ISSUE 13 • SPRING 2003

Counting on IT

MATHEMATICS AND SCIENTIFIC COMPUTING

Progress made on Continuous Modelling projects

NPL has made progress on SS*f*M-2 projects 1.4 (continuous modelling for metrology) and 2.2 (testing continuous modelling software). The aim of project 1.4 is to provide guidance on using continuous modelling techniques in metrological applications, with particular emphasis on model validation and uncertainty determination. Project 2.2 aims to provide methods of testing continuous modelling software, and its deliverables will include the results of tests run on commonly used finite element packages.

The first step in the projects was to determine

- the uses of continuous modelling in metrology,
- methods and software packages being used,
- where more guidance is needed

This was done using an on-line questionnaire (available until December 2002) from the SS*f*M website. (Paper copies can still be obtained by contacting louise.wright@npl.co.uk)

The responses to this questionnaire have helped define the direction of the future project work. Respondents seemed particularly interested in

- knowing the accuracy of their models,
- improving their model validation methods,
- using their models to determine uncertainties.

These three concerns are strongly linked, since both validation and uncertainty evaluation involve assessing the accuracy of results. Issues connected with these concerns are now being investigated, and

continued on page 2

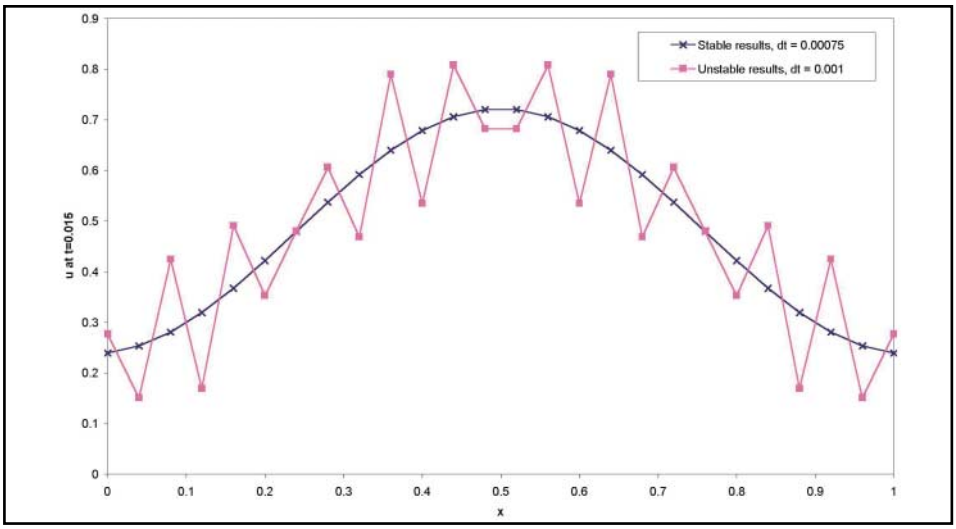


Figure 1: Two calculated solutions to the one-dimensional heat equation. Both calculation methods passed a check for conservation of energy, but one was generated using an unstable time step.

Contents

NPL National Physical Laboratory

Progress made on Continuous Modelling projects *(continued)*

information about suitable techniques that address them will be included in the project deliverables.

The model validation deliverable suggests a range of techniques suitable for validating continuous models, and illustrates the pros and cons of each technique with simple examples. A well-validated model will generally have been checked using several techniques so that the deficiencies in one method will be covered by the strengths of a different one.

An example of this is shown in figure 1, which shows two calculated solutions to the one-dimensional heat equation. Both methods used to produce these results passed a check for conservation of energy, but the method producing the oscillating results failed a check for a stable time-step. If conservation of energy had been checked but time-step stability had not, the oscillating results may have been accepted erroneously.

The development of a testing methodology for continuous modelling software is now well advanced, and work has begun on using simple benchmark examples to test the accuracy of popular packages. The methodology consists of two parts: simple tests for the correctness of element formulation, and larger tests of the matrix algebra, preferably using problems that can be parameterised so that a measure of degree of difficulty can be estimated.

