NPL Report CISE 32/99

**Report**

**to the National**

**Measurement System**

**Policy Unit, Department**

**of Trade & Industry**

# INTERIM STATUS REPORT ON THE PHOTONICS AREA

## FROM THE SOFTWARE SUPPORT FOR METROLOGY PROGRAMME

**BY**

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**October 1999**

# *Software Support for Metrology*

# Interim Status Report
# on the
# Photonics Area

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## Abstract

This report describes the status of the mathematics and software used to support the Photonics area of metrology, particularly as used within the NMS Photonics 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 Photonics programme projects applying SSfM outputs to specific problems in the Photonics area.

ISSN 1361-407X



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# Contents

# 1. Introduction

The purpose of this status report is to inform the NMS Software Support for Metrology (SSfM) programme about the status of the mathematics and software used to support the **Photonics** area, concentrating on the use of mathematics and software within the NMS **Photonics Metrology Programme**. This and the companion status reports for the other metrology areas will inform the first annual review of the SSfM programme and will help in the identification of best-practice to be disseminated, and suitable topics for case studies and feasibility studies. It should also lead to appropriate linkage between the Photonics 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.

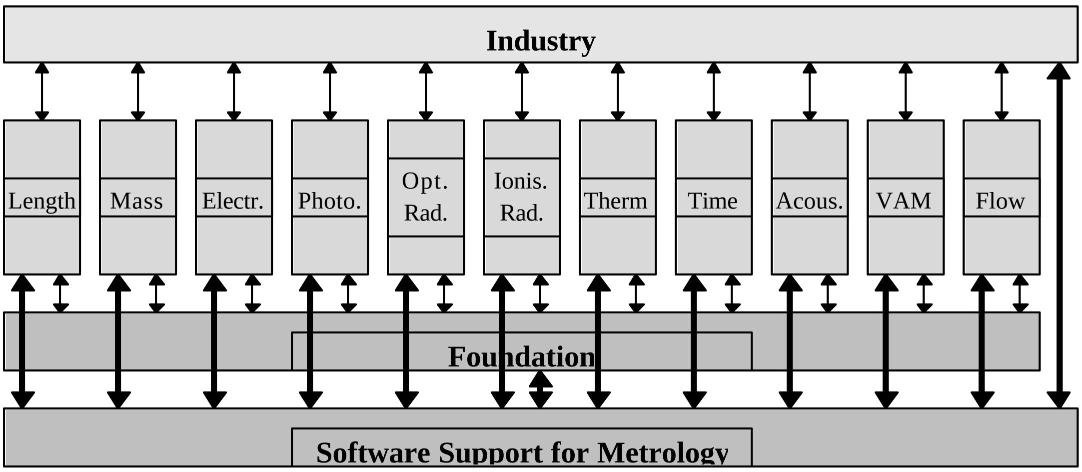


**Figure 1. Relationship of SSfM to other NMS Programmes and Industry**

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 Photonics area which are not addressed by the current 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 [4]. A summary of the differences from the initial Photonics status report is provided at the end of this report.

## 2. Scope of the Area Covered

The Photonics Metrology programme is a newly established programme that brings together all DTI funded measurement activities relating to the photonics industry. The programme includes three technical themes that are outlined below:

*Optical Fibres and Components*

Work in this area includes:

- Provision of measurement services for optical fibre parameters
- Development of measurement techniques for distributed measurements in fibres
- Development of measurement techniques for fibre components and gratings
- Fibre coating geometry

*Test Equipment, Amplifiers, Sources and Detectors*

Work in this area includes:

- Provision of calibration services for fibre optic test equipment including OTDRs, power meters and spectrum analysers
- Development of measurement techniques for fibre optic amplifiers
- Provision of wavelength standards for WDM application

*Optical Properties of Materials*

Work in this area includes:

- Optical properties of displays
- Refractometry of photonic devices

In addition, *technology transfer* is an important activity within each of these themes. It provides the enabling mechanism by which traceability and the concepts of good measurement practice are taken up within UK industry, enabling industry to make measurements that are fit for purpose, to meet regulations, to trade, to improve the efficiency of processes and to remain competitive. One of the key technology transfer platforms for much of the photonics work is the Optical Fibre Measurement Club (OFMeC).

