NPL National Physical Laboratory

Counting on IT

A National Measurement Newsletter

Autumn 2004 | Issue 16

Contents:

NPL, SS*f*M and Dave Rayner – moving on

A new era for NPL has begun. Serco, in conjunction with Sira, won the contract to manage the Laboratory for the next ten years on behalf of DTI. The new contract came into force on 1 April 2004.

A major internal reorganisation has taken place: the new structure comprises three Divisions. Dave Rayner and the NMS Software Support for Metrology programme are also moving on. Dave writes:
"It has been a great pleasure and a privilege for me to have led Mathematics and Scientific Computing (MSC), and SS*f*M over the past seven years. I have steered the programme through its first three formulations and its first two programme cycles.

"In the inevitable round of 'musical chairs' that accompanies company reorganisations, I have moved to become the Business Leader for the Radiation Dosimetry team in the Quality of Life Division. Meanwhile, MSC has remained intact but now as a Group within the Electrical and Software team in the Division of Enabling Metrology. Bernard Chorley, with whom I've worked for many years, and especially closely over the past seven, has taken over responsibility for both the Group and the SS*f*M programme.

"I wish Bernard well in his new role and feel confident that the programme will continue to go from strength to strength, not just because of his leadership, but also because of the excellence of the technical staff he has to support him. Work on discrete modelling, uncertainty evaluation and numerical analysis could hardly be led by a stronger team than Maurice Cox, Alistair Forbes and Peter Harris. The programme's work on continuous modelling now moves confidently towards a good practice guide in the

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Figure 1: *Photo above:* Dave Rayner with SS*f*M staff. Left to right: Peter Harris, Mike Stevens (editor), Dave Rayner, Bernard Chorley, Alistair Forbes, Graeme Parkin

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very capable hands of Louise Wright and Trevor Esward. Trevor will also lead the new work on modelling for nanotechnology, signal processing and distributed computing, with significant contributions to the latter from my new team. Graeme Parkin and Robin Barker will continue to assist Bernard to provide excellent leadership on software engineering, particularly in software validation and internet-enabled metrology.

"I will certainly miss having close involvement with all these areas of work and the links we forged with almost all other NMS programmes; but more especially I shall miss working with this excellent team of people. Keep up the good work."

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European Network *SofTools_MetroNet*

***SofTools_MetroNet* is a European Thematic Network, focused on computational tools for measurement, including the mathematical and statistical foundations for such tools.**

The network was started in 2002 and will run until July 2005. It is coordinated by IMGC (the Italian National Measurement Institute). Its aim is to promote collaboration between National Measurement Institutes, industry, software developers and academia across Europe, in the areas of:

- Software for instrumentation
- Mathematics and statistics
- Databases and software validation

Towards the end of 2003, the network launched six *co-operative projects* (COPs), two for each of the themes listed above, in the following areas:

- Data acquisition and virtual instruments
- Internet-enabled measurement
- Best practice in uncertainty evaluation
- Discrete modelling, data fusion and data fitting
- Databases in metrology
- A validation framework for metrology software

Collaboration in these projects is expected mainly to involve short visits between participants to work jointly on specific problems, leading to submission of procedures and software for consideration by the network. NPL has put forward a number of SS*f*M best-practice guides and reports for adoption or endorsement by the network, with the aim of achieving appropriate international recognition of these documents. In addition, NPL is leading two of the above co-operative projects: COP2 on internet-enabled measurement and COP3 on best practice in uncertainty evaluation.

COP2 aims to provide good-practice in the implementation of internet-enabled measurement software, a commonly agreed specification for an application-programming interface (API) for such software, and an inventory of the applicability of internet-enabled measurement.

COP3 includes tasks on uncertainty evaluation in the context of testing, methods for expressing and evaluating uncertainties, methods for interlaboratory (including key) comparison data evaluation, and methods for expressing and evaluating uncertainties for multivariate models, including spectral quantities. As part of this project, NPL led a *SofTools_MetroNet* special session at the recent international conference *Computational and Mathematical Methods in Science and Engineering* (see www.fysik.uu.se/cmmse/).

