ISSUE 9 • SPRING 2000

Counting on IT

MATHEMATICS AND SCIENTIFIC COMPUTING

A year of achievements for SS*f*M

SS*f*M stream at NMC 99 well attended

The second year of the first National Measurement System (NMS) Software Support for Metrology (SS*f*M) programme (April 1998 - March 2001) has been a year full of achievements.

The year began very well with the hosting of the Advanced Mathematical and Computational Tools for Metrology conference in Oxford on 13-15 April 1999. This was a well attended international event at which the SS*f*M programme was seen to be the envy of those with similar interests in other countries. The UK was seen to be taking the lead in co-ordinating generic software and mathematics support for metrology, right across the NMS and in international co-ordination of such activities.

Within the year, several workshops have been held. These included one on uncertainties and statistical modelling, one on data fusion and related topics, and one on continuous modelling. There were also two SS*f*M Club meetings, one within the National Measurement Conference (NMC 99) in Brighton in November and one hosted by Glaxo Wellcome in March. However, by far the most impressive workshop was the one on Statistical Analysis of Inter-laboratory Comparisons held at NPL on 11-12 November. This is reported on elsewhere in this newsletter. NMC 99 provided the SS*f*M programme with an important platform by having one of the parallel streams devoted almost exclusively to SS*f*M topics.

An annual membership fee was introduced for full members of the SS*f*M Club. This full membership is a fully transferable corporate membership. As expected this had the effect of initially causing a drop in membership, but we are pleased to say that membership has built up steadily throughout the year. At the end of the previous year there had been 124 individual members plus 19 international associates, a total of 143 members. By the end of this second year there were 38 full members (representing 30 organisations), 50 NPL (individual) members and 44 international associates, a total of 132 members.

One particularly attractive development for club members has been the addition, within the SS*f*M web site, of restricted web pages for club members only. Through these pages draft guides are made available for comment and other unpublished material, such as slides of presentations, is provided for downloading. The public SS*f*M web site has also developed, particularly with the addition of a discussion forum on uncertainties for key comparisons, framework 5 project suggestions, and the formulation of SS*f*M-2.

This year has seen the production of five best

Contents

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practice guides, at least in "draft for comment" form. These are as follows:

Guide 1: Measurement System Validation, by NPL, now finalised
Guide 2: Virtual Instruments, by Adelard, now finalised
Guide 3: Guide to the Development of Software for Metrology, by Logica
Guide 4: Discrete Modelling, by NPL, now finalised
Guide 5: METROS, the Software Reuse Library, by NAG and NPL

The two that are not yet finalised are currently being evaluated and feedback is sought from initial experience in using them. In the case of the Virtual Instruments guide, there is an accompanying training course which has been run both at NPL and publicly. Feedback received indicates that this is a most valuable practical guide and course. It covers the general principles of developing virtual instrument software, as well as the specific implementation of such software in LabView or in Visual Basic.

Other publications include a large set of status reports reviewing the use of software and mathematics in each area of NMS metrology, and similar activities world wide. There have also been reports on Y2K issues, legacy software, the generalisation of the "Virtual Co-ordinate Measuring Machine" concept, data visualisation, format standards for metrological data, and statistical analysis for key comparisons. However, the most significant of the other reports are three on numerical software testing, particularly as applied to mathematical and statistical functions within Excel. This work is the subject of a major item within this newsletter. In addition to all these reports, there have been many presentations at conferences, workshops, club meetings and to industrial groups on various aspects of the SS*f*M programme.

We now look forward to the final year of the programme, including the production of another five best practice guides and the development of three more training courses.

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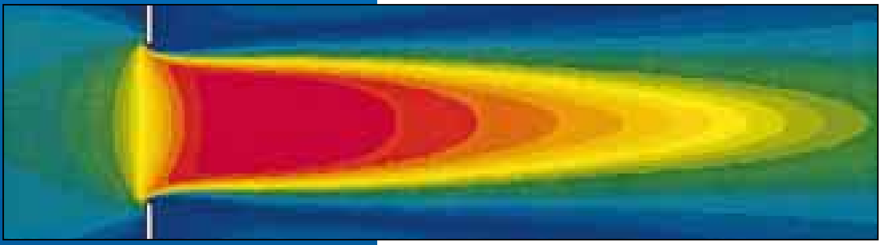

Velocity magnitude downstream of an orifice plate

Continuous Modelling

In many metrological experiments, the behaviour of the system is best described by a set of ordinary or partial differential equations - a continuous model. Typical applications of these models are to gain an understanding of the physics of the metrological process, give guidance on experimental design or determine estimates of system parameters.

There are a number of aspects that must be considered in a continuous model: the physical model as a system of equations, the discretization of that model by a particular method, the sensitivity of the solution to the boundary conditions, and the implementation as a piece of software. Among barriers to the use of continuous modelling are problems in obtaining the boundary conditions, the time to build the model, and the costs of validating the model.

As part of the SS*f*M "Methods of Modelling Measurement Data", NEL is writing a report on modelling continuous data, aiming to guide the development and promotion of best practice and to enable different parts of the metrology community to learn from one another. The report in addition provides a survey of continuous modelling in metrology and presents several case studies.

Two successful workshops have been held at which many of the issues of continuous modelling were addressed. A third and final workshop will be held later this year, bringing together metrologists and experts in partial differential equations to discuss methods for solution validation and uncertainty estimation. These are key areas to be addressed if continuous modelling is to reach its potential in metrological applications.

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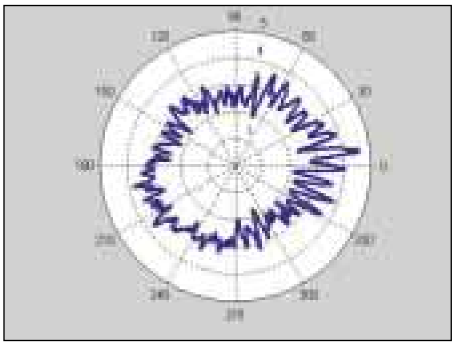
Mathematical modelling and ultra-high accuracy roundness measurement

The Talyrond 73HPR roundness instrument has been developed by NPL and Taylor Hobson Limited as part of the NMS Programme on Length Metrology. It is used to establish the form of nominally-circular sections of an artefact. It incorporates a precision rotary stage, which permits the component being measured to be rotated through arbitrary angles. Measurement traces taken for each position of the stage are combined to estimate both the component form errors and the instrument spindle errors.

The use of techniques of the type being promulgated by the SS*f*M programme were used to formulate a mathematical model of the measurement process. Least-squares methods, the Fast Fourier Transform and other numerical techniques were employed to derive a solution. Detailed statistical error analysis provided a Type A evaluation of the solution uncertainties. Software implementing the solution process forms an integral part of the ultra-high roundness-measurement service to customers.

The main outputs of the software are the Fourier representations of the component form error, the peak-to-valley roundness error, and the uncertainties in these quantities. The estimated instrument spindle error is also provided as a check on the temporal stability of the instrument.



The form error of a component determined using the indicated approach

The Talyrond 73HPR roundness instrument

The model-based approach is general, being applicable to any set of indexing angles, avoiding the harmonic-suppression effects present in many roundness systems, and providing automatic validation of the quality of the results by "reconstructing" the measurement traces from the model.

