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of Trade & Industry

INTERIM STATUS REPORT ON THE IONISING RADIATION AREA

FROM THE SOFTWARE SUPPORT FOR METROLOGY PROGRAMME

BY

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Software Support for Metrology

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Abstract

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

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1. Introduction

The purpose of this status report is to inform the NMS Software Support for Metrology (SSfM) (1998-2001) programme about the status of the mathematics and software used to support the **Ionising Radiation** area of metrology, particularly what is used within the NMS **Ionising Radiation 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 Ionising Radiation 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 has some direct impact upon industry, 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.

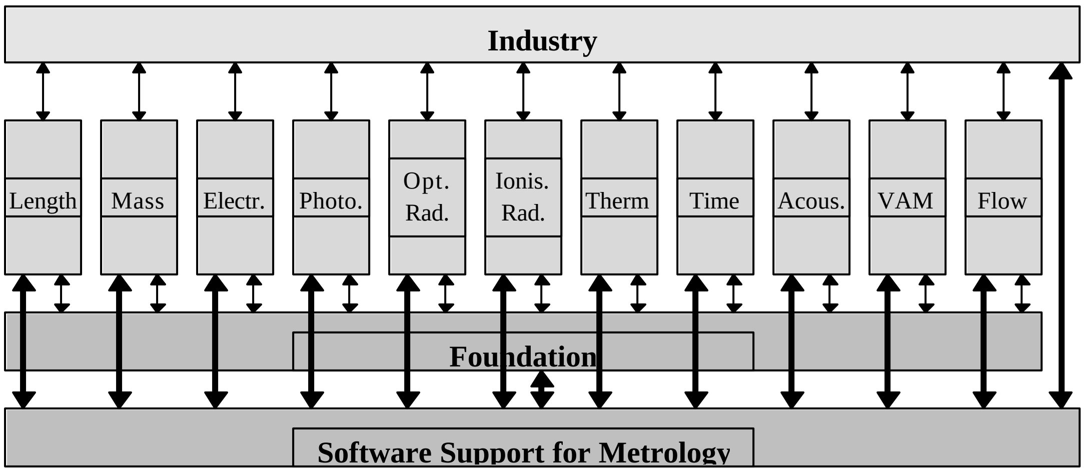

Figure 1. Relationship of SSfM to other NMS Programmes and Industry

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 Ionising Radiation area which are not addressed by the current SSfM programme or which need to taken further in the next SSfM programme.

This report is an update of an initial restricted status report produced in November 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 [3]. A summary of the differences from the initial Ionising Radiation status report is provided at the end of this report.

2. Scope of the Area Covered

The current NMS Ionising Radiation programme is carried out by the NPL Centre for Ionising Radiation (CIRM). It covers the following themes:

a) radiation dosimetry

b) radioactivity measurements

c) neutron measurements.

Much of the requirement for the work arises in connection with health and safety in the uses of x-rays, gamma-rays, beta-rays, electrons, neutrons, and radionuclides; also for environmental and health monitoring. As part of this work CIRM manage three large accelerator facilities.

The NMS Ionising Radiation Metrology Programme carried out at NPL provides the basis for the following services :

1. maintenance of primary standards for:
   a) beta-ray, X-ray and gamma-ray dosimetry at environmental, protection, therapy, sterilisation and industrial processing dose rates;
   b) the standardisation of a wide range of radionuclides and the provision of standardised radioactive source material at environmental, protection and therapy activities;
   c) neutrons with energies from thermal to 20 MeV, primarily for radiation protection purposes;
2. development of new techniques;
3. calibration and measurement services.

Typically, the DTI acts as proxy customer for 1) and 2) whereas 3) is offered directly to customers, both in the UK and overseas.

Software is used extensively in the Ionising Radiation Metrology Programme ranging from instrument control, through data manipulation, to mathematical problem solving. These relate as follows to the SSfM Themes:

a) modelling, Monte Carlo simulation and data visualisation (in SSfM Theme 1);

b) numerical software testing and measurement system validation (in SSfM Theme 2);

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

d) 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.

