COMMODO – COMPLEX MATERIAL MODELLING OPERATIONS

A COMPREHENSIVE APPROACH TO THE MODELLING OF COMPLEX MATERIALS WITH MACHINE LEARNING MODELS WITHIN FINITE ELEMENT SIMULATIONS

Andreas Kuhn, Toni Palau, Gerolf Schlager[a], Helmut J. Böhm, Sergio Nogales[b], Victor Oancea, Ritwick Roy[c], Andrea Rauh, Jürgen Lescheticky[d]

[a] ANDATA GmbH, Hallein, Austria
[b] Institute of Lightweight Design and Structural Biomechanics, Vienna University of Technology, Vienna, Austria
[c] ABAQUS SIMULIA, Providence, RI, USA
[d] BMW AG, Munich, Germany

[a] {andreas.kuhn, toni.palau, gerolf.schlager}@andata.at,
[b] {hjb, snogales}@ilsb.tuwien.ac.at,
[c] {victor.oancea, ritwick.roy}@3ds.com,
[d] {andrea.rauh, juergen.lescheticky}@bmw.de

ABSTRACT

Due to the increasing usage of complex materials in lightweight design the development of proper material models for the prediction of damage and failure within Finite Element simulations has become an extensive task. Other fields of application already have shown that the introduction of Soft Computing and Machine Learning methods can be very beneficial for getting the complexity under control. The contribution aims at sketching a systematic approach to the application of machine learning methods in the field of material modelling. The focus is put not only on the definition of well performing mathematical models, but also on process aspects of generating and maintaining the mathematical models within reproducible, requirement-driven and controlled iterative environments for Computer Aided Engineering.

Keywords: material modelling, finite element simulation, soft computing, machine learning, artificial neural networks

1. INTRODUCTION

The Finite Element Method (FEM) is a well established technique in a wide range of disciplines, most successfully applied in mechanical engineering. In the automotive and aerospace industries the FEM is commonly used for structural design and development of new products. It enables modern lightweight designs and facilitates the development and usage of new and highly specialized materials (composites, advanced aluminium alloys, high strength steels, etc.) as well as joining technologies (spot welding, adhesive bonding, etc.).

The quality of FEM results depends strongly on the availability of appropriate material models that describe the nonlinear behaviour and failure of these materials. The development and identification of new material models has become an increasingly complex and expensive process, partly as a consequence of the conventional approach of using purely analytical, physically motivated mathematical models for predicting material behaviour. Other fields of application have shown, however, that example based approaches, such as Machine Learning and Pattern Recognition, may outperform conventional methods and significantly reduce the development effort (Bishop 2006). Furthermore, their superiority even increases with the complexity of the problem.

At present the application of Machine Learning and Soft Computing methods to material modelling in computational mechanics, see, e.g., Lefik and Schrefler (2003), Hashash, Jung and Ghaboussi (2004), Aquino and Brigham (2006), or Kessler, El-Gizawy and Smith (2007), is rather marginal. The research project *CoMModO (Complex Material Modelling Operations)*, which is funded by the Austrian Research Promotion Agency and the Austrian Federal Ministry of Transport, Innovation, and Technology under the initiative *"ModSim Computational Mathematics"* within the program *"Research, Innovation and Technology in Information Technology"*, is intended to overcome this deficit. The proposed solution strategy is the smart combination

- of Machine Learning as well as Soft Computing methods (example based modelling)
- plus the interpretation of experimental data in the framework of time-series classification and forecasting problems
- with an object-oriented design approach in order to develop a requirements-driven process,

for the modelling of material behaviour in FEM simulations.

The present paper aims at giving an overview of several points of attack where Soft Computing and Machine Learning techniques can be used for achieving improvements in the modelling of complex material behaviour to be applied in Finite Element Methods. A number of approaches to tackling this problem are summarised, which can be understood as escalating steps in a controlled process for developing and building material models. Although here applications to the modelling of weld spots are presented as examples for most of these steps, the basic CoMModO idea and methodology are applicable to other complex material types and joining technologies as well.

2. ESTIMATING THE KEY FEATURES OF MATERIAL BEHAVIOUR

When carrying out material tests one typically obtains a number of curves like the one shown in Figure 1, where the applied force is plotted against the displacements of a test specimen. In the first run we describe the curve via parameters that characterize its key features. In the case of Figure 1, these parameters could be the elastic stiffness, E, of the initial slope of the curve, the maximum force F_{max}, or some integral associated with energies, e.g., W_{max}. Such parameters may have a physical meaning and are often used as key parameters and coefficients in conventional analytical material models. Nevertheless, their prediction and estimation based on material specifications and load conditions can be challenging.

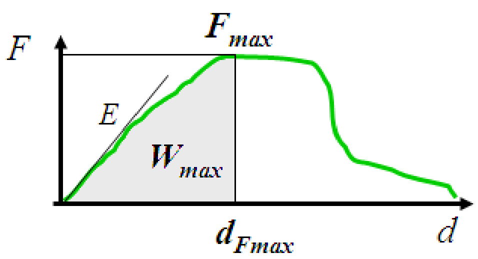

Figure 1: Generic force-displacement curve from a material test.

