

**Report
to the National
Measurement System
Policy Unit, Department
of Trade & Industry**

**INTERIM STATUS REPORT
ON SOFTWARE ACTIVITY
WORLD-WIDE**

**FROM THE UK SOFTWARE SUPPORT
FOR METROLOGY PROGRAMME**

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September 1999

Software Support for Metrology

Interim Status Report on the Software Activity World-wide by M G Cox

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Abstract

This report describes the status of mathematics and software world-wide in support of metrology. It is one of a set of status reports produced for the NMS Software Support for Metrology (1998-2001) programme mid-way through the current programme to inform the formulation of the next SSfM programme (2001-2004). The different aspects of mathematics and software are reviewed under the headings of the themes and project topics of the current SSfM programme. The SSfM programme is identifying best practice where it exists and disseminating guidance on that best practice to other metrology areas. The outputs of the SSfM programme will be generic, applicable to a range of metrology disciplines. This report, therefore, not only identifies problems to be tackled and best practice to be disseminated by the SSfM programme, but also possible future projects, the results of which are applicable to more than one area of measurement science.

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1. Introduction to the SSfM programme

The UK National Measurement System Policy Unit (NMSPU) commissioned the Software Support for Metrology (SSfM) programme with the aim of improving mathematical and software support for metrology, largely by organising workshops, undertaking case studies, publishing best-practice guides and providing clubs to act a forum in which issues relating to mathematics and software, across all metrology areas, can be discussed. The programme started in April 1998 and is scheduled for completion in March 2001. Key requirements of the programme are that it should

- add to the resources available to metrologists in the UK and hence should not duplicate work elsewhere and, where possible, it should seek
- collaboration with related activity elsewhere in the world to complement its resources and impact.

For details of the programme, its expected deliverables and the results already produced, see the SSfM web site: <http://www.npl.co.uk/ssfm/>.

2. This report

2.1 Scope

This report covers the breadth of software used in metrology, from instrument control to theoretical simulation, from the determination of fundamental constants to applied tasks such as industrial inspection, quality control and the production of certificates. It addresses SSfM issues in a global context, by reporting on a survey of international concerns in such issues.

2.2 Aims

This report is intended to summarise the status of related activity world-wide at a point half-way through the SSfM programme, key requirement of which is that it should benefit work across metrology. It is an update of an initial status report with the same scope produced in December 1998 [1]. It is a companion report to a set of interim status reports, one for each metrology area covered by the UK National Measurement System (NMS), being produced to update the initial status report which gave a synthesis of the status on the use of software and mathematics in these metrology areas in the UK [2].

Input has been sought from metrologists and organisations around the world, including national measurement institutes (NMIs), standards organisations, certification agencies and similar bodies. Additional information has also been obtained from publications, the World-Wide Web, conferences and other meetings.

In addition to this status report, companion status reports are being produced for the main metrology areas (mass, length, time, etc.). The NMSPU is the direct customer for this work.

Given the broad definition of software in metrology in the SSfM programme, the aims of the report are as follows:

- 1) to survey the state of software support for metrology in key National Measurement Institutes (NMIs) and related organisations
- 2) to survey the views of metrologists, world-wide, on the issues addressed in the SSfM programme

- 3) to determine areas of synergy and/or overlap and thereby to identify possible areas of collaboration between the SSfM programme and similar activity world-wide.

2.3 Structure

The structure of this report is derived from the aims above; it

- a) reports on an international survey of metrologists, who were asked questions relating to the themes and projects of the SSfM programme, and
- b) draws conclusions concerning areas of overlap and/or synergy.

The survey questionnaire appears in Appendix 1 of this document.

3. Survey methodology

3.1 Preparation of questionnaire

The questionnaire was structured hierarchically into three sections, with progressively finer detail:

- 1) questions at the programme level
- 2) questions at the theme level
- 3) questions at the project level

Typical of questions from each section are:

- 1) Is there any programme of activity in your country or organisation which aims to tackle general problems relating to the use of software and mathematics in metrology?
- 2) Is there any programme of activity in your country or organisation which aims to study the modelling of measurement data?
- 3) Which off-the shelf software packages (spreadsheets and others) are used for the numerical processing of measurement data?

Questions at Level 1 were designed to determine whether the correspondent is engaged in activity which overlaps with that of the SSfM programme. If such activity is under way, participation in the survey can be seen as the first step in building a relationship between that programme and SSfM.

Questions at Level 2 were designed to probe deeper, looking at activity themes. It serves both

- a) as a test of SSfM coverage (i.e., key activities which are missing from the SSfM programme, and possibly covered elsewhere) and
- b) helps to identify links at a more detailed level.

Questions at Level 3 were designed to elicit technical views from the survey correspondents. As such, this section of the questionnaire can be seen as complementary to the other status reports, which attempt to determine the same information by metrology area.

3.2 Contacting correspondents

NPL already has extensive contacts with many NMIs. Where possible, known contacts were used in the first instance, and invited to forward the questionnaire to colleagues as appropriate.

Use was made of the NIST web site which contains an index of NMIs at the Web address <http://www.nist.gov/oiaa/national.htm>.

Survey questionnaires were sent to 41 correspondents in metrology institutes outside the UK. Apart from BIPM, with its direct international responsibilities, all were either national measurement institutes or accreditation bodies.

Where e-mail addresses were known, questionnaires were sent as Word 95 attachments. Otherwise, messages were sent to fax numbers, requesting e-mail addresses. If these e-mail addresses were provided, the questionnaires were sent as attachments, as before. Otherwise, the questionnaires were sent by fax. Regardless of the mode of transmission, the covering note

- a) introduced the SSfM programme
- b) explained the purpose of the attachments: the survey questionnaire and SSfM brochure (the latter being included for information)
- c) explained the purpose of the survey and its dissemination: to members of the SSfM DTI customer group, the SSfM programme team and the survey participants
- d) provided the address of the SSfM web site, in particular the download area for Word 95 and PDF versions of the survey questionnaire
- e) invited recipients to participate in the survey
- f) requested the approval of the respondents to include their names and affiliations in the report
- g) invited them to become International Associate Members of the SSfM Club.

At least one reminder was sent to those who did not reply or who promised to reply. A series of deadline dates was provided, generally two to four weeks from the date of invitation or reminder.

4. General survey results

Formal replies were received from 16 of the 41 invitees. Each invitee has agreed that his name and affiliation should appear in the report; hence they are listed in Table 1.

Table 1: Survey participants

Country	Organisation	Contact Name	Receipt Mode	Contact Mode
Australia	CSIRO	Dr Mike Blanco	Email	E-mail
Austria	BEV	Dr Michael Matus	Fax	Fax
Brazil	UNIMEP	Dr Alvaro Abackerli	E-mail	E-mail
Denmark	DFM	Dr Lars Nielsen	E-mail	E-mail
Germany	PTB Berlin	Prof. Dieter Richter	E-mail	E-mail
Greece	EIM	Dr Chris L Mitsas	E-mail	E-mail
Indonesia	KIM-LIPI	Dr Husein Avicenna Akil	E-mail	E-mail
International	BIPM	Dr Richard S Davis	Letter	Fax
Ireland	NML	Dr Paul Hetherington	E-mail	E-mail
Italy	IMGC	Prof. Alessandro Balsamo	E-mail	E-mail
Japan	NRLM	Dr Isao Kishimoto	E-mail	E-mail
The Netherlands	NMi	Dr Gert Rietveld	E-mail	E-mail
Russia	CSRI Elektropribor	Dr Valery Granovsky	E-mail	E-mail

Singapore	NMC	Dr Sze-Wey Chua	E-mail	E-mail
South Africa	NML, CSIR	Dr Chris Matthee	E-mail	E-mail
Taiwan	ITRI	Ms Hui-Chung Ma	E-mail	E-mail

Furthermore, each invitee has become an International Associate Member of the SSfM Club, in order to be kept informed of developments within the SSfM programme and, where appropriate, interact with it.

The list of participants indicates the global interest in SSfM-related issues, particularly within the EU, the Pacific Rim, and the more advanced developing countries.

Although NIST did not contribute formally to the survey, a meeting was held with their Prof. Norman Belecki to discuss the SSfM programme and related matters. The main points arising from that meeting were

- a) the USA has several projects, managed by NIST, addressing many of the subjects of the SSfM programme. However, there is no single programme in the USA with the breadth of the SSfM programme.
- b) Prof. Belecki approved of the “ambitious” aims of the programme and indicated suitable contact points at NIST for the development of technical links.
- c) Prof. Belecki leads an IT “technology foresight” exercise within NIST and could envisage future links between spin-off/development projects both from the NIST exercise and from SSfM.