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 Ionising Radiation Programme

Typically, data in Ionising Radiation arise from observations of continuous phenomena and hence *continuous models* are important. Where these observations are sampled at discrete points, *discrete models* also play an important role.

Significant effort, and in-house expertise, is devoted to Monte Carlo computational techniques. These techniques provide a bridge between measurements and analytic calculations. These three techniques provide complementary descriptions and each would be less useful or credible without the contribution of the other two. Experimentation and simulation result in the distillation of insight by a careful choice of parameters to be measured in one case and 'scored' or tabulated in the other. Monte Carlo calculations provide a benchmark for analytic calculations and a verification of results obtained in difficult or impossible measurement situations. In turn, Monte Carlo calculations are built on the foundation of measured and calculated probability distributions, for example, those describing scattering or energy loss.

Many problems in radiation dosimetry and radiation protection are being addressed by Monte Carlo techniques because the complexity of atomic particle transport in materials renders analytical solutions intractable. The use of these techniques in these fields has increased dramatically in the last few years for a combination of reasons. One is the rapid increase in speed and decrease in cost of data processing. At the same time, large, general purpose software packages have become available. It is now possible to Monte Carlo model situations in which physical measurements are difficult or impossible, i.e., 'virtual measurements'. For example, whilst in principle, the spectra of high energy linear accelerators can be measured, such measurements are inordinately difficult, whereas, Monte Carlo calculated spectra can be obtained relatively easily.

The majority of this work is based on two well respected FORTRAN based public domain codes which have been bench-marked and have a documented long development history:

(i) The EGS4 (Electron Gamma Shower) suite of computer codes is a general purpose package for the Monte Carlo simulation of the coupled transport of electrons and photons in a user-defined geometry in any element, compound or mixture, for particles with an energy above a few keV up to several TeV. The suite of codes originated from the Stanford Linear Accelerator (SLAC) and National Research Council of Canada (NRCC), from whom it is freely available. The EGS4 codes are used for photon and electron radiation transport through a wide range of materials, complimenting experiments, and is also used to predict instrument response outside the experimental regime. To date it has been used to compute correction factors for the primary standards (free air chambers and cavity ionisation chambers) as well as to model the NPL linear accelerator and the response of ionisation and Fricke dosimeters in water phantoms. Based on this in-house expertise, CIRM has hosted three training courses on the EGS4 software and have made a number of presentations at international meetings on the use of the codes.

(ii) MCNP (General Monte Carlo N-Particle Transport Code) is a continuous energy, generalised geometry, time dependent, coupled or de-coupled neutron, photon and electron Monte Carlo code. It was developed at Los Alamos National Laboratory (LANL) and is freely available from Oak Ridge National Laboratory (ORNL) or via the NEA data bank in Paris. MCNP is used for neutron and photon radiation transport through a wide range of materials, complimenting experiments, but is mainly used to predict radiation field parameters or instrument response outside the experimental regime. To date it has been used to compute the response functions of the Bonner sphere neutron spectrometry systems and the NPL secondary standard long counters for neutron fluence measurements, to model room and air scattering within the NPL experimental hall and to derive correction factors for calibrations of area and personal neutron monitoring equipment. Based on this in-house experience, CIRM has contributed to a number of training courses on the use of MCNP and has been actively involved in drafting a review of Monte Carlo and deterministic codes for applications in radiation protection and dosimetry for the European Commission. Other examples of modelling codes in use in the Ionising Radiation area are the following:

1) Finite Element Analysis: this code is being used to model the heat flow through calorimeters. This is to investigate corrections to measured temperature rises from radiation. Currently this is done using Pafec on a site machine.

2) Finite Difference methods: using CIRM-developed code and DiffPack. This code is being used for a purpose similar to the finite element code.

The techniques used for discrete modelling include data approximation, using spreadsheets and other third-party software.

