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New Directions – Future Directions in Mathematics and Scientific Computing: recommendations for the Software Support for Metrology programme 2004-2007

T J Esward, A B Forbes, A J Mansfield
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ABSTRACT

New developments in applied mathematics and computing are reviewed to identify the research that will be needed to meet future challenges within the National Measurement System. Topics under review include simulation, modelling over more than one length scale, molecular modelling, distributed computing, parallel co-ordinate systems, risk and uncertainty, and data mining. In each case, new research areas are suggested for the Software Support for Metrology programme that are of importance to metrologists and the report identifies the key mathematical challenges that those new topics present. Each section of the report makes specific recommendations for activities that might be undertaken in the next Software Support for Metrology programme.

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

Approved on behalf of the Managing Director, NPL
by Dr Dave Rayner,
Head of the Centre for Mathematics and Scientific Computing

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1. INTRODUCTION

1.1 THE BACKGROUND

This report sets out the conclusions of a study into new developments in mathematical and software engineering research that will be needed to meet future challenges within the National Measurement System (NMS). It forms part of the "New Directions" project, in the current Software Support for Metrology (SS*f*M) programme. The "New Directions" project encompasses a wide range of topics: legal metrology, digital signal processing, bioinformatics and measurements for biotechnology, soft metrology, and the subject of the current report, future directions in mathematics and software engineering. Separate reports are being produced for each of the five topic areas and it is the intention that each report should stand alone and that overlap between the topic areas should be avoided. The intention is that the reports should provide useful input to the process of formulating the 2004-2007 SS*f*M programme. Further information about the SS*f*M programme can be found at the website address: www.npl.co.uk/ssfm/.

1.2 METHODOLOGY

During the formulation of the current SS*f*M programme, a number of potential topics were identified for the subject of this study, including for example, optimisation methods, analysis of data from remote sensors, data mining, and the analysis and simulation of chaotic systems. Since then two significant events occurred which led to the re-appraisal of the original list of topics.

The first of these was the publication in April 2002 of a report by the Smith Institute entitled *Mathematics: Giving Industry the Edge* [6]. The Smith Institute is a Faraday Partnership organization, supported by the Department of Trade and Industry and the Engineering and Physical Sciences Research Council, which aims to build links between industry and academics to tackle applied mathematical and computing challenges that are faced by UK industry. Their report, which the Institute characterizes as a "roadmap", aims to identify the needs of UK industry over the next ten-year period for new developments in mathematics and computing.

The second important event that influenced the range of topics to be discussed in this report was an internal strategic research review of mathematical modelling activities at NPL. The review, which was carried out by a group of senior scientists representing all NPL's scientific centres, recognised that there was a planned strategic growth in NMS programmes in nanotechnology, functional materials and measurements for biotechnology (the subject of a separate New Directions study) and that this growth would lead to new mathematical challenges. For example, one key problem highlighted was the need to be able to produce mathematical models that are valid for more than one length scale, the aim being to carry out what has been characterized as "seamless modelling from atoms to structures".

In addition to these two specific sources, recent reviews of the relationship between mathematics and industry in the USA were studied (SIAM [7], Wright and Chorin [9]). The analysis set out in these reports, particularly the report by Wright and Chorin, identified as future mathematical challenges many of the topics discussed in the Smith Institute roadmap and thus helps reinforce many of the Institute's conclusions.

Other sources of information that have been taken into account include DTI's e-Science Grid Outreach programme and the outcomes of recent conferences on future trends in mathematics and metrology, for example, the September 2002 joint BIPM/NPL workshop on the *Impact of Information Technology in Metrology*. Finally, during the drafting stage, the key conclusions of this report were made known to representatives of industry, academia, and within NPL, to obtain comments and suggestions, and to ensure that the conclusions had a measure of general support.

1.3 STRUCTURE OF THE REPORT

The report contains chapters on the mathematical and software challenges in the fields of simulation, modelling over more than one length scale, distributed computing, the understanding of multi-variate data sets, risk and uncertainty, and data mining. The aim has been to avoid defining detailed work packages or project milestones, but rather to suggest new topic areas for the SS*f*M programme that are of importance to metrologists and to identify the key mathematical challenges which those new topics present. Nevertheless, each chapter makes specific recommendations for activities that might be undertaken in the next SS*f*M programme and these recommendations are summarised in the final chapter of the report.

2. SIMULATION

The Smith Institute roadmap [6] identified simulation as an essential component of modern science and engineering, particularly given the development of cheaper and more powerful computers, so that simulation is used not only to support but often to replace experimentation. The traditional manner in which scientists and engineers attempt to validate their theories and the results of model predictions is the comparison of theoretical predictions with experimental results. When no experiment exists or when the modelling and simulation is done to replace experimental work, this practical approach to validation is no longer available. However, there is a continuing need for greater physical realism in simulations, the Institute argued, but many simulations lack sufficient realism because good models do not exist, or because model data are uncertain or incomplete. However, as the report's authors point out, improving the realism of a simulation usually leads to a longer time being needed to carry it out. Expensive models on fine scales often need to be replaced with effective coarse-scale descriptions when computation on the fine scale is not feasible. Thus, hierarchical models may be of use so that a small, fine-scale simulation may be used to verify a much larger coarse-scale model.

In industry traditional approaches to new product development have involved the use of the 'make and test' philosophy, which necessitates expensive and time-consuming activities of prototype manufacture and testing, followed by a number of design iterations. It has long been recognised by industry that competitiveness could be substantially improved if it were possible to develop computer-based methods of modelling, simulating and optimising the manufacture and performance of products before prototypes are manufactured. Such simulations are currently wide-ranging, for example, casting of metals, impact assessments of vehicles, gait analysis of the human form, to name a few. Simulation is also used to train humans in complex tasks, for example, flight simulators for the training of aircraft pilots. Such simulations lead to the need to generate realistic 'virtual worlds' through the use of virtual reality (VR) software.

2.1 SIMULATION IN METROLOGY

Two examples of the current use of simulation in metrology at NPL are provided by the Watt balance project and by the Monte Carlo simulation of ionising radiation processes in NPL's Centre for Acoustics and Ionising Radiation (CAIR).

2.1.1 WATT BALANCE

A Watt balance is currently regarded as providing the most accurate method of comparing electrically generated and gravitationally generated forces. The outcome of this comparison is a highly accurate determination of the Planck constant. Once the value of the constant has been fixed, the balance also provides a means of realising the kilogram without reference to an artefact such as one of the copies of the standard kilogram that is currently maintained at the BIPM in Sèvres, France. NPL's Watt balance project has been running for many years and is now close to realising its aim of being able to establish the kilogram to an uncertainty of one part in 10^8 or better. Whether this aim can be achieved or not depends crucially on improvements in the technical and engineering quality of the Watt balance. With the support of the DTI, NPL is aiming to carry out the necessary improvements between now and 2005.

Mathematical simulation of the Watt balance apparatus is crucial to the achievement of the project's technical objectives. The key component in the Watt balance is the electrical coil and magnet system and it is essential to know the forces and torques exerted on the coil as a result of the applied magnetic field. The potential torques and velocities that arise from misalignments are important both in setting up and operating the balance and in the assessment of measurement uncertainties. These effects are believed to be the main source of the drift in measurements that has been observed in recent years. A mathematical simulation of the behaviour of the balance coil in applied magnetic fields is required and initial work has begun to establish such a model using the computing algebra software *Mathematica*. Analytical solutions are required which can accurately predict the forces and torques on real coils from variations in the applied magnetic field. Future work required for the Watt balance project includes the simulation of the effect of a magnetic shield to be used to surround the magnet and coil to try to eliminate the effects of stray magnetic fields. It is likely that commercial finite element software will be employed for this simulation. Finally, simulations of thermal and mechanical processes will be needed to support the engineering design of the laboratory's temperature control system and vibration isolation system.

