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Report

to the National

Measurement System

Policy Unit, Department

of Trade & Industry

INTERIM STATUS REPORT ON THE OPTICAL RADIATION AREA

FROM THE SOFTWARE SUPPORT FOR METROLOGY PROGRAMME

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Software Support for Metrology

Interim Status Report on the Optical Radiation Area

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Abstract

This report describes the status of the mathematics and software used to support the Optical Radiation area of metrology, particularly as used within the NMS Optical Radiation programme. This 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 more than one metrology area. This report, therefore, not only identifies problems to be tackled and best practice to be disseminated by the SSfM programme, but also if appropriate possible future Optical Radiation programme projects applying SSfM outputs to specific problems in the Optical Radiation area.

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Contents

1. Introduction

The purpose of this status report is to inform the NMS Software Support for Metrology (SSfM) programme (1998-2001) about the status of the mathematics and software used to support the **Optical Radiation** area, concentrating on what is used within the NMS **Optical Radiation Metrology programme**. This and the companion status reports for the other metrology areas will inform the formulation of the next SSfM programme (2001-2004). It may also lead to appropriate linkage between the Optical Radiation Metrology programme and the SSfM programme.

The SSfM programme is an underpinning programme that provides generic support in the use of software and mathematics to the NMS programmes for each metrology area. For details of the programme, its expected deliverables and the results already produced, see the SSfM web site: http://www.npl.co.uk/ssfm/.

The NMS programmes for specific metrology areas provide metrological support to industry. The SSfM programme in contrast has relatively little direct impact upon industry, although there is some as evidenced by the SSfM Club membership. This relationship is depicted in Figure 1. It is because of this relationship that the Status Reports concentrate primarily on the use of software and mathematics in the other NMS programmes.

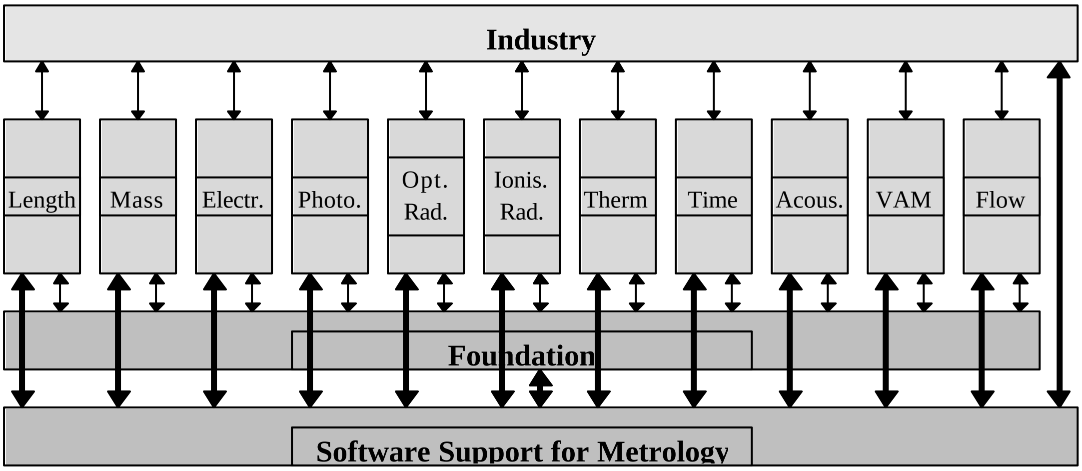

Figure 1. Relationship of SSfM to other NMS programmes and industry

In particular, this report addresses each of the themes within the SSfM programme and describes the status concerning the topics covered by each of the relevant projects. It also considers whether there are any important software or mathematics issues in the Optical Radiation area which are not addressed by the current SSfM programme or which need to be taken further in the next SSfM programme.

This report is an update of an initial restricted status report produced in December 1998. That initial report was one of a set of restricted status reports which were synthesised into an overall status report for all metrology areas [5]. A summary of the differences from the initial Optical Radiation status report is provided at the end of this report.

2. Scope of the Area Covered

The NMS Optical Radiation Metrology programme covers the following technical themes:

a) improved underpinning of primary optical radiation scales, including those for visible light and colour;

b) maintenance and dissemination of optical radiation scales, including those for visible light and colour;

c) development of improved transfer standards;

d) development of new or improved measurement techniques and facilities;

e) development of new scales of measurement for vision and the appearance of surfaces.

In addition, as usual in NMS programmes, there is also a technology transfer theme.

