

# NAG SMP Library

## Introduction to the NAG SMP Library

### 1 What is the NAG SMP Library?

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

The NAG SMP Library contains all the routines currently available in the NAG Fortran Library. Routine interfaces are identical to those of the NAG Fortran Library; this makes the migration from using the NAG Fortran Library to using the NAG SMP Library trivial.

Many routines, including those in the key areas of dense and sparse linear algebra and FFTs, have been specially coded for this Library to make optimal use of the processing power and shared memory parallelism of SMP systems. Many other routines in the NAG SMP Library benefit from this increased performance.

### 2 The Features of the NAG SMP Library

The main feature of the NAG SMP Library is that it maximizes the processing power potential of SMP machines in the key areas of

- Dense Linear Algebra

- Sparse Linear Algebra

- 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 the user programs can achieve high levels of performance and scalability simply by linking with the high performance NAG SMP Library routines.

Further details and listings of the specially tuned and enhanced routines are given in the Mark 21 News – NAG Fortran SMP Library document.

### 3 How to Use the NAG 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 NAG SMP Library (in place of the NAG Fortran Library) to benefit from the optimized performance of the tuned NAG 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 machines, 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 SMP Library.

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

### 3.2 How to Maximize the Performance of Your Application

There are a number of things 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 Tuned and Enhanced Routines in the NAG SMP Library 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 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.

Sparse Iterative Solvers (Chapter F11): when running the sparse iterative solvers with preconditioning on multiple processors, it may be beneficial to reduce the action of the preconditioner, e.g., by decreasing LFILL, or by increasing DTOL with  $LFILL < 0$  in F11DAF or F11JAF. This will tend to increase the number of iterations required to obtain a converged solution, but allow a greater percentage of the computational work to be spent in the parallelized iterative solvers, resulting in a lower overall time to solution. There is unfortunately no choice of the various preconditioner parameters which is optimal for all types of matrix, and all numbers of processors, and some experimentation will generally be required for each new type of matrix encountered.

## 4 Structure of the Documentation

The NAG SMP Library is the same collection of routines as available in the NAG Fortran Library which have been parallelized or enhanced and are intended for use on Symmetric Multiprocessor (SMP) machines and the document entitled 'Essential Introduction' is essential reading for NAG SMP Library users.

### 4.1 Marks of the Library

The NAG SMP Library was released as a **Release** at Release 1 and Release 2. The NAG SMP Library now contains the full suite of user-callable routines as provided by the NAG Fortran Library with parallelized and enhanced routines as listed in the document entitled 'Tuned and Enhanced Routines in the NAG SMP Library'. We have consolidated the two products and will now refer to new releases of the NAG SMP Library as a **Mark**. At a new release of the NAG SMP Library, new routines are added, corrections and/or improvements are made to existing routines; and occasionally routines are withdrawn if they have been superseded by improved routines.

At each Mark, the documentation of the Library is updated. You must make sure that your documentation has been updated to the same Mark as the Library software that you are using.

The current Mark is Mark 21.

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