

NAG Update

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Experts in numerical software and
High Performance Computing

The Numerical Algorithms Group Ltd, Inc and KK

- ▶ Global software and services company with headquarters in Oxford, UK
 - Subsidiaries in USA and Japan, staff in France, Germany, Egypt.
 - Around 70 staff worldwide
- ▶ Specialists in:
 - Numerical Algorithms
 - High Performance Computing applications and technology advice
 - Software Engineering for Science and Technology
- ▶ Not-for-profit Company
 - Founded as inter-University project in 1970
 - Became independent Company in 1976
 - Collaborates with world-leading mathematicians and computer scientists

NAG Customers

- ▶ Broad range of industries and academic areas
- ▶ Key markets:
 - Financial Services (investment banking)
 - Very keen on bitwise reproducibility
 - Energy (oil & gas)
 - Very keen on improving throughput/productivity
- ▶ NAG code licensed to many ISVs
 - DemandTec, OriginLab, Maplesoft, ...
- ▶ Involved in BLAS/LAPACK etc. for many years
 - MKL, ACML, ARM Performance Libraries

The NAG Library

- ▶ Focus on high-level functionality
- ▶ Documented interfaces in Fortran, C and Matlab
 - Bindings for Java, Python, R, VB, ...
- ▶ Parallelism via OpenMP
- ▶ Implemented on multiple hardware platforms, operating systems, compilers ...
 - x86, Power, Xeon Phi, ARM v8, ...
 - Linux, MacOS, Windows
- ▶ Extensively tested, supported and maintained code
- ▶ Where possible, call into vendor libraries (MKL, APL,...)

Mark 26: 1872 user-callable routines covering:

- ▶ Optimisation
- ▶ Differential Equations
- ▶ Root Finding
- ▶ Quadrature
- ▶ Wavelets
- ▶ Linear Algebra
- ▶ Special Functions
- ▶ Data Fitting
- ▶ Multivariate Methods
- ▶ Analysis of Variance
- ▶ Random Number Generation
- ▶ Univariate Estimation
- ▶ Time Series Analysis
- ▶ Correlation & Regression Analysis
- ▶ ...

Mark 26 NAG Library: New functionality

- ▶ Semidefinite optimization (SDP)
- ▶ Interior point method for large-scale nonlinear optimization (NLP)
- ▶ NAG Modelling Optimization Suite
- ▶ New quadrature functionality
- ▶ Improvements to ODE Runge-Kutta routines – with reverse communication
- ▶ New correlation matrix functionality
- ▶ LAPACK 3.7.0

Future Plans: Randomized Numerical Linear Algebra

- ▶ For solving very large problems
- ▶ Sample the data and solve a smaller (denser) problem
- ▶ Extrapolate back to an approximation of solution to original problem
- ▶ Algorithm guarantees that if successful the distance between the approximate and real answer is bounded
- ▶ Initial suite under development for a customer
 - Based on work of Xi , Xia , Cauley & Balakrishnan

Future Plans: Algorithmic Differentiation

- ▶ Produce a variant of an application that computes the sensitivities of the output to variations in the input
- ▶ Can sometimes automate but:
 - Often run-out of memory because of storing large intermediate expressions
 - May be more efficient to formulate the derivative of a routine symbolically
- ▶ Working with University of Aachen
 - To develop tools to automate differentiation of C++/Fortran/CUDA code
 - To develop AD-enabled NAG routines (around 60 expected later in 2017)
 - To offer consultancy to customers
 - To enable efficient use of BLAS etc.

Other plans

- ▶ More support for Python
- ▶ More algorithmic functionality
 - Optimisation
 - Bayesian Statistics
 - ...
- ▶ More support for data analytics

Summary

- ▶ NAG continues to develop new Library content, in collaboration with our international network of experts
- ▶ NAG work to make its Library more accessible from new languages and on new hardware platforms
- ▶ Strong demand for bitwise reproducibility from big finance customers

Experts in High Performance Computing, Algorithms and Numerical Software Engineering

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