Information about the network can be found at www.amctm.org/index.asp Other events include a workshop on the co-operative projects, held on 13-15 September 2004, and the seventh in the series of conferences *Advanced Mathematical and Computational Tools in Metrology*, 27-30 June 2005.

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Visualisation of uncertainties

The interpretation of statements of measurement uncertainty can be difficult when there are several input quantities and several output quantities involved in the model of measurement.

The use of appropriate ways of visualising uncertainty information can be helpful in this regard.

As part of SS*f*M-2, NPL studied the visualisation of uncertainty for vector and multidimensional data. Two case studies from the areas of electrical metrology and electrical engineering were considered. One study concerned co-ordinate system transformations, as arise in converting measurements from Cartesian (real and imaginary) co-ordinates to polar (magnitude and phase) co-ordinates. The other concerned microwave power meter calibration, particularly the determination of comparison loss, as is necessary when testing a power sensor for use at RF and microwave frequencies with respect to a specification limit.

A number of visualisation techniques were explored, including static two- and three-dimensional plots (such as scatter plots, contour plots, elevated surfaces and histograms), movies, three-dimensional plots in which the user can control the viewpoint for the visualisation, and scenes viewed using a web browser which allow the user to modify the data for the object displayed.

A report, with associated visualisations, is available for download on the publications page of the SS*f*M website (see www.npl.co.uk/ssfm/download/nplreports.html). As part of SS*f*M-3, it is planned to revise SS*f*M Good-Practice Guide No 13 on *Data visualisation* to include further material on the visualisation of uncertainties.

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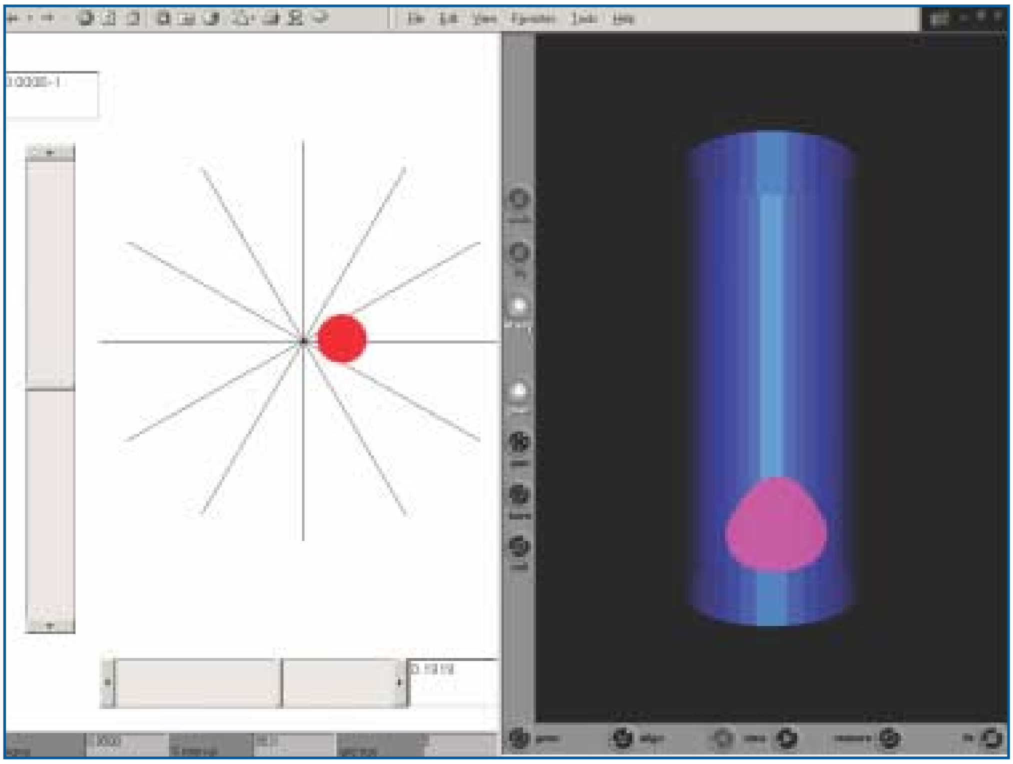