One of the most important features is an explicit uncertainty formula expressed in terms of the main measurement parameters (the number of points per trace, the number of traces and the indexing angles). The advantage of the formula is that it can be used to predict the uncertainty associated with any candidate measurement strategy.

A short paper on the technique was presented at NMC 99 and a full version is in preparation. Further work is in hand which will refine the approach to permit full account to be taken of any serial correlation present in the measured data and thus reduce further the already very small uncertainties evaluated for this measurement process.

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Uncertainties and Statistical Modelling

The major "event" in recent months within this project was a workshop held at NPL on 11-12 November 1999 on the Statistical Analysis of Inter-laboratory Comparisons.

The objectives were to:

- Deliver EUROMET Project 504 on the same topic
- Consider implementation aspects of the Technical Supplement to the Mutual Recognition Arrangement (MRA) signed in Paris in October 1999
- Discuss appropriate statistical techniques
- Propose a way forward

"The workshop was attended by over 120 delegates from 27 countries"

The workshop was attended by over 120 delegates from 27 countries, including in particular, representatives from all main CIPM Consultative Committees (CCs) and statisticians concerned with the analysis of inter-laboratory comparisons.

Presentations were given by the CIPM CCs and by statisticians who develop and apply analysis tools to metrological data. Discussion sessions centred on the features of the CIPM key comparisons (KCs) and on relevant statistical tools and their applications.

Maurice Cox addresses the Workshop at NPL

The main emphases of the meeting concerned:

- the MRA, especially its interpretation and implementation using statistical methods to determine the KC reference value and the degrees of equivalence of national measurement standards
- mathematical models of KCs, to account for KC design and provide a framework for analysis which included correlation effects
- the ISO Guide to the Expression of Uncertainty in Measurement (GUM) and its application to KCs
- relevant statistical tools including outlier tests, least-squares and other fits, estimators such as the weighted mean, median and total median, and the estimation of sampling distributions
- quality aspects of KCs
- the determination of defensible and objective solutions.

The highly interdisciplinary nature of the meeting was found to be of considerable value, enabling everyone to appreciate both the similarities and the differences between KCs in diverse metrology areas. A detailed workshop report is available.

Other aspects of the project are concerned with producing a best-practice guide and software specifications, due to be published in June 2000. Some users, especially in conforming to their organisations' or clients' quality procedures, need to be sure that the main approach advocated in the GUM is applicable for their purposes. Therefore, an important aspect of the guide will be the provision of a validation procedure, with specifications of software tools to support it. The procedure will also be capable of use in its own right to provide uncertainty statements when the conditions of the main GUM approach do not apply. Finally, discussions at international level start in Spring 2000 to consider possible enhancements and extensions to the GUM, especially to permit improved industrial usage. The SS*f*M project team, containing staff from NPL and the National Engineering Laboratory, will play a leading role in these deliberations.

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Modelling Discrete Data - a Best Practice Guide

To extract knowledge from measurements, we need a mathematical model of the system. For an (apparently) simple measurement task such as using a steel rule to measure the length L of a wooden rod, there is may be a straightforward relationship between the measurements and the quantities of interest, e.g., the reading x from the ruler scale is an estimate of the length L. In more complicated measurement experiments the relationship between the measurements and the parameters of interest is generally less straightforward.

If we are interested in an accurate estimate of the rod length, we must take into account the effect of temperature and bending on the rule and rod, the squareness of the ends of the rod, the effect of humidity on the wood, etc.

In general terms, the mathematical model predicts the response of the system y (e.g. scale reading) as a function of the variables $\mathbf{x} = (x_1,\ldots,x_p)$ (e.g., temperature, humidity) and the unknown model parameters $\mathbf{a} = (a_1,\ldots,a_n)$ (e.g., length of the rod): $y = f(\mathbf{x}, \mathbf{a})$. The goal of a measurement experiment is to determine estimates of $\mathbf{a}$ from measurements of responses y_i of the system corresponding to variables $\mathbf{x}_i$. This is usually done by solving a set of equations involving the parameters $\mathbf{a}$ and data $(y_i,\mathbf{x}_i)$.

The equations relating the response of the system to variables and parameters represent one aspect of the model. A second aspect arises from the fact that measurements have uncertainties associated with them which feed through to uncertainties in the parameter estimates. This means that in solving for the parameters $\mathbf{a}$, it is necessary to take into account the uncertainties in measurements in order to determine estimates that are most consistent with and make best use of the data.

We can assess the effectiveness of different estimation approaches by using Monte Carlo simulation to examine the variation in parameter estimates. Suppose a system is modelled as a linear response $y = a_1 + a_2x$ depending on one variable and two parameters: estimates of the parameters a_1 and a_2 can be found from fitting a best fit line to data (see Figure 1). Figure 2 shows the variation in the estimates of parameter a_1 for three estimation algorithms, the first using an optimal approach (least variation), the second using inappropriate weights for the data, and the third using only two of the data points (most variation). Designing a good parameter estimation approach is a crucial step in getting the most from the data.

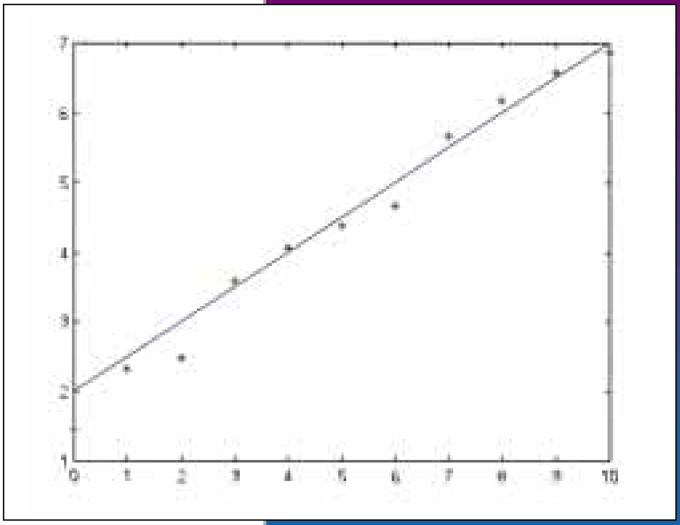

Figure 1: Estimating parameters from a best fit line

The Best Practice Guide for discrete modelling covers all the main stages in experimental data analysis: construction of candidate models, model parameterization, error structure in the data, uncertainty of measurements, choice of parameter estimation algorithms and their implementation in software, with the concepts illustrated by case studies. A www version of the Guide will allow for further chapters on models, algorithms and case studies to be added as an ongoing activity within the Metrology Software environment METROS within the next programme.

