

**Report to the National
Measurement System
Policy Unit, Department
of Trade & Industry**

**INTERIM STATUS REPORT
ON THE LENGTH AREA
FROM THE SOFTWARE SUPPORT
FOR METROLOGY PROGRAMME**

**BY
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Software Support for Metrology

Interim Status Report on the Length Area

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Abstract

This report describes the status of the mathematics and software used to support the Length area of metrology, particularly as used within the NMS Length Programme. This is one of a set of status reports produced for the NMS Software Support for Metrology (1998–2001) Programme (SSfM) mid-way through the current programme to inform the formulation of the next SSfM Programme (2001–2004). The different aspects of mathematics and software are reviewed under the headings of the themes and project topics of the current SSfM Programme. The SSfM Programme is identifying best practice where it exists and disseminating guidance on that best practice to other metrology areas. The outputs of the SSfM Programme will be generic, applicable to more than one metrology area. This report, therefore, not only identifies problems to be tackled and best practice to be disseminated by the SSfM Programme, but also if appropriate possible future Length Programme projects applying SSfM outputs to specific problems in the Length area.

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1. Introduction

The purpose of this status report is to inform the NMS Software Support for Metrology (SSfM) Programme (1998-2001) about the status of the mathematics and software used to support the **Length** area, concentrating on what is used within the NMS **Length Programme**. This and the companion status reports for the other metrology areas will inform the formulation of the next SSfM Programme (2001-2004). It may also lead to appropriate linkage between the Length Programme and the SSfM Programme.

The SSfM Programme is an underpinning programme that provides generic support in the use of software and mathematics to the NMS programmes for each metrology area. For details of the Programme, its expected deliverables and the results already produced, see the SSfM web site: <http://www.npl.co.uk/ssfm/>.

The NMS programmes for specific metrology areas provide metrological support to industry. The SSfM Programme in contrast has relatively little direct impact upon industry, although there is some as evidenced by the SSfM Club membership. This relationship is depicted in Figure 1. It is because of this relationship that the Status Reports concentrate primarily on the use of software and mathematics in the other NMS programmes.

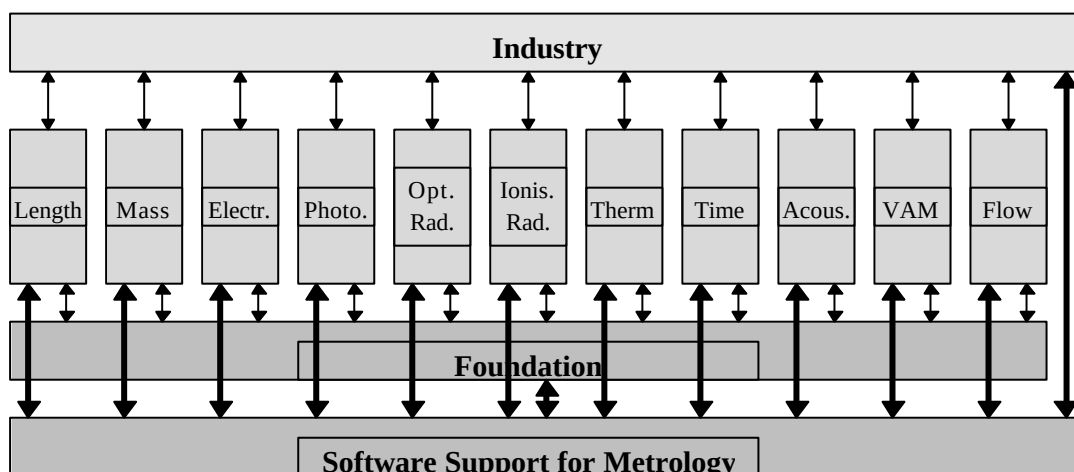


Figure 1. Relationship of SSfM to other NMS Programmes and Industry

In particular, this report addresses each of the themes within the SSfM Programme and describes the status concerning the topics covered by each of the relevant projects. It also considers whether there are any important software or mathematics issues in the Length area which are not addressed by the current SSfM Programme or which need to be taken further in the next SSfM Programme.

This report is an update of an initial restricted status report produced in December 1998. That initial report was one of a set of restricted status reports which were synthesised into an overall status report for all metrology areas (Rayner (1999)). A summary of the differences from the initial Length status report is provided at the end of this report.

2. Scope of the Area Covered

Length metrology is of direct importance to manufacturing industry. It is also a main building block of the international system of units (SI). However, length metrology has a feature other metrological areas lack, that of dimensionality. Thus, the Length area encompasses

measurement in 1-, 2- and 3-dimensions involving a large number of geometrical features such as roundness/circularity, cylindricity, conicity, screw and gear metrology as well as dimensionless quantities such as angle. Length metrology also covers a vast range of scales, from X-ray interferometry at approximately 10^{-11} m to surveying at 10^3 m. (In astronomy, units such as the lightyear involve distances of the order of 10^{16} m.). In two or three dimensions, it is not unusual for different axes to involve different scales, e.g. millimetres in one or two dimensions, micrometres in the remaining dimension.

Corresponding to the vast range of measurement activity in the Length area, there are a large number of technologies and instruments used in length metrology, many of which are mature and sophisticated, including X-ray and optical interferometry, atomic force microscopy (AFM), co-ordinate measuring machines (CMMs), roundness measuring machines (e.g. Talyrond), surface characterisation (e.g. Talysurf), theodolite and photogrammetric systems.

Uncertainties associated with the definition of the metre and wavelength standards are a few parts in 10^{11} , those with gauge block calibration, one part in 10^7 , while uncertainties required by precision engineering are typically a few parts in 10^6 .

The 1996 – 1999 Length Programme was organised into a number of projects, and the main technical projects are listed in Table 1. As indicated, these projects cover a wide range of activity and technologies. This report concerns all these project areas. For reference the main themes in the 1999 – 2002 are given in Table 2.

