Numerical Algorithms for Metrology

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NPL and NAG

1 Abstract

Numerical algorithms are key for almost all areas of metrology. Ensuring that good quality algorithms are available to metrology practitioners, are documented in readily understandable terms, and are available within their chosen work environment, is a real challenge.

The major premise here is that most metrology practitioners are better employed doing metrology rather than becoming embroiled in numerical computation. This premise was recognised and acted upon as part of the Software Support for Metrology (SSfM) programme with a project on Software Reuse. The project sought ways to provide world-class numerical software to the Metrology community in an easy-to-use manner. The project identified the web as the key delivery mechanism and developed an embryonic website to be the initial delivery vehicle for the METROlogy Software (METROS) concept. Under SSfM-2 this idea is being extended with the aim of further populating METROS and making it the delivery vehicle of choice for all numerical software within Metrology.

This talk will look briefly at the METROS Environment and most importantly how it can be best populated with solution software. We will take time to look at the range of commercial software available and how NPL are working towards having a core of numerical software available for use from all of the major computing environments in use within the organisation. NPL are seeking to have a high level of confidence in the underlying numerical software rather than having to rely on the numerical components offered by each of the computing environments in use - which in some cases have been proven to be lacking (e.g. [2]).

2 The Challenge

Most metrology practitioners have no real interest in numerical computation, they simply want to use best practice calculations from within their favourite environment in order to analyse their data. In practice this means that many simply use the tools available to them in the environment in which they are most familiar. This is simple human nature – why look for 'something better' when what you already have works – or at least it seems to?

The challenge is to define best practice and then make that best practice solution available in an easy-to-use manner for the metrologists. Of course, this is just the high-level challenge. Working out what is best practice for a myriad of problems, documenting the solutions in such a way that metrologists with vastly differing backgrounds find easy to follow, and making the solutions available in a wide-range of end-user environments are just some of the underlying challenges.

3 The Solution – METROS

3.1 Background

METROS exists to promote best practice in the design, development, use and re-use of software for metrology. The web site is primarily a means of accessing information about functions and their implementations, which form the Metrology Software library. There are separate web pages for the different components of METROS, the information for each component being provided in a tabular form. The overall structure and content of METROS at the end of the first SSfM programme is described in the METROS user guide [1].

The current version of the web site was populated by function and implementations from NAG and NPL, but contributions from elsewhere are necessary for METROS to mature. Any contributions of software are welcomed but the emphasis is on software based on sound numerical analysis, reflecting best practice in mathematical modelling, which is well written and which has undergone thorough appropriate testing. Contributed software will include an indication of its status: whether or not it has been tested/validated and by whom. The METROS user guide includes procedures and criteria for the acceptance of contributions. NPL will be setting up a service for testing and reviewing contributed software. METROS will also include guidance material; initially this material will be best practice guides, reports and case studies from the SSfM programmes.

The intention is to include material that is relevant to the application of modelling, algorithms, uncertainty estimation, numerical analysis, software development, and testing and validation to software for metrology.