Figure 2: Visualising co-ordinate system transformations. Under a co-ordinate transformation, the Cartesian uncertainty region (left) is mapped onto a polar uncertainty region, depicted in the surface of a cylinder.

On-line testing services

Members of the SS*f*M Club have access to online data generators for obtaining reference data and corresponding reference results for testing the numerical correctness of software for a number of computations important in metrology.

The generators can be used to obtain data sets to mimic those that are likely to be encountered in the user's own application by permitting the user to control various properties of the data and corresponding results. For example, for testing software for straight-line regression, the user may control the number of points in the data set, the signal-to-noise ratio for the data, and the slope and intercept of the solution straight-line.

The data generators form the basis of an online testing service soon to be made available. When using the service, reference results will *not* be provided to accompany a reference data set. Instead, the reference results will be held at NPL and will be compared with test results submitted by users, who will obtain them by applying their test software to the reference data. Users will be informed automatically of the result of the comparison. Such an approach provides an independent validation of the test software.

Whereas the data generators are currently available as applets that run on the user's machine, the new testing service will be based on servlets that run on the server. They can be accessed through the EUROMETROS website (see www.eurometros.org/). NPL is keen to receive feedback on these, as well as suggestions for new data generators.

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Distributed computing: harnessing the power of desktop PCs

By installing the United Devices Grid MP platform on two hundred top-performing networked desktop PCs, NPL has established a site-wide distributed computing system that utilises the spare computing capacities of the machines to create a virtual supercomputer.

NPL is now able to perform much larger calculations than were possible before, and to speed up the computation of many metrology applications.

To assist metrologists in getting the best out of distributed computing systems, SS*f*M-3 is funding the production of a Good-Practice Guide on the selection and optimisation of mathematical models to use parallel computing in a distributed computing environment.

What is distributed computing?

The term *distributed computing* refers to collaborative initiatives in which large numbers of users of PCs allow some of their networked computers' spare computing capacity to be used to tackle a large computing problem, with the collaboration often being co-ordinated by means of the Internet. A well-known example of this is *SETI@home* in which computer owners offer their machines to work on the *Search for Extraterrestrial Intelligence* project to download and investigate radio telescope data.

In organisations such as NPL, large numbers of networked PCs are used on the desktop or in the laboratory, but their full processing capability is very rarely utilised: the unused capacity is typically as high as 80%. Distributed computing is a way of accessing this unused power to tackle large computing problems. By running a program on many machines in parallel and in a co-ordinated manner, the computing task can be completed many times faster than is possible with serial computing.

In distributed computing, individual PCs do not have access to shared memory, in contrast to some other types of parallel computing, and all communication is routed via a central server machine. A parallel task is split up into work units (parcels of data) and a 'donor' PC communicates with a central server to receive a work unit and send back a result. Inter-process communication is not possible because there is no certainty that a given machine will be computing a required work unit at a given time.

The most commonly run applications, e.g. Monte Carlo simulations, are often "data parallel". These are ideal for distributed computing, as the same program will run on each machine in the network but with a different input control file sent from the central server. It may be that a serial program can be transferred directly to a distributed computing system. Where this is not possible, the planned Good-Practice Guide will provide advice on how to make the best use of the system.

