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Counting on IT

MATHEMATICS AND SCIENTIFIC COMPUTING

SSfM-2 delivers as SSfM-3 firms up

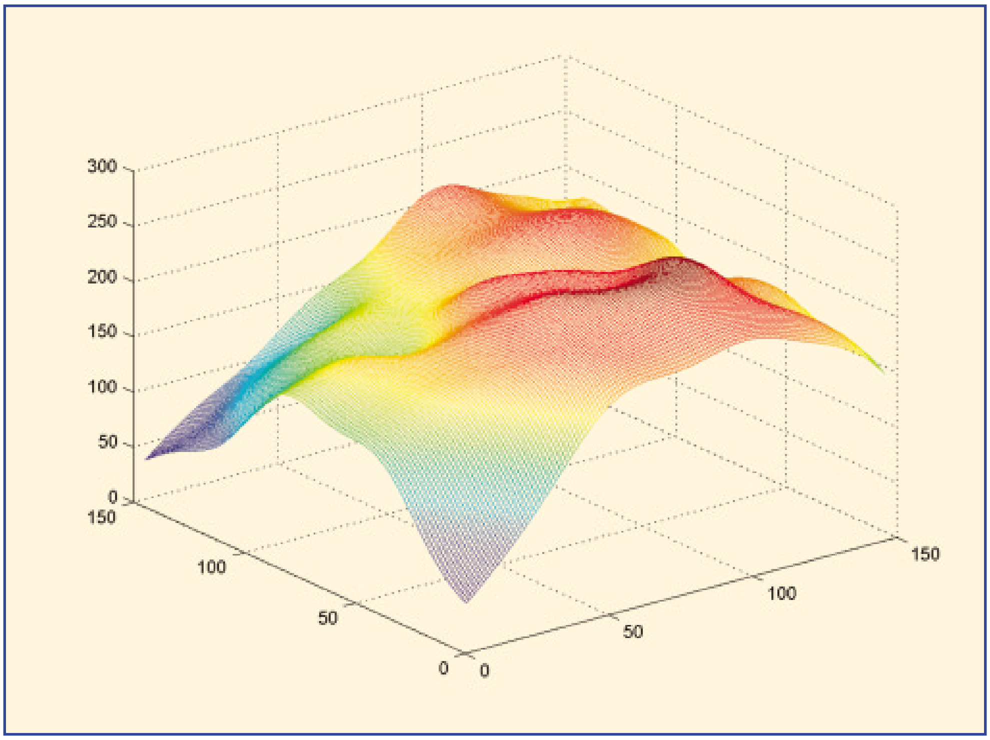
As we near the end of the current Software Support for Metrology programme (SSfM-2), many projects are coming to completion and delivering new reports. At the same time, the content of SSfM-3 (April 2004 to March 2007) has been decided, subject to ministerial approval. The new reports and programme document are available for download at the SSfM website www.npl.co.uk/ssfm/download/.

In this issue of *Counting on IT*, you will find a major article on the continuous modelling work, which has delivered three new reports: on validation, uncertainties and a guide to finite element and finite difference software.

Work on data fusion has resulted in two new reports: *Classification techniques and their application in metrology* and *Parameter estimation methods in data fusion*. Both reports contain results from particular case studies.

Other recent reports include: *Multivariate empirical models and their use in metrology* (see figure 1), *The comparison of algorithms of type A1 surface texture reference artefacts*, and *International activities during the second SSfM programme 2001-2004*.

Figure 1. Gaussian Radial Basis Function fitted to interferometric data, illustrated in the report "Multivariate empirical models and their use in metrology"



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NPL National Physical Laboratory

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The programme's Internet-enabled metrology activities have resulted in a new report, *Use of the Internet for calibration services – protecting the data – final report*, to complement the earlier report, *Survey of international activities in Internet-enabled metrology*. The new report covers issues of data security, firewalls, electronic calibration certificates and data warehousing.

