

FINAL PUBLISHABLE REPORT

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TABLE OF CONTENTS

1	Executive summary	3
2	Need for the project.....	4
3	Objectives	5
4	Results	6
5	Impact	9
6	Website address and contact details	14

1 Executive summary

Introduction

This project demonstrated, to a major developer of software development and analysis tools, how components of its products, which implement mathematical calculations, can be independently verified via the internet. By developing verification services for example calculations, this project showed how to investigate the numerical correctness of implementations of these calculations. Verification can be undertaken even if the environment, within which the software under test is running, is unable to communicate via the internet.

The Problem

Developers of software products, which contain components that implement mathematical calculations, increasingly require verification of their products by an independent organisation such as a National Measurement Institute (NMI). National Instruments, the primary supporter of this project, recognised the potential value of the calculations implemented in its products, such as LabVIEW and DIAdem, being independently verified, after being made aware of the outputs of EMRP JRP NEW06 TraCIM. Therefore, the consortium aimed to apply the TraCIM approach to the calculations implemented within National Instruments products. Furthermore, products such as LabVIEW allow users to develop implementations of further calculations, for example, by combining a number of the calculations that are “built-into” LabVIEW. Such users of National Instruments products also need to verify their implementations. Therefore, this project also considered taking advantage of this functionality within LabVIEW to facilitate this verification.

The Solution

The project’s partners and the primary supporter selected calculations, from those considered within EMRP JRP NEW06 TraCIM, which could be used for the development of software verification services. As far as possible, calculations were selected that were implemented in more than one National Instruments product. For each of the selected calculations, a demonstration software verification service was developed. An example “standalone TraCIM client” was also developed: this is a software component, implemented by the service provider, which allows users to communicate with the “TraCIM server” via the internet. The calculations implemented in the National Instruments products LabVIEW and DIAdem were then verified. The project’s partners then selected further calculations, again from those considered within EMRP JRP NEW06 TraCIM, for implementation in LabVIEW. Software verification services were established for demonstration purposes and example “LabVIEW integrated TraCIM clients” were developed. These calculations were then verified.

Impact

This project created impact as National Instruments used the TraCIM-based demonstration software verification services to verify calculations implemented in both LabVIEW and DIAdem. To maximise the impact for National Instruments, the standalone TraCIM clients were specifically developed to simplify the verification of calculations implemented in DIAdem i.e. American Standard Code for Information Interchange (ASCII) files were generated from, and written to, the eXtensible Markup Language (XML) files that are used for data exchange. Integrated TraCIM clients are also of interest to National Instruments for verifying the calculations implemented in LabVIEW. National Instruments recognises that the provision of software evaluation reports for calculations implemented in its products will enhance the credibility of, and user confidence in, its products.

Further impact will be achieved through the project’s engagement with additional software developers and through the provision of software verification services for more calculations. The training of the project’s partners, in particular, on the development of expert extensions to the TraCIM server, will prove to be vital for the provision of such additional services. An important component in the provision of software verification services is the provision of example TraCIM clients, in both executable and source code formats. The partners will continue to investigate the verification of calculations implemented in additional software environments.

A project website has been developed that will be populated with both the outputs of the project and with material developed beyond the end of the project (<http://empir.npl.co.uk/valtrac/>).

2 Need for the project

Developers of software and programming tools need to have their products validated, i.e. to ensure that the products undertake the tasks for which they were intended and that they perform as expected. Increasingly, there is a requirement or desire for the validation of (components of) products to be undertaken by an independent organisation such as a National Measurement Institute (NMI). For software developers, independent validation will ensure the reputation of their products is maintained, and for software users, independent validation will provide greater reassurance on the quality of their applications.

A common approach when validating software that implements mathematical computations involves the use of reference pairs, comprising reference data and reference results. The software under test is applied to multiple reference data sets and for each reference pair, the test results are compared, in an appropriate way, with the corresponding reference results. The results of the comparison obtained for each reference pair can then be combined to provide the overall assessment of the software that is needed.

EMRP JRP NEW06 TraCIM developed a complete ICT infrastructure – the “TraCIM system” – which allows software to be validated online using reference pairs. The approach that underpins the TraCIM system is applicable to any mathematical software for which the use of reference pairs is appropriate. In order to validate software for implementing a particular computational aim, three steps need to be completed:

1. Reference data pairs need to be generated for the computational aim.
2. A software module (referred to as a “TraCIM client”) needs to be written that allows the software under test to communicate with the TraCIM server using the internet, e.g., to request reference data, to send test results, etc.
3. A software module, referred to as an “expert extension” to the TraCIM server, needs to be written that implements the comparison of the test results with the reference results.

