The Numerical Algorithms Group

Combining mathematics and technology for enhanced performance

Numerical Algorithms for Posterity

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Over 30 years of mathematical excellence

NAG Numerical Libraries

- §Re-usable, application-neutral code
- §Each piece of algorithmic code supported by:
  - §examples
  - §test material
  - §user-level documentation
  - §programmer-level documentation
- §Different language implementations of same algorithm
  - §Ada, Algol-68, C, Fortran-77, Fortran-90, Pascal, …

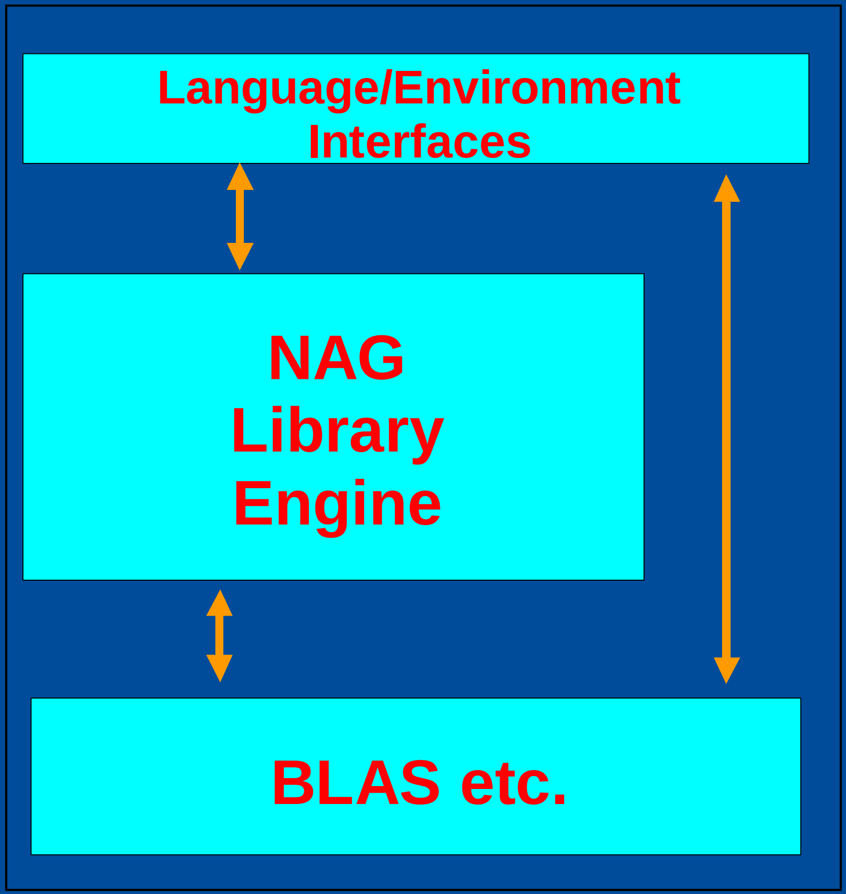
Advantages

- Interfaces exploit strengths of host language
  - Fortran-77: arrays, no dynamic memory allocation
  - C: arrays, structs, dynamic memory allocation
  - Fortran-90: arrays, derived types, generic interfaces, dynamic memory allocation
  - …
- Documentation and examples oriented towards host language

Disadvantages

- Developers waste time re-inventing wheels
- Support effort spread across multiple versions
  - testing, bug-fixing, documentation etc.
- Not all languages can make efficient use of performance-enhancing technology such as BLAS, vendor maths libraries etc.
  - e.g. BLAS 2-D arrays in column order so C programmes must transpose before calling them
- Not all languages optimise well for numerical computation

The New NAG Library Architecture



Software:

- Language-independent algorithmic core
- Interfaces customised to host environment
- Ability to make efficient use of BLAS etc.

