Counting on

A third successful year for SSfM

The third and final year of the first Software Support for Metrology (SSfM) programme (April 1998 -March 2001) has again been full of achievements.

The set of SSfM best-practice guides has been extended from the five produced by the end of the second year to ten at the end of the programme. The following table lists all ten best-practice guides, which together with other SSfM reports are being included on a single CDROM, providing a "road map" to the outputs of the programme: There were also reports on guidelines for software selection and software tools for uncertainty evaluation, which were supplemented by conference and journal papers on topics such as data fusion, model validation, and uncertainty evaluation.

In addition, three training courses have been developed on measurement system validation, advanced uncertainty evaluation and statistical modelling, and testing the numerical accuracy of scientific software.

Guide No.	Title	Originator	Status
1	Measurement System Validation	NPL	Published
2	Development of Virtual Instruments	Adelard	Published
3	Developing Software for Metrology	Logica	Finalised
	The Guide		
4	Discrete Modelling	NPL	Published
5	Software Reuse: Guide to METROS	NAG & NPL	Published
6	Uncertainties and Statistical Modelling	NPL & NEL	Final Draft
7	Testing Spreadsheet Models	NPL	Published
8	Mixed Language Programming	NAG	Published
9	Selection and Use of LIMS	Sira Test &	Finalised
		Certification	
10	Discrete Model Validation	NPL	Final Draft

A number of other reports were published during the year. NEL produced one on continuous modelling in metrology, and NPL produced a set of reports on numerical software testing, including the results of testing functions in MathCAD and S-Plus and comparative studies of various implementations of standard deviation and linear regression algorithms.

Measurement Systems Validation Training Course



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This year we have held a joint workshop on mathematical and statistical modelling, a workshop on data fusion, and a joint workshop on discrete and continuous modelling. We also participated very fully in the Advanced Mathematical and Computational Tools for Metrology conference held in Portugal in May.

The SSfM Club remains very active with 31 full members, 41 UK associates, 62 international associates and 81 NPL members.

Two Club meetings were held in the year. The University of Huddersfield hosted the first in September 2000, at which the topics covered were numerical analysis, continuous modelling, and uncertainty evaluation. The second meeting was held at NPL in February 2001, and the topics covered were statistical modelling, LIMS, looking back, and looking forward. Reports on club meetings are available to members via the SSfM web site, which also provides information on all the projects, and gives access to all publications and to the METROS web site.



Mathematical modelling workshop



AMCTM 2000 Meeting audience

For further information contact: Dave Rayner, extension 7040, e-mail: dave.rayner@npl.co.uk

Genetic algorithms in metrology

Traditionally, optimisation problems within metrology are solved by a variety of methods, including gradient-based or other direction search approaches. These techniques can be effective and accurate for finding a local minimum. However, in problems where a global minimum is required these methods can be somewhat limiting, as once they find an appropriate solution they terminate, and will thus not find anything other than the local minimum.

In order for a solution method to find global minima effectively when required, searches must take place throughout the solution space rather than just in the vicinity of a potential minimum. Since a search in this manner by definition needs to be less focused, such techniques lose out in terms of efficiency. However, a trade-off may be made in the ability to find global solutions, and it is often possible to combine a global search followed by a more localised one to obtain the accuracy required.

Among a number of promising techniques that can be used to assess global minima is the application of genetic algorithms. These computational methods mimic evolutionary processes in nature to obtain the most favourable, or *fit*, solution.

Genetic algorithms work in the following way: the system under analysis is firstly characterised in terms of a population of "chromosomes" made up of a string of binary numbers. Each string characterises a particular state of the system. The population of possible candidates for global minima is then subjected to a number of "evolutionary" processes governed by probabilistic rules. A check for convergence is performed after the application of the algorithms, and the process continues until a suitable convergence is achieved.

PA<u>GE</u>2

Random testing - bridging the gap

Recently we faced the task of testing software that "bridged" two tools: taking the output of one and applying a complex transformation to produce input for the other. The two tools were *NP-Tools*, which models systems and automatically proves their properties, and *FaultTree+*, a reliability analysis tool.

The techniques used to generate random self-checking programs were used to generate random fault trees for *FaultTree+*, which were then used to test the software bridge. The self-checking of the results was done by using the automatic proof capabilities of *NP-Tools*.

A test suite for the transformation was developed manually. However, the sizes and the usefulness of the tests were limited, because each test required the construction of a complex data structure. The problem was to develop sufficiently large data structures to test the correctness and efficiency of the transformation. To do this manually would have taken too long and would have been error prone.

