QuantaPlus Manual and User Guide

Mustafa Ahmed Ali Ahmed

Department of Physics, Faculty of Pure and Applied Sciences,
International University of Africa, Khartoum, Sudan

Mohammed Maher Abdelrahim Mohammed

Dipartimento di Fisica dell'Università della Calabria
I-87036 Arcavacata di Rende, Cosenza, Italy

INFN - Gruppo collegato di Cosenza
I-87036 Arcavacata di Rende, Cosenza, Italy

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Abstract

QuantaPlus is a modern general-purpose multi-threaded quantum computing mechanics written in C++17 and composed solely of header files.

Contents

Introduction

High-performance numerical algorithms play a central role in theoretical calculations and analysis of experimental data in (non-relativistic) quantum mechanical problems, which is the problem of predicting the properties of systems of several quantum particles at a much larger scale [**?**]. The latter is a crucial ingredient in the field of today's computational physics due to its technological interest and potential applications in various problems of fundamental importance in quantum chemistry, condensed matter physics, and materials science.

Files, installation and testroutines

The package can be downloaded from github repository. There are ready to install libaries there for some cases, but in general it is better to compile it for your own system. C++ can have a large overhead in calling classes and functions compared to FORTRAN. Therefore always compile the library with optimization. The interfaces are as much as possible defined with the keyword const to allow the compiler to optimize more efficiently.

Files

The gzipped tarred file (chiron.vvvv.tar.gz) will produce a directory chiron.vvvv with a number of subdirectories. vvvv is version information. The created directory is called the main directory in the remainder. The main directory contains the files COPYING, INSTRUCTIONS, GUIDELINES and a Makefile.

The subdirectory doc contains the documentation. The latest published article about CHIRON, this manual (manual.tex), a list of files (filelist.txt) and a summary of things added since earlier versions (Changelog.vvv.to.www.txt). The subdirectory lib will after compiling contain the compiled libraries libjbnumlib.a and libchiron.a.

The subdirectory include contains all the needed header files. The subdirectory src contains the source files. test contains the testing and example programs. testoutputs contains the output the testprograms should produce. Typically for each subject xxx there are files xxx.h, xxx.cc, testxxx.cc and testxxx.dat in the respective directories. There are a few extra files around as well. These typically contain inputs needed or large sets of constants.

Installation

The main steps are to run make in the main directory. This should produce the files libjbnumlib.a and libchiron.a and also copy them to the lib subdirectory. You might have to change the variables CC, CFLAGS and CFLAGTESTS. CC should specify the C++ compiler and the options to be used for everything. CFLAGS can be used to specify addi- tional options in compiling the libraries and CFLAGTESTS to specify additional options for the testing programs. "make clean" can be used to remove many of the files created during compiling. The actual installation is by putting the contents of the include directory somewhere in the include path of your compiler and the two files libjbnumlib.a and libchiron.a somewhere in the library path. For many C++ compilers the paths are given in the environment variables CPLUS INCLUDE PATH and LIBRARY PATH respectively.

testroutines

For every file xxx.h and xxx.cc included for chiron there is a testing/example code testxxx.cc in the subdirectory test. These can be compiled using "make testxxx" in the main directory. Executing the resulting file a.out should then produce output identical (up to the precision specified and possible randomly generated cases) to the file testxxx.dat in the subdirectory testoutputs.