IMSL(®) Fortran Numerical Library, Version 7.0.0
January 2012 (revised)

This document contains release notes for IMSL Fortran Numerical Library, Version 7.0.0.

This document has the following parts:

1. **Introduction**
2. **Improvements**
3. **Routines New to IMSL Fortran Numerical Library 7.0.0**
4. **Code Fixes and Improvements for IMSL Fortran Numerical Library 7.0.0**

Part 1: Introduction

This document contains information on improvements made with IMSL Fortran Numerical Library 7.0.0.

Part 2: Improvements

- Users have the option of using Basic Linear Algebra Subroutines (BLAS) which take advantage of the computational power of NVIDIA graphic cards through the use of the NVIDIA CUDA Toolkit. (platform dependent).
- Integration of vendor supplied FFTs into IMSL code.
- Online documentation is provided as HTML files in addition to Adobe Acrobat PDF files.
- The ARPACK package is incorporated in the product with a Fortran 2003 interface. (platform dependent).
- By default the LINK environment variables link with the supported high performance library. Refer to the description of the LINK options in the accompanying Readme.txt file.

Part 3: Functions New to the IMSL Fortran Numerical Library 7.0

FNL Math Library

Chapter	Description
2: Eigensystem Analysis	**ARPACK_SYMMETRIC** - Computes the eigenvalues and eigenvectors of a generalized real symmetric eigenvalue problem.

Chapter	Description
	ARPACK_SVD - Computes the singular values and the left and right singular vectors of a real rectangular matrix. **ARPACK_NON SYMMETRIC** - Computes the eigenvalues and eigenvectors of a generalized eigenvalue problem. **ARPACK_COMPLEX** - Computes the eigenvalues and eigenvectors of a generalized eigenvalue problem.
3: Interpolation and Approximation	**SURFND** - Multidimensional interpolation and differentiation.
4: Integration and Differentiation	**QDAG1D** - Integrates a function with a possible internal or endpoint singularity. **QDAG2D** - Integrates a function of two variables with a possible internal or end point singularity. **QDAG3D** - Integrates a function of three variables with a possible internal or endpoint singularity.
5: Differential Equations	**DAESL** - Solves a first order differential-algebraic system of equations, g(t, y, y') = 0, with optional additional constraints and user-defined linear system solver. **IVOAM** - Solves an initial-value problem for a system of ordinary differential equations of order one or two using a variable order Adams method. **MMOLCH** - Solves a system of partial differential equations of the form ut = f(x, t, u, ux, uxx) using the method of lines. The solution is represented with cubic Hermite polynomials. **FEYNMAN_KAC** - Solves the generalized Feynman-Kac PDE on a rectangular grid using a finite element Galerkin method. Initial and boundary conditions are provided. The solution is represented by a series of C2 Hermite quintic splines. **HQSVAL** - This rank-1 array function evaluates a Hermite quintic spline or one of its derivatives for an array of input points. In particular, it computes solution values for the Feynman-Kac PDE handled by routine FEYNMAN_KAC.
7: Nonlinear Equations	**ZUNI** - Finds a zero of a real univariate function.
8: Optimization	**DDJAC** – Approximates the Jacobian of M functions in N unknowns using divided differences. **TRAN** - Solves a transportation problem.
9: Basic Vector/Matrix Operations	**SSPMV/DSPMV** – Performs the matrix-vector operation y := alpha*A*x + beta*y where alpha and beta are scalars, x and y are n element vectors

