Abstract  The identification of the proper parameters of material models plays a crucial role in the design of production technologies, especially in the case of modern materials with diversified properties under different boundary conditions. The procedure of identification is usually based on an optimization algorithm that uses sophisticated numerical simulations as a part of the goal function and compares the obtained results with experimental tests. Despite its reliability, such an approach is numerically inefficient. This paper presents the concept of how to replace the most numerically-demanding part of the identification procedure with metamodels, allowing us to maintain uniform result quality. The computer system, which allows us to manage input data, metamodels, and calculations, is proposed and described in detail in this paper. Finally, the proposed approach is validated on the basis of tests performed in the laboratory.

Keywords  Inverse analysis, identification of model parameters, computer system, rings compression

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1. Introduction

When manufacturing metallic products, modern heavy industry requires fast numerical simulations based on reliable data that supports the design of new production technologies. However, the acquisition of proper input data for numerical simulations is very time consuming. This process includes the following steps:

- performance of laboratory tests based on a standardized material sample under different conditions (various temperatures and/or strain rates),
- parsing and analyzing the data gathered, which is usually available as a multi-element set of text files,
- preparation of a numerical test (virtual experiment) representing a real laboratory test with the same geometry of tools and samples as well as the same boundary conditions,
- selection of a material model that will be identified during calculations,
- performance of inverse analysis based on a selected optimization procedure aimed at determining the most-suitable parameters of the material model.

Nevertheless, multi-iterative optimization joined with numerical simulations of experiments is very time consuming, which is unacceptable to the industry. Poor efficiency of computational procedures can be improved by the parallelization of particular methods or by the application of High Performance Computing (HPC) architectures to distribute calculations. These methods work efficiently only when calculations without barriers can be applied to obtain optimal parallelization. Such an approach improves the computational efficiency of inverse analysis; however, the time required for calculations is still unsatisfactory. In this paper, we propose replacing computationally-inefficient numerical simulations with less-sophisticated metamodels based on Artificial Neural Network (ANN), Kriging, or Response Surface methods. Then, the overall computing cost will be related to the configuration of metamodel background methods; e.g., training of ANN, which is performed only once to create a reliable metamodel. Such a solution allows us to maintain a high quality of obtained results and significantly reduce computing time. A hybrid computer system supporting metamodel creation and its application in inverse analysis is the main subject of this work. The first part of the paper is devoted to a definition and short review of different hybrid computer systems [18], which is followed by a description of the inverse analysis idea as well as a presentation of material models and metamodels. These approaches are combined in the form of one computer system. Design and implementation details of this system are described in the fourth section of the paper. Finally, the results of our case studies are presented.

2. Hybrid systems

Hybrid computer systems are usually defined as software covering more than one different functionality; e.g., optimization, numerical simulation, or an embedded expert
system. Such hybrid systems supporting Design of Experiments (DOE), data analysis, or the design of production planning systems (PPS) that play an important role in the industry. These systems manage supply chains, optimize the work of employees, maximize incomes, or plan the use of space in warehouses. Commercial versions of such systems were developed in the early 1990s and were based on task schedulers or management of Gantt charts [11]. This simple functionality was being constantly developed by the implementation of the following ideas [1]: mass production, flexible manufacturing, computer integrated manufacturing, lean manufacturing, and material resource planning (MRP). These steps were necessary to achieve the milestone in the lifecycle of planning systems; i.e., from MRP (mentioned earlier) to Enterprise Resource Planning (ERP) conversion. Further evolution of the functionality of PPS systems focused on the implementation of methods supporting concurrent engineering and, finally, to increase the agility of manufacturing. The latter systems were created to manage production processes held in unstable environments and to satisfy individual fast-changing customer needs. Following the development of PPS, systems were modified and extended by including algorithms based on artificial intelligence and soft computing in an effort to create the so-called Intelligent Manufacturing Systems (IMS). One of the first examples, proposed by Giachetti [4], was based on a formal multi-attribute decision model and relational database. The created system was helpful in the selection of materials and manufacturing processes. Nowadays, such approaches often use expert systems [10] or knowledge bases [5]. The former proposed a framework to create a customized rule-based system that utilize a semantic net and edges between its nodes. The computation of semantic hulls allows us to obtain solutions and to determine optimal decisions. Halevi and Wang suggest creating a knowledge-based "road-map", which facilitates decision making in production planning by introducing flexibility and dynamics to the manufacturing process.