Optical Radiation at NPL involves the following services:

i) measurement of visual and optical properties of materials that transmit, reflect or absorb light;

ii) measurement of visual and optical properties of sources of optical radiation;

iii) measurement of detectors of optical radiation;

iv) calibration and production of certificates;

v) consultancy, advisory and training services.

There is optical radiation involvement in both the Photonics and Foundation NMS programmes, but these aspects are covered in the SSfM Status Reports for those programmes, and hence are excluded from the scope of this report.

Software is used extensively, chiefly for data manipulation, and mathematical problem solving. Typical applications are as follows:

1) interpolation between points using simple mathematical routines and models;

2) least-squares fitting algorithms to determine best fits to data points;

3) mathematical manipulation, weighting and analysis of spectral measurements on sources and materials;

4) simple statistical analysis;

5) uncertainty analysis (involving correlated quantities);

6) modelling of integral transforms for determination of diffraction patterns produced by apertures, ray tracing within cavities, etc.

The Optical Radiation Metrology programme has concerns which relate to each of the themes of the SSfM programme:

a) improvement in uncertainty estimations (SSfM Theme 1);

b) numerical software testing (SSfM Theme 2);

c) metrology software development techniques (SSfM Theme 3);

d) support for measurement and calibration processes, particularly the use of Laboratory Information Management Systems (LIMSs) (SSfM Theme 4).

3. Modelling Techniques

3.1 Methods for Modelling Measurement Data

3.1.1 Types of data

There are three categories of measurement data sets:

1. discrete measurement data, which means:
   a) data obtained by sampling a discrete variable: e.g., a variable that may take only integer values such as in counting processes, and
   b) data obtained by sampling a continuous variable.
2. continuous measurement signal, which means an analogue signal prior to any analogue to digital conversion, which would result in data of type 1 b).
3. hybrid measurement data composed of both discrete and continuous data sets.

In the Optical Radiation area, many of the measurements made are expressed in terms of values at discrete wavelength points. However, this is simply a convenient way of expressing what are actually continuous (but not necessarily smoothly or predictably varying) quantities which vary with wavelength across the spectrum. Sometimes, when spectral techniques are used, the raw data is an analogue signal. This analogue signal may be used directly as a continuous signal or may be fed into an A/D converter, resulting in large amounts of discrete data. In addition, occasionally, hybrid data may be needed for some applications.

3.1.2 Modelling

Types of model

There are three categories of model:

1. discrete models in which the outputs of the measurement system are related to measurements of its inputs by a system of algebraic equations;
2. continuous models in which the outputs of the measurement system are related to measurements of its inputs by a system of differential equations;
3. hybrid models in which the outputs of the measurement system are related to measurements of its inputs by a system composed of both algebraic and differential equations.

It is appropriate to distinguish here between the nature of the model and the approach to solving the model (which for a continuous model typically also involves solving algebraic equations).

Given infinite precision arithmetic, the set of equations derived from a discrete model can be solved exactly. This is not the case for a continuous model which typically requires approximations to be made, for example, in terms of domain discretisation.

Models used in the Optical Radiation Metrology programme

Examples of modelling used in the Optical Radiation Metrology programme include:

a) Least-squares fitting of polynomial functions;

b) Statistical modelling for uncertainty estimation;

c) Interpolation of data values and subsequent analysis, including some statistical calculations;

d) Processing of spectral detector data;

e) Fourier transforms and their inverses.

Modelling has had some success, particularly in areas where the physics is well understood.

Where there is a need to interpolate between data points, this is frequently done empirically, not based upon proper modelling of the physics. There is concern that as uncertainties are reduced, by reduction in systematic errors, problems with interpolation will begin to show up. Thus, there may be a need for a better approach towards interpolation based upon a model of the physics involved.

In some situations (e.g. when calibrating the wavelength scale of a spectrometer using a small number of emission lines from a discharge lamp) it is not possible to develop a suitable model of the physics; in such cases there is often a need to fit splines to the data.

There is a serious research and development problem regarding the uncertainties in some types of Optical Radiation measurement (e.g. colour measurements). The issue is how to integrate an array of spectral data with a weighting function. Three numbers are obtained, for the three primary colours, rather than many spectral points, but there is no agreed procedure for how to assess the uncertainty associated with these three numbers from the uncertainties in the spectral values. See the related case study suggested in section 7.2.

See Appendix 3 for a summary of the characteristics of typical modelling used in the Optical Radiation area.

3.2 Uncertainties and Statistical Modelling

The estimation of uncertainty is important in all work in the Optical Radiation area. Some of the most complex analyses relate to the estimates of uncertainties for continuous quantities such as the distribution of power output with wavelength and the subsequent calculation of integrated, spectrally-weighed data (see above). Uncertainties in wavelength calibration of the spectroradiometer, linearity of the detectors, noise, stray light, voltage calibration of the digital voltmeters etc. can all make significant contributions to the uncertainty budgets for such measurements.