During EMRP JRP NEW06 TraCIM, as part of step 1, the partners developed reference pairs for specific calculations from the Length and Chemistry metrology domains as well as some common, more generic, calculations that occur within several metrology domains. Within EMRP JRP NEW06 TraCIM, the main focus was on the validation of software developed by manufacturers of coordinate measuring machines, such as for the fitting of geometric elements, e.g., spheres, cones, to data. For these calculations, the partners developed TraCIM clients and expert extensions, and a fully-operational validation system, along with extensive guidance on its use, was put in place.

National Instruments recognises the benefits to its own products, as well as to its customers who develop software using these products, that can be achieved through the use of the TraCIM system as a means of providing independent validation of mathematical software. Therefore, National Instruments is keen to adopt the TraCIM system.

The requirement for implementations of mathematical calculations to be validated applies to all developers of software and tools that undertake such calculations. The applicability of the TraCIM approach is therefore widespread and the TraCIM system is potentially of great use to many software companies.

3 Objectives

The overall aim of this project was to allow both developers and users of software development and analysis tools to benefit from the outputs of the previous project, EMRP JRP NEW06 TraCIM, irrespective of the domain at which the tools are aimed.

In order to do this, two distinct types of TraCIM client needed to be considered. The first type is referred to as a “standalone” client. A standalone client enables communication with the TraCIM server for software development and analysis tools that cannot connect to the server directly. Standalone clients are generally appropriate for developers of software development and analysis tools, who may be interested in undertaking validation of a function throughout the software development process. The second type of TraCIM client is referred to as an “integrated” client. An integrated client enables communication with the TraCIM server directly from within a software development and analysis tool. Integrated clients are generally appropriate for users of software development and analysis tools, including third-party software developers.

To meet the overall aim of the project, the specific objectives were:

1. To provide guidelines for developers of mathematical software development and analysis tools on how to use the TraCIM system to undertake independent validation of their mathematical functions by using standalone TraCIM clients. This mechanism will be demonstrated for a number of calculations implemented by “built-in” mathematical functions within products developed by National Instruments.
2. To provide guidelines for users of software development and analysis tools on how to use the TraCIM system to undertake independent validation of their mathematical functions by using integrated TraCIM clients. This mechanism will be demonstrated for a number of calculations implemented by “user-generated” mathematical functions developed using National Instruments products.

4 Results

Objective 1: To provide guidelines for developers of mathematical software development and analysis tools on how to use the TraCIM system to undertake independent validation of their mathematical functions by using standalone TraCIM clients. This mechanism will be demonstrated for a number of calculations implemented by “built-in” mathematical functions within products developed by National Instruments.

The partners, in conjunction with the primary supporter, selected three calculations for which demonstration software verification services would be made available, using the following criteria:

- The calculations had been considered during the EMRP JRP NEW06 TraCIM.
- The calculations are from three different metrology areas.
- The input and output parameters of the calculations involve different combinations of scalars, vectors and matrices.
- The calculations map directly to (built-in) calculations implemented within National Instruments software tools LabVIEW and DIAdem.

The following calculations were selected:

1. Least squares fitting to data of the sum of an exponential decay function and a constant (short name “LSEXP”). This calculation was from the metrology area **QM** (amount of substance – metrology in chemistry). The calculation involves input and output parameters that are scalars and vectors.
 - Within LabVIEW, the calculation is implemented using the “Exponential Fit” VI (a VI can be thought of as being equivalent to a function or subroutine in other programming languages). The input parameter “parameter bounds” of the VI can be assigned to align as closely as possible with the constraints on the output parameters listed in the specification of the computational aim.
 - Within DIAdem, the calculation can be implemented using the function “ChnNonLinearFitY” and the setup function “ $b + c \cdot \exp(-x/a)$ ”.
2. Weighted least squares polynomial regression (“WLSPR”). This calculation is from the **INT** (interdisciplinary) metrology area, i.e. it arises in more than one metrology area. The calculation involves input parameters that are scalars and vectors and output parameters that are vectors and matrices.
 - Within LabVIEW, the calculation is implemented using the “General Polynomial Fit” VI.
 - Within DIAdem, the calculation can be implemented using the function “ChnNonLinearFitYWeighted” and a setup function corresponding to the degree of the polynomial function required to be determined.
3. Principal component analysis (“PCA”). This calculation is from the **INT** (interdisciplinary) metrology area. The calculation involves input parameters that are scalars and matrices and output parameters that are vectors and matrices.
 - Within LabVIEW, the calculation is implemented using the “TSA Principal Component Analysis” VI (requires access to the Advanced Signal Processing Toolkit).