Software is used extensively within the programme for data manipulation, instrument control and, to a lesser extent, mathematical problem solving. A common use for mathematical solutions is in calibration and control processes where, for example, various forms of least-squares fitting algorithms are used (see Section 3.1).

The programme has concerns which relate to three main areas associated with the SSfM programme:

a) numerical software testing (SSfM Theme 2),

b) metrology software development techniques (SSfM Theme 3), and

c) support for measurement and calibration processes (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.

Wavelength is usually considered to be a continuous property, in the sense that it varies across the spectrum. However, wavelength data is collected and recorded as discrete data by digital sampling, so that the measurement data that is subsequently processed will consist of discrete values. Another example of this type of consideration is the measurement of the geometric parameters of fibres which can be considered as continuous also, but often are recorded as discrete quantities with interpolation between points. A specific example of this is the major and minor axes of an ellipse which are considered as discrete quantities. The radius or curvature of the internal region of the fibre are the derived quantities that are of interest. The length of an optical fibre is, of course, always considered as a continuous property.

### 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 Photonics area**

The techniques used in discrete modelling include:

a) Simple data manipulation.
b) The fitting of polynomial functions to data. This is achieved by the use of linear least-squares regression models.

c) Least-squares fitting of ellipses. This is achieved by linear least-squares regression models and orthogonal distance regression with quadratic constraint conditions.

d) Fitting of approximately parabolic functions. This is also achieved by linear least-squares and orthogonal distance regression techniques.

e) Reconstruction of three-dimensional geometric representation of fibre parameters from cross-sectional data, which is essentially two-dimensional in nature.

f) The use of Hankel transforms in the modelling of discrete diffraction data.

Continuous modelling also includes the use of integral transforms, including Hankel transforms, to transform from direct images to diffraction patterns and vice-versa.

Other examples of continuous modelling are the mathematical models used to model two- and three-dimensional objects that are geometric representations of optical fibres and the effect that these have on attenuation of travelling waves.

Modelling has had some success, in certain well-defined areas of Photonics, specifically where the physics of the underlying models is well-understood. The success may be hampered if the mathematics of the underlying physical model is highly complicated and/or possibly non-linear.

There has also been success in understanding processes using models where the physics has not been understood initially. This has been achieved by the development and validation of empirical models which may then feed into improved knowledge of the physical model. For example, this has been seen in the working out of field distributions in fibres under bending conditions, which has a direct impact on measurements of certain fibre parameters.

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

## 3.2 Uncertainties and Statistical Modelling

Uncertainty estimation associated with derived measured quantities, such as length and wavelength, arises most commonly in the measurement services within the Photonics area. An interpretation of the ISO Guide to the expression of Uncertainty in Measurement (GUM) [1] and UKAS document M3003 [2] is used for such estimation processes.

Uncertainties in wavelength are commonly analysed and evaluated using spreadsheet packages and their intrinsic statistical functions. Correlation of errors is a factor that could be considered in the analysis, but its effect on the final results are not felt to be an important issue, and is not usually considered. The size of each statistical contribution to an output is estimated and combined in accordance with the ISO GUM. It is acknowledged that this method of uncertainty estimation will provide an overestimate of the uncertainty and a more rigorous treatment could possibly be used to reduce the effects of correlation.

Non-Gaussian statistics feature highly in some parts of the Photonics area. For example, there are applications where it is necessary to

- take account of the Maxwellian nature of the distributions, and
- to establish and characterise the type of distribution from which a histogram originates.

An International Electrochemical Commission document gives guidelines on how to achieve this by comparison with the procedure for Maxwellian or Gaussian distributions. Much of the theory in this area has been only been tested by making assumptions of uncorrelated data, and it is recognised that more research in this area would be of benefit.

Confidence intervals are usually considered at the 95% level. Work does not presently consider levels other than this.

### 3.3 Visual Modelling and Data Visualisation

Visual modelling and data visualisation is seen as having potential application in the Photonics area, for example for the reconstruction of three-dimensional surfaces from sets of two-dimensional measurements. No specific packages for visual modelling and data visualisation are used at present.

### 3.4 Data Fusion

It is generally acknowledged that data fusion techniques may be of use in the Photonics area, for example relating to distributed stress measurements in fibres. Other applications of data fusion techniques may be identified in the future.

