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VForm-xSteels: virtual materials database

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Abstract. Nowadays, most of the product designs rely on the aid of simulation software, particularly Finite Element Analysis (FEA) programs. However, an accurate simulation requires a proper virtual/numerical material behavior reproduction, meaning a precise material characterization through constitutive models and their parameters. To numerically characterize a material, particularly a metal, (i) experimental tests, (ii) model selection and (iii) inverse procedures are required. All these three tasks can be expensive and time-consuming. Therefore, product development engineers resort to materials databases to obtain the virtual materials, i.e. the constitutive models and their parameters adequate for the desired material. However, the information provided by the materials databases does not include experimental data nor provide information on the testing procedures. Due to this absence, users cannot verify the information nor its accuracy on the material database. Moreover, data related to material constitutive models, required for accurate simulations seems to be absent [1]. This work presents the development of a new material database that revises the previous problem. This database has the focus on virtual materials and their importance in product simulation and design. The presented VForm-xSteels material database includes (a) mechanical models and their implementation in FEA software, (b) experimental data and (c) the parameters identified for each material, and (d) indications concerning the quality of the material behavior reproduction associated with each model/parameters set. This database can be enlarged by the contributions of all users and present the following benefits for the engineering community: (i) increasing the precision and reliability of numerical FEA simulations by providing accurate input data, filling then a gap of the FEA market and answering to the request of the FEA users; (ii) reducing the development lead-time of metallic parts and the development of robust technological solutions with highly improved quality, consequently decreasing cost and time in the overall development process.

Introduction

Nowadays, the use of numerical simulation and particularly Finite Element Analysis (FEA) has become a mandatory step of material processing optimization [2]. According to the TechNavio "Global Simulation and Analysis Software Market" report (2023) [3], FEA software dominates around 50% of the simulation market and for the automotive industry alone, FEA is likely to exceed $968 million by 2024 (see Fig. 1). Despite the size of the FEA market and the regular use of FEA in the engineering design industry, the problem of obtaining reliable FEA input data, especially the description of non-linear material behavior, is a constant and has not been answered yet by the FEA software market. A solution for this problem is required for both the FEA users and providers.

Fig. 1. The market for simulation and analysis software is expected to grow at a CAGR of 14.22% between 2022 and 2027, with a forecasted increase of USD 9,680.14 million. This growth is driven by factors such as the rising demand for simulation and analysis software, the integration of advanced safety technologies in luxury cars to achieve higher safety ratings, and the increasing developments related to autonomous vehicles by OEMs (adapted from [3]).

Reliable virtual forming would lead to stiffer, stronger, safer and lighter industrial parts through using advanced models, capable of accurately predicting the thermo-mechanical response and ductile failure behavior of materials when subjected to complex loading conditions. Simple constitutive models do not present any difficulties to be calibrated to known metals. However, these models do not provide accurate and robust results, such as the ones demanded by manufacturing, automotive, aerospace, etc. industries. Additionally, the continuous development of new materials, such as Advanced High Strength Steels (AHSS) that allow higher performance at lower weight, urgently requires (well calibrated) complex models to reproduce their behavior in FEA programs. An additional complexity is that the stiffness and yield stress of these materials are so high that their forming processing is frequently done in warm conditions.

Therefore, the characterization of materials has received increasing attention due to the need for precise input data to computational analysis software at a lower cost. Simulation software uses complex material constitutive models, and the successful prediction of the real thermo-mechanical and ductile failure behavior is inherently dependent on the quality of the model and the related material parameters. In general, these parameters are determined using multiple and different standard tests. However, the homogeneous thermal, stress and strain fields generated in these relatively simple tests do not fully represent the complex heterogeneous thermal, stress and strain fields occurring in warm metal forming operations. Additionally, inverse methodologies commonly used, e.g. minimization of experimental vs FE model, are not reliable enough, due to the non-uniqueness of the solution. Furthermore, for complex constitutive models with many parameters, a high number of classical standard tests must be included in the experimental database, leading to an expensive and time-consuming experimental characterization and identification processes.

