ONLINE VALIDATION OF NUMERICAL ALGORITHMS IN THE FIELD OF METROLOGY

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Abstract:

Numerical algorithms used in metrology can be online validated based on testdata and corresponding reference results in order to improve the reliability of measurement results. An established realization of the online validation is named Traceability for Computationally-Intensive Metrology (TraCIM). It allows service user to validate their software at the point of use. The service is operated by European national metrology institutes (NMIs).

TraCIM is based on three pillars, the technical implementation, the legal aspects, and the commercial requirements. The technical implementation provides a client-server concept. It allows a direct link between the NMIs and the service users. It is a fundamental principle that the TraCIM service is provided and hosted only by a NMI or an authorized organization. These institutions assume del credere liability and finally guarantee for the correctness of the results.

Meanwhile, TraCIM is registered as a wordmark. It is operated as a legal non-profit association under German law and allows only NMIs and designated institutes (DIs) to become members. The TraCIM association has been established with its main mission to provide quality rules for the TraCIM service. The business concept and the income of the TraCIM service are strictly uncoupled from the TraCIM association.

An example allowing to validate a least square fit for regular geometries such as cylinders, cones, planes and spheres is used to explain an application. This example is developed at the Physikalisch-Technische Bundesanstalt (PTB). A detailed focus is given on the TraCIM organization and the client server application.

Keywords: Software test, validation of algorithms, Gaussian test, TraCIM

1. INTRODUCTION

Today, a significant – and partly dominant – contribution to measurement uncertainty is due to the processing of the measurement data. Its causes are varied and the analysis algorithms used can practically not be traced back to metrology institutes at all. The errors often come from the incorrect or insufficient implementation of formal mathematical requirements. More often than not, seemingly trivial problems are the cause.

One of these seemingly trivial differences may, for instance, occur when numbers get rounded. Software engineers will often use the rounding function provided without thinking about the rounding rules it implies. But beware, this can already lead to significant differences in different applications, as shown in the following example.

Let us consider the series 1.5, 2.5, 3.5, 4.5. The task now consists in rounding the result to integral numbers and afterwards calculating the sum of the numbers. For this purpose, two different rounding rules are applied. In [1, 2], it is shown that the variety of rounding rules is even wider [3].

First case: "Half up rounding" round towards nearest neighbor unless both neighbors are equidistant as described in [4]. It behaves as rounding up if the discarded fraction is >= 0.5; otherwise, it behaves as rounding down. Note this is the rounding mode commonly taught at school. In the examples the numbers became 2, 3, 4, 5 and the mathematical sum of the numbers becomes 14.

Second case: "Half even rounding" round towards the nearest neighbor unless both neighbors are equidistant. In this case it depends on the digit left of the discarded fraction. If this digit is odd rounding down has to be used. If the digit left of the discarded fraction is even rounding up is the qualified option. Note that this rounding mode statistically minimizes cumulative error when applied repeatedly over a sequence of calculations. In the examples the numbers became 1, 3, 3, 5 and the mathematical sum of the nubmers becomes 12.

Comparing the results 14 and 12 of the two different rounding rules shows a systematic difference of 15% which finally contributes to a measurement uncertainty if clear instructions are missing.

In order to address these sources of errors, some metrology institutes already supply possibilities of checking analysis algorithms. These checks are often available for free. Industry, willing to demonstrate that its products can be trusted, is increasingly calling for a certificate issued by a trustworthy organization. Driven by this incentive, activities aimed at an online validation under the supervision of European metrology institutes have begun. To this end, not only technical, but also commercial and monetary preconditions had to be met in order to set up a complete and sustainable system.

2. THE TraCIM SERVICE

In association with and under the supervision of European metrology institutes, TraCIM aims to validate analysis algorithms in the field of metrology. In the following, they will be referred to as "algorithm tests" or simply "tests". Similar to the well known calibration chain which is related to physical standards the NMIs transfer the numerical accuracy of evaluation algorithms from the highest metrological authority to the individual application.

Computations are addressed which are used to analyse measurands of the International System of Units (SI) and their derived units. The medium of choice for communication between the service provider and the user is the Internet. The principle is shown in Figure 1. On the left, the service provider is represented as the association of metrology institutes. This is of paramount importance, since the algorithm tests are to be carried out – or at least monitored – by the supreme metrological authority of a country. The metrology institutes are organized with each other under the umbrella of the TraCIM association. TraCIM's main task consists in describing quality guidelines and defining the technical infrastructure under which the algorithm tests are to be run. Each service provider is, however, solely responsible – and therefore held liable – for the extent of the algorithm tests provided, for the business workflow, for the maintenance of the datasets, for consultation upon installation as well as for running the tests. For this reason, each metrology institute runs its own server within the TraCIM association, i.e. each server has to be addressed individually, which leads to a different extent of services depending on each metrology institute. The metrology institutes, however, have the possibility of mutually providing algorithm tests as subcontractors, which allows a service provider to enhance the extent of services provided.