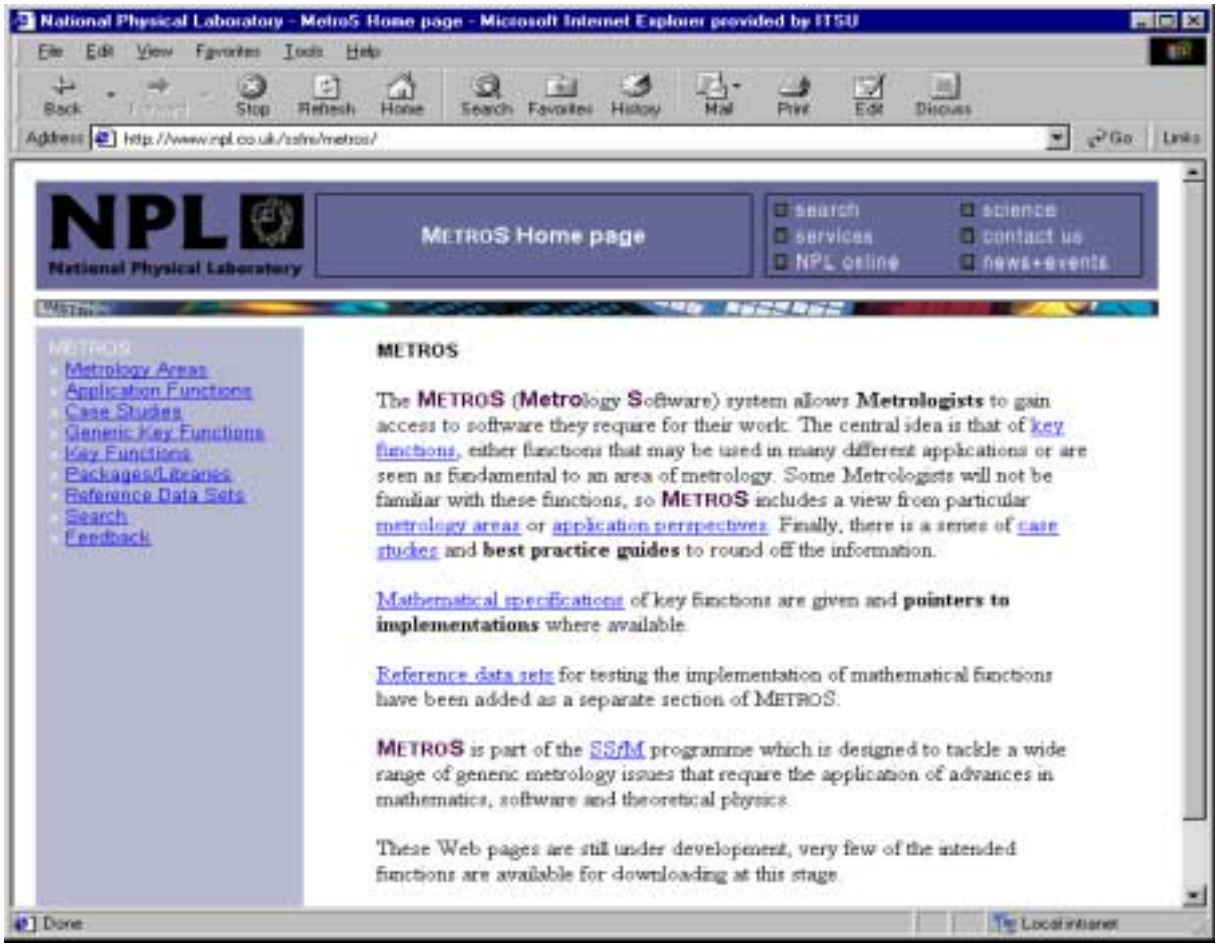

Figure 1 METROS home page at **www.npl.co.uk/ssfm/metros**

3.2 Current Status

Central to METROS is the key function, a mathematical specification of a piece of functionality required by metrologists, the specification gives the input and output parameters and the computational aim (equations describing the relationship between the input and output parameters). The key function definition can also include the algorithms to be used in implementing the key function. On the web site the key functions are grouped by mathematical category: polynomial, spline and other series evaluation and fitting; geometric elements and fitting; statistical functions, distributions, and routines; numerical solver routines; and functions giving properties of materials (e.g. refractive index and density of air) that are given by empirical mathematical formulae.

The main items of software in METROS are the implementations of key functions. The description of the implementations shows how they relate to the key functions, their input and output parameters, with pointers to the documentation and the code. Software may be supplied free or as commercial software: free software implementations can be downloaded directly from the website, commercial implementations will include information about how the software can be obtained. It is intended that commercial software included in METROS should be available for download from the appropriate commercial e-commerce site.

The implementations in METROS include NAG functions for fitting a circle to data which is built on NAG library routines for solving non-linear least squares problems. This function is available in a DLL, which can be accessed via an “add-in” and called in an Excel spreadsheet (see Figure 2). Fitting circles to data is important in roundness assessment of physical artefacts. Less obviously, circle fitting is used in network analysers, where the data are complex numbers representing electrical quantities.

Other implementations in METROS include the NPLFIT library of fitting routines developed by NPL: this provides functions for fitting curves as polynomials and splines, and calculating statistics of these fitted curves. The ability to fit curves to data and understand the uncertainties in the fit is needed in all branches of metrology.