1	The metre and wavelength standards Frequency stabilisation of gas, diode and solid state lasers, trapped ion standards, measurement of wavelength/optical frequency, calibration of laser interferometric systems
2	Maintenance and development of dimensional metrology standards Calibration of end standards, gauge blocks, length bars, step gauges, reference length artefacts, calibration of internal and external diameter standards and reference screw threads, including API standards, calibration of angle standards, nanometrology and surface texture measurement, optical profilometry, atomic force and scanning tunnelling microscopy, X-ray interferometry
4	Micro-and optical metrology Form and deformation using Moiré and photogrammetry, 1- and 2-dimensional micrometrology, linewidth standards, photomasks and wafer metrology, graticules and metrology gratings, displacement transducers, gas and liquid refractometry, optical fibre metrology, diffracting optics and gratings
5	Gear metrology National Gear Metrology Centre, University of Newcastle-upon-Tyne
8	Nanorond-2 roundness instrument Collaborative project with Taylor-Hobson Ltd to develop an accurate roundness measuring facility
9	Small angle generator Collaborative project with Renishaw plc.
12	National primary co-ordinate measuring machine Collaborative project with Brown & Sharpe and Cranfield University to develop two CMMs based on interferometry.

Table 1. 1996 – 1999 Length Programme main projects

1	The metre and wavelength standards
2	Large scale co-ordinate metrology
3	Dimensional metrology, including gears
4	Form Metrology
5	Metrology for miniaturisation
6	Environmental factors affecting traceable length metrology

Table 2. 1999 – 2002 Length Programme main technical themes

3. Modelling Techniques

3.1 Methods for Modelling Measurement Data

3.1.1 Types of data

There are three categories of measurement data sets:

1. discrete measurement data, which means: a) data obtained by sampling a discrete variable: e.g., a variable that may take only integer values such as in counting processes, and b) data obtained by sampling a continuous variable.
2. continuous measurement signal, which means an analogue signal prior to any analogue to digital conversion, which would result in data of type 1 b).
3. hybrid measurement data composed of both discrete and continuous data sets.

Examples of the type of measurement data encountered in the Length area include:

Counts. Interferometry works on the basis of counting fringes, similar in principle to counting the number of peaks in a simple harmonic signal. Given a sufficiently accurate signal, the data can be analysed to produce counts of fixed fractions of a fringe. The error in the estimate of the associated displacement arising from fringe fractioning is bounded by a fixed fringe fraction.

Discretely sampled, finitely represented. In co-ordinate metrology, the co-ordinates of points are sampled at discrete locations on a continuous profile or surface. The measurands are a finite array of real numbers and the measurements are finite precision representations of these arrays.

Continuously sampled, discretised, and finitely represented. In a number of areas such as roundness and surface texture, the instrument probe is in continuous contact with the profile or surface providing a continuous sensor signal. Thus the measurand is generally a continuous curve C , and the measured data a finite representation of a discrete sample of points on this curve. In interferometry, the fringe pattern can be a continuous two dimensional image describing the phase of the wavefront as a function of two spatial co-ordinates.

3.1.2 Types of model

There are three categories of model:

1. discrete models in which the outputs of the measurement system are related to measurements of its inputs by a system of algebraic equations;
2. continuous models in which the outputs of the measurement system are related to measurements of its inputs by a system of differential equations;
3. hybrid models in which the outputs of the measurement system are related to measurements of its inputs by a system composed of both algebraic and differential equations.

It is appropriate to distinguish here between the nature of the model and the approach to solving the model (which for a continuous model typically also involves solving algebraic equations).

Given infinite precision arithmetic, the set of equations derived from a discrete model can be solved exactly. This is not the case for a continuous model which typically requires approximations to be made, for example, in terms of domain discretisation.

3.1.3 Models used in the Length Programme

The wide range of activity within the Length area is reflected in the wide range in the type of models, as indicated below.

Discrete modelling examples

A common calculation in length metrology involves finding the best-fit curve or surface to a discrete set of co-ordinate data. The curves and surfaces can be represented by geometric elements such as circles and cylinders, each with a well-defined set of parameters (e.g., for a circle, its centre co-ordinates and radius) or by empirical functions expressed in terms of basis functions such as polynomials, splines, Fourier components, wavelets, etc. The fitting criteria can involve least squares, minimax (Chebyshev), and related criteria. For data which is subject to sporadic wild points caused by a crack in a surface, for example, robust methods are appropriate.

The calibration of instruments often require fitting calibration curves to data. For example, in the calibration of an autocollimator (Project 12¹), the relationship between angle and voltage output by a photodiode is modelled by a cubic polynomial. In the calibration of the small angle generator (Project 9), the relationship between angle of a prismatic body and change in path length of light passing through the body is modelled by a polynomial of degree up to approximately 20. In this latter example, the use of an orthogonal basis to represent the polynomial is absolutely essential in order to preserve numerical stability².

In CMMs, the scale readings can be converted straightforwardly into probe co-ordinates. However, in many systems, the determination of the target estimates from the sensor reading is a nontrivial task requiring relatively sophisticated models and optimisation tools. A related area is the modelling of machine behaviour. For example, CMMs exhibit systematic errors due to their imperfect geometry. These systematic errors are described by the kinematic error model involving the functions describing the straightness, orthogonality, roll, pitch and yaw of the motion along each axis. These errors are determined either from direct measurement designed to determine the individual error components or from the repeated measurements of calibrated artefacts. The design of methods to simultaneously determine machine error, system configuration parameters and the parameters associated with the artefact being measured present significant modelling problems, some of which have been successfully tackled in recent

¹ Unless stated otherwise, project numbers refer to the 1996 – 1999 Length Programme.

² See http://www.npl.co.uk/ssfm/tt/ssfm_interactive_examples/orthfit/orthFit.html for a demonstration of numerically stable polynomial fitting using orthogonal polynomial basis functions.

years (see, e.g. Cox *et al.* (1998,1999), Downs, Forbes and Siddle (1998), Evans, Hocken and Estler (1996), Forbes, Johnson and McCarthy (1999)).

In a number of systems, a controller is used to maintain the system in a preferred state and modelling and simulation is also used in the design of such systems, working from first principles or in configuring a commercial control system.

Continuous modelling examples

Continuous modelling is important in the calculation of machine and artefact deflection. For example, in the calibration of a 5 m long reference artefact (Corta *et al.* (1998), Forbes and Peggs (1997)) the deflection of the artefact due to gravitational loading introduced significant changes in the distances between targets on the artefact. In order to compensate for these deflections, a finite element model of the artefact was used to estimate the deflection during the artefact's calibration and subsequent use for various support regimes. Finite element (FE) models are also used in experimental design to predict material properties such as stiffness. Continuous modelling is used to estimate temperature distribution in artefacts. For example, in gear metrology FE analysis is used to provide data for the specification of minimum stabilisation times for artefacts used on site, transported by air freight, etc.