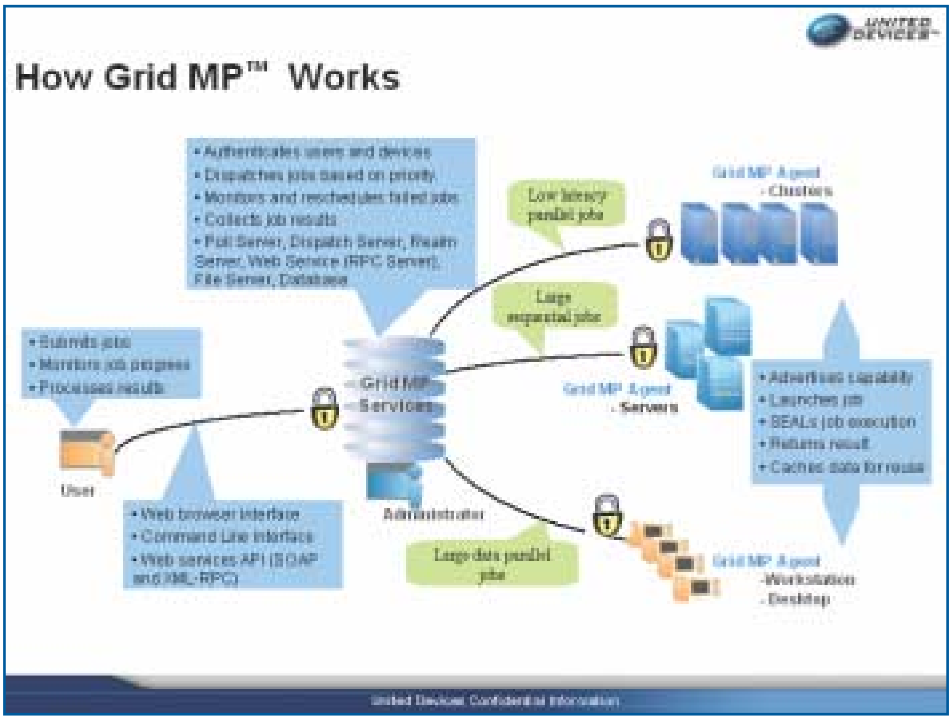

Figure 3: Schematic representation of United Devices Grid MP system (reporduced by permission of United Devices)

NPL's United Devices system

NPL is working in partnership with United Devices to develop its MP Grid distributed computing software into a system suitable for running and developing metrology applications (figure 3).

The user interacts with the central server to submit jobs and collect results. The server controls the submission of work units to the agents (the available computing resources) and is responsible for all communication; the agent machines typically do not communicate with each other unless the distributed application employs Message Passing Interface (MPI). The agent machines can be heterogeneous, including desktops, other servers and clusters, and they can run under different operating systems.

Proton Beam Energy (MeV)	Number of jobs	Average CPU, hours	200 Node grid, hours	Speed-up factor
60	100	84.6	1.17	73
100	300	192.9	1.77	109
150	500	393.1	3.09	127
200	1000	730.7	4.70	156

Table 1: Performance improvement for a 200 node grid: CPU time in hours for the average PC (~Pentium IV 2 GHz), compared with average wall-clock time on the NPL distributed system

Applications

The new distributed computing system has already led to substantial performance improvements in NPL software systems and opened up many new possibilities for research. The ionising radiation application described here shows how the system speeds up lengthy calculations, and the materials example shows how a new project has been started to tackle problems that would previously have been intractable.

Monte Carlo calculations for ionising radiation applications

Certain cancers can be treated by irradiation, by focusing high-energy particles on the cancerous cells to destroy them. For a successful treatment, it is necessary to measure both the dose delivered and its distribution in the body. Air-filled ionisation chambers are used to measure the dose distribution in a water bath (mimicking the patient), but the introduction of an ionisation chamber itself affects the dose pattern. To ensure accurate measurement we simulate in detail the movement of the proton particles through the geometry of the water bath and the ionisation chamber.

The software uses the Monte Carlo method, in which the paths of a large number of particles are simulated. For each particle history, the simulation is based on the same interaction data, but random numbers control one or more of the interaction parameters, resulting in a different path for each individual particle.