The observed variation in Watt balance measurements is very small when consistent experimental procedures are adopted. The purpose of the simulation work described in this section of the report is to identify and quantify systematic effects, which are often those of most interest to the metrologist who is attempting to design high-quality measurement equipment and systems.

The key mathematical issues that arise from Watt balance work are:

- How does one validate simulations of complex experimental systems, especially when those systems may be unique?
- Minimising sources of uncertainty for primary measurement standards can be an extremely challenging task. If simulations are to be used in helping to establish uncertainties, what contribution to uncertainty budgets do simulations themselves make?
- The simulations frequently rely on the output of complex commercial software packages. What contribution to the "simulation uncertainty" arises from the use of these software packages? The current SS*f*M programme is studying methods of validating continuous modelling software, and in particular finite element and finite difference software. This work should be extended to cover other software packages that are in common use in metrology.

2.1.2 VISUALISATION IN IONISING RADIATION AND MATERIALS METROLOGY

Virtual reality technology is now being used very widely to assist in the presentation of the results of mathematical models. At NPL, for example, NPL's Materials Centre (MATC) has itself developed a 'virtual testing' system for composite laminates that enables scientists and engineers to use their PCs (over the web) to define laminates, observe them using 3D visualisation techniques, and to generate the engineering properties that they need for design.

A specific application of the combined use of simulation and visualisation methods at NPL is provided by the numerical dosimetry group in the Centre for Acoustics and Ionising Radiation (CAIR). The practical realisation of radiation dosimetry standards at NPL is supported by theoretical and computational studies. CAIR uses Monte Carlo techniques based on the Electron Gamma Shower radiation transport code EGS4 to simulate the irradiation facilities and radiation detectors used at NPL as part of a programme to establish improved dosimetry standards. The EGS software is a general-purpose package for the Monte Carlo simulation of the coupled transport of electrons and photons in an arbitrary geometry for particles with energies from a few keV up to several TeV. It is frequently considered to be the *de facto* gold standard for clinical radiation dosimetry simulation. CAIR is also interested in visualising the particle tracks and geometries in its Monte Carlo simulations and for this purpose uses the Virtual Reality Modelling Language (VRML). This is an ISO standard language for representing a virtual world of three-dimensional objects on the World Wide Web, which allows the user to navigate through the virtual world. VRML aims to include features such as perspective, lighting, and transparency to make virtual worlds look realistic. To take advantage of the functionality of VRML, the numerical dosimetry group produced their own software utility for converting graphical output from EGS4 to a format that could be used by VRML.

It would be of benefit to other metrology areas within the NMS to extend the combined use of mathematical modelling and three-dimensional visualisation to simulate measurement systems. The CAIR example is concerned with particle tracks in complex measurement apparatus. Other potential uses include the simulation of wave propagation in confined spaces, for example, in microwave antenna measurements and in underwater acoustics. A good example is provided by NPL's acoustic pressure vessel (APV), which aims to allow underwater acoustic measurements in simulated ocean conditions. For any particular measurement the vessel may contain several hydrophones, a source transducer, material test panels and acoustic filters, all of which have their own mounts and supports and which may be moved (translated or rotated) both during and between measurements. The interior of the vessel is, of course, not accessible to the metrologist during measurements. Major sources of uncertainty in pressure vessel measurements include those due to misalignments of transmitters and receivers and materials under test, echoes from walls and supports with the pressure vessel and diffraction around objects that the acoustic beam intercepts. Mathematical modelling of acoustic wave propagation and scattering within the APV combined with a three-dimensional visualisation of the interior of the instrumented vessel would allow optimisation of the measurement configuration and minimisation of the sources of uncertainty. A similar example is the simulation of the acoustics in a free-field chamber to model and visualise where structures, instrumentation and their associated echoes interfere.

It is necessary, however, to appreciate that fundamental to these types of simulation are the mathematical models that describe the geometry and appearance of objects, govern the dynamics of their structural performance, and the constitutive models that define the properties of the materials used in the construction of the objects. It is vitally important that the physically-based mathematical models used in the simulation, visualisation and optimisation procedures are robust, have been thoroughly validated, and are fit for purpose. The development of simulation techniques leads to demands for an ever-growing array of mathematical models, design methods, and measurement methods that provide the reliable input data needed by the models. In addition, as was pointed out by speakers at the joint BIPM/NPL workshop on the *Impact of Information Technology in Metrology* held at NPL in September 2002 and at the SS*f*M Club meeting in October 2002, although it is now becoming easier to present data in the form of three-dimensional graphics, it can be difficult to choose an effective visualisation that is metrologically accurate and does not mislead the viewer.

- It is therefore recommended that a study be carried out of the potential benefits to metrology of the combined simulation and visualisation of measurement systems, with the aim of assisting metrologists who believe that their measurement problem may benefit from such an approach, and of transferring existing good practice from the numerical dosimetry group and from NPL's Materials Centre to other NMS metrologists.

3. MODELLING OVER MORE THAN ONE LENGTH SCALE

One of the most important questions facing metrologists, particularly those working in nanotechnology, biotechnology and in materials science, is the problem of validating and testing mathematical models which describe phenomena that manifest themselves over several length scales. The understanding of multi-scale phenomena, and especially of those properties of matter which are sensitive to structure, poses a significant challenge to physicists and mathematicians.

As Wright and Chorin point out [9], quantum mechanics has not always been able to deal effectively with some of the most useful and interesting characteristics of materials, especially where these properties are structure-sensitive, that is, they are affected by the microstructure of the material in question. These authors list a number of examples of such structure-sensitive properties: strength, plasticity, magnetic hysteresis, dielectric constant, optical properties of liquid crystals, and superconductivity, among others. They also emphasise the wide range of time scales over which processes of interest to materials metrologists occur.

To understand the nature of challenge to be faced in this field it is useful to examine modelling requirements and methodologies in the field of nanotechnology, which was a topic that was studied in detail in the recent NPL internal mathematical modelling review. One aspect of this study was an attempt to identify the new mathematical modelling requirements needed to tackle measurements activities associated with nanotechnology and materials science. The observations on molecular dynamics and continuum mechanics below (sections 3.1.2 and 3.1.3 respectively) are taken from this NPL study.

3.1 MODELLING FOR NANOTECHNOLOGY

Nanotechnology occupies the physical size region that involves structural building blocks that are usually at the molecular or crystallographic level. It is concerned with the region between atomistic structures (length scale in Ångstroms) and microscopic structures of materials whose length scales are measured in micrometres. Modelling at the nano-level is possible using a variety of techniques, ranging from quantum mechanics, through molecular dynamics, to continuum approaches, and the key features of these methods are summarised below. A useful account of the various approaches can be found in [4] (Schlick).

3.1.1 QUANTUM MECHANICS

Quantum mechanics methods rely on the solution of the Schrödinger equation. Three-dimensional structures, energies and other properties are calculated directly using fundamental principles of physics – the nuclear and electronic structure of atoms – without the need for experimental data. In the past such calculations could only be carried out for small systems but recent developments in computing have made such calculations possible for large systems of atoms and molecules, usually with the employment of various approximation methods.