Further information was discerned from the detailed NIST Web site.

In addition, contact has been established with Jerry Stenbakken of NIST concerning SSfM participation in their Workshop on Software-Embedded Systems Testing (WSEST) to be held on 8-9 November 1999. Contact has also been established with Keith Eberhardt of NIST concerning their participation in the Statistical Analysis of Interlaboratory Comparisons Workshop being organised under SSfM to take place at NPL on 11-12 November 1999. Indeed, Keith Eberhardt has agreed to speak on the subject “Quantifying laboratory comparability with, and without, the use of key comparison reference values” at that workshop. Thus, communication between the SSfM programme and NIST is now firmly established.

5. Analysis of survey results

The survey responses were collated and entered in a Microsoft Access database for analysis. The questions and their analysis have been grouped according to level and are treated in the following three sections.

5.1 Programme level

The most important question at the programme level relates to whether there is already a programme in the organisation or country which is equivalent to SSfM. Ten of the 16 participants said there was no such programme. Of the remaining six, it became clear that these organisations had (at least) one of

- a) sponsorship from industry to address particular topics within an SSfM-like programme
- b) internal funding in support of cross-divisional projects within the organisation which were not intended for dissemination outside the organisation. As an example, one organisation provided

the following indicative list of topics: Software Engineering, Data Bases, Communication, Data Acquisition, A/D Conversion, Mathematical Algorithms for Measurement Data Processing, Type approvals for (Software-Intensive) Special Apparatus (Cash-Gambling Machines, Voting Machines). Another organisation made use of general techniques (data fusion, data processing quality evaluation, etc.), but applied them to a narrower range of metrology disciplines.

- c) a major review of mathematics and software in preparation for third-party certification of its operations.

Of those 10 participants who had no SSfM-like programme, six had not considered establishing a programme such as SSfM. Of the rest, it would appear that securing resources had been a stumbling block. All 10 participants believed SSfM could be beneficial, though two were less-enthusiastic supporters. Seven of the 10 wanted two-way interaction; the remainder were content to receive reports.

Several participants commented on the programme, all favourably, e.g.,

Australia: A very useful initiative that will benefit metrologists who need to use and/or create software to deal with sophisticated computer-controlled instrumentation and ever-increasing quantities of data. The expertise required to make the right decisions in the form of technology transfer from software-engineering professionals will be welcomed. The publication of outcomes as general publications and web-based documents with interactive menus will be well received.

The Netherlands: The main advantages of an SSfM-like programme are:

- providing coherence in software use and development in a broad range of metrology activities*
- a stimulus for good practices in software (re)use*
- a platform for discussions and exchange of information on a local (NMI), national, and international scale.*

Although NMI does not yet have a coherent SSfM-like programme, it recognises the importance of the subject and intends to start one as soon as government funding becomes available. At present there are different activities spread over its whole institute, without much interaction between them. It is believed that an SSfM-like programme would be of benefit to the institute, mainly because of the exchange of information between groups, which will increase the general level of software activities at NMI. NMI would like, and in fact already has, two-way interaction with the SSfM programme. NMI hopes to learn from and contribute to the UK SSfM programme.

The SSfM programme is unique in many aspects. Stimulated by the UK initiative, NMI has also proposed a similar programme for VSL (its standards laboratory). When approved for funding by the government, it will not have the broad scope of the SSfM programme, but focus on a few aspects that are most useful for VSL, or where VSL has specific knowledge already. Items envisaged currently are:

- good software-development practice (including documentation),*
- greater unification in (technical) automation software*

- *better laboratory management systems (LIMS) throughout the whole of VSL*
- *research on measurement-system validation, the evaluation of embedded software, and the evaluation of “self-calibrating” instruments.*

Russia: *The SSfM programme is considered as a most valuable programme with great international significance. There is much interest in collaborating with the programme. Some extensions and specific problems within the limits of the corresponding themes of the SSfM programme are proposed.*

In Russia there is particular emphasis on the MDPN (Measurement Data Processing in Navigation and Motion Control) programme. It contains a number of research themes, including the methodology of data processing in measurements, methods for estimating the accuracy of measurements results (precision), and the quality evaluation of algorithms and software for data processing in measurements. Further, since the field of navigation measurements is so vast and diverse, almost all modern metrological tools are employed in it. Moreover, this field also demands extensions of the traditional metrological tools in some respects. These extensions may also be useful later for other complicated measurement problems. In particular, the basic methodology that is under development for the evaluation of the quality of software and algorithms may be applied to the wider scope of precise and complicated measurements, including metrological procedures used in traceability and calibration.

5.2 Theme level

The four themes of the SSfM programme are:

- 1) Modelling Techniques
- 2) Validation and Testing
- 3) Metrology Software Development Techniques
- 4) Support for Measurement and Calibration Processes.

Questions at this level had the same format as those at the programme level.

5.2.1 Modelling techniques

Only two participants had no activity in any of the modelling project areas. Of the rest,

- a) Twelve had activity in Modelling Techniques
- b) Eight in Uncertainties and Statistical Modelling
- c) Three in Visual Modelling and Data Visualisation
- d) Five in Data Fusion.

The breakdown of activity is surprising, in that questions at Level 3 relating to uncertainties and statistical modelling generally received more attention than those relating to modelling techniques. One explanation might be that uncertainty estimation is seen as part of the larger problem of modelling experimental data, i.e., that modelling projects generally include uncertainty estimation (applied statistical modelling) as an important issue and that there are relatively few projects relating to uncertainty estimation in its own right. This explanation is supported by supplementary questions on scope of the work.

The relatively small number of organisations which had projects relating to visual modelling and data fusion reflect the fact that such topics represent “new technology” and that those that have such projects are to be considered “early adopters”.

Funding sources for such projects include

- a) a levy on metrology projects
- b) operating funds of the organisation
- c) an academic research fund.

Therefore, it is recognised that research on modelling is a supporting activity, benefiting many areas of metrology. Funding is provided either from within the organisation (possibly budgeted), or from applied academic research funds. There is no instance of its being funded by an industry or trade association. One of the consequences of the generally-internal nature of funding this activity is that there is no formal dissemination programme, other than publication of papers and reports, as witnessed by the general lack of references¹ to programme outputs.

Another relevant aspect is that such projects are generally undertaken by “metrologists” within the organisation, the implication of which is that mathematics and IT personnel are dispersed among metrology groups, or that mathematics and IT are performed by metrologists with a particular interest in such issues. The larger laboratories have generally resisted the drive towards greater integration of this kind, perhaps recognising the benefits of generic (though metrology-focused) IT and mathematics research and consultancy, while being aware of the danger of poor communication between professional groups. One large NMI has stated that, at directorate level, it strongly regrets it has been unable to maintain a central group such as that at NPL to provide mathematical and computational support to its metrology workforce and to benefit its country’s metrological requirements.

Of those that considered themselves to have little or no generic modelling projects, three of the four had not considered this activity, but all considered it worthwhile. Therefore, it would appear that lack of activity might well be caused by lack of resource, rather than by lack of demand. This aspect is confirmed when all four indicated their willingness to collaborate with the SSfM programme.

5.2.2 Validation and testing

While spreadsheets and other packages with mathematical content are widely used in metrology, it is rare to find a generic project addressing their validation². Nine of the organisations have at least some activity in validation and testing but, again, this is largely focused on internal requirements, particularly in preparation for third-party certification of their operating practices, e.g., to ISO 9001.

There was just one instance of a model-validation project, though it was noted by five organisations that model validation forms part of modelling or even of metrology generally. The same observation applies to measurement-system validation and validation of simulated instruments. The organisation with a programme of work in the area covers model validation and measurement-system validation, choosing to categorise the former here rather than under modelling techniques because of its central role in modelling. Moreover, it considered this theme, and especially the problem of model validation, to be of prime importance for all the domain of

¹ A notable exception is CMIS, part of CSIRO Australia, which provided a reference to its web site.

² The exception is the Software Practices Group at NML Australia, which is at an early stage of reviewing spreadsheet usage within metrology.

data processing in measurements, since it determines the quality of the measurement result and its practical importance.

Generally, participants were less forthcoming on supplementary questions relating to funding, scope, etc., than they were in the case of modelling techniques.

Of the six organisations that considered themselves to have no activity on validation and testing, two had considered such activity. The five organisations which expressed a view believed it might be beneficial, and four of the five were willing to collaborate with the SSfM programme on this topic.

