SimTKlapack README

Version 1.2.1

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1 What is SimTKlapack

SimTKlapack is a high performance linear algebra library for C/C++ and FORTRAN programmers. SimTKlapack implements version 3.1.1 of the LAPACK (Linear Algebra PACKage) [1] and BLAS (Basic Linear Algebra Subprograms) [2] standards and provides routines for solving systems of simultaneous linear equations, eigenvalue problems, singular value problems and least-squares solutions of linear systems of equations. SimTKlapack also provides the LU, Cholesky, QR, SVD, Schur, generalized Schur matrix factorizations and operations for estimating condition numbers. It supports both dense and banded matrices and can operate on real and complex matrices in single or double precision. SimTKlapack is internally threaded and will automatically take advantage of multiple processors.

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2 What is in this download

The download file includes the SimTKlapack shared library, header file, and example programs for using SimTKlapack. The download file is organized into 4 directories: lib, include, doc and examples. The lib directory contains the SimTKlapack shared library. On Linux systems this is named libSimTKlapack.so and on Mac it is named libSimTKlapack.dylib. On Windows there are two files; SimTKlapack.dll and SimTKlapack.lib. The include directory contains the SimTKlapack.h header file which contains the function declarations for C and C++ programs to call the LAPACK FORTRAN routines. The doc directory contains this file. The examples directory contains example programs that use the SimTKlapack.h header file and the SimTKlapack shared library.

3 How to use SimTKlapack

SimTKlapack implements the standard FORTRAN 77 interface for LAPACK and BLAS which can also be called from C and C++ programs. Instructions on how C and C++ programs can call SimTKlapack are provided in the README file in the examples directory of this download.

4 Where to go for more information

To learn more about using the LAPACK API a good place to start is the "LAPACK User's Guide" third edition. You can either buy a hardcopy version (ISBN: 0898714478) or use the online version at: http://www.netlib.org/lapack/lug. Also the Numerical Algorithms Group (NAG) [4] has a nice set of FORTRAN example for using LAPACK. UNIX man pages can also be downloaded from http://www.netlib.org/lapack/manpages.tgz.

6 SimTKlapack performance

The performance of SimTKlapack vs. coding it yourself if very good. For example, a matrix multiply of a 2000x2000 single precision matrix is over 200 times faster in SimTKlapack on a 4 processor AMD opteron than using the code from Numerical Recipes [5] compiled with all optimizations. SimTKlapack is optimized

for large problems (matrices larger than 50x50). If your application does many linear algebra operations on small problems, other linear algebra packages may give better performance.

5 Known Limitations

The current version of SimTKlapack is not thread safe during its initialization. The work around is to make a single call to each of the LAPACK routines your application will use in a single thread. After the routines have been called once, they can then be safely called from multiple threads.

6 Changes to the LAPACK API

In order to make SimTKlapack thread safe arguments needed to be added at the end of the parameter list for routines that were doing reverse communication with the calling routine. The values of the additional arguments are set in the routine itself and should be initialized to zero in the calling routine before the first time the routine is called. The routines which have additional arguments are: (s/d/c/z)lacon which added: J, JUMP, ITER. The (s/d)lasq4 routines which added the argument G. The (s/d)lasq3 routines added the TTYPE, DMIN1, DMIN2, DN, DN1, DN2, TAU arguments

Also note that the auxiliary routine slamch returns a double value when called from C programs.

7 Compiler flags used to build SimTKlapack

The following table lists the compiler flags that were used to build SimTKlapack

OS	C compiler	C flags	FORTRAN compiler	FORTRAN flags
Linux	gcc 4.2	-O3 –fPIC –fomit-frame-pointer -mfpmath-387	gfortran 4.2	-ff2c –fPIC –O3 -funroll-all-loops
Mac	gcc 4.0.1	-O3 –fPIC –fomit-frame-pointer	gfortran 4.3	-ff2c –fPIC –O3 -funroll-all-loops
Windows	gcc 3.4.4	-O3 –mno-cygwin –fomit-frame-pointer -mfpmath-387	g77 3.4.4	-funroll-all-loops –O3 –mno-cygwin

8 References

[1] http://www.netlib.org/lapack

[2] http://www.netlib.org/blas

[3] http://math-atlas.sourceforge.net

[4] http://www.nag.com/lapack-ex/lapack-ex.html

[5] “Numerical Recipes in C++: The Art of Scientific Computing”, Cambridge University Press; 2 edition