In the Born-Oppenheimer approximation, for example, the behaviour of the atoms in the molecule is considered in two stages. Electronic and nuclear motions are considered separately. This is thought to be reasonable because nuclei are very much heavier than electrons and so can be regarded as fixed with respect to the electrons. At the same time electrons are modelled as reacting instantly to changes in the position of the nucleus.

The motion of the electrons in a field of fixed nuclei in calculated first to obtain an effective nuclear potential function. This is then used to derive the vibrational, rotational and translational states of the nuclei.

Two basic methods of applying quantum mechanics techniques employ the Born-Oppenheimer approximation: *ab initio* methods and semi-empirical methods. As the name implies, ab initio methods solve the Schrödinger equation from first principles. However, it is not solved exactly but a method is chosen which can lead to a reasonable approximation to the solution, where "reasonable" means adequate for the purpose of the calculation. A wide range of *ab initio* techniques exists but the most commonly used technique is the molecular orbital method in which molecular orbitals are approximated by a linear combination of atomic orbitals. The coefficients that describe the linear combination are derived by minimising the electron energy of the system for a given set of orbitals. This energy – the Hartree-Fock energy – and the related coefficients are obtained by means of an iterative calculation in which the positions of the nuclei are considered fixed – the Self Consistent Field procedure. Such methods can be computationally demanding, as many integral calculations have to be evaluated.

Another variant of *ab initio* methods is Density Functional Theory (DFT), which is based on the theorem that the density of any system determines all the ground-state properties of the system. Instead of considering the interactions of individual electrons with nuclei as is required for the Hartree-Fock approach, DFT considers the entire electron system. It is assumed that at each point in a molecule there exists a well-defined electron density and that, by making simplifying assumptions, the many-body interactions between particles (the exchange correlation energy) can be calculated by performing a volume integral to sum the contributions from each volume element.

An alternative class of quantum mechanics solutions is described as semi-empirical. These methods parameterise the Hamiltonian operator by fitting it to experimental data or the results of first-principles calculations. Semi-empirical calculations are less computationally demanding than first-principles methods, but are usually less accurate. They cannot be applied to systems that are radically different from those used in the parameterisation procedure. These methods provide practical solutions to studying many of the properties of molecular systems from reactivity to UV spectra. It is important to recognise for all the methods discussed here that the quality of the results depends on the quality of the approximations made [4] (Schlick).

3.1.2 MOLECULAR DYNAMICS (FORCE FIELD METHODS)

Classical atomistic simulation assumes that a molecular system can be described using the laws of classical mechanics. It provides a fast, though approximate, way of studying molecular structure, energetics, and motion. Alternative quantum mechanics methods are usually more accurate but also much more computationally expensive. The methods differ in the manner in which they compute the energy of the molecular system. Classical mechanics uses the concept of the force field. A molecule is modelled as a collection of atoms connected by bonds (springs), and its potential energy can be described by knowing the mass of all of the entities and the 'spring' constants of all of the bonds. Computing the arrangement corresponding to the lowest energy gives the most likely geometry of the system. Dynamic behaviour in response to any disturbance can also be calculated by applying the laws of classical mechanics. In reality, molecular systems are far more complex than this simple picture, but the principle of molecular mechanics is similar. The system is described by summing all of the relevant energetic components. This energy expression is the basis of a force field - so called because it enables the calculation of the forces on the system by differentiating the energy function. A force field provides a relatively simple and extremely fast method of computing the energy of a molecular system or material. According to Schlick [4], such methods work well for describing molecular structures and processes, except for bond-breaking events.

Molecular mechanics finds the geometry that corresponds to a minimum energy for the system - a process known as energy minimization. A molecular system will generally exhibit numerous minima, each corresponding to a feasible conformation. Each minimum will have a characteristic energy, which can be computed. The lowest energy, or global minimum, will correspond to the most likely conformation. Molecular mechanics calculations can be performed on molecular systems including isolated molecules in gas phases, systems in solution, and macromolecules. Introducing periodic boundary conditions, which use a unit cell to represent the behaviour of an infinite or semi-infinite system, enables calculations on crystalline materials, bulk amorphous solids, and surfaces. The information these calculations provide is invaluable in explaining and controlling crucial processes and properties including synthesis, chemical reactions, stereo-chemical effects, solubility, the binding of drugs or chemical additives, the structure of crystals, and the behaviour of bulk materials, including fracture processes.

Molecular dynamics applies the laws of classical mechanics to compute the motion of the particles in a molecular system. This allows the study of molecular and conformational stability, the likely effects on reactions or properties, the thermally averaged molecular structure, and any other property dependent upon molecular motion - examples include diffusion, permeability, binding mechanisms, and vibrational modes (leading to prediction of IR spectra).

3.1.3 CONTINUUM MECHANICS

Classical approaches to mechanics and thermodynamics involve the use of an equation of state relating an energy function (e.g. Helmholtz, or Gibbs) to state variables such as the thermodynamic temperature, and the stress or strain tensors. For fluids, the density or pressure are used as state variables. This approach has been very successful when applied to systems that are large enough to behave as continua. When applying the principles at small length scales in the nanometre range, especially when a free surface (possibly contaminated or oxidised) or an array of interfaces are present, the classical continuum approximation is likely to break down owing to the direct effects of the atomistic structure of the material system being modelled. To bridge the gap between atomistic models, such as molecular dynamics, and the classical continuum approach, continuum mechanics methods have been modified to include the effects of gradient terms (spatial or temporal dispersion) in the equation of state, thus defining one possible application of the subject known as non-local continuum mechanics. For fluids, for example the interface between a gas and liquid, the density gradient would be included as a state variable in addition to the density. This leads to a self-consistent model that automatically includes surface or interfacial energy effects within a bulk model. For solids, strain or stress gradients would be taken as state variables. A very brief look at the literature for this field suggests that strain gradient modelling techniques might successfully deal with the problem of establishing a rigorous bridge between atomistic modelling and classical continuum mechanics. Current applications of non-local continuum mechanics have included analyses of stress and strain fields associated with dislocation cores and cracks in elastic materials, and the development of models of localisation phenomena such as slip-band formation during plastic flow. One issue is that gradient theories introduce additional materials properties that need to be defined and measured.

3.1.4 KEY QUESTIONS FOR NANO-SCALE MODELLING

The three techniques outlined above, namely, quantum mechanics, molecular modelling and non-local continuum mechanics, have great potential for overlap in the nano-scale size region. The recent Materials Foresight exercise [5] (Shercliff) referred the concept of "seamless modelling from atoms to structures". If this can be achieved then it will have a revolutionary effect on the way in which we perceive the importance of measurement science. For example, in the materials field it might be possible to predict the thermo-elastic constants of a crystal from first principles, removing all need for measuring these properties.

The question which then arise for all the modelling methods outlined above are:

- How many atoms can be handled?
- How many different properties and material types can be handled together?
- How well do the various approaches overlap - if at all?
- How is it possible for nano-scale models to be validated and benchmarked?
- Are the approximations used in a particular technique are reasonable for the problem of interest?
- Are current computing resources adequate to tackle large calculations or is there a need to move to parallel processing, Grid or distributed computing techniques to speed up computation times?