Chapter	Description
	and A is an n by n symmetric matrix, supplied in packed form **SSPMV/DSPMV –** Performs the matrix-vector operation y := alpha*A*x + beta*y where alpha and beta are scalars, x and y are n element vectors and A is ann by n symmetric matrix, supplied in packed form **SSPR/DSPR –** Performs the symmetric rank 1 operation A := alpha*x*x' + A where alpha is a real scalar, x is an n element vector and A is an n by n symmetric matrix, supplied in packed form. **SSPR2/DSPR2 –** Performs the symmetric rank 2 operation A := alpha*x*y' + alpha*y*x' + A where alpha is a scalar, x and y are n element vectors and A is an n by n symmetric matrix, supplied in packed form **STPMV/DTPMV –** Performs one of the matrix-vector operations x := A*x, or x := A'*x where x is an n element vector and A is an n by n unit, or non-unit, upper or lower triangular matrix, supplied in packed form **STPSV/DTPSV –** Solves one of the systems of equations A*x = b, or A'*x = b where b and x are n element vectors and A is an n by n unit, or non-unit, upper or lower triangular matrix, supplied in packed form **CHPMV/ZHPMV** - Performs the matrix-vector operation y := alpha*A*x + beta*y where alpha and beta are scalars, x and y are n element vectors and A is an n by n hermitian matrix, supplied in packed form. **CHPR/ZHPR** - Performs the hermitian rank 1 operation A := alpha*x*conjg (x') + A where alpha is a real scalar, x is an n element vector and A is an n by n hermitian matrix, supplied in packed form. **CHPR2/ZHPR2** - Performs the hermitian rank 2 operation A := alpha*x*conjg (y') + conjg(alpha)*y*conjg(x') + A where alpha is a scalar, x and y are n element vectors and A is an n by n hermitian matrix, supplied in packed form. **CTPMV/ZTPMV** - Performs one of the matrix-vector operations x := A*x, or x := A'*x, or x := conjg (A')*x where x is an n element vector and A is an n by n unit, or non-unit, upper or lower triangular matrix, supplied in packed form. **CTPSV/ZTPSV** - Solves one of the systems of equations A*x = b, or A'*x = b, or conjg (A')*x = b where b and x are n element vectors and A is an n by n unit, or non-unit, upper or lower triangular matrix, supplied in packed form.

MATH LIBRARY Special Functions

Chapter	Description
4: Airy Functions	**PSI1** -Evaluates the second derivative of the log gamma function.
11: Probability Distribution Functions and Inverses	**BETNDF** - Evaluates the noncentral beta cumulative distribution function (CDF).

Chapter	Description
	BETNIN - Evaluates the inverse of the noncentral beta cumulative distribution function (CDF). **BETNPR** - Evaluates the noncentral beta probability density function. **FNDF** - Evaluates the noncentral F cumulativedistribution function (CDF). **FNPR** - Evaluates the noncentral F probabilitydensity function. **FNIN** - Evaluates the inverse of the noncentral F cumulative distribution function (CDF). **TNPR** - Evaluates the noncentral Student's t probability density function. **CSNPR** - Evaluates the noncentral chi-squared probability density function.

FNL Stat Library

Chapter	Description
2: Regression	**PLSR** - Performs partial least squares regression for one or more response variables and one or more predictor variables. **SEASONAL_FIT** - Determines an optimal differencing for seasonal adjustment of a time series.
7: Test of Goodness of Fit	**ADNRM** - Performs an Anderson-Darling test for normality. **CVMNRM** - Performs a Cramer-von Mises test for normality.
8: Time Series and Forecasting	**REG_ARIMA** - Fits a univariate, non-seasonal ARIMA time series model with the inclusion of one or more regression variables. **TS_OUTLIER_IDENTIFICATION** - Detects and determines outliers and simultaneously estimates the model parameters in a time series whose underlying outlier free series follows a general seasonal or nonseasonal ARMA model. **TS_OUTLIER_FORECAST** - Computes forecasts, associated probability limits and weights for an outlier contaminated time series. **AUTO_ARIMA** - Automatically identifies time series outliers, determines parameters of a multiplicative seasonal ARIMA model and produces forecasts that incorporate the effects of outliers whose effects persist beyond the end of the series. **AUTO_PARM** - Estimates structural breaks in non-stationary univariate time series.
17: Probability Distribution Functions and Inverses	**BETNDF** - Evaluates the noncentral beta cumulative distribution function (CDF). **BETNIN** - Evaluates the inverse of the noncentral beta cumulative

Chapter	Description
	distribution function (CDF). **BETNPR** - Evaluates the noncentral beta probability density function. **FNDF** - Evaluates the noncentral F cumulative distribution function (CDF). **FNPR** - Evaluates the noncentral F probabilitydensity function. **FNIN** - Evaluates the inverse of the noncentral F cumulative distribution function (CDF). **TNPR** - Evaluates the noncentral Student's t probability density function. **CSNPR** - Evaluates the noncentral chi-squared probability density function.
18: Random Number Generation	**RNMVGC** - Given a Cholesky factorization of a correlation matrix, generates pseudorandom numbers from a Gaussian Copula distribution. **RNMVTC** - Given a Cholesky factorization of a correlation matrix, generates pseudorandom numbers from a Student's t Copula distribution. **CANCOR** - Given an input array of deviate values, generates a canonical correlation array. **MLE** - Calculates maximum likelihood estimates for the parameters of one of several univariate probability distributions.