There are some legal issues related to uncertainties, where the measurements have safety and cost implications.

3.2.1 Derivation of statistical models

Measurement uncertainty estimation in the Optical Radiation area follows the principles of the ISO Guide [1] (GUM).

Disseminated measurement uncertainties are typically at around the 1% level, which is comparable to those claimed by other NMIs but often higher than customers require. The level of agreement seen in international comparisons generally supports the claimed uncertainties. There is some instability of results within the error bars which, although to be expected, still worries some customers. Changes of scale, even within the uncertainties, is generally unwelcome to customers. There therefore needs to be very robust analysis before such changes are made. Nevertheless, several key changes to scales are expected to be made in the near future.

In some areas (e.g. the calibration of the colour temperature of lamps), there is no rigorous treatment of correlation among the errors. It is considered that, despite efforts to reduce uncertainties, there may be an overestimate of the uncertainties in such areas and that a more rigorous treatment of correlations could reduce the uncertainties even further. Results from intercomparisons with other NMIs indicate that NPL scales for these quantities agree well with those elsewhere. There is also some recognition internationally of a need for more robust treatment of the statistics.

3.2.2 Determination of the statistical distribution of measurement results

Within the Optical Radiation area the statistical distributions of measurement results are generally considered to be Gaussian, apart from a few cases where a uniform distribution is assumed. These assumptions are not known to cause any real problems.

3.2.3 Levels of confidence other than 95%

Results are usually quoted at a level of confidence of 95%, although this is often calculated simply in terms of two standard deviations. Some research and development work, however, uses only one standard deviation (equivalent to 68% confidence).

3.2.4 Supporting software

Statistical calculations are usually made using spreadsheets, typically Excel, and their in-built functions (e.g. LINEST).

3.2.5 Supporting documentation

The ISO Guide to the Expression of Uncertainty in Measurement is the base document in the area of uncertainty estimation. UKAS document M 3003 [2] is also used in the Optical Radiation area in relation to the measurement and calibration services provided.

3.2.6 Training

Basic training in uncertainty estimation, such as that provided by UKAS, is sufficient for most staff in the Optical Radiation area. However, in one or two cases, training in techniques to handle correlations and in robust statistics may be useful in future.

3.3 Visual Modelling and Data Visualisation

Visualisation is seen as potentially valuable in relation to the measurement of appearance properties, such as texture, in order to deal with 4^{th}, 5^{th} and 6^{th} dimensions. The work on appearance is very new, so it is too early to develop a case study in this area, but those working on appearance may well benefit from the output of the SSfM Visual Modelling and Data Visualisation project or related projects in the next SSfM programme. The timescale for this potential application of visualisation is about 5 or 6 years.

3.4 Data Fusion

3.4.1 Applications

The following list identifies the typical areas of application of data fusion, with an indication of the extent to which each is applicable to the Optical Radiation area. Note that there has been some use of neural networks in this field in the past (e.g. in the development of models of the human visual system), but not at NPL.

1. *Processing and reconciling measurements from an array of sensors*

   Photodiode and CCD arrays are being used increasingly by the optical radiation industry, for spectral measurements and image processing applications. Indeed one project within the Optical Radiation Metrology programme deals specifically with the development of best practice for key aspects of the calibration of such systems, particularly for spectrometry. Data fusion is likely to be of only limited relevance to the analysis of spectral data, but it may be applicable to image processing (see also point 6 below).

2. *Patching together measurements corresponding to different sets of parameters*

   This does not seem to be applicable to the Optical Radiation area.

3. *Fault and error detection/diagnosis by multivariate statistical process control*

   This does not seem to be applicable to the Optical Radiation area.

4. *Combining results from several very different measurement processes*

   This does not seem to be applicable to the Optical Radiation area.

5. *Dealing with predictive data from models, or historical or archive data, in tandem with current measurement data*

   There are some projects in the Optical Radiation area for which this is applicable e.g. work which compares results from colour specification models with others obtained by human experimentation and measurements of the performance of filtered detectors designed using models of the absorption, reflection and diffraction effects of various components.

6. *Handling numerical, image, and/or qualitative data within a single framework*

   This is potentially applicable to the analysis of appearance parameters, for example to measure how healthy hair is from its appearance.

3.4.2 INTErSECT awareness

There is good awareness of INTErSECT within NPL, including within the Optical Radiation area. There are already planned collaborations in this area within INTErSECT.

