2nd INTERNATIONAL WORKSHOP

ON

VALIDATION OF COMPUTATIONAL MECHANICS MODELS

5th November 2013

At the British Museum, London

PROGRAMME & ABSTRACT BOOKLET

Supported by the VANESSA (Validation of Numerical Engineering Simulations: Standardisation Actions) project which has received funding from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement nº319116

The first international workshop on Validation of Computational Solid Mechanics Models was held at Shanghai Jiao Tong University in October 2011 by Professor Shan Fu, Shanghai Jiao Tong University, China and Eann Patterson, University of Liverpool. A series of papers based on the work presented at the workshop were published as a special issue of the Journal of Strain Analysis for Engineering Design in January 2013 (see: http://sdj.sagepub.com/content/48/1.toc).

A number of free copies of the special issue will be available for attendees at the 2nd Workshop in London on November 5th, 2013 on first-come-first-served basis.

Second international workshop on Validation of Computational Mechanics Models is organised as part of the VANESSA (Validation of Numerical Engineering Simulations: Standardisation Actions) project which has received funding from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement nº319116.

Conference Chairs:

Eann Patterson, University of Liverpool, UK [eann.patterson@liverpool.ac.uk]

Erwin Hack, EMPA, Switzerland [erwin.hack@empa.ch]

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SECOND INTERNATIONAL WORKSHOP ON VALIDATION OF COMPUTATIONAL MECHANICS MODELS

5TH NOVEMBER, 2013 AT THE BRITISH MUSEUM, LONDON

PROGRAMME

10.00 Registration and Coffee

10.20 Introductory Remarks: Eann Patterson, Workshop Chair

TOPIC ONE: ***Solid mechanics model validation*** Chair: Eann Patterson (University of Liverpool)

10.30 Keynote Lecture 1: **Quantifying model quality using measured strain fields**
ERWIN HACK (EMPA, Switzerland)

11.10 **Application of 3D DIC for calibration of FEM model of graded metal plate arches**
Malowany K, (Warsaw University of Technology), Piekarczuk A, (BRI, Warsaw), Więch P, (BRI, Warsaw), Kujawińska M & Malesa M, **(**Warsaw University of Technology)

11.30 **Uncertainty quantification and robust design optimisation**
Sönke Klostermann (EADS Innovation Works)

11.50 Plenary Discussion 1: **Solid mechanics model validation**
Panel: Erwin Hack (EMPA), George Lampeas (University of Patras) & Sönke Klostermann (EADS Innovation Works)

12.20 **LUNCH** [not provided but plenty of choice locally]

TOPIC TWO: ***Acceptable evidence for engineering decisions*** Chair: Erwin Hack (EMPA)

13.45 Keynote Lecture 2: **What constitutes evidence and its role in calibration & confirmation**
CHARLOTTE WERNDL (LSE, UK)

14.25 **A principal component analysis decomposition based validation metric for use with full-field measurement situations**
Allemang RJ (University of Cincinnati), Eason TG (USAF), Spottswood SM (USAF)

14.45 **Accommodating the Effect of Sparse Data Input in Engineering Modelling Applications**
Graham S, Taylor R (National Nuclear Laboratory)

15.05 Plenary Discussion 2: Acceptable evidence for engineering decisions
Panel: Charlotte Werndl (LSE), Randy Allemang (University of Cincinnati) & Alex Ihle (High Performance Space Structures GmbH)

15.35 **TEA BREAK**

TOPIC THREE: ***Fluids mechanics model validation*** Chair: George Lampeas (University of Patras)

15.50 Keynote Lecture 3: **Validation Challenges in Industrial Computational Fluid Dynamics**
ALTHEA DE SOUZA (Tridiagonal Solutions Ltd, UK)

16.30 **Quantifying turbulence-model inadequacy with Bayesian-Model Averaging**
Dwight R (TU Delft), Edeling W (TU Delft), Cinnella P (ENSAM, ParisTech)

16.50 **Validation of a rheological model for non-Newtonian fluid flow**
Widmer-Soyka RP (ETH Zurich), Lopez A, Persson C (Uppsala University), Cristofolini L (Rizzoli Orthopaedic Institute, Bologna), Ferguson SJ (ETH Zurich)