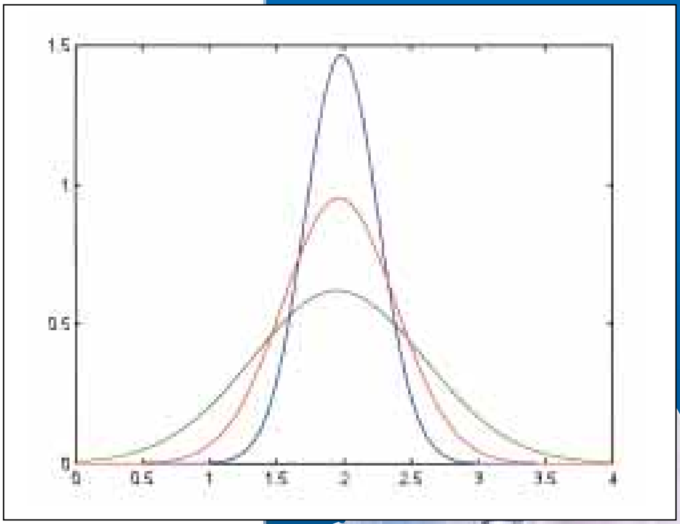

Figure 2: Estimates obtained from three estimation algorithms

Further Reading:

SSfM Best Practice Guide 4: Discrete Modelling, by NPL

SSfM Best Practice Guide 5: METROS, the Software Reuse Library, by NAG and NPL

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Reference Data for Testing the Numerical Accuracy of Software Tools

A requirement exists, driven to some extent by Quality Management Systems, to demonstrate that the scientific software used in metrology is fit for purpose, and especially that the results it produces are correct, to within a prescribed accuracy, for the problems purportedly solved. To meet this need, a general methodology for testing the numerical accuracy of scientific software has been proposed [1].

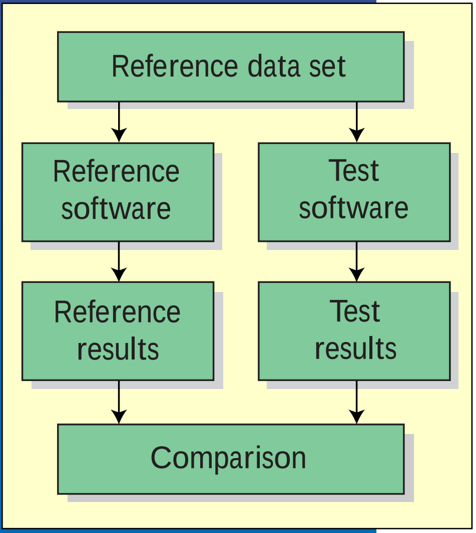

Figure 3: Using reference software to test the numerical accuracy of scientific software

The basis of the approach is the design and use of *reference pairs*, i.e., reference data sets and corresponding reference results, to undertake “black-box” testing. A reference pair may be produced either by starting with a reference data set and applying *reference software* to it to produce the corresponding reference results, or by starting with some reference results and applying a *data generator* to them to produce a corresponding reference data set. Procedures for undertaking software testing in these ways are illustrated in figures 3 and 4.

Both approaches are adopted in [1] although, where possible, a data generator is used to construct reference data sets which have known solutions, i.e., solutions specified *a priori*. Where a mathematical *characterisation* of the solution exists, data generators can generally be implemented, and this applies to a wide range of calculations used in metrology.

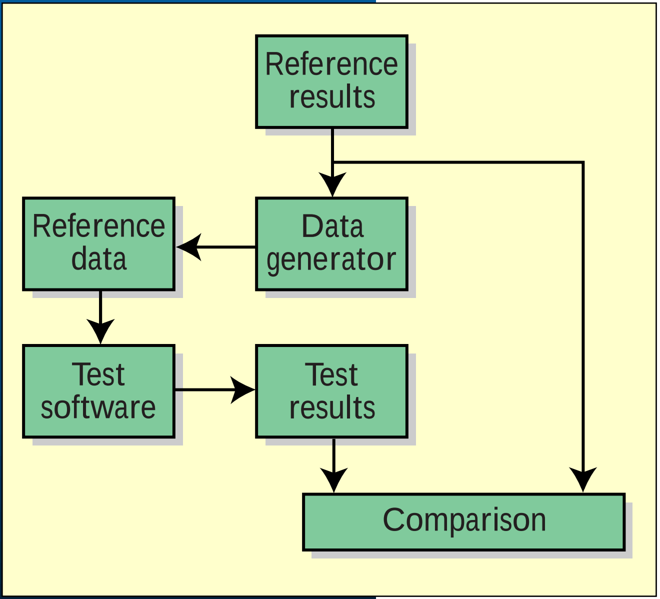

Figure 4: Using a data generator to test the numerical accuracy of scientific software

The alternative approach relies on the availability of reference software. Reference software must be written to an extremely high standard, and consequently it cannot be produced without a great deal of effort. It is akin to a *primary standard* in measurement, such as a kilogram mass, to which secondary standards are compared for calibration purposes. We have found that a data generator can be produced with only a small fraction of the effort required to write reference software. It is usually a much more compact operation with fewer numerical pitfalls, and it has the advantage that the theory is generic, and the software is reusable. The testing overhead is significantly less than that of reference software for the forward calculation (where the reference results are determined from the reference data sets).

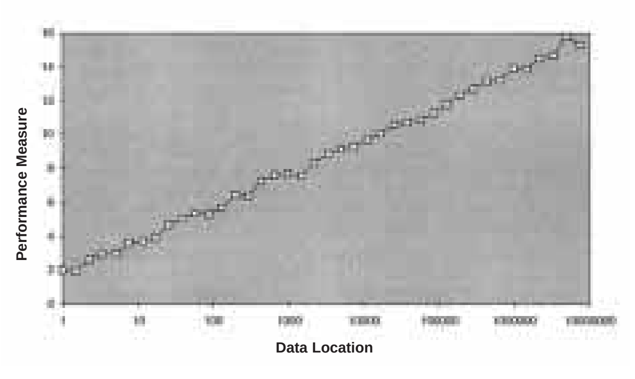

Figure 5: The numerical performance of the TREND function for a suite of reference data sets

Testing the Intrinsic Functions of Excel

The general methodology for testing the numerical accuracy of scientific software described in [1] has been applied to the in-built functions of the spreadsheet package Microsoft Excel for Windows 95 (version 7.0a), and the results are reported in [2]. The results of testing the accuracy of statistical procedures taken from Microsoft Excel 97 are also presented in [3, 4]. Here, we highlight some of the conclusions taken from [2].

The numerical performance of some of Excel’s “regression” functions can be *poor*, with results accurate to only a small number of significant figures for certain data sets. This can be caused by the use of a mathematical formula (as in the *STDEV* function) or a model parametrisation (as in the *LINEST* and *TREND* functions) that exacerbates the natural ill-conditioning of the problem to be solved, i.e., leads to results that are not as accurate as those that would be returned by alternative stable algorithms. The poor performance can also be a consequence of solving a substitute problem that approximates to the one required to be solved (as in the *LOGEST* and *GROWTH* functions). In figure 5 we illustrate the numerical performance of TREND as a function of data location using data sets obtained from a data generator.

The numerical performance of Excel’s mathematical and trigonometric functions is generally *good*. The exception is the inverse hyperbolic sine function, *ASINH*, for which the algorithm used is unstable for negative values of its argument.

For Excel's statistical distributions, graphs of the quality metrics used to summarise the numerical performance of these functions exhibit *systematic* behaviour, *discontinuities,* and large values, at *critical* values of their arguments. These features are illustrated in figure 6 where the *CHIDIST* function is compared against the equivalent function taken from the IMSL library.

References

[1] *A methodology for testing spreadsheets and other packages used in metrology.* SS*f*M web site, publication 299.

[2] *Testing spreadsheets and other packages used in metrology: testing the intrinsic functions of Excel.* SS*f*M web site, publication 273.