Several hybrid systems were already designed and implemented by the authors of this paper. Many of the systems were based on similar software architecture; however, their final functionality differed slightly from each other. The first attempt to create a hybrid system dedicated to support the design of production technologies was proposed in [20]. The system was dedicated to specific processes of the manufacturing of fasteners; e.g., screws, bolts, or anchors. This concept of hybrid system was further developed and adapted for the needs of flat rolling processes. A series of papers have been published in this area. The first system was proposed for the ArcelorMittal company [19] for a new hot-rolling mill in Krakow. This system was further extended with functionality that allowed for the design of production processes in a collaborative environment [16]. Another hybrid system for flat rolling was dedicated to the pilot-rolling mill that LPS described in [3]. Since the prediction of the properties of products is essential to the effectiveness of such systems, advanced modelling methods based on either internal variables or discrete techniques were applied. The selection of the relevant method and presentation of the details of modelling were particular objectives of the previous research. The functionality of system modules
and the results of the calculations were presented in [17]. Both systems were equipped with knowledge bases and a reasoning module, which allowed for the application of case-based reasoning on real industrial data. Additionally, the hybrid systems were extended with functional modules dedicated to modern steels and alloys. The case of DP steel was analyzed in [9], while multiphase steels were the main subject in [15]. Finally, the generic hybrid system ManuOpti was proposed in [21], which covers the flexible design of various industrial processes by using external software for numerical simulations and internal modules for optimization and sensitivity analysis. The ManuOpti system also works with e-infrastructures such as HPC architectures, realized by communication with the Scalarm system [6].

3. Inverse analysis

3.1. Basic idea

Inverse analysis is applied in numerical simulations to determine the most accurate parameters of material models. Details of the inverse algorithm developed by Szeliga et al. were presented in [24]. It is based on an optimization loop, where experimental data gathered from laboratory tests is compared to the results obtained in the numerical approach. The optimal coefficients in the model are determined by searching for a minimum objective function, which is defined as the Euclid norm between measured and predicted loads in the experiment:

$$\Phi = \left[ \frac{1}{Npt} \sum_{i=1}^{Npt} \left[ \frac{1}{Nps} \sum_{j=1}^{Nps} \frac{F_{cij}(x,P_i) - F_{mij}}{F_{mij}} \right] \right]^{1/2}$$

(1)

where: $F_{mji}$, $F_{cji} –$ measured and calculated loads, $Nps –$ number of stands, $Npt –$ number of tests, $p –$ vector of process parameters (strain rates, temperatures), $x = \{A,n,q,m,B\} –$ vector of coefficients in the flow stress model.

To maintain a high reliability in the identification process, the numerical approach has to reflect laboratory test in detail. In the inverse-analysis simulation of the laboratory test is often called the formulation of a direct problem. The direct-problem model is usually based on the thermal-mechanical finite element method [17,18], which is computationally costly and very time-consuming. The approach presented in this paper assumes replacing the finite element method with a metamodel based on one of the artificial intelligence methods. The material models analyzed by the system as well as the concept of metamodels are presented in the next sections.

3.2. Material models

The approach developed in this work can be applied to various materials and various material models. However, this paper is focused on models that are used in the simulation of processing metallic materials. These models and the experimental tests performed for their identification are listed in Table 1.
The models, which can be identified using the developed system, are described briefly below, and a reference is made to the relevant publications where detailed descriptions of these models can be found. The models were identified for DP600 steel containing 0.071%C, 1.45%Mn, 0.25%Si, 0.55%Cr, 0.03%Mo, 0.005%V, 0.002%Ti, 0.01%P, and 0.006%S.

### 3.2.1. Rheological models

Material rheological models of various complexities of formulation were considered. Models with external variables (temperature, strain, and strain rate) used as independent variables were the simplest ones (4 coefficients – top curve in Figure 1). Models accounting additionally for softening due to recrystallization (5 coefficients – central curve in Figure 1) and for softening and saturation (7 coefficients – bottom curve in Figure 1) were also investigated. Reviews of these models can be found in [14]. Typical responses of these models are shown in Figure 1.