Work on numerical correctness testing has also resulted in two new reports: *Testing the numerical correctness of software* and *Testing methods of Java libraries*. The former compares results of arithmetic mean, standard deviation, linear regression and polynomial regression functions in several different packages and libraries. The latter reports on the results of testing a wide variety of mathematical and statistical "methods" in Java libraries.

There is still more to come - the new best practice guide on numerical analysis is nearing completion, and several of the existing best practice guides are being updated.

Finally, the SSfM-3 programme document describes all the projects for the new programme. All the core SSfM topics are still there. The largest new topic is Signal Processing. Other new topics include modelling for nanotechnology and uncertainties associated with simulations. Two projects provide new technical advice services to user organisations and NMS programmes, and many collaborative case studies will be conducted jointly with other NMS programmes.

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Mathematics for Measurement

A colloquium, *Computational Mathematics for Measurement*, organised by the Numerical Algorithms Group (NAG) Ltd and NPL, and the NAG AGM Invited Lecture took place at the Oxford University Computing Laboratory on 12 December 2003.

Dr Richard Field, Chairman, NAG Council of Management (left), Dr Brian Ford, Director, NAG Ltd (centre) and Professor Maurice Cox.

The theme of the colloquium was the mathematics, especially the numerical aspects, that supports the measurements that impact on all our lives, from the fuel delivered at the local garage pump to the sophisticated inertial navigation systems in commercial and military aircraft. NPL's measurement capability has to surpass that of industry because the measurements must be traceable. The high accuracies required are today generically underpinned by mathematics, statistics and numerical computing. The demands on mathematical solution capabilities are becoming ever-more challenging as the state of the art in metrology advances in response to practical requirements.

The colloquium conveyed the flavour of the mathematics undertaken in this regard, through presentations in a number of areas. The opening talk, "*... and express it in numbers*", by Dr Seton Bennett, Deputy Director & Director of International Metrology at NPL, constituted an introduction to the way measurements are expressed. The remaining presentations covered mathematical aspects from academia, NPL and industry. These contributions were from Professor John Mason, School of Computing and Mathematics, University of Huddersfield, on "*Novel approximation estimators*", Professor Alistair Forbes, NPL, on "*Gauss-Markov regression*", and Dr Stephen Kyle, Metrology Division, Leica Geosystems, on "*Analysing optical instrumentation and measurement networks in large-scale metrology*".

The NAG AGM Invited Lecture, "*Mathematics in support of measurement*", was given by Professor Maurice Cox, NPL, who illustrated some of the main principles through two applications: *ultra-high- accuracy roundness measurement* and *interlaboratory comparisons*.

Key aspects of measurement that were emphasised by the speakers, and that can benefit from the application of sound mathematics were measurement models, measurement strategies, contaminated measurements, uncertainty structures and uncertainty evaluation, numerical algorithms and software, and consistency of the manner in which measurements are expressed and compared.

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Area under a curve defined by measurements

The area under a curve defined by a mathematical function is a basic concept in texts and courses on integration. Given a function $f(x)$ defined over an interval $a \leq x \leq b$, it is required to evaluate the definite integral $I = \int_a^b f(x)dx$. Tables of integrals exist for cases that can be treated analytically. Otherwise, *quadrature rules* are applied to obtain I numerically, ideally to within a user-prescribed accuracy. A basic rule is the *trapezoidal rule*. The interval [*a*, *b*] is partitioned into *n* sub-intervals of equal width and f evaluated at the resulting *n* + 1 partition points. f is approximated by the piecewise straight-line function joining the function values at these points (figure 2). The area under this approximation is determined. Higher-order rules are possible based on approximating f by a piecewise cubic function, for example.

What can be done if f is not given analytically, but by measurement at a number of points? What can be done if these points are not equally spaced? What can be done about the uncertainties associated with the measurements? The SSfM best-practice guide, *Numerical analysis for algorithm design in metrology*, addresses these issues and other metrology problems requiring numerical considerations.