Part 4: Code Fixes and Improvements for IMSL Fortran Numerical Library 7.0

MATH Library

Chapter 1: Linear Systems

- **C_LIN_SOL_LSQ** – Corrected the calculation of the sign for the imaginary part.

Chapter 3: Interpolation and Approximation

- **CSIEZ** - Modified so that the reordering of the XVEC argument does not occur.

Chapter 4: Integration and Differentiation

- **QDAGI** - Added a comment to the Comments section of the documentation explaining transformation limitations.

Chapter 6: Transforms

- **FFT2B** - Corrected code so as to yield correct results when input array COEF is 1 by N.

Chapter 8: Optimization

- **QPROG** - Added optional arguments MAXITN and SMALL which allows users to set the maximum iterations allowed and the convergence criteria of a constraint violation.

  The default values for MAXITN and SMALL have been changed. These values were not previously accessible to the user.

- **NNLPF** - Added optional arguments LGMULT and CONSTRES providing access to the Lagrange Multipliers and Constraint Residuals respectively.

  Changed an internal COMMON block name so NNLPF and NNLPG do not use common blocks with the same name.

- **NNLPG** - Added optional arguments LGMULT and CONSTRES providing access to the Lagrange Multipliers and Constraint Residuals respectively.

- **UNLSF** - Code modified to prevent infinite looping.

Chapter 10: Linear Algebra Operators and Generic Functions

- **.DET.** - Resolved wrong sign issue in the imaginary part of the return value.

- .**IX.** - Recompilation with newer compiler resolved segmentation fault issue occurring on some environments.

- **SPARSE_LINEAR_OPERATORS** - Improved performance and accuracy of optional (hbc_sparse%options%accumulate) sparse matrix accumulation algorithm.

MATH Library Special Functions

Chapter 3: Exponential Integrals and Related Functions

- **CI** - Corrected an equation in the documentation.

Chapter 4: Gamma Function and Related Functions

- **BETAI** - Complementary probabilities are used to calculate BETAI only when a direct CDF calculation demonstrates that the BETAI value is in the extreme right tail (i.e. very close to 1) to improve accuracy.

Chapter 11: Probability Distribution Functions and Inverses

- **CHIDF** - Added optional argument COMPLEMENT to indicate the complement of the distribution function is to be determined.
  Modified the algorithm to increase accuracy.

- **CHIIN** - Modified the algorithm to increase accuracy.

- **CSNDF** - Modified the algorithm to increase accuracy.
- **FDF** - Added optional argument COMPLEMENT to indicate the complement of the distribution function is to be determined.
  Modified the algorithm to increase accuracy.
- **TDF** - Added optional argument COMPLEMENT to indicate the complement of the distribution function is to be determined.
  Modified the algorithm to increase accuracy. STAT Library

Chapter 1: Basic Statistics

- **UVSTA** -Added code to set stat(15,:) to stat(10,:) when iwt = 0.
  Before, it was not initialized.

Chapter 2: Regression

- **RNLIN** - Modified code to prevent possible infinite looping.
- **RBEST** - Code was added to prevent an out-of-bounds exception. Added a warning message in the case of an almost exact fit with Mallows CP criterion calculations. Initialized data which would sometimes cause a "Terminal Error".

Chapter 5: Categorical and Discrete Data Analysis

- **CTGLM** - Changed the default allocation size of optional argument CLVAL to adjust according to values of NCLVAR.
  Added documentation to clarify the differences in log-likelihood values between models.

Chapter 7: Test of Goodness of Fit and Randomness

- **KSTWO** - Corrected an equation in the documentation.

Chapter 8: Time Series Analysis and Forecasting

- **AUTO_UNI_AR** - Reduced memory requirements.
- **NSBJF** - Corrected an equation in the documentation.

Chapter 17: Probability Distribution Functions and Inverses

- **CHIDF** - Added optional argument COMPLEMENT to indicate the complement of the distribution function is to be determined.
  Modified the algorithm to increase accuracy.
- **CHIIN** - Modified the algorithm to increase accuracy..
- **CSNDF** - Modified the algorithm to increase accuracy.
- **FDF** – Added optional argument COMPLEMENT to indicate the complement of the distribution function is to be determined.
  Modified the algorithm to increase accuracy

- **TDF** - Added optional argument COMPLEMENT to indicate the complement of the distribution function is to be determined.

Chapter 19: Utilities

- **SROWR** - Corrected sort when NCOL is not equal to LDX.

Chapter 20: Mathematical Support

- **CHFAC** - Corrected TOL argument in interface to be double precision.