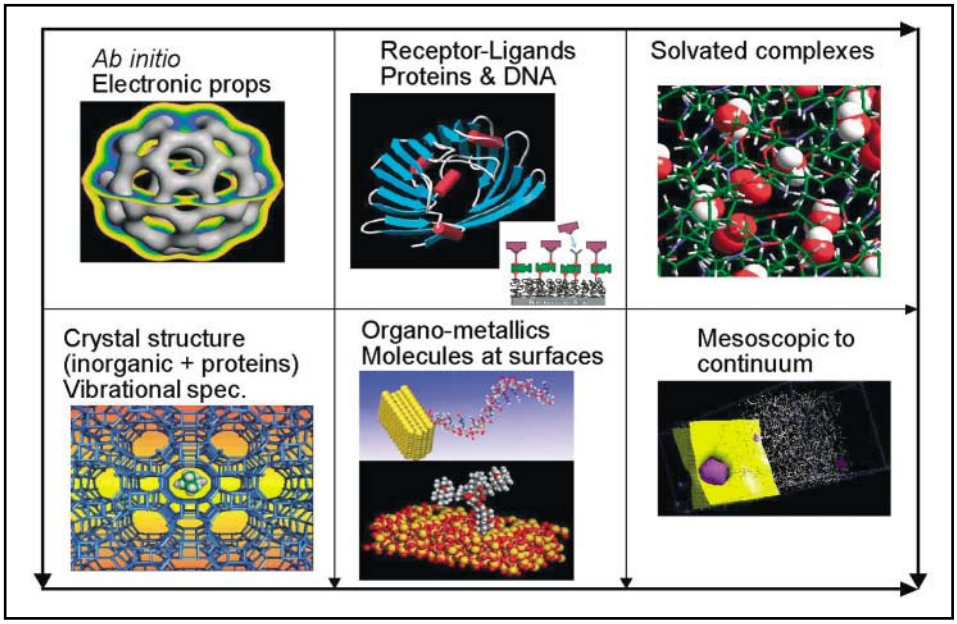
There are opportunities for SS*f*M Club Members to gain an early benefit from the projects. Several of the reports will require input from regular users of various packages, either by running small software tests on a packages or by briefly describing their experiences of the package. Anyone contributing to the project will receive draft copies of the relevant deliverables prior to publication. Members wishing to be involved should contact Louise Wright.

For further information contact:
Louise Wright, extension 6466
e-mail: louise.wright@npl.co.uk

Multiscale Modelling: a new challenge for physicists and mathematicians

One of the most important questions facing metrologists, particularly those working in nanotechnology, biotechnology and materials science, is the problem of validating and testing mathematical models which describe phenomena that manifest themselves over several length and time scales. The understanding of multiscale phenomena, especially those properties of matter that are sensitive to structure, poses a significant challenge to physicists and mathematicians. As micro-electro-mechanical systems (MEMS) and nanoscale devices become commonplace in metrology, understanding materials behaviour over a range of length scales is essential if one wishes to develop reliable models of device performance. This is one of the main conclusions from a study of "New Directions in Mathematics and Scientific Computing", which forms part of the current SS*f*M programme formulation exercise.

The aim of multiscale modelling is to predict the behaviour of complex materials, including biomaterials such as proteins, across a range of length and time scales. At the molecular scale, quantum mechanics methods are required to describe the interactions between atoms and electrons. As one moves from the atomic scale towards the macroscale in solids, for example, the performance at the micrometre scale is governed by the behaviour of defects and dislocations. At the next larger scale, the effects of grain boundaries and ensembles of defects become important. Finally, at the macro or continuum scale, the behaviour of materials may be dominated by environmental or loading factors such as applied stresses or temperature gradients.



Graphical demonstration of the range of problems to which multiscale modelling can make a contribution, from the electronic scale of ab-initio methods to the meso- and continuum scale and from the study of DNA and proteins, to crystal structures, and to bulk materials properties.