Documentation:

- Customised to host environment

QA Material:

- Separate testing of different components

The NAG Library Engine

- Base material written in extended Fortran-77
  - Simple language which is relatively easy to
    - interface with other languages
    - transform into other languages
    - process with software tools
  - Highly optimisable, very efficient for numerical computation
  - Extensions allow for dynamic memory allocation
    - mechanism works with all modern Fortran compilers
  - Substantial body of existing, tested material which can be adopted (e.g. NAG Fortran Library Mark 20)

The NAG Library Engine contd.

- Engine code can be automatically translated to other languages as necessary
  - to remove Fortran run-time dependencies
  - in principle, to provide platform independent code (Java, C#)
- Clear software guidelines for authors
  - Enforced by tools and by peer review
  - Emphasis on clarity and efficiency of code
    - e.g. dynamic memory allocation only used in engine when it is more efficient
- Routine interfaces designed to simplify interfacing to other languages
- *While the engine is derived from the old NAG Library, it is fundamentally different!*

Customising the Engine for a Language or Environment

- For each routine we need to create
  - an interface or wrapper
  - end-user documentation
  - examples
- As far as possible, this is an automatic process
- Wrappers are non-trivial. In general they:
  - transform between interface data-structures and engine data-structures
  - ensure that all arrays are in engine-order (column-major to allow for efficient use of BLAS)
  - allocate and de-allocate memory for workspace (and sometimes output parameters)
  - check constraints on all parameters they use
  - construct error messages to be returned to the user

Simple Example: Engine, Fortran-77 & C

```
SUBROUTINE C06PFFN(IEMODE,DIRECT,NDIM,L,ND,N,X,WORK,LWORK,ERRBUF,IFAIL)
     INTEGER              IEMODE, IFAIL, L, LWORK, N, NDIM
     CHARACTER            DIRECT
     CHARACTER*200        ERRBUF
     COMPLEX *16          WORK(LWORK), X(N)
     INTEGER              ND(NDIM)

SUBROUTINE C06PFF(DIRECT,NDIM,L,ND,N,X,WORK,LWORK,IFAIL)
     INTEGER             IFAIL, L, LWORK, N, NDIM
     CHARACTER           DIRECT
     COMPLEX *16         WORK(LWORK), X(N)
     INTEGER             ND(NDIM)

void c06pfc(Nag_TransformDirection direct, Integer ndim, Integer l,
            const Integer nd[], Integer n, Complex x[], NagError *fail)
```

Engine Interface

- IEMODE
  - determines whether the routine is being asked to check constraints and calculate workspace required or to perform the algorithm
- ERRBUF
  - is used to return diagnostic information (type of error, point where algorithm failed etc.)
- Helper Routines
  - are used to mediate between user-supplied call-back functions and the engine

