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REPORT

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

INITIAL STATUS REPORT ON SOFTWARE ACTIVITY WORLDWIDE

FROM THE UK SOFTWARE SUPPORT FOR METROLOGY PROGRAMME

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1. Introduction to the SSfM programme

The UK National Measurement System Policy Unit (NMSPU) has 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 guidelines 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 completes 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 leverage its resources and impact.

2. This report

2.1 Scope

This report covers the breadth of software used in metrology, from instrument control through to theoretical simulation, from determination of fundamental constants to such applied tasks as geometric dimensioning and tolerancing. 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 report on the status of related activity world-wide at the beginning of the SSfM programme. Subsequently, an interim report will be produced to provide up-to-date status information to inform decisions in the programme. Input has been sought from metrologists and organisations around the world, including metrology institutes, standards organisations, certification agencies and similar bodies.

In addition to this status report, which looks at what is happening in mathematics and statistics in support of metrology across the world, companion status reports are being produced for the main metrology areas (mass, length, time, etc.). The UK National Measurement System Policy Unit is the direct customer for this work. However, A key requirement of the SSfM programme is that it should benefit work across metrology.

Given the broad definition of software in metrology, which corresponds with the definition used in the SSfM programme, the aims of the report is 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 UK Software Support for Metrology (SSfM) programme, and

b) draws conclusions concerning areas of overlap and/or synergies.

The survey questionnaire is to be found in Annex 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

Example questions from each section include:

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?....
2) Is there any programme of activity in your country/organisation which aims to study ... modelling 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 a bit deeper, looking at activity themes. It serves both

a) as a test of SSfM coverage (i.e., is there any key activity which is 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 draw out 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.

The NIST website has an excellent index of national metrology institutes 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, which has direct international responsibilities, all were either national measurement institutes or accreditation bodies.

Where email addresses were known, questionnaires were sent as Word 95 attachments. Otherwise, messages were sent to fax numbers, requesting email addresses. If these 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 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) indicated the address of the SSfM web home page, in particular the download area for Word 95 and PDF versions of the survey questionnaire
e) invited correspondents 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 2-3 weeks from the date of invitation or reminder.

4. General survey results

Formal replies were received from 14 of the 41 invitees. Each has agreed that his/her name and affiliation should appear in the report, hence they are listed in Table 1 below.

Table 1: Survey participants

Country	Organisation	Contact Name	Receipt Mode	Contact Mode
	CSIRO	Dr Mike Blanco	Email	Email
Austria	BEV	Dr Michael Matus	Fax	Fax
Brazil	UNIMEP	Dr Alvaro Abackerli	Email	Email
Denmark	DFM	Dr Lars Nielsen	Email	Email
Germany	PTB Berlin	Prof. Dieter Richter	Email	Email
Greece	EIM	Dr Chris L Mitsas	Email	Email
Indonesia	KIM-LIPI	Dr Husein Avicenna Akil	Email	Email
International	BIPM	Dr Richard S Davis	Letter	Fax
Ireland	NML	Dr Paul Hetherington	Email	Email
Italy	IMGC	Prof. Alessandro Balsamo	Email	Email
Japan	NRLM	Dr Isao Kishimoto	Email	Email
Singapore	NMC	Dr Sze-Wey Chua	Email	Email
South Africa	NML, CSIR	Dr Chris Matthee	Email	Email
Taiwan	ITRI	Ms Hui-Chung Ma	Email	Email

Furthermore, each has agreed to become an International Associate Member of the SSfM club, in order to be kept informed of developments within the SSfM programme.

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, the author met Prof. Norman Belecki of NIST and discussed 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 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 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.

5. Analysis of survey results

The survey responses were collated and entered in a Microsoft Access database for easier 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 relates to whether there is already a programme at the organisation/country which is equivalent to SSfM. Nine of the fourteen participants said there was not such a programme. Of the remaining five, it became clear that these organisations had either

a) sponsorship from industry to address particular topics within an SSfM-type 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)"
c) a major review of mathematics and software in preparation for third-party certification of its operations.

There appears to be only one such organisation (CSIRO) which has a reasonably comprehensive programme which is *not* for in-house development, or directly funded by industry.

Of those nine participants who said No, six had not considered setting up a programme such as SSfM. Of the rest, it would appear that winning resources had been a stumbling block. All nine participants believed SSfM could be beneficial, though two were less enthusiastic supporters. With regard to interaction, the picture was mixed: six of the nine wanted two-way interaction, the remainder were content just to receive the reports.