17.10 Plenary Discussion 3: Fluids mechanics model validation
Panel: Althea de Souza (Tridiagonal Solutions Ltd, UK), Richard Dwight (TU Delft) & Steve Graham (NNL)

17.40 End of Workshop

18.00 Museum closes

ABSTRACTS

and

BIOGRAPHICAL DETAILS OF SPEAKERS

(in order of presentation)

Quantifying model quality using measured strain fields

Erwin Hack, Empa, Electronics/Metrology/Reliability Laboratory, CH-8600 Dubendorf, Switzerland
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Abstract

The term „stress test“ has received a special meaning as a consequence of the financial crisis. Yet its basic meaning originates in solid mechanics where stress is used to study the behaviour of a structure, component or design under load. Since the stress-induced deformation or strain in a test object is related to potential damage it is common practice to measure or simulate strain fields during design, manufacturing or service of a structure. Only the surface strain field is readily available, since full volumetric strain data inside solid bodies are rarely accessible, e.g. through x-ray computed tomography.

There is an implicit expectation that a numerical model should faithfully represent the component under service load. In a first step, it should reproduce the behaviour of the component in a specifically designed test environment, viz. a validation test. The use of camera-based instrumentation to measure deformations and surface strains has led to the availability of strain field data similar in point density to the numerical model output. It is generally accepted that the assessment of the model quality is deduced from a comparison of the simulated to the measured data. We describe how data rich strain fields from experiment and simulation can be compared in a quantitative manner with reasonable effort. Instead of comparing a million points, matched onto a common coordinate grid by interpolation, a hierarchical comparison of image descriptors furnishes evidence for consistency, and, in addition, allows one to define a quantitative measure of data consistency together with a confidence limit. In turn this methodology allows one to define an acceptance band beforehand which is an indispensable step in solid mechanics model validation.

Short Biography: Erwin Hack

Erwin Hack holds a diploma in theoretical physics and a PhD in physical chemistry, both from the University of Zurich, Switzerland. Since 1998, he is deputy head of the Electronics/Metrology/Reliability lab at Empa, the Swiss Federal Laboratories for Materials Science and Technology. His research interests are in full-field measurement techniques including speckle interferometry, thermography, and THz imaging. He coordinated the European FP7 project ADVISE and was partner in several other research projects on optical techniques. Erwin lectures at ETH Zurich on optical methods in experimental mechanics. He is associate editor of *Optics and Lasers in Engineering*, vice-chair of CENWS 71 – “Validation of computational solid mechanics models using strain fields from calibrated measurements”, vice-president of the „Swiss Society for Non-destructive Testing“, and member of both EOS and OSA.

Application of 3D digital image correlation for calibration of FEM model of graded metal plate arches

K. Malowany[1], A. Piekarczuk[2], P. Więch[2], M. Kujawińska[1], M. Malesa[1]
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Abstract

The lack of sufficient engineering knowledge, particularly when a new, specific design is applied in an inadequate environment are one of main cause of a building failure, next to negligence in process of design and construction. For reduction of the building cost, many innovation solutions have been developed. One of them are graded metal plate arches, which were used for military application as temporary buildings. To extend the area of use of such structures to large building structures for public use, a formal regulation should be prepared (including guidelines regarding: calculation, design, monitoring), preceded by proper tests. Uncommon geometry of the metal plate (plastic deformations, cross section of a trough, goffer pattern) is difficult to be modeled numerically, and hence, the local loss of stability can occur in unexpected regions. In order to enable numerical modeling, the hybrid experimental-numerical methodology should be elaborated for the processes of design, construction and operation. Another aspect is the need for optimization of mechanical, material and technological parameters. Steel halls are used in many different environments which might be associated with stochastic loads applied by wind, snow or temperature. Thus proper construction project depends on many factors and is crucial both for safety and for reducing costs of construction.

Development of the multi-camera 3D digital image correlation (DIC) measurement methodology (with distributed fields) for the analysis of large building constructions will introduce a new quality comparing to solutions being currently used throughout the world, both in terms of research of constructions based on graded metal plate arches and of creating numerical models of them. The preliminary measurements have been performed in 2011 at Building Research Institute. On the basis of them, the innovative methodology of validation numerical models by the measurements based on the 3D DIC have been proposed in a project 'Opt4Blach'.

