Development of MPACK (MBLAS/MLAPACK) library: Multiple precision arithmetic versions of BLAS and LAPACK

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Overview

- Why Linear algebra is important?
- BLAS and LAPACK.
- We matter accuracy.
- Applications
- MPACK (MBLAS/MLAPACK)
- How I create?

Why Linear Algebra is important?

- Linear Algebra is a key tool for science, industry and engineering, etc.
 - (basically) Solving linear equation Ax=b.
 - 雉兎同籠 (孫子算経) -> 鶴亀算 (江戸)
- Many applications
 - Linear programming (operations research)
 - Quantum mechanics (partial differential equation)
 - Sound analysis, Fast Fourier Transformation..

BLAS and LAPACK

- Many interesting problems are formulated as linear equations.
 - Usually we cannot solve linear equation by hand -> use computer!
- BLAS/LAPACK are widely used linear algebra libraries.
 - A high quality "building block" routines for performing basic vector and matrix operations.
 - Eigenvalue problem, singular value decomposition...
 - Big libraries: BLAS 151 routines, LAPACK 1582 routines.

We matter Accuracy

- We just want to solve Ax = b!
- But... size of A becomes large ...solution becomes meaningless.
 - More precisely, "condition number".
 - IEEE 754 double: 16 significant digits.
 - We need more digits!
- Do not trust your results without error analysis!

Applications

- SemiDefinite programming...condition number becomes infinite at the optimal. (at most 7-8 digits with IEEE754 double)
- Elementary particle physics; solving large scale ill-conditioned problems, Feynman diagram...etc.
- Qunantum chemistry. Reaction energy can underflow.

MPACK (MBLAS/MLAPACK)

- To solve
 - Linear equations which have large condition number.
 - Numerically unstable problem.
 - Check your mathematical theorem.
- How we solve
 - Just add precision.

MPACK (MBLAS/MLAPACK) http://mplapack.sourceforge.net/

- MPACK (MBLAS/MLAPACK) is a multiple precision version of BLAS and LAPACK
- Provide Application Program Interface.
- 0.6.0 (2009/11/24); 50 MLAPACK routines (666 routines), 76 (all) MBLAS routines.
- Highly portable.
- Written in C++; rewrite from FORTRAN77.
- LGPL; everyone can use my library.

How I create?

- Total 666 MLAPACK routines...
- Transform original FORTRAN77 routines to C code via "f2c".
- Using "sed" heavily to make the translated code readable.
- Pass compilation by hand editing.
- Input random values and compare with the results of BLAS/LAPACK.
- Keeping motivation and mental strength are important.