Few participants chose to comment on the programme, but the comments received were favourable. An example follows:

> *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 coming 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.* [CSIRO]

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) 10 had activity in Modelling Techniques
b) 6 had activity in Uncertainties and statistical modelling
c) 3 had activity in Visual Modelling and Data Visualisation
d) 3 had activity 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 is supported by supplementary questions on scope of the work.

The relatively low number of organisation 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 either from within the organisation (possibly budgeted), or from applied academic research funds. There is no instance of it 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 references[1] to programme outputs.

Another interesting feature is that such projects are generally undertaken by "metrologists" within the organisation. This implies that mathematics and IT staff would appear to be dispersed among metrology groups, or 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.

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

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[1] A notable exception is CMIS, which is part of CSIRO Australia, which provided a reference to its website.

appear that lack of activity might well be caused by lack of resource, rather than by lack of demand. This is confirmed when all four indicate their willingness to collaborate (in a manner as yet unspecified) 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 validation[2]. Seven of the organisations have at least some activity in this area, but again, this is largely focused on internal requirements, particularly on preparation for third-party certification of their operating practices, e.g., to ISO 9001.

There was no instance of a model validation project, though it was noted by four 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.

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 (we assume the sixth did not), and four of the five were willing to collaborate with the SSfM programme on this issue.

5.2.3 Metrology software development techniques

Only three of the fourteen had any project relating to software development methods. This was generally seen as an internal activity[3]. Of those that had not, one comment was that the software group was small and hence a formal methodology was not required.

Only one organisation 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.

Two organisations had a project addressing development of virtual instruments, but it became clear from the comments of one of the two organisations that the correspondent had mistaken virtual instrument for simulated instrument. Therefore, it would appear that software development for virtual instruments (in the National Instruments/LabVIEW meaning of the term) is not seen as presenting unique problems.

There were no replies to supplementary questions regarding funding, scope, etc., for existing projects. Three of eight organisations had considered such projects; all eight believe such projects could be beneficial, one noting that "the quality of the results depends on the software". Six of seven were willing to collaborate with SSfM project activity in this area.

Only one organisation ventured a reference to related activity[4].

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

[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 webpage.

5.2.4 Support for measurement and calibration processes

Four of ten organisations had activity on automation of measurement and calibration processes, one adding that it related to "automation of calibration and certificate generation". Only two of the ten had any activity on format standards for measurement data.

As regards funding, it appears as an internal activity, with "Technicians and Researchers" as customers.

There were no replies 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.

Only one organisation (ITRI) was willing to refer directly to its activity in this area, referring to its installation of a LIMS for supporting the automation of its measurement and testing services.

5.3 Project level

Since questions at this Level were more detailed, hence more time-consuming to answer, and 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 two participants answered all the 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

Five of the participants provided information on some of the phenomena, of which they have knowledge, modelled at their organisations. These include

a) dimensional phenomena
b) pollutants in the upper atmosphere
c) transfer functions of transducers, measuring instruments, piezo-electric actuators
d) optical tomography, biomagnetic fields, heat dissipation, accelerometer excitation, shearing interferometry
e) corrections for temperature and humidity

The models were based on "as much of the underlying physics as possible", though supplemented by "empirical polynomials and by differential equations which are able to take into account hysteresis effects" and where possible "implemented in standard mathematical software".

The main modelling concerns relate to

1) "the selected model is not as good as I think";
2) "understanding, simulation, controlling, solving inverse problems (it depends on the context)";
3) "the model should be rich enough to permit a full uncertainty analysis".

The last point provides strong evidence in favour of the observation made in Section 4.2.2.1 that uncertainty estimation and physical modelling are very closely linked.

5.3.1.2 Uncertainty estimation and statistical modelling

Ten of the fourteen participants were involved in uncertainties and statistical modelling. It could be argued that this means that ten of the participants are practising metrologists!

All use the GUM, though one participant also mentions EAL-R2.

Of the eight that expressed a view, three admitted to problems in applying the GUM. All of these three referred to difficulties with regard to statistical assumptions, two of the three had difficulties with software support and with difficulty of understanding. Interesting, this means that one organisation (ITRI) had problems applying the GUM relating to statistical assumptions, and claimed not to have difficulty in understanding it. Hence, it must be concluded that, for that organisation, the difficulty lies in the nature of the statistical assumptions in the GUM itself. As evidence of difficulty of understanding, one organisation points to the popularity of its internal courses for uncertainty estimation according to the GUM.