![Figure 1](image-url). Rheological models as dependency between flow stress and strain.
A model with internal variable (dislocation density) and time used as independent variables [12] was considered as well. In this model, the evolution of dislocation populations is described by the differential equation:

\[
\frac{d\rho(t)}{dt} = \frac{\dot{\varepsilon}}{bl} - k_2\dot{\varepsilon}\rho(t) - \frac{3\mu b^2 k_3}{2D}\rho(t)^{\alpha_s} R[\rho(t) - \rho_{cr}]
\]  

(2)

where: \(\dot{\varepsilon}\) – strain rate, \(b\) – length of the Burgers vector, \(\rho\) – dislocation density, \(l\) – average free path for dislocations, \(\mu\) – shear modulus, \(k_2, k_3\) – recovery coefficient and grain boundary mobility, respectively, \(\rho_{cr}\) – critical dislocation density for dynamic recrystallization (DRX), calculated as a function of the Zener-Hollomon parameter \(Z\), \(D\) – grain size, \(t\) – time. Function \(R\) in equation (5) is:

\[
R[\rho(t) - \rho_{cr}] = 0 \quad \text{for} \quad \rho \leq \rho_{cr}
\]

\[
R[\rho(t) - \rho_{cr}] = \rho(t - t_{cr}) \quad \text{for} \quad \rho > \rho_{cr}
\]

where: \(t_{cr}\) – time to the beginning of DRX.

The Zener-Hollomon parameter is defined as:

\[
Z = \dot{\varepsilon} \exp \left( \frac{Q_{DEF}}{RT} \right)
\]

(3)

where: \(Q_{DEF}\) – activation energy for deformation, \(R\) – gas constant, \(T\) – temperature in K.

Flow stress in the internal variable model is calculated in the following equation:

\[
\sigma = \sigma_0 + \alpha b \mu \sqrt{\rho_{av}}
\]

(4)

where: \(\mu\) – coefficient, \(\rho_{av}\) – average dislocation density, \(\sigma_0\) – initial stress accounting for the elastic deformation.

3.2.2. Microstructure evolution models

Microstructure evolution models describe the kinetics of recrystallization, grain size after recrystallization, and grain growth during interpass between subsequent deformation. The kinetics of recrystallization is described by the model known as JMAK (from the names Johnson, Mehl, Avrami, and Kolmogorov). In this model, the volume fraction of a new phase is:

\[
X = 1 - \exp(-kt^n)
\]

(5)

where: \(X\) – volume fraction of a new phase, \(k, n\) – coefficient.

Adaptation of this model to the case of recrystallization was made by Sellars [23], who proposed the following equation:

\[
X = 1 - \exp \left[ \ln(0.5) \left( \frac{t}{t_{0.5}} \right)^n \right]
\]

(6)
where: \( t_{0.5} \) – time for 50% of recrystallization.

A full description of the microstructure-evolution model used in the present work can be found in [8]. Results of the identification of that model for steel DP600 investigated in this work are given in that paper as well.

### 3.2.3. Phase transformation models

Phase transformation models describing kinetics of ferritic, pearlitic, bainitic, and martensitic transformations in steels (up to 23 coefficients) were considered in the system as well. These models are also based on the JMAK equation (8); however, coefficient \( k \) is introduced as a function of temperature. A detailed description of this model for all transformations is given in [13]. Results of the identification of the phase transformation model for steel DP600 investigated in this work are given in [8].

### 3.2.4. Fracture criteria

In the modeling of material processing or calculation of material-related parameters, the finite element method [28] or alternative methods are used. The continuum of the material is the main assumption in this approach. The modeling of fracture in material processing is generally based on the fracture criteria [2], which predict the moment of fracture by integration with respect to strain of a term dependent on the ratio between the first invariant of the stress tensor and flow stress. These criteria are implemented in finite element (FE) codes and currently use local values of strains and stresses as independent variables. More-advanced models of fracture based on CAFE (Cellular Automata – Finite Elements) or xFEM are not discussed in this paper. These methods have extensive predictive capabilities, but they require long computing times. This limits their application in practical industrial simulation.

