NAG C Library

Mark 8 News

1 Introduction

At Mark 8 of the NAG C Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1006 user-callable routines of which 990 are documented and 146 are new at this mark.

A new chapter on large scale eigenproblems has been introduced, and new algorithms have been included in the areas of optimization, dense and banded linear algebra, direct solution of large scale linear systems, regression, random numbers, time series and the NAG interface to BLAS.

The new chapter on Large Scale Eigenproblems (f12) has functions for the solution of symmetric and nonsymmetric standard and generalized large scale eigenvalue problems. Chapter f11 has been renamed as Large Scale Linear Systems, and new functions for the direct solution of sparse problems have been added.

Chapter e04 (Minimizing or Maximizing a Function) has been updated with new functions for the solution of LP, QP and nonlinear programming problems with sparse linear constraints.

A comprehensive suite of driver functions for the solution of dense and banded linear equations has also been added to Chapter f04 (Simultaneous Linear Equations).

New functions for stepwise regression and mixed effects regression have been included in Chapter g02 (Correlation and Regression Analysis), and a number of new random number generators, including Copulas and improved quasi-random number generators have been added to Chapter g05 (Random Number Generators) and Chapter g13 (Time Series Analysis).

Chapter f16 (NAG Interface to BLAS) now covers the full BLAS specification.

The NAG Boolean type has been withdrawn and replaced by Nag_Boolean (see Section 2.2.1.1 of the Essential Introduction). The change had to be made in order to avoid a clash of types with those compiler vendors who also use Boolean.

Individual function documents have been provided at this Mark for Chapter a00 (Library Identification), Chapter a02 (Complex Arithmetic) and Chapter f06 (Linear Algebra Support Functions).

2 New Routines

The 146 new user-callable routines included in the C Library at Mark 8 are as follows.