We will describe the methodology of the FEM model calibration realized by means of date obtained from 3D DIC method, which include 3 steps: (1) analysis of the segments (1 m high) of different kinds of graded metal plate arches, to assess how mechanical parameters are influenced by technology used to achieve a desired geometry; (2) laboratory analysis of the full-dimensional elements, for development of calibrated and experimentally verified numerical models of single-surface objects made of graded metal plate arches in natural scale; (3) *in-situ* analysis of the multi-segment, full-dimensional object, for development of the guidelines for the design of constructions based on metal plate arches, as well as the systems of monitoring and control for an objects being in their exploitation phase. We will also present the results obtained in the first step and describe the multi-camera 3D DIC instrumentation devoted to measurements of graded metal plate arches.

Short biography: Krzysztof Malowany

Krzysztof Malowany is a PhD student of applied optics at Warsaw University of Technology. His areas of interest include: full-field optical metrology in civil engineering and power engineering industry, hybrid opto-numerical methods in mechanics, image and data processing, design of novel photonics systems. Current research focuses on the development of a method for calibration of FEM models with utilization of full-field optical methods (in particular with digital image correlation).

Uncertainty quantification and robust design optimisation

Sonke Klostermann (EADS Innovation Works)

Abstract

System behaviour is influenced by a high number of uncertainties in the early stages of development when technical innovations have been included. A key source of uncertainty is the scatter of physical boundary conditions and system characteristics that influences the behaviour of real systems to a high degree. These uncertainties may be represented by a scatter of: Geometry (tolerances in shape or measure), Material properties (density, Young's modulus), Loads and boundary conditions (initial velocities, forces).

Since real tests are time-consuming and expensive it is highly desirable to predict system behaviour by means of simulation. However, regardless of the simulation method a deterministic model cannot incorporate the uncertainties mentioned above. It is therefore impossible to assess and to quantify the numerical robustness of the model as well as the robustness of the system's behaviour. In order to increase the reliability of predictions about real system behaviour, probabilistic models can be created that take uncertainties into account by modelling individual aspects of the system and the environment as a realisation of stochastic influences.

One way to consider uncertainties is to describe a parameter as a random variable that is defined by its distribution type and statistic moments. As random variables are independent of time and space it is evident that they can only be a global approximation of real scatter. It is impossible to account for local, spatial or temporal effects. For a consideration of local effects the uncertainties can be modelled by so called random fields. For a random field the parameter is a function of the position vector in the n-dimensional feature space.

An approach to simulate the consequences of scatter is stochastic simulation of the system using the Monte Carlo method. The post processing of stochastic simulations is performed by means of statistic methods like arithmetic mean, standard deviation, correlation coefficients, histograms and scatter plots. This way only values of selected points in space and time can be evaluated and the associativity to the geometric model is lost.

To overcome these limitations a new concept to visualise the geometric scatter from stochastic simulation results was developed. Therefore a non-parametric density estimation using multi-dimensional kernel smoothing of the Monte Carlo samples is performed. Based on this the expected value geometry can be derived, representing the most probable shape of the mesh.

The visualisation of the expected value geometry and surrounding probability envelopes as superimposed transparent geometry constitutes a first approach to evaluate the geometric variation in a holistic way. The method is a part of robust design optimisation which enables designs with performances less sensitive to the uncertainties conditioning their operation, and for which the risks related to their operation envelope are minimized, reducing hereby the risks of failure.

Short Biography: Sönke Klostermann

Sönke Klostermann is a mechanical engineer specialising in aircraft systems engineering. He received his diploma degree from the Hamburg University of Technology and has been with EADS Innovation Works since 2008. His work focuses on nonlinear dynamic simulation and stochastic simulation techniques. This includes stochastic modelling of random fields, uncertainty quantification and robust design optimisation.

What constitutes evidence and its role in calibration & confirmation

Charlotte Werndl (London School of Economics)

Abstract

It is widely held that double-counting is bad and that separate data must be used for calibration and confirmation. This paper argues that this is far from obviously true. According to a Bayesian/relative-likelihood approach to incremental confirmation, double-counting is entirely proper. It is argued that scientists' worries about double-counting are most charitably reconstructed as the failure of confirmation or double-counting because (i) past evidence is irrelevant for assessing models that concern the medium-run future; (ii) the model has a good fit with any arbitrary evidence; (iii) there is radical uncertainty whether other models could explain the evidence better. Examples from engineering and climate science will be used to illustrate the main claims.