3.2 MULTIPLE LENGTH SCALES IN "TRADITIONAL" METROLOGY

It might be thought that multiple length scale modelling problems arise mainly in new areas of metrology. However, such challenges also occur in more traditional metrology areas. A good example of such a case occurs in pressure metrology.

Piston-cylinder pressure balances are used to generate accurately known static pressures in the pressure range from 0.1 MPa to 1 GPa. Pressure balances consist of a piston located within a closely fitting cylinder. The radius of the piston is typically a few mm and the external radius of the cylinder may be several times that of the piston. The clearance between the piston and cylinder is typically of the order of 1 μm or less. The gap between the piston and cylinder is filled with fluid, which flows along the gap under the influence of a pressure gradient. This pressure gradient arises because the lower end of the piston and cylinder assembly is connected to a pressurised reservoir of fluid (in practice this may be another pressure balance) and the top of the assembly is exposed either to atmospheric pressure or to a vacuum. The force on the piston generated by the application of the pressurised fluid is balanced by the force from a mass applied to the top of the piston. The calculation of the pressure generated by a piston-cylinder pressure balance or deadweight tester requires one to know both the forces applied to the piston and the area over which they act. However, the piston and cylinder assembly is itself distorted by the pressure generated in the pressure balance fluid, and accurate determination of the generated pressure requires this distortion to be taken into account. In other words, it is necessary to know the effective area over which the force is applied in practice. Traditionally, finite element methods have been used to study both the flow of fluid along the gap and the manner in which the balance distorts under pressure.

At the low-pressure range of operation, gas-operated balances are used to generate static pressures from approximately 0.1 MPa to 20 MPa. It has been observed by many National Metrology Institutions that there are differences in nominally identical devices of the order of several parts per million per MPa. Furthermore, different devices exhibit different degrees of linearity. This is becoming increasingly unacceptable to primary standards laboratories and to end-users, as the uncertainties associated with these non-linearities are virtually of the same magnitude as the claimed accuracy of the primary standards. It is believed that nanometric flow effects in the annular gap between the piston and cylinder, which can be in the range 50 nm to 2000 nm, are responsible. Existing finite element methods are unable to tackle such a problem and there are no existing theories which can be used to calculate the frictional drag forces on the piston/cylinder, and the local pressures along the gap, which cover the range from the high pressure end of the piston/cylinder gap where continuum/viscous flow predominates, through to the low pressure end where the molecular flow regime predominates. This is essentially a transition flow problem. Furthermore, there is no existing method of accounting for differences in surface texture. There is a need for new mathematical models which can address this problem of modelling over several length scales, from nano flow to viscous continuum flow, and which can also model the effect on the flow pattern of surface irregularities. It is interesting to note that conventional pressure balances use rotating pistons/cylinders, hence there is potential for rubbing and therefore changing the surface texture. Understanding flow at the nano-scale level along channels with realistic surfaces will become increasingly important in achieving further improvements in primary pressure standards.

3.3 CHALLENGES OF MULTISCALE AND MULTI-PHYSICS MODELS

It is in fact not surprising that multiscale modelling is of importance in mechanical metrology. As the USA's Laurence Livermore Laboratory emphasise on their multiscale modelling web-site (www.llnl.gov.str/Moriarty.html) mechanical properties of materials and systems are inherently multiscale, depending on phenomena at all length scales. It is therefore necessary to be able to produce computer models that can predict and explain material properties over three main length scales: the atomic scale (nanometres), the micro-scale (micrometres) and the meso-scale (millimetres and above). For this approach to be successful, fundamental physical and mathematical principles first have to be applied rigorously at each length scale and then the same rigour is necessary to ensure that the model at each scale connects with its neighbouring scales.

The Shercliff Report [5] which reviewed UK activity and requirements in the modelling of materials and processes made a number of observations relevant to the problems of multiscale modelling that have been discussed in this section of the report. These are summarised below:

- Centres of excellence in each industrial sector are needed to offer advice and training in modelling, to transfer expertise to industry (particularly SMEs), and for benchmarking software.
- Industrial modelling problems are no less demanding academically than purely scientific research.

- Increased computer power is absorbed far too readily in added complexity, rather than in the more thorough use of an existing model.
- Choosing the appropriate level of complexity is an essential element of all model building.
- Finite element methods are largely mature. Much more can be achieved by integrating microstructural and damage modelling with FE.
- The data needs of a modelling activity, both for input and to validate the output, should be considered (and costed) from the start.
- Interface properties, friction and heat transfer in particular, are critical in all materials process modelling. There is a need for research on micro-modelling of interfacial conditions, and the coupling of these models to macroscopic FE computations and to experiment.

In setting out these conclusions, Shercliff made a number of important comments. He argued that multi-physics models and modelling over several length scales required the development of numerical methods to tackle the solution of problems with many coupled boundary conditions. Shercliff argues that micro-level models are not actually connected to a macro-model for much commercial work, but that a micro-level model is used to generate a higher-level approximation to the phenomenon of interest and that this approximation is then passed on the next higher-level model.

Occasionally, limitations in macro-modelling generate work in associated micro-modelling. Shercliff's example is of current research on friction and heat transfer, where average values use in macro-models are accepted as inadequate, but that improved information needs a combined programme of micro-modelling and experiment. Similar requirements exist in the modelling of piezoelectric materials, where the use of average properties (which are themselves often the subject of large uncertainties), means that the real behaviour of piezoelectric components is not captured by finite element models, for example.

He also criticises the inadequate validation of complex computer code. He argues that multi-physics codes create a huge demand for parallel computing and increased computing resources. His view is that as the complexity of code goes up it becomes more open to criticism. He asked three questions:

- Has the code been sufficiently validated?
- Could the increased computing power be used for sensitivity analysis to identify "first-order" effects so that "reduced modelling" could be carried out?
- How many industrial users can really benefit from multi-physics codes?

Shercliff also argues for the importance of a "centre of excellence" in modelling that is concerned primarily with technology transfer. Its role should be to link modelling closely to real applications and exploit parallels between processes. Commonality of much physical behaviour of software structures suggests potential for technology transfer in mathematical modelling between widely different processes.

3.4 USA STUDY ON COMPUTATIONAL CHEMISTRY

In 1999 the USA's Council for Chemical Research (CCR) published a report on the future of computational chemistry in which it attempted to forecast the challenges that would need to be overcome in the field of molecular modelling in the first 20 years of the 21st century [2]. The report reviewed the start of the art at the quantum scale, the atomistic scale and the meso-scale and also considered the problems that exist in trying to bridge these length scales. The authors identified a number of computational issues that are relevant to the subject of this chapter. At the quantum scale they argued, amongst other things, that there is a need for accessible benchmark calculations for selected "gold standard" reference molecules and that more usable robust software was needed. Another major barrier to the development of molecular modelling at this scale was lack of validation of results, and of inadequate methods for predicting uncertainties in calculations. They are also critical of current modelling capability at the meso-scale and they argue that there is a need to develop methods for applying statistical and stochastic methods to meso-scale phenomena.

In a discussion of bridging techniques for joining together the various spatial and temporal scales involved in molecular modelling, they argue for the increased use of seamless data interfaces which permit interactions between calculations performed at different size scales. They also consider coarse-graining techniques, which allow knowledge gained from calculations at a small scale to be usefully applied at a larger scale. Lack of good statistical techniques is seen as a critical computational limit for the development of bridging techniques. More research is needed on stochastic methods, including Monte Carlo methods, which are regarded as being able to provide a basis for the techniques needed for moving from scale to scale.