NPL has over the years developed a means to generate random self-checking programs, of any size, to test the object code produced by compilers, in particular for PASCAL (including variants), Ada and several other languages. This technique has produced program generators, which have found many bugs in commercial compilers, and has been used to give assurance for compilers in a safety-critical context. Bridges can have complex structures

The technique described above is very good in generating complex tests. It can be applied when the tests require complex structures, have relatively simple semantics, and there is a means to check the results automatically. It has been applied to the testing of compilers and software bridges. It is thought it could also be applied to the testing of interfaces.

For further information contact: Graeme Parkin, extension 7104, e-mail: graeme parkin@npl.co.uk

Due to the probabilistic nature of the process, it is possible to obtain a number of distinct near-optimal solutions that may be further analysed as necessary.

The basic rules governing the "evolution" of the population are as follows:

selection, where a new population is obtained by weighted probabilistic selection from the previous population,

crossover, where members of the population are crossed with each other to produce "child" strings,

mutation, where a new population is created by randomly changing bit values, at a very low probability.

The three stages ensure that the overall "fitness" of the population improves probabilistically, but the search is maintained throughout the function space and is thus done in a truly "global" sense. Genetic algorithms are a useful and straightforward method of treating global optimisation problems. They are particularly useful when applied to discrete problems, or problems that can be readily discretised. The techniques can be further manipulated to give a predefined number of minima, which may then be further distinguished by alternative qualitative criteria that are beyond the scope of the objective function.

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

GUM - The next generation

The Guide to the Expression of Uncertainty in Measurement (GUM), published by ISO, has been very widely used and accepted. Its release in the mid-1990s has had a dramatic effect in improving the evaluation and reporting of measurement uncertainty.

Although the GUM is an extraordinarily rich document, it has generally been implemented in software in ways that can sometimes lead to invalid results. Moreover, GUM users are seeking further guidance, particularly for the more complicated situations or when the uncertainties are large. Further work, with SSfM involvement, is aimed at addressing these issues.

Current GUM. Use of the current version of the GUM (or UKAS M 3003) is widespread. A measurement model is developed that relates the inputs (quantities that can be measured or obtained from suppliers' data, calibration certificates, etc.) and their uncertainties to the output (the measurand or physical quantity) and its uncertainty. These input values and their uncertainties are then propagated though the model to provide a measurement result and its uncertainty. Finally, an expanded uncertainty, viz., an interval likely to cover say 95% of the values that could plausibly be ascribed to the measurand, is obtained.



A North Sea oil export metering system. Courtesy of FLOW Ltd., which has developed a range of generic models as the basis for evaluating the uncertainty of typical metering systems. With regular calibration of the meters and other instrumentation the overall measurement uncertainty is better than 0.25% of the reading to comply with Department of Trade and Industry and Norwegian Petroleum Directorate regulations.

So where's the problem? First, it is often difficult to assign appropriate distributions (rectangular, normal, etc.) to the inputs, from which the input uncertainties are obtained. Second, the propagation has to be carried out reliably. If the first part can be carried out satisfactorily, then usually there will be no problem, since the GUM gives a clear but approximate prescription for uncertainty propagation. The difficulty is that it is hard to say when this prescription will give us the answers we want and when it might let us down. Generally, we want to determine a measurement result and its associated coverage interval to a particular number of figures. Typically, we would be looking for just one correct figure in the uncertainty, e.g. a result of the form (50.000 84 \pm 0.000 06) mm. Can we be sure of the 0.000 06? Should it be 0.000 04 or 0.000 08, for

example? The importance of this point depends on the application, but in terms of the credentials of a laboratory or in a competitive environment, the differences can be very relevant.

GUM revision. The revision will assist in deciding whether the limitations of the GUM apply in any particular circumstance. It will cover what the validity of results means, and how valid results can be obtained. The current GUM concentrates on a certain class of models; the revision will cover a wider range of model types:

- (a) measurements where there is more than one output, e.g. the parameters of a calibration curve
- (b) circumstances where it is not possible to express the output explicitly in terms of the inputs, e.g. in some flow measurement models
- (c) measurements involving complex variables as arise in electrical, acoustical and optical metrology

Two phases. GUM revision will handle the problem of the correctness of the output uncertainty by dividing the process into two phases:

• Phase 1 (formulation): developing the model, deciding its inputs, and assigning their distributions.

• Phase 2 (evaluation): the propagation of these distributions through the model to obtain the distribution of the output. The central 95% of this distribution gives the required expanded uncertainty.