Short Biography: Charlotte Werndl

Charlotte Werndl is Associate Professor at the Department of Philosophy, Logic and Scientific Method at the London School of Economics. Previously, she was a Junior Research Fellow at the Queen's College, University of Oxford. Her doctoral degree is from the University of Cambridge. She has a background in both philosophy and applied mathematics. Her research interests lie in questions on evidence and the philosophy of statistics, the philosophy of climate science, the philosophical foundations of physics and in general philosophy of science.

A Principal Component Analysis (PCA) Decomposition Based Validation Metric for Use with Full Field Measurement Situations

R.J. Allemang (UC-SDRL, USAF AFRL/SSC)
T.G. Eason (USAF AFRL/RQHF), S.M. Spottswood (USAF AFRL/RQHF)

Abstract

A validation metric that involves principal component analysis (PCA) decomposition of simulation and test data is developed for potential use in the quantification of margin and uncertainty (QMU) for model validation applications. This validation metric allows for use of nearly full-field, simulation and test data over a wide range of spatial realizations (3-D responses over multiple input conditions) and temporal (time or frequency) information, as needed. While 3-D response information has been readily available in model simulations, only recently has 3-D response information been available in test data based upon the use of laser scanning and/or photogrammetry methods such as digital image correlation (DIC). A demonstration example utilizing two datasets explains how the validation metric is formed and how it can be used to quantify the margin between the simulation and the test data as well as how it can quantify the uncertainty. The primary advantage of the proposed PCA validation metric is that it preserves the engineering units (EU) of the original data so that the quantifications of margin and uncertainty can be made in EU. A second advantage of the PCA validation metric is that it can be used over a wide range of temporal information. One final advantage is that the aerospace industry already has experience with using PCA based methods to compare sets of experimental data with large numbers of DOFS so acceptance of a similar validation metric can be anticipated. While the proposed method shows considerable promise, future work is identified in terms of exploring other decomposition methods and the problem of comparing simulations and experimental data sets with mismatched data matrix dimensions.

Short Biography: Randall J. Allemang

Dr. Allemang is a member of the faculty of the Mechanical Engineering Program in the Department of Mechanical and Materials Engineering, University of Cincinnati, where he currently also serves as Director of the Structural Dynamics Research Laboratory (UC-SDRL). Dr. Allemang has been actively involved in the area of experimental structural dynamics and modal analysis for over thirty five years, pioneering the use of multiple input, multiple output estimation of frequency response functions, developing the concept of cyclic averaging, formulating the modal assurance criterion (MAC) and the enhanced frequency response function and reformulating modal parameter estimation algorithms into the unified matrix (coefficient) polynomial approach (UMPA). During this period, Dr. Allemang has authored or co-authored over 160 technical articles, including chapters for 2 different handbooks and numerous refereed articles. Dr. Allemang is currently involved as Senior Collaborator for the AFRL Structural Sciences Center at USAF-AFRL/WPAFB and has been awarded a Summer Faculty Fellowship with the USAF (ASEE) for the summers of 2011-2013 in the area of verification and validation (V&V) of structures including quantification of margin and uncertainty (QMU). Dr. Allemang has been recognized by three professional societies as a Fellow (SEM, SAE and ASME) and has also served as President for the Society of Experimental Mechanics (SEM), 2003-2004, and on the Executive Board of SEM from 1998-2006.

Accommodating the Effect of Sparse Data Input in Engineering Modelling Applications

S. Graham, R. Taylor (National Nuclear Laboratory)

Abstract

In the civil nuclear power industry the predictive capability of mathematical models is often used to provide an understanding of the behaviour of plant and processes. Outputs from the models form part of safety cases and need to be sufficiently robust to satisfy the requirements of a regulatory environment. Due to the nature of the process conditions data is often sparse and incomplete. This provides a challenge to deliver a full set of conditions to adequately solve for the physics and chemistry that govern these processes. In many cases simplifications are made which use pessimisms to deal with the uncertainty in the modelling approaches. The presentation will show how these issues are typically tackled with reference to where key input was provided to a safety case for decommissioning the fire damaged Windscale Pile 1 reactor on the Sellafield site.