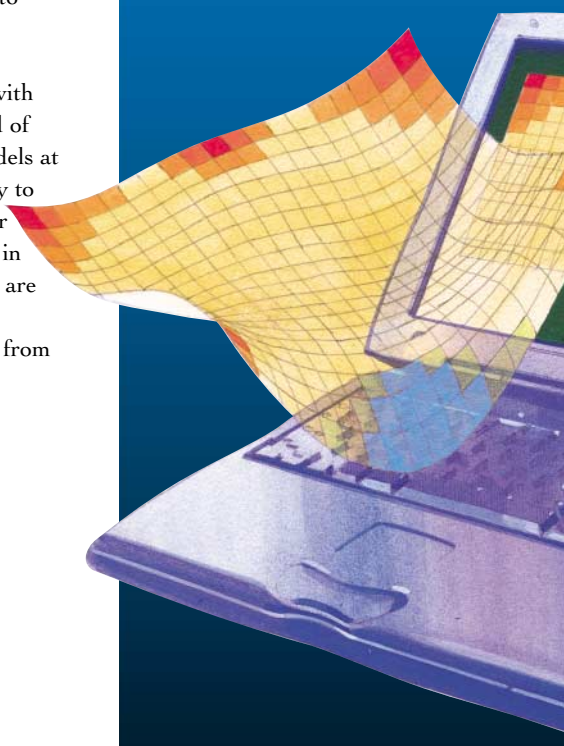
The key questions for mathematical modellers are:

- how does one develop a range of computational techniques which can tackle this wide range of scales?
- how does one ensure that the results of modelling at one length (or time) scale can be connected to results at the next higher or lower scale?

Ideally one would like to begin at the quantum mechanical level and perform calculations on electrons and nuclei, using only the tools of theoretical physics, that is, knowledge of the particles present and the interactions between them. In the past, such calculations could only be performed for relatively small systems, but modern computing developments have made them tractable for large systems of atoms and molecules, usually with the employment of various approximation methods. Currently researchers are developing new quantum-mechanics-based modelling techniques for simulating large systems containing many thousands of atoms.

Such large quantum mechanics systems are still a long way from what is required to understand materials at the micro and mesoscales. The final goal is "seamless modelling from atoms to structures", with quantum mechanics models at one end of the length scale and finite element models at the mesoscale and beyond. On the way to this goal mathematicians and computer engineers will have a vital role to play in ensuring that computational resources are used efficiently and that the results of models can be trusted and transferred from one length scale to the next.

For further information contact:
Trevor Esward, extension 6883,
e-mail: trevor.esward@npl.co.uk



SSfM Training Courses

Several training courses have been developed during the current and previous SSfM programmes. In the past we have tended to run a course as soon as it has been developed, and then repeat it only if there is a particular demand. This year we have decided to do things differently – we are planning a schedule of eight SSfM courses in which each will be run at least once.

We will be running the courses at NPL as follows:

- *Visualisation of data*, delivered by Sira Ltd & NAG Ltd, 11 June 2003. This is intended for metrologists and others who need a greater understanding of their data, particularly physically-based data, and who are interested in maintaining accuracy in visualisation.
- *Software validation in measurement systems*, delivered by NPL, 18 June 2003. This focuses on software to be embedded within scientific instruments or measurement systems.
- *Discrete modelling and data fitting*, delivered by University of Huddersfield, 24-25 September 2003. This is aimed at scientists & engineers involved in experimental data analysis.
- *Testing numerical correctness of scientific software*, delivered by NPL, 2 December 2003. This will give insight into the importance of numerical correctness of scientific software and how to conduct objective testing to ensure fitness for purpose.
- *Uncertainty evaluation and associated statistical modelling*, delivered by NPL, 19-20 January 2004. This is directed at practitioners concerned with more difficult measurement models. It is a more advanced course than those offered by UKAS or NWML.
- *Development of measurement software*, delivered by Adelard, two-day course, 10 - 11 November 2003. This is aimed at developers of virtual instrument software for controlling equipment, especially for users of LabView or Visual Basic.
- *Scientific computing in FORTRAN 90/95*, delivered by University of Hertfordshire, two-day course, date to be announced. This is intended for scientists & engineers involved in developing algorithms & software for scientific computation.
- *Reliable numerical computing*, to be delivered by lecturers drawn from NPL,

The SSfM Club

The Spring Meeting

The spring Club meeting was hosted by NAG Ltd, Oxford, on 4th March 2003, and had a slightly different flavour from previous meetings. The theme for the morning session was formulation of the next SSfM programme, reflecting the fact that the consultation phase of formulation had begun. Following presentations describing new directions in mathematics and scientific computing, and formulation topics, there was a very useful open discussion on potential projects for the 2004-07 programme. The other main themes of the meeting were numerical analysis and modelling. Feedback from the 20 attendees showed widespread agreement that the formulation discussion was most useful. The full report on the meeting can be found at www.npl.co.uk/ssfm/news/events/20030304/report.html.