Hybrid modelling

Often the continuous modelling involves the incorporation of discrete data. For example, in the calculation of the deflection of the large reference artefact mentioned above, the stiffness coefficients were determined from measurements providing discretely sampled data. In an ideal approach, the uncertainties associated with these measurements would be taken into account in estimating the uncertainties in the deflection corrections.

Discussion

Because of the rich interplay between Length metrology (and co-ordinate metrology in particular) and geometry, many of the modelling issues that arise in Length are naturally the subject of past and current applied mathematics research. There is a long history of collaboration between co-ordinate metrologists and numerical mathematicians at NPL on modelling and software development; see, for example, Forbes (1989), Anthony, Anthony, Cox and Forbes (1991), Butler, Cox and Forbes (1994), Butler, Forbes and Harris (1994), Anthony *et al.* (1996).

This collaboration continues. Projects in the 1996 – 1999 Length Programme generated a number of similar computational problems for which a common algorithmic approach was developed. The analysis of data from multi-station co-ordinate measuring systems all involve the solution of systems of linear equations with block sparsity structure, linear equality constraints, covariance in the uncertainties associated with the observation equations and (prior) calibration information (Forbes (1999)). A generic regression algorithm has been developed to solve these types of problems by transforming them to a standard nonlinear least squares problems. The algorithm has been implemented in Matlab (Forbes, Fossati and Smith (1999)). In the self-calibration of 1- and 2-dimensional reference artefacts, the regression problem potentially involves thousands of observation equations in thousands of parameters for which a full matrix approach would be completely impractical. Fortunately, the matrices involved are sparse and sparse matrix techniques can be applied (Paige and Saunders (1982), Cox and Forbes (1998)). These have been implemented in Fortran 90 to solve any sparse nonlinear least squares problem subject to linear equality constraints (Forbes, Johnson and McCarthy (1999)).

There are a number of areas where further work on modelling and algorithm development is required or of potential benefit. These include:

Geometric tolerance assessment. There are a large number of unresolved modelling problems associated with geometric tolerance assessment:

- Development of algorithms that successfully take into account form and measurement error. Chebyshev methods take into account form error only, least squares methods usually only take into account measurement error.
- Development of algorithms that take into account the correlation in the co-ordinate estimates that arises in laser tracking, theodolite and photogrammetry systems. This is currently being addressed; see Forbes, Fossati and Smith (1999), Forbes, Fossati and Clarke (1999).
- Data approximation using parametric curves and surfaces, important in tolerance assessment using CAD models; see Turner *et al.* (1999), Watson (1999).
- Robust (outlier resistant) data approximation methods; see Ross *et al.* (1999).

Error separation techniques. In the calibration of reference artefacts it is important to separate the systematic error behaviour of the measuring instrument from the deviation from nominal form associated with the artefact. Reversal and error separation techniques have a long history in length metrology, for example in straightness measurement and in angle calibration (Evans, Hocken and Estler (1996), Estler (1998)). These methods can be extended and applied to other situations. For example in roundness measurement, the spindle error can be separated from the form error of the sample (Cox (1999a); see also Forbes, Lewis *et al.* (1999), Forbes, Johnson and McCarthy (1999)). Further work could be done on developing the general principles and in their application, for instance, to determining the form error in the reference spherical wave front in interferometry.

Combining physical and empirical models. Often an empirical model is used to describe systematic departure from nominal behaviour specified by a physical (or empirical) model. For example, the form error of a lobed circle may be described by a Fourier series. However, when the models are combined, parameters may become convolved with each other leading to stability problems when the model is used. For example, the circle centre coordinates are no longer independent of the radial deviation when the Fourier terms are added.

Empirical models in higher dimensions. While polynomials, splines, etc., can be used efficiently and effectively to model empirical functions in one dimension, they are less well adapted to two and higher dimensions. For example, refractive index of air can be represented by a real valued function of three spatial co-ordinates. It may be that technology based on radial basis functions, when sufficiently developed, will provide a solution.

Image analysis. In the optical measurement of gratings, pin holes, etc., the system response depends in a complicated way on the optical and geometrical properties of the sample. This means that determining unbiased estimates and their uncertainties is difficult.

Models for surface roughness. There are many modelling problems associated with 2-dimensional and more especially 3-dimensional roughness measurement, many of them associated with the definition, calculation and interpretation of the various roughness parameters³. In particular, the use of different form error and waviness subtraction algorithms along with different data filters places barriers to producing traceable roughness measurement as evidenced by large discrepancies in round-robin exercises.

³ See http://www.hud.ac.uk/schools/engineering/research/ultrap/surface/project_open.html for information on an EU project examining some of these issues.

3.2 *Uncertainties and Statistical Modelling*

Many systems have comprehensive uncertainty budgets derived following the ISO Guide (ISO (1993)) and UKAS M 3003 (UKAS (1997)). Often, there is an informal template for such uncertainty budgets, covering typical sources of uncertainty such as air refractive index, temperature, material constants etc., with 10's of components identified. These error budgets are presented in tables, the entries calculated either by hand, calculator, spreadsheet, Mathcad or other scientific software packages. The Guide and M 3003 are generally seen to cover many aspects adequately and scientists are sufficiently trained in applying their principles. Uncertainties are assumed to have normal or rectangular distributions and coverage factor $k = 2$ corresponding to 95% confidence limits is the norm. For a low number of degrees of freedom, other k -factors are sometimes used.

Often in response to UKAS reviews or instrument development, uncertainty budgets are refined to take into account more factors, more realistic assumptions about underlying distributions or a better analysis of the degrees of freedom. These refinements can lead to a better understanding of the system as a whole and improvements in measurement strategies.

NPL's Centre for Information Systems Engineering has collaborated with the Centre for Basic, Thermal and Length Metrology (formerly the Centre for Length Metrology) in the statistical modelling of many of the measurement systems. For example, in the CMM projects (Project 12), the mathematical models allow uncertainties associated with the probe positions to be estimated from the covariance matrix of the fitted parameters determined from the linearisation about the solution of a nonlinear optimisation problem. There are many possible estimation approaches, and much effort has gone into ensuring that all sources of measurement uncertainty are adequately incorporated.