Three of seven organisations use confidence levels other than 95%, one referring to 99%.

The main concerns relating to uncertainties and statistical modelling are very informative. The list of concerns from the five organisations which expressed a view is as follows:

1) "the GUM is not general enough to cover many common measurement situations."
2) "gaining information from measurement data, parameter estimation, uncertainty estimation"
3) "how do we use the statistical tools correctly?"
4) "the number of parameters in uncertainty budgets"
5) "that they reflect reality"

The first and last of these relate to dissatisfaction with the GUM. The first might be addressed by extensions to the GUM (now being considered by the JCGM). The last falls in the domain of model validation: by definition, if the model is suitable, the associated uncertainty estimates will be believable. The other points relate to difficulty in practical uncertainty estimation, from the viewpoint of a metrologist who is not overly concerned with the details (2), to difficulties with the complexity of the analysis and available tools (4) and 3), respectively). Each of these indicates a weakness of the GUM and allied 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

Five of nine participants are involved with sensor fusion, the same proportion in fusing data by location etc. Four of nine use intercomparison between measurements for online fault and error detection/diagnosis, and a further participant is soon to join that group. Two organisations attempt to incorporate predictive and/or archive data with measurement data. Four organisations are looking to incorporate qualitative and image data with quantitative measurement data. The concerns relate to

a) "the errors sometimes do not come from the normal distribution. When we check against the Measurement Assurance Program (MAP), the measurement standard has drifted"
b) "use of bought-in software and how it combines measurement data"
c) "When weighing data from different sources, generally, we take the advice of Consultative Committees composed of experts"

Generally, data fusion is used at the larger laboratories. Taking the concerns listed above in turn, data fusion 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.

5.3.2 Validation and testing

5.3.2.1 Testing spreadsheets and other mathematical packages

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

1) MatLab and Mathematica
2) Excel, Mathematica, MatLab, LabWindows, C/C++
3) IMSL, IDL, Statistical software packages, in-house bespoke software
4) Excel, in-house bespoke software
5) Data-acquisition: LabVIEW, HP – VEE, Visual Basic, Visual C, Turbo 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

The software can be classified as follows:

a) Office suites, particularly spreadsheet packages: overwhelmingly Microsoft Office and Microsoft Excel, respectively
b) general numerical and symbolic packages: MatLab, Mathematica, MathCAD
c) statistical/graphing packages: IDL, SAS, SPSS, Sigmaplot
d) data acquisition: LabVIEW, HP -VEE
e) bespoke: (Visual, Turbo) C/C++, IMSL, Visual Basic

Two of the six 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 used of spreadsheets. Of the remainder, the main use was for computing combined uncertainties according to the GUM. One organisation also used spreadsheets "to record the calibration history of instruments". The latter 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.

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 is of concern because such functions might be expected to used in estimating 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 might vary.

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.

5.3.2.2 Model validation

It became clear from many of the replies that participants see close links between model validation and both modelling and measurement system validation. Two of the six participants who expressed a view on model validation (intend to) incorporate model validation formally as part of their quality system, with one identifying it as part of method validation in the context of ISO Guide 25. Methods of model validation include:

1) "compare with experimental data"

2) "use the scientific method, i.e., try to establish the limitations of the model by experiments"
3) "use two or more measurement methods to check the validity of each of the models of measurement"
4) "submit to peer review".

All but the last of these blurs the distinction with measurement system validation.

The degree of information and analysis from model validation is variable. Comments include

a) "useful for diagnostics"
b) "if the models fails, you know where it fails, and some times you get a hint why"
c) "Models are proved whether they are fit for the problem using physical and mathematical properties"
d) "tests are as full as possible, but limited by resource constraints"

Note that c) implies that some questions of model validity can be resolved by numerical (non-experimental) means and that d) implies that model validation is sometimes limited, not by technical difficulties, but by resource limitations.

Of the five participants who replied to the question, all are aware of the distinction between model correctness and (software) implementation correctness. One adds that the software generally has 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 seven participants who replied, 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.

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) "statistical process control".