Short Biography: Dr Steve Graham

Dr Steve Graham has over 25 years experience working in the nuclear industry the field of mathematical modelling of fluid flow and heat transfer. After completing his PhD in Computational Fluid Dynamics at the University of Sheffield he spent 7 years at the National Nuclear Corporation in Warrington applying predictive methods to Advanced Gas Cooled Reactors and Fast Reactors. After joining BNFL he became the lead CFD Technologist, becoming increasingly involved in technical quality. This led to Steve representing BNFL in the European 5th Framework initiative QNET-CFD where a case study was provided to the best practice guidelines. As the BNFL R&D Division evolved into the UK National Nuclear Laboratory, Steve now chairs two Working Groups associated with technical quality in Modelling & Simulation and has been awarded a Laboratory Fellowship for his work in Engineering Modelling.

Validation Challenges in Industrial Computational Fluid Dynamics

Althea de Souza
Principal Engineer, Tridiagonal Solutions
and Chairman of the NAFEMS CFD working group

Abstract

Validation of an engineering simulation has been defined fairly widely in the analysis community and although the phrasing differs, it can be summarised as the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. Purists, working in the early days of (structural) engineering analysis might claim that validation requires the precise analytical solution against which the results of a simulation may be compared. This is however unhelpful for many classes of problem and engineering applications and some may even argue that if we can calculate a precise analytical solution, then a simulation is unnecessary.

The fundamental requirement is to determine how closely a simulation represents the behaviour it is attempting to capture. If we can determine that behaviour in some way, it can be used as a comparison for the simulation results. The most obvious solution is to take measurements of what happens in the physical world. However this in itself can be problematic. For the flow of fluids and heat transfer, the behaviour can be difficult to observe. For example it is fairly straight forward to observe the surface of a river but much less easy to see what is happening at a distance beneath the surface or to the air-currents around a building or the mixing of two different fluids in a stirred tank. In many cases the introduction of measurement equipment can alter the behaviour of the flow so unless the measurement equipment can remain in place during operation and also be included in any simulations, it may be considered of limited use.

These challenges have led engineers to develop a variety of techniques for validation and often to use a number of them in combination to provide confidence in the results of their simulations. If the behaviour of interest is difficult to measure, it may be that other features of the flow can be measured which can provide confidence in the simulation as a whole. Alternative simulation tools and approaches may be used and compared. Hand calculations can provide insight into expected behaviours and ball park values. Where measurements of the industrial application are not possible due to size or safety issues, smaller scale controlled experiments can prove useful. This presentation was discuss these issues in the context of industrial requirements for Computational Fluid Dynamics (CFD).

Short Biography: Dr Althea de Souza

Dr Althea de Souza has been using engineering simulation to support and improve industrial design for 18 years. She has worked in and managed analysis and qualification teams, integrated within engineering design departments and as a consultant on industrial simulation and optimisation and is currently Principal Engineer at Tridiagonal Solutions. Dr de Souza is also chairman of the NAFEMS CFD working group, which strives to encourage the effective use of computational fluid dynamics methods for industrial applications. She is a Chartered Engineer, a Fellow of the Institution of Mechanical Engineers, a member of the Royal Aeronautical Society, a FEANI accredited EurIng and a founder member of the NAFEMS Professional Simulation Engineer scheme.

Quantifying Turbulence-Model Inadequacy with Bayesian-Model Averaging

R. Dwight (TU Delft), W. Edeling (TU Delft), P. Cinnella (ENSAM, ParisTech)

Abstract

Reynolds-averaged Navier-Stokes (RANS) simulations form an important part of the analysis and design methods used in industry. Methods exist for the quantification and control of discretization error (a *posteriori* error estimation, goal oriented adaptation), and parametric uncertainty (polynomial chaos, global sensitivity analysis), but in many simulations the dominant error source is likely to be the turbulence closure model. We aim to develop *a posteriori* estimates of this component of the error which we denote *model error.* Our estimate is based on variability in the space of model closure coefficients across multiple flow scenarios. This coefficient uncertainty is estimated using Bayesian calibration against experimental data for the scenarios, and Bayesian model averaging (BMA) is used to collate the resulting posteriors to obtain an error estimate for a Quantity of Interest (QoI) in a new flow. We demonstrate it for wall-bounded flows at a variety of favourable and adverse pressure gradients.

