Some particular advantages using *NAG* in applied mathematics

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I gained my PhD in the Laboratory of Mechanics and Acoustics in Marseilles (France). The objective was to define a numerical algorithm able to recover some properties of an immersed body (density, elastic coefficients, size or shape). Experimentally diffraction of ultrasonic pulses was used: measurement was done all around the body and the experimental acquisition was already so efficient that a huge number of measurements could be done.
In order to reconstruct obstacles (the inverse problem), a classical method consists of comparing measurements with numerical simulations of the wavefield built with some a priori knowledge on the geometrical and material properties of the body. The estimation is then defined as the set of parameters for which the error between simulation and measurement is a minimum. Hence, these types of algorithm are optimization processes.
Inverse problems are known as ill-posed problems in the sense that the solution may not exist, or be multiple or unstable. In view of these difficulties a reliable and fast numerical model was necessary.
All my colleagues advised me to use the NAG library and its compiler (it's remarkable in the sense that unanimity is not so common in a research team). I will give here some steps where NAG has been useful during these three years[1].

Bessel functions

If we consider an acoustic problem (celerity c and angular frequency ω), the pressure field $p(\mathbf{x})$ satisfies a linear partial differential equation called the Helmholtz equation:

$$(\triangle + k)p(\mathbf{x}) = 0 \qquad ; \qquad k = \frac{\omega}{c}$$

The diffracted pressure field $p^d(\mathbf{x})$ caused by a centred cylindrical obstacle with constant radius is analytical and can be expressed as a series of Bessel functions. At a distance r and in the direction ϕ :

$$p^d(\mathbf{x}) = \sum_{n=-\infty}^{+\infty} i^n a_n H_n^{(1)}(kr)e^{in\phi} \tag{1}$$

[1]In the following, some simplifications and omissions will be assumed in order to focus on the main objective of this paper

The Hankel function $H_n^{(1)}$ (S17DLF) is part of the family of Bessel functions (S17DEF, S17DCF for example).

The Hankel function is singular at the origin ($r = 0$ or $\omega = 0$) and the evaluation of its values is not straightforward for $kr \neq 0$; some approximate forms can be used for extreme cases $kr \gg n$ or $n \gg kr$. Note that the infinite sum is not numerically possible - the solution is to truncate this sum in a proper way. (Some particular laws for n_{max} according to kr can be found in the literature.) Moreover even if all is done in a rigorous way, we observe that the sum must be performed for critical values for which the estimation of the Bessel functions must be particularly accurate. Using the NAG libraries allows us to avoid introducing approximate forms in the numerical algorithm.

LU decomposition of ill-conditioned matrix

In the diffracted field expression (Eq.1), the a_n coefficient is a parameter evaluated thanks to the boundary conditions at the interface between the body and the surrounding medium: continuity of stress and displacement. For canonical bodies (spheres, cylinders) these boundary conditions can be expressed through a transfer matrix for each mode n and each angular frequency ω. Then, a_n (but also the corresponding coefficient for the transmitted wave) can be obtained by inverting this matrix.

If we consider a sound-soft cylinder for example this matrix is simply a 2×2 matrix, which does not introduce difficulties. But for a more complex body such as an elastic multilayer tube in an elastic surrounding medium, the boundary conditions introduce a $4L \times 4L$ matrix (where L is the number of layers). For a 2D problem, each element of the matrix can be expressed via cylindrical functions (Bessel functions). At low or high frequencies this complex matrix is particularly ill-conditioned. However the inversion can be made numerically thanks to $F07ARF$ and $F07AWF$ (LU-factorisation) without any trouble.

Some numerical examples

A good way to evaluate the efficiency of the NAG libraries is to perform the following test (based on the inverse problem). First a diffracted (measured) field $p^{d,m}(\mathbf{x})$ is numerically evaluated. In a second step, this measured field is compared with an estimated field $p^{d,e}(\mathbf{x}; c^e)$ depending on an estimated parameter, for example the celerity of the medium (c^e). We can define an error function depending on the estimate $\mathcal{F}(c^e) = \|p^{d,m}(\mathbf{x}) - p^{d,e}(\mathbf{x}; c^e)\|$. Of course when $c^e \equiv c$ we have $\mathcal{F} \equiv 0$, and the celerity can be reconstructed by a minimization algorithm on $\mathcal{F}$.
But the most interesting thing here is that the diffracted field is a C^1 function of c (continuous and continuous derivative), therefore $\mathcal{F}(c^e)$ must be a C^1 function. Evaluating this error function with various libraries, or with an algorithm using explicit approximation[2] shows that the error function is numerically not C^1 : this can be explained by errors on estimation of the Bessel function in the libraries or by introduction of approximate forms by the programmer; it can also be explained by errors during transfer matrix inversion.

[2] as I did initially

From my knowledge, only the NAG libraries have been able to give me a satisfactory C^1 error function. This property clearly helps the implementation of minimization techniques to find the solution of the problem.