The TraCIM server developed during the EMRP JRP NEW06 TraCIM was first installed at NPL. Subsequently, for each calculation, the partners carried out the following activities:

- Data generation software, developed within the EMRP JRP NEW06 TraCIM, was employed to generate twenty-five sets of reference pairs to be used within a demonstration software verification service by the partners and the primary supporter. The reference pairs have different properties, e.g. they involve different numbers of data points, different levels of noise in the data, etc.
- An expert extension, a software component that allows reference results to be compared with results returned by the software under test, was developed.
- The expert extension was incorporated into the TraCIM server at NPL and the demonstration software verification service was made available to the partners and the primary supporter.

- A standalone TraCIM client, that allows the user of a software verification service to communicate with the TraCIM server using the internet, was developed. Although service users are free to develop clients for themselves in the language of their choice, this TraCIM client allows those who are unfamiliar with web communication and/or eXtensible Markup Language (XML) parsing to use the services without the need to undertake significant software development themselves. The TraCIM client:
 - Requests and receives reference data, in the form of a “reference data XML message”, from the TraCIM server.
 - Extracts the reference data from the reference data XML message to ASCII files.
 - Extracts test results, generated by the user applying the software under test to the reference data, from ASCII files, and constructs a “test results XML message”.
 - Submits the test results XML message to the TraCIM server, and receives a “software evaluation report XML message”.
- The standalone TraCIM client was successfully used to undertake verification of the implementation of the calculation in LabVIEW and, where appropriate, DIAdem.
 - For the implementation of calculation LSEXP within LabVIEW, verification was repeated a number of times, varying the value of tolerance used to determine the estimates of the solution parameters, and using different criteria to compare test and reference results.
 - For calculation LSEXP implemented within DIAdem, verification was repeated using different initial estimates of the solution parameters (default initial estimates, and user-selected initial estimates), different values for the maximum number of iterations of the parameter fitting routine, and using different criteria to compare test and reference results.
 - For the implementation of calculation WLSPR within LabVIEW, verification was repeated using different choices of algorithm (SVD, Givens, Givens2, Householder, LU Decomposition, and Cholesky), and using different criteria to compare test and reference results. For calculation WLSPR implemented within DIAdem, verification was repeated in the same manner as for calculation LSEXP.
 - For the implementation of calculation PCA within LabVIEW, verification was undertaken using different criteria to compare test and reference results.
 - For calculations LSEXP and WLSPR, the outcomes of the verification exercises allowed comparisons to be made between LabVIEW and DIAdem implementations of those calculations.
- A user manual for the corresponding demonstration software verification service was written. The user manual is available to registered users of NPL TraCIM services and can be obtained by logging into the NPL TraCIM webshop (<https://tracim.npl.co.uk>).

The partners developed guidance material on the use of the TraCIM software verification services using standalone TraCIM clients and disseminated it to the primary supporter.

Objective 2: To provide guidelines for users of software development and analysis tools on how to use the TraCIM system to undertake independent validation of their mathematical functions by using integrated TraCIM clients. This mechanism will be demonstrated for a number of calculations implemented by “user-generated” mathematical functions developed using National Instruments products.

The partners selected a further three calculations for which demonstration software verification services would be made available, using the following criteria:

- The calculations had been considered during the EMRP JRP NEW06 TraCIM.
- The input and output parameters of the calculations involved combinations of scalars, vectors and matrices.

- The calculations did not map directly to (built-in) calculations implemented within National Instruments product LabVIEW, but could be implemented by combining built-in LabVIEW functions.

The following calculations were selected:

- Least squares plane fitting (short name “LSPLANE”). This calculation involves input parameters that are scalars and vectors and output parameters that are vectors.
- Generalised distance polynomial regression (“GDPR”). The calculation involves input parameters that are scalars and vectors and output parameters that are vectors and matrices.
- Least squares 3D line fitting (“LS3DLINE”). This calculation involves input parameters that are scalars and vectors and output parameters that are vectors.