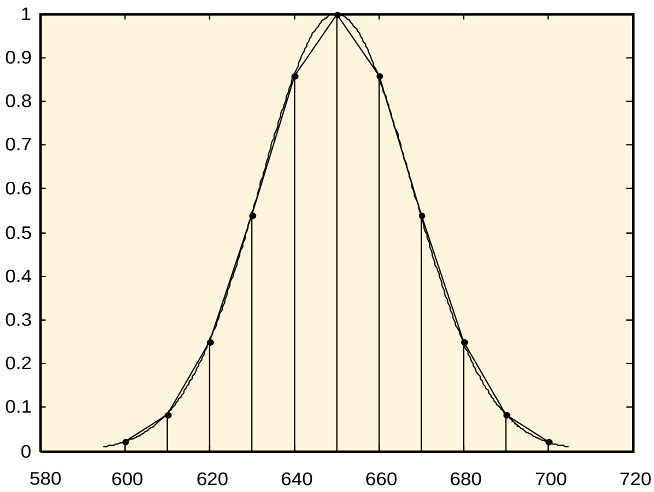

Figure 2. The trapezoidal rule applied to spectral data

One of the applications considered in the guide relates to climate change. The total radiant energy associated with the Earth's Radiation Budget is the difference between (a) the incoming radiation from the sun and (b) the outgoing reflected and scattered solar radiation plus the thermal infrared emission into space. High accuracy in the determination of (a) and (b) is essential because their difference is relatively small, but important in the context of global warming. The total radiant energy associated with (a) is the energy given by integrating the incoming radiation from the sun over the relevant spectral region. To calibrate satellites that measure this data, NPL has supplied large-area uniform radiance sources. The data points in figure 3 relate to NPL's calibration of such a source, prior to using it to calibrate a satellite's on-board instrumentation. Uncertainties associated with these measurements are available.

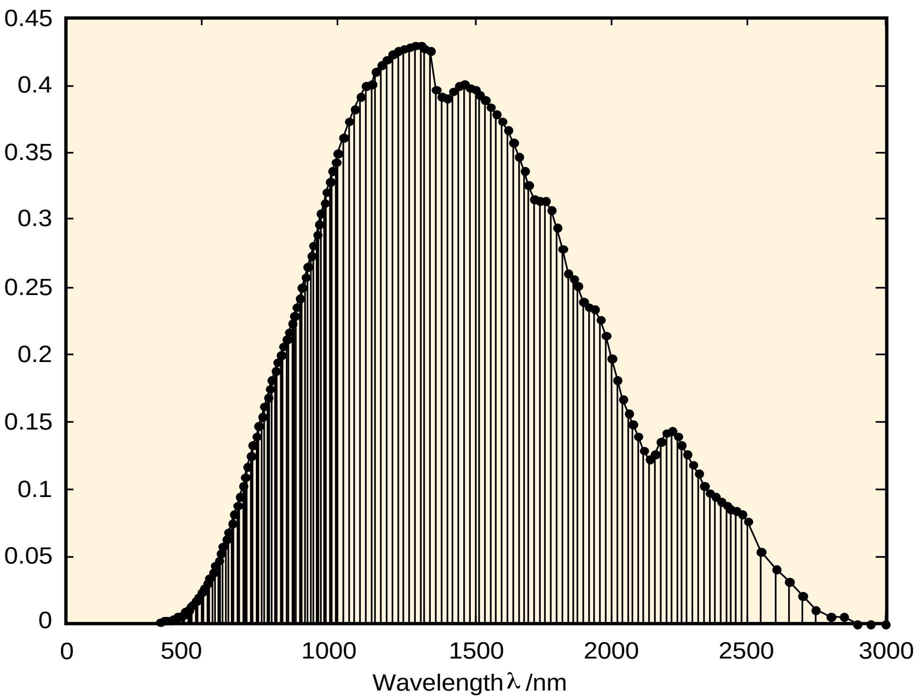

Figure 3. Measurement of a rediance source and interval sub-division for numerical quadrature

The application of several quadrature rules (based on approximations ranging from piecewise-linear to piecewise-quintic) gave estimates of the integral as 515.29, 515.28, 515.29, 515.27 and 515.30 W m^{-2} sr^{-1}. The standard uncertainties associated with these estimates were evaluated in accordance with the law of propagation of uncertainty (as described in the Guide to the Expression of Uncertainty in Measurement) and found to be 0.74, 0.75, 0.75, 0.75 and 0.76 W m^{-2} sr^{-1}. It was deduced with a high degree of assurance that the required integral is 515.3 W m^{-2} sr^{-1} with an associated standard uncertainty of 0.8 W m^{-2} sr^{-1}, or 0.2 %.