3.2 Uncertainties and Statistical Modelling

CIRM are competent in the estimation of uncertainties in their field. There is no problem in applying the ISOGUM [1] or UKAS M3003 [2]. It has been agreed with UKAS that CIRM will be responsible for drafting a new appendix to M3003 devoted to radiation physics to replace UKAS NIS 0825 which has been withdrawn. The new appendix to be published later this year will include worked examples of a number of typical calibration situations explaining in each case the uncertainty budget and the derivation of the quoted uncertainty based on a standard uncertainty multiplied by a coverage factor k=2, which provides a level of confidence of approximately 95%. The examples include the calibration of (i) photon dosimeters in terms of air kerma, (ii) therapy-level dosimeters in terms of absorbed dose, (iii) neutron survey meters in terms of neutron ambient dose equivalent, (iv) large area sources used for calibrating surface contamination monitors in terms of emission rate, and (v) surface contamination monitors in terms of emission rate. UKAS plan to use this document as a submission to a guidance document to be published by the European Co-operation on Accreditation (EA). Also, included within the 1998/2001 NMS Ionising Radiation programme is the provision of two courses on uncertainties appropriate to measurements and calibrations of radiation sensitive instruments used for radiation protection purposes; the first course is planned for late 1999 and will be based to a large extent upon the content of the M3003 appendix mentioned above.

One outstanding uncertainty problem area is spectrum unfolding involving a 52 X 52 vastly underdetermined uncertainty matrix. When Bonner spheres (BSs) are used at NPL to determine a neutron spectrum over the full energy range from thermal energies to 20 MeV (nine orders of magnitude), the derived spectrum is usually presented in an energy group structure of 52 bins of equal width on a lethargy scale, with five bins per decade. Since there are only nine or ten measured responses and 52 bins, the unfolding problem is underdetermined. This is the usual case for BSs, but evidence from various international spectrometry and unfolding intercomparisons has shown that very reasonable results can be obtained, although some additional information, e.g., smoothness, non-negativity, etc., is often used. The approach to BS unfolding at NPL is to use the public domain software code STAY'SL. This requires an *a priori* estimate of the spectrum to be given by the user. However, since this estimate is given with uncertainties, and these can be large, only very approximate *a priori* information is needed. The process is essentially one of adjusting the *a priori* spectrum in the light of the measured BS data. Although it is certainly true that the more accurately the *a priori* spectrum is known, the more accurate will be the final spectrum, provided it is consistent with the measured sphere responses, experience has shown that STAY'SL will provide reliable results even when the *a priori* information is very limited. A reliable uncertainty analysis for the fluences in the various energy bins of the spectrum is not at present possible. The mathematical tools to provide this information are in place, but it requires reliable estimates of variances and co-variances for both the *a priori* spectrum and the sphere response functions, as well as for the measured BS sphere data. All these data are not presently available, and uncertainty estimation for spectra unfolded from BS measurements remains an unsolved problem at the present time.

3.3 Visual Modelling and Data Visualisation

CIRM is interested in visualising particle transport and interactions and the user-defined geometry in its Monte Carlo simulations. Such an ability would be useful to not only enhance the understanding of the processes involved but would also enable the rapid identification of errors and/or wrongly defined geometries and input specifications.

In the past, visualisation has required special-purpose software, preferably running on expensive workstations. However, the graphics performance of standard PCs has improved so much recently that much cheaper solutions are now possible. CIRM has therefore produced software to convert the standard graphical output of particle tracks in EGS4 into VRML (Virtual Reality Modelling Language) which has recently emerged as the standard language in which to represent 3-D graphics. So far, only the EGS4 showers are converted to VRML; the solid objects with which the electrons and photons interact are added manually using a VRML world-building tool.

VRML is an ISO standard language for representing a virtual world of three dimensional (3-D) objects on the world wide web. Such virtual worlds can be navigated using freely available VRML browsers. VRML provides many features to make worlds look realistic, including perspective, lighting, transparency effects, etc. A number of visual examples have recently been set up enabling users to navigate around the simulation.