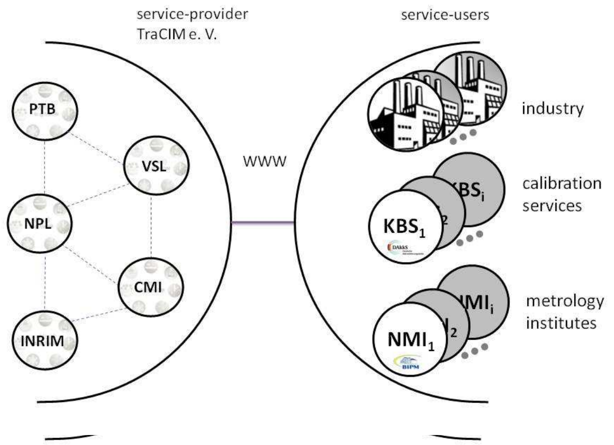

Fig. 1: TraCIM service

The service users are essentially manufacturers of analysis software or measuring instruments. This algorithm test service allows them to have their analysis algorithms validated by an independent metrology institute. This mainly serves to increase confidence in the products they offer on the market. In principle, they can have this service unlocked for their customers in order to have, for example, updates validated directly. Software engineers can already test their algorithms during the development phase to be on the safe side and, thus, make development faster. Each registered user which supports the specifications of the client-server interface can access individual tests via the Internet. The service is available 24 hours a day on every day of the year at each location on the globe to which internet is provided. Furthermore, the response times are considerably shorter than with the existing validation capabilities.

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3. THE BASIS OF THE TraCIM TEST

A full test dataset includes test data as input quantities of an algorithm test, reference results and their assigned numerical uncertainties. Hereby, the test data are defined as being error-free. In contrast, the indication of the reference results, by analogy with the indication of measurement results, is defective in the case of geometrical measurements [5]. Hereby, it is up to the metrology institutes to develop procedures as long as these meet the requirements.

The following is a description of the approach followed by PTB. To this end, all test datasets are computed, tested and archived in a database when setting up an algorithm. This database – also called "golden dataset" – thus contains all sensitive test data and must therefore be protected from unauthorized access. Contrary to a reference software in which test data can be specified externally, PTB's approach, consisting in the one-time computation of test datasets, is far more secure, since the correctness of a software can never be guaranteed. In addition, specified datasets are practically not subject to ageing. Reference algorithms, in contrast, depend on the state of the art of the programming language, of the operating system, of the processor properties and, thus, need maintenance and are short-lived.

Yet, the test data do not represent an inflexible system. They can be adapted to an individual application without losing their accuracy. This can mean, for example, that an SI unit or a derived unit is indicated. In the case of geometrical measurands, the test data can be represented with additional SI prefixes such as "nano-", "micro-", "milli-" etc. This does not affect the numerical presentation – and, thus, the accuracy. The same applies to the scaling of measuring ranges which may only be done in the form of decimal powers (i.e. $\times 10$; $\times 100$, etc.).

The confidence across the measurement trueness of the reference results is yielded by means of comparative computations. Thus, the reference results of at least three independent software implementations are computed and compared with each other. The numerical accuracy is determined by varying the test data by means of a Monte Carlo simulation. For this purpose, the last decimal digits of the test data are randomly varied, and the dispersion of the corresponding reference results is determined. After ignoring another two decimals for safety's sake, this value is deemed the assigned numerical uncertainty.

The presentation of the test datasets is geared to the technical applications in question – and not to what is mathematically feasible. The test datasets are supposed to simulate frequent technical situations. Exceptions which require a high degree of development and consultation effort should, as a rule, be avoided.

4. TraCIM IT'S ARCHITECTURE

TraCIM's IT architecture consists of four central modules. These are represented in Figure 2

The server is the core module. As a management module, it is operated by a competent metrology institute. It manages all of the operating data and controls the data flow to the other modules.