5.2.3 Metrology software development techniques

Only four of the 16 participants had any project relating to software-development methods. Such a project was generally seen as an internal activity³. Of those that had no such project, one comment was that since the software group was small no formal methodology was required.

Only two organisations had a project relating to software reuse. A comment in the majority group was that there was limited use of common libraries because many languages are used. Hence, this might be one area in which there are technical barriers to its wider adoption.

Three organisations had a project addressing the development of virtual instruments, but it became clear from the comments of one of these organisations that the correspondent had mistaken “virtual instrument” for “simulated instrument”. Therefore, it would appear that software development for virtual instruments (in the LabVIEW meaning of the term) has not (yet) been identified as a particular problem for metrologists.

There were few responses to supplementary questions regarding funding, scope, etc., for existing projects. Four of nine organisations had considered such projects; all nine believe such projects would be beneficial, it being noted that the quality of the results depends on the software. Six of seven participants were willing to collaborate with SSfM project activity in this area.

Only two organisations mentioned related activity⁴.

One laboratory reported that as far as it was aware only the “normal operation” of software is conventionally tested. Hence, the development of methods for the quality evaluation of software is very important for metrology. For investigations into virtual instruments, the main problem is an extension of the metrological characteristics of measuring devices to complicated devices including software. The development of the quality evaluation of software would provide the basis for addressing this problem.

5.2.4 Support for measurement and calibration processes

Five of 12 organisations had activity on automation of measurement and calibration processes, related to the automation of calibration and certificate generation. There is much activity at NMI in this area, including automatic certificate generation, the reliability of the data used in certificate generation, and the availability of the latest certificate value for its own equipment. Only two of the ten organisations mentioned activity on format standards for measurement data.

³ The CMIS SEI webpage contains some useful information.

⁴ ETL, within NRLM Japan, has some activity on metrology software development techniques, which is described on its web page. In Russia, related activity to develop “software for measurements” takes place in several organisations.

As regards funding, the topic appears as an internal activity, with technicians and researchers as customers.

There was no reply to supplementary questions regarding funding, scope, etc., for existing projects. Two of seven organisations had considered such a project; one added that it did not proceed owing to lack of funding. Five of six saw it as being beneficial, and the same organisations were willing to collaborate with the SSfM activity in the area. Perhaps mindful of its earlier experience, one laboratory expressed caution about receiving funding for such activity.

Two organisations referred to the use of a LIMS for supporting the automation of its measurement and testing services.

5.3 Project level

Since questions at the project level were more detailed, and hence more time-consuming to answer, and since not all of the participants were practising metrologists, this section of the questionnaire was made optional. Consequently, not all participants completed this section, and only four participants answered all questions. Hence, the information is limited, but is valuable because of the insight it gives into the concerns of metrologists, who are self-selecting in the sense that they are making input on issues of *real* concern or success.

5.3.1 Modelling techniques

5.3.1.1 Modelling measurement data

Eight of the participants provided information on some of the phenomena modelled at their organisations. These phenomena include

- a) dimensional phenomena
- b) pollutants in the upper atmosphere
- c) crystal growth, molecular dynamics, foams, polymers, fluid flow
- d) transfer functions of transducers and piezo-electric actuators
- e) optical tomography, magnetic and biomagnetic fields, electromagnetic waves, heat dissipation, mechanical motion, accelerometer excitation, shearing interferometry
- f) corrections for temperature, humidity and other environmental effects
- g) measuring instrument properties including dynamic characteristics, calibration curves and parametric errors.

The models were based on the underlying physics where possible, yielding algebraic and differential equations which take into account effects such as hysteresis. Empirical modelling is also used, in its own right and to supplement physical models (i.e., hybrid models). The models are fitted using numerical and statistical models (including some heuristic approaches). Where possible, standard mathematical software is used.

The main modelling concerns relate to

- 1) inadequacies of the selected model
- 2) satisfactory simulations
- 3) sensible balance between model complexity (giving difficult algebraic and numerical problems) and model adequacy (providing sufficient realism)
- 4) a sufficiently rich model to permit a full uncertainty analysis
- 5) inverse problems
- 6) approximations: linearisation, curve fitting, etc.

There is further strong evidence in favour of the observation made in Section 4.2.2.1 that uncertainty evaluation and physical modelling are closely linked.

5.3.1.2 *Uncertainty estimation and statistical modelling*

Twelve of the 16 participants were involved in uncertainties and statistical modelling. All but one use the GUM [3], though two participants also mention EAL-R2 [4].

Of the 10 that expressed a view, four admitted to problems in applying the GUM. Of these, three referred to difficulties with regard to statistical assumptions, two had difficulties with software support and with difficulty of understanding. As evidence of difficulty of understanding, one organisation pointed to the popularity of its internal courses for uncertainty estimation according to the GUM.

For the complicated measurement problems treated in CSRI Elektropribor, the GUM does not generally provide the required tools for the error estimation required at the earlier stages of analysis. In particular, the GUM is applied only for the final stage of the data processing. At the earlier stages of data processing, it is necessary to apply richer and more profound concepts of error analysis, e.g. based on random and systematic components. So, generally, reliance is placed on ISO documents for error evaluation, which are based on the traditional approach (using systematic errors), since these provide broader application and prove to be more appropriate for the measurement problems under consideration. Although error and uncertainty are useful concepts in metrology, uncertainty is not introduced instead of error. Measurand and error estimates are valid only within the limits of the assumed measurement model. So it is reasonable to use uncertainty as the quality characteristic of the assumed model inadequacy. This view closely parallels that within the SSfM Uncertainty and statistical modelling project, where “uncertainty” is seen as the GUM-like activity and “statistical modelling” as relating to aspects such as those here concerning error structures.

Four of nine organisations use confidence levels other than 95%, two referring to 99% and one to 90%.

The main concerns relating to uncertainties and statistical modelling are very informative, those from the six organisations which expressed a view being

- 1) the GUM is insufficiently general to cover many common measurement situations
- 2) formal adoption of the GUM may result in or cause a decrease in the level of uniformity and reliability in data processing
- 3) there are several approaches for statistical modelling, but they should be based on a uniform methodology
- 4) the final testing of the adequacy of the model is essential in all respects
- 5) gaining information from measurement data, parameter estimation, uncertainty estimation
- 6) the correct use of statistical tools
- 7) the number of parameters in uncertainty budgets
- 8) the adequate reflection of reality
- 9) there is too much attention paid to the use of mathematical tools compared with developing a better understanding of physical (Type B) error sources and even identifying error sources that were not addressed previously.

The first and second of these concerns relate to dissatisfaction with the GUM. The first might be addressed by extensions to the GUM (now being considered by the JCGM). The second is a profound issue with political sensitivities that is being tackled elsewhere. Several concerns fall in the domain of model validation: by definition, if the model is suitable, the associated uncertainty estimates will be valid. Some points relate to difficulty in practical uncertainty evaluation, from the viewpoint of a metrologist who is not overly concerned with the details to difficulties with the complexity of the analysis and available tools.

5.3.1.3 *Visual modelling and data visualisation*

Only one of eight participants is involved with visual modelling or data visualisation. The participant uses packaged software of various types, with the concern being “clarity”.

5.3.1.4 *Data fusion*

Six of 10 participants are involved with sensor fusion, the same proportion in fusing data by location, etc. Four use intercomparison of measurements for online fault and error detection or diagnosis, and a further participant is soon to join that group. Three organisations attempt to incorporate predictive or archive data with measurement data. A LIMS is used by one organisation to archive calibration data and to facilitate the comparison of current and previous calibrations. Four organisations are looking to incorporate qualitative and image data with quantitative measurement data. The concerns relate to

- a) the errors sometimes not originating from a Gaussian distribution
- b) unstable measurement standards
- c) use of bought-in software and the manner in which it combines measurement data
- d) weighting data from different sources.

Generally, data fusion is used at the larger laboratories. It is seen as

- a) an adjunct to traditional modelling
- b) being implicit in modern data analysis packages, hence requiring validation
- c) being addressed not only in software but by means of measurement protocols agreed by metrology experts.

One organisation gave the following useful definition of the general data-fusion problem, viz., the creation of a composite model based on the different partial models of the elements of the system under investigation, or equivalently the development of a comprehensive model into which the partial models could be embedded.