4. Validation and Testing

4.1 Spreadsheets and Other Mathematical Software Packages

4.1.1 ‘Off the shelf’ software

Several different ‘off the shelf’ mathematical software packages are used in the Optical Radiation area: particularly, Excel, LabVIEW and MathCad.

4.1.2 Spreadsheets

Spreadsheets, particularly Excel, are commonly used for statistical modelling for uncertainty estimations. Generally, the spreadsheets used are not particularly complicated, but they do rely on in-built statistical functions, such as mean and standard deviations, as well as linear fitting routines such as LINEST. Processing is done by way of cell formulae and by manipulation by macros.

4.1.3 Awareness of limitations

Within the Optical Radiation area, there is awareness of the potential limitations in spreadsheets and other software packages arising from inaccurate or unstable numerical algorithms.

4.1.4 Testing and validation

Testing and validation of spreadsheets and other software packages is usually by comparison of results with those obtained by hand calculation or other software.

4.1.5 Supplier advice

NPL metrologists in the Optical Radiation area use off-the-shelf software which is recommended by NPL's IT Support Unit and do not see a requirement to demand additional assurances from suppliers of this software that it is fit for purpose. Where bespoke software is purchased, the required performance is specified.

4.2 Model Validation

There is a very high awareness of model validation, and an acceptance that it is vital to the success of modelling in the Optical Radiation metrology programme. In particular, it is an issue as new models and methods of modelling are considered. Model validation is usually made by comparison with previous approaches.

4.3 Measurement System Validation

4.3.1 Embedded software

Most modern instrumentation contains embedded software and this is certainly true in the Optical Radiation area, where embedded software can be considered endemic in the measurement instrumentation used (e.g. digital voltmeters). Since this software cannot generally be accessed by the user such equipment tends to be validated as part of the complete measurement system.

4.3.2 System validation

Measurement systems in the Optical Radiation area are tested as complete systems. The users expect to notice anomalous results if the system is not performing correctly. The results are compared against previous results and data from international comparisons. They are also checked for self-consistency. In the spectrophotometry area, NPL's own reference materials are used to validate the systems.

4.3.3 Reference data

Reference data sets that are provided with embedded software are used for validation purposes.

Previous data sets (for which the right answers have been calculated) are used to validate the measurement systems.

4.3.4 Validating embedded software

There is a general lack of user validation of embedded software which is supplied with the hardware (because this cannot be accessed by the user) and this means that there is no detection of any errors in the outputs that might be caused by software errors.

4.3.5 Supplier assurances

In general, in the Optical Radiation area, assurances are not requested from suppliers of commercial software packages, although assurances of adequate testing are required from suppliers of bespoke software (see section 4.1.5). Spreadsheet functions are generally assumed to operate correctly, a view which has been reinforced by the occasional comparisons which have been made with results obtained using other packages or systems.. LabVIEW has not been validated by users in the Optical Radiation area; the supplier is relied upon to have got it right. Of course, the continuing successful use of the software confirms and increases the confidence that users have in it.

4.3.6 Supplier validation of embedded software

Suppliers should validate embedded software as part of the design and implementation process. Current recommendations on software qualification require a ‘design qualification’ to verify that the design meets requirements; this is necessary but not considered sufficient. Most suppliers use a specification-design-code-test process through implementation; in conjunction with a design qualification, the specification/test pair constitutes validation. In addition, software needs to be tested in situ and under normal performance conditions.

Development and testing in general are almost certainly best carried out within recognised software development systems, such as TickIT, which allow suppliers to choose their own processes to achieve fitness for purpose.

4.3.7 Access

Ideally, scientists should have sufficient access to embedded software to satisfy themselves that it meets their own requirements. Unfortunately, manufacturers do not generally provide such a facility. Comments from those involved in the Optical Radiation area suggest that they are satisfied with their validation of the software by checking the outputs of the measurement system; hence, they do not see that access to embedded software is a particularly important requirement.

4.4 Validation of Simulated Instruments

There is currently no use of simulated instruments within the Optical Radiation area, although there is some use of simulation in related work in the Foundation programme. Furthermore, there is little likelihood of being able to apply the ideas of the Virtual Co-ordinate Measuring Machine within this area.