How will this help? Phase 1 is the province of the metrologist, perhaps with statistical support. Phase 2 can be carried out, using software or by hand, but without any metrological knowledge. Once the metrologist has finalised the model and the inputs, phase 2 can be undertaken as accurately as required *in terms of that information*. There is no *further* source of *uncertainty* as a result of approximations, as in the GUM today.

The solution process is designed to return a valid answer for the *posed* problem. It is then down to the metrologist to investigate the effects of his assumptions, perhaps by varying an input distribution to see the changes in the output and its uncertainty. Whatever he does will be under his control, and not exacerbated by numerical effects that are unknown to him.

No change! There will be *no* change to the GUM as we know it, in order to protect the considerable implementation investment made by many organisations. The GUM revision will take the form of supplemental guides. The first, concerned with the propagation of distributions, will promote the two-phase process described above, especially providing approaches for obtaining the output distribution. The recommended tool is Monte Carlo Simulation (MCS), a computer-intensive process that samples many times from the input distributions, and, by evaluating the model for each sample, provides a distribution for the output. Unless the model is very complicated, a valid answer for phase 2 can be established in minutes, or even seconds in simple cases.

Models. The second supplemental guide will provide a classification of models: one or more than one output, formula for the output or an equation to be solved for it, real or complex variables; 2 by 2 by 2 = 8 categories in all. Advice on how to handle each category will be given, plus an example, with formulae or an approach that is readily implemented.

not deliver results that are fit for purpose. The modelling guidance will expedite GUM usage to a wider range of models, but leave matters unaffected in terms of "conventional" models.

The SSfM angle. A major part of the first SSfM programme was concerned with the development, application and promotion of sound uncertainty principles. We have been strongly guided by four workshops, attended by over 250 delegates, themed sessions at conferences such as the international Advanced Mathematical and Computational Tools



GUM validation. An important aspect of MCS is that it can be employed to validate the use of the GUM. If the GUM and MCS results agree in the above sense, the GUM approach can be taken as valid for the application and for sufficiently similar applications. If there is disagreement, there is a cause for investigation. A conclusion could be that the GUM is inapplicable for the problem and MCS should be considered instead.

User impact. MCS can be introduced alongside the current use of the GUM. Only if the GUM is producing inadequate results need any change be made. Of course, a change should be necessary in any circumstance where the approach used does in Metrology series, national and international committee work, and numerous additional contacts. This emphasis will continue in SSfM-2. A best-practice guide resulting from SSfM is available from the SSfM web site, and a training course has been developed.

Applications of the SSfM work, in the MCS and the modelling senses, have been made to a large number of projects. They range from inter-laboratory comparisons through co-ordinate measuring machines to radiation emitted by domestic appliances. The MCS principle has been applied by industry to large-scale flow metering in the oil industry and other areas.

The future. The Joint Committee for Guides in Metrology (JCGM) is responsible for GUM revision. BIPM, OIML, ISO, IEC, IUPAC, IUPAP, IFCC and ILAC are represented on JCGM. Experts from the national measurement institutes, all concerned with the needs of users, also sit on JCGM. The UK, benefiting greatly from the SSfM programme, has made and will continue to make substantial input to this work.

EMC radiated emission measurement of a substitute electronic product inside a fully anechoic chamber at NPL over the frequency range 30 MHz to 1 GHz. The cables simulate a mains supply and a connection to peripheral equipment.

For further information contact: Maurice Cox, extension 6096, e-mail: maurice.cox@npl.co.uk



Model validation - best practice

The quality of the information we extract from experimental data depends on the quality of the mathematical model used to describe the system. If the mathematical model inadequately represents the actual behaviour of the system, or the way we analyse the measurement data is not appropriate for the model, then the results we derive could be invalid. As part of the SSfM validation theme, we have looked at case studies to examine validation issues in all aspects of modelling including:

- a) the specification of the functional model in terms of equations relating the various parameters and variables
- **b)** the specification of the statistical model for the measurement errors
- c) the method of solution for the model parameters
- d) estimation of the uncertainties of the fitted parameters



One suite of case studies concerned roundness assessment of manufactured artefacts from measurement data. While the basic functional model is easy to define, the complete model depends crucially on the systematic behaviour of the measuring instrument and the form errors of the artefact, and if these are not modelled appropriately the estimated parameters and their uncertainties can be wildly unrealistic.

A second suite of case studies concerned models of measurement systems where the focus of attention was on taking into account the measurement sensor behaviour and the multiple correlation in the measurement errors.

These case studies feature in the Best Practice Guide on Discrete Model Validation.