[3] L. Knusel. *On the accuracy of statistical distributions in Microsoft Excel 97.* Computational Statistics and Data Analysis **26** (1998), 375-377.

[4] B.D. McCullough and B Wilson. *On the accuracy of statistical procedures in Microsoft Excel 97.* Computational Statistics and Data Analysis **31** (1999), 27-37.

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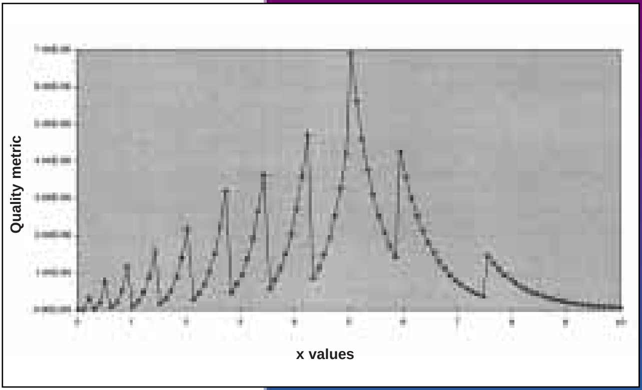
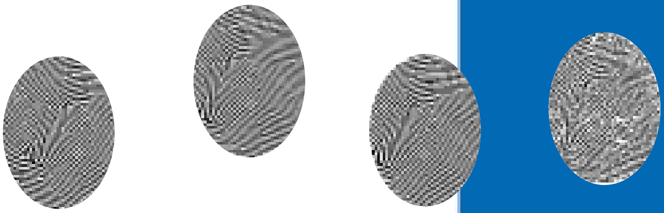
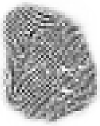


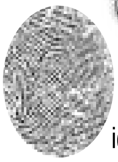
Figure 6: The numerical performance of the CHIDIST function measured against an alternative software implementation

Best Practices for Performance Evaluation of Biometric Systems



In real life, fingerprint images are given in different positions and rotations, and suffer from noise, cuts, and distortions. Often only a partial image is captured



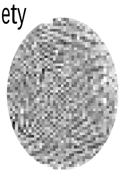


NPL has been working jointly with the UK Government's Biometrics Working Group, and the National Biometric Test Center in the USA, to develop best practice guidelines for the performance testing of biometric systems.

Biometric systems identify individuals from their physiological and behavioural characteristics. An intrinsic performance measure is the likelihood of identification errors in terms of "false matches" and "false non-matches". These, and other error rates must be determined by tests on real data.

A review of previous performance tests of biometric devices reveals a wide variety of conflicting and contradictory testing protocols. Even single organisations produce multiple tests, each using a different test method. Protocols vary because test goals and available data vary from one test to the next. However, another reason for the various protocols is that no guidelines for their creation exist. The inconsistencies between tests make it difficult, if not impossible, to compare performance or to determine likely performance on new applications - difficulties which are acknowledged by the biometrics industry.

Biometric testing can be of three types: technology, scenario, or operational evaluation. Each type of test requires a different protocol and produces different results. Further, even for tests of a single type, the wide variety of biometric devices, sensors, vendor instructions, data acquisition methods, target applications and populations makes it impossible to present a precise "standard" testing protocol. On the other hand, there are specific philosophies and principles that can be applied over a broad range of test conditions. These principles are described in the biometric testing best practice document, available at *www.afb.org.uk/bwg/bestprac.html.*



The guidelines cover all the main phases of performance evaluation: selection of volunteers, enrolment, collection of test data, analysis of data, dealing with uncertainties, and how results should be reported. Possible pitfalls at each stage are explained.

Though it may not be possible to follow best practice completely in any test, we believe that the concepts can serve as a framework for the development of scientifically sound test protocols for a variety of devices in a range of environments.

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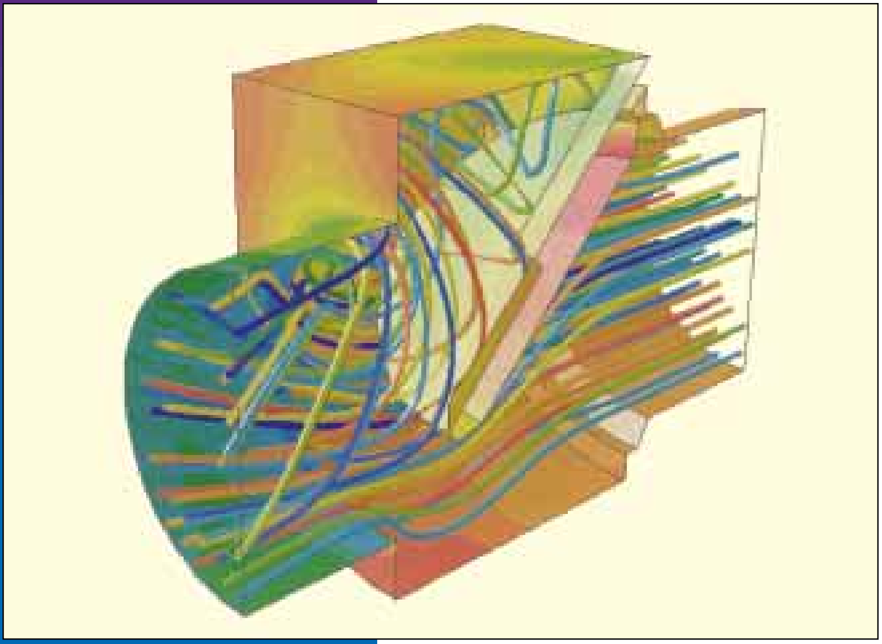
Visualisation in Metrology

Visual modelling and data visualisation are rapidly developing technologies, with a wide range of applications in science, industry and commerce. Sira has recently completed a year long study on the application of these techniques in metrology, as part of the SS*f*M programme.

Six case studies highlighted metrological applications, which consisted either of designing new visualisation solutions, or of publicising the value of existing work. A diverse range of applications requiring solutions of varying complexity was purposely chosen, in order to stimulate those directly involved, and to give the work appeal to a wider audience.

Visualisation of X-ray production using the NPL electron linear accelerator



Pathlines superimposed on contours of fluid pressure

Virtual instruments and uncertainty estimation

Many measuring instruments undergo periodic calibration, a process that generally involves using the instrument to measure a number of calibrated artefacts (traceable to national standards) and, from these measurements and the calibration information, deriving a calibrated model of the instrument response. This response model relates that output from the instrument to units traceable to standards, for example converting a voltage to a temperature measurement. The response $\mathbf{y}$ is modelled as a function $\mathbf{y} = f(\mathbf{x}, \mathbf{b})$ of the variables $\mathbf{x}$ and calibration parameters $\mathbf{b} = (b_1,\ldots,b_n)$, for example, the coefficients of a polynomial representing a calibration curve.

These calibration parameters, determined from measurements, will have an associated uncertainty. Often, when the instrument is re-calibrated, there is a significant change in the calibration parameters as behaviour of the instrument drifts with time (due to wear, etc.). Both these effects need to be taken into account when evaluating the uncertainty associated with the measurements produced by the instrument.