5. Metrology Software Development Techniques

5.1 Software development methods

5.1.1 Software Quality

1. Quality systems

NPL is certified to ISO 9001 plus TickIT, so any software NPL sells is produced in accordance with the requirements of TickIT. Although much of the bespoke software used within the Optical Radiation area would not meet the requirements for new production software (software integrity level 3), because it is generally production software produced before the introduction of a formal quality system (i.e. software integrity level 3 extant), it has been validated in practice over several years of operation. New software is developed according to NPL’s quality management system, complying with ISO 9001 and TickIT but not necessarily to software integrity level 3 if the software is only for use within NPL.

Sometimes, new software is developed by external software specialists using LabVIEW. Although this has produced good results in terms of cost, timeliness and quality, the lesson is that considerable effort needs to be put into writing the functional specification to ensure that the requirements are tightly specified. Indeed, more training on how to write functional specifications would be helpful.

Where new software is developed in-house, the discipline of using the quality system has improved documentation, particularly the specifications.

2. Reliability records

Where the reliability of software impacts the quality of a measurement service, software reliability records are kept. However, no formal records of software reliability are kept for software used in the research and development activities in the Optical Radiation area beyond (usually) notes in lab-books.

3. Reliability

The methods used for checking software reliability are considered to provide sufficient reliability appropriate to the use to which particular software is put. There is, however, concern over the reliability of some corporate software, such as certificate macros.

4. Version Control

Configuration and version control of software are used consistent with the requirements of the NPL quality management system. This is important if results need to be reproduced.

5.1.2 Management issues

1. Maintenance

Legacy software developed for instrument control of old hardware needs to be maintained for the life of the hardware. This can potentially give rise to the usual problems associated with maintaining legacy software: inadequate documentation, loss of contact with the original software developer, and use of obsolete languages for which training is no longer available. However, in practice, good quality support has been available for maintaining most of the legacy software; instead, the main problem found with continued use of legacy software is its slow speed. The current Optical Radiation Metrology programme includes the updating of much of the legacy software to improve its speed and reliability and bring it fully in line with the requirements of the NPL quality management system.

2. Development costs

Current software development costs are considered to be reasonable. However, the quality of service provided by the software developer is considered to be more important than the initial development cost, because it is recognised that the effectiveness, reliability and flexibility of the software all have a major impact on the lifetime costs of the software. As a result, some software is developed externally, some by software professionals within NPL, and some by the scientists themselves.

3. Problems

The main problem is that some of the software used requires too much specialist training. It is considered important that the scientists should be able to make effective use of software without having to continually call upon the services of professional software engineers. To obtain more user-friendly software, there will need to be better requirements capture at the outset.

There have also been problems with some corporate software, such as certificate macros, being delivered late and inadequately tested.

4. Quality attributes

The most important software quality attributes in the Optical Radiation area are reliability and usability.

5. Risks

The importance of software risk analysis is recognised. The risks from software errors in the Optical Radiation area are highest in the measurement services provided, since this is where any mistakes would be most visible to the 'outside world' and where reliance on automated (software-controlled) systems is highest.

5.1.3 Technical issues for software developers

1. Development methods

Developers use both the V model (design-code-test) approach and prototype refinement. The V method is sometimes used to develop a working prototype and then that prototype may be refined as requirements change.

The main languages used in the Optical Radiation area are as follows:

1) HT-Basic, BBC Basic, Quick Basic and Commodore Basic, particularly in legacy software for instrument control;
2) Visual Basic, for instrument control;
3) MathCad, for simple algebraic manipulation;
4) Pascal, for data processing and manipulation;
5) SQL statements and configuration utilities for the LIMS;
6) LabTalk, the input language of LabVIEW, for instrument control (see section 5.3).

There is a gradual shift towards using LabVIEW or Visual Basic in new software for instrument control, although there are cases where this is either not possible or inappropriate e.g. for control of some of the spectrophotometers which have their own, in-built, programming language.

2. Software testing methods

Checks that software is correct are carried out by verifying results by hand and/or using a spreadsheet. Software is often checked by isolating parts of the software at places which form a natural break or interface in the calculation.

3. Independent testing

Instrument control software is tested in combination with the hardware. Independent testing of such software is rarely considered practical.

4. Development problems

The scientists working in the Optical Radiation area are generally satisfied with their current software development methods, reporting that they are not aware of any significant problems.

5. NPL Measurement Good Practice Guide 5, Software in Scientific Instruments

The scientists working in the Optical Radiation area are not generally aware of NPL Guide 5. The software professionals within NPL are very much aware of it and do use it as appropriate. It is not clear whether or not the external software developers used in the Optical Radiation area are aware of NPL Guide 5.

5.2 Software reuse

5.2.1 Management issues

1. Importance

Generally, externally-supplied HT-Basic and LabVIEW instrument drivers are used where possible and appropriate. Software is re-used extensively, partly as a way of reducing maintenance costs.