2.1. Description of Physical Parameters

In our first process step we use Machine Learning methods for the definition and construction of models that describe such physical parameters. Assuming that a suitable number of test results are available, the first step consists in evaluating the measurements extracted from them. This process step can also be seen as a first Data Mining session on all the material data of the given test set. This way one gains insight into the necessary parameters and material specifications that contribute to the problem, as to which material properties are important for the description of physical parameters of the material behaviour. This first step constitutes a method for describing the material behaviour, which works at least for materials that are not excessively complex.

An example of this can be seen in Figure 2, where the response of a model for estimating the maximum axial force sustained by weld spots under different loading conditions and for different combinations of sheet materials and sheet thicknesses is plotted against the values measured in a series of some hundred experiments. Each dot represents a test case. Blue dots indicate that the sample was used for training the Machine Learning model. Red and green dots denote test and validation samples, which were not seen by the model during the training and tuning phase and therefore can be used for validation to assess the generalization properties of the model.

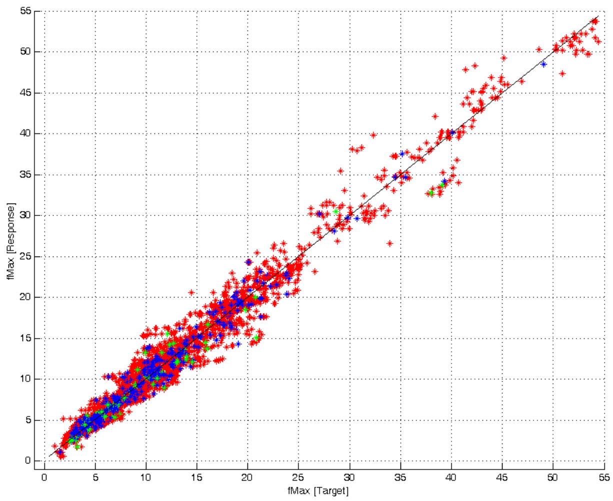

Figure 2: Estimates of maximum force sustained by a weld spot.

The resulting models can be employed for estimating the material parameters for various conditions and may be inserted accordingly into the Finite Element material description.

2.2. Process Scheme for Material Model Design

It is a very important point that the generation and maintenance of the prediction models are embedded into a proper process scheme.

Of course, the models cannot predict behaviour that has not been seen before and that is not represented by the test cases and the parameterisation in some way. However, the adaptation of the models to new data can be done very quickly if this behaviour is already described by the given or measured parameters. In case parameters are missing from the model one gets the confirmation that additional parameters are required. The process also automatically supports the identification of these parameters. In the case that some candidate parameters are available and measured in the data set, the identification of these parameters can be performed with the help of so called feature selection algorithms (Kittler 1986, Somol and Pudil 2000).

The flow chart shown in Figure 3 represents a standard procedure within Data Mining processes. The important issue is that it should be implemented as a standard procedure in material modelling as well.

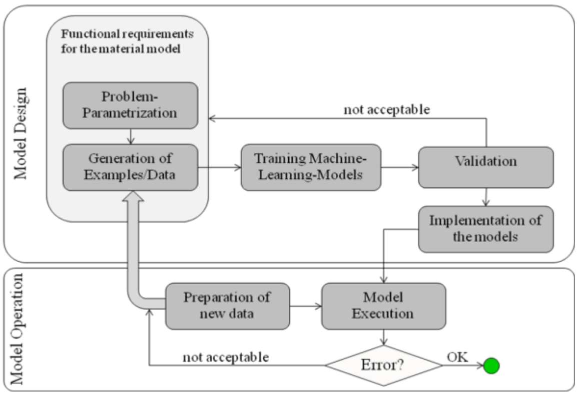

Figure 3: Machine Learning based process for material modelling.

When executing a series of material tests, one needs a good guess of the parameters required for the description of the desired behaviour to start with. These parameters then need to be measured and collected consistently during the material tests. It is important to support this procedure at a strategic level, so that the test data sets collected over time and different test runs and organizations can be put into one common context and database. Then Data Mining methods can be applied by generating Machine Learning models. The general Data Mining procedures (Witten and Frank 2005), with their accompanying validation processes, provide feedback about which parameters are relevant for describing and predicting the desired material behaviour. The methods give referable evidence whether the chosen parameters and test cases are sufficient or if new parameters are needed for a correct prediction of the material behaviour. Once the resulting models meet the performance goals, they can be implemented for daily use. When new material test data is available, the model predictions should be promptly evaluated and assessed. If the predictions do not match the experimental data, the models can be easily adapted by including the new data in further training of the prediction models. If the new data shows behaviour that cannot be described with the given parameterisation, the design process described above needs to be started from the beginning.

Among the major advantages of the Machine Learning based approach are its capabilities for preserving and reusing given knowledge. Also, it can be adapted to new experience much more quickly and efficiently than is generally possible with purely analytical approaches. If models are formulated analytically, it commonly happens that one has to begin from scratch if new data does not fit the existing model structure, so that the danger of running into extensive trial and error scenarios increases with the complexity of the problem.

2.3. Material Model Validation using Monte Carlo methods

The best prediction of the key parameters is of little use if the underlying material model is not sufficiently flexible for describing the behaviour of the material under study. If the estimated key material parameters are inserted into the material model, a validation of the model's performance still has to be carried out. If the performance goals are not met, further efforts are required.