For each calculation, the partners carried out the following activities:

- Data generation software, developed within the EMRP JRP NEW06 TraCIM, was employed to generate twenty-five sets of reference pairs to be used within a demonstration software verification service, by the partners and the primary supporter. The reference pairs have different properties, e.g. they involve different numbers of data points, different levels of noise in the data, etc.
- An expert extension, a software component that allows reference results to be compared with results returned by the software under test, was developed.
- The expert extension was incorporated into the TraCIM server at NPL and the demonstration software verification service was made available to the partners and the primary supporter.
- A LabVIEW implementation of the calculation was developed.
- An integrated (into LabVIEW) TraCIM client, that allows the user of a software verification service to communicate with the TraCIM server using the internet, was developed. Although service users are free to develop clients for themselves, this TraCIM client allows those who are unfamiliar with web communication and/or XML parsing in LabVIEW to use the services without the need to undertake significant software development themselves. The TraCIM client:
 - Requests and receives reference data, in the form of a “reference data XML message”, from the TraCIM server.
 - Extracts the reference data from the reference data XML, calls the LabVIEW implementation of the calculation to process the reference data, and writes the test results to a “test results XML message”.
 - Submits the test results XML message to the TraCIM server, and receives a “software evaluation report XML message”.
- The integrated TraCIM client was successfully used to undertake verification of the implementation of the calculation in LabVIEW.
 - For the GDPR calculation implemented in LabVIEW, verification was repeated a number of times, varying the value of the tolerance used to determine the estimates of the solution parameters, and using different criteria to compare test and reference results. For calculations LSPLANE and LS3DLINE implemented in LabVIEW, verification was undertaken using different criteria to compare the test and reference results.
- A user manual for the corresponding demonstration software verification service was written. The user manual is available to registered users of NPL TraCIM services and can be obtained by logging into the NPL TraCIM webshop (<https://tracim.npl.co.uk>)

The partners developed guidance material on the use of TraCIM software verification services using integrated TraCIM clients and disseminated it to the primary supporter.

5 Impact

Overview

This project built on the outputs of the EMRP JRP NEW06 TraCIM, which was primarily concerned with the verification of metrology software, through the development of six demonstration software verification services for calculations that are generally of interest beyond the metrology community. For the primary supporter (National Instruments), this project provided the opportunity to understand how software components within its products can be independently verified. Three of the six calculations were selected as they are implemented within built-in functions in National Instruments products LabVIEW and DIAdem. These functions were verified using the demonstration software verification systems and the results were discussed with National Instruments. The other three calculations were selected as they are not implemented in National Instruments product LabVIEW, but they that can be implemented in LabVIEW by combining built-in functions. An implementation of each calculation was developed in LabVIEW, and verification was undertaken using the corresponding demonstration software verification service.

NPL, PTB and Ostfalia-HAW delivered an oral presentation at the British Computer Society (BCS) Software Quality Management Conference in April 2017. A corresponding paper was published in the conference proceedings. A further oral presentation took place at the Metromeet International Conference on Industrial Dimensional Metrology in March 2018 following successful submission of an abstract. An article on the TraCIM approach, discussing both standalone and integrated TraCIM clients was published in The Tester, the newsletter of the BCS Specialist Group in Software Testing. A case study on the use of the clients that were integrated into LabVIEW will be submitted for publication on the National Instruments website.

Summary of the main outputs of EMRP JRP NEW06 TraCIM

Within EMRP JRP NEW06 TraCIM, the partners focused on 34 calculations that they had selected from four different metrology areas. For each calculation:

- A specification was written for the computational aim (often referred to for brevity as a “computational aim”), which provided information, in a number of fields, on the calculation to be undertaken. The fields included the Input parameters, the Output parameters, and the Mathematical model.
- Software was developed to generate the reference pairs. These play a fundamental role in the verification of mathematical software. A reference pair comprises reference data and reference results. The software under test is applied to multiple reference data sets and for each reference pair, the test results are compared, in an appropriate way, with the corresponding reference results (Figure 1).
- The results of the comparison obtained for each reference pair can then be combined to provide the overall assessment of the software that is needed (Figure 2).
- Approaches for determining performance metrics, i.e. numerical values that provide an assessment of the performance of the software, were developed.