Short Biography – Richard Dwight

I'm an assistant prof. at TU Delft leading a small group (5 PhDs) in the aerodynamics department. The common theme is data assimilation for fluids in engineering. Previously I worked at the German Aerospace Center (DLR) in Braunschweig, on solvers for compressible flow, and optimization methods for aircraft design.

My work focuses on the reliability and trustworthiness of numerical predictions in fluid dynamics. Working in UQ it quickly became clear that the bottleneck lay not in our ability to propagate uncertainty, but our poor knowledge of uncertain inputs. On the other hand, there are very few projects in which experiment and simulation do not coexist. Since then I have been working in stochastic data-assimilation, and with applications in fluid-structure interaction; turbulence modelling; compressible flow; and post-processing of PIV data. My attack on simulation error is two pronged: the first prong is post-processing experimental data with simulation, to reduce and estimate simulation error by using measurements as a reference. This employs physics-based covariance structures. The second prong (this presentation) aims at the original goal of simulations which quantify their own error with zero input of data (though data at related conditions is needed).

Validation of a rheological model for non-Newtonian fluid flow

R.P. Widmer-Soyka (ETH Zurich), A. Lopez, C. Persson (Uppsala University), L. Cristofolini (Rizzoli Orthopaedic Institute, Bologna), and S.J. Ferguson (ETH Zurich)

Abstract:

Bone augmentation is the process of injecting bone cement into osteoporotic or fractured bone in order to relieve pain and/or to stabilize the fracture. The bone cement (more generally the biomaterial) injected is typically a type of poly(methyl methacrylate) (PMMA) cement used more commonly to fix joint prostheses to bone. A computational model that can predict pre-operatively the flow of this biomaterial through the porous bone matrix during the augmentation process has been developed in order for supporting clinicians to maximize the treatment outcome and avoid complications. A validation of the proposed numerical models was performed either by injecting non-Newtonian fluids into surrogate bones (N=2) or human vertebrae (N=9). Radiographs of the specimens were acquired using fluoroscopy or computed tomography scanners prior and after the fluid injection and co-registered to the corresponding Finite Element (FE) models. Error estimates were derived by computing position differences of the fluid interfaces either directly on the 3D CT data (human cadavers) or the 2D fluoroscopy data (surrogate bones). Local errors up to 10 mm and root-mean-square (RMS) errors in the order of 2-3 mm have been found. The errors moreover differed statistically significant ($p<0.01$) between spine levels (thoracic/lumbar) and Newtonian/non-Newtonian fluid models. In the in-vitro experiments, the principal source of error is uncertainty in the location of the cannula. Our findings highlight (a) the importance of validating computational models generally, (b) the relevance of incorporating the non-Newtonian fluid properties in computational models of porous media at the appropriate length scale and (c) that surrogate bones are not a replacement yet for cadaveric bones both in terms of quality and sample costs.

Short biography: René Widmer

René Widmer received his B.Sc. in Electrical Engineering in 2004 and, after several years of working in industry, his M.Sc. in Biomedical Engineering in 2009 from the University of Bern, with a special focus on the musculoskeletal system. In his Master Thesis, he implemented a Darcy Rheology model to simulate the flow of biomaterials in vertebral trabecular bone and porous media generally. In 2009, he joined Prof. Stephen Ferguson's group at the Institute for Surgical Technology and Biomechanics, University of Bern and completed his PhD Thesis at the Institute for Biomechanics, ETH Zurich, in July 2013. His research focuses on the study, characterization and validation of the nonlinear biomaterial rheology using multi-scale statistical finite element approaches.

Notes

Members of the VANESSA consortium

University of Liverpool

Dantec Dynamics GmbH

Materialpruefungs-und Forschungsanstalt (EMPA)

University of Patras

High Performance Space Structure Systems GmbH

Schweizerische Normen-Vereinigung (SNV)

Centro Ricerche FIAT SCPA

National Nuclear Laboratory Limited