NAG Update

Mike Dewar
Chief Technical Officer

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
- ...

nag®
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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