## 4. Validation and Testing

### 4.1 Spreadsheets and Other Mathematical Software Packages

The following off-the-shelf software packages are used in the Photonics area:

1) HP-Basic and HT-Basic, for instrument control, data acquisition and data processing;
2) LabVIEW, also for instrument control, data acquisition and data processing;
3) MathCad, in particular for simple algebraic manipulation;
4) High-level languages such as C, C++, Pascal, FORTRAN and Visual Basic;
5) Spreadsheet packages, in particular Microsoft Excel and Lotus 1-2-3 for basic data processing in the measurement services area;
6) Desktop calculators, for basic data processing;
7) Mathematica;
8) Word and WordPerfect macros for production of calibration certificates.

Software developed in-house is tested in accordance with NPL’s Quality System using test data. Records of past data are kept for this purpose, and allows regression testing of software.

Effort has been made, particularly over the last year or so, to standardise all software that performs instrument control, data acquisition and processing tasks on either HT-Basic or LabVIEW. This development has been done in-house. Older applications that were written using Pascal and HP-Basic have been moved over to HT-Basic, and newer applications are being developed in LabVIEW. The reason for this is three-fold:

1) Corporate NPL policy to move over to the use of LabVIEW for these such tasks;
2) An attempt to reduce the number of packages that are used within the area so that training in software development can be streamlined;
3) Many systems on which Pascal and HP-Basic were used were possibly not Y2K compliant, and it was felt that this point in time was a good opportunity to address this.

The second two reasons are considered to be customer, as well as centre motivated.

Generally, the spreadsheets used are not particularly complicated, but they do rely on in-built statistical functions such as the mean and standard deviation, as well as linear fitting routines such as the Microsoft Excel function LINEST. Processing is done by way of cell formulae as opposed to manipulation by macros.

For many applications usability of the functions from software packages is not an issue as these are only used at relatively low-levels within the area. For example, least-squares solving subroutines written in HP-Basic have been incorporated into more complicated instrument control software by in-house development of the basic subroutines.

There is a high level of awareness of the limitations of the packages used with regard to useful parameter ranges. However, there is no evidence that metrologists in this area *demand* assurances from software suppliers that their software is fit for purpose.

### 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 Photonics area. In particular, it is an increasingly important issue as new models and methods of modelling are considered.

### 4.3 Measurement System Validation

Some hardware systems used in the Photonics area include embedded software. Reference data sets provided with the software are used for validation purposes.

## 5. Metrology Software Development Techniques

### 5.1 Software development methods

Older software used within the Photonics area was generally classified as "Level 3 extant", i.e., it was developed before the introduction of NPL's formal quality system, and validated in practice over several years of operation. However, with the increased recent use of new software packages, the movement has been towards development according to NPL's Quality System. In many cases the development of software involves the refinement of prototype software and/or its adaptation into LabVIEW and HT-Basic.

Verification that software is giving correct answers is achieved by checking results by hand and/or using a spreadsheet. If there are clearly defined intercept points at which numerical values may be observed and extracted software that satisfies this criterion can be checked in isolation.

The most important aspects of ISO 9001 [3] identified in the development of software are reliability and usability. The analysis of risk is also considered.

Problems previously encountered included lack of training for software packages which might assume the programming ability of a software engineer. This was not always appropriate. However, it is felt that this has been adequately addressed by training of staff, in particularly in the use of LabVIEW.

### 5.2 Software reuse

Software is re-used extensively, partly as a way of reducing maintenance costs. Where necessary, the modification of programs involves the development of existing programs and reuse of compiler subroutines. For example, externally-supplied HT-Basic instrument drivers have been used and adapted where necessary. In some cases it may have been necessary to replace these drivers with LabVIEW routines.

Mixed-language programming is chiefly necessary when hardware comes with its own programming language, in which case simple interfaces are developed in-house. This use of software manifests itself as sequential processing, where data is written out into files at each interface to allow further processing. Issues concerning the need for data to be in the correct format have been noted in the past and are addressed as and when is necessary.

The issue of legacy software is presently being addressed, particularly in the context of Y2K. The use of software packages on PCs that were known not to be Y2K compliant has been phased out.