Further Reading:

Software Support for Metrology Best Practice Guide 4: Discrete Modelling, M G Cox, A B Forbes and P M Harris, National Physical Laboratory.

Software Support for Metrology Best Practice Guide 10: Discrete Model Validation, R M Barker and A B Forbes, National Physical Laboratory.

See the SSfM website for published guides.

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Measurement strategy can have a large effect on roundness assessment

CMM software standard approved for publication



Co-ordinate measuring machines (CMMs) are widely used in industrial metrology as part of the inspection of manufactured components. They return co-ordinate measurements of points on the surface of a real feature. In order to yield useful information from these measurements, a common requirement is to fit an associated geometric feature, such as a line, circle, plane or cylinder, to a data set consisting of such points. The parameters of the fitted feature that describe the size, shape, position and orientation of the feature, are compared with design tolerances in order to decide the extent to which the feature satisfies dimensional and positional specifications. Typically, the fitting of geometric features to co-ordinate data is undertaken using software. Consequently, the reliability of the information derived from the measurement data that crucially impacts on the decision to accept or reject a part is influenced by the quality of the software for computing these features.

Using a CMM to inspect a manufactured component

LIMS - best practice

Laboratories produce a vast amount of information, which, because of the regulatory climate, needs to be retained for long periods and must be readily retrievable for processing at any time. The information can be disparate - it might include test data, staff training and workload records, for example. Laboratory Information Management Systems can bring major benefits in terms of productivity, resource management, reduction of paperwork and the efficient handling of customer enquiries.

Selecting and implementing a LIMS is a non-trivial task. Bespoke software or off the shelf packages may be used, the trend being to choose packages that can be configured to meet the laboratory's needs. Thorough preparation of the system specification is essential, and it is recommended that a laboratory audit be undertaken to define what will be required. This will include a review of the workflow, the instruments, the reports, security, and the systems to which the LIMS will have to interface. The specification will also consider the retention of records in electronic or paper format, the control of the software itself and the medium on which it is stored.

Thought will also need to be given, and assurances received about an upgrade and development path: to obtain a return on the substantial investment required, a LIMS should be seen as a long term tool lasting at least eight years.

The performance of a LIMS is vital to the laboratory, and one of the keys to realising the desired performance is to build a good partnership relationship with the supplier. Planning, an agreed scope, and flexibility are also important in getting the best from the system.

It can take at least six months, and often much longer to install, prove and adopt a LIMS system, and it is crucial that supporting documentation and training offered by the vendor are of high quality. The requirements will change, not least because

ISO committee TC213/WG10 (whose meetings are attended by NPL) has approved a standard concerned with testing software for computing best-fit geometric elements [1]. The standard is expected to be published in Summer 2001, and will underpin NPL's work in testing and validating such software. The new standard utilises the methodology promoted in the SSfM software testing project for the use of reference data sets and the comparison of test and reference results.

Reference

 ISO 10360-6:2001(E), Geometrical Product Specifications (GPS) - Acceptance test and reverification test for coordinate measuring machines (CMM), Part 6: Estimation of errors in computing Gaussian associated features.

For further information contact: Peter Harris, extension 6961, e-mail: peter.harris@npl.co.uk users will become more aware of the capabilities of the system, and there needs to be a scheme for change management.

The system needs to be validated, and problems can arise here. In most cases it is not possible fully to understand the intricacies of the software, and the 'black box' approach needs to be implemented. This treats the system as an entity, and provides inputs (test data) and validates the outputs. Consideration needs to be given to 'what if' tests, as well as thorough preparation of usual scenarios. Calculations, including roundings need to be closely checked.

The product alone will not guarantee a successful installation. The right approach and methodology must be followed, and the chosen system should be based on future technology needs, selected after a thorough search to find a supplier with the desired interpersonal

skills. With this in mind, once commissioning is complete, there are enormous benefits to be gained from the installation of a LIMS.

Further Reading:

Software Support for Metrology Best Practice Guide 9: Selection and Use of LIMS, Sira Test & Certification

This is available from the SSfM website.

For further information contact: Steve Lower, 020 8467 2636, e-mail:smlower@siratc.co.uk



LIMS can bring benefits to a wide variety of measurement laboratories



Wavelets in metrology

Traditionally, in spectral analysis, techniques based on the Fourier transform are used to relate a signal that varies in time or space to its frequency-domain representation. However, such methods have limitations when applied to non-stationary signals.

Within the last 20 years, an approach using "wavelets" has been developed. This uses a different set of basis functions from those used in Fourier analysis. Wavelets provide a general set of basis functions that are localised both in time and frequency.