The main goal of the VForm-xSteels project [2] is to develop an efficient and accurate methodology for determining the material parameters of advanced mechanical and ductile damage models from a dedicated single test that involves non-homogeneous strain fields. Indeed, this non-homogeneity leads to richer information than more traditional approaches with quasi-homogeneous tests, thus leading to a decrease in the number of experiments and therefore to a cost-effective solution. However, this methodology requires performing a suitable mechanical test using Digital Image Correlation (DIC) technique and using post-processing numerical tools for the precise calibration of the constitutive models. Several numerical tools and strategies have emerged to solve the inverse calibration problem, such as the Finite Element Model Updating (FEMU) [4], the Virtual Field Method (VFM) [5], Constitutive Equation Gap Method (CEGM) [6], the Equilibrium Gap Method (EGM) [7], and very recently, with the explosion of data-driven methods, Machine Learning (ML) and Artificial Intelligence (AI) techniques [8]. A commercial numerical tool available to straightforwardly calibrate constitutive numerical models, which uses some of the previously listed methodologies, is MatchID [9]. Nevertheless, expertise on both experimental mechanical tests and inverse calibration is required. Therefore, a more straightforward solution should be available for most FEA users.

FEA software's libraries of material properties and material databases could be the solution for the need of material models and their parameters. However, the included materials are generic or the most common and do not represent the entire materials market, and these databases do not include experimental data nor provide information on the testing procedures [1]. Due to this absence, users cannot verify the information or its accuracy on the material. Moreover, data related to material constitutive models, required for accurate simulations seems to be absent.

Therefore, the only solution is the creation of a new database of material constitutive models calibrated to a large number of materials, which include (a) thermo-mechanical and ductile damage models and their implementation in FEA software (as user subroutines), (b) experimental data and (c) the parameters identified for each material, and (d) indications concerning the quality for reproducing the material behavior of each model/parameters set. This database should be enlarged by the contributions of all users even after the conclusion of the project. This solution is also an outcome of the vForm-xSteels project, as illustrated in Fig. 2.

Recently, this need was also highlighted by ANSYS Granta, launching their product called Granta Materials Data for Simulation (Granta MDS) [10], using sources like MaterialsUniverse™ database and the JAHM [11] simulation data set.

Development methodology

In the design stage, it was decided to build a web platform, including the online open database, instead of a desktop application. This task is critical because this platform must be ready for easy upscaling, storage and management of a very large amount of data (the experimental full-field data of a single non-linear mechanical test can easily reach 5Gb without thermal data), be intuitive (in access, retrieving information, download and upload data) for an engineer, technician, or scientist and well documented. This platform must show a long longevity and must be developed by an expert engineer in the thematic of this project.

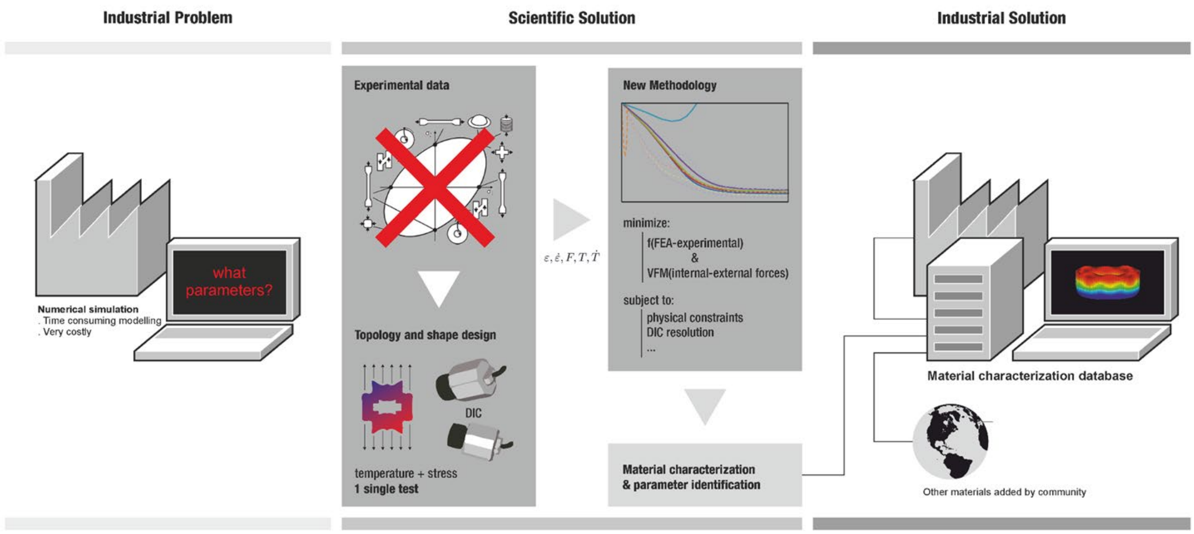

Fig. 2. Graphical abstract of the project proposal VForm-xSteels. While full-field mechanical tests and calibration methodologies are scientifically sound, they may not be practical for industrial and FEA users. Instead, a material database can provide engineers with accurate and readily available data, enabling them to create more reliable simulations.

