Robotics methods for beam line instrument simulation and control

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ABSTRACT

The majority of sample positioning systems in use at neutron and synchrotron beam line facilities around the world, may be accurately described as serial robot manipulators, i.e. they comprise a series of rotating or translating links connected together in a chain, with the tool or sample that is to be manipulated attached to one end. This characterization suggests that the methods of serial robot kinematic modeling might be usefully applied to the task of simulating and controlling beam line positioning systems.

We describe how this approach is being developed within the planning, simulation and control software, SScanSS. The advantages of using the robotics approach are shown to include the ability to: i) model any number of disparate positioning systems from within one software (and hence one user interface), with a minimum of instrument specific code, ii) accurately and speedily position and orientate samples of arbitrary complexity, and iii) provide options for automatically optimizing other important experimental parameters, such as the measurement count time.

The possible extension of this technique to include parallel robotic systems, such as Stewart Platforms, is also discussed.

1 Introduction

The Strain Scanning Simulation Software (SScanSS) was first presented at the 2002 NOBUGS conference, [1]. At that time the remit of the software was to provide comprehensive support to users of the new engineering diffractometer ENGINX, based at the ISIS spallation neutron source in the UK [2]. The need for enhanced computer support for instrument scientists and users was seen, from the start, as essential if the scientific output of the instrument was to realize its potential. In particular the time spent with the tasks associated with sample positioning and machine control were considered likely to take up a disproportionate amount of beamtime given the order of magnitude faster count times of the new machine, [3].

The SScanSS software, which was developed by the Materials Engineering group at the Open University in close collaboration with the ENGINX instrument scientists, utilizes Virtual Reality (VR) computer techniques to provide tools for planning, optimizing and executing experiments, [4]. The software generated interest at a number of other facilities and a comprehensive re-formulation was undertaken to enable other instruments and positioning systems from within one code. The theoretical basis of this formulation, which utilized the methods of robotic kinematic modeling, was reported in [5].

In this paper we provide a brief overview of SScanSS methodology and functionality before describing some recent developments. The paper continues with a description of the practical implementation of the software and ancillary hardware at two strain scanning facilities and concludes with a discussion of future directions.

2 Overview

2.1 Core functionality

The sample and hardware models used by SScanSS take the form of general polygon meshes, (usually though not exclusively triangular). The advantage of this form of model, which is common within VR applications, is that it allows the representation of arbitrarily complex objects. Sample and instrument models of this form are manipulated within SScanSS to provide the following core functionality;

Pre-beamtime

Facilities are provided to support the generation and testing of detailed measurement plans. These facilities include:

- Provision for generating or importing accurate sample models, for example from a CAD drawing or LASER scanner.
- A realistic (kinematic) instrument model which accurately reproduces the action of the instrument hardware.
- Graphical, and other, means for accurately specifying the position of measurement points within the sample model and the strain component(s) that are to be measured at each point.
- Provision for combining the sample and instrument models to enable the accurate simulation of the entire experiment including the calculation of instrument movements, neutron path lengths, count times and possible collisions.

During beamtime

Given a detailed and proven measurement plan, the priority is to minimize the time spent on activities that must be performed during beamtime but which are other than making measurements, i.e. finding the position of the sample and calculating the instrument motor commands. The time spent on these tasks is minimized by providing:

- The facility to accurately measure and input the sample position into the software and hence automatically generate the instrument motor commands required to complete the measurements.
- The means to speedily modify a measurement plan by moving existing, measurement points or adding new points without the needing to re-align the sample.

Post Beamtime

At the end of the beamtime the software and associated files contain a comprehensive description of the entire experiment. This information may be of considerable help during measurement analysis and is retained for future use by offering:

- The option to archive an entire experiment to a single (HDF) project file, thereby enabling instrument configuration, motor positions, sample model, measurement points and strain components to be recovered for future reference or analysis.

2.2 Ancillary tasks

The functionality described above is delivered from the SScanSS code, however input from external systems is also required at two key points: i) the generation of sample models and ii) the determination of the sample position on the instrument. The approaches to these tasks vary between facilities (some details are given below), but the basic requirements are held on common.