Accuracy of numerical simulation can also be highlighted during comparison of models. In Fig.1 we observe the following error function :

$$\mathcal{F} = \frac{\|a_1 - \tilde{a}_1\|}{(k_0 r_0)^2}$$

where $k_0 = \omega/c_0$ is the wave number in the surrounding medium and r_0 is the exterior radius of the body. Here a_1 has been evaluated exactly with the NAG libraries (inversion of transfer matrix and evaluation of Bessel functions) and $\tilde{a}_1$ has come from an approximate model for a very small argument $0 < k_0 r_0 \ll n$ (here $n = 1$). This last model is explicit and does not introduce numerical difficulties.

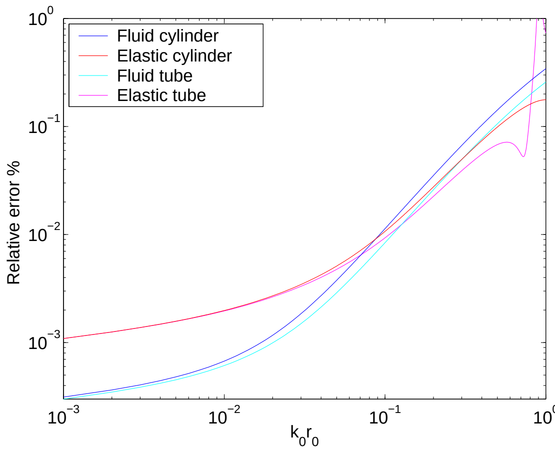

Figure 1: Error function $\mathcal{F}(k_0 r_0)$ for various bodies.

Evaluation is performed for elastic and fluid bodies (cylinder or tube) immersed in a fluid medium. We observe that the error function is clearly C^1 in spite of the vicinity of the singularity for the Hankel functions.

Optimization

The last step for inversion consists of finding the minima of the error functions between measurements and estimations. We have shown that theoretically the solutions correspond to a zero of the function. Moreover, because the inverse problem is ill-posed, this zero may be not unique. In the case of real measurements (or if the estimation and synthetic measurements are performed with a different model) the solution is no longer defined as a zero of the error function but by a simple minimum.
Generally the error function is defined by a sum of squares function, for example:

$$\mathcal{F}(\boldsymbol{\tau}) = \sum_{\mathbf{x}} \sum_{\omega} \|p^{d,m}(\mathbf{x}) - p^{d,e}(\mathbf{x}, \omega; \boldsymbol{\tau})\|^2$$

where $\boldsymbol{\tau}$ is a vector containing all the unknown parameters. For a typical elastic cylinder, 4 parameters are unknown : the density ρ, the pressure and shear celerity c_p and c_s, and the external radius r_0.
For such problems NAG suggests various minimization algorithms according to the type of function (sum of squares or not) and the number of unknowns. The same routine can generally be used with or without introducing the first derivative.
For these types of routines, NAG gives a lot of advantages. First, each *Routine Document* finishes with an example for which input and source code are given. This is a good introduction for new users. Second, each NAG routine gives a lot of additional information that can be used in order to evaluate the quality of the results. Third, the user can improve the efficiency of his algorithm by testing first easy-to-use subroutines (for example E04KZF) before using more specialized subroutines (for example E04KDF).

These routines are particularly efficient and well adapted for physical problems. Keeping the same example of acoustic imaging, and supposing that r_0 is known, we want to reconstruct the following parameters ρ, c_p and c_s. In a general configuration the programmer uses traditional bounds such as $\rho_{min} \leq \rho \leq \rho_{max}$, $c_{p,min} \leq c_p \leq c_{p,max}$ and $c_{s,min} \leq c_s \leq c_{s,max}$. Moreover physical consideration informs us that these celerities can also been expressed via Young modulus E and Poisson coefficient ν or in terms of Lamé coefficients λ and μ :

$$\begin{aligned} c_p &= \sqrt{\frac{E(1-\nu)}{\rho(1+\nu)(1-2\nu)}} = \sqrt{\frac{\lambda+2\mu}{\rho}} \\ c_s &= \sqrt{\frac{E}{\rho 2(1+\nu)}} = \sqrt{\frac{\mu}{\rho}} \end{aligned}$$

Then non linear bounds can be used in order to constrain the problem, for example $0 < \nu \leq 1/2$.
The NAG routines are very useful for such configurations. Practically the efficiency is increased by reducing the variation domain which avoids finding unphysical results, but the main advantage is clearly the detailed information available as output.

Conclusion

These are just some basic examples of the advantages I found in using NAG software during my PhD. After my PhD, I was lucky enough to be always able to find a NAG compiler and libraries in order to continue my work. This is important: the numerical tools you need must be common enough for you to be able to continue with the work already done without any additional transfer tasks.
So far NAG has always been able to give me the best numerical tools to do my job, and it's with pleasure that I share my research with NAG products.