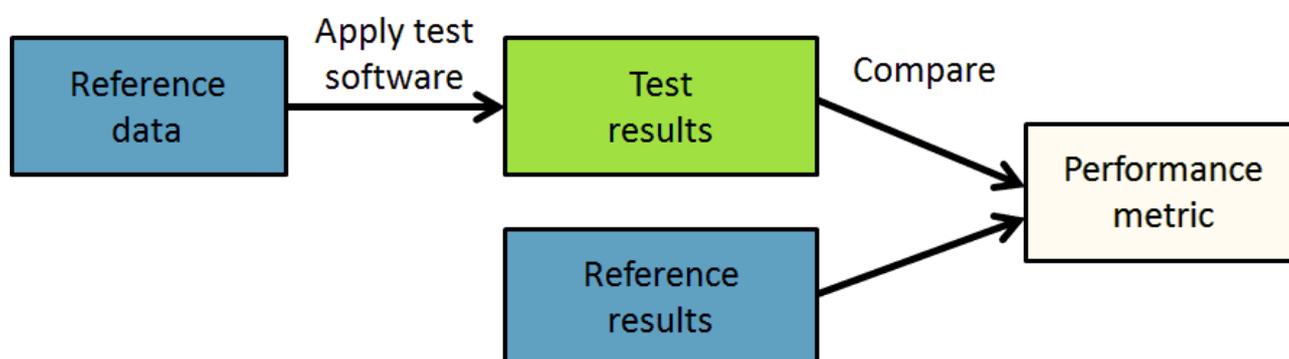


Figure 1: Assessing the performance of software using a single reference pair.

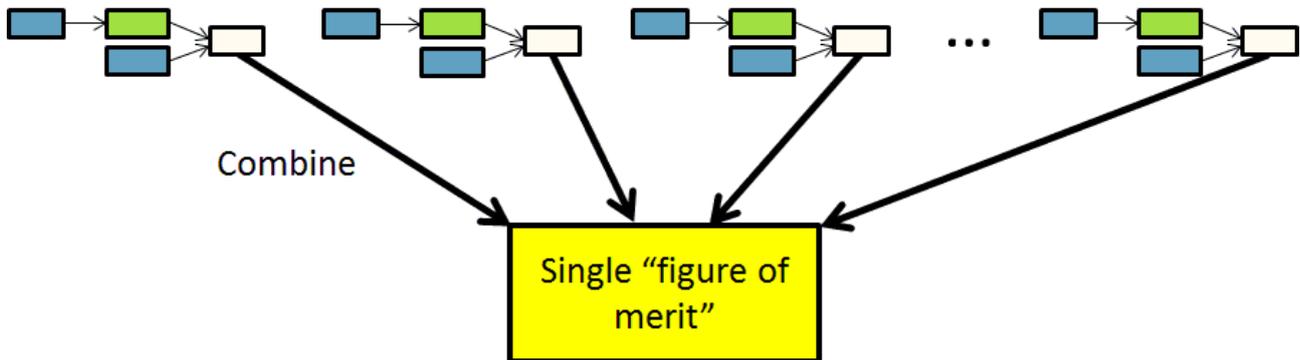


Figure 2: Assessing the performance of software using multiple reference pairs.

The “TraCIM system” is an information and communications technology (ICT) infrastructure that was developed to allow software verification services to be provided. The TraCIM system comprises two elements (Figure 3): the “TraCIM server” is the core module that manages all of the operating data and controls the flow of data to other modules, and the “TraCIM client” is a software module that allows the user of a software verification service to communicate with the TraCIM server via the internet.