However, there are many problems associated with determining calibration uncertainties associated with length artefacts. While mathematically, length can be realised as the distance between two points, artefacts involve real surfaces with form error, roughness and hardness characteristics and change shape due to temperature, gravitational loading, etc. This means that associating a unique length with a real artefact is not straightforward. In practice, the calibrated lengths are often derived from a sample of measured points and the calibrated value and its uncertainty depends on the sample chosen.

In other areas, such as form assessment, the measurand is a function of the complete real surface. When a real feature on an industrial part is measured with a CMM, the estimates of the feature parameters (diameter, angle etc.) will depend on the probing strategy, i.e., the number and placement of the measurement points. If a probing strategy is inadequate, these parameter estimates may differ considerably from the correct values and therefore possess large uncertainties (which cannot readily be quantified). Moreover, the estimate of the form error of the feature is almost certain to be optimistically small. In many circumstances, it is expected that the uncertainties due to the probing strategy, as a consequence of form error, constitute the major contribution to measurement uncertainty. This point has also been forcibly made at the International Standards Organisation Committee TC/213/WG10, Co-ordinate Measuring Machines. However, the relationship between probing strategy and the reliability of the resulting estimates is often complex. This leads to the fundamental problem of how to assess the uncertainties associated with a given choice of probing strategy and this problem is only recently being addressed; see e.g., Butler, Cox and Forbes (1999). Similar issues arise in surface roughness.

This problem is also important in gear metrology. Many of the gear artefacts at the National Gear Metrology Laboratory have deliberate form errors introduced during manufacture in order

to “exercise” the measurement and evaluation system. The influence that these form errors have, when combined with the errors in the measuring instrument, are at present unquantified.

A related problem concerns the treatment of systematic errors and correlation in the measured co-ordinates and their influence on the uncertainty of parameters associated with the substitute feature. For example, if a mathematically perfect cylinder is measured by a co-ordinate measuring machine in a number of different locations and orientations within its working volume different estimates of the radius will be obtained, reflecting systematic and random measurement error. Quantifying this in terms of an uncertainty on the estimated radius is an extremely difficult task. Furthermore, there are a vast number of parameters associated with substitute elements and determining a method to calculate such task specific uncertainties is a major challenge. In a number of institutions, e.g., IMGC, NPL, and PTB, the Virtual CMM concept has been developed and implemented to tackle this problem (Cox, Forbes and Peggs (1999), Trapet and Waldele (1996)). By modelling all the systematic errors simulating all the main sources of measurement uncertainty associated with a CMM, it is possible in principle to estimate these uncertainties. However, to be successful, it is necessary to ensure the model of CMM behaviour is valid, a major task in itself (see, e.g., Cox *et al.* (1998, 1999)).

These problems also arise and are further complicated in multi-station measuring systems such as theodolite, photogrammetry and laser tracker systems. If the correlation between estimates of target co-ordinates are not properly taking into account, the estimates of the uncertainty of simply defined quantities such as the distance between two targets can be hopelessly inaccurate (Forbes (1999), Forbes, Fossati and Clarke (1999)).

In determining uncertainties there are many grey areas where the influence of some factors is not perfectly understood and are assigned an uncertainty on the basis of experience, often erring on the side of pessimism. In some instances, UKAS assessors have indicated that the uncertainties have been significantly (100%) overly pessimistic.

There is a need for software support tools for calculating uncertainties for “standard” experiments, something like a uncertainty budget “wizard” that guides the user through the various stages and performs the calculations. However, many uncertainty calculations, for example, in co-ordinate metrology are task specific and require a bespoke analysis. For instance, in order to gain more accuracy from a CMM the comparator principle is used in which measurements of the test artefact are compared with before-and-after measurements of similar reference artefact, perhaps a gauge block or a plain-setting ring gauge. The uncertainty budget for the test artefact has to take into account the uncertainty in the calibration of the calibrated artefact, repeatability and drift in the measurements of the calibrated artefact, before and after, repeatability of the measurements of the test artefact, effects of mounting and remounting artefacts on the artefact and measuring system as well as the measurements of temperature, etc.

Another example where a non-standard approach is required is in the assessment of uncertainties associated with physical quantities that can only be positive such as form error, concentricity, co-axiality and roughness. The standard approach can lead to confidence limits straddling zero. A related issue is the compatibility of go/no-go tolerancing with confidence limits. Does the part pass if a (small) part of the confidence interval lies outside the confidence band?

Guidance for these non-standard problems is sought.

3.3 Visual Modelling and Data Visualisation

Data visualisation is used extensively in graphing sensor outputs, roundness profiles, residual errors, etc., and is important in monitoring system performance and understanding system behaviour. In analysing the measurement strategies for determining CMM systematic errors,

visualisation was used to analyse the modes of artefact and system distortion that were undetectable from the data. This led to a clearer understanding of the systems and ultimately to the design of better measurement strategies. Visualisation is also important in understanding artefact deflections estimated from finite element modelling. Many optical systems involve imaging directly, in particular fringe maps⁴.

Mathematica, Matlab and Excel are used in data visualisation and graphing. Graphical tools are also used in instrument design and description. In the calibration of 2-dimensional photomasks, special purpose software modules have been written to provide high-quality visualisation of the calibration results.

Commercial tolerance assessment packages use visualisation to display the CAD data. There are opportunities to extend this to portray tolerance information, recommended measurement strategies, actual measurements taken and tolerance assessment results.

In multi-station systems such as multi-lateration, theodolites, etc, given a CAD representation of the object to be measured, visual modelling could be used to design system configuration and measurement strategy to take into account line-of-sight and other configuration constraints. Visualisation tools could also be used to show how the uncertainty in target locations (the *uncertainty map*) changes as a function of position. Since the uncertainty information is represented by an ellipsoid defined by nine parameters, the uncertainty map is essentially a map from 3-dimensional space to 9-dimensional space, presenting a visualisation challenge.