"Model and simulate... sources of measurement error"

In recent years a number of laboratories, including NPL, PTB and IMGC, have developed approaches based on numerical simulation to estimate uncertainties associated with co-ordinate measuring machine (CMM) measurements. A Virtual CMM attempts to model and simulate all the main sources of measurement error and, in particular, how the uncertainty and drift in the calibration parameters contribute to the uncertainty in assessing the quality of manufactured parts, such as the circularity of a cylindrical shaft. As part of the SS*f*M programme

The areas of metrology which were involved were Electromagnetic, Thermal, Ionising Radiation Dosimetry, Computational Fluid Dynamics, Remotely Operated Vehicle guidance and Composite Material Testing. Contributions were made by the National Physical Laboratory, the National Engineering Laboratory, University College London and Sira itself.

Visualisation should begin from a clear specification of the problem to be solved. In designing a solution the user has to consider carefully the type of effects which it would be useful to view, the software and hardware tools which are available, and the way in which visualisations are presented and accessed. It is possible to visualise data in many ways, so finding the best way to make the visualisation accessible is vitally important. This project has demonstrated how careful use of available technology can provide measurement specialists with tangible benefit.

A workshop describing each of the case studies was held at NMC 99 in November 1999, and a project report has been distributed to metrology practitioners. A training course on the subject is planned for later this year.

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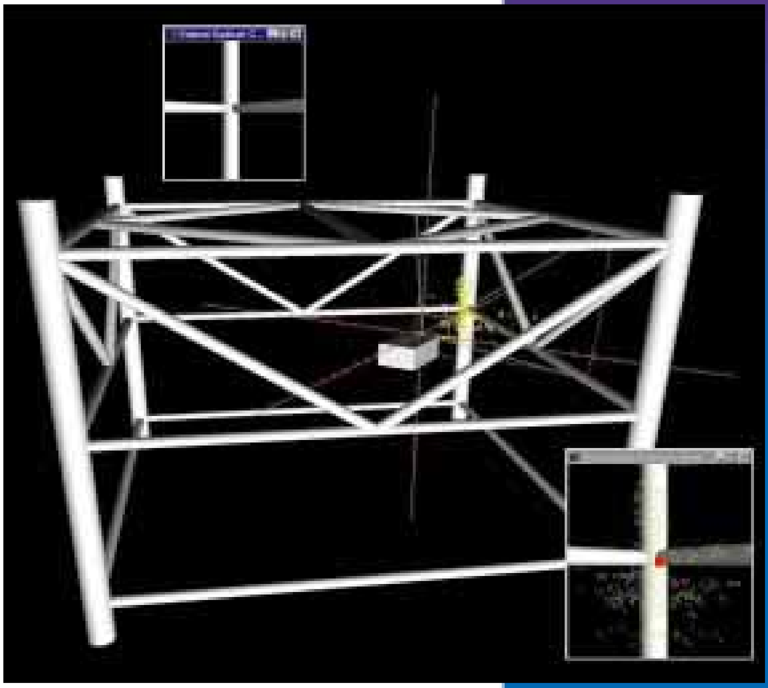

Visualisation of an underwater oil rig structure

Small co-ordinate measuring machine

NPL have completed a report on how the Virtual CMM concept can be generalised to models of other measuring instruments, providing a general methodology to take into account prior calibration information in uncertainty estimation.

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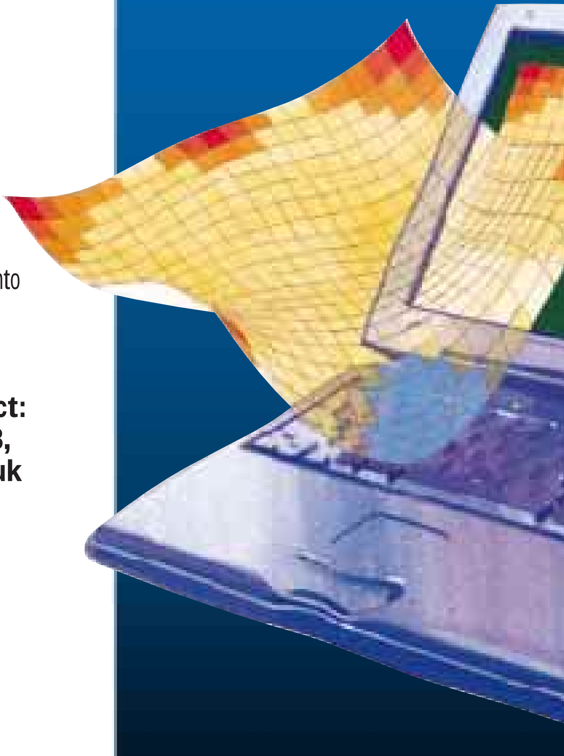


Interactive web pages

In the Spring 1999 issue of Counting on IT we outlined our plans for two pieces of work related to the use of the world wide web in metrology. The first of these, a report "Guidance and tools for interactive web pages", was published in September 1999 [SS*f*M web site, publication 480]. It reviews the technologies presently available, providing a resource for anyone wishing to develop interactive web pages, and briefly looks ahead to what may be just over the horizon.

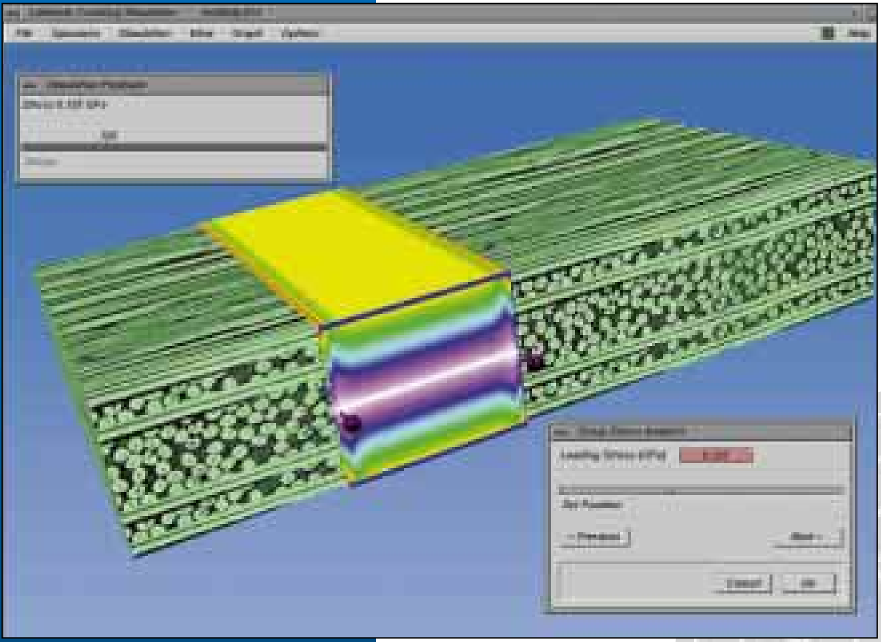
> *"the applets use various "plug-in" reusable components"*

The second piece of work, aimed at providing examples of the kind of interactive web pages that can be developed to support metrology, is also complete now, and samples of the output can be seen on the next page. Two applets have been developed, demonstrating a number of software components and concepts in the design and use of interactive web pages:

- they implement user interfaces allowing the user to control the system parameters;
- the interfaces are designed to be as straightforward as possible, using colour and common conventions, such as grey buttons, white or colour coded text boxes etc. to present the controls;
- the applets use the Java event model to implement the interfaces, allowing. the user to manipulate the various parameters of the system with an immediate effect;
- the applets utilise the sophisticated graphics handling capabilities of Java to provide a visual environment for the user to explore or manipulate the system implemented. This adds value to the data, information, or service being presented to the user;
- the applets use various "plug-in" reusable components.