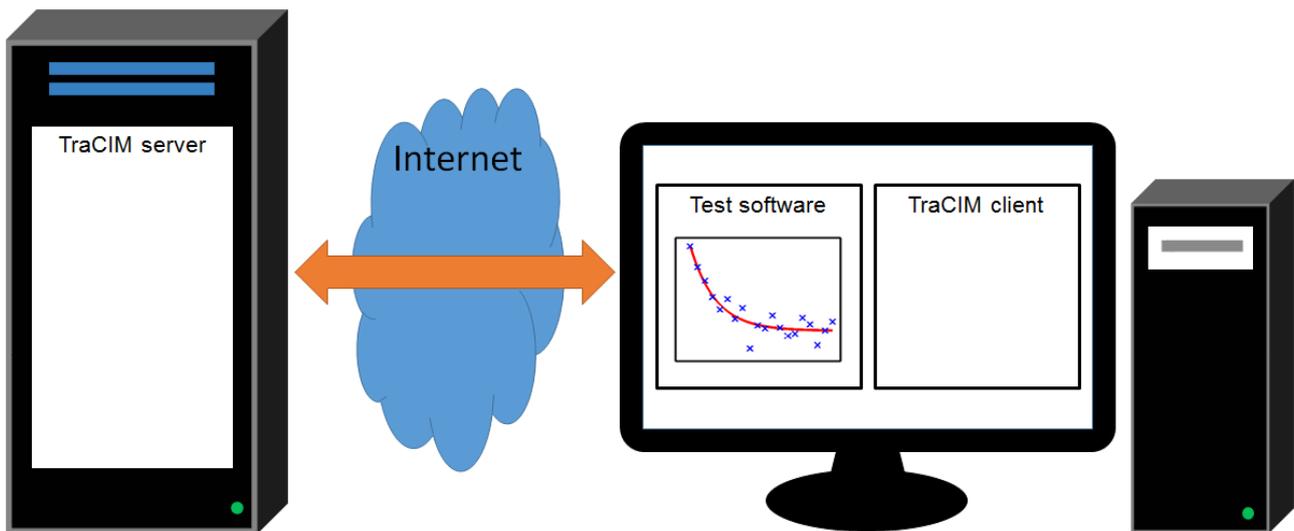


Figure 3: Elements of the TraCIM system.

Communication between the server user and the service provider, via the TraCIM client and the TraCIM server, takes place as follows:

1. The service user submits a request for reference data for a particular computational aim to the service provider.
2. The service provider supplies the service user with the required reference data.
3. The service user applies the software under test to the reference data and submits the test results to the service provider.
4. The service provider undertakes a comparison of the test and reference results and supplies the service user with a software evaluation report.

In the final three steps, information is provided in eXtensible Markup Language (XML) format.

From a software verification service user's point of view, the TraCIM client plays a key role. There are two distinct types of TraCIM client:

- “Standalone” TraCIM clients – in some cases the software environment, within which the software under test is running, is unable to connect directly to the TraCIM server. Therefore, a TraCIM client that runs outside of that particular software environment, but within a software environment that does allow communication with the TraCIM server, must be used.
- “Integrated” TraCIM clients – in other cases the software environment, within which the software under test is running, is able to connect directly to the TraCIM server. Therefore, a TraCIM client can be implemented within that software environment.

Software verification services for a total of six calculations (viz., LSEXP, WLSPR, PCA, LSPLANE, GDPR and LS3DLINE) were made available by NPL to the partners and the primary supporter.

Impact for developers of mathematical software development and analysis tools

Impact was initially achieved through the development and application of demonstration software verification services for calculations implemented within built-in functions in National Instruments tools, using standalone TraCIM clients. From the calculations considered within EMRP JRP NEW06 TraCIM, three calculations were selected: least squares fitting to data of the sum of an exponential decay function and a constant (short name “LSEXP”), weighted least squares polynomial regression (“WLSPR”), and principal component analysis (“PCA”). All three of these calculations are implemented within built-in functions in LabVIEW and two of the calculations, LSEXP and WLSPR, can be implemented in DIAdem.

To maximise the impact for the primary supporter, the partners made the following decisions:

- Where appropriate, the demonstration software verification services would be developed to allow a subset (as opposed to all) of the calculation outputs to undergo verification. This decision reflects the fact that not all of the output parameters listed in the computational aim are generated when the calculations are implemented in LabVIEW and DIAdem.
- The example standalone TraCIM clients would be developed in such a way as to make the verification of implementations of calculations in DIAdem more straightforward. Since XML parsing in DIAdem is not possible, TraCIM clients were developed that:
 - Extract the reference data provided in XML format (step 2 above) to ASCII files (that are more easily processed using DIAdem).
 - Take test results obtained using DIAdem and stored in ASCII files, and generate the required XML message (step 3 above).
- Therefore, the need for the verification service user, who may not be at all familiar with XML parsing, to work with XML is removed.