5.3.2 Validation and testing

5.3.2.1 *Testing spreadsheets and other mathematical packages*

Nine of the participants listed the key metrology software packages used at their organisations:

- 1) Mathematica, MatLab
- 2) C/C++, Excel, LabWindows, Mathematica, MatLab
- 3) IDL, IMSL, statistical software packages, in-house bespoke software
- 4) Excel, in-house bespoke software
- 5) Data-acquisition: HP-VEE, LabVIEW, Turbo C, Visual Basic, Visual C; data-processing/reports: Excel, SAS, SPSS, Word
- 6) Corel Office suite, to be replaced by MS Office. The organisation is evaluating mathematical packages in a general move to improve precision of calculations.
- 7) Excel, SigmaPlot
- 8) Excel, MathCAD, MatLab
- 9) Calculations: Maple, MatLab; graphs: Axum, SigmaPlot; spreadsheets: Excel, Quattro Pro; word-processing: LaTeX, Word, WordPerfect, Word; automation of measurements: Basic, C/C++, LabVIEW, Testpoint, Turbo Pascal, Visual Basic.

The software can be classified as follows:

- a) word processing: LaTeX, Word, WordPerfect, Word
- b) spreadsheet applications: Excel, Quattro Pro
- c) analysis and data processing: C/C++, Excel, Maple, Mathematica, MathCAD, MatLab

- d) statistical/graphing packages: Axum, IDL, SAS, SigmaPlot, SPSS
- e) data acquisition: HP-VEE, LabVIEW, Turbo C, Visual Basic, Visual C
- f) bespoke: (Visual, Turbo) C/C++, IMSL, Visual Basic.

Two of the seven organisations which expressed a view stated that spreadsheets were *not* used for processing measurement data. Clearly, that must have been a policy decision, possibly relating to concerns about the uncontrolled use of spreadsheets. Of the remainder, the main use was for computing combined uncertainties according to the GUM. Two organisations also used spreadsheets to record the calibration history of instruments. The last-mentioned point is interesting, since a database package might seem more appropriate for such a task (with its greater security features and support for logging transactions). Hence, the emphasis of the SSfM programme on numerical correctness *and* configuration control would appear to be well-placed. One organisation made extremely wide use of spreadsheets, for measurement automation, data fusion, data analysis, uncertainty analysis and a record of calibration history.

Five of seven organisations were aware of deficiencies in the available software packages. One participant singled out the standard deviation (stdev) and inverse t-distribution (tinv) functions within some versions of Microsoft Excel as requiring care in their use. This aspect is of concern because it is expected that such functions would be used in evaluating combined standard uncertainty, etc. from the GUM. Six of eight participants have performed some formal testing of the packages they use, though it appears that the level of detail of such testing varies.

Three of eight participants have sought advice from software suppliers about the “quality” of the mathematical software they use. One of the three added that this advice is often lacking or unsatisfactory. One of the remaining five has offered advice to others concerning the validity of mathematical software used.

NIST is especially aware of the need for well-tested software and in recent times has developed a testing and evaluation methodology. Specifically, NIST has developed a web service that provides reference data sets with certified computational results which permit objective evaluation of statistical software. Interestingly, this NIST methodology is complementary to that being developed within SSfM, the concentration being more on highly-accurate reference data sets rather than on the explicit determination of fitness for purpose. NIST is currently working on the automatic generation of specification-based tests. This approach parallels that of the methodology employed in the current SSfM Testing Spreadsheets and Other Mathematical Packages theme, where reference data sets are derived using a mathematical characterisation of the problem determined by the functional specification of the task purportedly performed by the software. NIST maintains a Matrix Market, a repository of test data for sparse linear algebra problems,⁵ and a Digital Library of Mathematical Functions, an online successor to the widely-used *National Bureau of Standards Handbook of Mathematical Functions*.⁶

5.3.2.2 Model validation

Participants see close links between model validation and both modelling and measurement-system validation. Two of the eight participants who expressed a view on model validation (intend to) incorporate model validation formally as part of their quality system, with one

⁵ Many models used in metrology give rise to sparse linear algebra problems from the fact that a large set of model equations usually contains only a relatively small subset of the problem variables in each model equation.

⁶ These mathematical functions range from basic statistical functions such as the normal (Gaussian) integral to the Bessel functions which frequently arise from models of sensors, etc., which exhibit radial symmetry.

identifying it as part of method validation in the context of ISO Guide 25. Methods of model validation include:

- 1) comparison with experimental data
- 2) use of the scientific method, i.e., establishing the limitations of the model by experiment
- 3) use of two or more measurement methods
- 4) comparison with results from a more comprehensive model
- 5) cross-validation within the given measurement-data set
- 6) tests using reference data sets
- 7) submission to peer review.

Some of these methods blur the distinction with measurement-system validation.

The degree of information and analysis from model validation is varied. Aspects include

- a) the usefulness of diagnostics, e.g., to understand in what sense a model fails
- b) the use of physical and mathematical properties to establish whether models are fit for the problem
- c) information that can be helpful in making improvements to the model
- d) validations that are as complete as possible, but limited by resource considerations.

Note that c) implies that some questions of model validity can be resolved by numerical (non-experimental) means and d) that a barrier to model validation can be resource limitations rather than technical difficulties.

Of the eight participants who responded, all are aware of the distinction between model correctness and (software) implementation correctness. One adds that the software generally provides sufficient numerical precision to be fit for purpose, even though it has deficiencies. Another adds that the host organisation offers consultancy on good numerical implementation of models.

5.3.2.3 *Measurement system validation*

Of the eight participants who replied to the questions on measurement-system validation, all have some smart measurement systems. The extent varies, and embedded-sensor intelligence is not always welcome. For example, one organisation (prefers) to use in-house software, and bypass smart options. Functions include data acquisition and control, though generally not higher-level functions such as analysis, although self-calibration was mentioned.

Eight organisations validate measurement systems as complete systems, by means of

- a) the measurement of well-known artefacts measured by other methods
- b) manual cross-checking
- c) comparison with peer laboratories
- d) validating the modules of a measurement systems separately and checking the data transferred between the modules
- e) type testing of the complete system including software, e.g., utility (kWh) meters
- f) testing of complete set-ups for reliability, including software, e.g., in legal metrology
- g) statistical process control.

Note that methods a) to c) relate to traditional calibration and traceability techniques within metrology. One approach to methods d), e) and f) is a “bottom-up” systems approach, which requires deep analysis of the system modules and interfaces to be effective. Method f) is intended to avoid external users changing measurement results or the software itself. Method g) is appropriate for routine measurement tasks.

Validation of embedded software is difficult; to quote one participant, who represents the common view:

Embedded software cannot be validated in most instances. Therefore, manufacturers' claims about testing software have to be relied upon when and if such claims can be extracted from the manufacturers.

Two of the eight participants who replied use manual or spot checks, while one participant states that the validation of embedded software is an active research topic in his organisation.

One organisation prefers to use in-house software because of the ability to check it. Apart from data acquisition and control, the data is almost always analysed with regard to stability and noise as a first indicator for the quality of the measurement. In the case of a “self-calibrating” instrument evaluation, in one case the manufacturer of the instrument gave confidential access to the source code of the software—which was essential in order to carry out more than the standard “black-box” evaluation (i.e., check against other methods or standards, or check with a manual method). The validation of embedded software is an active research topic at NMi, which finds that a focus on functionality is very helpful: dividing the instrument into relevant functional blocks aids the structuring of the evaluation. Reliance is not placed by NMi on the claims of suppliers that the software has been sufficiently tested. However, tests are very difficult to perform in general. For specific calibration software some tests are always performed, mainly based on checking with other, manual methods.

5.3.2.4 Validation of simulated instruments

Three participants claimed to be aware of simulated instruments. Of these, it became clear that one has mistaken simulated instruments for virtual instruments, referring to LabVIEW and Visual Basic. Clearly, there is a problem of terminology in this area.

The two participants who had genuine awareness of simulated instruments quoted the Virtual CMM and a virtual biomagnetic measurement system as examples.

With regard to their benefits to metrology, one participant did not believe that simulated instruments were cost-effective. Another commented on the strengths of LabVIEW, the third felt unable to comment in general, while the fourth was an enthusiastic supporter, stating that simulated instruments

... allow the user to simulate measurements off-line, saving money and time. Also they enable the user to estimate the instrument's performance, to help select the best measurement conditions within the constraints of a specific measurement problem.