Generating sample models

Some elementary options are provided within SScanSS for generating simple sample models, however sample models will generally be obtained from either, i) other CAD software, or ii) LASER scans of the actual sample. Typically a CAD model may be used for initial planning or feasibility studies, but the exact sample geometry is often invaluable for precisely positioning measurement points within complex or distorted samples.

Initialising the sample position

In order for the motor positions generated by SScanSS to be accurate the initial position of the sample on the instrument must be precisely determined. The measurement of the sample position is achieved by identifying fiducial points on the sample and sample model and by measuring the coordinates of these points in both the sample and instrument coordinate systems. The measured positions of these fiducial points are input into the software and the transformation which relates the sample and instrument coordinate systems calculated.

3 Software design principles

3.1 Minimising Instrument Specific code

In order to provide a common interface to multiple instruments while retaining manageable software it was considered paramount that the amount of instrument specific code be kept to an absolute minimum. This goal has been achieved through the use of the robotics framework described in [5]. In summary, using this approach requires that an instrument is constructed as one or more serial robots, for example an x, y, z, omega positioning table would be one robot, and a moveable detector with retractable arm would be a second. Each robot comprises a number of mesh models, with each mesh model representing a separate moveable component or link of the robot (for example an x-stage of an x,y,z,Ω positioning system). The robots required to model a particular instrument are written as structures with elements that include: pointers to the relevant mesh models, details of rotation or translation axis, hardware limits, directions of movement, default positions, etc. Each of these instrument robots is an example of a generic class of robot, for example a 'detector robot' or 'positioning system robot'. All of the SScanSS code, apart from the instrument setup routines is written entirely in terms of these generic robot types.
Figure 1 shows the SScanSS virtual models of two instruments; ENGINX at ISIS in the UK and NRSF2 at ORNL in the US, [6]. Control panels for the various moveable instrument components are generated automatically when each instrument is selected.

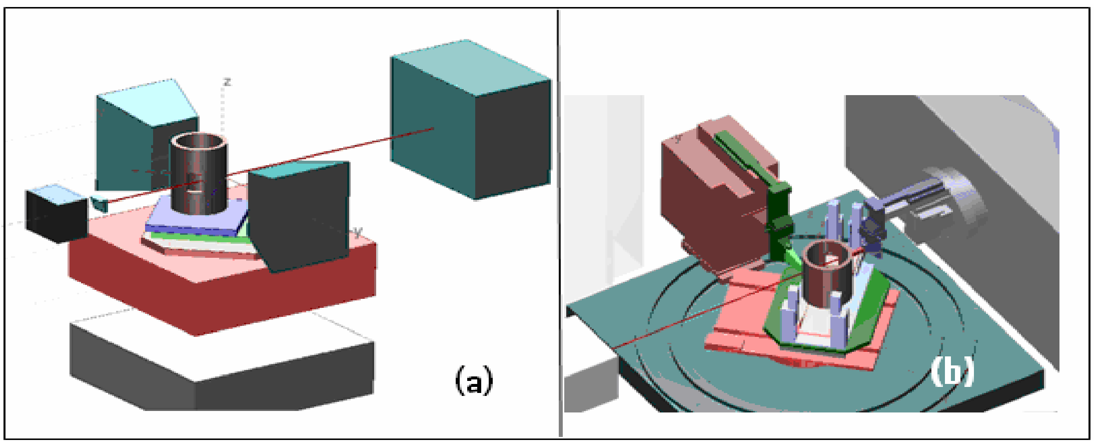

Figure 1. The robotics formulation enables the accurate modelling of arbitrary positioning systems and detectors. A pipe sample with neutron access hole mounted for measurement on (a) ENGINX at ISIS, UK, and (b) NRSF2 (Neutron Residual Stress Mapping Facility) instrument at HFIR, Oak Ridge National Laboratory, USA.

3.2 Interactions with hardware

The nature of the link between the SScanSS software and an instrument's hardware has been considered. Four options may be identified:

1. **No direct link**: the software generates the motor commands which are written to a file which is then passed digitally to the instrument for execution.
2. **Direct forward link only:** the output from the software is passed directly to the instrument which executes the commands without any further intervention.
3. **Direct backwards link only:** there is no direct forwards link, so motor positions for instrument control would be passed to the instrument manually as in option 1, however a direct backwards link would exist so that the software would read the motor positions from the instrument and reproduce the position of the actual sample and hardware within the simulation.
4. **Both forward and backwards direct links:** Both forward and backward direct links, as described above would exist.