3.4 Data Fusion

The Length area is rich in certain categories of data fusion examples:

- Multi-station measuring systems require fusing sensor data from more than one station in order to determine target co-ordinate estimates in a common frame of reference (see, e.g., Butler, Forbes and Kenward (1998), Forbes, Fossati and Clarke (1999)).
- In the comparator principle, measurements of an artefact to be calibrated are fused with measurements and calibration information associated with a similar, high quality artefact (possibly obtained using a different system) in order to reduce uncertainties arising from systematic machine errors.
- In determining CMM behaviour, prior calibration information about an artefact has to be fused with current CMM measurements. Once the systematic errors have been estimated, this information can be fused with ongoing measurements in order to monitor system stability (see, e.g. Cox *et al.* (1998, 1999), Forbes (1999)).
- Gear calibration is the result of fusing the measurements from the calibration machine, temperature compensation data, differential level and laser compensation and other measurement data.
- In theodolite and photogrammetry systems measurements of a calibrated length artefact have to be fused with the sensor information in order to determine the scale for the target co-ordinates.
- In the combined optical and X-ray interferometry instrument, X-ray fringe counts are fused with optical fringe fractioning data.

⁴ An example image associated with gauge block interferometry can be viewed at <http://www.npl.co.uk/npl/sections/dmet/flap.html>.

- In optical interferometry, temperature, pressure and humidity measurements are fused with fringe counts via refractive index corrections in order to determine estimates of displacement.

While these examples can legitimately be viewed as data fusion, it is fair to say that the data fusion angle is not particularly stressed within the Length community. Many models involve some sort of data fusion. One can view co-ordinate metrology as 'the data fusion of tactile sensors'. However, many of the problems above do have common characteristics, e.g., involve structured matrix systems, and a generic approach, whether labelled data fusion or not, could bring benefits in terms of efficiency, improved understanding and, ultimately, more accurate measurement systems; see Forbes (1999), Kelly (1999).

A problem not to be underestimated is that practical data fusion depends on the easy transfer of data from one system/package to others. Data format compatibility problems (in particular, implementing secure data transfer) are common.

4. Validation and Testing

4.1 Spreadsheets and Other Mathematical Software Packages

A number of mathematical software packages are used within the Length area:

- *Excel*. Used to calculate uncertainty budgets, modelling, data visualisation.
- *Quatro-Pro*. As Excel.
- *Matlab*. Used in a range of modelling and application software development, data visualisation.
- *Mathematica*. As Matlab. Also the control systems toolbox is used to design and model control systems.
- *Mathcad*. As Matlab.
- *LabView*. Used for instrument interfacing and modelling.
- *Pafec*. Used for finite element modelling.
- *Co-ordinate measuring system in-built functions*, e.g. Quindos
- *Image analysis packages*

In general, these packages are accepted as fit-for-purpose by virtue of their widespread use but viewed with varying degrees of scepticism. Usually, no validation of the packages as a whole is undertaken. However, software written using these packages is usually tested in accordance with software development quality procedures, for example, by comparing calculated results with reference results or results determined using other software. This is probably the only way to proceed with these packages which have a large number of functions. For example, Matlab has thousands of in-built functions and it is clearly impractical for a single user to test each function. Furthermore, the quality of these functions can vary and good results for one set of functions is no guarantee that another set are reliable.

While the use of packages such as Excel in Length is probably similar to its use in other metrology areas, many measurements in Length rely on complex in-built functions associated with measurement systems, CMMs in particular. These functions determine best-fit substitute features such as spheres and cylinders to co-ordinate data and calculate the parameters such as radius associated with these elements. These calculations are a key component in the chain from measurement data to measurement result. In the 1980's, it became apparent that not all software

performing these calculations gave reliable results and two EU projects undertook a test of such software. The results of the first exercise showed that many implementations produced inaccurate results (Porta and Waldele (1986)). The second exercise, a few years later, demonstrated that for least squares calculations (Gaussian substitute features), most software (but not all) performed satisfactorily (Drieschner *et al.* (1991)). These exercises led to the draft of an ISO standard for testing substitute feature calculations and also third party testing services at PTB, NIST⁵ and NPL⁶ and elsewhere.

In view of the large number of different calculations associated with co-ordinate metrology, it is clear that further work on validating the software performing these calculations is necessary, covering, for example,

- Calculation of Chebyshev substitute features and more general tolerance assessment.
- Target location estimation algorithms in laser tracking, photogrammetry, theodolite and portable (flexible arm) CMMs.
- Image analysis software.

In order for this activity to bring most benefit, a standards framework is required so that tests of software performed by different organisations can be seen to be compatible (Anthony *et al.* (1993)).

4.2 Model Validation

Many models are generated from first principles and validated by comparing quantities predicted by the model with results that can be measured independently or calculated from other considerations. A common approach is to look at the residual errors associated with the computed fit (Butler *et al.* (1999)). The model is (partially) validated if these errors are appear random and free from systematic behaviour.

There are a number of model validation issues that arise in Length metrology.

Selection from a family of empirical models. In the use of empirical functions such as polynomial or spline curves and surfaces to model profiles and surfaces, it is important the select the degree or number of terms that produces an adequate fit to the data. Statistical techniques such as examining the RMS residual as a function of degree can be used more widely to supplement more subjective approaches. For example, the kinematic error model for CMMs use empirical functions to describe the 18 error components. The choice of degree is often determined on the basis of custom, experience, constraints on the number of variables the software can handle or the number of measurements required to determine the model parameters rather than from strict model validation principles. The kinematic model itself requires validation as it makes assumptions about the independence of the errors components. One validation approach suggested in Cox *et al.* (1998) is to embed the kinematic error model in a more comprehensive empirical model and determine if the larger model provides a better prediction of behaviour.

Measurement strategy validation. To validate a model from measurement data, it is necessary to have enough data to in order to make a sensible judgement. It follows that the measurement strategy used in the model validation must itself be validated. As discussed in section 3.2, the

⁵See http://www.mel.nist.gov/div826/msid/sima/ia_cmm.html for some information about the NIST testing service. See also <http://www.nist.gov/itl/div898/strd/> for the NIST data sets for testing statistical software.

⁶ <http://www.npl.co.uk/npl/sections/sss/services/index.html>

calculation of form error is heavily dependent on measurement strategy. In determining roundness (circularity) a measurement strategy consisting of just three points produces an (invalid) estimate of zero form error. While this example is clearly absurd, in much more complicated situations it is not so simple to specify a measurement strategy that is guaranteed to test the validity of a model and there are model validation or verification procedures implemented that provide only partial information. Much of the focus of Cox *et al.* (1998, 1999) and the NPL work in the Jigless Aerospace Manufacturing (JAM) project is providing a theoretical and numerical basis for measurement strategies that adequately test the model assumptions (Forbes, Fossati and Clarke (1999)). The main approach is the use of estimates of the uncertainties of the fitted parameters as a measure of adequacy of the measurement strategy.