Note that methods a) to c) relate to traditional calibration and traceability techniques within metrology. Method d) is based on a 'bottom-up' systems approach, which requires deep analysis of the system modules and interfaces to be effective. Method e) is appropriate for routine measurement tasks.

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

> *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/spot checks, while one participant notes that validation of embedded software is an active research topic in his organisation.

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 they 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 they

> *... allow the user to simulate their 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 nine 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 redesigns of software developed in-house". This trade-off of costs is examined further in the next question, when six of seven participants believe developing new systems is reasonable, though expensive. One participant makes the point that

> *After all, you do not develop if it does not pay off within a reasonable time scale.*

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

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/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 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, namely 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 of 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) Does it do what I want?
3) Will it cost a lot over its lifetime?

Perhaps even more interesting is the lower priority given to other attributes, such as usability, efficiency and portability. This 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 growth of computer performance has outstripped need in many areas of metrology in the recent past. This 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 quantum 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 five of the seven 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 runtime system needs to treat the legacy software as a black box, hence the programmer has less control over program execution. Not alone does the programmer need to know several languages, he/she 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) "we recommended a strong software documentation rule for software developed at [the organisation] to avoid problems in future. It became part of an internal guide"
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).

Four participants were willing to divulge their plans for becoming millennium-compliant. Strategies include

1) "[We are working] with the help of the best advice we can get. We have reason to believe our level of risk is minimal"
2) "We taking part in a project with our government on this subject."
3) "Special considerations, declarations of conformity by vendors, etc."
4) "The system manager has studied potential Y2K problems"

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 OK, although the same cannot always be said for legacy software. Organisation 4) has chosen to view this as a management problem, and 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.

5.3.3.3 Virtual instruments

Only three of six who replied make use of virtual instruments. Uses include

1) "to set-up computer automated measurement facilities"
2) "to control the processing of the data."
3) "occasionally, e.g., for 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 use 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.

No participant identified a particular development method for developing virtual instruments, apart from the use of National Instruments' software tools. Nor did they consider 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 six 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.

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/ processing; embedded software for collection/ 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 automatic 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.

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

1) "Errors are spotted by cross-checking between steps. The main disadvantage is that it is time consuming"
2) "Too many data have to be entered more than once. We are trying to eliminate that right now."
3) "Purpose-written software/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 do backups"
4) "Advantage: components are well understood. Disadvantage: development is time-consuming"
5) "The main advantages are to manage all of the measurement areas in our labs, and to offer better services to our customers. There are no special disadvantages now."

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 implementation might have had some initial difficulties, but that the system has settled down and is now satisfactory.

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

1) "Plan to combine 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 stream-lined mass calibration system"
2) "developed using a standard Excel spreadsheet. Software developed using C++"
3) "The members of our Quality Assurance Section develops/modifies our LIMS in-house."

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) "We set the specification in order to meet requirements from our self, our customers and the accreditation/certification body and then verify that the specifications are met."
2) "We have established standard documents."
3) "Consultation with peers"

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 benchmarking.

5.3.4.2 Format standards for measurement data

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

a) "Time and Frequency"
b) "biomagnetical and bioelectrical measurement data"
c) "Need data for calibration history (at least 5 years' worth for periodic recalibration); use comma-separated variable for transfer within the organisation"

Time and frequency is a well-known example, since time transfer is an important function of many national metrology institutes. Bioelectromagnetic data transfer is probably a less well-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.

Six of eight 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 email attachments, in common database formats, etc. One participant referred to the agreed protocol for time transfer, which the organisation uses to communicate with BIPM and USNO.

Five of seven participants indicated a need for a common international format for calibration records (picking up use 3) 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 have a need for standard data formats argued that data formats should be standardised at the record level, not at the bit level. As an example of their current use, another participant cited regulatory bodies such as the Federal Aviation Administration in the USA.

Six of eight participants already use a common format for electronic exchange of measurement data, including one participants 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

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. Thus 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 started during the consultation exercise for this report should be strengthened. 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. This gives some hope that the problems and solutions might be similar, and hence that international collaboration would be mutually beneficial.

There are also 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 metrology needs of the metrology areas within the UK's National Measurement System.

Annex 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?

2. 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 you 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 you 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 you 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 process, 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?

Annex 2: Glossary of Abbreviations

Abbreviation	Expansion
A/D	Analogue to Digital conversion (of a signal)
ASCII	American Standard Code for Information Interchange
DTI	Department of Trade and Industry (UK)
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
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)