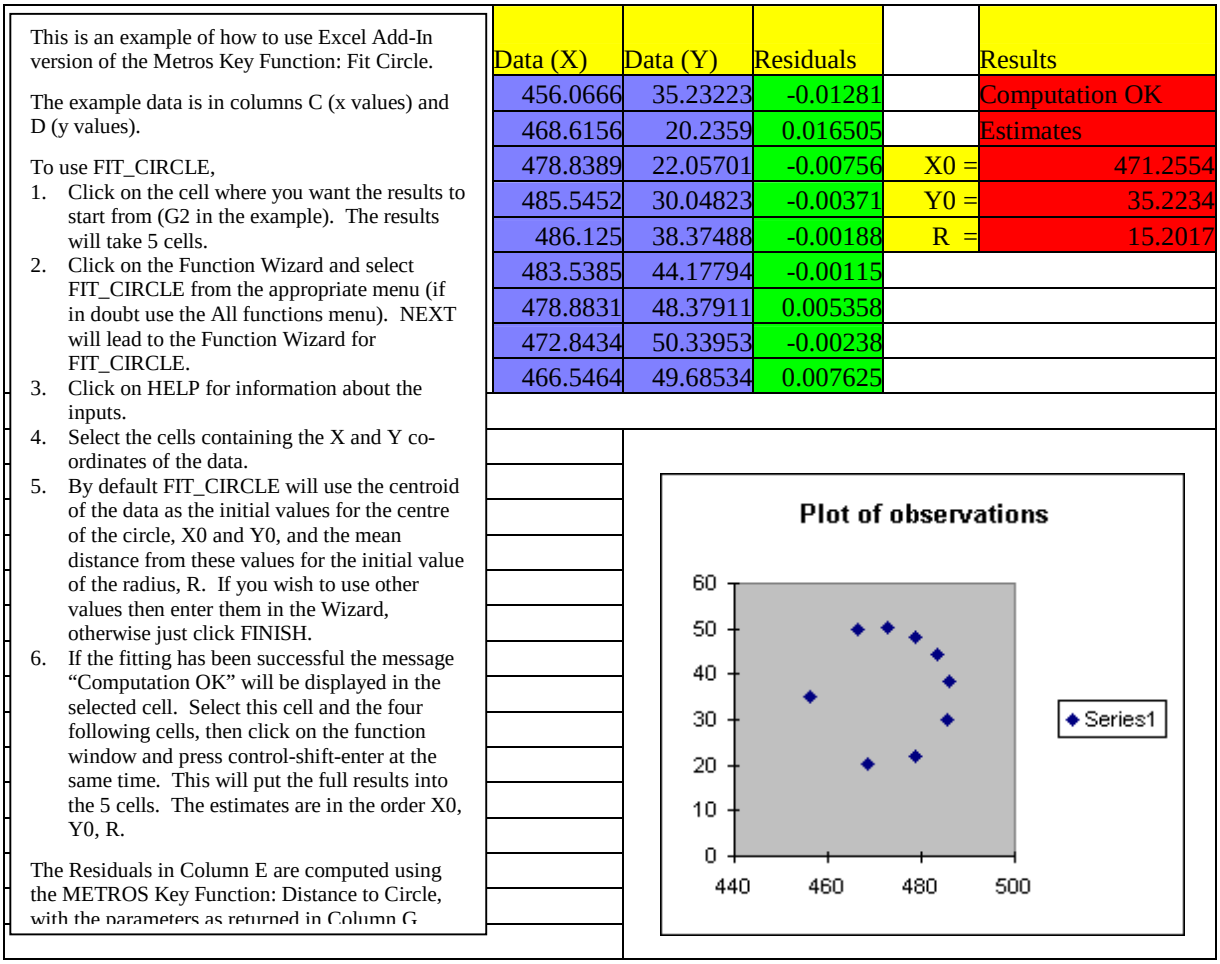

Figure 2 Example of an Excel spreadsheet using the METROS key function circle via a NAG "add-in"

3.3 Testing

The METROS approach to software testing is based on the use of reference data sets, as developed and promoted by the SSfM programme. The reference data sets are sets of inputs for a particular function together with the reference result; implementations of the function can be tested by applying them to the input data set and comparing the output with the reference result. Methods of generation of reference data sets, based on null-space methods, allow the data set to be generated for a predetermined result. METROS includes reference data sets for a number of key functions and are being extended to include more data sets during the current SSfM programme. These data sets will be used in the testing and validation of software contributed to METROS and other software. By making the data sets available on METROS we hope to demonstrate the openness of the process of accepting and validating contributions to METROS. Data sets available in METROS (not necessarily with reference results) can be used for comparing the efficiency of different algorithms and implementations of the same function.