The expert modules are developed by experts responsible for a particular individual test. Each expert module operates basically autonomously and deals with all logical processes in connection with a test. It makes the test datasets available on request, compares the test results computed by the users with its own reference results and, finally, issues the test report. Since the individual tests may vary significantly from one application to the other, only few input parameters have been defined by TraCIM for the data traffic. This applies, for instance, to the support of a software interface in JAVA which allows the expert system to be logged into the server system. Indispensable operating data such as the order number must also be transmitted via this interface. Since the formats of the test data can be freely selected, the expert is, to a large extent, free to design the test according to his needs. Furthermore, existing tests and test data structures can easily be integrated into the TraCIM system.

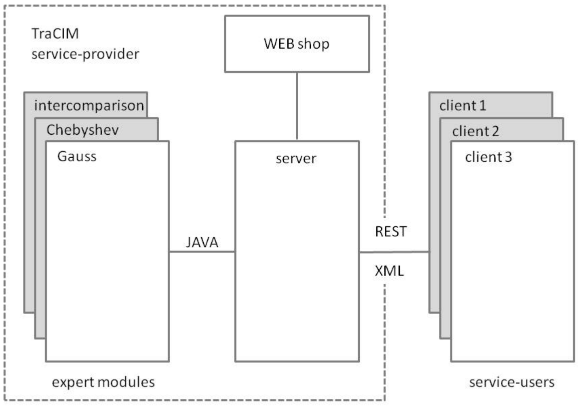

Fig. 2: TraCIM modules

The formal specifications of the TraCIM server with regard to the user are, in contrast, more restrictive. The server-client communication runs via a REST interface. Hereby, the data are embedded into an XML structure. Then again, within this structure, free formats of test data (such as binary formats or established test data structures) can be defined, depending on the application. The expert is solely responsible for the test data format, the test data and the test results.

The interface is available externally via a webshop which is also connected to the server module. At the current stage of implementation of the system, this interface is, however, not yet available. Similar to online shopping, interested users will be able to register via the Internet and to order individual tests. The precondition for running the test is, however, that the REST interface is supported. Until the webshop has been set up, interested users can contact the TraCIM secretariat directly in order to register.

5. COSTS

The validation of analysis algorithms is subject to charges. This has several reasons: firstly, the service user will obtain an official report, secondly, the management and maintenance of the TraCIM system are expected to generate costs, and, last but not least, the development costs for the system need to be refunded in the long run. Figure 3 explains the costs of the so-called "Gaussian test" which is already offered by PTB. There are different offers for this test. Besides an individual test, also test packages of 10 and 50 tests are available. Purchasing test packages makes sense, for example, in the case of a software-developing company willing to have its updates or upgrades validated.

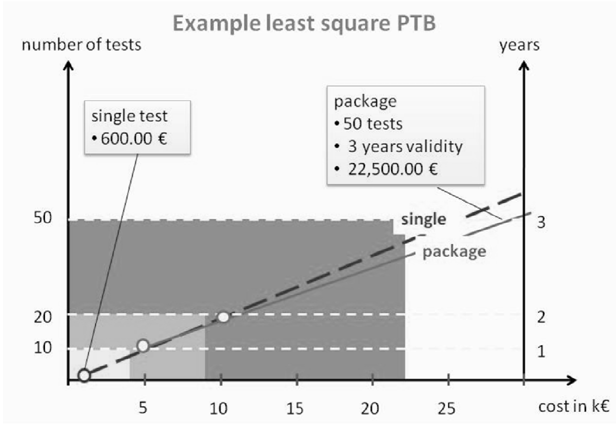

Fig. 3: Business concept Gaussian test of PTB

Strictly speaking, a validation is valid only for the software used during the test. Only the software manufacturer can appraise when a modification of a complex analysis software has an influence on the algorithms to be validated. It is therefore his responsibility vis-à-vis his customers to assess whether the validation is still valid.

6. THE TraCIM ASSOCIATION

The TraCIM association under German law offers a number of possibilities to fit best for the needs of an international cooperation. The organization structure is very flexible and can be adjusted according to the needs of the association and its members by the general assembly. Furthermore, the structure chosen for TraCIM is similar to the well-known EURAMET-structure but not as detailed and complex. Figure 4 shows the TraCIM structure. The statutes are dealing with regulations concerning especially the membership, the chairpersons, the general assembly, technical committees, membership fees and the secretariat.