Finally, at all length scales they see the need for increased computing power including parallel and distributed computing systems. Distributed and parallel computing can itself assist in bridging length scales simply by allowing very large-scale calculations to be carried out.

3.5 RECOMMENDATIONS

In the light of the observations made in this section of the report, the following recommendations are made for the next SS*f*M programme.

- Three or four areas of metrology from NMS science programmes should be identified where modelling over several length scales and multi-physics modelling is currently used or has the potential for future use. Metrologists in these areas will need assistance in deciding whether potential problems are tractable with existing modelling techniques and on the choice of software packages, and also in identifying potential academic and commercial collaborators. Such support could be provided specifically through the SS*f*M programme.
- A study of methods of validating modelling software at the boundaries between length scales should be carried out. This study should not only make recommendations concerning validation techniques but should also identify those areas of metrology in which gaps in current scientific knowledge prevent the development of models which are valid over several length scales or which link different physics disciplines.

- A review of molecular modelling software and computation techniques should be carried out with the aim of identifying the specific contribution the SS*f*M programme might make to the development of statistical techniques for molecular modelling and to the incorporation of predictions of uncertainty into molecular models.

4. DISTRIBUTED COMPUTING AND GRID COMPUTING

Distributed computing can be defined as the use of a network of computers to process a particular task in a concurrent or parallel manner. Whereas distributed computing systems can be implemented within one system domain or using computers which are under the control of one administrator, Grid computing refers to the use of networks of computers, but with the additional requirement that one is linking computers over more than one domain or administrative unit. Both developments will provide challenges for the SS*f*M programme.

NPL metrologists have recently investigated the benefits of distributed computing by means of a pilot study and their experience provides the foundation for sections 4.1.1 to 4.1.3 of this chapter. In relation to Grid computing, the UK Department of Trade and Industry is one of the main sponsors of the UK's e-Science initiative through its Grid Outreach programme (www.Gridoutreach.org.uk/). It is important that the NMS is in a position to take advantage of the benefits that will arise from these new developments in the use of the Internet.

4.1 DISTRIBUTED COMPUTING

In the past the limited power of desktop personal computers and the unreliability of their operating systems meant that they were often not suitable for distributed computing applications. However, the speed of currently available processors and high bandwidth computer networks are such that the computing power which is available from linking together large numbers of desktop personal computers can often be comparable to that available from supercomputer systems.

Distributed computing systems are able to farm out to desktop personal computers tasks which are run in the background while the PC is used for other computing tasks. In this way efficient use is made of all the computing power of the PC and there are no additional hardware costs, as the PC network is already in existence. As United Devices, one of the leading providers of software for distributed computing, point out, desktop PCs are usually the most plentiful computing resource in a company or organization and they are consistently the most under-utilised.

The distributed computing project which has received substantial publicity and which is well known to many is the SETI@home project. This project originated at the University of California at Berkeley to process the very large amounts of data received by the Arecibo Radio Telescope in Puerto Rico and to attempt to identify possible signs of extraterrestrial intelligence in signals received from space. As Trunnell [8] explains, users of Internet-connected computers were encouraged to donate idle processing power by means of a special screensaver application. In this way it has been possible to use these donations to provide over 700,000 years of CPU time to analysing data from the telescope. Trunnell also points out that just 250 Pentium II machines at average utilisation have a total idle capacity equal to two 64-CPU Sun Enterprise 10000 servers. This comparison clearly identifies the potential benefits to be gained from the introduction of distributed computing.

4.1.1 IMPLEMENTING A DISTRIBUTED COMPUTING SYSTEM

There are a number of general issues that must be considered whenever a distributed computing system is introduced. These are summarised briefly below.

- ***System reliability***. As there is no guarantee that particular desktop machines or laptops may be available perform calculations at any specific time (they may have been disconnected, or switched off, or the CPU may be heavily committed to a locally-running application), it is necessary to ensure that the number of potentially available machines is large enough to allow the central controller or server to be able to find alternative machines to run tasks or to be able to give the same task to more than one machine. The minimum useful network size and the optimum network size will both depend on the size of the computing task to be carried out, the degree of parallelism which is possible, and the length of time each task takes on the machines to which it has been farmed out. Of course, it is very likely that individual networked PCs will vary in their computing power and speed. Criteria are needed to help users of distributed computing systems determine their minimum and optimum network sizes for particular computing tasks.
- ***Security.*** Two security questions arise. The first is the concern of the user or administrator of a distributed computing system. Is it possible to be sure that the application itself and the data sent to and returned from individual desktop machines are secure? The second is for the owners and users of each desktop machine. Are their own local data and applications secure from intrusion by the distributed applications they are asked to run from time to time? Much of the intellectual property of the providers of software to manage distributed computing systems is related to the solution of these security questions. One important question to be considered here is whether encryption might be necessary on Grid systems to protect intellectual property rights, as it may be argued that sharing data and software with other computing systems is equivalent to making public the results of potentially patentable work.
- ***What are the characteristics of applications that are most suited to distributed computing?*** To gain most benefit from distributed computing, the task which it is planned to implement should be one in which there is only limited need for the transfer of files or data between the central server and the desktop machine in question. Ideally, such transfers of data should be required only at the beginning and end of each work task and these transfers should take a relatively short time compared with the computing time needed for the task in question. In addition, the task should not need to take up large amounts on memory on the desktop computer. There should be no need for communication between individual desktop machines and the application must be one which can be easily divided into small pieces [8] (Trunnell).

4.1.2 A PILOT STUDY AT NPL

NPL itself carried out a pilot study to determine the possible benefits of distributed computing in metrology in the autumn of 2002. This employed control software from United Devices and was hosted by NPL's Materials Centre (MATC) with financial contributions and support from other NPL centres, including the Centre for Ionising Radiation Metrology (CIRM) as it was then known (it has now become the Centre for Acoustics and Ionising Radiation (CAIR)) and the Centre for Mathematics and Scientific Computing (CMSC). Three applications were converted to run on the distributed computing system. The trial demonstrated that it was possible to use up to 80% of the available computing resource of desktop PCs for distributed computing applications. Users of host machines reported no problems caused by running the distributed application and no disruption to the network was observed.

The project allowed NPL to identify what expertise would be needed to develop parallel applications suitable for distributed computing, including expertise in the optimisation of parallel software. The pilot study suggested that there was the potential to speed up computationally intensive calculations many hundreds of times if the system could be implemented site-wide.

A study of metrology applications suggested that a number could benefit immediately from distributed computing. These include work on thermophysical calculations, composite laminate damage modelling and image correlation in MATC, radiation simulation in CAIR, numerical simulation of highly resonant enclosures in microwave antenna calibration, Monte Carlo simulation of measurement and uncertainties, and predicting the far field of underwater acoustic transducers. The pilot study also identified areas that might benefit in the future: molecular modelling, simulation, and finite element modelling both of acoustic transducers and of piston-cylinder pressure balances.