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Continuous Modelling for Metrology

Three reports comprising the deliverables of the SSfM project on *Continuous Modelling for Metrology*, are now available for downloading from the SSfM website www.npl.co.uk/ssfm/download/. Their titles are:

- Model validation in continuous modelling
- Uncertainty evaluation in continuous modelling
- Guide to the use of finite element and finite difference software

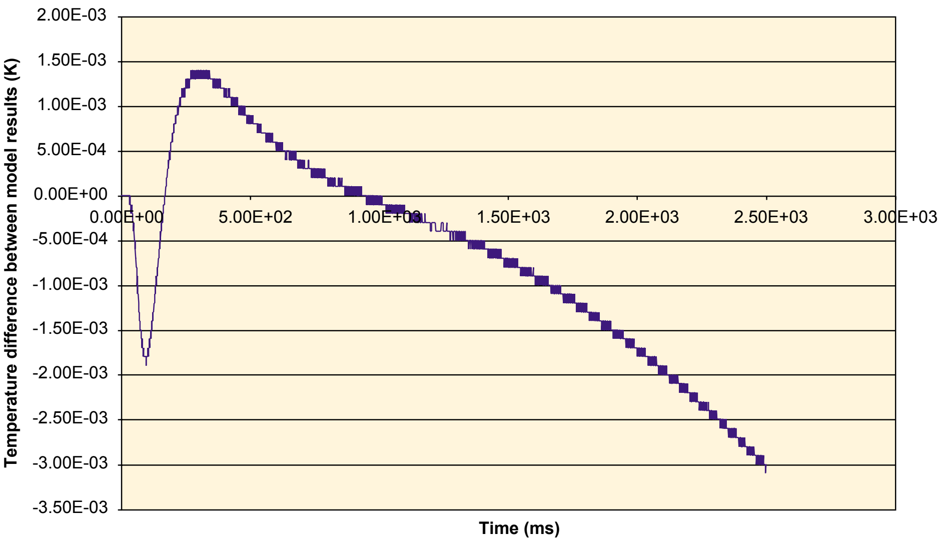

Figure 5: Difference between the results of three-dimensional and axisymmetric models of the same problem.

Model Validation In Continuous Modelling answers Club members' requests for advice on error estimation in continuous models. The report provides a description of a wide range of validation methods, ranging from checking that results "look right" to use of *a posteriori* error estimation techniques. The strengths and weaknesses of the validation methods are illustrated by examples throughout the text. Figure 4 shows an example of the pitfalls of relying on results "looking right": the plot from the post-processing software (a) implies that the two components overlap, whereas the plot of the numerical results in a different package (b) shows that they do not touch.

As well as describing individual methods, a set of recommendations for a general validation strategy is provided, since there are often several aspects of a model that need to be validated before it can be used. A detailed worked example, applying many of the methods to a single problem, is used to illustrate use of the methods as well as some of the general strategy points. An example of the results of one of the methods used is shown in figure 5: the three-dimensional model being validated was compared to an equivalent axisymmetric model, and the figure shows the difference in results of the two models.