- a00acc nag_check_licensing
  Check availability of a valid licence key
- e01sgc nag_2d_shep_interp
  Interpolating functions, modified Shepard’s method, two variables
- e01shc nag_2d_shep_eval
  Interpolated values, evaluate interpolant computed by nag_2d_shep_interp (e01sgc), function and first derivatives, two variables
- e01sjc nag_2d_triang_interp
  A function to generate a two-dimensional surface interpolating a set of data points, using either the method of Renka and Cline or the modified Shepard’s method
- e01skc nag_2d_triang_eval
  A function to evaluate, at a set of points, the two-dimensional interpolant function generated by nag_2d_shep_interp (e01sgc)
- e02dac nag_2d_spline_fit_panel
  Least-squares surface fit, bicubic splines
- e02zac nag_2d_panel_sort
  Sort two-dimensional data into panels for fitting bicubic splines
- e04npc nag_opt_sparse_convex_qp_init
  Initialization function for nag_opt_sparse_convex_qp_solve (e04nqc)
e04nqc  nag_opt_sparse_convex_qp_solve
LP or QP problem (suitable for sparse problems)
e04nrc  nag_opt_sparse_convex_qp_option_set_file
Supply optional parameter values for nag_opt_sparse_convex_qp_solve (e04nqc) from external file
e04nsc  nag_opt_sparse_convex_qp_option_set_string
Set a single option for nag_opt_sparse_convex_qp_solve (e04nqc) from a character string
e04ntc  nag_opt_sparse_convex_qp_option_set_integer
Set a single option for nag_opt_sparse_convex_qp_solve (e04nqc) from an Integer argument
e04nuc  nag_opt_sparse_convex_qp_option_set_double
Set a single option for nag_opt_sparse_convex_qp_solve (e04nqc) from a double argument
e04nxc  nag_opt_sparse_convex_qp_option_get_integer
Get the setting of an Integer valued option of nag_opt_sparse_convex_qp_solve (e04nqc)
e04nyc  nag_opt_sparse_convex_qp_option_get_double
Get the setting of a double valued option of nag_opt_sparse_convex_qp_solve (e04nqc)
e04vge  nag_opt_sparse_nlp_init
Initialization function for nag_opt_sparse_nlp_solve (e04vge)
e04vhe  nag_opt_sparse_nlp_solve
General sparse nonlinear optimizer
e04vje  nag_opt_sparse_nlp_jacobian
Determine the pattern of nonzeros in the Jacobian matrix for nag_opt_sparse_nlp_solve (e04vge)
e04vke  nag_opt_sparse_nlp_option_set_file
Supply optional parameter values for nag_opt_sparse_nlp_solve (e04vge) from external file
e04vlc  nag_opt_sparse_nlp_option_set_string
Set a single option for nag_opt_sparse_nlp_solve (e04vge) from a character string
e04vmc  nag_opt_sparse_nlp_option_set_integer
Set a single option for nag_opt_sparse_nlp_solve (e04vge) from an Integer argument
e04vnc  nag_opt_sparse_nlp_option_set_double
Set a single option for nag_opt_sparse_nlp_solve (e04vge) from a double argument
e04vrc  nag_opt_sparse_nlp_option_get_integer
Get the setting of an Integer valued option of nag_opt_sparse_nlp_solve (e04vge)
e04vsc  nag_opt_sparse_nlp_option_get_double
Get the setting of a double valued option of nag_opt_sparse_nlp_solve (e04vge)
e04wce  nag_opt_nlp_init
Initialization function for nag_opt_nlp_solve (e04wce)
e04wde  nag_opt_nlp_solve
Solves the nonlinear programming (NP) problem
e04wec  nag_opt_nlp_option_set_file
Supply optional parameter values for nag_opt_nlp_solve (e04wce) from external file
e04wfc  nag_opt_nlp_option_set_string
Set a single option for nag_opt_nlp_solve (e04wce) from a character string
e04wgc  nag_opt_nlp_option_set_integer
Set a single option for nag_opt_nlp_solve (e04wce) from an Integer argument
e04whc  nag_opt_nlp_option_set_double
Set a single option for nag_opt_nlp_solve (e04wce) from a double argument
e04wkc  nag_opt_nlp_option_get_integer
Get the setting of an Integer valued option of nag_opt_nlp_solve (e04wce)
e04wlc  nag_opt_nlp_option_get_double
Get the setting of a double valued option of nag_opt_nlp_solve (e04wce)
f04bac  nag_real_gen_lin_solve
Computes the solution and error-bound to a real system of linear equations
f04bbc  nag_real_band_lin_solve
Computes the solution and error-bound to a real banded system of linear equations
f04bcc  nag_real_tridiag_lin_solve
Computes the solution and error-bound to a real tridiagonal system of linear equations
f04bdc  nag_real_sym_posdef_lin_solve
Computes the solution and error-bound to a real symmetric positive-definite system of linear equations
f04bec nag_real_sym_posdef_packed_lin_solve
Computes the solution and error-bound to a real symmetric positive-definite system of linear equations, packed storage

f04bfc nag_real_sym_posdef_band_lin_solve
Computes the solution and error-bound to a real symmetric positive-definite banded system of linear equations

f04bgc nag_real_sym_posdef_tridiag_lin_solve
Computes the solution and error-bound to a real symmetric positive-definite tridiagonal system of linear equations

f04bhc nag_real_sym_lin_solve
Computes the solution and error-bound to a real symmetric system of linear equations

f04bjc nag_real_sym_packed_lin_solve
Computes the solution and error-bound to a real symmetric system of linear equations, packed storage

f04cac nag_complex_gen_lin_solve
Computes the solution and error-bound to a complex system of linear equations

f04cbc nag_complex_band_lin_solve
Computes the solution and error-bound to a complex banded system of linear equations

f04ccc nag_complex_tridiag_lin_solve
Computes the solution and error-bound to a complex tridiagonal system of linear equations

f04cdc nag_herm_posdef_lin_solve
Computes the solution and error-bound to a complex Hermitian positive-definite system of linear equations

f04cec nag_herm_posdef_packed_lin_solve
Computes the solution and error-bound to a complex Hermitian positive-definite system of linear equations, packed storage

f04cfc nag_herm_posdef_band_lin_solve
Computes the solution and error-bound to a complex Hermitian positive-definite banded system of linear equations