In order to assess the flexibility of a given material model, a standard approach is to use Monte Carlo Simulation (Metropolis and Ulam 1949, Rubinstein and Kroese 2008). In such an analysis, material model parameters are scattered within suitable ranges to test if the material model is sufficiently flexible for covering the behaviour measured in a set of experiments. If this flexibility is found to be sufficient, the rest of the required material model parameters that were not estimated in the previous step can be identified by means of an optimisation process, for example an Evolutionary Algorithm (Bäck 1996) that seeks to minimise the deviation from the experimental measurements. The search space for this optimisation has been covered by the exploratory Monte Carlo Simulation carried out before, ensuring that this optimisation is able to achieve the required parameter identification.

An example of such an analysis is presented in Figure 4, which shows several performance parameters for the resulting Monte Carlo samples (black dots) and some results from material tests (red dots). The cloud of

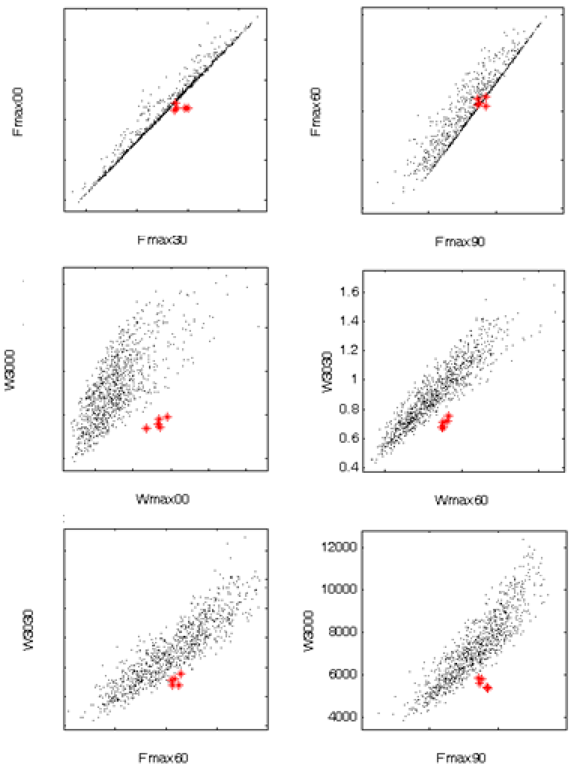

Figure 4: Validating a model by means of a Monte Carlo Simulation approach.

black dots identifies the region of parameter space that can be reached with a given analytical model. In the example shown, the analytical model lacks sufficient flexibility for concurrently reaching the material test results for several key parameters. It can be concluded that this analytical model is not capable of satisfactorily reproducing the targeted material behaviour.

3. EXAMPLE BASED DESCRIPTION

In the case of complex material behaviour, analytical approaches may reach their limitations in providing suitable descriptions or models, and example based approaches like Machine Learning may in principle be the better choice or at least a valuable complement. For example, the universal approximation properties shown by Artificial Neural Networks allow the reproduction of any given functional relationship (Hornik, Stinchcombe and White 1989), as long as a sufficient number of neurons are used in the hidden layer(s).

3.1. Interpretation as a Time-Series Problem

In order to extract the maximum information out of experimental data, the problem is formulated as a time series prediction. From this point of view, each one of the samples constituting, for example, an experimental force-displacement curve can be seen as a training example for the Machine Learning models.

This different view of the problem helps in overcoming the main counterargument used against Machine Learning models as well, namely that such approaches require excessive amounts of data and numbers of tests for proper models to be trained. This line of reasoning comes from the practical use and mindset of Design of Experiments approaches, where the main features of the results are already determined by the choice of the model's structure in the beginning. The test data are then only set up and used for fixing some coefficients of the predetermined assumption. When using analytical models, most aspects of their behaviour are already predetermined by the choice of ansatz functions.

With the interpretation as a time series problem the rate effects and path dependent behaviour become conceptually uncomplicated, too. Historic values, accumulated signal features or special filter values can be introduced as input parameters in an easy way. A further alternative is using recurrent Artificial Neural Networks for the incorporation of history dependent behaviour.

3.2. Example based description of weld spot behaviour

For the special case of modelling the behaviour of weld spots, the force-displacement curves obtained in some hundred experimental tests were used to train a neural network that models the responses of specimens that were obtained by spot welding sheets of different compositions and thicknesses and were subjected to different load cases. The quality of one of the resulting "global" models can be seen in Figure 5. There, the black lines are the measured results from the material tests, whereas the red lines and red and green crosses depict validation and test curve samples that were not used in the training process. Note that this figure shows only 20 out of about hundred similar curves with comparable performance, the generalization properties of the neural network being excellent in this case.

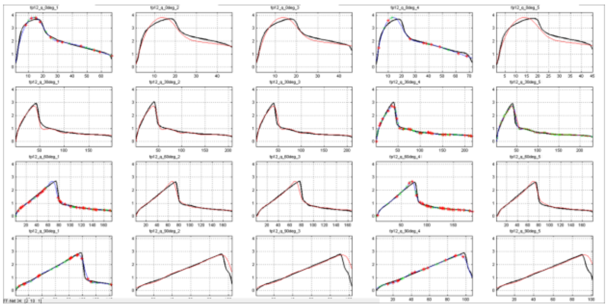

Figure 5: Example based training of a global model of a spot weld specimen.