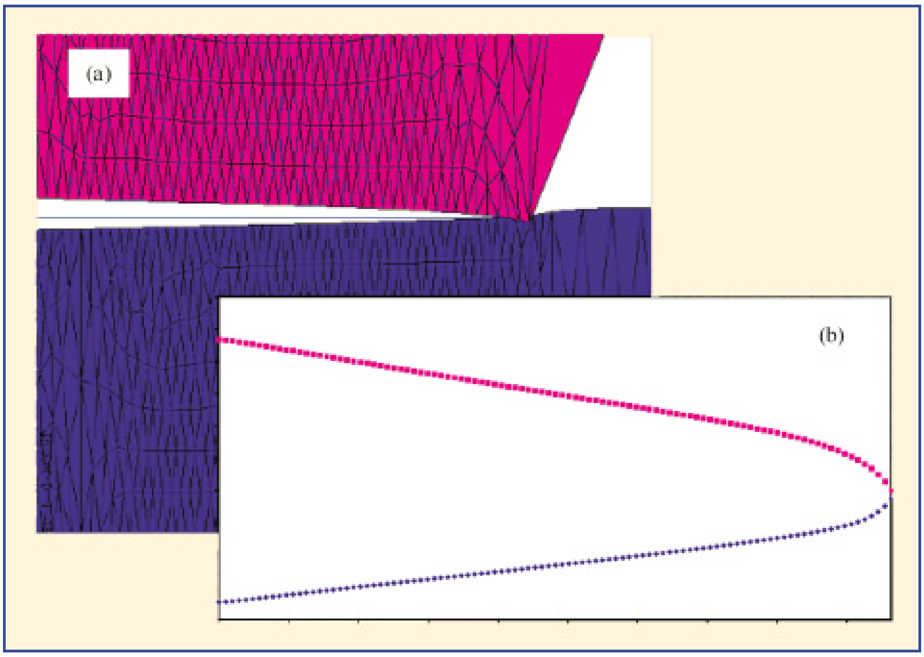

Figure 4: Visualisations of the distortion of two stressed components. 1a is the output from an FE package's post-processing software, which incorrectly shows the components overlapping. 1b plots the numerical results for the displacement of the outer surfaces in another package and correctly shows no overlap.

Uncertainty Evaluation in Continuous Modelling surveys the methods that are available for evaluating uncertainties associated with continuous models, and illustrates the findings with three case studies. Particular emphasis is given to sampling methods and to the use of stochastic differential equations. Figure 6 shows some results produced during the case studies using different sampling methods. Some sampling methods have been identified that provide good approximations to distributions based on fewer data points. These approximations cannot provide information at high confidence levels, but they may be more suitable for studying computationally expensive models.

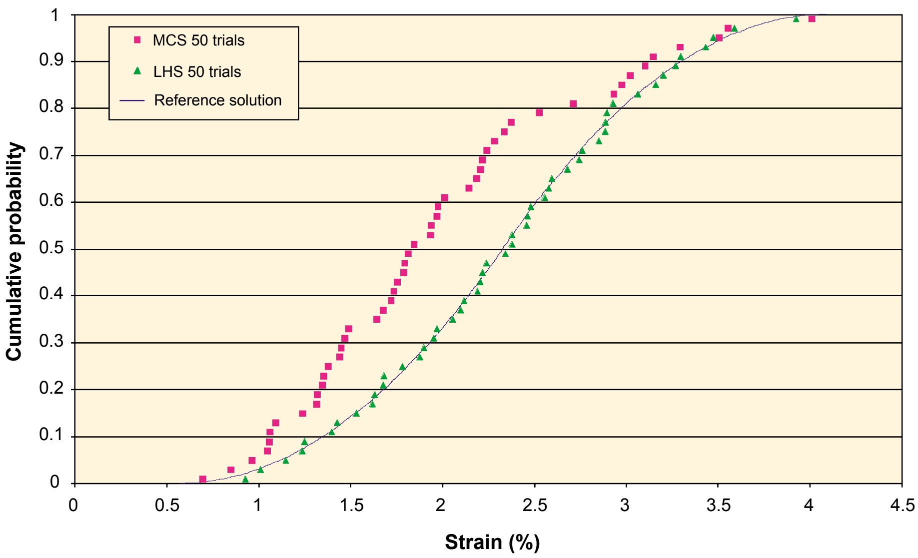

Figure 6: Distribution functions produced using 50 samples chosen with the Monte Carlo Simulation method (pink) and the Latin Hypercube Sampling method (green), compared to the reference distribution function.

