

Quad Double computation package
Copyright (C) 2003-2012

=====
Revision date: 13 Mar 2012

Authors:

Yozo Hida U.C. Berkeley yozo@cs.berkeley.edu
Xiaoye S. Li Lawrence Berkeley Natl Lab xiaoye@nersc.gov
David H. Bailey Lawrence Berkeley Natl Lab dhbailey@lbl.gov

C++ usage guide:

Alex Kaiser Lawrence Berkeley Natl Lab adkaiser@lbl.gov

This work was supported by the Director, Office of Science, Division of Mathematical, Information, and Computational Sciences of the U.S. Department of Energy under contract number DE-AC02-05CH11231.

This work was supported by the Director, Office of Science, Division of Mathematical, Information, and Computational Sciences of the U.S. Department of Energy under contract numbers DE-AC03-76SF00098 and DE-AC02-05CH11231.

*** IMPORTANT NOTES:

See the file COPYING for modified BSD license information.
See the file INSTALL for installation instructions.
See the file NEWS for recent revisions.
See the file README.pdf for additional information. The file is mostly identical, but
 but includes additional tables on constructors and constants.

Outline:

- I. Introduction
- II. Directories and Files
- III. C++ Usage
- IV. Fortran Usage
- V. Note on x86-Based Processors (MOST systems in use today)

I. Introduction

This package provides numeric types of twice the precision of IEEE double (106 mantissa bits, or approximately 32 decimal digits) and four times the precision of IEEE double (212 mantissa bits, or approximately 64 decimal digits). Due to features such as operator and function overloading, these facilities can be utilized with only minor modifications to conventional C++ and Fortran-90 programs.

In addition to the basic arithmetic operations (add, subtract, multiply, divide, square root), common transcendental functions such as the exponential, logarithm, trigonometric and hyperbolic functions are also included. A detailed description of the algorithms used is available in the docs subdirectory (see docs/qd.ps). An abridged version of this paper, which was presented at the ARITH-15 conference, is also available in this same directory (see docs/arith15.ps).

II. Directories and Files

There are six directories and several files in the main directory of this distribution, described below

src This contains the source code of the quad-double and double-double library. This source code does not include inline functions, which are found in the header files in the include directory.

include This directory contains the header files.

fortran This directory contains Fortran-90 files.

tests This directory contains some simple (not comprehensive) tests.

docs This directory contains two papers describing the algorithms.

config This directory contains various scripts used by the configure script and the Makefile.

C++ Usage:

Please note that all commands refer to a Unix-type environment such as Mac OSX or Ubuntu Linux using the bash shell.

A. Building

To build the library, first run the included configure script by typing

```
./configure
```

This script automatically generates makefiles for building the library and selects compilers and necessary flags and libraries to include. If the user wishes to specify compilers or flags they may use the following options.

CXX	C++ compiler to use
CXXFLAGS	C++ compiler flags to use
CC	C compiler to use (for C demo program)
CFLAGS	C compiler flags to use (for C demo program)
FC	Fortran 90 compiler
FCFLAGS	Fortran 90 compiler flags to use
FCLIBS	Fortran 90 libraries needed to link with C++ code.

For example, if one is using GNU compilers, configure with:

```
./configure CXX=g++ FC=gfortran
```

The Fortran and C++ compilers must produce compatible binaries. On some systems additional flags must be included to ensure that portions of the library are not built with 32 and 64 bit object files. For example, on 64-Bit Mac OSX 10.6 (Snow Leopard) and 10.7 (Lion) the correct configure line using GNU compilers is:

```
./configure CXX=g++ FC=gfortran FCFLAGS=-m64
```

To build the library, simply type

```
make
```

and the automatically generated makefiles will build the library including archive files.

To allow for easy linking to the library, the user may also wish to install the archive files to a standard place. To do this type:

```
make install
```

This will also build the library if it has not already been built. Many systems, including Mac and Ubuntu Linux systems, require administrator privileges to install the library at such standard places. On such systems, one may type:

```
sudo make install
```

instead if one has sufficient access.