5.3.3 Metrology software development techniques

5.3.3.1 Software development methods

Six of 10 participants claim to develop software using processes which are compatible with an ISO 9000-like quality system. Of these, one admits that they are at the early stages of implementation, with the implication that these processes are under review. Another refers to ISO Guide 25 as being the relevant “standard” for its activity. Yet another claims to be operating to its own standards which are equivalent to ISO 9000 and its ilk. Of those three participants who do not claim to use such processes, two claim they will “soon”.

Five of eight participants claim that their quality practices give them the accuracy they require. Generally, these are the same organisations which have some formal quality system. The

organisation operating to its own internal standards claims that reliability of software developed in-house is kept under review.

Three of five find maintenance of old software too expensive; one of these takes a pragmatic approach and notes that “whenever the opportunity arises and resources permit we encourage migration to new software or complete re-designs of software developed in-house”. This trade-off of costs is examined further in the next question, when six of seven participants believe that developing new systems is reasonable, though expensive. One participant makes the point that development is not undertaken if it is not expected to pay off within a reasonable time scale.

This aspect also introduces the wider question of capital-investment decisions which take into account lifetime costs, and not just the choice between maintenance of software versus development of new software. There are important management decisions to be made in this regard.

One organisation states that it has no internal strategy for software-development quality, but recognises this as one of its weakest points. It claims that it is one of the most difficult to implement since staff want to develop software in their own way, and not everybody sees the added value of good software documentation (or wants to make time for it). All developers carry out checks of the software written, but in general do not document the test results very well. The current introduction of a quality system based on ISO 17025 [5] is expected to improve this situation. Functionality is the most important aspect of software, with reliability close following.

The five participants who identified their most pressing problem(s) with software listed the following:

- 1) the IT industry-driven changes in software and hardware platforms is a problem especially in relation to the archiving of data, programs, and records
- 2) to have a firm computer and software strategy within the company
- 3) validation; obtaining adequate software for performing specific functions; linking software packages—e.g. purpose-written software to “Windows-based systems”
- 4) the variety of professional software-engineering methods to develop software and their limited ability to ensure adequate software quality
- 5) resource shortages (time and personnel).

The first two issues relate to management of change, particularly in an area as fast-moving as IT. Quite often, rapid change elsewhere in IT, driven by demand from major industry sectors can have large effects on smaller sectors such as metrology. This aspect impacts on procurement, training, interoperability and flexibility to be adapted to meet evolving requirements. The third issue relates closely to two projects elsewhere in the SSfM programme, viz., Testing Spreadsheets and Other Mathematical Packages (in the Validation Theme), and Software Reuse (in the Metrology Software Development Techniques theme).

The fourth issue relates to choice of method, given that it is unlikely that any one method will be optimal (across all quality attributes) for the task. In turn, the task is rarely easily defined. Therefore guidance is needed to find a suitable method for a task, where no single method is ideal and the choice of method is complicated by lack of precision in the requirements specification.

The fifth issue relates to a perennial difficulty in any form of applied research, namely (the management problem of) how to deploy scarce resources effectively.

Of the eight who replied to the question asking which quality attribute of the six identified in the ISO standard is most important,

- a) three chose not to select a subset; one of these noted that the most important attributes depend on the context of use
- b) two chose functionality
- c) two chose reliability
- d) one chose reliability and maintainability.

Given that there is a case to be made for incorporating all the six attributes in metrology software, the prioritisation is interesting. The most important questions for metrologists appear to be

- 1) Does the software operate as expected?
- 2) Will it cost a large amount over its lifetime?

Perhaps even more interesting is the lower priority given to other attributes, such as usability, efficiency and portability, which suggests that

- a) The human-computer interface is not a concern, even though it has been estimated that a large proportion of errors in metrology are due to user error [see *Measurement Good Practice Guide 8: Human Factors in Measurement and Calibration*, by C Thomas, O Daly-Jones and A Harry, NPL].
- b) The lack of emphasis on efficiency is a consequence of the fact that the growth of computer performance has outstripped need in many areas of metrology in the recent past. This aspect is not guaranteed to continue, as data capture rates are set to rise and more powerful models and software are developed to improve measurement capability.
- c) The low rating given to portability would appear to be a consequence of the fact that most metrology software is installed on dedicated computers, which remain stable until there is a significant leap in technology, as occurred in the move from DOS to Windows. Also, while the new computer language, Java, has many advantages, the portability advantages are less important in metrology-software development.

There are many method of testing software for correctness. Five of the seven who replied check the results using another instrument, although one notes that this is not always possible. The same applies to checking software by hand calculation or by using an alternative software package. Several participants noted that it was best to use as many validation tests as possible, probably because individual validation tests often have poor coverage, and it would be hoped that an ensemble of tests would test most of the domain of use of the software.

5.3.3.2 Software reuse

Software reuse is supported, as a matter of policy, by six of the nine who replied to the question; two of these note that this is not always convenient.

Five of the six state that their organisations use mixed-language programming (presumably in support of software reuse). Attitudes vary: one participant saw no special problems with mixed language programming; another saw it as a last resort, to be tried when other methods failed. Others identified some of the difficulties as being

- a) the programming may become less transparent and the management of files needed to run the program may be more difficult for the user
- b) the main problem is the need to be expert in many languages.

Mixed programs arguably lack clarity (because of the need for interface procedures and features of one language which intrude on the other). Also, there are development difficulties if the run-time system needs to treat legacy software as a black box; hence the programmer has less control over program execution. Not only does the programmer need to know several languages, he also needs to be aware of unusual language or compiler features which are

intended for experts. Therefore, mixed-language programming is probably best tackled by persons with a software-engineering background.

Recommendations for dealing with legacy software include

- 1) where resources permit by redesigning or upgrading
- 2) an old program compiled with a previous compiler will be transcribed to the current compiler if changes to the programme are needed
- 3) a strong software-documentation rule for software developed [at the organisation] is recommended to avoid problems in the future
- 4) programmers study the source code until they understand it.

Recommendations 1) and 2) relate to planned obsolescence of software. In particular, old software is used while still convenient, but eventually the time comes to replace it. At that stage, good documentation and close scrutiny of the source code assist the user to upgrade to a new system (compiler, language, or hardware).

Five participants divulged their plans for becoming millennium-compliant. Strategies (by participant) include

1. making use of the best advice available to minimise the level of risk
2. participation in a government project on the subject
3. obtaining declarations of conformity by vendors, etc.
4. system manager-led study of potential Y2K problems
5. extensive analysis of all hardware and software at the organisation.

Clearly organisation 1) has performed a risk assessment, and is now working to iron out the difficulties. Organisation 2) is part of a government scheme; the implication is that it is intended to lead by example. Organisation 3) has identified problems in its supply chain, such that recent and new software can be guaranteed to be conformant, although the same cannot always be said for legacy software. Organisation 4) has chosen to view matters as a management problem; this could be an efficient way to proceed provided there is good visibility of the software at management level, supported by motivated staff at more junior grades to ensure that management is and remains fully aware of the software in use. Organisation 5) had completed an extensive project on the Y2K problem. It found that (i) most problems reside in administrative programs, (ii) few problems arise with software dealing with measurements, since they normally do not rely on the computer date, (iii) most problems relate to old computers and old software which were scheduled for replacement and for which the Y2K project was the stimulus to complete it, (iv) suppliers were included in the project.

Mathematical-software libraries are seemingly not as widely used compared with the times when much metrology computation was carried out remotely on main frame computers with library support. NIST, however, maintains a “virtual repository” of mathematical and statistical software, nominally for “use in computational science research”, but it clearly is of value to metrology.

5.3.3.3 *Virtual instruments*

Four of seven who replied make use of virtual instruments. Uses include

- 1) to set up computer-automated measurement facilities
- 2) to control data processing
- 3) special purposes, e.g., for the spectral analysis of noise.

Uses 1) and 2) would appear to be classical uses of LabVIEW, taking advantage of its data-flow programming paradigm. Use 3) is not an obvious application of LabVIEW, since users might be expected to use specialised analysis packages if such were available. However, it serves as a

reminder that virtual instruments can include appreciable intelligence and analysis capability, in which case questions of software correctness are not trivial.

One laboratory reported that it has many virtual instruments in the sense that almost all its measurement facilities are automated, including some data-processing aspects. The electrical department uses Testpoint heavily for this purpose and also LabVIEW. The latter is also found very useful for the simulation of measurement processes. LabVIEW will be the main tool in the near future. Documentation is very poor in general.

No participant identified a particular development method for developing virtual instruments, apart from the use of National Instruments' software tools. Nor did they consider that there are any special problems with documenting, testing or maintaining the design. Hence, the consensus would seem to be that, despite their different approach to programming, conventional software-development techniques are likely to have the same degree of success with producing virtual instruments as they have with producing modules of Visual Basic, C or MatLab, say.