f04cgc nag_herm_posdef_tridiag_lin_solve
Computes the solution and error-bound to a complex Hermitian positive-definite tridiagonal system of linear equations

f04che nag_herm_lin_solve
Computes the solution and error-bound to a complex Hermitian system of linear equations

f04cjc nag_herm_packed_lin_solve
Computes the solution and error-bound to a complex Hermitian system of linear equations, packed storage

f04dhe nag_complex_sym_packed_lin_solve
Computes the solution and error-bound to a complex symmetric system of linear equations

f04dhc nag_complex_sym_packed_lin_solve
Computes the solution and error-bound to a complex symmetric system of linear equations, packed storage

f06fec nag_drscl
Multiply real vector by reciprocal of scalar

f06kec nag_zrscl
Multiply complex vector by reciprocal of real scalar

f11mdc nag_superlu_column_permutation
Real sparse nonsymmetric linear systems, setup for nag_superlu_lu_factorize (f11mec)

f11mec nag_superlu_lu_factorize
LU factorization of real sparse matrix

f11mfc nag_superlu_solve_lu
Solution of real sparse simultaneous linear equations (coefficient matrix already factorized)

f11mge nag_superlu_condition_number_lu
Estimate condition number of real matrix, matrix already factorized by nag_superlu_lu_factorize (f11mec)

f11mhc nag_superlu_refine_lu
Refined solution with error bounds of real system of linear equations, multiple right-hand sides

f11mke nag_superlu_matrix_product
Real sparse nonsymmetric matrix matrix multiply, compressed column storage
f11mlc  nag_superlu_matrix_norm
1-norm, \(\infty\)-norm, largest absolute element, real general matrix

f11mmc  nag_superlu_diagnostic_lu
Real sparse nonsymmetric linear systems, diagnostic for nag_superlu_lu_factorize (f11mec)

f12aac  nag_real_sparse_eigensystem_init
Initialization routine for (nag_real_sparse_eigensystem_iter (f12abc)) computing selected eigenvalues and, optionally, eigenvectors of a real nonsymmetric sparse (standard or generalized) eigenproblem

f12abc  nag_real_sparse_eigensystem_iter
Implements a reverse communication interface for the Implicitly Restarted Arnoldi iteration for computing selected eigenvalues and, optionally, eigenvectors of a real nonsymmetric sparse (standard or generalized) eigenproblem

f12acc  nag_real_sparse_eigensystem_sol
Returns the converged approximations (as determined by nag_real_sparse_eigensystem_iter (f12abc)) to eigenvalues of a real nonsymmetric sparse (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace

f12adc  nag_real_sparse_eigensystem_option
Set a single option from a string (nag_real_sparse_eigensystem_iter (f12abc)/nag_real_sparse_eigensystem_sol (f12acc)/nag_real_banded_sparse_eigensystem_sol (f12agc))

f12aec  nag_real_sparse_eigensystem_monit
Provides monitoring information for nag_real_sparse_eigensystem_iter (f12abc)

f12afc  nag_real_banded_sparse_eigensystem_init
Initialization routine for (nag_real_banded_sparse_eigensystem_sol (f12agc)) computing selected eigenvalues and, optionally, eigenvectors of a real nonsymmetric banded (standard or generalized) eigenproblem

f12age  nag_real_banded_sparse_eigensystem_sol
Computes approximations to selected eigenvalues of a real nonsymmetric banded (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace

f12anc  nag_complex_sparse_eigensystem_init
Initialization routine for (nag_complex_sparse_eigensystem_iter (f12apc)) computing selected eigenvalues and, optionally, eigenvectors of a complex sparse (standard or generalized) eigenproblem

f12apc  nag_complex_sparse_eigensystem_iter
Implements a reverse communication interface for the Implicitly Restarted Arnoldi iteration for computing selected eigenvalues and, optionally, eigenvectors of a complex sparse (standard or generalized) eigenproblem

f12aqc  nag_complex_sparse_eigensystem_sol
Returns the converged approximations (as determined by nag_complex_sparse_eigensystem_iter (f12apc)) to eigenvalues of a complex sparse (standard or generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the associated approximate invariant subspace