There is also the requirement for software in scripting languages to enable the use of spectral photometers sourced from two different suppliers. The software (scripts) is tied to a particular make of instruments and as such there is little chance of reuse. If the scripts contain functionality which is needed on future spectral photometers, there is clearly a legacy problem in moving the software. There are similar problems for many other programmes here these is equipment which is locked into a particular supplier's software.

Another example of legacy software has been the change in production macros for certificates. This was originally implemented once in WordPerfect and then in Word. It was generally accepted at the time that this process could have been managed better, with improved co-ordination across NPL. Another issue of this type has been the move away from applications such as the NAG library on the NPL mainframe as the bulk of the software has been ported to PCs.

Although there have been legacy problems in this area, the situation has improved with the adoption of BPL software procedures (applied to some software development from 1992, and all development from 1995 onwards).

### *5.3 Virtual Instruments*

The concept of virtual instruments is not generally used in the Photonics area, but it is acknowledged that this could change in the future.

LabVIEW is beginning to be used for applications and may become more important in the future. The need for guidelines in its use, which could involve a training course, is acknowledged. It is felt that further increase in the use of LabVIEW within the Photonics area would be dependent on developments such as this. In addition, the use of library routines in LabVIEW is seen as vital to its future development.

## 6. Support for Measurement and Calibration Processes

### *6.1 Automation of Measurement and Calibration Processes*

At present, Laboratory Information Management Systems (LIMS) are not used widely in the measurement services within the Photonics area, but it has been implemented on one service as an initial test example. The service that this applied to can now be considered standardised, but it is felt that the process led to an increase in administration. However, it is not yet properly linked to the equipment database. There is a general intention to bring in a more extensive use of LIMS over the next six months. At present, there are still some concerns about flexibility and how the system would handle exceptions. There is already some automation of the production of calibration certificates.

### 6.2 Format Standards for Measurement Data

Format standards are not identified as an issue within the Photonics area. Standards impose the processing of data to some extent, which tends to ensure the data is transferable. Other format standards are tied to the software packages which operate on the data.

# 7. Suggestions for Future Activities

### 7.1 Expected Benefits of the SSfM Programme

The key benefits that the Photonics Programme might be expected to gain from the SSfM programme include:

a) guidance and seminars on modelling and validation, particularly of continuous/hybrid models,

b) guidance on uncertainty estimation, in particular for correlated data,

c) guidance on testing third-party packages, and

d) guidance on visual modelling.

### 7.2 Case Studies and Feasibility Studies

The potential for a specific case study in the area has been identified. A number of issues need to be addressed in the development of software for a measurement service for the effective area of optical fibres.

Under an NMSPU Photonics contract won by NPL, there is a requirement to develop a service to measure the effective area of the core of optical fibre, that is typically $6 - 10mm$ in diameter. A system already exists that measures the mode field diameter of the core and the same raw data will be used to calculate the effective area.

Presently, the data is acquired using one machine, and binary data files from this system are converted into ASCII text files that need to be stripped down before further processing on a different machine can take place. This is performed using a routine written in C, and then the relevant data is passed to a MathCad sheet for analysis.

A number of important issues need to be addressed as part of this process:

- the use of separate machines/operating systems;
- time-consuming nature of conversion of data between differing formats;
- data processing issues that are specific to effective area calculation.

All three of these issues would be of considerable interest as a case study within the SSfM programme, but it is the third of these that is considered as the most suitable at present.

The effective area is calculated from the angular intensity of the distribution of light leaving the end of the test fibre, sampled at angular increments. The raw data consists of measured intensity at angular sample points, typically in steps of 4 degrees. The far-field amplitude is taken as the square root of the intensity data. This produces graphs of data that contain sharp dips which correspond to points where the amplitude has changed sign, but the information has been lost in the squaring process. At present, these dips are located manually and the sign of the amplitude distribution is then reversed at these points for further processing. An interpolation routine is then applied to the two halves of the amplitude data, and then both halves are Hankel transformed to a near-field distribution at the fibre endface. The effective area can then be finally calculated from the near-field distribution using the following formula,

$$A_{eff} = \frac{2p\left(\int_0^\infty |E(r)|^2\, rdr\right)^2}{\int_0^\infty |E(r)|^4\, rdr} .$$

For both halves of the far-field scan, the process of centring, interpolating, transforming to the near-field and calculating the effective area takes approximately 15 seconds using MathCad 8 on a 350MHz Pentium 2. The manual selection of the points at which it is necessary to invert the far-field amplitude distribution adds an approximate 30 seconds onto this time and thus an automatic method of selection of the location of these dip-points at which inversion is necessary would be of considerable advantage. Methods of automatic selection have been tried initially but without much success due to the presence of noise in the data.