2. Mixed language programming

Much of the programming can be regarded as sequential mixed-language, in the sense that it involves development of results in one language, followed by processing of the results in another. Commonly, the second "language" is actually Excel, although sometimes LabVIEW is used for the processing. There are two reasons for this approach:

a) the pre-processing is often done by trusted legacy software written in a language which is now considered obsolete (e.g. HT-Basic); or

b) the hardware may come with its own programming language which is not suitable for the further processing of the results.

3. Responsibility

The details of software reuse and mixed language programming tend to be left to the scientists concerned or their suppliers. The use of LabVIEW or Visual Basic is, however, a management policy for new instrument control software in much of the Optical Radiation area, where this is possible and appropriate. Examples of situations where LabVIEW or Visual Basic would not be used include:

a) where similar software is already available which has been written in another language and on which the new software can be based;

b) for the control of instrumentation or systems which have their own, in-built, programming language.

4. Legacy software

Most of the legacy software is instrument control software, e.g., written in BBC or HT Basic, which is used to control old instruments. There is still some need for maintenance and further development of such software (e.g. when it becomes necessary to incorporate a new piece of instrumentation or to improve the reliability of the measurements).

5. Year 2000

The Year 2000 problem has been recognised for some time. NPL has a task group working on this issue, testing every piece of appropriate equipment. A Y2K co-ordinator has been appointed for the Optical Radiation area and he has ensured that all instrumentation has been reviewed to assess the risk and identify items which might cause problems. No major problems have been identified and it is not anticipated that Y2K issues will have significant impact on the delivery of NMS milestones.

5.2.2 Technical issues for software developers

1. Producing similar programs

When it is necessary to produce a program very similar to an existing one, any of the following approaches may be used depending upon circumstances:

a) copy the existing program and make the changes needed;

b) add an additional module to the existing program to cater for small changes;

c) start from scratch using an appropriate language (often LabVIEW), for instrument control software which was previously produced in an old development environment.

All these approaches are used in the Optical Radiation area.

2. Software reuse strategies

As more instrument control software gets written in LabVIEW, the scope for software reuse will increase. Common Virtual Instruments are readily available for downloading from the Internet. There are separate sites for ones produced by National Instruments and ones produced by third parties. There is an implication, but no guarantee, that the ones produced by National Instruments have been validated and hence should be preferred.

3. Extent of mixed language programming

There is little true mixed language programming in the Optical Radiation area, only that described above in section 5.2.1 item 2.

4. Year 2000 problems

No significant Y2K problems have been identified with instrumentation used in the Optical Radiation area. With all bought-in software, the scientists concerned are relying upon the suppliers to fix any Y2K problems that those packages contain.

5.3 Virtual Instruments

LabVIEW is being used increasingly for applications such as instrument control. An example of this would be control of measurements taken from a Digital Voltmeter. There are no perceived problems with the approach and it is expected that it will soon become the dominant approach used for new instrument control software in much of the Optical Radiation area.

Software development for some instrument control in LabVIEW is outsourced. The specification is developed in-house (typically 3-4 days work) and this is passed to the developers who produce the code. The software is tested in-house and bug-fixes and enhancements may be done in-house or are passed back to the developers, as appropriate. This method of operation relies on the developers gaining an understanding of the experimental application so they can interpret the requirements reliably. The developer must also know how the LabVIEW instrument drivers are accessed, especially as the drivers may have been developed in-house. This has proved to be very cost-effective where the developer has achieved a close working relationship with the scientists involved.

Instrument control software is tested at the level of individual software components (for LabVIEW these are components of virtual instruments (“sub-VIs”)). The software is designed so that the components are stand-alone and can be tested and demonstrated in isolation.

Current LabVIEW training courses, run at NPL or in Reading, are considered to be quite good and sufficient for the needs of the Optical Radiation area.

6. Support for Measurement and Calibration Processes

6.1 Automation of Measurement and Calibration Processes

Over the past few years, a LIMS has been developed within the Optical Radiation Metrology programme, but its routine use in the measurement and calibration services has only recently begun in earnest, following a period of about 6 months during which it was run in parallel with the previous, paper-based system. This development was begun prior to the NPL corporate study of LIMS, and provided considerably input to this study. Indeed the collaboration is continuing, following the corporate decision to use the same commercial package, Matrix Plus. The Optical Radiation LIMS development has tried to accommodate more complex requirements than those likely to be required corporately, and further refinement of the system is taking place within the current Optical Radiation Metrology programme. The experience to date is that it is important to keep field definitions flexible, avoiding over-constraining them. In contrast, the NPL corporate LIMS is seen as being too simplistic for use with Optical Radiation measurement services. A remaining concern with the Optical Radiation LIMS is how to handle non-standard (bespoke) measurement services. It has been decided that it is inappropriate to try to use the full functionality of a LIMS for these measurement services, although less ambitious automation within LIMS is being used to beneficial effect.