The directory "tests" contains programs for high precision quadrature and integer-relation detection. To build such programs, type:

```
make demo
```

in the "tests" directory.

B. Linking

The simplest way to link to the library is to install it to a standard place as described above, and use the `-l` option. For example

```
g++ compileExample.cpp -o compileExample -l qd
```

One can also use this method to build with make. A file called "compileExample.cpp" and the associated makefile "makeCompileExample" illustrate the process.

A third alternative is to use a link script. If one types "make demo" in the test directory, the output produced gives guidance as to how to build the files. By following the structure of the compiling commands one may copy the appropriate portions, perhaps replacing the filename with an argument that the user can include at link time. An example of such a script is as follows:

```
g++ -DHAVE_CONFIG_H -I. -I../include -I../include -O2 -MT $1.o -MD -MP -MF
.deps/qd_test.Tpo -c -o $1.o $1.cpp
mv -f .deps/$1.Tpo .deps/$1.Po
g++ -O2 -o $1 $1.o ../src/libqd.a vèlm
```

To use it, make the link script executable and type:

```
./link.scr compileExample
```

Note that the file extension is not included because the script handles all extensions, expecting the source file to have the extension ".cpp" .

Similarly, a script for compiling fortran programs may be constructed as follows. In the fortran directory, type "make quadts". This compiles the Fortran program tquadts.f, links with all necessary library files, and produces the executable "quadts". As this is being done, all flags and linked libraries are displayed. For instance, on many Mac systems, presuming g++-4.0 was defined for C++ and gfortran for F90, the following is output:

```
gfortran -O2 -ffree-form -c -o tquadts.o tquadts.f
g++-4.0 -O2 -Wall -o quadts tquadts.o second.o libarprec_f_main.a
libarprecmod.a ../src/libarprec.a
-L/usr/local/lib/gcc/i386-apple-darwin9.0.0/4.3.0
-L/usr/local/lib/gcc/i386-apple-darwin9.0.0/4.3.0/../../../../ -lgfortranbegin
-lgfortran
```

Thus a general compile-link script (which could be saved in an executable file named "complink.scr") is the following:

```
gfortran -O2 -ffree-form -c -o $1.o $1.f
g++-4.0 -O2 -Wall -o $1 $1.o second.o libarprec_f_main.a \
libarprecmod.a ../src/libarprec.a \
-L/usr/local/lib/gcc/i386-apple-darwin9.0.0/4.3.0 \
-L/usr/local/lib/gcc/i386-apple-darwin9.0.0/4.3.0/../../../../ -lgfortranbegin \
-lgfortran
```

Note that if the .f90 suffix is used for Fortran-90 source files, the -ffree-form flag can be omitted, and the first line above ends with "\$1.f90". Remember to type "chmod +x complink.scr". Then, for instance, a program named "prog.f90" could be compiled and linked by merely typing "./comlink.scr prog".

C. Programming techniques

As much as possible, operator overloading is included to make basic programming as much like using standard typed floating-point arithmetic. Changing many codes should be as simple as changing type statements and a few other lines.

i. Constructors

To create dd_real and qd_real variables calculated to the proper precision, one must use care to use the included constructors properly. Many computations in which variables are not explicitly typed to multiple-precision may be evaluated with double-precision arithmetic. The user must take care to ensure that this does not cause errors. In particular, an expression such as 1.0/3.0 will be evaluated to double precision before assignment or further arithmetic. Upon assignment to a multi-precision variable, the value will be zero padded. This problem is serious and potentially difficult to debug. To avoid this, use the included constructors to force arithmetic to be performed in the full precision requested.

For a table with descriptions, please see the included file README.pdf

ii. Included functions and Constants

Supported functions include assignment operators, comparisons, arithmetic and assignment operators, and increments for integer types. Standard C math functions such as exponentiation, trigonometric, logarithmic, hyperbolic, exponential and rounding functions are included. As in assignment statements, one must be careful with implied typing of constants when using these functions. Many codes need particular conversion for the power function, which is frequently used with constants that must be explicitly typed for multi-precision codes.