Estimator validation. It is appropriate to consider estimator validation as a component of model validation. In determining system parameters from measured data, it is often the case that the computational aim (for example, the minimisation of an error function) is correctly formulated but that an estimate is determined by solving a simplified computational problem. In determining the Gaussian substitute circle or sphere, an approximation is often used to convert a nonlinear problem into a simpler, linear problem. It has been shown that this is a safe approximation for data distributed uniformly around a circle but introduces significant bias for data on a small arc of the circle (Cox and Forbes (1992), Forbes *et al.*, (1999)). In the determination of form error, the Gaussian substitute feature can be calculated instead of the more difficult Chebyshev substitute feature, generally without introducing significant bias into the subsequent analysis. In co-ordinate metrology using interferometric transducers, the correction for refractive index effects properly leads to a generalised regression problem, but an ordinary regression estimator is implemented instead. In implementing approximate estimators, it is important to be able to quantify the resulting bias, if any, over the applicable range of problem domains. In recent years, the null space techniques developed to generate reference data and results to test software implementations (Cox and Forbes (1992), Butler *et al.* (1997)) have been successfully adapted to validating estimators and used in a number of Length applications, including the analysis of theodolite data, National Primary CMM (Project 12) and geometric tolerance assessment.

4.3 Measurement System Validation

A large number of instruments used in the Length area have significant amounts of software performing nontrivial calculations, a main example being CMMs. The software is embedded in the sense that the user has no access to the source code and may have limited means of inputting test data and intercepting intermediate calculations. Since much of the intellectual property associated with these systems is bound up in the software, there is no likelihood that users will have access to source code in the future. This means that validation has to be based on a black box test of the software. Both users and suppliers recognise the need for validation of such software and there is a draft ISO standard in place for testing software for calculating Gaussian substitute features. This addresses a significant area but there are many other areas for which a similar approach could be applied. The NIST algorithm testing service also includes testing Chebyshev substitute features (but uses an approach that could be problematical). The JAM project includes a work package to develop a methodology (based on black box testing) to validate software for calculating target locations from sensor reading for theodolites and similar systems.

Complete measurement systems are verified through measurements of calibrated artefacts. For example, ISO 10360 (ISO (1995)) describes a procedure for verifying the length measuring capabilities of CMMs from measurements of calibrated length artefacts. Composite artefacts have been designed and used to test a system's capabilities on a range of standard features such as cylinders and cones. These tests are an indirect test of element fitting software.

Systems are also tested against each other. For example, CMM's ability to measure circularity can be tested against a roundness instrument, again involving a (partial) test of the embedded software.

4.4 Validation of Simulated Instruments

Numerical simulation has been an important tool in Length metrology, used in instrument design and configuration, the design of control systems, the selection of measurement strategies and the evaluation of measurement uncertainties. Simulation was used extensively in analysing the behaviour of multilateration systems and the design of the new National Primary CMM. A novel feature of this activity is the use of actual measurement data from a single laser tracking station to build a simulation of a multistation system (Hughes and Wilson (1999)). A large European project led by PTB has as its focus the implementation of an online Virtual CMM which takes actual measurement data and uses a comprehensive numerical simulation of the CMM and its main sources of uncertainty to estimate through Monte Carlo techniques the measurement uncertainty associated with the measurement task (Trapet and Waldele (1995), Cox, Forbes and Peggs (1999)). However, there are many issues relating the approach adopted, some of which will be discussed in the Validation of Simulated Instruments report (Forbes and Harris (1999)). Simulation and Monte Carlo techniques are also important in determining uncertainties due to sampling error in form assessment (Butler, Cox and Forbes (1999)).

5. Metrology Software Development Techniques

5.1 Software development methods

A wide variety of software is written in the Length Programme. At NPL, the software is written in accordance with NPL quality procedures and following the guidance explicit or implicit therein. (NPL is certified to ISO 9000 plus TickIT.) There is no formal development methodology in widespread use and software development methods reflect application, software language, operating system, hardware interface requirements, personal experience, training and preference. The size of software applications run from a few lines to over 1 million (Flapack software). Issues related to software development include:

Number of languages in use, including Basic, BBC Basic, Quick Basic, HP Basic, HT Basic, Visual Basic, Pascal, Turbo Pascal, Delphi, Fortran, Fortran 90, C, Borland C++, Builder, Visual C++, Mathematica, Mathcad and Matlab, many in different versions associated with different operating systems.

Training. People are generally expected to pick up the rudiments of a new language/software environment as part of project work, with little formal training. It is not unusual for someone to have to program in three or more languages at any given time.

Benefits of formal development methodology. The use of many software languages is probably inevitable and there is a large potential benefit of having a language independent description of the software design as part of a formal development methodology, helping users familiar with one language to understand software in other languages and aiding the upgrade of application modules from one language to a later release or to a completely different language as hardware and/or operating systems become obsolete.

Benefits of object oriented approaches. Visual C++ and other object oriented systems have software development tools that in theory help the user design and implement software in a structured and re-usable way, providing another method of capturing a high level description of the software design.

In many situations, software is directly involved in the traceability chain. A full range of methods are used test software including checking against published results, hand calculations, other software (or previous versions of the same software) and, in the case of CMM software, reference results for reference data. The Flapack software, written in Borland C++, was specifically designed to allow all components to be tested using test data, a good example of best practice.

5.2 Software reuse

While software reuse is seen as worthwhile, there are a number of factors that work against it. The move from mainframe to work station to PC often implies a change in supported languages, leaving large amounts of software that have to be re-implemented or discarded. Many instruments support or have supported nonstandard languages leading to further incompatibility. Legacy software is being translated into modern languages such as Visual Basic, but with the realisation that further updating may be required as new versions are released. Many instruments have an operational lifetime of ten years or more and have proprietary hardware interfaces. Data acquisition software has to support these interfaces putting very real constraints on what software language, computer and operating system can be used.

Software libraries are used mainly through functions in packages such as Matlab and Mathematica and CMM packages such as Quindos. The use of object oriented languages such as C++ promote reusability. Many of the objects within the Flapack software (such as temperature measurement data acquisition) are completely reusable. The move away from mainframes has resulted in less use of libraries such as the NAG library.