4.1.3 BUILDING ON THE PILOT STUDY

To consolidate the achievements of the pilot study there are some specific contributions needed from computer scientists that could help metrologists make the most of distributed computing technology. These include:

- Guidance for metrologists on how to develop parallel computing applications and how to convert existing serial applications to make them suitable for distributed computing.
- Assistance in identifying applications that would benefit from using parallelism.
- Optimising the performance of the distributed computing system, including identifying the optimum size of the network for specific tasks, the optimum size of work tasks to be sent to desktop machines and minimising communications tasks between the server and the networked PCs.
- Ensuring that the chosen server software meets all necessary requirements for data and application security.
- For metrology applications traceability is important, as is the need to be confident that any particular calculation will yield the same result no matter on what specific set of networked desktop machines it is run. In a large network it is likely that there will be a range of operating systems and versions of those systems installed on the networked machines and that these systems and versions will be subject to constant change as PCs are upgraded or replaced. Metrologists will need detailed advice on how to maintain traceability in the context of distributed systems.
- Development of test programs to identify faulty machines on the network or problems with arithmetic precision for example. These could include the solution of systems with known ill-conditioning, random number generation routines and chaotic systems, all of which would be sensitive to small numerical errors.

It is therefore recommended that the next SS*f*M programme include a specific project related to distributed computing in metrology to allow the above issues to be addressed.

4.2 GRID COMPUTING

The Grid computing initiative "will exploit the next-generation, high-bandwidth Internet to enable flexible, secure and co-ordinated resource sharing among dynamic collections of people, institutions, scientific facilities and computers", in the words of Dr Anne Trefethen, the Deputy Director of the UK's e-Science Core programme. In effect, it will allow the creation of virtual organisations and institutions, which will be linked by access to shared data sets and databases, shared software and shared hardware. The e-Science initiative recognises that increasingly science research will be carried out through distributed global collaborations with access to very large data sets, the most advanced computing resources and with high performance visualisation and simulation software.

The technology that will enable this new development in science is the Grid (the terminology arises through an analogy with electrical power supply), which can be regarded as an information utility to store, access and communicate large quantities of data. These developments will inevitably have an impact on the SS*f*M programme. It is likely that metrological uses of the Grid will include:

- Modelling and simulation;
- The next generation of Internet-enabled metrology;
- Delivery of NMS knowledge and best practice to users of the Grid and those taking part in e-Science initiatives.

One important area where the SS*f*M programme can make a specific contribution is in the area of acceptability of Grid-based methods of operation. For the Grid to be successful users have to have a degree of trust in the system. It has to be seen to be dependable, and fault-tolerant. To ensure that information is always available it may be necessary to duplicate information and hold copies it in different locations and to replicate services so that there is more than one route to data of interest. In addition, data must be shown to be secure, especially when it consists of sensitive personal information such as may exist in medical databases, for example, or if its disclosure could have detrimental commercial consequences. Data must also be available in a timely manner, as and when required.

In the light of these developments, it is recommended that the next SS*f*M programme should include the following activities related to Grid computing:

- Undertake a small study of the potential impact of the Grid on the NMS.
- Develop a demonstrator of Grid services as a means of delivering knowledge transfer within the NMS.
- Consider whether the development of a metric or benchmarking process for computing power sold over the Grid is within the scope of the NMS. Such a benchmarking system should also take into account issues such as reliability, security and fault tolerance of Grid services.

5. UNDERSTANDING MULTI-VARIATE DATA SETS

As the Smith Institute roadmap [6] points out, large data sets require careful investigation to discover and explain patterns, special features and causal connections. New techniques are needed to help understand complex systems and processes, especially when mathematical models cannot represent every aspect of the process. In fact, one of the key features of modelling in the physical sciences is that the physicist seeks to make models that are as simple as possible. However, many modern measurement systems are extremely complex and it can often be difficult to quantify the interactions between the various parts of the measurement system and between the system and its environment, which includes, of course, those who are responsible for operating and maintaining the system itself. In such circumstances, it may be beneficial to be able to investigate the performance of a system without the need to produce a comprehensive mathematical model. This may have particular benefits in the early stages of experimental design, when one is investigating how best to establish a measurement system or define a measurement procedure.

One approach to this type of modelling which has gained some publicity in recent years, and which has generated substantial interest in those attending SS*f*M club meetings, is the use of parallel co-ordinate transformations. In conventional Euclidean geometry axes are orthogonal to each other, limiting the presentation of information to three dimensions. However, if one employs parallel co-ordinates one is not limited to three axes and further axes may be added so that one has an axis for each variable in the data set. Whereas in a conventional three-dimensional graph a point indicates those axis values which belong together, in parallel co-ordinate systems a line links the points on each parallel axis that belong together. This approach has an inherent flexibility: further parallel axes may be added to the plot, allowing the line to be extended further. To identify which value from each axis belongs to one realisation of the "measurement" one merely traces the line across the set of parallel axes.

This form of parallel co-ordinate representation allows the user to explore experimental results visually, and to manipulate data without the need for detailed mathematical analysis. Every aspect of an experimental process that can be measured is represented on one of the parallel co-ordinate axes. By observing the behaviour of sets of lines, how they group together, which sets of lines relate to acceptable and which to unacceptable results, one can identify the key variables in processes and experiments in a straightforward manner. Note, too, that the axes can all be scaled independently, so that it possible for large multi-variate data sets with extreme variability in scale from one parallel axis to the next to be represented straightforwardly.

One commercial software package that implements parallel co-ordinate data analysis techniques is marketed by Curvaceous Software Ltd (www.curvaceous.com). The software has been used successfully in chemical and other process plants to understand and monitor large sets of complex experimental data and to assist plant operators in optimising the output of process plants. It is likely that such software could also be of benefit in the development and monitoring of complex calibration experiments. In particular, it may be able to identify correlations amongst experimental variables and sets of variables that were previously treated as uncorrelated. Another benefit may be in the design of calibration and measurement procedures. Typically, written measurement procedures employed in the delivery of calibration services are lengthy and specify in detail how each part of the equipment is to be set up and how measurements are to be performed and analysed. Measurement procedures should be robust enough to withstand potential small changes in methodology, which might arise from differing practices by different calibration staff, for example, or from experimental modifications, which might be needed to accommodate particular devices undergoing calibration. Parallel co-ordinate techniques offer the possibility of studying such factors with the aim of strengthening and simplifying calibration procedures.

It is recommended that:

- A detailed case study be carried out to help clarify the possible benefits to metrologists of employing parallel co-ordinate systems for representing complex experimental data and that the beneficial results of the study be published and made known as widely as possible.

6. RISK AND UNCERTAINTY

6.1 MANAGING CALIBRATION AND MEASUREMENT FACILITIES

Limited resources must be used efficiently and effectively. Calibration and measurement activities are no exception to this rule. The maintenance of equipment needed for the provision of calibration services and especially for the maintenance of primary calibration standards can be both expensive and time-consuming. Where complex measurement systems exist (and this complexity can also include software which is used to control equipment or to calculate the results of calibrations) substantial costs can be incurred ensuring that equipment and indeed the calibration systems themselves are in working order and available to meet customers' needs. Metrology programme costs in many of the scientific areas covered by the NMS have a substantial percentage devoted to the maintenance of primary and secondary standard calibration facilities.

In calibration systems one is not only concerned with the availability and performance of the equipment itself but also with the operational environment required for accurate results. Typical environmental requirements for measurement systems may include specifications concerning temperature, air-flow, humidity, freedom from dust, electromagnetic interference, ionising and non-ionising radiation, vibration and noise (both electrical and acoustical). Thus, optimising the performance of measurement systems requires attention not only to the measurement hardware and software but also to the environment in which the measurement is carried out. It is of interest to note that failure to meet environmental specifications has been a cause of some considerable delay in commissioning the new laboratories that are currently being completed for NPL. A further point that arises from the move to the new NPL building is that calibration facilities have to be re-installed in new laboratories, with consequent changes in environment, experimental layout and apparatus, so that what happened in the past is not necessarily a guide to what future requirements might be.