Despite being very satisfactory, these results do not provide a solution to the problem of modelling the material behaviour of weld spots, because the load-displacement curves in Figure 5 pertain to whole specimens (and thus include the responses of the two sheets plus some influence of the testing apparatus) rather than to the weld spots.

3.3. Classification and Hybrid Modelling

Another way of benefiting from the advantages of Machine Learning approaches in the modelling of material behaviour can take the form of using them only for some components of an existing analytical model. For example, the indication of the presence of damage or the classification of the damage mode may be done via a time series classification model. Such a model may take as inputs strain and stress states, with some history values, and a number of additional material and load specifying parameters, to return values 1 or 0, indicating whether or not a given integration point shows damage. It is then up to the analytical model, into which the classification model is embedded, to make appropriate use of this information.

The advantage of this approach is the fact that normally classification problems are technically much easier to solve than regression problems. However, in practice the onset of damage is very difficult to detect in material tests. In addition, care must be taken of the issue that the measured curves incorporate the effects of damage, whereas damage classifiers require data that is free of damage.

Before going more deeply into the issues of example based models for weld spot behaviour, however, a short discussion of some general aspects of weld spot models for FE analysis will be presented in Section 4.

4. WELD SPOT MODELS

Finite Element models of weld spots fall into two groups. On the one hand, detailed models have been proposed, see, e.g., Lamouroux et al. (2007), which are outside the scope of the present discussion. On the other hand, "simplified" weld spot models have been developed explicitly for use in large scale analysis, such as crash simulations. Such models must combine computational efficiency, the capability of handling nonlinear behaviour with sufficient accuracy for general load paths, and features that facilitate automatic mesh generation. The latter issue leads to the demand of supporting the use of non-congruent meshes for the sheets to be joined by spot welding.

The present work is based on the Finite Element code ABAQUS/Explicit (SIMULIA, Providence, RI), which comes with a simplified weld spot model in the form of the FASTENER option. This combines connector elements, which allow modelling various types of nonlinear material behaviour including plasticity, damage and failure, with coupling constraints for consistently handling a mesh-independent connection to the sheets, which are modelled by shell elements. Material responses of weld spots are introduced in terms of forces and displacements, i.e., they do not describe a material behaviour in the strict sense, but rather a "structural behaviour" of the weld spot and the closely neighbouring regions of the sheets (for brevity, however, the expression "material behaviour" is used throughout the present work). The path dependences of plasticity and damaged behaviour are handled via status variables, damage indicators and damage evolution algorithms. The resulting, highly robust material descriptions are complex analytical models in the sense of Section 3, and their parameters must be identified from suitable experiments.

Such experiments involve testing to destruction standardized test specimens, such as the KS-II specimen (Hahn et al. 2000) shown in Figure 6, which consists of two U-shaped sheets that are joined, e.g., by a spot weld. When suitable fixtures are employed, a universal testing machine can be used to carry out tests for different load cases, such as normal, shear and mixed loading as well as peeling.

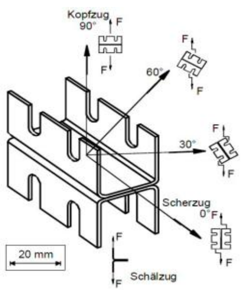

Figure 6: KS-II test specimen used for characterising weld spots.

The results of experiments of this type are global force-displacement curves that contain contributions from the weld spot, the test fixtures and the metal sheets, with the latter dominating the displacement responses in most cases. If the sheets are very stiff, such data can provide reasonable approximations to the behaviour of the weld spot proper. In general, however, these global force-displacement curves characterise the behaviour of the whole test setup rather than the local responses of the weld spot.

Therefore, the global results cannot be used directly for describing the material behaviour of any type of weld spot model. This also holds true for FE-based simplified weld spot models of the type discussed above, considerably complicating their practical use. In analogy, when a neural network is trained with the global force-displacement curves, as is the case for the approach introduced in Section 3.2 and the data shown in Figure 5, the resulting model in general does not represent the local behaviour of the weld spot and cannot be used in Finite Element models of the latter.

Some additional complications have to be kept in mind. On the one hand, radial loading at the global level (i.e., keeping constant the direction of the force acting on the specimen) does not necessarily imply locally radial loading of the weld spot due to geometrical effects of the deformation of the sheets. On the other hand, the weld spot model not only must be capable of describing the failure of the weld spot proper (e.g., "nugget fracture" or "nugget pullout") but also failure of the sheets in the immediate vicinity of the weld spot ("sheet tearing").

To overcome the issue of global vs. local behaviour, a solution in the form of introducing an indirect training procedure is proposed, which accounts for the differences between behaviour at the local (element) and the global (component) levels.

5. INDIRECT TRAINING OF A NEURAL WELD SPOT MODEL FOR RADIAL TENSILE LOADS WITHIN A FINITE ELEMENT SIMULATION

In order to account for the complex and nonlinear behaviour of weld spots, the local material description in the connector part of an ABAQUS FASTENER is to be modelled by a neural network. This neural network is to be trained with the only data available, the global load-displacement curves obtained from a series of experiments. Once trained, the neural network is expected to reproduce the behaviour encoded in these data.