f12arc  nag_complex_sparse_eigensystem_option
Set a single option from a string (nag_complex_sparse_eigensystem_iter (f12apc)/nag_complex_sparse_eigensystem_sol (f12aqc))

f12asc  nag_complex_sparse_eigensystem_monit
Provides monitoring information for nag_complex_sparse_eigensystem_iter (f12apc)

f12fac  nag_real_symm_sparse_eigensystem_init
Initialization routine for (nag_real_symm_sparse_eigensystem_iter (f12fbc)) computing selected eigenvalues and, optionally, eigenvectors of a real symmetric sparse (standard or generalized) eigenproblem

f12fbc  nag_real_symm_sparse_eigensystem_iter
Implements a reverse communication interface for the Implicitly Restarted Arnoldi iteration for computing selected eigenvalues and, optionally, eigenvectors of a real symmetric sparse (standard or generalized) eigenproblem
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f12fcc nag_real_symm_sparse_eigensystem_sol
Returns the converged approximations (as determined by nag_real_sparse_eigensystem_iter
(f12abc)) to eigenvalues of a real symmetric sparse (standard or generalized) eigenproblem and,
on Optionally, the corresponding approximate eigenvectors and/or an orthonormal basis for the
associated approximate invariant subspace

f12fdc nag_real_symm_sparse_eigensystem_option
Set a single option from a string (nag_real_symm_sparse_eigensystem_iter
(f12fbc)/nag_real_symm_sparse_eigensystem_sol
(f12fcc)/nag_real_symm_banded_sparse_eigensystem_sol (f12fgc))

f12fec nag_real_symm_sparse_eigensystem_monit
Provides monitoring information for nag_real_symm_sparse_eigensystem_iter (f12fbc)

f12ffc nag_real_symm_banded_sparse_eigensystem_init
Initialization routine for (nag_real_symm_banded_sparse_eigensystem_sol (f12fgc)) computing
selected eigenvalues and, optionally, eigenvectors of a real symmetric banded (standard or
generalized) eigenproblem

f12fgc nag_real_symm_banded_sparse_eigensystem_sol
Computes approximations to selected eigenvalues of a real symmetric banded (standard or
generalized) eigenproblem and, optionally, the corresponding approximate eigenvectors and/or
an orthonormal basis for the associated approximate invariant subspace

