Moving SCA/LAPACK to Higher Precision

without *too much* work

Yozo Hida

yozo@cs.berkeley.edu

Computer Science Division
EECS Department
U.C. Berkeley

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Outline

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Motivation for higher precision

- LAPACK and SCALAPACK are widely used.
- User survey revealed small but significant portion of users wanted precision higher than double precision.
  `http://icl.cs.utk.edu/lapack-forum/survey/`
- We want to support codes like

  n_digits $\leftarrow 32$
  repeat
    n_digits $\leftarrow$ n_digits $\times 2$
    Solve with n_digits
  until error $<$ tol
- We want to do the least amount of work to support multiple precision.

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Gap between CPU performance and memory speed has been increasing exponentially.

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Do more computation per unit data.

- solve problems more accurately,
- debug problems without waiting too long.
  - Numerical instability can be ameliorated with higher precision.

More work per unit data

- Speeds of matrix-vector multiply:

	time (s)	mop/s	time ratio
double (MKL)	0.052	965	1
double-double	0.27	189	5.1
quad-double	5.85	8.55	113

Dimension 5000.
Ran on 1 core of dual quad-core "Cloverton" Intel Xeon 2.33 GHz.

  - Double-double uses 17.5 times more flops but only twice as much data. Matrix-vector multiply runs only 5.1 times slower.
  - Quad-double uses approx. 200 times more flops but only four times as much data. Matrix-vector multiply only runs 113 times slower.

- Greater effect for sparse and parallel codes, where flops is even "cheaper".

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Some Implementations of Higher Precision

- Fixed precision
  - Compiler supported quad
  - Double-double, Quad-double
- Arbitrary precision
  - GMP / MPFR
  - ARPREC

Double-double and quad-double numbers

Store higher precision numbers as an unevaluated sum.
`http://www.cs.berkeley.edu/~yozo/`

- $2^{100}+1$ is stored as the pair $(2^{100}, 1)$ in double-double.
- Can represent about 32 / 64 digits of precision,
- Highly efficient algorithms due to their fixed, small size.
- Simple representation: fixed size array of doubles.
  Makes it easy to allocate arrays and use MPI.
- $\pi \approx 3.14159265358979323846264338327950288419716939937510582097494$
  is stored as

$$\begin{array}{rll}
3.1415926535897931160 \times 10^{0} & (\quad 1 & 1100100100001111110110101010001000100001011010001100\\
1.2246467991473532072 \times 10^{-16} & (-\ 53 & 1000110100110001001100011001100010100010111000000011\\
-2.9947698097183396659 \times 10^{-33} & (-109 & 1111100011001011101101011011111101101100011111011110\\
1.1124542208633652815 \times 10^{-49} & (-163 & 1010011001111100110001110100000000100000101110111110\\
\end{array}$$

  in quad-double.
- Peculiar precision: $1+2^{-1000} \neq 1$ in double-double arithmetic.

Double-double and quad-double numbers

- C, C++ and Fortran 95 interfaces.

```
use qdmodule
type (qd_real) a, b
a = 1.d0
b = cos(a)**2 + sin(a)**2 - 1.d0
call qdwrite(6, b)
```

- Support for complex data types recently added.

GMP/MPFR

- Multiple-precision floating-point computations with correct rounding.
- `http://www.mpfr.org/`
- Uses integer arithmetic instructions.
- Highly optimized for variety of platforms.
- Somewhat complicated data structure, mixing various types in a C struct.
  This makes inter-language operation, porting, and message passing somewhat harder.
- C, C++ interfaces. No Fortran 95 interface.

ARPREC

- `http://www.cs.berkeley.edu/~yozo/`
- Uses simple floating point array to represent data.
  This makes inter-language operation and message passing easier.
- Slower than GMP.
- C, C++, and Fortran 95 interfaces.

```
use mpmodule
type (mp_real) a, b
a = 1.d0
b = cos(a)**2 + sin(a)**2 - 1.d0
call mpwrite(6, b)
```