As noted above, extracting the local behaviour of weld spots from measurements of the global responses lies at the root of a major complication in the use of simplified weld spot models. The most common expedient in such situations is to make recourse to involved calibration methods for finding suitable parameters for the weld spot model. In contrast, a systematic indirect training process applicable to weld spot models is proposed in the following, in which the material behaviour is described by neural networks. In this process the neural network model for the weld spots' material behaviour is embedded in a Finite Element simulation during training and thus contributes to predicting the global behaviour of the whole component of which the spot weld is a part. Comparing the results of a given simulation with the experimental data obviously allows assessing the performance of the full model. Because the local behaviour of the weld spot, described by the neural network, is the only variable part of the global model of the sample, the latter's performance allows drawing conclusions on the performance of the local model. On this basis, in turn, the weights and biases of the neural network can be updated, i.e., training can be carried out.

In a first step, discussed in the following, the use of the neural network model is restricted to globally radial and monotonic load cases, so that issues of the path dependence of plasticity and damaged behaviour are of little relevance. The extension of the approach to non-radial and non-monotonous load paths is ongoing work.

Even though this problem may sound very specific to weld spots and their test configurations, the problem pattern is generic and occurs in many types of material tests, namely that the material behaviour cannot be measured directly at the same level of interface as, required for the Finite Element formulation. Once we find a method for training Machine Learning models not for their direct output but for the effect of their output at a higher level of abstraction (such as the behaviour of the whole test configuration), the problem is formulated in a way that any type of test can be used to train the models. For the special case of weld spots this may imply testing not only specimens with a single weld spot but also test structures containing several ones, so that a sufficient variety of load paths can be sampled

5.1. Integration into the Finite Element Simulation as User-Defined Element

As mentioned above, in ABAQUS/Explicit the standard tool for modelling weld spots is the FASTENER option, within which the proper place for integrating new material descriptions – including models based on neural networks – are the connector elements. At present, however, ABAQUS/Explicit does not provide a user subroutine interface for specifying the mechanical behaviour of connectors, so a workaround had to be used. This took the form of combining kinematics appropriate for weld spots, as defined by SIMULIA's BUSHING connector type, with a user defined element (VUEL) having two nodes with three translational and three rotational degrees of freedom each. The neural network was integrated as a code sequence within this VUEL. To complete the FASTENER surrogate, the weights of the coupling constraints to the shells are required, which can be extracted from the output of an analysis employing a standard FASTENER. Bushing kinematics was provided by SIMULIA as linked functions.

The task of the neural network implemented within the user defined element consists in returning a set of suitable generalized force increments for any set of increments of the generalized displacements passed in from the Finite Element code. Here, both force and displacement vectors are given in the connector's local coordinate system. Because an explicit time integration scheme was chosen, there is no need for providing Jacobians.

Within this framework, the weights and biases of the neural network can either be specified as parameters within the user defined element or they can be provided via the ABAQUS input file. Both of these options fully support dynamic updating in the course of training of the neural network.

5.2. Assessment of Model Performance

For the task at hand the performance of a given neural network model is assessed by comparing the force-displacement curve measured in a suitable experiment with the one predicted by a model of the whole sample which incorporates the VUEL containing the neural network. The task of the performance assessment function is to formalise the computation of such a performance, i.e., to provide an algorithm for computing a performance value that correlates with how well the simulated material behaviour used for the weld spot allows matching the experimental measurements.

Performance is assessed by combining several criteria, each one focusing on a specific aspect of the general performance. The assessment criteria used are the following:

- Difference between experimental and simulated force-displacement curves using a *mean squared error (MSE)*, evaluated at discrete points chosen with consideration of the shape of the curve.
- Agreement in terms of maximum force: The simulation should predict a similar value for the maximum force as the one measured in the experiment.
- Agreement in terms of displacement at maximum force: The simulation should achieve the maximum force at a similar value of total displacement as measured in the experiment.
- Agreement in terms of displacement at failure: The simulation should predict a similar value for the displacement at total failure of the weld spot as the one measured in the experiment.
- Characteristics of the local curve can be taken into account as well, for example maximum force reached, convexity, etc.

For each one of these assessment criteria, an error value normalised to the interval [0, 1] is generated, with 0 denoting the most desirable outcome, i.e. corresponding to the best performing model. Then a single scalar error measure is obtained from these normalised errors by means of a weighted average. This allows for a dynamic adjustment of the relative importance of some of the assessment criteria with respect to others.

Once a performance assessment function has been defined, it can be used as objective function for an optimisation process that considers the weights and biases of the neural network as optimisation variables and seeks to minimize the error value. This optimisation constitutes, indeed, the training of the neural network.

5.3. Indirect Training of the Neural Material Model

In general, the training of a neural network can be understood as the solution of an optimisation problem in which values of weights and biases are sought, which minimize the network error obtained by comparison of the network's response and the available targets. By minimizing the network error through this optimisation, the neural network is trained to reproduce the behaviour represented by the target data.

The same interpretation can be applied when the network's response cannot be directly compared to the available target values. In such cases, the definition of a suitable performance assessment function that is able to map the local (element) network responses into global (component) curves comparable to the targets turns out to be the key to make this kind of training feasible.