To date only the first option has been implemented, i.e. SScanSS output is written to a simple ASCII file before being passed manually to the instrument. One advantage of this approach is that it simplifies the inclusion of a new instrument within the software as only modification of the format of the output file is required, rather than complex interfaces to different instrument hardware. Advantages of the second option are readily apparent, particularly for instruments where the sample environment may not be visible from the control area.

4 Recent developments

4.1 Collision prevention

There are a number of direct and indirect ways through which simulation software may help in the important task of preventing collisions between the sample and components of the instrument hardware. Firstly, because the software enables an experiment to be planned in detail, many of the possible collision scenarios will have been discovered and circumvented. Secondly, if the user has planned the experiment using the software they will already have some degree of familiarity with the operation of the instrument, in particular with the directions and limits of travel of the various components. Thirdly, simulating a proposed sample movement before it is made on the real instrument will readily show the user whether a collision is likely to occur; in most cases by simple visual inspection of the simulation but also via specific software collision detection.

Software collision detection

A basic level of software collision detection was provided in the earliest implementation of the software, however, with the use of increasing large LASER generated sample models, a more advanced method was required if the computational expense was to be kept down and the smooth running of the simulation maintained.
Mathematically a collision is considered to have occurred if any pair of polygons comprising the models of the bodies in question intersects. Given the potential size of LASER generated models it is generally prohibitively expensive to explicitly test every polygon pair in a multi-component environment and alternative methods are required. Collision detection is a generic problem in computer graphics, and many different schemes have been devised to optimize this process, [7]. Collision simulation within SScanSS is an example of a general method which utilizes a tree of nested bounding boxes to reduce the number of polygon combinations that have to be tested explicitly. The root of the bounding box tree is an ‘axis aligned bounding box’ (AABB) that encloses the complete object (sample or instrument hardware component model). This AABB is repeatedly subdivided and the polygons contained within each subdivision determined at each step. If no polygons are contained within a particular box then that box is eliminated. The result of this process is shown in Figure 2.

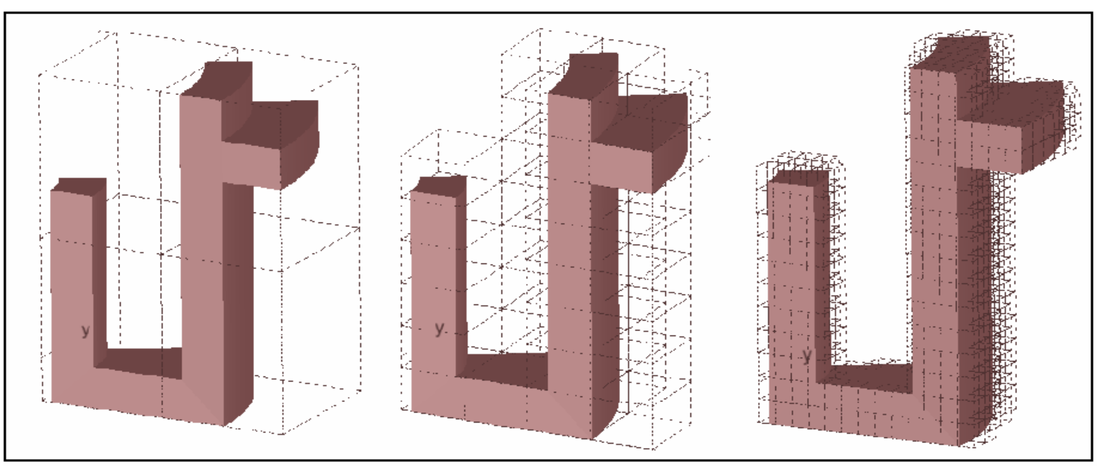

Figure 2. An object bounded by successively smaller boxes, providing an efficient means to check for collisions.