One of the projects within the SSfM programme is concerned with visual modelling and data visualisation. The initial status report identified CIRM as having a need for improved software in this area. Subsequently, SIRA have been awarded a competitively tendered contract to conduct the SSfM visual modelling and data visualisation project. SIRA have decided to adopt this CIRM application as one of their case studies; CIRM is providing data to enable SIRA to undertake the project, and discussing with SIRA the progress made and difficulties encountered. It is too early to comment on the success or otherwise of this case study.

3.4 Data Fusion

Data fusion is not seen as relevant to much of the Ionising Radiation Metrology Programme. One area, however, that might benefit is the examination of the low dose radiation of a pellet with large background noise. Note, that some data fusion is practised as part of routine measurements, for example combing results from thermistors or analysing a mix of two chemicals to correct for temperature variations.

4. Validation and Testing

4.1 Spreadsheets and Other Mathematical Software Packages

The principal off-the-shelf software packages used in Ionising Radiation metrology are:

1. HT-Basic and HP-Basic (for instrument control and data acquisition)
2. Excel (for data analysis and curve fitting, not directly for external customers)
3. Sigmaplot (for graphics, calibration curve fitting and curve fitting)
4. MathCad (for routine analysis of measurement data)
5. Origin (for graphics)
6. MatLab
7. LabVIEW
8. Mathematica (light usage)
9. NAG Library (FORTRAN - rarely used now)
10. Instat (based on the statistical software package Minitab), used in the analysis of primary standard measurements.
11. Pafec: a finite element package (used by the Centre for Information Systems Engineering (CISE) for CIRM)
12. Staysl (least squares code for fitting spectrum unfolding for ill-determined problems)
13. Visual Basic (for database customisation)
14. FORTRAN 77, FORTRAN 90 and the related SLAC language MORTRAN
15. Collection of software developed in CIRM with some software contributed from external sources (such as SLAC and PTB). These tend to be written in FORTRAN. In CIRM FORTRAN calling routines are written for the Monte-Carlo simulation software.

External software, such as the public domain software, is tested as far as possible as the majority has safety aspects and dosimetry errors in radiotherapy and in radiation protection have a high public profile.

There has been a move away from FORTRAN based code towards the use of spreadsheets. Generally, the spreadsheets used are not particularly complicated, but they do use in-built functions such as max and min (these are not quoted externally).

At present approximately 50 CIRM programs are registered by NPL's Quality System as Level 3 Level i.e. software that has effective support and may be delivered to a customer, developed with a design process and errors are logged and corrected. Level 1 (performs no vital function) and Level 2 software (software that is used for development and feasibility) is also produced.

Independent checks are performed on software. Results are compared with experimental data and independent calculations are made (for example graphs are checked and spreadsheets are verified by hand).

In CIRM there is an awareness of the limitations of the packages with regard to useful parameter ranges and some concerns over sophisticated functions (for example minimisation in spread sheets).

4.2 Model Validation

Within CIRM there is a high awareness of the need to validate models, particularly because many of the applications have an impact upon health and safety. Techniques for model validation vary - but whenever possible simulations are checked against known experimental data.

For photon and electron dosimetry applications based on the use of EGS4, calculations are made within the range of experimental measurements as well in regions inaccessible to experimental measurement in order to ensure that the theoretical and measured results agree within the uncertainties. Such checks have been performed for Fricke dosimetry within water phantoms and for depth dose profiles for both photons and electrons within a water phantom. Calculated correction factors for primary standards have been confirmed using other computational techniques and by comparison with results generated by other laboratories.

For neutron dosimetry applications based on the use of MCNP, similar attempts to compare theoretical and experimentally measured results are routinely performed. Typical examples are the response of the NPL long counters for neutron fluence measurements, the anisotropy of neutron emission from commercially available radionuclide neutron sources and the room and air scattering components within the NPL neutron experimental hall. The neutron spectrum unfolding codes have been bench-marked and validated through intercomparisons with other national laboratories for neutron spectra determined around specific radiation environments as part of an international effort funded principally by the European Union.