Within the scientific community, wavelet analysis has been applied successfully to a wide range of problems, including the recognition of features in signals, signal compression and de-noising. Wavelets have also been used as a basis in numerical schemes. To date these techniques have not, however, generally been exploited in metrology.

While the traditional Fourier-based signal processing techniques have proved effective for the majority of applications, a capability in wavelet analysis would significantly add to the available techniques and enable more general forms of signal to be studied.

The last eighteen months have seen research undertaken at NPL to investigate the potential for using wavelets in the metrology environment, and to increase awareness within NPL of their usefulness. In addition, the application of wavelets to a specific acoustic application, namely the calibration of underwater electroacoustic transducers in reverberant laboratory tanks, is being investigated. Potential applications of wavelets in this acoustics area include de-noising and estimation of echo-arrival times (an example of feature recognition). Figure 1 shows a sample signal originating from the calibration of a hydrophone, while Figure 2 shows the signal obtained after de-noising using wavelets. Figure 3 contains a visualisation of a so-called "continuous wavelet transform", usually abbreviated to CWT and analogous to the Fourier transform, of the original signal, which illustrates its non-stationary characteristics.



The aim throughout the research project is to combine the strengths of wavelet analysis (e.g. sparse representation of signals, feature detection, etc.) with existing techniques, to form a more complete set of analytical tools.





Figure 3

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Near-field to far-field prediction for underwater acoustics

Manufacturers of underwater acoustic transducers want to know the performance characteristics of their devices in the acoustic far-field. However, for some transducers, direct measurement in the farfield requires a large volume of water such as a lake or reservoir, which means making test measurements is an expensive and time-consuming task. As a solution to this problem, NPL has been investigating methods for predicting the far-field response of a transducer from measurements made in the near-field in a laboratory tank. NPL operates a large open tank (5.5 m diameter, 5 m deep, see figure 4) equipped with a high-resolution positioning system, which is used for the near-field measurement scans.



Figure 4

The propagation of acoustic waves of constant frequency in homogeneous media may be described using the Helmholtz equation, which can be reformulated as an integral equation over a closed surface. This means that if the pressure distribution over a closed surface is known, the pressure value anywhere else can be calculated.



Figure 5



Boundary element methods provide a numerical technique for solving the Helmholtz integral equation, and NPL has carried out an investigation of such methods. An initial study identified two techniques that were suitable for this problem, and work has concentrated on the validation and comparison of these two methods. Software is currently being developed that will process the scanning device output and calculate results at user-specified points in the far-field.

The pictures show a typical example of a measurement data set on a cylinder (figure 5) made up of about 29000 points and a far field prediction (figure 6) on a cylinder with a radius 20 times larger, calculated using about 7200 values. The next areas of investigation will be uncertainty estimation and understanding how the results depend on the number and distribution of measurement points.

For further information contact: Louise Wright, extension 6466, e-mail: louise.wright@npl.co.uk



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METROS expands

The SSfM Software Re-use project is now complete, with the prototype METROS library for re-usable software as its major output. The METROS website, www.npl.co.uk/ssfm/metros/, contains specifications of over 50 keys functions, and implementations of some of those key functions, provided as source in languages such as Fortran and MATLAB, and as compiled DLLs which allow them to be called from Excel, for example.

The METROS website will be central to the delivery of various outputs from the next SSfM programme. Algorithms for discrete modelling and for uncertainty analysis will be included as key functions, and existing and new software from NPL will be included as implementations of these key functions. We will also extend METROS to include bundled software such as packages and libraries, guidance material such as the existing SSfM best practice guides, and reference data sets and results for testing mathematical software, including results from a project to test contributions to METROS.



Figure 7 'Choices and Visualisation' window

The software testing project has made extensive use of reference data sets and these are already available through METROS at:

www.npl.co.uk/ssfm/metros/reference_data_sets/. The structure is similar to the rest of METROS: there is a page for each function to be tested, and these pages point to the individual reference data sets, which are indexed by various parameters. There is also guidance on how the data sets should be used and reference material on how they were produced.

NPLFIT

A software package, NPLFIT, has been available for some time for fitting calibration curves and other experimental data. In its original file-based version it had some limitations, but an enhanced version has just been released which provides a graphical user interface to the package having a Windows "feel".

NPLFIT will be made available on METROS in various forms. Implementations of particular functions from the library are implementations of key functions. The library as a whole will be made available as DLLs, and the NPLFIT-GUI will be

available as a package, providing a user interface to the library functions.