At each point in the simulation when either a piece of hardware or the sample moves, the collision detection routine searches successively down through the bounding box tree for collisions and only if the lowest level bounding boxes are found to collide does the routine search the actual model polygon meshes, and then only the few polygons contained in the particular pair of colliding bounding boxes. Potentially each instrument allows a different set of possible collisions, hence a collision test list, denoting which pairs of objects need to be tested, forms a part of the instrument specification. The most obvious application of the collision prevention capability is to guard against the collision of sample and instrument hardware, however if the geometry of experimental setup is complex it may also be useful for the software to check for 'collisions' between the beam and the positioning system hardware upstream of the detectors.

4.2 Automatic path length minimization

When supporting an actual experiment, SScanSS positions the measurement point at the centre of the instruments gauge volume and orientates the sample so that the requested strain component(s) are correctly aligned. This is done by finding the motor positions that minimize a cost function based on the sample position and alignment errors, [5]. In addition to this standard procedure, it may be possible, by utilising spare degrees of freedom in the sample positioning process, to simultaneously find the alignment that minimizes the neutron path length. For example, considering a measurement at one particular point; if a single strain component is required, it is clear that the measurement could be made with the sample in any orientation for which the required strain component lies parallel to the Q-vector, (the Q-vector is the vector bisecting the incident and diffracted beam). Hence, by rotating the virtual sample about the Q-vector and continuously monitoring the changing path length, the orientation corresponding to the minimum path length can be found. Once this orientation has been determined the software will, if the positioning system is able to 'reach' that position, position the sample accordingly. If the positioning system is not able to reach this optimum position then the user will be able to use the information to manually position the sample if wished.

Figure 3 illustrates the implementation of this approach for the ENGINX positioning system augmented with the optional goniometer. Figure 3b shows the result of the path length calculation as the sample is rotated about the Q-vector. It may be seen that in this example the minimum path length occurs for a relatively narrow range of rotation angle, indicating that the sample needs to be positioned accurately to avoid un-necessarily long measurement times.

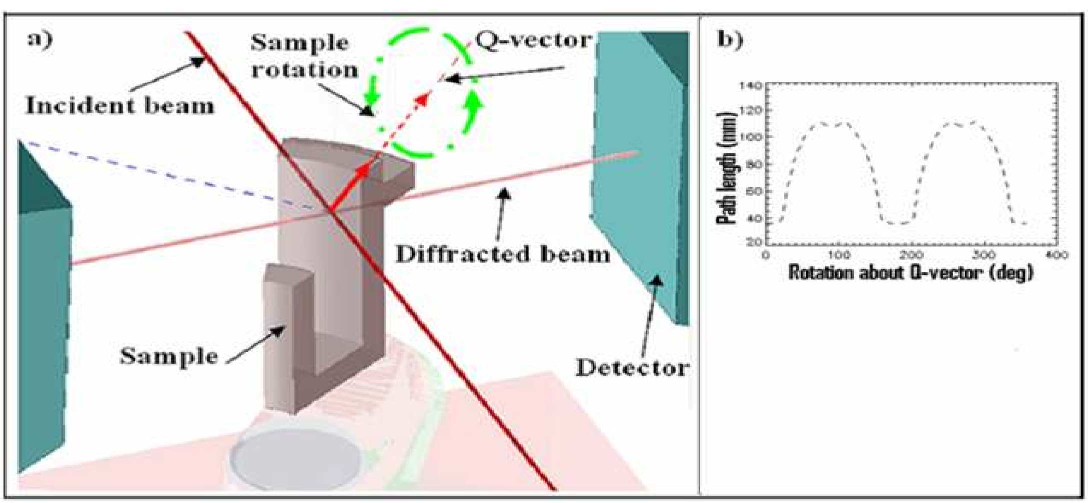

Figure 3. Automatic path length minimization.
(a) The virtual sample is aligned so that the required strain component lies parallel to the Q-vector and is rotated while the neutron path length is monitored. (b) The output from the path length minimisation process; the orientation associated with the minimum path length is selected and the sample positioned accordingly if possible.

It may be noted that the path length calculation currently calculates the path length of a single ray passing along the centre of the incident and diffracted beams. When used in the context of an area detector a more advanced approach is required where proper account would be taken of the varying path length between the centre of the gauge volume and different points of the detector. It is expected that this more accurate scheme will be implemented in the near future.