The questions that arise from the above observations are:

- How does one ensure that equipment is available when it is required?
- How does one ensure that environmental issues do not prevent a useful measurement being made?
- How does one maximise the availability of equipment and the existence of the required measurement environment, while minimising the cost of maintenance and environmental control activities?
- To what extent are opportunities to perform calibrations, and thus earn money from customers, limited by both maintenance and environmental failures?
- Has the move to new experimental facilities allowed metrologists to improve the performance of measurement systems with consequent service benefits to customers and financial benefits to NPL? Can the lessons of this experience be generalised to assist other calibration and measurement laboratories that may need to re-locate?

To answer these kinds of questions there are two basic requirements: data on the performance of measurement systems and their environments, and mathematical models that allow one to study the operation of such systems and their optimisation. In the first instance there is a need to design and develop databases on equipment maintenance and failure and on environmental performance of calibration laboratories, which can be combined with information of an economic or logistic nature (number of customers, timing of calibration work, cost of calibration work, prices charged for work, work scheduling etc). Laboratory Information Management Systems (LIMS) are the main database tools that measurement laboratories use to control their work and such databases could be extended to include the information required for optimising the performance of calibration facilities. This is a topic that is also addressed in the following chapter, which considers the contribution which modern data mining techniques may be able to make to the practice of metrology.

Mathematical models are needed which can be used to study the reliability of complex systems and which can be used to assist managers in making decisions, including financial decisions, about the operation of such systems. The previous chapter pointed out the usefulness of parallel co-ordinate systems for the study of complex processes with many variables to be monitored and it may be that such methods have a contribution to make here. In addition, it may be of assistance to extend modelling methods that are applied in the field of business and finance to the task of optimising the operation of complex measurement systems. Simulations of measurement system performance could allow one to study the effects of equipment and environmental failures and maintenance downtime on work scheduling and on the economic operation of laboratories.

It is therefore recommended that:

- A study be carried out of the database and mathematical modelling requirements which are needed for optimising the performance of complex measurement systems and calibration facilities, with the aim of assisting managers of such facilities to minimise risk and maximise earnings.

6.2 STOCHASTIC DIFFERENTIAL EQUATIONS

Another topic that is becoming of interest to metrologists is that of the application of stochastic differential equations to metrology tasks. Statistical modelling and stochastic PDEs have featured as a topic of high interest among metrologists who attended a December 2002 mathematical modelling seminar and software demonstration at NPL.

Many problems in applied physics are characterized by uncertainties in boundary conditions or initial conditions, nonstationary (transient) response, noisy excitation signals, finite correlation times, and uncertainties in system parameters. In all these cases, a proper solution for evolution of the process of interest in space or time requires solving the associated stochastic ordinary or partial differential equation (SODE/SPDE) for a physical quantity or its distribution function. This goes beyond simple estimation of (time-independent) standard deviations and correlations for the equilibrium state.

Solving stochastic differential equations is more difficult than solving the associated deterministic equation. Stochastic calculus, for example, has many peculiarities and does not conform to the rules of classical calculus. As a result, special novel solution methods are required compared to conventional (deterministic) ODEs and PDEs. This has repercussions on both analytical and numerical solution techniques.

SDE analysis and application to physical disciplines is a relatively young but fast growing area with substantial work left to be done particularly for realistic (non-idealized) situations and environments. It is important that the SS*f*M programme be able to provide assistance to metrologists in this developing area, especially as stochastic differential equation methods rarely form part of the mathematical training of applied scientists and engineers.

- The current SS*f*M programme contains a range of activities associated with continuous modelling. It is recommended that in the new programme this activity be extended to include support for metrologists who are applying stochastic differential equation methods in their work.

7. DATA MINING

Data mining can be regarded as a means of extracting useful information from large quantities of data, using highly flexible models and minimal assumptions [1] (Butler). In recent years such techniques have become of interest in a number of fields of activity including biological data analysis and bioinformatics, in financial and business applications, for example, to gain a better understanding of the behaviour of specific groups of customers, and in criminology to examine offending patterns and identify possible perpetrators of particular crimes. As yet there seem to be no reported applications of data mining that are specifically concerned with metrology issues. However, it appears clear that metrologists have potentially much to gain from a better understanding of data collected during the course of calibration activities.

7.1 POTENTIAL BENEFITS OF DATA MINING IN METROLOGY

In a survey of recent industrial trends, the journal Nature Biotechnology [3] reviewed recent trends in data mining for biological and chemical applications. However, a number of observations made concerning data mining methodologies are relevant to metrology applications. One of these is time-delay data mining. This refers to the fact that the data set is not available immediately in complete form but is collected over time. Data mining software that is designed for such data sets must be able to identify patterns that are confirmed or rejected as the data set increases and becomes more robust. Calibration activities are of exactly this nature. An artefact is periodically returned to NPL or to a UKAS calibration laboratory for a new calibration. In the meantime its performance may have changed; its components wear and age; the standard against which it may have been calibrated in the past may itself have been recalibrated; it may perform differently from identical devices owned by different customers; the staff performing the calibration may have changed; the calibration procedure may have been updated or modified. It is common practice for calibration laboratories to check the current calibration of a device against the most recent previous calibration certificate. Data mining may allow the extraction of information that is not noticed during such simple checks.

Butler [1] quotes an example of how this type of approach could benefit metrologists by aiding in the quantification of type B (systematic) uncertainties. As he points out, type B uncertainty evaluation is often a difficult modelling task. Such uncertainty contributions can be regarded as arising from an incomplete deterministic model. Instrument drift over time, for example, may contribute to type B uncertainties, but if calibration records existed for batches of instruments it might be possible to derive a model of drift which could be employed in reducing type B uncertainties within the particular calibration process of interest.

Data mining techniques are particularly suited to analysing trends in data sets that are collected over time. They are also often employed for predictive purposes, that is, to forecast or simulate future data sets. In the context of calibration, it may be possible to take the calibration histories of particular classes of instrument, make a prediction of expected behaviour at the next calibration and then compare the prediction with what was actually measured. These techniques offer the potential to diagnose hitherto unnoticed trends within calibration data sets.

7.2 RECOMMENDATIONS

The question arises as to how best to incorporate data mining techniques into metrology practice. At present LIMS are often used to records details of the calibration process from the first contact with the customer, the preparation of the quotation for the work, the arrival of the artefact at the calibration site, its progress through the calibration process and the despatch of the artefact and the associated calibration certificate back to the customer. In the case of LIMS at NPL the system does not record detailed scientific or technical information about the calibration process, nor does it record the actual results of the calibration (the content of the calibration certificate including the uncertainties associated with each value quoted on the certificate).

- It is recommended that the question of extending the range of data captured by LIMS be investigated with a view to applying data mining techniques in those areas of calibration in which it may be of most use (large throughput, many customers, many types of devices to be calibrated, changing calibration methodologies etc.).
- A pilot project be set up in a small number of metrology areas, or with one of two large UKAS-accredited laboratories with substantial numbers of calibration customers to test the benefits of data mining in metrology with the specific aim of better understanding of sources of type B uncertainties.