f16pac nag_dgemv
Matrix-vector product, real rectangular matrix

f16pbc nag_dgbmv
Matrix-vector product, real rectangular band matrix

f16pcc nag_dsymv
Matrix-vector product, real symmetric matrix

f16pde nag_dsbmv
Matrix-vector product, real symmetric band matrix

f16pec nag_dspmv
Matrix-vector product, real symmetric packed matrix

f16pfc nag_dtrmv
Matrix-vector product, real triangular matrix

f16pgc nag_dtbmv
Matrix-vector product, real triangular band matrix

f16phc nag_dtpmv
Matrix-vector product, real triangular packed matrix

f16pkc nag_dtbsv
System of equations, real triangular band matrix

f16plc nag_dtpsv
System of equations, real triangular packed matrix

f16pnc nag_dger
Rank-1 update, real rectangular matrix

f16ppc nag_dsvr
Rank-1 update, real symmetric matrix

f16pqc nag_dspr
Rank-1 update, real symmetric packed matrix

f16pdc nag_dspr2
Rank-2 update, real symmetric matrix

f16sac nag_zgemv
Matrix-vector product, complex rectangular matrix

f16sbc nag_zgbmv
Matrix-vector product, complex rectangular band matrix

f16sec nag_zhemv
Matrix-vector product, complex Hermitian matrix

f16sdc nag_zhbmv
Matrix-vector product, complex Hermitian band matrix

f16sec nag_zhpmv
Matrix-vector product, complex Hermitian packed matrix
f16sfc  nag_ztrmv
Matrix-vector product, complex triangular matrix
f16sgc  nag_ztbbmv
Matrix-vector product, complex triangular band matrix
f16she  nag_ztpmv
Matrix-vector product, complex triangular packed matrix
f16skc  nag_ztbsv
System of equations, complex triangular band matrix
f16slc  nag_ztpsv
System of equations, complex triangular packed matrix
f16sme  nag_zger
Rank-1 update, complex rectangular matrix, unconjugated vector
f16spc  nag_zher
Rank-1 update, complex Hermitian matrix
f16sqc  nag_zgpr
Rank-1 update, complex Hermitian packed matrix
f16src  nag_zher2
Rank-2 update, complex Hermitian matrix
f16ssc  nag_zgpr2
Rank-2 update, complex Hermitian packed matrix
f16tac  nag_zsymv
Matrix-vector product, complex symmetric matrix
f16tcc  nag_zspmv
Matrix-vector product, complex symmetric packed matrix
f16yac  nag_dgmm
Matrix-matrix product, two real rectangular matrices
f16ycc  nag_dsyr
Matrix-matrix product, one real symmetric matrix, one real rectangular matrix
f16ycf  nag_drmm
Matrix-matrix product, one real triangular matrix, one real rectangular matrix
f16yfc  nag_dsyrk
Rank-k update of a real symmetric matrix
f16yrc  nag_dsyr2k
Rank-2k update of a real symmetric matrix
f16zac  nag_zgemm
Matrix-matrix product, two complex rectangular matrices
f16zcc  nag_zhemm
Matrix-matrix product, one complex Hermitian matrix, one complex rectangular matrix
f16zfc  nag_ztmm
Matrix-matrix product, one complex triangular matrix, one complex rectangular matrix
f16zpc  nag_zherk
Rank-k update of a complex Hermitian matrix
f16zrc  nag_zher2k
Rank-2k update of a complex Hermitian matrix
f16ztc  nag_zsymm
Matrix-matrix product, one complex symmetric matrix, one complex rectangular matrix
f16zuc  nag_zsyrk
Rank-k update of a complex symmetric matrix
f16zwc  nag_zsy2k
Rank-2k update of a complex symmetric matrix
f02efc  nag_full_step_regsn
Stepwise linear regression
f02ewc  nag_full_step_regsn_monit
Monitor function for full stepwise regression
f02jac  nag_reml_mixed_regsn
Linear mixed effects regression using Restricted Maximum Likelihood (REML)
f02jbc  nag_ml_mixed_regsn
Linear mixed effects regression using Maximum Likelihood (ML)
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3 Routines Scheduled for Withdrawal

The routines listed below are scheduled for withdrawal from the C Library, because improved routines have now been included in the Library. Users are advised to stop using routines which are scheduled for withdrawal immediately and to use recommended replacement routines instead. See the document ‘Advice on Replacement Calls for Withdrawn/Superseded Functions’ for more detailed guidance, including advice on how to change a call to the old routine into a call to its recommended replacement.

The following routines have been superseded, but will not be withdrawn from the Library until Mark 10 at the earliest.

**Superseded Routine**

<table>
<thead>
<tr>
<th>Routine</th>
<th>Replacement Routine(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>nag_2d_scat_interpolant (e01sac)</td>
<td>nag_2d_shep_interp (e01sgc) or nag_2d_triang_interp (e01sjc)</td>
</tr>
<tr>
<td>nag_2d_scat_eval (e01sbc)</td>
<td>nag_2d_shep_eval (e01shec) or nag_2d_triang_eval (e01skc)</td>
</tr>
<tr>
<td>nag_2d_scat_free (e01szc)</td>
<td>No replacement document required</td>
</tr>
<tr>
<td>nag_opt_bounds_no_deriv (e04jbc)</td>
<td>nag_opt_nlp_solve (e04wdc)</td>
</tr>
<tr>
<td>nag_opt_bound_deriv (e04kbc)</td>
<td>nag_opt_nlp_solve (e04wdc)</td>
</tr>
<tr>
<td>nag_opt_sparse_convex_qp (e04nkc)</td>
<td>nag_opt_sparse_convex_qp_solve (e04nqc)</td>
</tr>
<tr>
<td>nag_opt_nlp (e04ucc)</td>
<td>nag_opt_nlp_solve (e04wdc)</td>
</tr>
</tbody>
</table>