One issue is the awareness and accessibility of key function implementations. (In the derivation of uncertainty budgets, the calculation of sensitivity coefficients require the evaluation of partial derivatives associated with these key functions.) There are many instances of key functions being used in different areas in different applications. For example ellipse fitting is required in the dimensional assessment of fibre optics, co-ordinate metrology and interferometry. Another example is the calculation of the refractive index of air from an Edlen-type equation. At present there is no obvious way that a metrologist working in one sub-area will know what key functions have been implemented in another sub-area.

A second issue has been the use of Matlab for developing prototype software to test concepts and help with algorithm design. Matlab is ideal for this and it is possible to write sophisticated and reliable software quickly. Unfortunately, it is generally impossible to develop a stand alone executable or dynamically-linked library (DLL) from Matlab and Matlab software will only run on a system with Matlab installed. This means that for many applications, the Matlab software has to be translated into another language. Experience with the Matlab "compiler" which converts Matlab software into C has not been positive. A similar situation exists with the large amount of reliable Fortran library software for which an interface is required to languages such as Visual Basic, LabView and Excel.

In the roundness instrument (Project 8), the problem arose of interfacing Fortran software performing polynomial approximation with the instrument control software written in Borland Builder. After much effort, the only available solution was to implement the approximation software in Builder. While it is quite possible that there is a way of designing a working interface, there was no clear route for the software engineers to find out what it might be. This type of problem is being addressed directly in the SSfM Software Re-use (Project 3.2).

Recent experience has shown that interfacing problems are potentially less troublesome with the advent of Fortran 90 (F90): i) F90 supports many of the features of Matlab, so that translation to F90 is very straight forward, ii) F90 DLLs can be interfaced with Visual Basic (VB), C++, Excel

through “add-ins”, etc. and iii) F90 is compatible with Fortran 77. It should be stressed that Fortran 90 is a language with a fixed specification and software written in it is, in theory, portable to any system that supports a F90 compiler. While in practice variants of the language may arise, as happened in the case of Fortran 66 and Fortran 77, the fixed specification removes the majority of the problems that plague other non-standardised, propriety systems in which version updates to any one of a whole range of components ultimately require changes in the user’s application source code. A number of projects in Length, including the Primary CMM projects (Project 12) have used or are using a Matlab–Fortran 90–VB interface paradigm to allow for rapid prototyping and efficient implementation.

A significant amount of software is written in the language of instruments, such as UMESS or Quindos in CMMs. This software controls the acquisition of the data (including the measurement strategy) and the analysis of the data (determining substitute features, for example).

The Year 2000 problem (Y2K) surfaces, for example, in the date-stamping of data and in the preparation of certificates. NPL has a task group working on this issue, testing every piece of appropriate equipment. The Flapack software, for example, has been tested specifically for Y2K anomalies. It is not anticipated that Y2K issues will have a significant impact on the delivery of NMS milestones. (The problematic date of 9th September 1999 passed without incident.)

5.3 Virtual Instruments

LabView is used in some areas of Length, for instrument interfacing, data acquisition, etc. Virtual instruments/numerical simulators exist or are being developed in other forms, including the Virtual CMM (NPL Matlab version), Virtual Multilateration CMM (NPL Matlab version) and Flapack. While Flapack is designed to work with a number of hardware systems, it can also work independently of any hardware, reading measurement data from files instead of acquiring it from sensors. Much of the methodology developed for verification of the performance of multi-station CMSs relies on numerical simulations using a “reference” model of the system. While these example are virtual instruments in the sense that they have a purely software representation, they do not properly embody the attributes of visual programming.

6. Support for Measurement and Calibration Processes

6.1 Automation of Measurement and Calibration Processes

There is no significant use of Laboratory Information Management Systems (LIMS) in the automation of measurement and calibration processes, although the need for a system has been recognised for a many years. There is a noticeable contrast between the sophistication of much of the metrology software (Flapack, Quindos, etc.) and the hand calculation and checking of certificated results and uncertainties. There is a clear need for automation in this area but there are obviously resource constraints. Moreover, simple approaches based, for example, on importing Excel spreadsheets into Word documents are fragile, often with unforeseen side effects. There are major concerns about data integrity using such systems as there are plenty of documented cases of data being wrongly interpreted or corrupted. In the experience of many, the manual transfer of data is still the safest and most robust method. Over fifty years into the computing age, this can hardly be a satisfactory state of affairs. Improvements are anticipated with the move to new laboratories and the adoption of a corporate LIMS.

6.2 *Format Standards for Measurement Data*

There are a number of data standards, relevant to Length, including the Dimensional Measurement Industry Standard (DMIS) for CAD and CMM data. This is a major activity promising the easy exchange between CAD, CAM and Computer Aided Inspection systems as well as graphics and visual modelling systems.

At the laboratory level, there are problems in converting instrument data files into suitable ASCII files for use by other systems and special software has to be bought (e.g., Zeiss CMM) or developed (e.g. roundness instrument) in order to perform the conversion. Post-editing is often required in order to extract the required data, a process subject to human error.

There are also issues concerning the specification of geometric elements, with different enterprises using different methods of specifying a cone, for example. This means that two sets of completely different numbers could specify the same geometric object according to different conventions and to compare these numbers properly, it is necessary to derive the correct conversion formulae, a significant and error-prone activity.

7. Suggestions for Future Activities

As discussed above, numerical mathematicians and metrologists have collaborated in the Length area for many years. Length continues to pose many problems which require new approaches to modelling, algorithm design and statistical analysis. As evidence of this, approximately one third of the papers at the Advanced Mathematical and Computational Tools for Metrology workshop held in Oxford in April 1999 (Pavese *et al.* (1999)) were Length related. Many of the numerical tools developed for Length projects are now being applied in other areas and, of course, techniques developed elsewhere often find ready application in Length.