Considering that the numerical characterization of a material requires experimental data and a selected constitutive model, and, consequently, the calibrated parameters of the model, the structure of the data is divided into these three groups, as illustrated in Fig. 3.

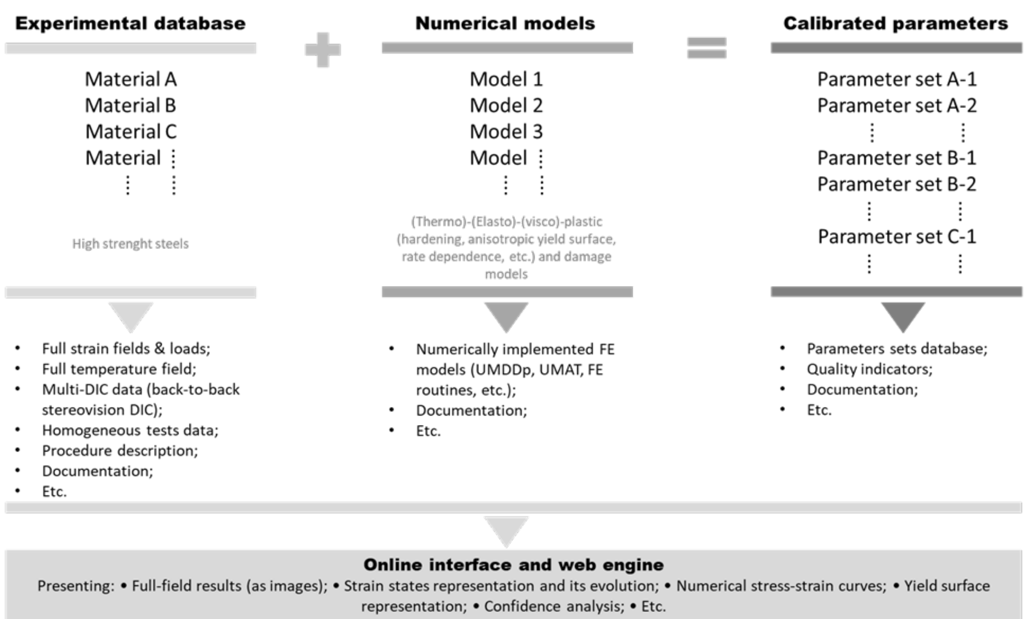

Fig. 3. Metadata of the open online platform.

However, the numerical material database must be prepared to effortlessly obtain the parameters using an inverse identification strategy. Nevertheless, the inclusion of these calibration software and codes in the platform is not practical in the sense that these require large computational effort to derive a precise result. Therefore, the structure of the database must be designed in a way of serving both the FEA users and the providers of calibration results. The solution found was the development of an API that could be used directly by parameter identification codes (for getting the experimental data and providing the results from/to the material database) and by the Front end (webpage) of the database. This solution is illustrated in

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Fig. 4. The use of API as backend and processing engine offers several benefits, including increased interoperability, improved efficiency, better user experience, increased flexibility, and new revenue streams.