Many constants are included, which are global and calculated upon initialization. The

following list of constants is calculated for both the `dd_real` and `qd_real` classes separately.
Use care to select the correct value.

For a table with descriptions, please see the included file `README.pdf`

ii. Conversion of types

Static casts may be used to convert constants between types. One may also use constructors to return temporary multi-precision types within expressions, but should be careful, as this will waste memory if done repeatedly. For example:

```
    qd_real y ;  
    y = sin( qd_real(4.0) / 3.0 ) ;
```

C-style casts may be used, but are not recommended. Dynamic and reinterpret casts are not supported and should be considered unreliable. Casting between multi-precision and standard precision types can be dangerous, and care must be taken to ensure that programs are working properly and accuracy has not degraded by use of a misplaced type-conversion.

D. Available precision, Control of Precision Levels,

The library provides greatly extended accuracy when compared to standard double precision. The type `dd_real` provides for 106 mantissa bits, or about 32 decimal digits. The type `qd_real` provides for 212 mantissa bits, or about 64 decimal digits.

Both the `dd_real` and `qd_real` values use the exponent from the highest double-precision word for arithmetic, and as such do not extend the total range of values available. That means that the maximum absolute value for either data type is the same as that of double-precision, or approximately 10^{308} . The precision near this range, however, is greatly increased.

To ensure that arithmetic is carried out with proper precision and accuracy, one must call the function `fpu_fix_start` before performing any double-double or quad-double arithmetic. This forces all arithmetic to be carried out in 64-bit double precision, not the 80-bit precision that is found on certain compilers and interferes with the existing library.

```
    unsigned int old_cw;  
    fpu_fix_start(&old_cw);
```

To return standard settings for arithmetic on one's system, call the function `ifpu_fix_end`.
For example:

```
    fpu_fix_end(&old_cw);
```

E. I/O

The standard I/O stream routines have been overloaded to be fully compatible with all included data types. One may need to manually reset the precision of the stream to obtain full output. For example, if 60 digits are desired, use:

```
cout.precision(60) ;
```

When reading values using `cin`, each input numerical value must start on a separate line. Two formats are acceptable:

1. Write the full constant
3. Mantissa e exponent

Here are three valid examples:

```
1.1
3.14159 26535 89793
123.123123e50
```

When read using `cin`, these constants will be converted using full multi-precision accuracy.

IV. Fortran-90 Usage

NEW (2007-01-10): The Fortran translation modules now support the complex datatypes `"dd_complex"` and `"qd_complex"`.

Since the quad-double library is written in C++, it must be linked in with a C++ compiler (so that C++ specific things such as static initializations are correctly handled). Thus the main program must be written in C/C++ and call the Fortran 90 subroutine. The Fortran 90 subroutine should be called `f_main`.

Here is a sample Fortran-90 program, equivalent to the above C++ program:

```
subroutine f_main
  use qdmodule
  implicit none
  type (qd_real) a, b
```

```

integer*4 old_cw

call f_fpu_fix_start(old_cw)
a = 1.d0
b = cos(a)**2 + sin(a)**2 - 1.d0
call qdwrite(6, b)
stop
end subroutine

```

This verifies that $\cos^2(1) + \sin^2(1) = 1$ to 64 digit accuracy.

Most operators and generic function references, including many mixed-mode type combinations with double-precision (ie real*8), have been overloaded (extended) to work with double-double and quad-double data. It is important, however, that users keep in mind the fact that expressions are evaluated strictly according to conventional Fortran operator precedence rules. Thus some subexpressions may be evaluated only to 15-digit accuracy. For example, with the code

```

real*8 d1
type (dd_real) t1, t2
...
t1 = cos (t2) + d1/3.d0

```

the expression $d1/3.d0$ is computed to real*8 accuracy only (about 15 digits), since both $d1$ and $3.d0$ have type real*8. This result is then converted to dd_real by zero extension before being added to $\cos(t2)$. So, for example, if $d1$ held the value 1.d0, then the quotient $d1/3.d0$ would only be accurate to 15 digits. If a fully accurate double-double quotient is required, this should be written:

```

real*8 d1
type (dd_real) t1, t2
...
t1 = cos (t2) + ddreal (d1) / 3.d0

```

which forces all operations to be performed with double-double arithmetic.