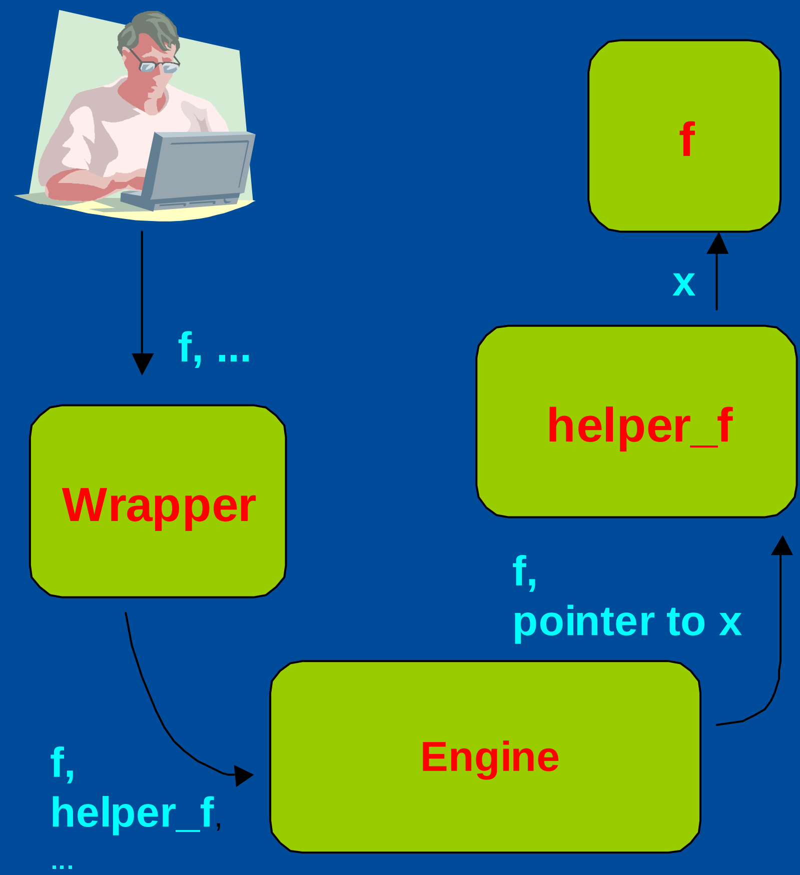
Call-backs

- Algorithms often ask the user to supply part of the problem data as a subroutine
- In our architecture this will naturally follow the semantics of the host environment and cannot necessarily be called directly from the engine, which uses Fortran-77 semantics
- A helper function is provided in the wrapper to mediate between the two
- For example, C naturally uses call-by-value and Fortran uses call-by-reference

Example of call-back and helper

```
double f(double x) {
  return(x^2);
}

double helper_f(
  double(*f)(double),
  double *x) {
 /* De-reference pointer */
  return f(*x);
}
```



NAG Routine Specifications

- Source from which wrappers and documentation (and eventually examples) are generated
- XML documents which include
  - user documentation
  - abstract specifications of each routine parameter
  - information about array dimensions, constraints, parameter dependencies …
  - information about error conditions including type of error, text to be displayed when error occurs etc.
- All text is environment-neutral
- Parameters which are created in the wrappers are distinguished from engine parameters
  - relationships between interface parameters and engine parameters can be specified

Parameter Descriptions

§ Every parameter may have the following information associated with it:

- § name (generic, language specific)
- § concrete engine type (integer, real, …)
- § abstract type (structured matrix, enumeration …)
- § intent (in, out, …)
- § purpose (data, algorithm, workspace, dimension …)
- § relationship to other parameters (*leading dimension of M*)
- § optional or required
- § constraints/recommended values
- § generic documentation
- § environment-specific documentation

Documentation

- Generic documentation can be processed to produce environment-specific version.
- Example: Fortran

X(M) – ***real*** array *Input*

On entry: X(i) must be set to the value of x_i, for i=1,2,…,m. The X(i) need not be ordered.

Constraint: $X_{MIN} \leq X(i) \leq X_{MAX}$, and the X(i) must be distinct.

- Example: C

x[**m**] – const double *Input*

On entry: **x**[i-1] must be set to the value of x_i, for i=1,2,…,m. The **x**[i] need not be ordered.

Constraint: $X_{MIN} \leq \mathbf{x}[\mathbf{i}] \leq X_{MAX}$, and the **x**[**i**] must be distinct.

