your own computing environment.

```
#PBS -q workq
#PBS -l select=3:ncpus=1:mpiprocs=1:mem=120gb:interconnect=fdr
#PBS -l walltime=72:00:00

### -----
### BEGINNING OF EXECUTION
### -----

cd $PBS_O_WORKDIR
module purge
module add gcc/5.4.0 mpich/3.1.4

export DELPHIEXEC=""

/bin/time -v mpiexec -n 3 $DELPHIEXEC <delphi_parameter_file> > <log_file>
```

## 2 Mac users

Current DelPhi C++ (Version 8.1) allows users to compile the DelPhi program on Mac systems. Ensure that the following software are installed before you compile DelPhi program:

1. C++ compiler such as GCC 5.4.0 and above
2. boost library installed in /usr/include and its path is recognized in the user environment

To compile the DelPhi C++, after downloading the DelPhi source code from DelPhi website, type the following:

```
$ tar -xf Delphicpp_v8.1_Mac.tar
$ cd Delphicpp_v8.1_Mac
$ cd Release_mac
$ make all
```

An executable named **delphicpp\_release** will be generated when the compilation process is finished.

**To developers using Mac:** Compilation folder (Debug) is also provided to developers so that DelPhi can be compiled into corresponding 'Debug' versions, which can be loaded into a debugger for finding the bugs, and studying how the program is executed, etc.

**Regular users are NOT suggested to compile the DelPhi program in these folders!**