The Monte Carlo simulation of ionisation chamber response is slow since:

1. a large number of particles must be simulated in order to lower the statistical fluctuations on the result below a pre-set limit;
2. the sensitive volume of an ionisation chamber is a small mass of air and the simulation needs a lot of particles interacting in this volume to achieve the desired accuracy;
3. the volume of an ionisation chamber is small compared to the size of the radiation field, which makes the calculation inefficient.

The distributed system allows us to generate a database for a large set of ionisation chamber types and proton beam energies, which would previously have been impossible.

Table 1 shows typical times to calculate the ionisation chamber response with a statistical uncertainty of less than 0.05% for some specific proton energy levels using the Monte Carlo code McPTRAN.CAVITY.

The number of particle histories needed was dependent on the beam energy, and the number of jobs for each simulation was determined such that the average calculation time of one unit was about one hour. From Table 1 it is obvious that, for these simulations, splitting a calculation into a larger number of work-units is more efficient – provided that the calculation time per work-unit is large compared to the system overhead time.

Modelling the behaviour of materials

Mathematical models are used in many areas of materials science, and often rely on ‘black box’ software in which the underpinning mathematics is hidden from the user. Commercial finite element software packages that are used to model material behaviour are good examples. To investigate how output quantities change as material input parameters are varied in these models requires a process of numerical experimentation, where the model is re-run for a range of input parameters, and the model outputs are recorded.

With complex models it is necessary to analyse a large range of cases that adequately represent the uncertainties associated with the input parameters. Such models may take a long time to reach a solution, and there may be insufficient time or computing resources available when operating in serial mode.

It can become difficult to compare the results of these models against experimental data. Additionally if a result of required accuracy is needed it is not clear how accurate the material property needs to be to guarantee this outcome.

Using distributed computing it is practicable to assess the input sensitivity of such models. A new project on uncertainty propagation in mathematical models of materials will identify the contribution that distributed computing methods can make to the study of the sensitivity of the output of complex models to changes in input parameters.

It can prove uneconomical to use commercial software in a distributed computing environment owing to the large number of licences required. However, negotiations with one software supplier have enabled NPL to obtain enough licences to run a commercial finite element package on the distributed computing system, and this will be studied under the new project.

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From *University of Genova* – UNCERT – A Package for the Probabilistic Expression of Measurement Results

The possibility of expressing the final result of a measurement with a probability distribution over the set, discrete or continuous, of the possible values of the measurand, is a very attractive option for metrology.

So at the Measurement Laboratory – University of Genova – DIMEC, Italy, (see www.dimec.unige.it/ PMAR/ pages/ research/measurement/ measurement.htm) a package, UNCERT, has been developed, within the EU Network AMCTM (see www.amctm.org), with the aim of providing the metrologist with a set of tools giving full support in that task.

The package is organised on the basis of a hierarchy of models, which allows a highly modular design, and is based on direct calculation of involved probability distributions, treating all variables as discrete. It has been developed according to quality assurance criteria, validated by wide testing, and is intended to be proposed as a *standard tool* for this kind of calculation. The expression of measurement results in probabilistic terms may be particularly beneficial whenever risk assessment or cost evaluation is required.

The package is at present not commercially available, but selected test cases from qualified laboratories may be submitted for treatment by contacting the authors.

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From *University of Huddersfield* – Standard surface texture parameters

An ESPRC CASE student project sponsored by NPL, at the University of Huddersfield, concerns the development of algorithms and software to compute standard surface texture parameters accurately with elements of numerical safety.

Two papers are available (see scom.hud.ac.uk/scomjkb): the first is an extended abstract of the project, and briefly details work completed, while the second is a research report concerning the ambiguities in the amplitude parameter set from ISO 4287: 1997.

The work described in these papers is timely because in a number of recent comparisons of surface texture measurements an alarming spread in the results has been shown, and it is difficult to say whether such variations are due to the instrument performance, the variation in shape over the surface or the software employed to calculate the parameters.