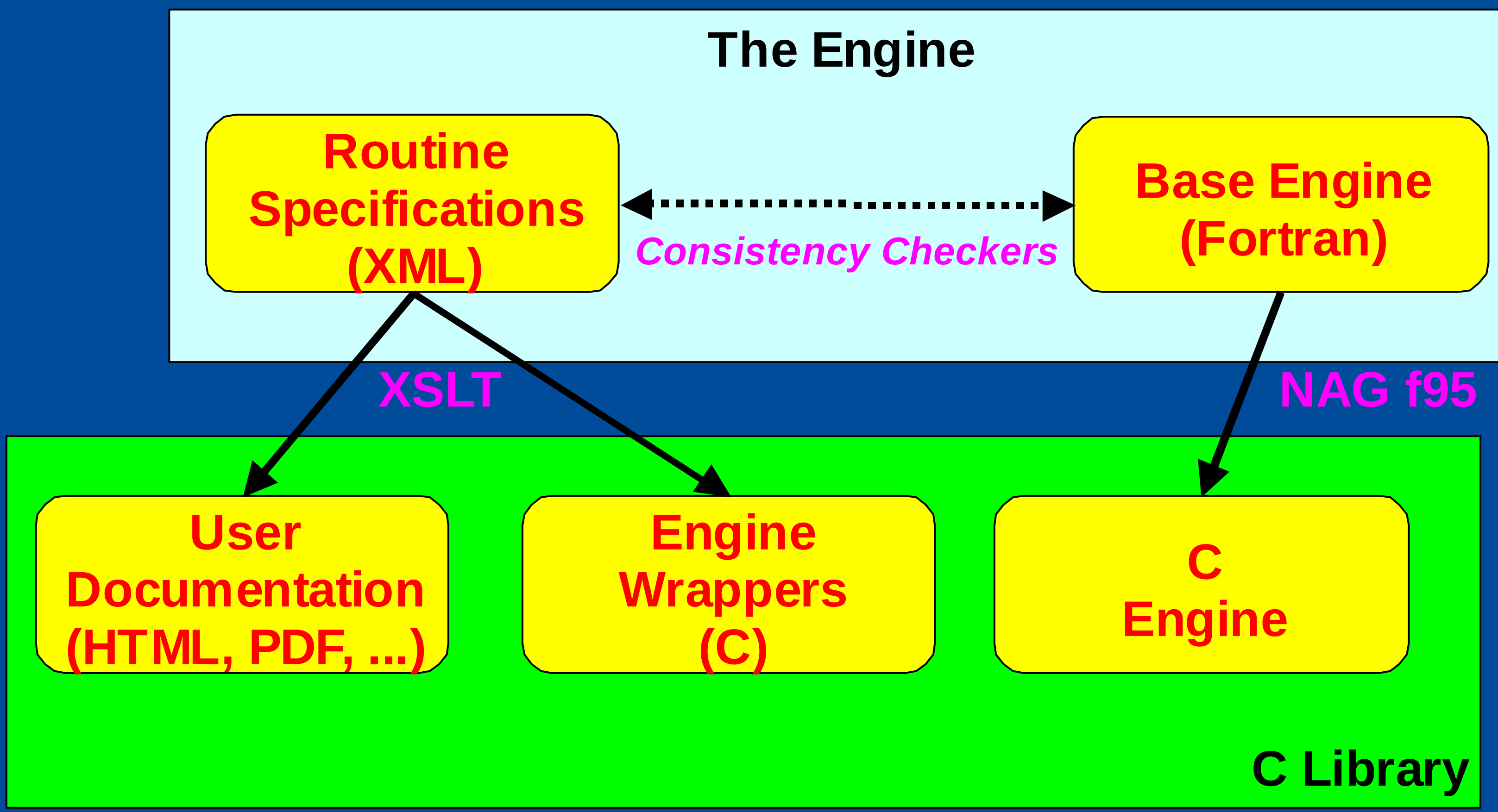
Example 1: NAG C Library Mark 7

- The first product to be based on the engine
- Over 400 fully-documented new routines introduced
- Interface customisations include
  - Use of existing NAG C structs and enumerated types
  - Introduction of new structs and enumerated types where necessary
  - Arrays may be provided in either row- or column-major order
  - Elimination of workspace arrays
  - Elimination of flags which determine whether an optional parameter is being used (in C they are set to NULL)
  - Error messages using C terminology
  - …

Production Process

- Engine delivered to users as C code
  - generated using NAG's f95 compiler technology
  - no dependencies on third-party compiler run-times
- Wrappers and documentation generated using XSLT
  - declarative information stored in specification files so can be re-used in other products
  - transformation to C material encoded as style sheets
- Test and QA material currently written by hand, although some tools were written to semi-automate the process

