Introduction to the NAG Fortran SMP Library

1 What is the NAG Fortran SMP Library?

The NAG Fortran SMP Library is a library of Fortran routines optimised for use on Symmetric Multi-processor (SMP) machines, which are multi-processor platforms with a (real or virtual) shared memory.

The NAG Fortran SMP Library contains all the routines in the NAG Fortran Library (at the Mark coincident with its release). It may also introduce some new optimised routines. The serial version of any such routine will appear in the next Mark of the NAG Fortran Library.

Routine interfaces are identical to those of the Fortran Library; this makes the migration from using the NAG Fortran Library to using the NAG Fortran SMP Library trivial.

Many routines, including those in the key areas of dense and sparse linear algebra, random number generators and FFTs, have been specially coded for this Library to make optimal use of the processing power and shared memory parallelism of SMP systems. In the area of dense linear algebra, routines are provided which considerably outperform all known LAPACK implementations. Many other routines in the Fortran SMP Library benefit from this increased performance.

2 The Features of the NAG Fortran SMP Library

The main feature of the NAG Fortran SMP Library is that it maximizes the processing power potential of SMP machines in certain key areas. These key areas include

Dense (real and complex) Linear Algebra

Sparse Linear Algebra

Random Number Generators

FFTs

Many routines in other areas have improved performance and scalability as a direct result of the tuning of key routines. The main areas affected are

Optimization

ODEs

PDEs

Linear Regression

Multivariate Statistics.

Additional features of the library are that the full functionality of the NAG Fortran Library is included, and that user programs can achieve high levels of performance and scalability simply by linking with the high performance NAG Fortran SMP Library routines.

Further details and listings of the specially tuned and enhanced routines are given in the News document.

3 How to use the NAG Fortran SMP Library

3.1 Linking and Executing Your Code

If your code currently contains calls to NAG Fortran Library routines then it is a simple matter of relinking your code to the SMP Library (in place of the NAG Fortran Library) to benefit from the optimized performance of the tuned SMP Library routines. On most platforms, parallelism is requested by setting an environment variable equal to the number of processors you wish the routines to run on and then running your linked code.

The steps required when compiling, linking and running programs on SMP platforms, in order to fully exploit their parallelism, are very much implementation specific. The particular details for your implementation are given in the **Users' Note** which should be read carefully before using the NAG Fortran SMP Library.

More general information regarding the conventions used in this Library is provided in the Essential Introduction to the NAG Fortran Library.

3.2 How to Maximize the Performance of Your Application

There are a number of things that you should consider when trying to maximize the performance of your code when linking to this Library. In the first instance you should be aware of the functionality of the Library and of which routines you should expect to achieve good levels of performance and scalability; for this you should consult the News document. There may be sections of your code which reproduce the functionality of a tuned/enhanced NAG routine or vendor BLAS routine; in such cases you should replace your sections of code with calls to the appropriate routines.

In addition there are areas of the NAG Fortran SMP Library that require further guidance.

FFTs (Chapter C06): in many implementations the vendors supply their own FFT routines that are optimized for their given platforms. Where possible the NAG FFT routines call these vendor routines for optimal performance. For details see the **Users' Note** for your implementation.

Random Number Generators (Chapter G05): a mechanism for generating independent sequences of random numbers in parallel has been incorporated into the Library. This mechanism should be the default for your implementation; however, you can explicitly set the mechanism used by an initial call to G05ZAF. It should be noted that sequences generated in parallel are not, in general, reproducible. If you require to reproduce sequences generated using the NAG Fortran Library with given seeds then an initial call to G05ZAF (see the G05ZAF routine document) is required in order to use the standard sequential algorithm.