As with the majority of applets, the example applications are downloaded to run on the user's machine. This and the platform independence of the Java language, give many benefits.

You can view these pages at *www.npl.co.uk/ssfm/tt/ssfm_interactive_examples/index.html.*



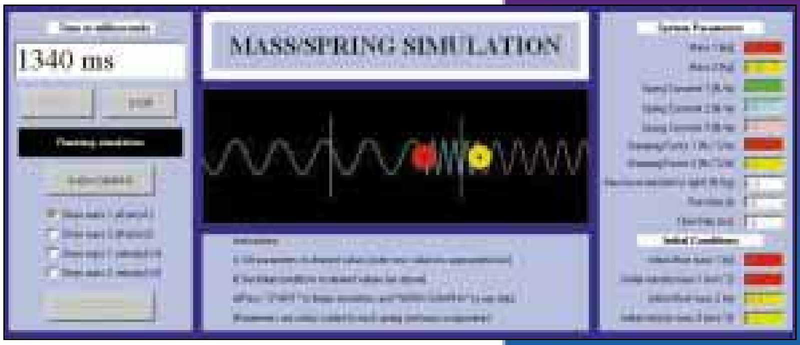
Visual Modelling Screen in an Interactive Web page

Flick through the pages of this newsletter for a moving image of the springies

Springies

In the first of the two example applications a mass spring system is modelled to demonstrate the modelling and visual display of a dynamic multi-component system. Mass spring systems are themselves used to model other dynamic systems, such as reflections and interference of radio frequency waves, AC electrical systems, materials behaviour etc.

The model of this system uses the 4th Order Runge-Kutta method to solve the ordinary differential equations describing the motion of the components over a specified time step. The results from this model are returned to the applet and used to animate a simulation of the motion of the system.

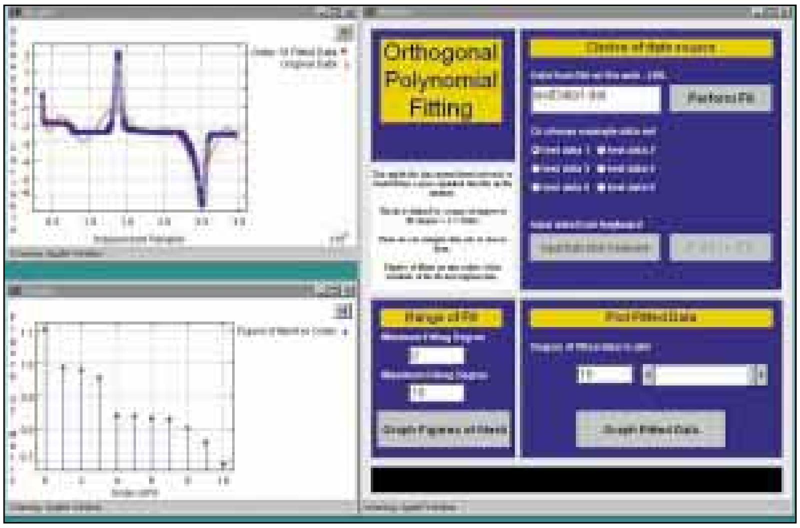


Data fitting

The second applet implements an orthogonal polynomial fitting algorithm and provides an interface to select or enter data for fitting. It allows the user to find an optimal fitting order for the data through setting a range of orders to fit and displaying a graph of figure of merit versus order for the data. From the graph, the minimum value can be selected if it is within the range of orders of fit.

The potential of this type of applet is the provision of a single system available over the internet allowing multiple users access to a range of fitting methods, the ability to explore the fitting parameters for each and the assurance of a well tested or verified algorithm with consistency of results with other users. This would give users a very high level of confidence in their results - that they have an optimal and reliable fit to their data.

For further information contact: Bernard Chorley, extension 7050, e-mail: bernard.chorley@npl.co.uk



Sample window from data fitting applet

Extending the numerical power of Excel

The issue of legacy software within numerical analysis is one that continually needs to be addressed. A number of software libraries have been written in various languages, such as Fortran and Pascal, to perform all manner of numerical tasks. However, problems are encountered when attempting to develop an application in one language and access software libraries written in another. Within metrology, if this problem is encountered, it is usually solved by communication between languages by way of data files, which is a potentially cumbersome process that may introduce I/O errors.

A prime example of this is the increasing use of Excel within metrology. The need to perform complicated data analysis using facilities that are beyond the scope of the intrinsic functions provided within this spreadsheet package may result in the need to import onto worksheets and export data to files in various formats. In addition, attention has already been drawn in a previous article about the need for care to be taken when the intrinsic functions are used. The numerical performance of some of the functions that are frequently used in metrology, such as LINEST and STDEV have been shown to be poor for certain choices of data [1].

"Minimal cost of development within VBA"

To circumvent these problems within metrology, a method of providing access to the extensive range of existing numerical libraries written in Fortran, by packaging them as dynamically linked-libraries (dlls) is recommended. This involves the compilation and linking of subroutine libraries such as the Basic Linear Algorithms Subroutine (BLAS), or other libraries provided by the developer. Subroutine libraries that are proven to be robust and efficient, and used widely in mathematical modelling are suited for this purpose. This avoids the need for detailed program development on the part of the user. The dlls, once compiled and linked may then be made available for call from within Excel via its development language, Visual Basic for Applications (VBA).

This technique is illustrated by a typical problem that can be solved by using numerical libraries in Fortran. In this case it is making of use of subroutines provided as part of the IMSL numerical Fortran library to obtain the solution of a non-linear least squares fitting problem. Two sine waves of identical frequency, but different amplitude and phase are fitted to two sets of measured data. Figure 7 shows raw data for the fitting purpose. Even by appropriate transformations of data values, this would not be possible using standard intrinsic functions within Excel.

Fitting data to straight lines and exponential curves is possible using the functions LINEST and LOGEST, but the approach recommended here allows more complicated fitting procedures to be made available. Supplying routines in this way permits the use of extant Fortran software of proven high pedigree, with minimal cost of development within VBA.

Reference:

[1] *Testing spreadsheets and other packages used in metrology: testing the intrinsic functions of Excel.* SSfM web site, publication 273.