The performance function requires an additional step to map the local network responses to global curves that are comparable to the targets, hence the name "indirect training" for this kind of process. In the case of the neural connector model, the Finite Element simulation of the whole specimen is part of the performance assessment function, as shown in Figure 7.

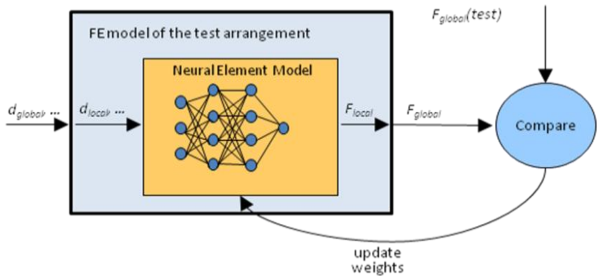

Figure 7: Schematic indirect training process.

In order to solve a generic optimisation problem, two steps must be performed:

1. *Initialisation*: Find one or more suitable initial points to start the optimisation from.
2. *Optimisation*: Apply an optimisation algorithm to find a point that minimises or maximises the objective function, starting from the given initial point(s).

In most applications, the initialisation step turns out to be at least as important as (and sometimes even more challenging than) the optimisation step itself in order to find an optimum of the objective function.

The heuristics used to initialise the neural network weights and biases comprised a pure random weight initialisation and the neural network specific *Nguyen-Widrow rule* (Nguyen and Widrow 1990), which takes into account network topology and ranges of inputs in providing initial values for the network weights and biases.

Depending on how many optima a given algorithm is designed to find, local and global optimisation methods can be distinguished. A *local optimisation* algorithm is able to find the local optimum closest to the current initial point. Other local optima, potentially better, cannot be found by a local optimisation algorithm. If a single optimum is known to exist, for example in the case of a convex objective function, a local optimisation algorithm may find the (unique) global optimum. For this reason, local optimisation is sometimes called *convex optimisation*. On the other hand, a *global optimisation* algorithm is designed to find several local optima and, from them, return the global optimum. These algorithms are often based on a population of quasi-independent agents that search for the global optimum, taking advantage of swarm intelligence based approaches.

As to the optimisation methods used for indirect training, the *Nelder-Mead simplex* algorithm (Lagarias, Reed, Wright and Wright 1998) was used for local optimisation, because it is a derivative-free method that does not require numerical estimates of the gradient of the objective function, which in the present indirect training setting includes the whole Finite Element simulation of the specimen. For global optimisation tasks *genetic algorithms* (Goldberg 1989) and *evolution strategies* (Bäck 1996) were used, all of which are derivative-free as well.

5.4. Software Framework for Indirect Training

For the sake of flexible testing of many different combinations of optimisation algorithms and initialisation heuristics, a generic optimisation software framework was devised that allows a very flexible replacement of the different modules thanks to its modular architecture.

In this software framework, *problems* and *solvers* are distinguished and kept independent from one another. A *problem* comprises a description of the search space (dimension, variable ranges, etc.) and an implementation of the objective function. A *solver* comprises an implementation of an initialisation strategy and an implementation of an optimisation algorithm. Applying a given solver to a given problem returns a solution, i.e., the optimum found by the solver starting from the specified initialisation of the objective function described in the problem.

For the indirect training of neural networks to be used as material models of a user-defined element within a Finite Element simulation of a spot weld specimen, the objective function was obtained by the following steps:

1. Set the current values of weights and biases in the neural network based user-defined element.
2. Perform a Finite Element simulation of the specimen using this parameterization of the user-defined element.
3. Compare the force-displacement curves obtained from this simulation with the

corresponding experimental measurements by means of the performance assessment function discussed above.

4. Return a value for the objective function based on the performance assessment function.

This software framework has been implemented using MATLAB (MathWorks Inc., Natick, MA), so that the existing and readily available MATLAB implementations of several optimisation algorithms (*Optimization Toolbox*, *Global Optimization Toolbox*) and initialisation heuristics for neural networks (*Neural Network Toolbox*) can be used.

5.5. Results from Indirect Training

In order to provide a proof of concept, an indirect training setup as presented above was tested against a synthetic problem for which both local and global load-displacement responses are known. The global behaviour for this test case was obtained by a Finite Element simulation, in which the local force-displacement behaviour was described by the standard ABAQUS FASTENER model for weld spots. This global force-displacement curve was then used as target for the indirect training of a neural material model.

Selected results of the indirect training process can be seen in Figure 8 andFigure **9**, where two different optimisation algorithms were used together with the Nguyen-Widrow weight initialisation rule. For both cases a feed-forward neural network topology with 5 neurons in the hidden layer was employed. As the plots show, such an indirect training setup can give rise to valid models of the responses of both weld spot and specimen. As shown by the examples this approach is well able to cover the gap between local and global behaviour in the case of a weld spot model.