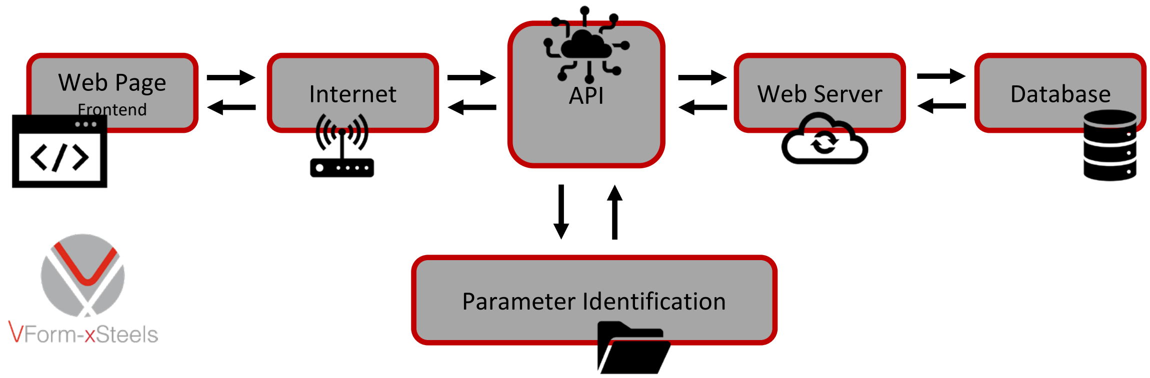


Fig. 4. Information and data processing structure. The use of an API allows to download and upload data for both the Front end and other inverse calibration codes, as well as some processing tasks.

Other difficulty on the development of the database is the structure for saving the data and an intuitive way to present to the user or even to access the database through the API. The chosen structure can be seen in the scheme of Fig. 5, where the hierarchy of the information was based on the file structure of a DIC test:

• material	>	• physical properties				
	>	• experimental data	>	• mechanical tests	>	• DIC data
	>	• behavior models	>	• parameters		

The result of the design phase has been developed in the last months. The actual stage of the VForm-xSteels Front end can be seen in Fig. 6. The database and its Front end include (i) documentation, scientific papers and description, (ii) FEA user routines (e.g. UMAT) with constitutive models, (iii) experimental data of mechanical tests for material characterization (see Fig. 6d), (iv) parameters identified for the available constitutive models and experimental data, and (v) Manual with instruction to use the database directly through the API. In this database, no files are saved, just data. However, the API engine can read all DIC files as well as write them to the user, which can reuse them for other purposes. The parameters resulting from the calibration operation are also presented to the user in a graphical manner, as shown in Fig. 7.

Results: the example of the VForm-xSteels benchmark

In the VForm-xSteels project, the inverse identification of the constitutive behavior of a dual-phase steel was benchmarked. It was assumed that the DP600 steel is well reproduced by a known hardening law and yield criterion (Swift + Yld2000-2D, respectively). Both the experimental and numerical stages required for the behavior characterization were analyzed and the current practices in the framework of MT2.0 were assessed. University-designed tools and equipment were used. In this example, only the results obtained by the University of Aveiro are exhibited as an example of the potential of the database, however, several partners have participated and all project consortium have contributed.