NPLFIT provides a coherent and usable interface to curve-fitting software representing the current best practice. The use of the package enables two important classes of models, polynomials and splines, to be fitted to data. These models offer considerable flexibility as the algorithms used allow polynomials of high degree, and splines with many knots. In particular, the "best fit" in terms of polynomial degree or number of spline knots can be reliably obtained. The fitting criteria available are 2-norm (least-squares), 1-norm (min-sum-mod) and infinity-norm (min-max).

The package has controls such as buttons and boxes, which are easily operated, to allow the user to select from a family of models the one that is most appropriate for the data, and to enable the fitted function to be evaluated, differentiated and integrated. This version is more versatile in that, for example, it allows the user to evaluate the



Figure 8 Window showing a graph of fitted spline

fitted function for any selection of points. For fits obtained using the 2-norm, measures of standard uncertainties can be extracted, and the choice of operations has been extended to include the analysis of features, such as extrema and points of inflexion, of the spline.

Figure 7 shows a window displaying the choices for a data file. The results are displayed graphically on a window and they can be plotted on a printer or saved to a file: see figure 8.

For further information on METROS contact: Robin Barker, extension 6348, e-mail: robin.barker@npl.co.uk on NPLFIT contact: Paul Kenward, e-mail: paul.kenward@npl.co.uk

Data fusion

The SSfM data fusion project recently sponsored a second workshop on data fusion in metrology. This was held at NPL on 31 October 2000 and, in contrast to the first workshop held a year earlier, was directed solely at NPL scientists. It consisted of three presentations on the data fusion work undertaken at NPL.

Alistair Forbes showed how data fusion was applicable in many metrology situations, and highlighted the prevalence of multiple-sensor measurements within the laboratory. For instance, with gauge block calibration using interferometry, air temperature, pressure, humidity, artefact temperature, and the coefficient of thermal expansion (and their uncertainties) can all be seen as factors that need to be fused to obtain a reliable measurement result. In this example, measurements are fused over attributes. There are other examples where fusion is made over a set of measurements taken over a time interval, or where the measurements come from many similar sensors, or are from overlapping parts of a physical spectrum.

figure 9, we show the results of using Bayesian priors to build into our uncertainty analysis the knowledge that a certain parameter is non-negative.

Finally, Robin Barker gave an overview of the work being carried out for the INTErSECT project, wherein a review of data fusion techniques is being undertaken. An early version of the resultant guide to data fusion techniques will soon be available at: www.datafusion.org.uk

For further information contact: Gavin Kelly, extension 6975, e-mail: gavin.kelly@npl.co.uk



The data fusion work was shown to be related to the discrete modelling best practice guide, and was described in terms of parameter estimation for multi-sensor systems.

Gavin Kelly presented some work on Bayesian statistics, and their role in data fusion. The case was argued that "Bayesian priors" are central to carrying out data fusion, as they provide an ideal way of carrying information from one experiment or calculation to the next.

If we make a series of measurements pertaining to mass, for example, then in a classical interpretation we would estimate the true mass to be the one that most likely explains the measurement data. In a Bayesian world, we update our prior belief using the measurement data, and can then find the value of mass that we have the most belief in. As we take more and more measurements, these views will generally converge.

The speaker argued that a Bayesian approach not only allowed us to carry measurement data between experiments, but it also allowed us to incorporate a wider range of information than just measurement data. For instance, in the graph in Figure 9 90 and 95% Bayesian confidence intervals for a positive parameter

Guidelines on selecting and using software in metrology applications

A report providing information and guidelines to help users select and use software in such a way that it is "fit for purpose", has been completed as part of the SSfM programme (CMSC Report 04/00). Fitness for purpose is defined in terms of meeting requirements relating to the numerical accuracy of the results returned by the software.

Four subjects are covered in the report:

- factors that affect how users decide fitness for purpose requirements, accounting for the possible ways that the results returned by scientific software may subsequently be used
- approaches for verifying or testing the numerical accuracy of scientific software
- how to make better use of existing software by pre-processing the input data and using appropriate model parameterisations
- help in locating software that is relevant to metrology applications

Figure 10 illustrates an example from the report. It shows some measurement data (as black circles) and a calibration curve (blue line) established as the least-squares best-fit quadratic to the data. Suppose we wish to communicate the calibration curve to a user by providing the values of the parameters defining the curve rounded to four decimal places (so that, for example, they fit on a calibration certificate). When the user comes to evaluate the calibration curve he obtains the curve shown as a red line, and the errors associated with this curve are evidently larger than the measurement errors associated with the data.