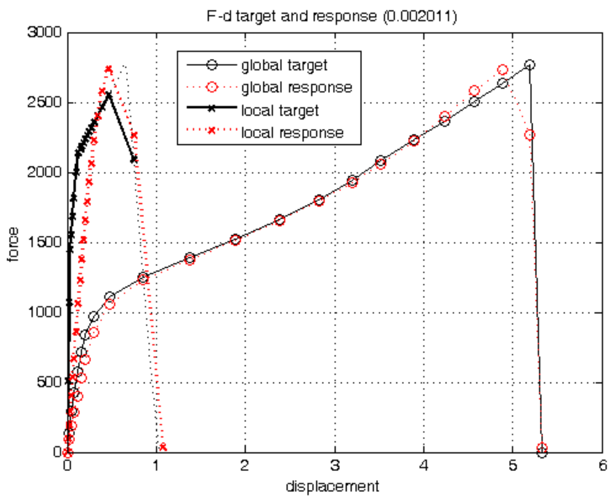

Figure 8: Global and local responses of a synthetic weld spot obtained by training with the Nelder-Mead simplex algorithm.

In general, local optimisation methods, such as the Nelder-Mead simplex algorithm, tend to reach slightly better solutions as long as the initialisation already shows an acceptable performance. Global optimisation methods, such as Evolution Strategies, may perform marginally worse, but in general show a higher probability of finding an acceptable solution, being less dependent on the quality of the initialisation.

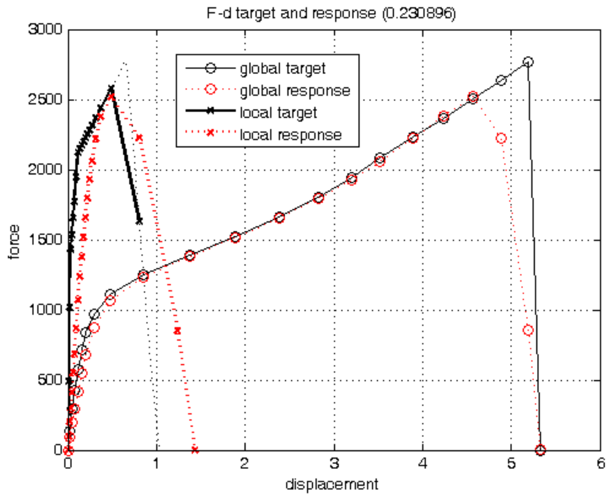

Figure 9: Global and local responses of a synthetic weld spot obtained by training with an Evolution Strategies algorithm.

When a model describing an actual weld spot, or any other kind of complex material or joint, is to be developed using this approach, the actual targets for the training process must, of course, be measurements obtained from appropriate experiments.

6. SUMMARY

The contribution discussed several approaches to using Machine Learning methods for material modelling within Finite Element simulation. A controlled process is sketched that ranges from the estimation and prediction of key feature parameters via descriptions of specimen behaviour at a global level to the use of Artificial Neural Networks for the direct description of material behaviour at the element level, escalating the use of Machine Learning models in dependence on the complexity of the material behaviour to be modelled.

For the example of weld spots a neural element model could be trained by introducing a scheme of indirect training. This approach allows evaluating the performance of the Machine Learning model at a higher abstraction level of the system, e.g., by using measurements involving the full test configuration. As a first step, the feasibility and prospective advantages of the approach were demonstrated for monotonous, globally radial loading. The generalization to arbitrary loads was under development at the time of writing the paper.

7. VISION AND OUTLOOK

The last major open issue in the presented approach is the extension to arbitrary loading conditions and histories. Once this is achieved, the method can be extended and applied to any kind of material behaviour, e.g., to the failure of CFRP and other composite structures, adhesives, etc,

This new approach requires changing the way of developing and carrying out material tests, which will have to represent operationally relevent loading conditions rather than test cases defined explicitly for identifying some specific material parameters. This is expected to allow avoiding the complexity trap of an exponential increase of development effort with increasing complexity of the target behaviour, which tends to bedevil analytical models. The interim results reported here support the assessment that this goal can, in fact, be reached.

ACKNOWLEDGMENTS

The paper presents interim results obtained within the research project *CoMModO (Complex Material Modelling Operations)*, which is funded and supported by the Austrian Research Promotion Agency and the Austrian Federal Ministry of Transport, Innovation, and Technology under the initiative *"ModSim Computational Mathematics"* within the program *"Research, Innovation and Technology in Information Technology"*.

The research work has benefited greatly from the unconditional support of the crash simulation department of BMW, Munich, Germany. This paper is also dedicated to the memory of Dr. Heinrich Werner, whose strategic foresight contributed considerably to the initiation and mentoring of the project. Unfortunately he is no longer with us to see and discuss the results.

REFERENCES

Aquino, W., Brigham, J.C., 2006. Self-learning finite elements for inverse estimation of thermal constitutive models. *International Journal of Heat and Mass Transfer* 49, 2466–2478.

Bäck, T., 1996. *Evolutionary Algorithms in Theory and Practice*. New York: Oxford University Press.

Bishop, C.M., 2006. *Pattern Recognition and Machine Learning*. New York: Springer.

Goldberg, D.E., 1989. *Genetic Algorithms in Search, Optimization & Machine Learning*. Reading, MA: Addison-Wesley.

Hahn, O., Besserdich, G., Dölle, N., Jendrny, J., Koyro, M., Meschut, G., Thesing, T., 2000. Prüfung und Berechnung geklebter Blech-Profil-Verbindungen aus Aluminium. *Schweissen & Schneiden*, 52, 266–271.

Hashash, Y.M.A., Jung, S., Ghaboussi, J., 2004. Numerical implementation of a neural network based material model in finite element analysis. *International Journal for Numerical Methods in Engineering*, 59, 989–1005.