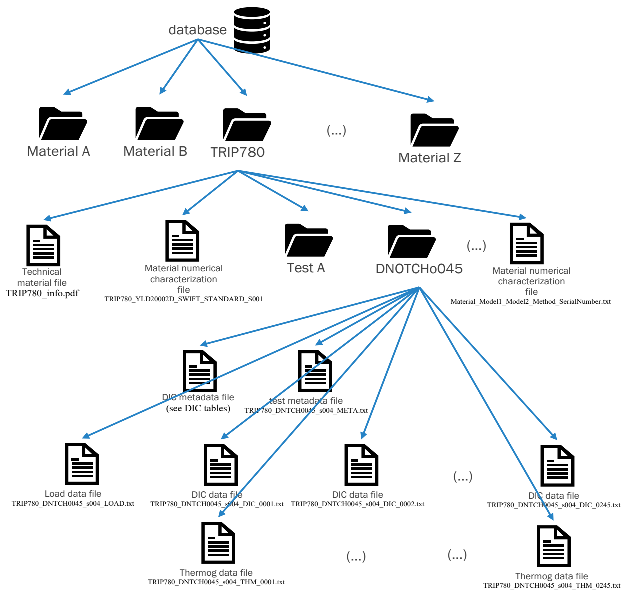
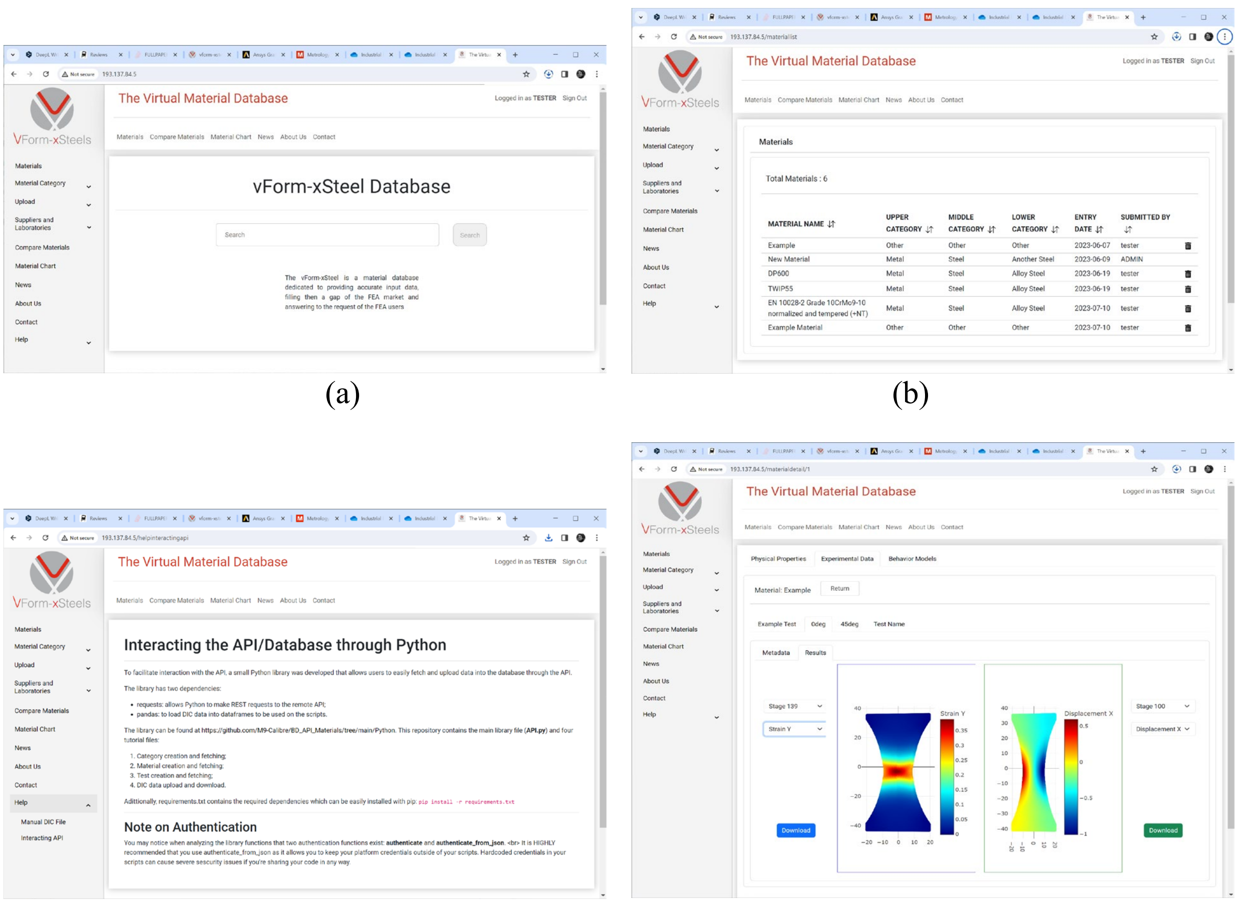


Fig. 5. Storage general view.



(a) (b)

(c) (d)

Fig. 6. VForm-xSteels database Front end. (a) Home page, (b) available material list, (c) instruction for the direct use of the API by external codes and softwares, and (d) DIC data exhibits as full-field results.

Fig. 7. Example of behavior model representation in the VForm-xSteels Front end. The model is composed of an elastic law, yield criterion and hardening law.

Using a known and simple specimen geometry (the heterogeneous dog-bone specimen, depicted in Figure 8) in a uniaxial tensile test at different material orientations (0, 45 and 90 degrees from the rolling direction), the hardening and anisotropy behavior of the DP600 steel must be characterized considering that these behaviors can be reproduced by the Swift's hardening model and the Barlat's yld2000-2d yield criterion, respectively. Therefore, the final goal of this exercise is to retrieve the parameters k, σ_0 and n of the hardening law and α_1-…-α_8 for the yield criterion (considering the yield's exponent a=6).