4.3 Measurement System Validation

Software is used for the control of measurement systems in CIRM and some instruments contain embedded software. Both internal and bespoke third party software is used to control the ensemble, with in the latter case a functional specification being provided by CIRM. The measurement system as a whole is validated against known calibrated reference instruments. Reference data sets are not used.

5. Metrology Software Development Techniques

5.1 Software development methods

CIRM follows the NPL Quality management system for software development and it is perceived that the current methods provide the reliability required, for example logs are kept of bug reports and enhancements. Maintenance of old software for enhancements is seen as costly and a current concern. Risks from software errors are considered small due to the number of checks performed. A variety of approaches are used for software development including structured design, data flow diagrams and object orientated design, however the most common approach is to refine a prototype. A recent innovation in CIRM is to use HTML and web browsers to develop and test both functional specifications and user requirements.

The air kerma measurement and calibration services rely upon calibration and control software running on obsolete HP workstations. This software is not 'Y2K' compliant and has been expensive to maintain. Work is under way to develop a replacement system which will better meet CIRM’s needs and will run on PCs. Web browsers and HTML have been used to mimic the user interface of the planned system. This has enabled useful feedback at an early stage and has increased our confidence that the system specification is appropriate before implementation began. It is expected that the web browser/HTML technique will be used again when the system specification is defined in more detail.

The results obtained from software are checked by other instruments, by hand and mathematical tools. There is only limited scope for testing software in isolation.

5.2 Software reuse

Software reuse is an ongoing issue, in particular for the control of instruments. Most instrument control is currently performed in HP-Basic and minor modifications to old code are required to control different instruments.

Year 2000 issues are being managed corporately and no great impact is currently envisaged on milestone delivery.

5.3 Virtual Instruments

At present little use is made of virtual instruments, although it is planned to review the application of LabVIEW to a particular problem as part of an evaluation in the near future.

6. Support for Measurement and Calibration Processes

6.1 Automation of Measurement and Calibration Processes

Each calibration and production of a certificate is often specific to the particular case in hand, although there has been some attempt to automate the process, for example in the interrogation of databases and merging of information.

The calibration service based upon the linear accelerator involves disparate measurements and a wide variety of data; it is very labour intensive to track data through summary sheets to certificates. CIRM has tried to use WordPerfect merge but this has proved expensive to maintain. A LIMS might prove to be of use in this area.

6.2 Format Standards for Measurement Data

There is no known requirement for format standards in the area of ionising radiation.

7. Suggestions for Future Activities

7.1 Expected Benefits of the SSfM Programme

Although CIRM is very conscious of the need for validation of continuous and discrete modelling it is possible that some improvements to the modelling and validation techniques may be made in continuous techniques.

As CIRM is about to investigate LabVIEW for instrument control some guidance and training might be of benefit.

7.2 Case Studies and Feasibility Studies

A case study has been identified to cover some aspects of visualisation of Monte Carlo simulation results for radiation transport and this has been taken up by SIRA within the current SSfM programme. It is too early at present to comment on the success of this project.

A feasibility or case study in the automation of calibration processes area could be the provision of an efficient data management system for the calibration service and the conversion of WordPerfect macros for certificate preparation to a more efficient alternative.

In addition, SSfM work on the validation of simulated instruments may benefit from consideration of the work done on the long counter. The recent use of HTML and web browsers for software development may also be of wider interest.

7.3 Future SSfM Topics

As stated previously, CIRM is at present engaged with CISE on the modelling of heat flow through calorimeters and with SIRA on a visualisation of Monte Carlo simulation results. There may be scope for follow-on work in the next SSfM programme in both these areas. Two other areas for future SSfM topics that arise from the Ionising Radiation area are as follows:

(a) Distributed Computing Resource

Most desktop computers are idle most of the time. Even if used for eight hours a day from Monday to Friday, they are idle 75% of the time. Considering the whole of NPL, this is a large computing resource and it is proposed to use this to develop a distributed computing resource which would enable work on significant problems in computational physics, across the full range of NMS programmes, and also open up new areas of potential research to the benefit of the UK metrological user-base.