"There are currently 38 full members"

Membership fees and Privileges

Membership categories and fees were revised in December 2002. UK membership is now set at £180 + VAT, but UK organisations numbering fewer than 250 people may join at a preferential rate of £140 + VAT as SME (small and medium enterprise) members. For non-UK members, the fee remains at £180 + VAT. SSfM collaborators in other NMIs and members of NPL or NMSD enjoy free Club membership.

Membership is for a named person, but members and collaborators may nominate any number of persons from their organisation to become associate members free of charge. One associate member may attend a Club meeting in place of the named member free of charge. Associate members may also attend in addition to a member for a fee of £75 + VAT.

UMIST and University of Huddersfield, date to be announced. This is a companion course to the FORTRAN 90/95 one.

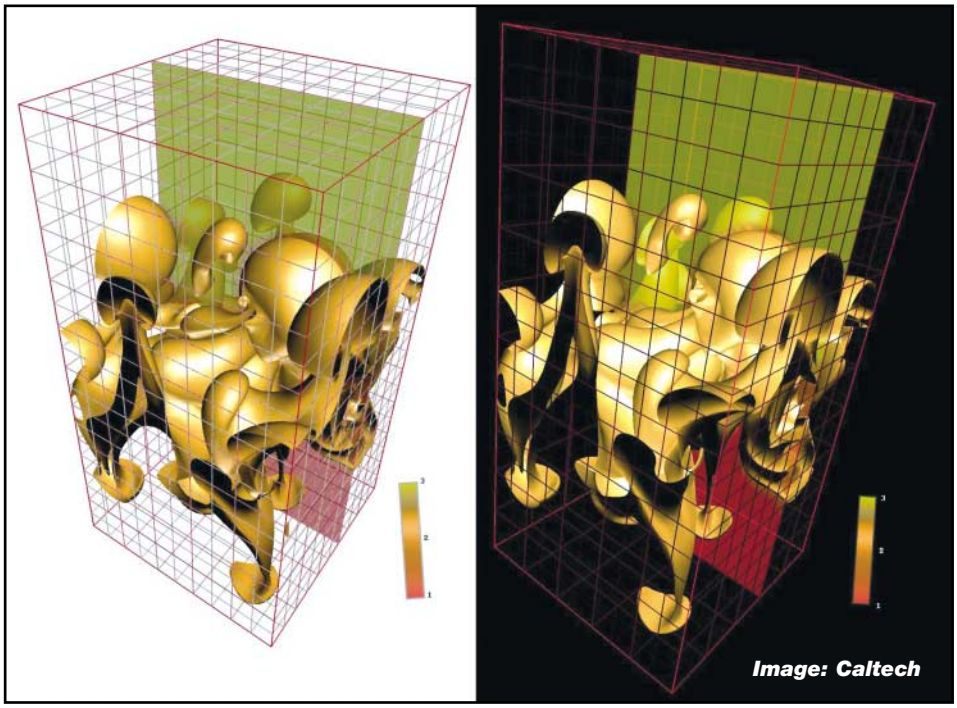
The prices range from £400 + VAT for a one-day course to £900 + VAT for a 2½-day course, with corresponding SSfM Club discount prices ranging from £350 + VAT to £810 + VAT.

Further information on course content, schedule and prices can be found on the SSfM website at:

www.npl.co.uk/ssfm/training

We are also willing to run any of these courses at customers' premises on request.

