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

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Main object: Scientists have been trying to elucidate mysteries of nature using computers and linear algebra is a basic and key tool for scientific computing. In this proposal, we would like to develop a general purpose **accurate** linear algebra library and define application program interface.

We solve linear equations, diagonalize matrices, and so on, even non-linear ones via linearization with iterations, arising from physics, chemistry and other areas of science, engineering, on computers. The BLAS (Basic Linear Algebra Subprograms) and LAPACK (linear algebra library) are popular and widely used linear algebra packages as building blocks.

However, since computers cannot handle real numbers, we usually calculate approximate manner. This causes inaccuracy and/or instability in the solutions. For example, the BLAS and LAPACK uses at most double precision, which can handle sixteen significant digits. This does not mean the solutions have such accuracy. Especially if the size of the problems becomes bigger, accuracy becomes worse. As a result, solutions become meaningless.

This is the reason why we have been developing general purpose MPACK (MBLAS and MLAPACK) multiple precision arithmetic version of BLAS and LAPACK. Development is ongoing at http://mplapack.sourceforge.net/ . Demands for multiple precision BLAS/LAPACK is very clear: Google search result with “multiple precision BLAS” returned 10400 pages, and top 20 pages point out ***ONLY*** our pages. In the 22nd pages we can find by other authors; “Design, implementation and testing of extended and mixed precision BLAS” in 2002 by Xiaoye S. Li, James W. Demmel, David H. Bailey *et al.*, mainly BLAS/LAPACK team members.

Features of MPACK are following.

- Providing basic building blocks for arbitrary or more accurate linear algebra.
- Arbitrary precision (GMP), quasi quadratic precision (DD) and quasi octuple precision (QD) are supported.
- Provide reference implementation to multiple precision versions of BLAS and LAPACK. No more re-invention of the wheel and others can concentrate on optimization.
- Having very similar API (Application Program Interface) to BLAS and LAPACK, so that we can try and migrate easily.
- Very portable, does not depend on operating system.
- MBLAS has been completed.
- Based on LAPACK 3.1.

Expected results:

1. We will provide reference implementation to multiple precision versions of BLAS and LAPACK.
2. In broad area of science, engineering, and industrial applications, users of MPACK will obtain accurate and/or correct results.
3. Some tuning for MBLAS packages using GPGPU or accelerator.
4. The number of supported LAPACK routines will increase; from 100 to 200.
    - Currently 50 MLAPACK routines are implemented and well tested.

Schedule:

Total approx. 670 MLAPACK routines will be implemented. In this period, we expect from 100 to 200 new routines will be implemented, and tested. To collaborate, we are planning to have meetings and discussions with regard to check implementation, algorithm and optimization.

Budget:

1. $6000; a workstation for developing.
2. $8000; travel expense. Usually takes $4000 to go U.S. to attend a conference for a week.

Using Microsoft technology:

None. We would like to provide a reference implementation; this should not depend on something as far as possible.

Related researches:
As far as we know, no attempts have been made to provide a general purpose library based on BLAS and LAPACK. There are some existing library using multiple precision and/or higher precision as follows.

1. BNCpack: a basic matrix and mathematical library which supports IEEE single, double and multiple precision arithmetic via GMP and MPFR by Kouya, Tomonori. Not compatible with BLAS and LAPACK. Supports parallel computation.
2. ALSQUAD: quasi quadruple precision vector operation packages by Ogata, Takamori and Kubo, Katsui, NEC HPC sector; optimized library, but this is not compatible with BLAS/LAPACK, and only supports quasi quadruple precision.
3. Extended and mixed precision BLAS; by Xiaoye Li et al., http://crd.lbl.gov/~xiaoye/XBLAS/ , just use higher precision arithmetic internally.

Our Results and results based on our software:
Original motivation came from quantum chemistry [2]. We solve quantum chemical problem using semi-definite programming solver and the results of semi-definite programming solver sometimes does not accurate (only one to four significant digits) for physically interesting cases (high correlation limit of Hubbard model).

We have published two referred papers.

1. “Strange Behaviors of Interior-point Methods for Solving Semidefinite Programming Problems in Polynomial Optimization”, Hayato Waki, *Maho Nakata*, and Masakazu Muramatsu, Computational Optimization and Applications (accepted).
2. “Variational calculation of second-order reduced density matrices by strong *N*-representability conditions and an accurate semidefinite programming solver”, *Maho Nakata*, Bastiaan J. Braams, Katsuki Fujisawa, Mituhiro Fukuda, Jerome K. Percus, Makoto Yamashita, and Zhengji Zhao, Journal of chemical physics 128, 16 164113 (2008).

Other published papers not by M.N., using MPACK via SDPA

1. “A new library of structured semidefinite programming instances.”, E. de Klerk, R. Sotirov, Optim. Methods Softw. 24, 959-971 (2009).
2. “High accuracy semidefinite programming bounds for kissing numbers.”, H. D. Mittelmann, F. Vallentin, arXiv:0902.1105v2 (2009).

Program packages:

1. MPACK 0.5.2 (2009/10/5). http://mplapack.sourceforge.net/
2. SDPA-GMP/-QD/-DD 7.1.2 (2009/10/5). http://sdpa.indsys.chuo-u.ac.jp/sdpa/software.html#sdpa-gmp