Hornik, K., Stinchcombe, M., White, H., 1989. Multilayer feedforward networks are universal approximators. *Neural networks*, 2 (5), 359–366.

Kessler, B.S., El-Gizawy, A.S., Smith, D.E., 2007. Incorporating neural network material models within finite element analysis for rheological behavior prediction. *Journal of .Pressure Vessel Technology*, 129, 58–65.

Kittler, J., 1986. Feature selection and extraction. In: Young, C.M., Fu, K.S., eds. *Handbook of pattern recognition and image processing*. New York: Academic Press, 60–81.

Lagarias, J.C., Reeds, M.H., Wright, M.H. and Wright, P.E., 1998. Convergence properties of the Nelder-Mead simplex method in low dimensions. *SIAM Journal of Optimization*, 9 (1), 112–147.

Lamouroux, E.H.J., Coutellier, D., Dölle, N., Kümmerlen, D., 2007. Detailed model of spot welded joints to simulate the failure of car assemblies. *International Journal on Interactive Design and Manufacturing* 1, 33–40.

Lefik, M., Schrefler, B.A., 2003. Artificial neural network as an incremental non-linear constitutive model for a finite element code. *Computer Methods in Applied Mechanics and Engineering*, 192, 3265–3283.

Metropolis, M., Ulam, S., 1949. The Monte Carlo method. *Journal of the American Statistical Association*, 44 (247), 335–341.

Nguyen, D., Widrow, B., 1990. Improving the learning speed of 2-layer neural networks by choosing initial values of the adaptive weights. *Proceedings of the International Joint Conference on Neural Networks*, 3, pp. 21-26. June 17–21, San Diego, CA.

Rubinstein, R.Y., Kroese, D.P., 2008. *Simulation and the Monte Carlo Method*. Hoboken, NJ: John Wiley & Sons.

Somol, P., Pudil, P., 2000. Oscillating search algorithms for feature selection. *Proceedings of the 15th International Conference on Pattern Recognition*, pp. 406–409. September 3–8, Barcelona (Spain).

Wegner, S., Hooputra, H., Zhou, F, 2006, Modeling of Self-Piercing Rivets Using Fasteners in Crash Analysis, *Proceedings of the 2006 ABAQUS Users' Conference*, pp. 511-526. May 23-25, Cambridge, MA, USA.

Witten, I.H., Frank, E., 2005. *Data Mining*. San Francisco, CA: Morgan Kaufmann Publishers.

AUTHORS' BIOGRAPHIES

Andreas Kuhn holds master's degrees in Technical Mathematics and Mechanical Engineering from Vienna University of Technology, where he also obtained his Ph.D. for work on the application of numerical simulation techniques to issues of satellite dynamics. After several years of experience in Computer Aided Engineering in the German automotive industry he founded the company ANDATA in 2004, where he currently holds the position of CTO. He is specialized in the application of Computational Intelligence and stochastic simulation techniques to the development and safeguarding of complex technical systems.

Toni Palau obtained his master's degree in Applied Mathematics at the Technical University of Catalonia (UPC-Barcelona Tech), Spain, and has occupied diverse technology related positions, covering the topics of Computer Vision, High Performance Computing and Parallelism, Optimisation, Monte Carlo Simulation, Machine Learning, Data Mining, Computational Intelligence and Finite Element Simulation. At present he works as a research engineer at ANDATA.

Gerolf Schlager studied Technical Physics at Vienna University of Technology. He was a doctoral student at the European Organization for Nuclear Research (CERN) in Geneva for more than four years and received his Ph.D. for his studies of the energy calibration of the ATLAS calorimeter system. At CERN he was introduced to stochastic simulation of particle collisions and the associated data mining techniques. Since 2007 he has been one of the principal research engineers at ANDATA on the topic of material modelling with Soft Computing approaches.

Helmut J. Böhm holds master's degrees in physics from Johannes-Kepler University in Linz, Austria, and Rutgers University, New Brunswick, NJ. He obtained his doctoral degree in Mechanical Engineering and his habilitation in Micromechanics of Materials at Vienna University of Technology, Austria, where he headed the Christian Doppler Laboratory for Functionally Oriented Materials Design from 1998 to 2004. At present he is associate professor at the Institute of Lightweight Design and Structural Biomechanics of Vienna University of Technology.

Sergio Nogales holds bachelor and master's degrees in Aeronautical and Materials Engineering from Technical University of Madrid (UPM), Spain. He obtained his doctoral degree at Vienna University of Technology, Austria. At present he is a post-doctoral researcher at the Institute of Lightweight Design and Structural Biomechanics of Vienna University of Technology.

Victor Oancea and **Ritwick Roy** both hold Ph.D. degrees and are Principal Development Engineers in the ABAQUS/Explicit development group at SIMULIA.

Andrea Rauh graduated in Mechanical Engineering from TU München, Munich, Germany. She joined BMW in 2009 and is currently working in the field of CAE method development for crash simulation with the focus on composite structures and joining technologies.

Jürgen Lescheticky studied Aerospace Engineering at the University of Stuttgart, Germany. After nine years of working as an engineering consultant, he joined BMW in 1995 as a project engineer for crash simulation. Since 1999, he has been head of the crash simulation department with the main responsibility for CAE method development.