NAG Library --> NAG Adjoint Library
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Advances In Numerical Linear Algebra: Celebrating the centenary of the birth of James H. Wilkinson

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Experts in numerical software and High Performance Computing
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NAG AD Library: Why, what and how

Why
▶ Because important NAG customers want it
  • Measure sensitivity of results to changes in inputs
  • Customers have large codes calling out to NAG Routines
  • New customers?

What
▶ AD versions of NAG Routines (Fortran C/C++) in:
  • Nonlinear systems, quadrature, Interpolation
  • Linear Algebra (Lapack, Blas, Sparse systems, nearest correlation)
  • Optimization
  • Statistics, special functions
  • Tangent Linear Derivatives and Adjoints (some symbolic)
NAG AD Library: How? -- From here

nagfor
Fortran compiler

Algorithmic
Engine
(Fortran)

NAG Lib Doc
(xml)

Generated:
Doc, wrappers
layers, headers
helpers

dco/c++
AD Tool for
C++
NAG AD Library: How? -- via

Source transformation tool
Klaus

AD
Algorithmic
Engine
(Fortran)

Fortran Modules:
Derived types,
Operator extensions
Intrinsic extensions

symbolic
adjoints
Viktor
dcof: C layer
instantiated types
Klaus

dco/c++
AD Tool for
C++
Johannes

Generate AD:
Doc, wrappers
layers, headers
helpers
Martin

Doc (xml)
DavidC – doc guru

MK27 Doc
NAG AD Library: Linear Algebra

• Adjoint from Bottom Up
  • AD Versions of BLAS (BLAS_AD Lib ?)
    • Relatively Easy, some symbolic adjoints trivial
  • AD versions of Lapack
    • can use algorithmic or symbolic BLAS_AD

• Performance
  • AD versions of common sub-tasks written as calls to BLAS
    • e.f. gemm, symm, trmm, trsm
  • PLASMA (OpenMP tasks, Tiled)
    • --> DAG of tasks + AD of tasks --> fast adjoint

• Primal code problems
  • BIGNUM = ONE / SMLNUM
    • 58 D & 53 Z Lapack routines
    • e.g. DGGEV3
NAG AD Library: Roadmap

- 2019 Dec
  - Another 64 routines adjoint and tangent linear
- 2020
  - Symbolic (Bottom up)
    - Most used BLAS, Linear solvers
  - Algorithmic
    - Lots
  - Second-order ? Mixed adjoint-tangent ?
- 2021
  - Symbolic
    - Further Linear Algebra
    - A few higher level routines
  - Algorithmic
    - Lots more (Good functionality coverage)
NAG AD Library - Summary

• Challenging task:
  • Square peg, round hole, big hammer, precision tools
  • Easy user migration from NAG Library to AD
  • Algorithmic and symbolic AD
  • C++ and Fortran

• It works 😊