6.2 *Format Standards for Measurement Data*

6.2.1 Need for standard data formats for measurement data

There is no apparent need for any standard formats for measurement data used in the Optical Radiation area. The use of Excel for processing measurement data is seen as diminishing the need for format standards for the data. In other cases, the formats used are determined by the software packages which operate on the data.

6.2.2 Need for sharing measurement data with other organisations

Measurement data from the Optical Radiation area is shared with other NMIs particularly in key comparison exercises. In these cases, simple text files and Excel spreadsheets are used at present, and there is doubt that any further sophistication is necessary.

6.2.3 Need for a common format for calibration records

There is no apparent demand for a common format for calibration records.

6.2.4 Need for a common format for exchange of measurement data

There is no apparent need for a common format for electronic exchange of measurement data.

6.2.5 Different data formats

There are currently no identified problems with the different proprietary data formats found in different measuring instruments.

7. Suggestions for Future Activities

7.1 Expected Benefits of the SSfM Programme

The areas of the SSfM programme which are most likely to benefit the Optical Radiation area are modelling techniques (interpolation of data values based upon modelling the physics), guidance on uncertainty estimation (for handling the integration of weighted spectral data, correlations, and interpolation between data points), visual modelling and data visualisation (for use with appearance), data fusion (also for use with appearance), the results of testing relevant software packages, and guidance and training on developing virtual instruments. However, it is recognised that the benefits expected in each of these areas, with the exception of uncertainty estimation, are either relatively slight or else several years away.

7.2 Case Studies and Feasibility Studies

There is a problem in how to deal with arrays of equally spaced spectral data that have to be integrated with a defined weighting function, particularly relating to the evaluation of uncertainties. The problem is compounded by issues of error correlation. Similar issues apply when trying to assess the uncertainty associated with measurements made by a detector which is designed to follow a defined weighting function (e.g. a photometer matching the response of the eye, or a colorimeter seeking to measure primary colours) but where the match is not perfect. This seems to be a good candidate for a case study.

In addition, it is clear that, within the Optical Radiation area, there is valuable experience in the use of LabVIEW and in the development of a LIMS. These experiences are likely to benefit the SSfM competitively tendered projects on “Virtual Instruments” and “Automation of Measurement and Calibration Processes”, possibly providing useful case studies.

7.3 Future SSfM Topics

There is scope for further work in the next SSfM programme on visual modelling, image data processing and data visualisation, and on data fusion, both applied to the measurement of appearance, probably as feasibility studies.

7.4 Future Optical Radiation Metrology Programme Topics

The uncertainties problem identified above in 7.2 is an unsolved problem to which the SSfM Uncertainties Best-Practice Guide will be particularly applicable. It is a problem requiring approaches outside the scope of “mainstream GUM” and the Best-Practice Guide is particularly directed at giving advice on such problems and reviewing the relevant techniques which can be used. It is therefore possible to consider this as a candidate project for the next Optical Radiation Metrology programme, applying the SSfM Best-Practice Guide to a problem of importance to Optical Radiation measurement.

8. Summary of changes

The principal changes from the initial restricted status report on the Optical Radiation area are as follows:

- updating the scope of the area covered to embrace the whole of the current Optical Radiation Metrology programme;
- giving more of a focus towards the formulation of the next SSfM programme;
- moving the tabulation of modelling characteristics to an appendix;
- updating text to reflect progress made in both the SSfM and Optical Radiation Metrology programmes;
- identifying the relevance of data fusion to image processing applications of photodiode and CCD arrays and to measurements of the performance of filtered detectors;
- clarifying the purpose of the Optical Radiation Metrology programme activity to update legacy software;
- clarifying why the risk of software errors is highest in the measurement services provided;
- clarifying the gradual shift towards using LabVIEW and Visual Basic;
- revising text concerning the Y2K problem to reflect the outcome of NPL’s Y2K investigations;
- updating the position on LIMS and how the Optical Radiation LIMS at NPL relates to the NPL corporate activity on LIMS;

- identifying an Optical Radiation application of the SSfM Best-Practice Guide on uncertainties as a candidate project for the next Optical Radiation Metrology programme.