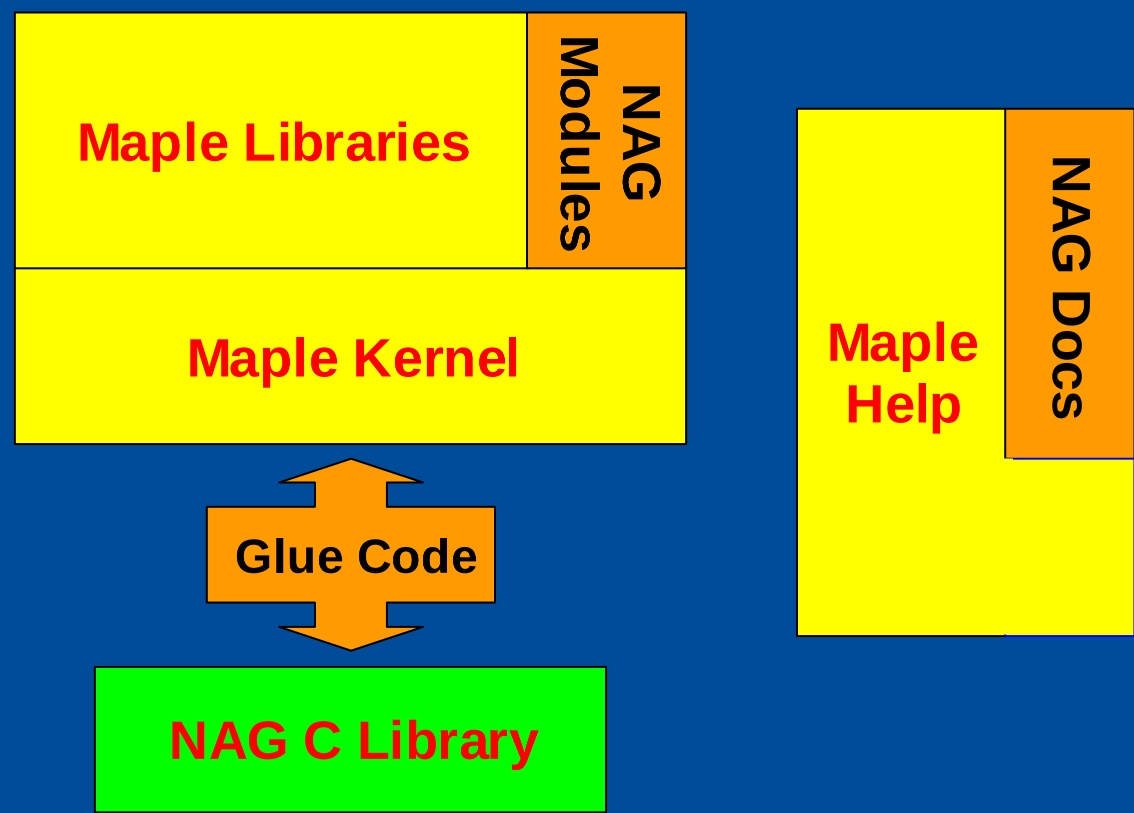
Creating The NAG C Library



Example 2: The NAG-Maple Connector Product

- Overview:
  - The Connector Product is a bridge between two existing products
  - Allow access to all NAG C routines from within Maple
  - Support prototyping
    - develop program calling NAG inside Maple
    - generate stand-alone C code for use outside Maple
  - Document all routines inside the Maple environment using Maple conventions and terminology

Connector Product Architecture



Conclusions

- New architecture is extremely flexible
  - major productivity gains for full-scale products such as C Library Mark 7
  - ability to produce lightweight interfaces such as Visual Basic very rapidly
  - opportunity to embed NAG products in other environments (such as Maple)
- Continued focus on correctness and efficiency
- Simplified, more effective maintenance
- A better service for our users