Guide to the use of Finite Element and Finite Difference Software is intended to be a starting point for people who have a modelling problem they believe could be solved using finite element (FE) or finite difference (FD) software. The first part of the guide describes the steps in developing an FE or FD model. It takes the reader through the issues that will have to be addressed when preparing a model, including:

- choosing a method
- constructing a mesh
- choosing approximations
- selecting material properties and boundary conditions
- interpreting results and post-processing

The second part of the guide is a compilation of user testimonies received from SSfM Club members, and aims to help potential users of FE and FD packages by giving an insight into the issues that have been encountered by experienced users. These testimonies describe people's experiences of using packages for real modelling problems, and cover a range of applications and packages.

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Training Courses

NPL is repeating all but one of the maths and scientific computing courses that were run in the last year. The course on "Software validation in measurement systems" was held twice, but will not be repeated in the coming year. Instead there will be a workshop on the application of measurement system validation to IEC61508 SIL4. The course on "Testing numerical correctness of scientific software" was cancelled, and it will now be combined with "Reliable numerical computing". Further details of the courses, and a schedule, can be found in the adjacent column and at www.npl.co.uk/ssfm/training/.

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SSfM Training Course and Workshop schedule

15-16 June 2004 ($1\frac{1}{2}$ days)
Visualisation of measurement data

Practical guidance in the effective visualisation of data.

Sept 2004 (2 days)
Discrete modelling and data fitting

Extracting quantitative information from data.

Oct 2004 ($2\frac{1}{2}$ days)
Reliable numerical computing

Understanding and use of the techniques of numerical analysis to develop algorithms and software that deliver reliable results.

Oct 2004 (Workshop)
Validation of safety-critical measurement software

How to give advice on best practice in software validation when applied to safety-critical measurement applications.

Nov 2004 (Workshop)
Best practice in uncertainty evaluation

To increase awareness of best practice in uncertainty evaluation and associated statistical modelling.

Dec 2004 (2 days)
Developing software for measurement

Includes human-computer interface design and organisational support for measurement software development.

Jan 2005 (2 days)
Scientific computing with Fortran 90/95

The main features of Fortran 90/95 important for scientific computing, plus interfacing to other software.

Feb 2005 ($1\frac{1}{2}$ days)
Understanding & evaluating measurement uncertainty – An advanced course

For those who need to go beyond the basics.

Club Members' Page

From *Zeeko Ltd.* – Deterministic Polishing with the Zeeko Intelligent Robotic Polisher

Craft-skill shortage and a need for ever faster prototyping in the optics industry induced the development of new technologies in the recent years for fast and predictable production of Optics with low reject and rework rates.

The Zeeko process (see figure 7) was originally conceived at University College London for the manufacture of large optics for astronomy applications, but it was subsequently developed for smaller optics.

The process utilises a variable geometry soft polishing tool controlled by a 7 axis CNC machine tool controller. The machine tool path is derived from an optimisation of polishing dwell times, based on the component's error profile as compared to its design profile, and the knowledge of the polishing effect of the tool.

This necessary information is collected from metrology equipment such as interferometers and profilometers (a number of interfaces have been implemented) that measures the footprint of the polishing tool, or influence function, and the error on the component to be polished.

Within the complex control software a varied use is made of mathematical tools such as NURBS for rapid handling and comparison of large data files or nonlinear least squares optimisation.

The latest developments of the technology have made some aspects of the process applicable to micro-optics, and some to problems outside the optics industry. The next development stage will also include freeform optics.

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From *National Institute of Standards & Technology* – NIST Updates Popular Web-Based Statistical Resources for Metrologists

The *NIST/SEMATECH e-Handbook of Statistical Methods* is now available on CD. The new CD format for the *e-Handbook*, which provides guidance on the use of statistical methods for physical scientists and engineers, supplements the original web-based format. The CD is ideal for people who need to use the *e-Handbook* when web access is not available. It is also convenient for organizations that would like to install a local copy on their own website. *Dataplot*, the statistical software integrated with the *e-Handbook*, is also included. The *e-Handbook* is at www.nist.gov/stat.handbook/, while information on obtaining the CD can be found at www.itl.nist.gov/div898/handbook/toolaids/cd.htm.