The fracture criteria are easy in application; however, on the other hand, their accuracy depends strongly on the accuracy of the evaluation of the critical value of parameter \( C \), which determines the moment of fracture. Evaluation of this parameter is difficult, and this is the reason why obtaining realistic results that quantitatively agree with experimental data is a challenge. In the present paper, the relation of the fracture criterion on process parameters (temperature, strain rate), proposed in [27], was introduced. The fundamental fracture criterion was upgraded to the following form:

\[
\int_0^{\varepsilon_f} F(\sigma_i, \sigma_m, \sigma_{11}, \dot{\varepsilon}, T) d\varepsilon \geq C
\]

where: \( \sigma_i, \sigma_m \) – effective and average stress, respectively, \( \sigma_{11} \) – maximum principal stress.

The identification of the fracture criterion (7) was performed in two steps. In the first step, function \( F \) was selected. Special software that evaluates the sensitivity of various functions from a certain class of functions with respect to the variables was developed, as described in [27]. The function with the highest sensitivity with respect to the variables was selected, and coefficients in this function were determined by
the computer system using SICO (Strain Induced Crack Opening) test results as an input. A description of the SICO test is given in [7].

3.3. Metamodels

The general idea of metamodelling relates to the postulate that a metamodel approximates the model of a considered process. A metamodel must correctly correspond to the model, and the metamodel output value has to be evaluated with a radically-lower computing time than when using the original model. Thus, metamodelling is the process of constructing an approximation of the analyzed model on the bases of different techniques. In other words, a metamodel is a model of the model. The accuracy of a metamodel is usually verified by the use of statistical methods. This accuracy of a metamodel depends on the metamodelling technique used as well as the number of samples generated by the model. Usually, the higher number of samples provides better metamodel accuracy. Among many artificial intelligence methods, the artificial neural network (ANN) is the most-commonly-used metamodelling technique. Examples of successful applications of artificial neural networks in metamodelling can be found in [28, 29]. The approach of applying a metamodel to solve an optimization task in the inverse analysis of plastometric tests was proposed in [26].

The most important issue in using metamodels is the possibility to achieve high efficiency. As mentioned in the introduction of this paper, computational cost is incurred only once during metamodel calibration, which is usually related to multi-iterative training or calibration of the procedure. The metamodels based on ANN are prepared by using data obtained from parameterized numerical simulations. This process can be performed inside the proposed system or with the use of external software. Finally, configured networks have to be described by using Predictive Model Markup Language (PMML). The system allows for the development of the metamodel for any of the models described in section 3.2 and for any of the tests listed in Table 1.

An example of this technique is presented in Listing 1. This metamodel was trained by using Multi-Layer Perceptron (MLP) with 8-16-5-1 architecture for the Handsel-Spittel model [equation (3) in Figure 1] with five parameters and for the ring compression test (see the case study in Chapter 5). Eight input parameters include five model parameters, temperature, strain, and strain rate. The output parameter is stress. The whole listing also contains other important description fields; e.g., header information, dictionary, transformation, biases, and weights. Due to the applied standard, the exchange of data describing metamodels is facilitated.

Listing 1. The example of neural network described in PMML.

```xml
<?xml version="1.0" encoding="UTF-8"?>
<PMML version="4.1" xmlns="http://www.dmg.org/PMML-4_1">
...  
</PMML>
```

1http://www.dmg.org/v4-1/GeneralStructure.html
4. Computer system

The system was designed as stand-alone application dedicated to the MS Windows OS with the possibility of local or remote database connection. A list of the most important modules in the system is presented in Figure 2, containing the following elements:

- **UI.Main** – the main project responsible for integration of all other modules together. It contains the startup manager, which allows us to execute the system and initialize crucial components.

- **Common.Core** – is the basic module in the whole hierarchy. It includes definitions of unified data types and classes, which are imported in other modules.

- **Common.MVC** – defines the abstract logic of all views inside the graphical user interface and manages the Model-View-Controller (MVC) pattern. The pattern is based on adapted idea of Model View ViewModel (MVVM) supported by MS. It is adapted to the specific needs of the system and implemented from the beginning.