5.3.4 Support for measurement and calibration processes

5.3.4.1 *Automation of measurement and calibration processes*

Of the seven who replied, two do not use LIMS of any kind, relying on *ad hoc* computer- and paper-based systems in support of their measurement and testing services. Two organisations have taken the first step to integrating several of their existing systems, e.g., Excel spreadsheets and a FAMIS database, but much more needs to be done. One organisation has a LIMS which was produced in-house and which is being upgraded to follow developments in commercial LIMS products. Only one organisation has a commercial LIMS which is fully integrated with its business practices. One organisation has developed a very advanced LIMS based on databases (implemented in Delphi) for temperature measurement, including automatic certificate generation. This organisation has also developed, CALCAS, a high-level LIMS which is available commercially. Further, there is a large variety of LIMS in use at this organisation, ranging from manual systems to completely automated. Again, here the value of an SSfM-like programme becomes clear: it will stimulate a higher overall level of software use, especially by upgrading the oldest (manual) systems. Most often, spreadsheets are used to process calibration data. The main advantage is the use of a general package. The disadvantage concerns reliability (prone to errors), and the difficulty of maintaining a good overview of the analysis.

Of those who claim not to use LIMS of any kind, the four who replied outlined the following alternative solutions:

- 1) Individual software for processing calibration data
- 2) Manual processing—word processing using MS Word; purpose-written software for data collection or processing; embedded software for collection or processing of results
- 3) Specific systems developed in-house
- 4) Software requiring a certain degree of manual input and output.

Solutions 1) to 4) represent the first steps in moving to automated calibration, where the software is tuned to perform discrete tasks, but problems may occur at the interfaces between the (software) modules. In addition to possible operational inefficiencies, the lack of integration often limits the business intelligence of the system, i.e., the ability to derive meaningful summary information. At one laboratory the automation of measurement set-ups is facilitated through the use of a variety of programming languages (Basic, Visual Basic, Pascal, C++) and object-orientated systems such as Testpoint and LabVIEW.

Five participants shared their perceptions of the advantages and disadvantages of the systems they used, as follows:

- 1) Errors are determined by cross-checking between steps. The main disadvantage is that it is time consuming.
- 2) Too much data has to be re-entered into different parts of the system.
- 3) Purpose-written software or embedded software is efficient and helps to reduce computational and other errors. It also ensures consistency but can be difficult to validate. Manual processing eliminates the need to validate software and carry out back-ups.
- 4) An advantage: is that the components are well understood. A disadvantage is that development is time-consuming.
- 5) The main advantages are to manage all the measurement areas in the laboratory, and to offer better services to customers. There is no special disadvantage.

Observations 1) to 4) were made by participants who do not use LIMS, and present the main advantages and disadvantages of the systems in place at the organisations. Many of the comments indicate a lack of trust in a completely-automated system. Observation 5) was made by a participant whose organisation has a commercial LIMS in place. There is an implication that its implementation might have had some initial difficulties, but that the system has stabilised and is now satisfactory.

Three participants provided information on how the calibration-management system was developed and modified at the organisation:

- 1) A combination of LabWindows, C/C++, Access (for storing and retrieving general information on a calibration task), Excel (for storing and presenting calibration history), and Word (for producing certificates) into a streamlined mass-calibration system
- 2) A standard Excel spreadsheet was integrated with software developed in C++
- 3) The in-house LIMS system is developed and modified by the Quality Assurance Section.

Note that 1) represents a plan for developing a custom LIMS, 2) represents a low-risk strategy and 3) represents the views of an organisation which has a LIMS in place.

Since LIMS and calibration systems generally are often costly to implement and maintain, a good business case is needed to win resources for their development. Three participants expressed the following views on how to ensure LIMS meet their objectives:

- 1) The specification was set in order to meet internal requirements and those of customers and the accreditation/certification body; verification that specifications are met was then undertaken
- 2) Standard documents have been established
- 3) Consultation with peers took place.

View 1) was offered by the same participant who described a plan to integrate LabWindows and MS Office to form a LIMS. It employs good software-engineering principles relating to requirements capture, etc. View 2) is from the participant whose organisation has a mature LIMS system which is well integrated with business practices. View 3) represents one form of requirements capture, using bench-marking.

5.3.4.2 Format standards for measurement data

Six of nine participants who replied use standard data formats for measurement data, providing the following examples of their use:

- a) time and frequency
- b) biomagnetic and bioelectrical measurement data
- c) data for calibration history (at least five years' worth for periodic re-calibration).

Time and frequency is a well-known example, since time transfer is an important function of many NMIs. Bioelectromagnetic data transfer is probably a poorer-known but vital application,

characterised by large data volumes and high security requirements (relating to data integrity and patient confidentiality). Calibration-history data is vital for traceability and also for estimating instrument drift. It is also a reminder of the importance of stored-data formats, in addition to data-transfer formats, and reflects an earlier concern about how changes in IT impact on metrology.

Seven of nine participants share data electronically with other metrology organisations. Of these, the most popular means are by standard IT protocols, e.g., as plain ASCII files, as e-mail attachments, in common database formats, etc. Two participants referred to the agreed protocol for time transfer, which the organisations use to communicate with BIPM and USNO.

Five of seven participants indicated a need for a common international format for calibration records (use c) above). One of the two participants who did not have a present need could foresee the need in the future. One of the participants who has a need for standard data formats argued that data formats should be standardised at the record level, rather than the bit level. As an example of their current use, another participant cited regulatory bodies such as the Federal Aviation Administration in the USA.

Seven of nine participants already use a common format for electronic exchange of measurement data, including one participant who includes the example of EC SMT collaborative projects, where results are shared between partners. Another participant states that

Until now the results of our measurement and calibrations are presented in paper certificates only. If our clients in the future should demand electronic certificates, a common data format at bit level would be desirable.

Only one of six participants had been prevented from using a package because it used a data format which was somehow incompatible with the systems used elsewhere in the organisation. Interestingly, that organisation was the organisation with the mature LIMS.

6. Conclusions

6.1 Recognition and position of SSfM

In the absence of any evidence to the contrary, the SSfM programme is unique world-wide, in the sense of being a single programme with such breadth. Other programmes either have narrower scope (but sometimes greater depth, by concentrating on a metrology area or a mathematical approach), or are focused on the internal needs of the organisation. For instance, several organisations have programmes focusing on software support for metrology, with a view to preparing for certification of their quality systems.

The degree of goodwill for SSfM is encouraging and the international links which have been established during the programme should be strengthened and existing links reinforced. Since the primary purpose of SSfM is the dissemination of guidelines for metrologists, the programme can benefit from collating best practice, wherever it occurs.

With regard to the more detailed technical discussions, it has become clear that the experience of the international metrology community is not too dissimilar from that of NPL's. This gives some hope that the problems and solutions might be similar, and hence that international collaboration would be mutually beneficial.

One aspect where there is less similarity is the lack of centralisation or networking of expertise at some NMIs in some of the SSfM areas. The result is poor communication across metrological disciplines in aspects that in fact have significant commonality. This point is recognised by some

NMIs, but difficulty has been experienced in gaining acceptance of cases for attracting the necessary support to remedy the situation.

There are some useful pointers to areas of overlap between projects, which might be addressed by appropriate choice of case studies within the programme.

Input from the Level 3 questions will also help to inform the SSfM technical programme, supplementing the information collected in the other status reports, which focus on the needs of the metrology areas within the UK's National Measurement System.

6.2 SSfM themes

6.2.1 Modelling techniques

1. There is generally greater emphasis internationally on uncertainty evaluation as opposed to modelling and model validation. In one sense this emphasis is surprising since the development of a valid model is a prerequisite to sound uncertainty evaluation.⁷ The SSfM programme recognises this fact by including Uncertainties and Statistical modelling within the Modelling theme. A further indication of the strong relationship between the two disciplines is reflected in the fact that NPL plans to make forthcoming workshops on discrete modelling and uncertainty evaluation a major *joint* event within the SSfM programme.
2. Difficulties with the interpretation and application of the GUM were experienced. This problem is also experienced in the UK and stated at the two uncertainty workshops already held as part of the SSfM programme. Within the Uncertainties and Statistical Modelling project, emphasis is being placed on validating the use of the GUM and applying other techniques beyond "mainstream GUM" where appropriate. Greater use is made of statistical modelling (also as part of the modelling generally), in order to obtain valid results.