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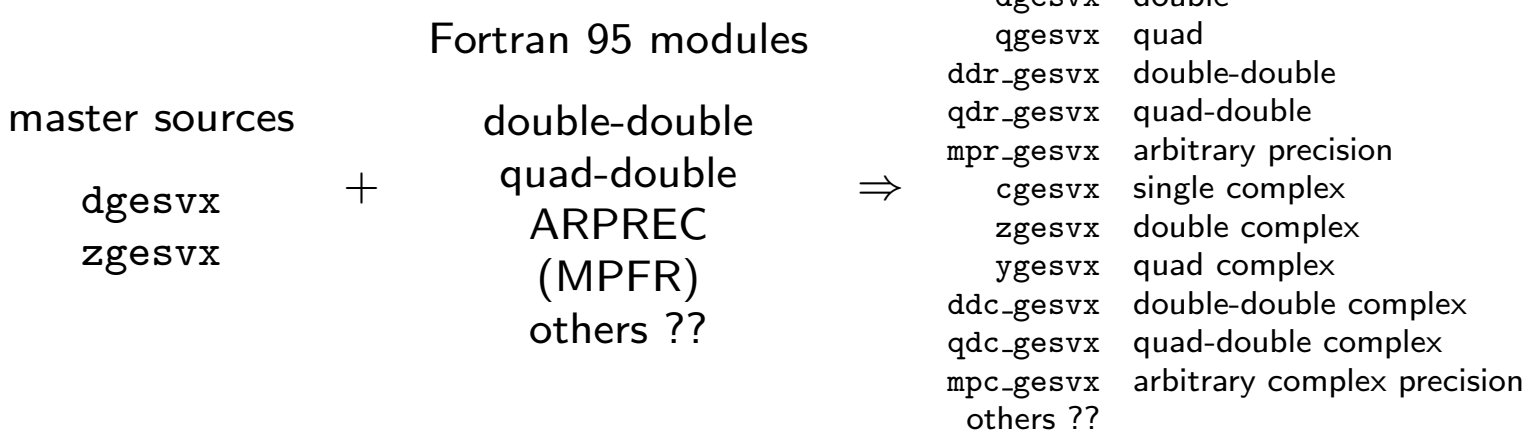
Source-to-source translator

- LAPACK contains $^3/_4$ million lines of FORTRAN 77.
  We do not want to rewrite LAPACK.
- Source-to-source translation:



Things to Consider

- Single source code for varying precision. This makes it much easier to maintain code.
- Workspace allocation. We need to tell the user how much workspace to allocate.
- Temporary variable allocation.
- Should we allow multiple precisions in one routine? Within one matrix?
- How to adjust precision.
- Can multiple versions co-exist? Naming issues.

Modules

The high precision library provides a module that declares what operators and functions are overloaded:

```
module mpmodule
  type mp_real
    sequence
    real*8 mpr(mpwds+5)
  end type

  interface operator (+)
    module procedure mpadd
  end interface

...

end module mpmodule
```

Modules

LAPACK source is then modified slightly:

```
subroutine some_lapack_routine
  !  Use module for arbitrary precision
  use mpmodule

  !  Declare variables in the desired format
  type (mp_real) a, b, c

  !  LAMCH must be provided by the
  !  arbitrary precision package provider
  smlnum = lamch(a, 'Safe minimum')

  !  ...the rest of the code ...
end subroutine
```

Assessment of Constants

Simple replacement of variable type is not enough:

```
x = 0.1d0 / 0.3d0
```

This line is interpreted by the compiler as double precision constants and computation. Needs to be replaced with something like,

```
x = mp_real("0.1") / mp_real("0.3")
```

This is the most common "bugs" reported to us when people convert their code to use our higher precision packages.

Naming Issues

How should a routine be named when using a new precision?

- Add a new prefix. DGESVX becomes QGESVX for quad, QD_GESVX for quad-double etc.
  Leads to name explosion, but easier for inter-language operations.
- Use generic names like "GESVX" and dispatch to correct routines using Fortran 95 module and interface facilities. LAPACK 95 does this.

Implementation

Currently implemented as a (rather ad-hoc) Perl script to convert LAPACK sources to perform

- use appropriate module file (provided by the dd / qd / arprec packages),
- constant literal substitutions,
- handle Fortran data declarations,
- use a new prefix for each LAPACK routines,
- substitute something appropriate for read / write statements, and
- declare variables in appropriate types.

Passes most LAPACK tests for Quad and QD precisions, including linear systems.

Current Work

More complete Fortran parser.

- Open Fortran Parser. Supports Fortran 2003.
- Parser from `ftnchek`. Mostly for Fortran 77.
- Gfortran or G95 frontend.

Variable precision LAPACK using ARPREC.

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Conclusion

Once the high-precision library provides the appropriate module file declaring the overridden functions, most of LAPACK code can be transformed to use them without too much effort.

Future Work

- Using ARPREC in LAPACK (current).
- Use more robust Fortran parser (current).
- Facilities for debugging numerical problems.
- Exception handling.
- How much performance can we buy from using multi-core BLAS?
- Apply same technique to SCALAPACK.
- Provide F95 interface to MPFR. Anyone?