For further information contact:
Jan Kane, extension 7100,
e-mail: ssfm@npl.co.uk



Visualisation of data: Simulation of Rayleigh-Taylor instability in the interface between two fluids. The upper fluid has a density of 3 units, the lower has a density of 1 unit, and the isosurface has been calculated for a threshold value of 2; thus, it follows the fluid-fluid interface, irrespective of its shape. The characteristic loops, spikes and bubbles in the surface are clearly shown in these two views of the cell at a given time step.

There are currently 38 full members, 69 collaborators, 80 associates, and 108 NPL/NMSD members, all of whom have privileged access to the Club Members' Page, allowing the downloading of draft and final reports, usually six months before they go public. Members also have access to data generators for testing the numerical correctness of software for some generic calculations used in metrology.

Members will receive new editions of the SSfM Roadmap CDROM, containing all the outputs of the SSfM Programme to date, whenever they are published. (The next one is due around Summer 2004.) In addition, members can obtain, by request, the NPLFit CDROM. NPLFit is a graphical user interface-based package, developed at NPL, for fitting calibration curves to experimental data using polynomials and splines, and evaluating uncertainties associated with fitted values.

The full list of Club benefits can be found on the Club website: www.npl.co.uk/ssfm/club. We look forward to welcoming you as a member if you have not yet joined.

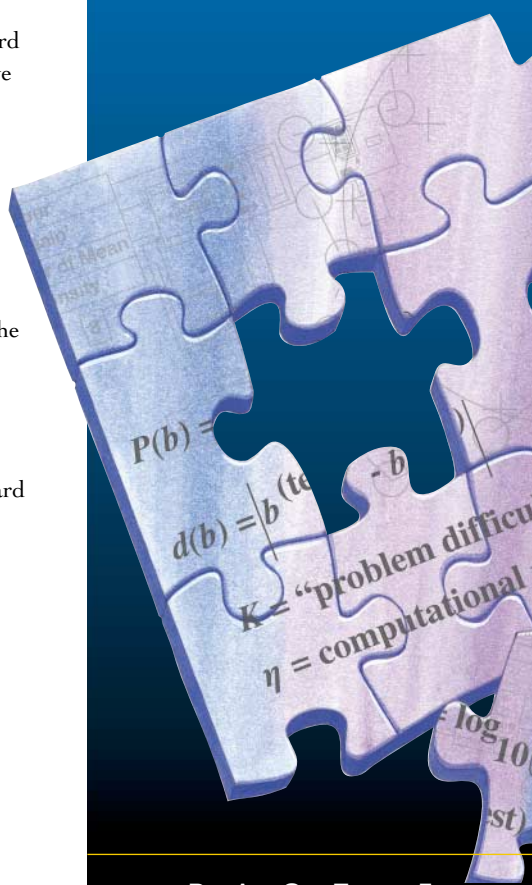
Articles for Counting on IT

Members may submit short articles for publication in this Newsletter. These should be e-mailed to mike.stevens@npl.co.uk. They must be relevant to SSfM. Publication will be at the discretion of the editor.

Future Meetings

Offers from Club members to host future Club meetings are welcome. To put forward your organisation as a potential host, contact Wendy Johnson via e-mail at ssfm@npl.co.uk.

For further information contact:
Ian Smith, extension 7071
e-mail: ian.smith@npl.co.uk



From *Analyticon Ltd.* - The Analytic Pointing Performance (APP) Software Tool & the European Space Agency (ESA) Pointing Error Handbook