In addition to the schemata for the XML messages (steps 2, 3 and 4 above), service users are also provided with detailed instructions on how to use the demonstration software verification services. An example standalone TraCIM client is also made available to service users (in both executable and source code formats).

The LabVIEW and DIAdem functions were verified using the demonstration software verification services and the results were discussed with National Instruments. Guidance material on the use of the TraCIM software verification services, using standalone TraCIM clients, was developed and disseminated to National Instruments.

Impact for users of software development and analysis tools

Further impact was achieved through the development and application of demonstration software verification services for calculations implemented by users of LabVIEW. From the calculations considered within EMRP JRP NEW06 TraCIM, three calculations were selected: least squares plane fitting (short name “LSPLANE”), generalised distance polynomial regression (“GDPR”), and least squares 3D line fitting (“LS3DLINE”). None of these calculations is implemented within built-in functions in LabVIEW, but they can be implemented by combining built-in functions. For example, the LSPLANE calculation can be implemented by combining the built-in VI SVD Decomposition.vi from the Linear Algebra Palette with a number of VIs from the Probability & Statistics, Array and Matrix Palettes (Figure 4).

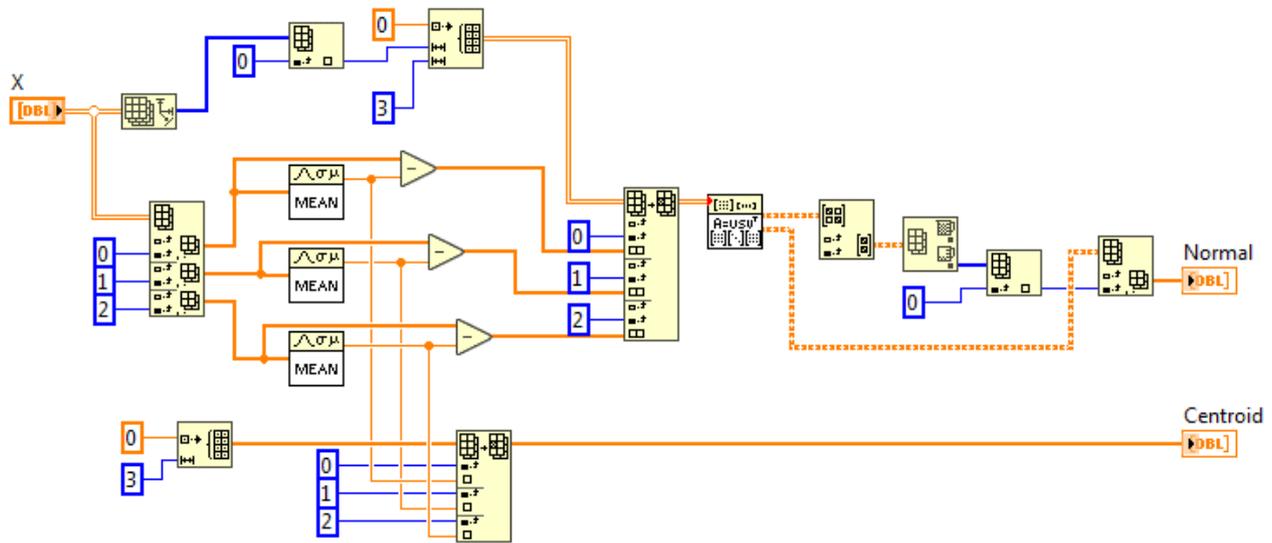


Figure 4: Block diagram showing an implementation of the LSPLANE calculation.

LabVIEW possesses functionality, viz. to allow XML messages to be parsed, and web requests to be sent, that makes it an ideal environment in which to employ integrated TraCIM clients.

In addition to scheme for the XML messages (steps 2, 3 and 4 above), service users are provided with detailed instructions on how to use the demonstration software verification services. An example standalone TraCIM client is also made available (in both executable and source code formats).

For each calculation, a LabVIEW implementation was developed. Subsequently, a TraCIM client was also integrated into LabVIEW, which calls the implementation of the calculation (Figure 5). Verification of the LabVIEW implementations was undertaken using the demonstration software verification services. Guidance material on the use of the TraCIM software verification services using integrated TraCIM clients was developed and disseminated to National Instruments.