The NIST Statistical Reference Datasets (StRD) website has recently been updated with the six new data sets for Bayesian model fitting using Markov Chain Monte Carlo (MCMC) algorithms. The StRD site, which provides data sets with certified values for assessing the numerical accuracy of statistical software, originally covered four areas of statistical computation: summary statistics, linear regression, non-linear regression and analysis of variance. The new data sets test the ability of MCMC software to compute accurately the parameters of the posterior distribution from a simple statistical model. Results obtained using these data sets challenge the conventional wisdom that longer simulations lead to improved approximation of the posterior distribution. The StRD web site is at www.nist.gov/strd/.

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Figure 7: The Zeeko Process: from metrology to corrective polishing

SSfM Club – membership fees and privileges revised

Club membership categories and fees have been revised for 2004/05. Corporate membership is available for £200 + VAT, while individual membership costs £150 + VAT. SSfM collaborators in other NMIs, enjoy free Club membership.

Corporate and individual memberships are for a named person, and corporate members and collaborators may nominate any number of persons from their organisation to become associate members free of charge. One associate member may attend a Club meeting in place of the named member free of charge. Associate members may also attend in addition to a member for a fee of £80 + VAT.

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Improve your software quality with a simple review

Recently, NPL conducted a review of software in a complex measurement instrument, and this brought to mind some simple things that all software developers can do to improve the quality of their software.

The instrument in question was developed about ten years ago – the software and documentation shows its age – and is still being sold. It includes a PC board and a digital signal processing board: the former manages the user interface, while the latter makes the measurements.

All the software was written in C, though two different compilers were required for the different processors.

No faults were found with the software that would affect the measurements, but our review found it was short of documentation and, where there was documentation, it was unclear whether it corresponded to the software in the instrument.

The main techniques we used to review the software were *static analysis* and *code review*.

The *static analysis* tool we used revealed unused variables, unused functions, unused parameters, unreachable code, incorrect comments, peculiar use of some C constructs, and parts of the code that could be simplified by splitting it into functions.

Code review needs to concentrate on important areas of the software. In this case, we selected the code that makes the measurement, performs the internal calibration, and calculates the measurement uncertainty.

Another technique we used was to re-implement parts of the code in another language, in order to compare the results with those produced by the instrument.

The tools we used are free and in the public domain. **Ctags** generates an index (or tag) file of language objects found in source files allowing these items to be quickly and easily located by a text editor or

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other utility – see http://ctags.sourceforge.net/. **Splint** is a tool for checking C programs statically for security vulnerabilities and coding mistakes – see www.splint.org/.

In summary, the simple things to do when reviewing software are:

- Ensure all aspects are fully documented and the documentation is retained.
- Ensure version control covers documentation of the delivered software.
- Review the code of selected critical parts of the software.
- Perform as much static analysis as is feasible, using general purpose tools.
- Where possible, compare the delivered implementation with a reference implementation.

For use of other more sophisticated techniques, see SS*f*M Best Practice Guide No. 1: "Measurement system validation: Validation of measurement software", at: www.npl.co.uk/ssfm/download/documents/ssfmbpg1.pdf.

Version 2.1 of this guide is now complete, and has been aligned with the standard for safety-critical software, IEC 61508, up to SIL 3.

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Forthcoming Events

27-28 April 2004, AMUM 2004 Conference. Advanced Metrology for Ultrasound in Medicine
Contact: adam.shaw@npl.co.uk

3-5 May 2004, McGill University, Montreal Canada
Advanced Workshop on Current Topics in Monte Carlo Treatment Planning
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15-16 June 2004, SS*f*M training course Visualisation of Measurement Data
Contact: CMSC_Training@npl.co.uk

27 June to 2 July 2004, Queen Elizabeth II Conference Centre, London
24th Conference on Precision Electromagnetic Measurements
Visit: www.cpem2004.npl.co.uk

Visit www.npl.co.uk/news-and-events/
www.npl.co.uk/ssfm/news/

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

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