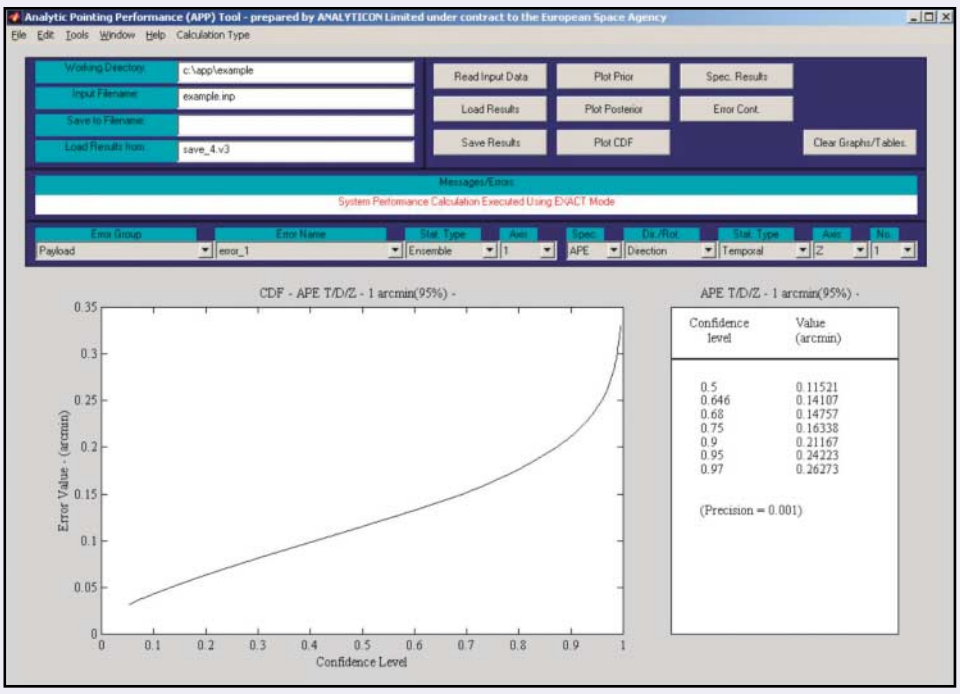
The problem of the statistical analysis of spacecraft pointing error performance has long been recognised within the European Space community, resulting in the development of a rigorous set of statistically correct procedures documented in the ESA Satellite Pointing Error Handbook. These methods are comprehensively implemented in APP, a software package that combines the effects of all identified sources of payload pointing error to produce overall pointing performance to stipulated confidence levels. Features include:

- Simple & consistent pointing budget management.
- Support for a wide range of component error PDFs.
- Full implementation of the Maximum A Posteriori (MAP) technique for combining PDFs with measured data.
- Use of statistically rigorous error combination methods, avoiding over- or under- design.

The methods within APP are generally applicable to statistical problems in science & engineering. For more information, please see www.analyticon.co.uk/APP_page.htm.

Contact:
Dave Dungate: +44 (0)1438 749886
e-mail: dave.dungate@analyticon.co.uk

Envisat



Screen shot showing the APP user interface

Software for Humidity Calculation

The support for humidity data analysis project is looking at software implementations of humidity calculations and conversions, where there are numerous quantities and units in use. To compare values of dew point with concentration units requires valid and accurate data in a usable form. As the graph in figure 2 shows, using three different software packages apparently to make the same calculation gives three different results.

The project aims to advise on suitable test data and methods, so users will be able to assess the fitness-for-purpose of humidity calculation packages, both purchased and written in-house.

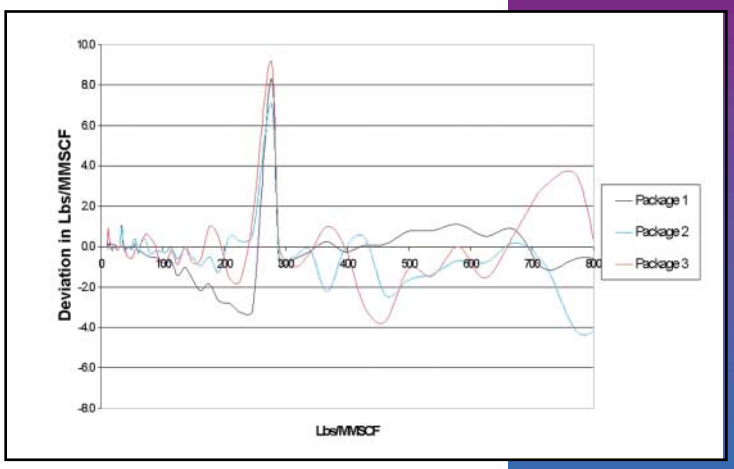


Figure 2: Deviation from ASTIM Tables for Moisture in Natural Gas of Three Different Software Packages

For further information contact:
Richard Gee, extension 6710
e-mail: richard.gee@npl.co.uk