5 Implementation of SScanSS at two facilities

5.1 ENGINX at ISIS

Instrument modelling issues

ENGINX is a third generation engineering diffractometer based at the ISIS spallation neutron source in the UK. The instrument comprises an x,y,z,Ω positioning table, two fixed detectors, ($2\theta=\pm 90^{\circ}$), various optional collimators and incident jaws with motorized position and aperture control.
The ENGHINX instrument is simply modeled as two robots; the first, the positioning system comprises three translational and one rotational link and the second, the jaws, comprises a single translational link, (the ability to set the jaws aperture is reproduced within the software but the associated moving components are not modeled).
The elements of both the positioning table and the collimators may be effectively approximated by simple geometric shapes thereby allowing for a very simple virtual model. In addition the instrument was designed such that no collisions can occur between elements of the standard instrument hardware, for this reason simulations in general and collision detection in particular are relatively economic computationally. The ENGINX instrument model is shown in Figure 1a.

Users on ENGINX have the option of adding a three axis goniometer to the x,y,z,Ω positioning table. The availability of optional hardware items on ENGINX (and elsewhere) is handled through the provision of drop down menus. Choosing to add the goniometer causes the re-generation of a single larger positioning system robot with three translational and four rotational links, a suitably extended control panel, with controls for each link is also simultaneously constructed.
The inclusion of the goniometer on ENGINX produces a flexible positioning system allowing suitable samples to be freely rotated and enabling, for example, the three strain components typically required for a stress calculation to be measured without remounting the sample. With this system the sample may also be automatically positioned in the orientation that produces the minimum path length, as described above.

Implementation

SScanSS has been available to users of ENGINX since the start of the project and ENGINX instrument scientists have been closely involved with the development of the software and, in particular, with establishing the practical methods required by the key ancillary tasks of generating sample models and measuring the initial position of the sample on the instrument.
The overarching principle is that techniques should be as speedy and simple to execute as possible, with the ideal being that they are accessible to new facility users with no previous experience. A brief outline of the current practice at ENGINX regarding the two key tasks of sample model generation and the measurement of the sample position is given below.

Sample model generation

- i) Attach a number (minimum 3 but more usually 4~8) of, typically 10mm diameter, stainless steel ball bearings to the sample to provide fiducial points.
- ii) Scan the sample using a LASER scanning head attached to an articulated arm, (Cimcore Portable Measuring Arm CMM Model No 5028SC-199) and measure the centre of the fiducial balls using a touch probe attached to the same arm.
- iii) Filter and mesh the sample model point cloud using the bundled software.

Sample position determination

i) Determine the position of the sample on the instrument by re-measuring the centres of the fiducial balls using a second identical arm and touch probe mounted on the instrument and close to the sample positioning table.

The approach described above has recently replaced earlier methods based on CMM and optical theodolites technology. Using the new techniques a sample can be changed and a new run instigated by a user within approximately 20 minutes, (full instructions for sample alignment and SScanSS applications are included in the ENGINX user manual, [8]). The proportion of strain scanning experiments that make use of SScanSS is currently estimated at about 65% [9].

5.2 Neutron Residual Stress Mapping Facility (NRSF2) at HFIR, ORNL

Instrument modelling issues

NRSF2 is a second generation neutron residual stress mapping instrument specifically designed for neutron residual stress measurement. The instrument comprises an x,y,z,Ω positioning table with optional z-stages, a position sensitive detector with a selection of retractable incident slits.

The NRSF2 instrument is modeled as three robots; the positioning system robot comprising three translational and one rotational link, the detector robot comprising one rotational link and one translational link and the incident slits robot comprising a single translational link. The NRSF2 instrument model is shown in Figure 1b.

The positionable detector introduces some degree of additional complexity, not merely through the need for an additional robot, but because the rotation of Q-vector rotation with changing detector position also needs to be modelled and taken account of in the automated sample alignment.

Users on NRSF2 have the option of adding a Huber circle to the x,y,z,Ω positioning table. The modeling of this additional item of positioning hardware is on-going but is expected to proceed similarly to the addition of the goniometer to ENGINX as described above. The inclusion of the Huber circle provides a flexible positioning system capable of allowing suitable samples to be freely rotated and enabling, for example, the three strain components typically required for a stress calculation to be measured without re-mounting the sample.