9. Acknowledgements

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Appendix 1: Glossary of Abbreviations

Abbreviation	Expansion
CCD	Charge coupled device
GUM	Guide to the expression of Uncertainty in Measurement
ISO	International Organization for Standardization
LIMS	Laboratory Information Management System
NMS	National Measurement System
SSfM	Software Support for Metrology
Y2K	Year 2000

Appendix 2: Bibliography

1. *Guide to the Expression of Uncertainty in Measurement,* International Organization for Standardization, 1993, ISBN 92-67-10188-9.
2. *M3003: The Expression of Uncertainty and Confidence in Measurement,* United Kingdom Accreditation Service, 1997.
3. *ISO 9001: Quality systems - Model for quality assurance in design, development, production, installation and servicing,* 1994, Geneva, Switzerland.
4. *Measurement Good Practice Guide 5, Software in Scientific Instruments*, NPL, 1997.
5. Rayner, D., *Initial Report on the Status of Software and Mathematics in each Metrology Area,* NPL Report CISE 18/99, February 1999.

Appendix 3: Summary of Modelling Characteristics

The following set of tables give a general characterisation of the typical modelling used in the Optical Radiation Metrology programme. There are, of course, some exceptions where more complex modelling is required or where the current models need improvement.

Table 1. Complexity of models used in the Optical Radiation Metrology programme

Simple	Score*	Complicated
Simple relationship between input and output.	2	Pages of equations to describe the system.
Small number of parameters.	3	Large number of parameters, with complicated inter-relationships.
Measurement errors limited to one measured quantity.	3	Many variables subject to significant measurement error.
Measurement errors consistent with Gaussian distribution.	2	Non-Gaussian behaviour, outliers likely under a Gaussian assumption.
Input quantities well controlled, understood.	2	Inputs estimated, not all influence factors have been identified.

** 1=First statement applies strongly; 5=second statement applies strongly*

Table 2. Maturity of models used in the Optical Radiation Metrology programme

Mature or Accepted	Score*	Developing or Speculative
Well understood and accepted physical theory.	2	A number of competing models or model incomplete.
Comprehensive theory adequately taking into account all main features.	2	Approximations employed, terms omitted to simplify model. Some components modelled by empirical functions, e.g., polynomials, splines. Behaviour of some components not understood and/or ignored.

** 1=First statement applies strongly; 5=second statement applies strongly*

Table 3. Incorporation of uncertainties in the Optical Radiation Metrology programme

Thorough treatment	Score*	Simplistic treatment
Measurement uncertainty modelled for all input quantities.	2	Measurement uncertainty modelled for only one or two input quantities. Other quantities either assumed to be exact or uncertainty contributions are assigned arbitrarily.
Variances and correlation amongst input quantities fully taken into account.	3	Possible variances and correlation among input quantities ignored.

** 1=First statement applies strongly; 5=second statement applies strongly*

Table 4. Comprehensiveness of solution methods for models used in the Optical Radiation Metrology programme

Comprehensive	Score*	Approximate
Solution method solves the computational problem posed by the model.	3	Approximations are employed. Some terms simplified/linearised/ignored.
Solution method takes into account all the sources of measurement error, variances and correlation amongst the input quantities.	2	Easiest method of finding a solution employed. All data treated as exact, independent and uncorrelated.

** 1=First statement applies strongly; 5=second statement applies strongly*

Table 5. Effectiveness of models in the Optical Radiation Metrology programme

Effective	Score*	Ineffective
Solutions consistent with those predicted by theory, established by other methods.	1	Solutions at variance with other results.
Method always returns a solution.	1	Method produces unrealistic solutions, fails to provide a solution, crashes.
Rerunning the method on perturbed data/ input quantities/ produces a nearby solution.	1	Small changes in the input data/quantities produces large changes in the output.
Iterative method converges quickly.	1	Method can make slow progress, fail to converge.
Estimate of statistical uncertainties consistent with the expected measurement error, noise in the data.	2	Unrealistic uncertainties calculated.

** 1=First statement applies strongly; 5=second statement applies strongly*

Table 6. Adequacy of model validation in the Optical Radiation Metrology programme

Good validation	Score*	Poor validation
Fit of model to the measurement data consistent with the expected measurement error.	1	Residual errors much larger than expected, have a systematic pattern.
Results agree with other methods of calculation.	1	Results inconsistent with other methods of calculation.
Results agree in situations for which an analytic/reference solution exists.	1	Solutions at variance with other results.
Numerical results in accordance with predicted behaviour of the algorithm (rate of convergence).	1	Behaviour at variance with prediction.

** 1=First statement applies strongly; 5=second statement applies strongly*