- **Common.MVC.WPF** – implements universal logic of the View layer integrated with Windows Presentation Foundation technology.
Common.NHibernate.Mapping – supports the creation of mapping between tables in the database and classes in the Model layer of the system.

MIS.Core – contains basic classes, interfaces used by the Controller layer as well as defined interfaces for plugins, which allows us to maintain increased flexibility of the system and openness for new functionality.

MIS.Database – defines the Model layer of the system.

Figure 2. Internal dependencies between the most important modules of the system.

The crucial components of the system (i.e., plugin managers) are hidden from the user inside the MIS.Core module. They allow us to add new functionality flexibly, while it is assumed that all of the functionalities in the system related to data processing, metamodeling, and optimization are treated as separated plugins. However, such a plugin can be imported into the system only when it implements one of the interfaces presented in Figure 3.

The system can be extended by using plugin interfaces in one of the following four directions:

• Data import – each of the machines used in laboratory testing generates output data, which describes material behavior under loading or temperature conditions. The data obtained from such tests are gathered in various formats, including text and binary files (e.g., results of plastometric tests generated by Gleeble3800 are exported to text in columns, while the data obtained from dilatometers is written in the MS Excel format). To assure the possibility of definition of the new machines and laboratory tests, IDataParserPlugin was implemented as a fundamental interface for these purposes.
• Data filtering – data obtained directly from laboratory test is usually very noisy and contains a lot of useless records that have to be omitted. The IDataFilterPlugin allows us to implement new filters dedicated to specific measurements. The most-commonly-used filters are: moving weighted average (data smoothing), screening (data selection), and inter-/extrapolation (data completing).

• Metamodelling – as mentioned previously, ANN metamodels have to be described in PMML; however, the system is open for other metamodelling approaches, such as Kriging or Response Surface Method. Metamodels based on such new
functionality can be imported to the system in the form of plugins implementing the IMetamodelPlugin interface. The methods of this interface allow us to receive input/output parameters and execute metamodelling.

- Optimization – the system is equipped with an internal software library with optimization methods. It includes conventional approaches as well as nature-inspired methods. However, similar to metamodelling functionality, the system stays open for new functionality. Therefore, new optimization procedures can be imported to the system in form of plugins implementing IOptimizationPlugin. The methods of this interface allow us to define optimization variables, objective function, and breaking conditions.

The plugins imported to the system are managed with PluginController, which is responsible for maintaining proper plugin configuration and data workflow. Due to such functionality, users are able to design a specific route of plugins, starting from data parsing and filtering up to the optimization loop with the selected metamodel. All of the data required by system modules is gathered in the database (Figure 4). After authorization, a user starts his work with the system by creating a new project (table Projects), where the type of laboratory experiment is selected (table Experiments). This choice determines the list of possible machines to be used in laboratory tests. The selected machine and type of experiment determine a list of possible material models (table Models) for which parameters can be further identified (e.g., the selection of a plastometric test on Gleeble 3800 would suggest a list of rheological models, including Hansel-Spittel, CEMEF, or Sellars models). Finally, the model selected by the user determines a list of possible metamodels (table Metamodels) that were virtually trained to reflect real experiments.

The configuration of the project is followed by import and analysis of the measurements. This functionality is realized by plugins that are composed into tree groups by the user (table PluginTree). Each node of that tree is described by a set of specific parameters (table ParamsTree). Such an approach starts optimization as the last major plugin, which uses a metamodel as a part of the objective function. Moreover, the plugin tree assures a fluent workflow of data between particular plugins and takes responsibility for data integrity. Results of the performed identification are presented on the main form of the graphical user interface (Figure 5). The system was implemented by using Microsoft .NET 4.5 framework with Windows Presentation Foundation (WPF).