3.4 Future Plans

There are a number of issues to be addressed in making METROS successful, making the algorithms and software in METROS accessible to all those who could use them. The main issues are encouraging contributions and promotion: getting people to access METROS. If METROS is to be useful and successful it needs a to reach a wide audience that will provide a large user community. Only from a large user base, can we expect sufficient contributions to allow METROS to grow and to become more relevant to its users. There will be contributions to METROS from projects in the current SSfM programme but we also need external contributions.

The users of METROS are measurement scientists and, equally importantly, the software developers who produce software and systems for measurement. Measurement scientists and their software developers are largely unaware of the particular issues to be addressed in software for metrology and tend to use common algorithms and software components that may not be fit for purpose in measurement. Therefore, they are not going out to look for support in developing software for metrology and we must find them. There is a project in the current SSfM programme aimed at the promotion of METROS. We will use the NPL and SSfM websites to draw people in to METROS and publicise METROS through NPL's network of industrial clubs (organisations aimed at a particular industrial sector or field of measurement).

Contributions to METROS will be validated using peer review of the algorithms employed by the software and reference data sets to test the software implementations. The validation status of software will be indicated on the web pages. Contributions and areas for development will be discussed on a discussion board; this will allow users to indicate the desire for new functions to be implemented and for developers to understand the users requirements.

METROS already has an international dimension through the European Metrology organisation (EUROMET): there is a EUROMET project to encourage contributions to METROS, as EuroMETROS. We have also received offers of software from Canada and New Zealand. As well as encouraging contributions from the rest of the world, we are also keen to avoid conflicts with similar web based software libraries. It is important that we liase and integrate sensibly with other related activities or web sites, so as not to duplicate effort nor develop pointless rivalries.

4 NPL's Underlying Solution

At the National Physical Laboratory, there is an understanding that best-practice solutions need to be delivered to a range of environments, including Microsoft Excel, LabView, Matlab and general programming. In order to provide a stable underlying framework for their best practice solutions they have turned to the Numerical Algorithms Group (NAG) and their libraries of numerical and statistical components. In particular, since NPL predominantly work in the Windows environment, NPL have chosen to take a site-wide license for the NAG DLLs and to work closely with NAG to ensure that these quality components are readily available from within these environments.

From NPL's perspective this means that they can rely on have the same underlying numerical and statistical components available for their best practice solutions. Hence, they don't have to rigorously test the underlying components of each of the front-end environments – some of which they know to have problems (see for example [2]) – they can test once and use many times.

5 Conclusions

The need to deliver top quality analytical algorithms to the metrology community in an easy-to-use manner is being addressed by the METROS environment as part of the Software Support for Metrology 2 Programme (SSfM-2). NPL and NAG are at the heart of those developments and will populate the METROS environment with a range of best practice solutions for a range of working environments.

The NAG-based solutions will not be the only solutions provided. Other software suppliers will be free to provide solutions, as will users. All solutions will all be made available on an equal standing with testing and validation information being made available where possible.

NPL have chosen internally to use NAG routines as their base for numerical and statistical calculations wherever possible in order to ease maintenance and to maintain high quality standards.

6 References

1. Robin Barker. Software Re-use: A Guide to METROS. Software Support for Metrology Best Practice Guide No. 5, National Physical Laboratory, September 2000.
   www.npl.co.uk/ssfm/download/documents/ssfmbpg5.pdf

2. H.R. Cook, M.G. Cox, M.P. Dainton and P.M. Harris. Testing spreadsheets and other packages used in metrology: Testing the intrinsic functions of Excel. Report to the National Measurement System Policy Unit, Department of Trade and Industry, from the UK Software Support for Metrology Programme. NPL Report CISE 27/99, September 1999.
   www.npl.co.uk/ssfm/download/documents/cise27_99.pdf