(a) (b)

Fig. 8. Heterogeneous dog-bone specimen in a uniaxial tensile test at 0, 45 and 90º from the RD. (a) Geometry of the specimen and measurement points and (b) samples of the specimen before and after the specimen manufacture.

This benchmark has several steps, however, here only the stages of experimental data analysis; parameter identification and parameter analysis are included to show the potential of the database, as the process illustrated in Fig. 9.

The use of the API by an external code can be made in an effortless manner using Python code. After performing the mechanical test using DIC techniques, the user can send all the data to the VForm-xSteels as exemplified in table 1. Then, the inverse calibration program can read the data in a similar proceeding and code, performing the parameter identification without requiring the multiple DIC files. In our example, a FEMU code named ParamID [12,13] was used and their

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results can be seen in Table 2. This inverse calibration code used a multistarting strategy to avoid the initial set dependence [13]. Then, the best parameter set, i.e. the ones that the difference between the strain full-field and force evolution is the lowest, can be directly written in the VForm-xSteels database using again the API and its Python scripts.

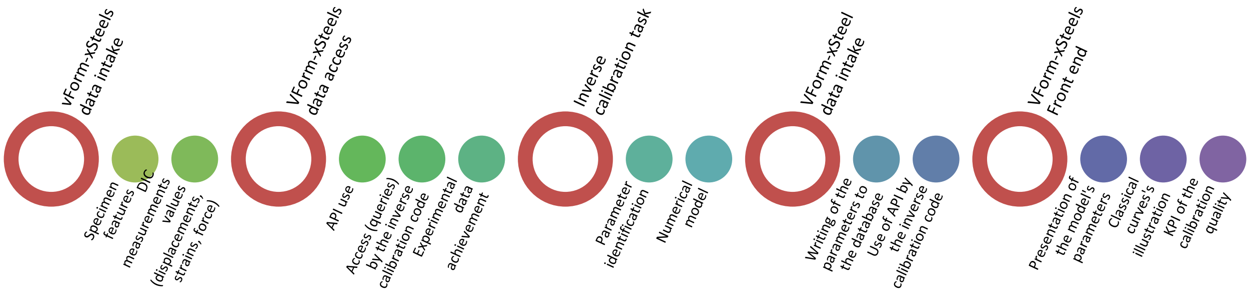

Fig. 9. Interaction stages of the inverse calibration process with the VForm-xSteels database. The advantages of the VForm-xSteels database are the inverse calibration process,the direct access to experimental data and writing of the achieved result with subsequent quality assessment.

Table 1. Code example for the VForm-xSteels data intake. Upload of DIC data. The file_mappings function reads the DIC files, writing in the most common format.

```python
from API import *
import os

token = authenticate("tester", "secretPass1234")

# Directory where the DIC files and load data are stored, consult the user manual for formatting and naming of the files
dir = "test\\"

# ID of the test we wish to populate
test_id = 3

f = []
for (dirpath, dirnames, filenames) in os.walk(dir):
    f.extend(filenames)
    break

file_mappings = {name : open(dir+name, "rb") for name in f}

test = get_test(test_id)

# Upload the data
test.upload_test_data(token, file_mappings, file_format=UploadFileFormat.MatchId, _3d=False)

# Download the data as a ZIP file
test.download_test_data()

# Download the data as a pandas dataframe
stages_df = test.load_test_data()

print(stages_df.keys())
print(stages_df[2])
```

Table 2. Results of the calibration of the elastoplasticity constitutive model (Yld2000-2D+Swift hardening) using a multistarting FEMU strategy and the heterogeneous dog-bone specimen.