6.2.2 Validation and testing

1. There is surprisingly little emphasis outside the UK on testing for numerical correctness the software that metrologists use on a day-to-day basis.⁸ There will be greater pressures in the future for such activity as organisations strive for certification to ISO 9001.
2. There is an awareness that some of the software packages used by NMIs are deficient and therefore require care in their use (superficially-simple functions such as standard deviation and the inverse t-distribution were mentioned).
3. Advice is generally lacking from software suppliers on the quality of their products. This fact raises difficulties in the context of quality systems used at the NMIs.

⁷ In another sense, it is possible to discern reasons for this attitude in particular metrology areas. For instance, the current UKAS publication on the treatment of uncertainty in electromagnetic compatibility (EMC) measurements (UKAS document NIS81, 1994), which is used in EMC circles world-wide, is *not* model-based. Formulae, etc., for estimating and reporting uncertainty are provided without reference to measurement models. The consequent problems of this attitude are recognised, particularly when conversions between units (linear and decibel) are required and measurement errors are large. Work is under way to re-present the material appropriately.

⁸ Exceptionally, NIST provides reference data sets for testing some of the software used by metrologists. The effort does not yet appear to be strongly integrated with metrologists' needs and with fitness for purpose. NML Australia is starting to review software usage within metrology.

6.2.3 Metrology software development techniques

1. Good practice in software reuse is lacking. There are inefficiencies world-wide because of the limited use across metrology disciplines of common libraries. One reason is that many languages are used. (Another is given in 2 below.) This barrier is starting to be addressed by the SSfM software reuse project. It would seem to be an important theme for the next SSfM programme also.
2. Mathematical-software libraries are not used as widely as they once were. A major reason is that previously much metrology computation was carried out remotely on a mainframe computer for which such libraries and support for their use were provided. The move to PCs, and their enormous advantages of integration with measurement systems, has not generally carried with it the libraries and their support. This aspect is recognised in the Validation and Testing projects and in fact is a primary motivation for the work. The Software Reuse project is making a start in addressing the problem through the Metrology Software environment (METROS) which being developed by NAG Ltd. and NPL.
3. Only one quarter of the participants had a project concerned with software-development methods. This aspect not only impacts on software reuse, but also on other aspects of the achievement of software quality.⁹
4. There is a need for the design of algorithms and the development of associated reusable software for the solution of problems for which a generic capability does not yet exist within metrology.

6.2.4 Support for measurement and calibration processes

1. An SSfM-like programme stimulates a higher overall level of software use, especially by upgrading the oldest (manual) systems and providing integration across the various aspects of measurement and calibration processes.
2. Such integration will help to produce records and certificates automatically, and therefore more reliably and more “traceably”. It will be important in this regard to pay attention to means for avoiding the re-entry of data into different parts of a LIMS, and the consequent problems of consistency and correctness.

6.3 Recommendations for the next SSfM programme

1. The involvement of software-engineering professionals in transferring coherent generic technology from their areas to the various metrology disciplines is seen as important. It would be necessary to tailor the documentation appropriately to suit particular disciplines. This aspect is also starting to be addressed by the SSfM software reuse project, and likewise would seem to be an important theme for SSfM2.
2. Generally there would be benefit from greater transfer of information at an international level. Important aspects of such transfer have already taken place through the Advanced Mathematical (and Computational) Tools for Metrology conferences and workshops that have taken place in 1993 (in Italy), 1995 (UK), 1997 (Germany) and 1999 (UK), with AMCTM2000 currently being organised (10-13 May 2000 in Portugal). The SSfM programme included support to host the 1999 conference and is also providing some support

⁹ NPL's Centre for Information Systems Engineering is deeply involved with the software aspects of many projects within NMS programmes through its relationships with other NPL Centres. Moreover, a stated requirement of NPL's Strategic Research programme is that projects having serious mathematical or software content are required to receive input from CISE.

to help organise the 2000 meeting. Such conferences are important as a mechanism to maintain and enhance international awareness and co-operation in this field.

3. Software aspects of metrology can benefit from concepts and tools in areas traditionally outside mainstream metrology. A good example is the Russian programme on Measurement Data Processing in Navigation and Control, in which most aspects of modelling, uncertainties, etc. appear. In recognition of the benefit of such knowledge transfer, NPL has recruited a professional statistician from the area of geostatistics who is applying his knowledge of modelling, data correlation, etc., in SSfM and other NMSPU programmes.
4. The current SSfM software reuse project is rightly perceived as seed-corn activity. Its continuation to the next programme should involve a maintenance phase (akin to maintenance of standards in other NMS programmes), in order to ensure that the existing methodology and software tools remain viable and applicable. It should also involve a design and development phase in which further contributions to and possibilities for a reuse library should be considered. International contributors to the library, which would be available on the World Wide Web, should be considered. NIST has reported that the increasing prevalence of computation in science and engineering has generated an acute need for accurate and robust computer software to solve frequently-occurring mathematical and statistical problems. The most important aspect of this would be the considerations needed to permit metrologists from all disciplines to access and make efficient use of generic quality software in their own areas.
5. There is scope for collaborative internationally activity, under Framework 5, for example, but a number of organisations, including industry, within the UK have also been identified with whom NPL and other NMS SSfM contractors could potentially work. There would be a considerable advantage in considering possible joint funding for some of these items, with the twin objectives of providing results generic to metrology and the NMS and a particularisation of them to the collaborating organisation.

7. Acknowledgements

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Appendix 1: The questionnaire

1. Questions at the programme level

1. Is there any programme of activity in your country/organisation which aims to tackle general problems relating to the use of software and mathematics in metrology?
 - a) If Yes to Q1:
 - i) How is it funded / who is the customer?
 - ii) Who is conducting the work?
 - iii) What is its scope?
 - iv) What is its duration?
 - v) What relation does it have to international metrology bodies (such as EUROMET or ISO, etc.)?
 - vi) Can you provide references to programme outputs?
 - vii) Can you provide contact details for the programme?
 - b) If No to Q1:
 - i) Was such a programme ever considered?
 - ii) Do you believe that such a programme would be beneficial?
 - iii) Are you interested in collaborating with the SSfM programme?
1. Do you have any general comments to make concerning the SSfM programme?

2. Questions at the metrology / software management level

2.1 Modelling Techniques

1. Is there any programme of activity in your country/organisation which aims to study any of the following:
 - a) modelling measurement data?
 - b) uncertainties and statistical modelling?
 - c) visual modelling and data visualisation?
 - d) data fusion?
 - e) If Yes to any one of Q1 a) to d):
 - i) How is it funded / who is the customer?
 - ii) Who is conducting the work?
 - iii) What is its scope?
 - iv) What is its duration?
 - v) Can you provide references to programme outputs?
 - vi) Can you provide contact details for the programme?

- f) If No to any one of Q1 a) to d):
 - i) Was such a programme ever considered?
 - ii) Do you believe that such a programme would be beneficial?
 - iii) Are you interested in collaborating with the corresponding SSfM project?
- 2. Is there any related activity in your country/organisation? If so, what is its scope?
- 3. Do you have any general comments to make concerning the SSfM programme theme concerned with modelling techniques?

2.2 Validation and testing

- 1. Is there any programme of activity in your country/organisation which aims to study any of the following:
 - a) testing of spreadsheets and other mathematical packages?
 - b) model validation?
 - c) measurement system validation?
 - d) validation of simulated instruments?
 - e) If Yes to any one of Q1 a) to d):
 - i) How is it funded / who is the customer?
 - ii) Who is conducting the work?
 - iii) What is its scope?
 - iv) What is its duration?
 - v) Can you provide references to programme outputs?
 - vi) Can you provide contact details for the programme?
 - f) If No to any one of Q1 a) to d):
 - i) Was such a programme ever considered?
 - ii) Do you believe that such a programme would be beneficial?
 - iii) Are you interested in collaborating with the corresponding SSfM project?
- 2. Is there any related activity in your country/organisation? If so, what is its scope?
- 3. Do you have any general comments to make concerning the SSfM programme theme concerned with validation and testing?

2.3 Metrology software development techniques

- 1. Is there any programme of activity in your country/organisation which aims to study any of the following:
 - a) software development methods?
 - b) software reuse?
 - c) virtual instruments?