8. CONCLUSIONS

8.1 INTRODUCTION

This report has reviewed recent developments in mathematics and computing to try to identify issues that are gaining in importance in metrology and particularly those in which the SS*f*M programme could make a substantial contribution. To understand the importance of the mathematician's contribution to metrology, it is perhaps useful to consider the distinction that needs to be made between computational physics or computational science and scientific computing. Computational science develops models and methods from the specific ideas associated with particular branches of science. It tends to use standard mathematical tools and problem-specific approaches that have priority over general reliability and robustness. Scientific computing on the other hand prefers not to take mathematical tools off the shelf but to develop new problem-specific and application-oriented methods, with an emphasis on general efficiency, reliability and robustness of algorithms, as well as quality guarantees for the results. The SS*f*M programme exists in part to bring the scientific computing approach, as it has been defined here, to metrology applications.

In preparing the report, particular attention has been given to recent studies of the role of mathematics in science and engineering (SIAM [7], Wright and Chorin [9], Smith Institute [6]) and to NPL's internal research on future mathematical modelling requirements, especially in relation to biotechnology, nanotechnology and materials science. It is these studies that have led us to emphasis the importance of simulation, molecular modelling and modelling over multiple length scales for future SS*f*M work. Validation of software is particularly important in these new areas. In addition, current developments in distributed computing and grid computing are producing new challenges in software engineering and the report aims to identify the effect these new technologies will have on metrology practice.

8.2 MAIN RECOMMENDATIONS OF THE CURRENT STUDY

Each chapter of this study has produced recommendations for topics and work packages to be considered for the next SS*f*M programme. The main recommendations are summarised below. As was emphasised in chapter one, the recommendations should not be regarded as detailed definitions of work packages for the new programme or of project deliverables, but as suggestions for possible new areas of work for the SS*f*M programme that are necessary to meet some of the new demands being placed on metrologists.

8.2.1 Simulation

Simulation has been shown to be an essential component of modern scientific and engineering practice, with a range of applications within metrology. This section of the report reviewed examples of the use of simulation in metrology and raised a number of questions to which the SS*f*M programme may be able to contribute answers. These include the following:

- How does one validate simulations of complex experimental systems, especially when those systems may be unique?
- Minimising sources of uncertainty for primary measurement standards can be an extremely challenging task. If simulations are to be used in helping to establish

uncertainties, what contribution to uncertainty budgets do simulations themselves make?

- The simulations frequently rely on the output of complex software packages. What contribution to the "simulation uncertainty" arises from these software packages? The current SS*f*M programme is studying methods of validating continuous modelling software. This work should be extended to cover other software packages that are in common use in metrology.

Key recommendation:

- A study should be carried out of the potential benefits to metrology of the combined simulation and visualisation of measurement systems, with the aim of assisting metrologists who believe that their measurement problem may benefit from such an approach, and of transferring existing good practice from the numerical dosimetry group and from NPL's Materials Centre to other NMS metrologists.

8.2.2 Modelling over more than one length scale and multi-physics modelling

For metrologists in the fields of nanotechnology, biotechnology and materials science who may be involved in modelling at the quantum, the atomic or the meso-scale, the question of modelling over more than one length scale and of bridging length scales can lead to substantial scientific and mathematical challenges. In this area, and in relation to the validation of the output of models, it will be necessary to develop close collaborations between mathematicians and software engineers and theoretical and experimental physicists and materials scientists. Recommendations for work that would assist in these fields are as follows:

- Three or four areas of metrology from other NMS science programmes should be identified where modelling over several length scales and multi-physics modelling is currently used or has the potential for future use. Metrologists in these areas will need assistance in deciding whether potential problems are tractable with existing modelling techniques and on the choice of software packages. Such support could be provided specifically through the SS*f*M programme.

- A study of methods of validating modelling software at the boundaries between length scales should be carried out. This study should not only make recommendations concerning validation techniques but should also identify those areas of metrology in which gaps in current scientific knowledge prevent the development of models which are valid over several length scales or which link different physics disciplines.

- A review of molecular modelling software and computation techniques should be carried out with the aim of identifying the specific contribution the SS*f*M programme might make to the development of statistical techniques for molecular modelling and to the incorporation of predictions of uncertainty into molecular models.

8.2.3 Distributed computing and Grid computing

A successful distributed computing pilot project carried out at NPL in the autumn of 2002 demonstrated the potential benefits of distributed computing for metrological applications. A number of activities were identified which would assist metrologists in getting the most out of distributed computing applications and also ensure that key questions relating to reliability, security and traceability were addressed. These should be incorporated into a distributed computing project within the next SS*f*M programme and include:

- Guidance for metrologists on how to develop parallel computing applications and how to convert existing serial applications to make them suitable for distributed computing.
- Assistance in identifying applications that would benefit from parallelism.
- Optimising the performance of the distributed computing system, including identifying the optimum size of the network for specific tasks, the optimum size of work tasks to be sent to desktop machines and minimising communications tasks between the server and the networked PCs.
- Ensuring that the chosen server software meets all necessary requirements for data and application security.
- For metrology applications traceability is important, as is the need to be confident that any particular calculation will yield the same result no matter on what specific set of networked desktop machines it is run. Metrologists will need detailed advice on how to maintain traceability in the context of distributed systems.
- Development of test programs to identify faulty machines on the network or problems with arithmetic precision for example. These could include solution of systems with known ill-conditioning, random number generation routines and chaotic systems, all of which would be sensitive to small numerical errors.

Specific recommendations for future work on Grid computing to enable metrologists to take advantage of current e-Science initiatives are:

- Undertake a small study of the potential impact of the Grid on the NMS.
- Develop a demonstrator of Grid services as a means of delivering knowledge transfer within the NMS.
- Consider whether the development of a metric or benchmarking process for computing power sold over the Grid is within the scope of the NMS. Such a benchmarking system should also take into account issues such as reliability, security and fault tolerance of Grid services.

8.2.4 Understanding multi-variate data sets

Parallel co-ordinate systems allow the efficient representation of multi-variate data, and also allow the user to explore experimental results visually without the need for detailed mathematical analysis. They are particularly useful in studying complex experimental processes typical of many calibration activities. It is therefore recommended that:

- A study be carried out of the possible benefits to metrologists of employing parallel co-ordinate systems for representing complex experimental data and that the beneficial results of such a study be disseminated as widely as possible.

8.2.5 Risk and uncertainty

This section of the report outlined the possible benefits to be gained from applying risk management and performance optimisation techniques to the control of complex engineering systems such as calibration and measurement laboratories. It also pointed out the growing interest that exists among metrologists in the application of stochastic differential equations to measurement problems. Two recommendations for future work arose from this:

- A study should be carried out of the database and mathematical modelling requirements which are needed for optimising the performance of complex measurement systems and calibration facilities, with the aim of assisting managers of such facilities to minimise risk and maximise earnings.
- The current SS*f*M programme contains a range of activities associated with continuous modelling. It is recommended that in the new programme this activity be extended to include support for metrologists who are applying stochastic differential equation methods in their work.

8.2.6 Data mining

Although there appear to be no reported applications of data mining in metrology, certain data mining techniques (time delay data mining and predictive data mining) have the potential to make a contribution to metrology and to the quantification of type B uncertainties.

It is recommended that:

- The question of extending the range of data captured by LIMS should be investigated with a view to applying data mining techniques in those areas of calibration in which it may be of most use.
- A pilot project should be set up in a small number of metrology areas, or with one of two large UKAS-accredited laboratories, to test the benefits of data mining in metrology with the specific aim of better understanding of sources of type B uncertainties.

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