Implementation

One of the guiding principles behind the NRSF2 approach to sample alignment is to provide a high degree of compatibility between the sample alignment and experiment control procedures used on NRSF2 at HFIR and the soon to be commissioned VULCAN instrument at SNS. To this end comprehensive off beam sample model generation and alignment procedures have been developed with the intention of facilitating easy movement of samples between the two instruments.

Sample model generation

Two distinct options for sample model generation are offered to users of NRSF2. The first is similar to that described above, i.e. the generation of LASER scanned models using a LASER scanning head and a touch probe attached to an articulated arm, [10]. The second method is to use a CAD sample model rather than a scanned model for the entire experimental procedure rather than just for the early planning stages. To support this option, work has been done on establishing the best methods for setting up fiducial points on the CAD model and on defining suitable coordinate systems and establishing accurate correspondence between the sample and the CAD model. Methods based on CAD sample models are a valuable new technique, in particular as they allow working with samples where measurements must be placed accurately in relation to internal sample features.

In addition to the scanning arm and touch probe, the alignment facilities at NRSF2 also include a LASER tracker system, [10]. The LASER tracker offers alternative options for sample and instrument alignment providing very quick and accurate measurements of reflective spheres which may be mounted in holders attached to the sample or instrument hardware. In the context of setting up the sample model this allows the possibility of using tracker spheres instead of precision steel balls as the fiducial markers.

<u>Sample position determination</u>
The measurement of the fiducial markers for the purpose of measuring the initial sample position is essentially the same as that used on ENGINX with the exception that a LASER tracker is used in place of the second touch probe.
Full instructions and options for sample model production and alignment are included in the comprehensive "Residual Stress Sample Alignment Laboratory Guidline" [11].

6 Future plans

6.1 Collaborations with other facilities

Collaborations are in place to setup SScanSS for the following instruments; i) KOWARI; (ANSTO), ii) VULCAN (ORNL) and iii) JEEP (DIAMOND).

6.2 Further developments

Extending methods to parallel robots

The methods on which SScanSS modelling is based are currently only applicable to serial robots, i.e. robots whose links are connected as a serial chain. The majority of beam line positioning systems belong to this category, however parallel robots such as Stewart tables, are also in use as positioning systems, (e.g. Hexapod which is used to position samples on the SALSA diffractometer at the ILL, [12]). Two approaches for including parallel robot positioning systems within SScanSS are to be considered;

1. Fully solve the parallel robot inverse problem and thereby enable the commands for the individual links (e.g. hexapod legs) to be generated.
2. Use the software in its current implementation to calculate the required translational and rotational movements and to pass these to the proprietary positioning system software for the calculation of the individual link commands.

The solution of the inverse problem for parallel robots is well documented. However taking into account the likely additional complexities of interfacing to the hardware and the need to consider dynamic as well as kinematic effects in modelling these types of robots, the most likely solution is to adopt the second approach outlined above.

Combined imaging and diffraction applications

Using LASER generated models in conjunction with SScanSS allows measurement points to be positioned accurately with respect the surface features of a sample. In some instances however measurement points would ideally be positioned with respect to internal sample features. Given the increasing use of Neutron tomography and, in particular, the likely development of joint imaging and diffraction instruments, [13], it is a natural extension of the approach to consider using virtual models derived from segmented tomography images in the place of the LASER scan models. Following this approach all the information on internal features yielded by tomographic imaging could be accessed from within the SScanSS model. Figure 4 indicates the possibilities of this approach; the figure uses illustrations taken from the field of cultural heritage research, however the same approach has many potential applications in the field of engineering, and elsewhere.

In addition to using tomography to provide the information required to position measurements with respect to internal geometric features, the use of energy selective methods, [14] is likely to yield information that would allow measurements to be accurately placed in relation to compositional features within the sample, for example, the position of the fusion boundary in weldments, or different compositional elements in cultural heritage objects. Research into these areas is under way within the Materials Group at the Open University.