The example shows how important it is for the requirements placed on the accuracy of the results returned by software to reflect their intended use: in this case four decimal places of accuracy is insufficient. Here, a better way to establish the calibration curve is to pre-process the data before fitting so that the *x*-values are normalised to lie in the interval [-1, +1], and then the curves defined by the parameters before and after rounding are (essentially) identical.



For further information contact: Peter Harris, extension 6961, e-mail: peter.harris@npl.co.uk

Testing the numerical correctness of scientific software

Two new reports (CMSC 07/00 and CMSC 08/00) have been completed as part of the SSfM programme concerned with testing the numerical correctness of scientific software used in metrology. Each report focuses on a particular numerical calculation and presents the results of testing functions for this calculation taken from a number of spreadsheet, statistical and scientific software packages used in metrology. The calculations considered are, respectively, sample standard deviation and straight-line linear regression, and the software packages covered are Excel, MathCAD, S-PLUS, Matlab, the NAG Fortran library and the IMSL Fortran library.

Figure 11 illustrates an example of the results obtained from testing the functions for sample standard deviation. A sequence of graded reference data sets is generated, where each data set has the same reference sample standard deviation but a larger sample mean than the previous set in the sequence. The sequence therefore mimics measurement data sets with increasing signal-to-noise ratio. The results illustrated in Figure 11 indicate that the IMSL, NAG, Matlab, S-PLUS and MathCAD packages provide reliable results for these reference data sets (albeit that MathCAD is slightly poorer than the others), whereas there is serious degradation in the performance of the function provided by Excel. The results suggest that the Excel function implements an unstable formula for calculating the sample standard deviation, whereas the other packages implement stable formulae for this calculation. The implementation of a common unstable formula for the standard deviation reproduced exactly the Excel results for the cases examined.

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Figure 11



Reference mean value

IMSL NAG Matlab Excel S-PLUS MathCAD

The reference data sets are applied as input to each test function and the results returned are compared with the reference results. A performance measure is used for this comparison: it measures the number of significant figures of accuracy that are lost by the test function over and above the number that can be expected to be lost by a reference algorithm for the calculation. The figure shows in the form of performance profiles the values of the performance measure for

profiles the values of the performance measure for the sequence of reference data sets and each test function. A near-flat performance profile is good. A strongly increasing profile is bad.



= computational

A global positioning system timing receiver

In recent years Global Positioning System (GPS) receivers have become relatively inexpensive. Recent improvements to the GPS have resulted in receivers costing £100 or less being capable of determining a user's position to within 20 m in real time.

GPS satellites have excellent on-board atomic clocks and this makes them superb sources of high quality timing signals. Primary timing laboratories use GPS for the inter-comparison of the clocks forming the national time scales; but expensive specialist receivers are required. Note here that the primary timing laboratories do not set themselves to GPS time! Instead, GPS is a convenient transfer standard: laboratories A and B compare their time against a satellite S. By recording the differences (A-S) and (B-S), and then subtracting, the time differences between the two laboratories (A-B) can be found. This method is known as GPS common-view.



The common-view receivers output data in a unique format developed by the Bureau International des Poids et Mesures (BIPM) in Paris, and require hardware modifications not normally available on standard GPS receivers, so that an external clock can be directly connected to the receiver.

Quartzlock Maser - UTC(NPL), GPS common-view, uncalibrated Quartzlock Maser - UTC(NPL) (ns) (uncalibrated) 270 265 260 255 250 245 240 235 230 225 220 215 210 51,871 51 872 51 873 51 874 51 875 51 876 MJD

Up until the mid-1990s, cost had prevented the widespread use of GPS receivers by UK users of time and frequency. However inexpensive GPS receiver engines have now been developed with timing capabilities that make them suitable for use not only by primary timing laboratories but also by top-level calibration laboratories within the UK.

NPL has been working in collaboration with a UK manufacturer, Time and Frequency Solutions, to develop a common-view receiver based on an inexpensive GPS receiver engine that can be used for the highest accuracy time and frequency disseminations within the UK. The new equipment allows users to compare their standards against the national time standard.

The software for this project has been produced by CMSC. It takes the form of a user-friendly package written in Visual Basic, to run in a Windows environment. The software both generates timing data in the internationally agreed BIPM format, and provides much additional receiver status information. It continuously reads and decodes satellite information and local clock timings from the receiver. Satellite time readings are corrected using orbital parameters from ephemeris readings, and further corrections are made for transmission delays through the earth's ionosphere and troposphere.

Following a prearranged schedule, readings are recorded in thirteen minute tracks, one reading being taken every second. At the end of each track, the data are sub-divided into fifteen-second blocks, and a result is obtained after applying quadratic and linear fits.