M fixed to 6		alpha 1	alpha 2	alpha 3	alpha 4	alpha 5	alpha 6	alpha 7	alpha 8	M	K	epsilon_0	n	Eval	CF
Run 0 (iso)	Initial set	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	6.000	1200.000	0.00550	0.200	1	1.20E-02
	Final set	1.029	0.855	0.664	0.914	0.983	1.497	0.868	0.677	6.000	1048.377	0.00471	0.236	276	3.60E-04
Run 1	Initial set	1.321	1.238	1.075	1.237	0.529	0.908	1.250	1.298	6.000	1610.791	0.00541	0.179	1	6.46E-02
	Final set	1.183	0.968	0.696	1.055	1.109	1.499	1.002	0.889	6.000	1261.792	0.00393	0.235	255	3.63E-04
Run 2	Initial set	0.963	1.038	0.876	0.560	0.917	0.783	0.812	1.076	6.000	1499.560	0.00334	0.280	1	6.89E-02
	Final set	0.648	1.434	1.231	1.081	0.975	0.500	0.963	1.040	6.000	1249.834	0.00374	0.233	230	3.81E-04
Run 3	Initial set	0.583	0.741	1.482	1.079	0.834	1.326	0.537	0.569	6.000	887.544	0.00636	0.252	1	1.45E-02
	Final set	0.809	0.702	0.502	0.744	0.768	0.965	0.702	0.658	6.000	817.292	0.00548	0.234	284	3.67E-04
Run 4	Initial set	1.207	1.390	0.500	0.705	1.267	1.104	0.934	0.728	6.000	695.224	0.00473	0.117	1	1.32E-01
	Final set	0.723	0.966	0.500	0.500	0.735	1.091	0.760	0.500	6.000	732.463	0.00275	0.189	276	2.04E-03
Run 5	Initial set	0.837	0.644	1.163	1.359	1.358	0.518	1.304	1.436	6.000	1103.603	0.007	0.21832	1	8.21E-02
	Final set	0.500	1.500	0.619	1.038	1.037	0.500	0.924	1.356	6.000	1331.195	0.004	0.23247	286	3.94E-04
Best run	Final set	**1.029**	**0.855**	**0.664**	**0.914**	**0.983**	**1.497**	**0.868**	**0.677**	**6.000**	**1048.377**	**0.004713**	**0.236**	**276**	**3.60E-04**

The identified parameters once kept in the database can be accessed by all users. Classical curves (yield surface, hardening curve, tensile test curve, shear test curve, etc.) are presented in the Front end to the user infer its general behavior (see Fig. 10). Other Key Performance Indicators (KPI), which evaluate the quality of both the model and their parameters, can be presented.

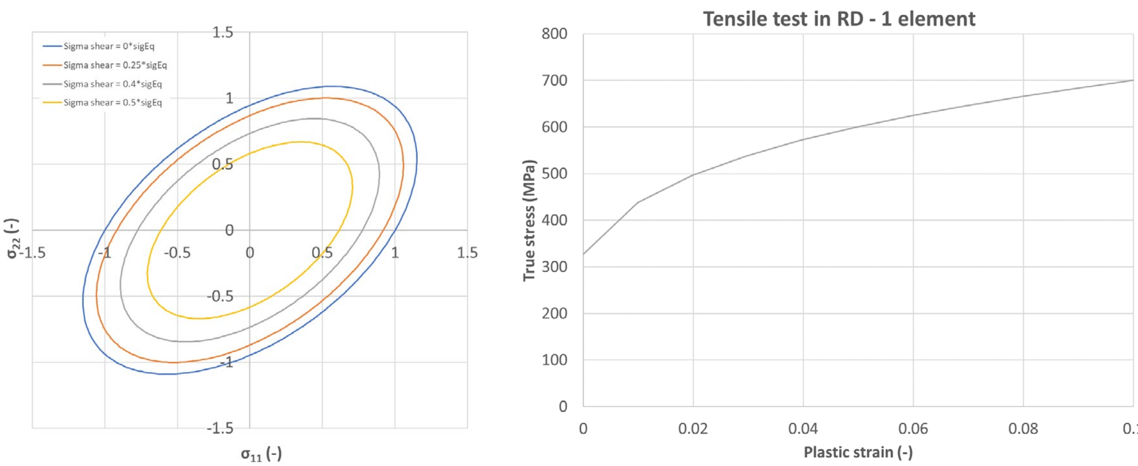

Fig. 10. Yield surface and hardening in the rolling direction of the constitutive model calibrated.

Conclusions

This paper presents the development of a numerical material database useful for FEA users. This database presents the following benefits for the engineering community: (i) increasing the precision and reliability of numerical FEA simulations by providing accurate input data, filling then a gap in the FEA market, and answering the request of the FEA users; (ii) reducing the development lead-time of metallic parts and the development of robust technological solutions with highly improved quality, consequently decreasing cost and time in the overall development process.

Disclaimer

The results reflect only the authors' view, and the European Commission is not responsible for any use that may be made of the information it contains.

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