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From *PTB* – Measurement Data Security: PTB strengthens its activities

Owing to the growing involvement of communication technology in measuring systems, the security of measurement data has become an important issue in metrology.

In particular, it is crucial when the underlying communication system turns out to be less secure than required in certain metrological applications. PTB has taken up the challenge by carrying out collaborative research and development projects with German industry.

One project, SELMA (Secure electronic exchange of measurement data), is primarily devoted to the exchange of meter data in the framework of legal metrology. The technology developed, however, is applicable to other areas (see www.selma-project.de).

Another project, SIMEDAKO (Secure measurement data communication), is oriented to the application of the WLAN standards 802.11x in measuring systems. Depending on the version of the standard used, the currently spreading WLAN technology may cause security problems, and needs therefore special attention (see www.simedako.de).
Both projects are funded by the German Government.

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Mesopic photometry

Photometry is concerned with the measurement of light in terms of human visual spectral sensitivity, i.e. in terms of how objects appear to a human observer.

The eye reacts differently to light at different wavelengths and its performance can be modelled in terms of a spectral luminous efficiency function $V(\lambda)$ that gives the efficiency of the eye response as a function of wavelength λ; see figure 4. In theory, the visual response to a given stimulus can be estimated by weighting the spectral density associated with the stimulus by the efficiency curve.

The eye response depends on the ambient light conditions and on the location of the stimulus in the field of vision. Research has shown that at low light levels (scotopic conditions), the eye responds better to blue light, relative to its response in bright light (photopic) conditions. This shift can be seen in the photopic efficiency curve $V_P(\lambda)$ and the corresponding scotopic curve $V_S(\lambda)$ in figure 4. The differences are due, at least partly, to the fact that the retinal cones are active in bright light but only the rods are active in low light conditions. The third curve $y_{10}(\lambda)$ in figure 4 is an estimated efficiency curve in photopic conditions for visual responses to stimuli 10° away from the line of sight. The difference between $y_{10}(\lambda)$ and $V_P(\lambda)$ reflects the fact that the cones are concentrated in the foveal (line of sight) region of the retina and the rods in the periphery.

While there is much research and reasonable consensus about visual response in photopic and scotopic conditions, the response in mesopic, i.e., half-light conditions, is less well understood. Mesopic photometry is of particular importance to lighting engineers providing street lighting, for example. NPL is taking part in a European project, led by Helsinki University of Technology, looking at mesopic photometry in relation to night time driving in urban environments. The research focuses on three questions: 'Can it be seen?', 'How quickly?' and 'What is it?'. A suite of experiments have been undertaken to record, for example, reaction times for different stimuli with different spectral content in a range of ambient light conditions. The main output from the project will be one or more efficiency curves for mesopic conditions that will allow lighting engineers to assess the effectiveness of lighting schemes. The SS*f*M programme is involved, through the data fusion project, in modelling the various experiments at different laboratories and analysing the resulting data gathered from a large number of observers.

Figure 5: Apparatus used to determine reaction times to visual stimuli in varying ambient light conditions. Courtesy of City University.