SS*f*M-3 Formulation

The process of formulating the next SS*f*M programme, to run from April 2004 to March 2007, is now well underway. DTI contracted PA Consulting to produce a "Trend spotting forward look" study, the results of which were presented at the "Orientation" meeting held at DTI on 14 January. This study identified the political, social, economic and technological drivers that SS*f*M should respond to. It identified the following topics for future SS*f*M activity:

- Internet-enabled metrology services
- Distributed computing
- Digital signal processing
- Embedded software validation service
- Data management and visualisation
- Modelling of complex problems
- Support for the CIPM mutual recognition arrangement
- Measurement uncertainty for regulatory compliance
- Support for soft metrology

In addition, we had the results of the New Directions project, with its five studies on:

- Support for Legal Metrology
- Digital signal processing
- Mathematics and computing
- Bioinformatics
- Support for Soft Metrology

Given these inputs, we embarked upon a consultation (requirements capture) phase that ran from February to the end of April. During this time we held a discussion at the SS*f*M Club meeting hosted by NAG Ltd on 4 March. We also held two open consultation meetings. The first at NPL on 10 March gathered requirements from other NMS programmes. The second hosted by Druck on 1 April gathered industry and public sector requirements.

Throughout this period we also collected views through a questionnaire on the SS*f*M website. This grouped the possible topics into the following categories:

- Modelling techniques
- Modelling tools
- Uncertainties and statistical techniques
- Data handling
- Validation
- Software development guidance
- Standards
- Networks
- Soft metrology
- Generic knowledge transfer

continued on page 8

SSfM-3 Formulation *(continued)*

We have been keen to identify projects that could be jointly funded by other NMS programmes or contributed to by industry or public sector users. Typically, this would mean generic work being funded by SSfM and application specific work being funded by the other NMS programme or contributed to by the industrial or public sector user.

This consultation phase will culminate in a presentation to DTI and their advisory group (MAC WG) at the SSfM Annual Review on 22 May. The presentation will cover the rationale, benefits and deliverables for roughly over 200% of the size of the eventual programme. Following this, the scope will be reduced to 115% of the final size and a public consultation document will be produced and mounted on the DTI and SSfM websites. "Public consultation" is expected to run from July to September.

Formulation is brought to a conclusion in the "Appraisal" meeting, probably in November, when DTI and their advisory group decide how to bring the 115% down to 100%. They will also decide which projects should be put out to competitive tender.

The final programme document will then emerge by about January 2004 and will be presented together with supporting documents for Ministerial approval.

For further information contact:
Dave Rayner, extension 7040,
e-mail: dave.rayner@npl.co.uk

Forthcoming Events

8-11 September 2003, CNR, Istituto di Metrologia, Torino, Italy
Advanced Mathematical and Computational Tools in Metrology (AMCTM 2003) conference

Contact:
Maurice Cox, extension 6096
e-mail: maurice.cox@npl.co.uk

14 October 2003, NPL
SSfM Club Autumn Meeting

Contact:
Wendy Johnson, extension 6106
e-mail: wendy.johnson@npl.co.uk

Centre for Mathematics and Scientific Computing (CMSC)
Making contact

You can contact any of the experts directly by using the direct dial number plus the extension or via e-mail.

Direct line +44 20 8943 + (extension)

Head of CMSC
Dave Rayner ext 7040 e-mail: dave.rayner@npl.co.uk

Software Support for Metrology Club
Wendy Johnson ext 6106 e-mail: ssfm@npl.co.uk
SSfM website: www.npl.co.uk/ssfm

If you have a general enquiry or do not know who you should contact please call our general enquires number and we will be pleased to help you.

General CMSC enquiries
+44 20 8943 7100 (direct line)
+44 20 8977 7091 (facsimile)
Website: www.npl.co.uk/cmsc

General NPL Helpline
For enquiries to NPL outside the scope of CMSC, please use:
+44 20 8943 6880 (NPL Helpline)
+44 20 8943 6458 (Helpline facsimile)

National Physical Laboratory
Queens Road, Teddington, Middlesex, UK, TW11 0LW

NPL/Aaron15523/2K/0503