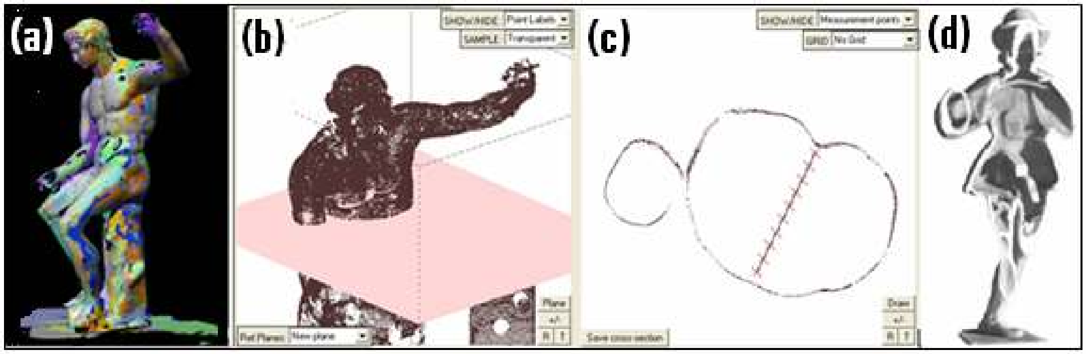

Figure 4. Potential use of tomography models within SScanSS, illustrated in the context of work taken from the field of cultural heritage research [1,2]. (a) A LASER generated virtual sample model of a complex sample. (b) Generating the cross-section through the virtual sample model on which the measurement points are to be placed – only surface information is available. (c) A line of measurement points placed in relation to the cross-sectional geometry. (d) A cross-section through a segmented tomography model of a similar object showing the internal information that would available for future study.

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8 References

1. J.A. James, J.R. Santisteban, M.R. Daymond, L. Edwards, *Use of a Virtual Laboratory to plan, execute and analyse Neutron Strain Scanning experiments*. Proc. NOBUGS, NIST, Gaithsburg, 2002.
2. J.R. Santisteban, M.R. Daymond, J.A. James and L. Edwards, *ENGINX: A Third Generation Strain Scanner:* J. of Appl. Crys, (2006), 39, 812-825
3. J.A. Dann, M.R., Daymond, L. Edwards, J.A. James, and J.R. Santisteban, *A Comparison between Engin and ENGINX, a new diffractometer optimised for stress measurement. ",.* Physica B: Condensed Matter (2004) 350, pp. 511-514
4. J. A. James, J. R. Santisteban, L. Edwards and M. R. Daymond, *A virtual laboratory for neutron and synchrotron strain scanning*, Physica B, Condensed Matter 350 E743-E746, (2004)
5. J.A. James and L. Edwards, *Application of robot kinematics methods to the simulation and control of neutron beam line positioning systems.* Nuclear Instruments and Methods in Physics Research A. (2007) 571, 709-718.
6. http://html.ornl.gov/uc_residual.shtml/
http://html.ornl.gov/documents/_vti_cnf/fs_rsuc.pdf/

7. *Collision Detection in Interactive 3D Environments (The Morgan Kaufmann Series in Interactive 3D Technology)*, Publisher: Elsevier Science & Technology Books, 2003, ISBN-13: 9781558608016.
8. E.C. Oliver, J.R. Santisteban, J.A. James, M.R. Daymond, J. Dann, *ENGINX Users Manual*, http://www.isis.rl.ac.uk/engineering/documentation/enginx_manual.pdf
9. Private communication: Dr A. Paradowska (ENGINX instrument scientist).
10. FARO International, http://www.faro.com/
11. J. Bunn, J. Schmidlin, C. Hubbard, *Residual Stress Sample Alignment Laboratory Guidline. 2008.*
12. G. Bruno, T. Pirling, P.J. Withers, W. Hutt, S. Rowe. *SALSA: Strain Analyser for Large and Small Scale Engineering Applications*. The Journal of Neutron Research (2003), 11, (4), 235-239
13. W. Kockelmann, E. C. Oliver, P. G. Radaelli*, IMAT- An imaging and materials science & engineering facility for TS-II*, http://ts-2.isis.rl.ac.uk/instruments/phase2-2007/IMAT_dec07_draft.pdf/
14. W. Kockelmann, G. Frei, E.H. Lehmann, P. Vontobel, J.R. Santisteban, *Energy-selective neutron transmission imaging at a pulsed source*. Nuclear Instruments and Methods in Physics Research A 578 (2007) 421–434