The first of the new GPS receivers is at present being used for NPL's GPS monitoring service, where the timing capability of the GPS system over the UK is being continuously monitored. The receiver automatically provides data, and a system of Real-time Autonomous Integrity Monitoring (RAIM) has been introduced to check for errors in the GPS system in real-time.

The main use of the GPS receivers will be in NPL's GPS common-view service that will be launched early in 2001. This will provide continuous monitoring of caesium clocks distant from NPL.

Comparison of a passive hydrogen maser at Quartzlock, Totnes, Devon, against UTC (NPL), the UK's national time scale. Each point represents a separate 13-minute GPS satellite measurement. Each GPS satellite measurement is plotted in a seperate colour. The x-axis plots the Modified Julian Day (MJD), a calendar that increments by one each day (i.e. the graph shows nearly six days of data).

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Sky map of GPS satellites observed at the National Metrology Laboratory in Dublin using the common-view receiver. Each satellite trajectory is traced using a seperate colour. The 'hole' to the north is an artefact of the GPS satallite constellation, but the rest of the sky shows a good spread of 'common-view' observations. These are important for reliable time comparisons

Biometric authentication performance

NPL has conducted a performance assessment of seven biometric authentication systems for the UK government Biometrics Working Groups run by the Communication Electronics Security Group (CESG). Each system used a different biometric technology: iris patten, vein patten, hand geometry, face image, fingerprint (using optical and capacitive chip imaging) and voice print.

The test scenario was one of access control in a normal office environment, and data was collected from over 200 volunteers using the systems several times over a three-month period. The test methodology followed the "Biometric Testing Best Practices" previously developed by NPL jointly with other biometric testing organizations (see: www.afb.org.uk/bwg/bestprac.html).

There are several performance measures, and systems can trade one aspect of performance against another. For example increasing the false acceptance rate, or the effort required of the user, might reduce the number of false rejections. Which is the "best" system will depend on application requirements, as illustrated by the Detection Error Trade-Off graph shown.

The results show typical levels of performance attainable by the technologies tested and, together with our testing experiences, are helping in the development of testable performance criteria for future security evaluations.







A typical voice print



Detection Error Trade-Off

Iris and iris code

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Looking forward to SSfM-2

The SSfM-2 programme (to run from April 2001 to March 2004) will have a substantial R&D content, with much work on modelling, uncertainties, validation and testing, which will build upon the successful work in these areas in SSfM-1.

The METROS website will be a major vehicle for disseminating the programme results. The programme will also coordinate international contributions to the website through the EUROMETROS EUROMET project. See article "METROS Expands" on page 10.

There will be a major uncertainties project, covering a wide spectrum of activities including:

- · international contributions to the GUM,
- analysis of results of key inter-laboratory comparisons,
 - research into statistical techniques new to metrology,
 - the development of an industrial uncertainty methodology to get the basic concept of uncertainty conveyed to those on the shop-floor who make and use measurements.

In addition, two projects will investigate uncertainties associated with visualisations and continuous models. Finally, two more projects will be devoted to contributions to standardisation, much of which will relate to uncertainty evaluation.

Continued on back page

Theme 1: Modelling techniques

Extension of empirical models
Algorithms for discrete modelling
Promoting best practice in discrete modelling
Continuous modelling for metrology
Uncertainties and statistical modelling
Data fusion
Visual modelling and uncertainties
Data visualisation
Theme 2: Validation and testing
Numerical software testing
Testing continuous modelling software
Testing algorithms in standards and METROS
Maintenance of measurement system
validation best practice
Validation of safety-critical measurement
systems
Validation of self-calibrating instruments
Theme 2: Metrology software and
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The work on validation and testing will include applying numerical software testing to continuous modelling software packages, such as finite element packages. Test services will be developed for the numerical testing of software in simple mass-market products, and for contributions to standards and METROS. The work on validating software in measurement systems will be applied to remote calibration situations, self-calibrating instruments, and safety-critical uses. The latter will be done in association with the DTI CASS scheme.

The programme will also tackle some important new topics. Firstly, it will provide generic support to and coordination of NMS activities on remote calibration over the Internet. Secondly, it will promote best practice in numerical analysis for algorithm design, raising awareness of the problems that can arise from not applying good numerical analysis. Finally, it will investigate new directions for future work, including new work to support legal metrology and digital signal processing, support for soft metrology, and the aspects of bioinformatics needed to support biotechnology measurement work.

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Overview of themes and projects in SSfM-2. Those in italics and highlighted orange are to be competitively tendered.

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