Along this line, a constant such as 1.1 appearing in an expression is evaluated only to real*4 accuracy, and a constant such as 1.1d0 is evaluated only to real*8 accuracy (this is according to standard Fortran conventions). If full quad-double accuracy is required, for instance, one should write

```

type (qd_real) t1
...
t1 = '1.1'

```


The quotes enclosing 1.1 specify to the compiler that the constant is to be converted to binary using quad-double arithmetic, before assignment to t1. Quoted constants may only appear in assignment statements such as this.

To link a Fortran-90 program with the C++ qd library, it is recommended to link with the C++ compiler used to generate the library. The Fortran 90 interface (along with a C-style main function calling f_main) is found in qdmod library. The qd-config script installed during "make install" can be used to determine which flags to pass to compile and link your programs:

"qd-config --fcflags" displays compiler flags needed to compile your Fortran files.

"qd-config --fclibs" displays linker flags needed by the C++ linker to link in all the necessary libraries.

A sample Makefile that can be used as a template for compiling Fortran programs using quad-double library is found in fortran/Makefile.sample.

F90 functions defined with dd_real arguments:

Arithmetic: + - * / **

Comparison tests: == < > <= >= /=

Others: abs, acos, aint, anint, asin, atan, atan2, cos, cosh, dble, erf, erfc, exp, int, log, log10, max, min, mod, ddcsshf (cosh and sinh), ddcssnf (cos and sin), ddranf (random number generator in (0,1)), ddrtf (n-th root), sign, sin, sinh, sqr, sqrt, tan, tanh

Similar functions are provided for qd_real arguments (with function names qdcsshf, qdcssnf, qdranf and qdnrtf instead of the names in the list above).

Input and output of double-double and quad-double data is done using the special subroutines ddread, ddwrite, qdread and qdwrite. The first argument of these subroutines

is the Fortran I/O unit number, while additional arguments (as many as needed, up to 9

arguments) are scalar variables or array elements of the appropriate type.

Example:

```
integer n
type (qd_real) qda, qdb, qdc(n)
...
call qdwrite (6, qda, qdb)
do j = 1, n
    call qdwrite (6, qdc(j))
enddo
```

Each input values must be on a separate line, and may include D or E exponents. Double-double and quad-double constants may also be specified in assignment statements by enclosing them in quotes, as in

```
...
type (qd_real) pi
...
pi =
"3.14159265358979323846264338327950288419716939937510582097494459230"
...
```

Sample Fortran-90 programs illustrating some of these features are provided in the f90 subdirectory.

V. Note on x86-Based Processors (MOST systems in use today)

The algorithms in this library assume IEEE double precision floating point arithmetic. Since Intel x86 processors have extended (80-bit) floating point registers, the round-to-double flag must be enabled in the control word of the FPU for this library to function properly under x86 processors. The following functions contains appropriate code to facilitate manipulation of this flag. For non-x86 systems these functions do nothing (but still exist).

fpu_fix_start This turns on the round-to-double bit in the control word.
fpu_fix_end This restores the control flag.

These functions must be called by the main program, as follows:

```
int main() {
    unsigned int old_cw;
    fpu_fix_start(&old_cw);

    ... user code using quad-double library ...

    fpu_fix_end(&old_cw);
}
```

A Fortran-90 example is the following:

```
subroutine f_main
use qdmodule
implicit none
integer*4 old_cw

call f_fpu_fix_start(old_cw)

... user code using quad-double library ...
```

```
call f_fpu_fix_end(old_cw)
end subroutine
```