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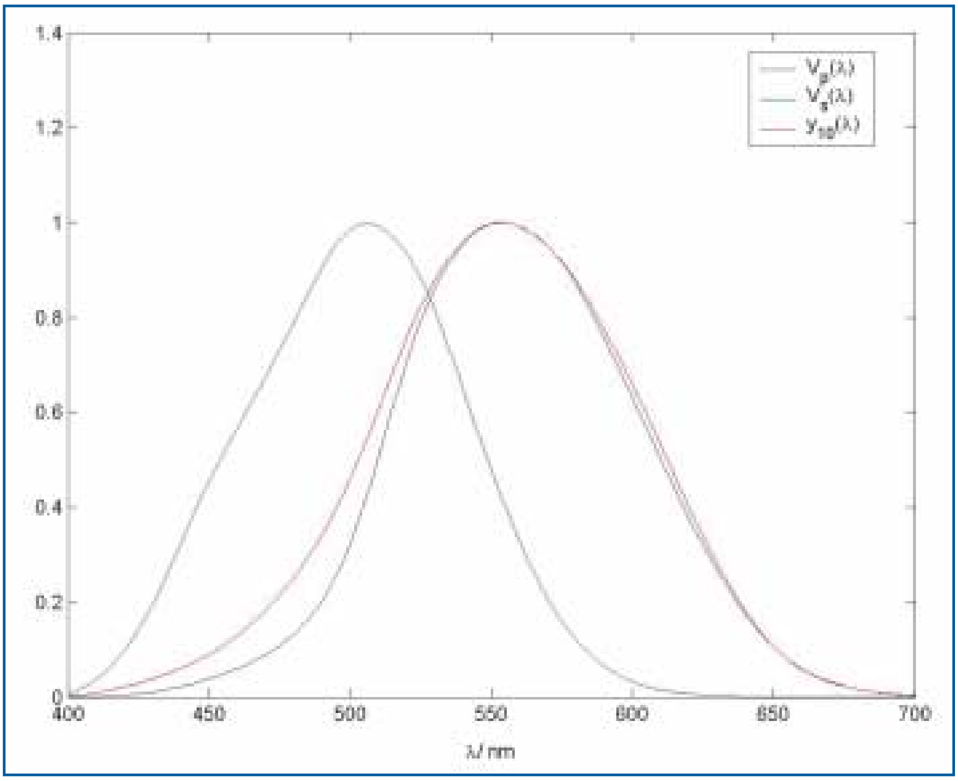

Figure 4: Examples of spectral luminous efficiency

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Dr. Brian Ford OBE retires

Dr. Brian Ford OBE, Director of the Numerical Algorithms Group Ltd., retired in July 2004.

NAG has been a major subcontractor to SS*f*M, and is expected to continue to provide valuable support to the programme. Brian has given invaluable service on the SS*f*M Working Group of the DTI's Measurement Advisory Committee. He was awarded the OBE for his work in building up NAG Ltd. from its inception in 1970 to become the world's foremost provider of top-quality mathematical software libraries.

A special one-day technical meeting under the title "NAG and Numerical Software – Achievements and Challenges" was held on 16 June 2004 at Oxford University, to mark Dr. Ford's retirement. Professor Maurice Cox delivered an invited address at the meeting with the title "NAG and NPL over the years". He concentrated on the collaboration between NAG and NPL over three and a half decades, covering the NPL contributions to the NAG Library in areas such as linear algebra, optimisation, data approximation and graphics, the Wilkinson Prize for excellence in numerical software, joint publications and co-organised conferences, and most recently the SS*f*M programme.

Dr. Ford will become a consultant to NAG Ltd., and it is anticipated that NPL and the SS*f*M programme will continue to benefit from his advice.

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Forthcoming Events

6 - 7 December 2004, NPL
Developing Software for Measurement
Contact: ssfm@npl.co.uk

8 December 2004, IEE Wheatstone Discussion Meeting focusing on "Measurement uncertainty in an industrial context".
Contact: www.iee.org/events/wheatstone.cfm

19 - 22 April 2005, Institute of Physics, London
The 4th CCM International Conference on Pressure Metrology from Ultra-High Vacuum to Very High Pressures
Contact: jasmina.bolfek-radovani@iop.org

18 - 20 May 2005, Advanced Industrial Science and Technology Institute
Second Workshop on the Impact of Information Technology in Metrology
Contact: alistair.forbes@npl.co.uk

20 - 23 June 2005, Lyon, France
12th International Metrology Congress
Contact: info@cfmetrologie.com

25 July 2005, Centre for Precision Technology, University of Huddersfield, UK
Seminars on the History and Future Prospects in the Field of Measurement Technology and Intelligent Instruments
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