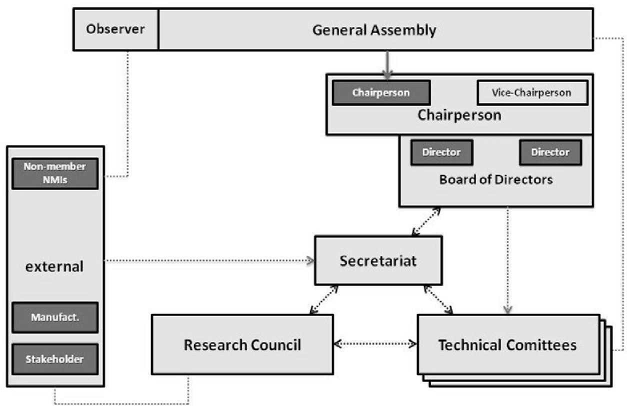

Fig. 4: TraCIM association

NMIs or DIs that are members of EURAMET e. V. may become full members of TraCIM as well as individuals who are active staff members of a NMI or DI.

NMIs or DIs who are members of EURAMET e. V., who – due to their legal provisions – may not become full members of TraCIM, may be nominated as extraordinary members. Other natural or legal persons (for example industry partners) may be nominated as sustaining members.

To become a member, the respective person/legal entity has to apply for membership in a written document to the committee of the association. The general assembly finally decides on the application. Every full member has the right to vote.

The committee consists of the chairperson and the vice-chairperson. They legally represent the association in and out of court. The committee is elected by and out of the general assembly.

The general assembly is held at least once a year. It may take place as a real meeting or via videoconference, depending on the topics to be discussed. All members have the right to participate. Each full member has one vote. The general assembly is responsible for the main decisions, for instance the election of the committee or the decision making of amendments to the statutes.

The technical work, especially preparing and implementing technical decisions and tasks, shall be done in the technical committees that will be open to all members as well as to non-members, if the committee (chairperson or vice-chairperson) has given its approval. They are not yet set up but may be established by the committee, depending on the need.

The secretariat has to deal with internal affairs (including the financial management) and to support the committee in external affairs. The first secretariat operates at PTB.

The association was established on 12th March 2014. Elected as chairperson is Frank Härtig, vice chairperson is Klaus Wendt. The application for registration of the association was submitted to the registration court and has been confirmed already. With the registration the association gets its own legal personality according to the undermentioned statutes.

Amendments may only be adopted by the members of the association having the right to vote in the general assembly.

As the offering of tests is not the business of the non-profit TraCIM association, each NMI keeps the possibility to offer tests by its own also with the consequence of the application of its respective national law. Meanwhile, the association opens up the legal framework for the international cooperation. It comprises in particular the contracting and licensing of the use of the TraCIM-logo and mark designation as well as the establishment and development of a common quality-management standard.

7. THE FIRST TraCIM APPLICATION

In the current state of implementation, PTB offers the so-called "Gaussian test". This test is used in the field of length measurement. It is used to check the correct determination of the parameters for the adjustment of geometrical elements, 2D straight line, 3D straight line, 3D circle, 3D plane, cylinder, cone and sphere, according to the least-square error fit. An individual test costs 600 Euros. Compared to the traditional test carried out manually by PTB via email correspondence, this has allowed costs to be cut by more than 50 %, but also to reduce time and effort. The first algorithm test was successfully carried out by the company Mitutoyo in May 2014.

8. TraCIM – THE RESEARCH PROJECT

The TraCIM system is being set up within the scope of the European Metrology Research Project (EMRP) under the denomination "Traceability for Computationally-Intensive Metrology". The project is coordinated by the National Physical Laboratory (NPL). Furthermore, it involves five other European metrology institutes, four partners from industry and four universities.

9. SUMMARY AND OUTLOOK

With the TraCIM system, analysis algorithms of metrological applications can be validated. This allows the – meanwhile significant – influence of the software on a measurement result to be considerably reduced. Validation takes place via the Internet and, thus, ensures direct traceability from industry straight to the metrology institute. The metrology institutes affiliated to the TraCIM association are solely responsible for complying with the quality rules.

After only half the project term, the association "TraCIM e. V." was registered. Shortly after that, the first test – the so-called "Gaussian test" – was implemented. After only two thirds of the project term, a project partner was able to validate its analysis algorithms via the Internet.
The remaining term of the project will be used by PTB to carry out further tests such as a Chebyshev test for geometrical elements and a test for the validation of analysis algorithms based on [6] for national and international comparison measurements. Moreover, the participating NMIs, DIs, institutes and partners from industry will start to establish technical committees in order to fix quality rules for the TraCIM services. In addition a public workshop held in November will teach interested software developers and instrument manufacturers how to operate the TraCIM system focusing on the technical implementation, the legal aspects, and the commercial requirements.

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