5. Case study

The system was validated for all material models described in this paper. The majority of results obtained from the system are published in other papers. Identification of the microstructure evolution model is described in [8], phase transformation models in [13], and identification of fracture criteria is described in [27]. Extensive application of the system to the identification of flow-stress models on the basis of uniaxial compression tests is presented in [26].
Figure 4. The main tables of the database.
Validation confirmed good efficiency of the system as far as the identification of material models is considered. In the present paper, the capabilities of the system are demonstrated for the compression of rings (Figure 6). Various disturbances make interpreting the results of ring compression (RC) tests very difficult. These tests are characterized by a large inhomogeneity of deformation (Figure 7), which is caused by the complex shape of the deformation zone and by the effect of friction. Beyond this, heat generated due to plastic work, friction and heat transfer to the tools and their surroundings causes strong inhomogeneity of temperature in the sample. Due to the fact that ring dimensions are very sensitive to friction after compression, this test is frequently used for the identification of the friction coefficient [22]. Since the above-mentioned inhomogeneities of strains, stresses, and temperatures make determining the flow stress from this test very difficult, researchers usually perform additional uniaxial compression tests to identify the flow stress model. This procedure is very costly; therefore, researchers searched for a possibility of applying numerical simulations to aid the interpretation of the RC test. Results of this research are described in [25]. It was shown in that paper that, when inverse analysis was applied, identical flow-stress models were obtained from RC and UC tests. Therefore, the ring compression test was selected as the case study in the present work. The ring samples used in laboratory tests are standardized; i.e., $R = 6$ mm, $R = 7$ mm or $R = 9$ mm and the ratio between $R$, $r$, and $H$ is 6:3:4 (Figure 6).
Numerical simulations reflecting the compression of rings with various radii were implemented. Besides the radius, the set of input parameters contained the following eight elements: $p_1-p_5$ (parameters of equation (3) in Figure 1), $\varepsilon$ (strain), $\dot{\varepsilon}$ (strain rate), $T$ (temperature). Five forces related to equal die displacement were the output parameters of the model (Figure 8). Finally, ten thousand virtual tests featuring randomized input parameters were performed to obtain a direct relationship between input and output values.

The set of results obtained was used to build ANN-based metamodels. Various architectures of MLP were verified, including variants with one and two hidden layers. The former networks (i.e., 8-6-1, 8-10-1, 8-14-1) were unable to obtain satisfactory accuracy. However, the architecture 8-18-13-1 with two hidden layers reached the lowest error value after training and validation. Fifteen networks were trained (i.e., for each of the three radii and for each of the five forces separately).

Particle Swarm Optimization (PSO) was used in searching for a minimum of the objective function (1). Optimization was performed for 10,000 particles, with inertia equal to 0.729 and for the same local and global accelerations equal to 1.49. During optimization, the effective number of required iterations was 100. The best thirty results from different cases of network learning were used to verify the effectiveness of the trained networks and optimization.
The obtained coefficients from the mentioned system were used in verification tests. The results obtained were verified by a comparison with inverse analysis with FEM. Results of this comparison are presented below. Figure 9a shows plots of flow stress obtained from conventional inverse analysis with the FE model and from inverse analysis with the metamodel. Figure 9b shows the comparison of forces measured in the tests and calculated by the FE code with flow stress equation (7) in the constitutive law with coefficients $p_1$–$p_5$ determined using the two inverse methods. The presented results confirm very good predictive capability of the system, and some discrepancies in Figure 9b are due to the lack of capability of equation (6) to properly describe the behavior of the material in a wide range of strain rates and temperatures.

Figure 9. The comparison of experimental data to the results obtained by using Finite Element Method with material model identified with ANN.
6. Conclusions

The hybrid computer system for the identification of metallic material models on the basis of laboratory experiments was described in this paper. The system was designed as a stand-alone application dedicated to the MS Windows OS with the possibility of local or remote database connection. Numerical tests of the system allowed us to draw the following conclusions:

- The presented system allows us to perform many simulations in a short time using a user-friendly interface with different plugins.
- Plugin-based applications allowed us to extend the existing system without writing new, often complicated and previously-developed core parts for new features. It is only needed to write a new plugin that implements the required interfaces.
- Plugins allow us to add new types of features such as subsystems for existing solutions, scatter computing plugins, etc.
- Stored informations with automated operations protect against often-made mistakes by human during manual reconfiguring before each simulation.
- The system allows us to decrease the time required to organize the work environment, like writing one’s own source codes and protecting against errors. Simulations can always be repeated to ensure correctness, and the obtained results can be saved for future analysis.
- The numerical tests performed for ring compression tests confirmed a very good predictive capability of the system.

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