The potential resource consists of more than 600 PCs whose specification lies in the range p/100 to pIII/550 or better, running Windows NT/2000, linked by 10 to 100 Mb/s Ethernet.

Several sites, including universities, NIST and other leading laboratories with comparable resources are now engaged in developing or using the software which enables such distributed computing resources to be used.

The first stages of development of such a system would be the identification of applications which would benefit from such a resource. It could then move on to one or more case studies based on existing NMS project work, and depending on the outcome of these studies, the final stage could be the realisation of an NPL-wide distributed computing resource.

(b) Improved Uncertainty Estimation for Spectra Unfolded from the Bonner Sphere

A significant outstanding problem is that mentioned in the second part of Section 3.2 above - the provision of a reliable uncertainty analysis following the spectrum unfolding involving a 52 x 52 vastly underdetermined uncertainty matrix. As noted, the mathematical tools are in place, but it requires reliable estimates of variances and co-variances for both the Bonner sphere response functions, as well as for the measured Bonner sphere data. All these data are not presently available but could be derived from available experimental and theoretical information, and uncertainty estimation for spectra unfolded from Bonner sphere measurements remains an unresolved problem at the present time.

The application of mathematical expertise could solve this problem and provide a sounder foundation for measurements which play an important role in radiation safety issues around the majority of UK nuclear facilities and workplace environments.

8. Summary of changes

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

- The description of modelling has been expanded and includes more details on the Monte Carlo simulations performed in the programme and the two main codes used.
- Further details have been included on the appendix to the GUM and a more detailed description given on the spectrum unfolding problem.
- Under visual modelling and visualisation, details have been included on CIRM's work on VRML. There is also discussion of the case study adopted by SIRA on the visualisation of the Monte Carlo simulations.
- Details have been added on developing a replacement for software that is not 'Y2K' compliant. As part of this work the user interface has been mimicked to represent the user interface and as a tool in software specification.
- Two potential areas for future investigation have been added: distributed computing and uncertainty estimation.

There are a number of areas where the Ionising Radiation Programme and SSfM programme may interact in the future. There are some interesting developments in software development using a web based approach and HTML that might be useful to incorporate elsewhere.

The setting up of a distributed network is an interesting idea that would be useful for improving Monte Carlo simulations both for CIRM and for other Centres. It is likely that there are other applications (such as high accuracy finite element simulations) for which this might prove a useful resource. The uncertainty estimation for spectra unfolded from Bonner sphere measurements is an exciting problem that would yield immediate benefits.

9. Acknowledgements

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Appendix 1: Glossary of Abbreviations

Abbreviation	Expansion
BS	Bonner sphere
CIRM	Centre for Ionising Radiation Metrology
CISE	Centre for Information Systems Engineering
EA	European co-operation on Accreditation
GUM	Guide to the expression of Uncertainty in Measurement
HTML	Hyper-Text Mark-up Language
ISO	International Organization for Standardization
LANL	Los Alamos National Laboratory
LIMS	Laboratory Information Management System
MCNP	General Monte Carlo N-Particle Transport Code
NAMAS	National Measurement Accreditation Service
NIS	NAMAS Information Sheet
NIST	National Institute of Standards and Technology
NMS	National Measurement System
NRCC	National Research Council of Canada
ORNL	Oak Ridge National Laboratory
PC	Personal computer
PTB	Physikalisch-Technische Bundesanstalt
SLAC	Stanford Linear Accelerator
SSfM	Software Support for Metrology
UKAS	United Kingdom Accreditation Service
VRML	Virtual Reality Modelling Language

Appendix 2: Bibliography

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