The issues to be addressed within the data processing step of this procedure are then:

- data centring and mid-point inversion;
- the possibility of automatic selection of location of the side-lobe inversion points in the presence of noisy data;
- accuracy of the Hankel transform process;
- reduction in the time taken for processing of each step.

### 7.3 Future SSfM Topics

There is scope for further work in the next SSfM programme on treatments of uncertainty, and possibly visual modelling and data visualisation. A concentration on software and instrumentation issues was considered to be of considerable future benefit to the Photonics programme. This may possibly also benefit from new techniques in the analysis of uncertainty and automatic/numerical differentiation.

Consideration should also be given to the inclusion of training courses in the development of software. These could perhaps be employed in conjunction with best practice guides.

## 8. Summary of changes

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

- inclusion of Hankel transform in discrete modelling section;
- inclusion of LabVIEW in software packages used, and a description of how Y2K issues within software have bee addressed by migration of software use to specific packages that run on machines that are fully Y2K compliant;
- discussion of the motivations towards more development of Level 3 software within NPL's Quality System;
- discussion of the fact that training issues, which were previously considered problematic, have now been addressed by a combination of standardisation of software packages used and training courses specific to those standardised packages;

- discussion of the implementation of LIMS and its future use;
- inclusion of a possible case study that could be used to address a number of software and mathematical issues.

# 9. Acknowledgements

The author gratefully acknowledges the help provided by Jerry Benson and Dave Rayner in providing input to this report and in reviewing drafts. The author also acknowledges the help given by Christine Wall, John Baines, David Ives, Andrew Hanson, Robin Barker, and Peter Harris in producing the initial restricted status report.

# Appendix 1: Glossary of Abbreviations

| | |
|---|---|
| ASCII | American Standard Code for Information Interchange |
| IEC | International Electrochemical Commission |
| ISO | International Organization for Standardization |
| LIMS | Laboratory Management Information System |
| NMS | National Measurement System |
| NMSPU | National Measurement System Policy Unit |
| NPL | National Physical Laboratory |
| OFMeC | Optical Fibre Measurement Club |
| OTDR | Optical Time Domain Reflectometer |
| PC | Personal Computer |
| SSfM | Software Support for Metrology |
| UKAS | United Kingdom Accreditation Service |
| WDM | Wavelength-Division Multiplexing |
| 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. 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 Photonics 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 Photonics programme**

| Simple | Score* | Complicated |
|---|---|---|
| Simple relationship between input and output. | 3 | Pages of equations to describe the system. |
| Small number of parameters. | 2 | 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 Photonics 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. | 3 | Approximations employed, terms omitted to simplify model. Some components modelled by empirical functions, e.g., polynomials, splines.<br>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 Photonics programme**

| Thorough treatment | Score* | Simplistic treatment |
|---|---|---|
| Measurement uncertainty modelled for all input quantities. | 3 | 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 Photonics 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. | 3 | 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 Photonics programme**

| Effective | Score* | Ineffective |
|---|---|---|
| Solutions consistent with those predicted by theory, established by other methods. | 3 | Solutions at variance with other results. |
| Method always returns a solution. | 2 | Method produces unrealistic solutions, fails to provide a solution, crashes. |
| Rerunning the method on perturbed data/ input quantities/ produces a nearby solution. | 2 | Small changes in the input data/quantities produces large changes in the output. |
| Iterative method converges quickly. | 3 | 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 Photonics programme**

| Good validation | Score* | Poor validation |
|---|---|---|
| Fit of model to the measurement data consistent with the expected measurement error. | 2 | Residual errors much larger than expected, have a systematic pattern. |
| Results agree with other methods of calculation. | 3 | Results inconsistent with other methods of calculation. |
| Results agree in situations for which an analytic/reference solution exists. | 2 | Solutions at variance with other results. |
| Numerical results in accordance with predicted behaviour of the algorithm (rate of convergence). | 3 | Behaviour at variance with prediction. |

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