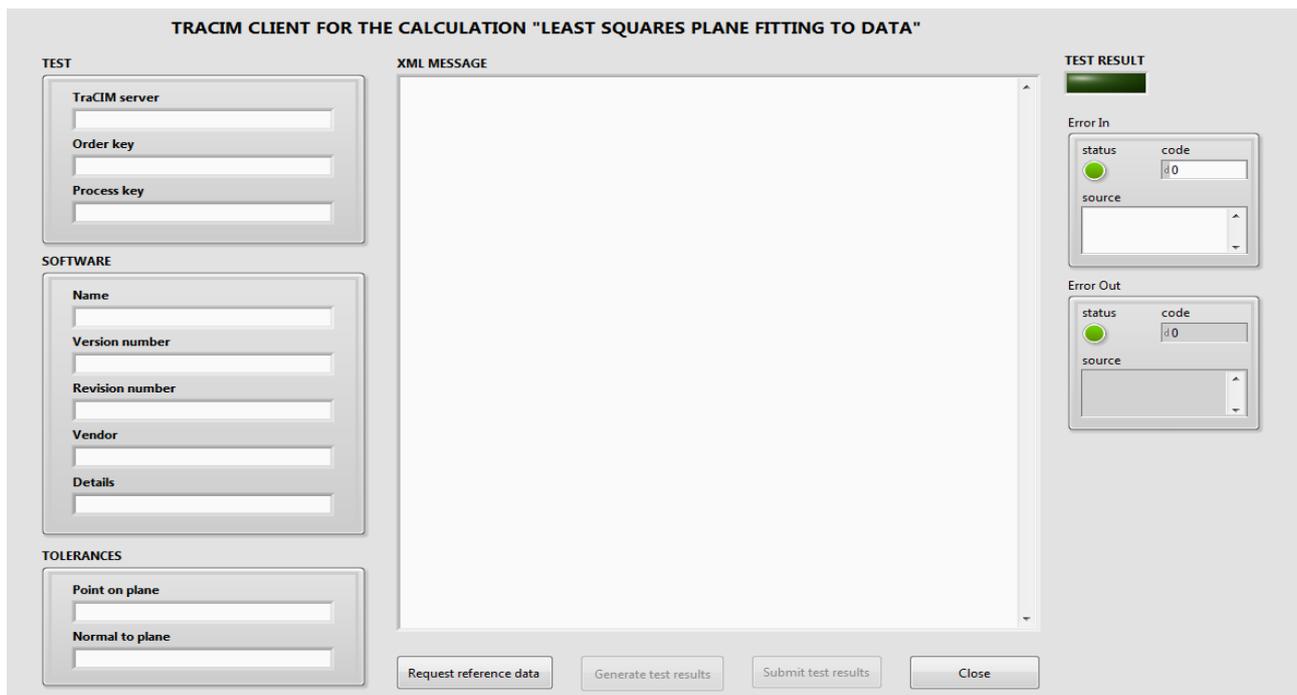


Figure 5: Front panel of a TraCIM client, which was integrated into LabVIEW, for the LSPLANE calculation.

Additional impact

NPL, PTB and Ostfalia-HAW were trained to help to ensure future impact of the outputs of EMRP JRP NEW06 TraCIM and EMPIR SIP 15SIP06 ValTraC. In particular, the training on the development of expert extensions will prove to be vital for the provision of future software verification services. Indeed, NPL, PTB and Ostfalia-HAW intend to develop and make further services available in the near future.

Future impact

Discussions regarding future interactions between the partners and the primary supporter is ongoing. National Instruments recognises the benefits to its products, as well as to its customers, of knowing how to develop software using these products. This can be achieved through the use of the TraCIM approach which provides independent verification of implemented mathematical calculations.

During the project, only the partners and the primary supporter had access to the demonstration software verification services. Access to these services will soon be given to other software developers. The provision of paid-for “advanced” software verification services is also being discussed.

While not a requirement, a project website has been created and this will be populated with both the outputs of the project and with material developed beyond the end of the project. For example, the partners are considering the verification of calculations implemented in other commonly used software environments. Existing guidance material will be extended and disseminated via the project website. A key aspect of the project was the provision of example clients in source code format, enabling service users to see how, e.g., XML parsing and communication via the internet is implemented.

A poster providing an overview of the TraCIM approach to the verification of mathematical software has also been developed to help publicise the outputs of EMRP JRP NEW06 TraCIM and EMPIR SIP 15SIP06 ValTraC (Figure 6). The poster can be downloaded from the project website.