7.1 Expected Benefits of the SSfM Programme

Benefits for the Length area arising from the SSfM Programme are being realised or are looked for in the following areas:

- *Modelling*: for example, the development of error separation techniques, empirical models in two or more dimensions, wavelet analysis of surface roughness, continuous modelling in instrument design.
- *Uncertainties and statistical modelling*, in particular software tools, best practice guide, uncertainty estimation for non-standard problems, the analysis of key comparison data in underpinning the equivalence in measurement standards (Cox (1999b)).
- *Data fusion*: for example, the development of generic approaches to fusing prior calibration information with current measurement data (Forbes (1999)). In particular, the models for multilateration systems in Length and global positioning systems (GPS) in Time (Chorley (1999)) have structural similarities and techniques developed for one could be equally applicable to the other, for example Kalman filter techniques (Kelly (1999)). Clearly there are opportunities to develop common approaches applicable to both areas.
- *Model validation*: for example, rules for selection from a family of empirical models, measurement strategy validation, estimator validation.
- *Metrology software development methods*.
- *Metrology software reuse and the creation of libraries of key functions*. The Length area is one in which there are a large number of key functions. Geometric tolerance assessment problems involve the calculation of the distance of a point to a curve or surface; these can be regarded as key functions. The solution of the tolerance problems require the application of solvers (i.e., optimisation software) that call the distance evaluation key functions. METROS, the METROlogy Software library being developed as part of the SSfM software re-use Project 3.2, is built around the concept of a key function and it is intended that many of the Length key functions will appear in the earliest releases of the library.

While METROS ultimately is concerned with software, it will be more than a software repository such as Netlib⁷ or a software guide such as GAMS⁸. The library will also give mathematical specifications of the key functions and contain test data and results with which to test implementations of the key functions.

⁷ <http://www.netlib.org/>

⁸ <http://gams.nist.gov/GAMS.html>

- *Automation of measurement and calibration processes*, particularly in the preparation of certificates and secure data transfer.

7.2 Case Studies and Feasibility Studies

Case studies and feasibility studies in the following areas have been identified and, where indicated, initiated:

- Analysis of roundness calculations from the point of view of model validation, measurement strategy validation, instrument validation, estimator validation and uncertainty evaluation: *discrete modelling best practice guide*, SSfM Project 1.1; *software re-use*, SSfM Project 3.2.
- Analysis of refractive index correction from the point of view of generalised regression, data fusion, high dimensional empirical modelling, estimator validation and uncertainty evaluation: *discrete modelling best practice guide*, *software re-use*.
- Visual modelling in designing measurement strategies that take into account line-of-sight constraints in multi-lateration systems.
- Visualisation of uncertainty maps associated with multi-station co-ordinate measuring systems.
- Data fusion relating to multi-station co-ordinate measuring systems and the incorporation of prior calibration information: *validation of simulated instruments*, SSfM Project 2.4 (Forbes and Harris (1999)).
- Substitute feature calculations, refractive index calculations, key functions in a metrology software library: *software re-use*.

7.3 Future SSfM Topics

The areas of strong interaction between the SSfM Programme and the Length Programme are indicated in sections 7.1 and 7.2. As mentioned above, the inherently geometrical nature of length metrology, co-ordinate metrology in particular, provides natural links to applied mathematics. The term *computational metrology* is used by some to encompass the modelling, algorithmic and computational part of co-ordinate metrology. New terms such as *geomatic engineering* are used to describe the acquisition, processing, analysis, display and management of spatial information⁹. It is safe to assume that mathematical modelling and numerical techniques will continue to play a role in Length metrology and dimensional measurement.

One issue being addressed by the software re-use project (SSfM Project 3.2) and which will need to be further considered in later SSfM programmes is access to the mathematical and computational techniques that exist or are being developed: where is the metrologist to find them and how is he/she able to use them? The central aim of METROS is to provide this access using the now universal world wide web interface to information stored in what can be modelled as a relational database. However, the interface can be deepened through the use of Java to perform calculations, etc., over the internet (McCormick (1999)¹⁰). There are now serious efforts being made to allow Java to be used in numerical computation as Fortran and C are currently used¹¹.

⁹ See, for example, <http://www.ps.ucl.ac.uk/>.

¹⁰ See also http://www.npl.co.uk/ssfm/tt/ssfm_interactive_examples.

¹¹ See, for example, <http://math.nist.gov/javanumerics/>.

7.4 Future Length Programme Topics

The main themes for the 1999 – 2002 Length Programme are given in Table 2. While much of the focus of the Programme is on establishing the traceability of high-accuracy length metrology, the use of co-ordinate measuring systems of novel design is increasing as the spatial representation of objects are required for a host of applications in medicine, architecture and heritage, film and virtual reality as well in engineering and manufacture. The traceability of these systems is also an issue and will call for new approaches in line with their novel designs. In this, mathematical modelling, simulation, statistical analysis and visualisation will play a part.

8. Summary of changes

The main changes from the initial restricted Length status report, summarised in Rayner (1999), are:

- the coverage has been extended to include the whole 1996 – 1999 Length Programme, including gear metrology;
- the text has been updated to reflect progress made in both the SSfM and Length Programme projects;
- additional text on potential future interactions between SSfM and Length, and the role of METROS;
- the inclusion of additional references and web page addresses.

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Appendix 1: Glossary of Abbreviations

AFM	Atomic Force Microscopy
API	American Petroleum Institute
ASCII	American Standard Character for Information Interchange
CAD	Computer Aided Design
CAM	Computer Aided Manufacture
CBTLM	Centre for Basic, Thermal and Length Metrology, NPL
CISE	Centre for Information Systems Engineering, NPL
CLM	Centre for Length Metrology, NPL
CMM	Co-ordinate Measuring Machine
CMS	Co-ordinate Measuring System
DLL	Dynamically Linked Library
DMIS	Dimensional Measurement Industry Standard
EU	European Union
F90	Fortran 90 computing language
GAMS	Guide to Available Mathematical Software: see http://gams.nist.gov/GAMS.html
IMGC	Istituto di Metrologia “G Colonnetti”, Italy
ISO	International Organisation for Standardisation
JAM	Jigless Aerospace Manufacturing (project supported by the EPSRC and DTI)
LIMS	Laboratory Information Management System
METROS	METROlogy Software Library, SSfM Project 3.2
NAG	Numerical Algorithms Group (Ltd.)
NIST	National Institute of Standards and Technology, USA
NMS	National Measurement System
NPL	National Physical Laboratory
RMS	Root Mean Square
PC	Personal Computer
PTB	Physikalisch-Technische Bundesanstalt, Germany
SI	International System of Units
SSfM	Software Support for Metrology
UKAS	United Kingdom Accreditation Service
VAM	Validation of Analytical Measurements
Y2K	Year 2000 (Millennium bug issues)

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