For further information contact: Mark Dainton, extension 7012, e-mail: mark.dainton@npl.co.uk

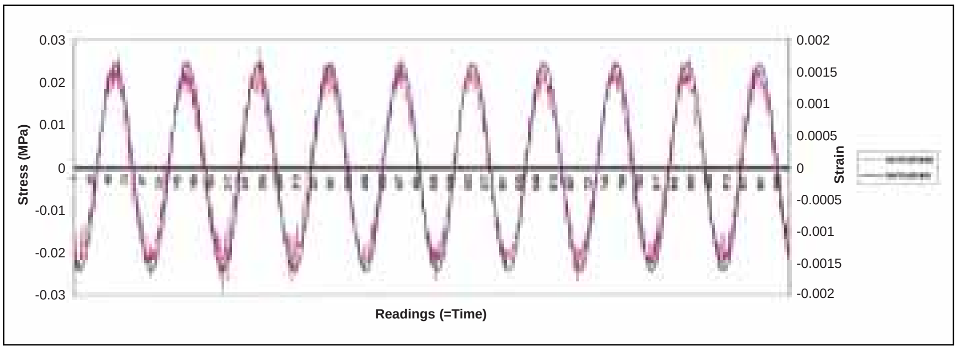


Figure 7. Stress/Strain Sinusoidal Wave

Identifying features in measurement data

A software package has been developed at NPL for identifying features (peaks and troughs, points of inflexion and elbow points) in measurement data. It forms an extension to the existing NPLFIT package. The software has been applied to thermal analysis data for the identification of temperature dependent material properties - see figure 8. This work was prompted by the need to determine these features as part of a project concerned with developing a "Measurement Good Practice Guide" on the use of thermal analysis techniques.

The approach is based on the following methodology. A spline curve is fitted to the data, and the first and second derivatives are evaluated. The zeros of the first derivative provide the peaks and troughs of the curve, and those of the second the points of inflexion. A decision is then taken by the software on which of these zeros are genuine and which are spurious. The algorithm for this decision selects as genuine zeros those that lie within a band which encloses the spline curve and which completely crosses the x-axis. The band is formed by calculating the expanded uncertainty of the appropriate spline derivative at each point on the curve. The elbow point is calculated differently as the intersection of tangents at the two selected points of inflexion. Uncertainty evaluation is carried out in accordance with the ISO Guide to the Expression of Uncertainty in Measurement.

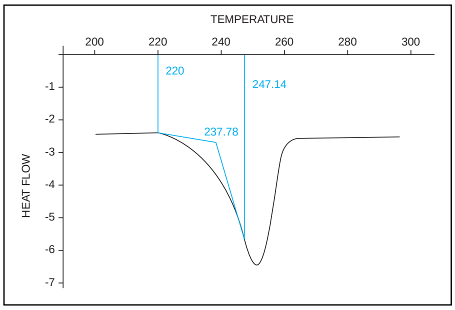


Figure 8: Extraction of elbow point

The software is interactive, so the user can select the range of data to be analysed, the type of feature to identify, the "important" features to display, and the two points to give the elbow point.

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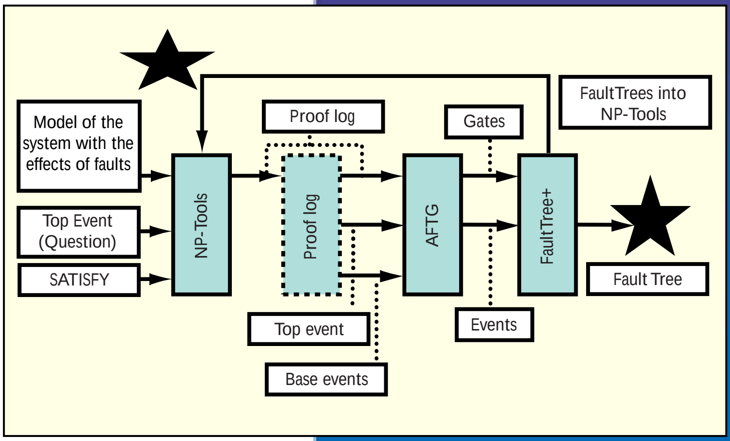
Automatic Fault Tree Generation with Logical Analysis

Over recent years algorithms for model checking have improved dramatically in terms of speed and ability to tackle large systems. They are beginning to be used in new application areas outside their traditional one of hardware. For example, commercial tools now exist in the railway industry. Fault trees are currently produced manually from specifications of a system and are then used to analyse the reliability of the system. This process is very error prone, and the fault trees can be very large, often including in excess of 2000 logical gates.



Tool for automatic fault tree generation

Under contract to AWE, NPL has developed a tool, *AFTG* - Automatic Fault Tree Generator (see diagram). This has two main functions:

1. Generating the fault tree. First a model of a system, including the effects of faults, is created using the tool *NP-tools*. A fault tree which is automatically generated from this is processed by a reliability tool *FaultTree+*. The resulting fault tree is complete and correct with respect to the model of the system.
2. Proving the fault tree. Fault trees developed in *FaultTree+* can be translated into *NP-Tools*. This allows logical properties of such fault trees to be proved.

AFTG also preserves names, splits fault trees into pages and pulls together gates of the same type. This is all done within the limits of *FaultTree+*.

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The METROS web site

METROS – the METROlogy Software environment – developed jointly by NAG Ltd and NPL is the main output of the SSfM *Software Re-use* project. The aim of METROS is to provide metrologists easy access to reliable and re-usable metrology software through a web interface. SSfM club members can preview METROS at the SSfM club site www.npl.co.uk/ssfm/members_only/metros. As well as metrology software, METROS will contain case studies illustrating the use of the software, methodologies for testing and validating the software, and information on commercial software packages. Developers of scientific software will also be able to use METROS to learn about the software requirements of metrologists and as a vehicle for providing software to the metrology community. METROS aims to be the main resource and delivery point for everything related to software for metrology.

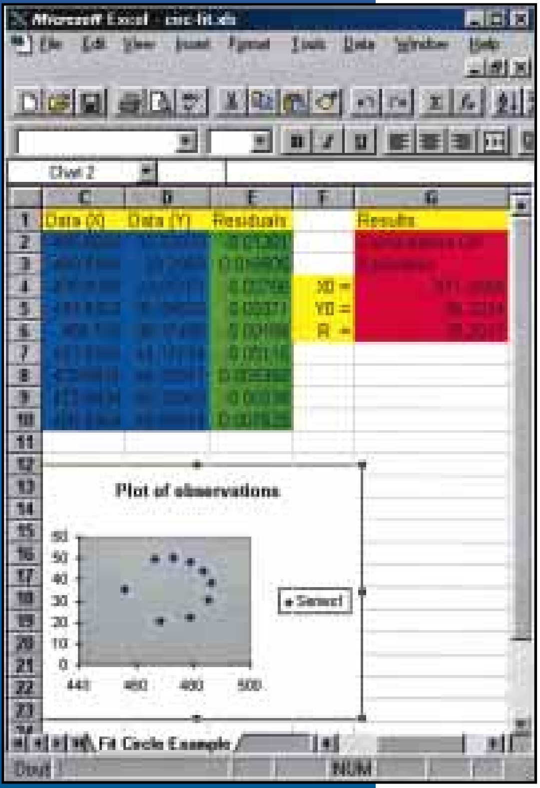

Figure 9: The METROS Key Function “Fit Circle”

METROS is built round the concept of a *key function*: i.e., a function that performs a basic calculation underlying a number of applications. *Application functions*, specific to an area of metrology, are built from key functions, promoting in a very direct way software re-use. Using the hyperlink facilities provided by the www interface, the user can move from a page describing the key function to pages concerned with software implementations or application functions which call it. Similarly, application functions will be linked to implementations and to case studies showing the use of these functions, as well as to pages describing key functions underlying the application.