- d) If Yes to any one of Q1 a) to c):
 - i) How is it funded / who is the customer?
 - ii) Who is conducting the work?
 - iii) What is its scope?
 - iv) What is its duration?
 - v) Can you provide references to programme outputs?
 - vi) Can you provide contact details for the programme?
- e) If No to any one of Q1 a) to c):
 - i) Was such a programme ever considered?
 - ii) Do you believe that such a programme would be beneficial?
 - iii) Are you interested in collaborating with the corresponding SSfM project?
- 2. Is there any related activity in your country/organisation? If so, what is its scope?
- 3. Do you have any general comments to make concerning the SSfM programme theme concerned with metrology software development techniques?

2.4 Support for measurement and calibration processes

- 1. Is there any programme of activity in your country/organisation which aims to study any of the following:
 - a) automation of measurement and calibration processes?
 - b) format standards for measurement data?
 - c) If Yes to any one of Q1 a) to b):
 - i) How is it funded / who is the customer?
 - ii) Who is conducting the work?
 - iii) What is its scope?
 - iv) What is its duration?
 - v) Can you provide references to programme outputs?
 - vi) Can you provide contact details for the programme?
 - d) If No to any one of Q1 a) to b):
 - i) Was such a programme ever considered?
 - ii) Do you believe that such a programme would be beneficial?
 - iii) Are you interested in collaborating with the corresponding SSfM project?
- 2. Is there any related activity in your country/organisation? If so, what is its scope?
- 3. Do you have any general comments to make concerning the SSfM programme theme concerned with support for measurement and calibration processes?

3. Questions at the metrologist or software developer level (optional)

3.1 Modelling Techniques

1. Are you or colleagues involved in modelling measurement data?
 - a) If Yes to Q1:
 - i) What phenomena do you model?
 - ii) How do you model your data?
 - iii) What are your main modelling concerns?
2. Are you or colleagues involved in estimating uncertainties and statistical modelling?
 - a) If Yes to Q2:
 - i) Do you use the GUM (*ISO Guide to the Expression of Uncertainty in Measurement*) and similar Guides?
 - ii) If yes to 2.a) i), Do you have problems applying the GUM? Do they relate to
 - a) statistical assumptions?
 - b) software support?
 - c) difficulty of understanding?
 - iii) Do you use levels of confidence other than 95%?
 - iv) What are your main concerns relating to uncertainties and statistical modelling?
3. Are you or colleagues involved in visualising multivariate data and/or interacting with complex simulations?
 - a) If Yes to Q3:
 - i) What methods of data interpretation do you use at present?
 - ii) What are your main concerns relating to visual modelling and data visualisation?
4. Are you or colleagues involved in
 - a) processing and reconciling measurements from an array of sensors?
 - b) patching together measurements corresponding to different sets of parameters (e.g. regions of an artefact's surface, local regions of a temperature spectrum, ...)?
 - c) fault and error detection/diagnosis by inter-comparison between measurements?
 - d) combining results from several very different measurement processes, because the target measurement was infeasible or inaccessible?
 - e) dealing with predictive data from models, or historical or archive data, in tandem with current measurement data (here, data fusion has similarities with hybrid data modelling)?
 - f) handling numerical, image, and/or qualitative data within a single framework?

- g) If Yes to any one of Q4 a) to f): What are the problems and how are they being overcome?

3.2 Validation and Testing

3.2.1 Testing spreadsheets and other mathematical packages

1. Which off-the shelf software packages (spreadsheets and others) are used for the numerical processing of measurement data?
2. What use is made of spreadsheets (in particular) to process measurement data in your area of expertise? Please indicate some example tasks, if possible.
3. Are you or colleagues aware of any limitations in the software packages used and/or in the in-built functions within these packages?
4. Do you or colleagues perform any testing and validation (both of in-built functions and spreadsheet solutions)?
5. Do you or colleagues seek (and receive) advice from software suppliers about the validity and/or applicability, accuracy and stability of the mathematical software they use?

3.2.2 Model Validation

1. In what ways do you or colleagues validate your models of measurement? Does (formal) model validation form part of your (or your colleagues') design review (in ISO 9000 terms)?
2. To what extent do model validation techniques provide more than pass/fail information?
3. To what extent are you (or colleagues) aware that an algorithm might be *mathematically* correct, yet have such poor *numerical* properties that much of the precision would be lost, were it to be implemented on a computer?

3.2.3 Measurement System Validation

1. To what extent do you or colleagues have measurement systems which contain embedded software, e.g. smart sensors, intelligent instruments, etc.?
2. In your experience, are measurement systems validated as complete systems, and if so by what means?
3. Do you or colleagues use any means of validating embedded software? Do you/they have to rely on supplier's claims that the software has been adequately tested?

3.2.4 Validation of Simulated Instruments

1. Are you aware of simulated instruments? If so, please give examples.
2. Do you believe that they have much to offer metrology (relative to cost) in your area of expertise? If they have, please indicate how.

3.3 Metrology Software Development Techniques

3.3.1 Software Development Methods

1. Do you or colleagues operate under an ISO-9001-like Quality Management System, where software development is concerned?
2. Do the current methods used give the reliability you require?

3. Do you find that maintaining old software is too expensive?
4. Does the cost of developing new systems seem reasonable?
5. What is your (or your colleagues') most pressing problem with software?
6. The ISO standard on software quality defines six key attributes (functionality, reliability, usability, efficiency, maintainability and portability). Which do you believe is most important?
7. How do you (or colleagues) check that the software is correct?
 - a. check the results by using another instrument
 - b. check the results by hand
 - c) use a mathematical tool/spreadsheet, etc.
 - d) other

3.3.2 Software reuse

1. Do you or colleagues employ software reuse as a means of reducing software maintenance costs?
2. Do you or colleagues use mixed-language programming? If so, what if any problems does this cause?
3. How, in your experience, are the problems of legacy software managed?
4. How is the Year 2000 problem being managed in your area of expertise?

3.3.3 Virtual Instruments

1. Do you or colleagues use virtual instruments? If so, what for?
2. Do you or colleagues use a particular development method for developing virtual instruments?
3. Are there any special problems with documenting, testing or maintaining the design?

3.4 *Support for Measurement and Calibration Processes*

3.4.1 Automation of Measurement and Calibration Processes

1. To what extent do you or colleagues use LIMS (Laboratory Information Management Systems)?
2. What other ways are used by you or colleagues to process calibration and test data?
3. What are the main advantages and disadvantages of the systems you use?
4. If you or colleagues developed/modified your LIMS in-house, how was this done?
5. How do you make sure that your systems adhere to appropriate standards and procedures, and are accurate and efficient for their users, your customers and your business processes?

3.4.2 Format Standards for Measurement Data

1. Do you or colleagues use (or need to use) standard data formats for measurement data?
2. Do you share measurement data with other organisations? If so, how is that data stored and/or transmitted?

3. In your field, is there a need for a common format for calibration records so one instrument can be calibrated in more than one country but still have a coherent and continuous calibration history?
4. In your field, is there a need for a common format for electronic exchange of measurement data?
5. Different measurement instruments and LIMS packages use different data formats - has this prevented you from using an instrument or package which you would otherwise have considered using?

Appendix 2: Glossary of Abbreviations

Abbreviation	Expansion
A/D	Analogue to Digital conversion (of a signal)
ASCII	American Standard Code for Information Interchange
CISE	Centre for Information Systems Engineering
DTI	Department of Trade and Industry (UK)
EA	European co-operation on Accreditation
EAL	European co-operation on Accreditation of Laboratories (now superseded by EA)
EC	European Commission
GUM	Guide to the expression of Uncertainty in Measurement [1]
IDL	Interactive Data Language, tool for Data Analysis and Visualisation
IMSL	(FORTRAN, C and Java) Mathematics and Statistics Libraries
ISO	International Organization for Standardization
JCGM	Joint Committee on Guides in Metrology (International)
LabVIEW	LabWindows with data flow programming interface
LabWindows	Data acquisition and instrument control package
LIMS	Laboratory Information Management System
MathCAD	General mathematics (particularly engineering) package
Mathematica	General mathematics package
MatLab	General mathematics package
METROS	Metrology Software environment
NIST	National Institute of Standards and Technology (USA)
NMI	National Metrology Institute
NMS	National Measurement System
NMSPU	National Measurement System Policy Unit (of DTI)
QMS	Quality Management System
SAS	General-purpose statistical analysis package
Sigmaplot	Curve plotting and fitting package
SMT	EC Standards, Measurement and Testing programme
SPSS	General-purpose statistical analysis package
SSfM	Software Support for Metrology
USNO	US Naval Observatory
Y2K	Year 2000 (millennium bug)

Appendix 3: Bibliography

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