Each function description will give the inputs and outputs of the function, the relationship between them (the computational aim) and, importantly, associated test data and/or validation criteria to be used to validate any implementation of the function. Implementation descriptions will specify the interface to the function, the target platform, and to what extent the implementation has been tested and validated. The software will be available either directly from the web pages (for example, as source code, dynamically linked library (DLL) or executable) or indirectly from a commercial supplier.

Implementations of a given function will often cover different languages and platforms. In many cases it will be possible to exploit a solution developed for one language/platform environment in another environment by using a “wrapper” for the implementation, again promoting software re-use. For example, it is possible to make functions implemented in FORTRAN available as user-defined functions in desk-top packages such as spreadsheets. (See the article “Extending the numerical power of Excel”.) The current METROS web site includes an example of a FORTRAN implementation of a circle-fit function that can be called from an Excel spreadsheet (see figure 9).

METROS users will have differing knowledge and skills and this will affect the way in which they interact with the system. For users with a programming/mathematical perspective the classification of key functions by category will be a suitable entry point. However, most users will have a metrological perspective and their entry point will be through their area of metrology.

It will be possible to perform a keyword search of METROS, to find an implementation of an application function, for example. If the users find that none is available, METROS may still be able to help. There may be a key function implementation which performs a more general calculation from which the required application can be developed (and subsequently submitted to METROS). If there is nothing which meets their needs, users can request the inclusion of a new key function.

The METROS web site is set to expand as new functions and implementations are added to fill out the existing structure. A wide range of supporting documentation on mathematical modelling and software development will be added as part of ongoing activity within the SSfM and other programmes in metrology. In particular, there will be support for the testing and validation of implementations of MetroS functions in a structure covering testing and validation.

MetroS is designed to be open and extensible. Users of MetroS, both individuals and commercial software developers, can contribute functions and implementations to MetroS and well as guide its development. How this material is added and updated will be co-ordinated as part of the web site maintenance but essentially, MetroS will be a resource owned by its user community, providing a focal point for finding solutions in metrology software.

The use of MetroS is explained in the draft best practice guide (see the article “A year of achievements for SS*f*M”).

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CRAFT Test Generation Tool

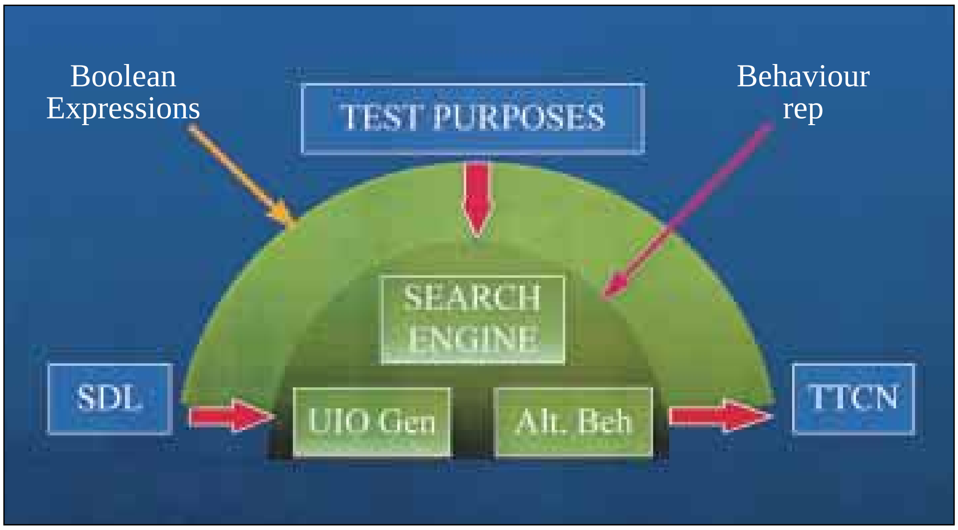

Figure 10: Test Generation - The conceptual outline

Figure 10 shows a conceptual view of the approach used by the EC sponsored *CRAFT* project. The project has developed a tool to produce TTCN tests (a standardised abstract test notation) from SDL (a system design language).

The *CRAFT* tool is based on the idea of modelling the SDL, the test purposes, and the resulting tester behaviour, in a common language - in fact in terms of a Boolean expression based on the system variables. The tool has generic routines for manipulating Boolean expressions, so it is then possible to answer questions such as “what is the simplest way of expressing this condition given that we know some other condition to be true?”

A second 'behaviour representation' is generated from the Boolean expression model. The behaviour representation is in some sense the simplest possible one needed to model the input and output behaviour of the SDL system, allowing the tool to investigate the overall system behaviour in an efficient manner.

The *CRAFT* test generation tool incorporates a very flexible state/event style test purpose input language, and sophisticated TTCN output. It can handle general data relations if needed, and it also knows about and deals sensibly with any sources of non-determinism, such as internal management interfaces, that might be encountered when testing.

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SS*f*M

Scientific Software

Techniques for High Integrity

Looking forward to SS*f*M-2: 2001 - 2004

We are now well advanced with the formulation of the next SS*f*M programme which is to run from April 2001 until March 2004. This new programme will retain the focus on generic mathematics and software activities in support of real needs of metrologists and industry throughout all the areas of metrology covered by the NMS. It will, however, change from the current programme's emphasis on technology transfer to a portfolio of projects which has a balance between technology transfer and research and development. The research content will rise from the current lowly 6% to nearer 50%.

Prior to the formal start of formulation we were attentive at the Foundations of Science Measurement (FSM 99) conference to listen out for the future requirements for mathematics and software support.

The formulation process began in October 1999 and has involved a lot of consultation, with particular emphasis on the SS*f*M Club membership and the Measurement Advisory Committee Software Working Group in the early stages. From July it will move on to a DTI public consultation phase.

It is proposed that the technical themes in the new programme should be as follows:

1. Modelling techniques
2. Validation and testing
3. Metrological software and algorithm development techniques

In discussion at FSM 99

4. Standards support and development
5. Support for NMS infrastructure

Many of the projects are expected to follow on naturally from the current programme. There are, however, suggestions for several completely new projects, including:

- Signal processing (theme 1)
- Intelligent technologies (theme 1)
- Numerical analysis for algorithm design (theme 3)
- Mathematical and statistical input to metrology standards (theme 4)
- Use of the Internet by calibration services (theme 5)

If you wish to comment on the formulation on this next programme, you can do so through the SS*f*M web site, particularly the related SS*f*M discussion forum.

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Centre for Mathematics and Scientific Computing (CMSC)

Making contact

You can contact any of the experts directly by using the direct dial number plus the extension or via e-mail.

Direct line +44 20 8943 + (extension)

Head of CMSC
Dave Rayner ext 7040 e-mail: dave.rayner@npl.co.uk

Software Support for Metrology Club
Jan Kane ext 7100 e-mail: jan.kane@npl.co.uk
SS*f*M web site: www.npl.co.uk/ssfm

If you have a general enquiry or do not know who you should contact please call our general enquires number and we will be pleased to help you.

(Note the new centre name)

General CMSC enquiries

+44 20 8943 7100 (direct line)
+44 20 8977 7091 (facsimile)

Web site: www.npl.co.uk/npl/cise

General NPL Helpdesk

For enquiries to NPL outside the scope of CMSC, please use:

+44 20 8943 6880 (NPL Helpline)
+44 20 8943 6458 (Helpline facsimile)

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