Proposal of Optimization and Neural Networks – related Workpackages In the Scope of a RFCS EU Project

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Contents:

1 Introduction

This is a proposal of optimization and ANN modeling tasks in a research project involving multiple academic and industrial partners in the field of steel making. The proposal was originally prepared for the RFCS (Research Fund for Coal and Steel) call in 2012. When preparing the call, COBIK was kick out of the project team because presumably it could not be a part of consortium together with Štore Steel because the company is one of the cofounders of COBIK. The proposal was thus further elaborated and is prepared for suitable future calls.

2 Suggested WP Tasks

2.1 About the Work Package

The “Optimization and Artificial Neural Networks modeling” work package will provide tools and methodologies for optimization of process parameters in steel production.

2.2 List of tasks

2.2.1 Optimization (WP leader & work: I. Grešovnik, COBIK):

- Framework
  - Basic infrastructure
  - Processing & presentation modules
- Algorithms
  - Modular library of basic tools
  - High performance algorithms for industrial applications
  - Taylor-made extensions for specific cases
- Testing environment
  - Benchmark tests with results
- Inverse identification of model parameters
  - Algorithms
  - Identification of cases suitable for inverse identification
    - Possibilities of industrial measurements
    - Possibilities of laboratory tests
    - Case studies
- Optimization cases
  - Continuous casting process
  - Rolling process
  - ...

2.2.2 Artificial Neural Networks (WP leader I. Grešovnik, work: T. Kodelja & I. Grešovnik, COBIK):

- Framework
- Testing infrastructure
  - Analytical benchmark tests
  - Numerical experiments
  - Investigative environment: Synthetic environment for generation of various data acquisition scenarios, with generated response surfaces similar in complexity to real life cases.
    - Suggestion: Based on combination of JMatPro & casting simulator. Feasibility must be discussed.
- Algorithms
- Connection with optimization framework

- Methods for error estimation
- Data filtering and validation
- Case studies
    - Process modeling - continuous casting (simulator generated response)
    - Process modeling – rolling (simulator generated response)
    - Actual response for chosen processes

2.3 Remarks and Explanations

The potential of optimization tools is primarily in use of numerical models to automatically find improved process parameters according to sensibly designed criteria. When criteria can be clearly stated (either in terms of possible problems that must be avoided, in terms of efficiency or in other terms directly related to economy of operation), which is usually the case in steel production, adequately designed automatic procedures will typically highly outperform manual experimentation with the same numerical model. On the other hand, adequate definition of criteria may itself be a difficult task, which requires harmonized work between numerical and industrial experts and is done in several iterations containing problem definition, problem solution and verification of side effects. Optimization WP will aim at maintaining flexible framework environment and set of tools that will enable manipulation of numerical models in an efficient and practically meaningful manner.

We will work on seamless integration of the optimization and the ANN modeling environments. This is possible because the ANN modeling environment will be built on top of the IGLib (the Generic Investigation Library), which was primarily designed as suitable code base for optimization environments and other umbrella applications in broader range of technical areas. Integration with external simulation software will be done on case to case bases by providing custom interfaces between simulation and optimization software. The requirement will be imposed on these interfaces to provide a higher-level layer compatible with the generic optimization interface. Such a generic approach will ensure interchangeability of ANN and physics-based numerical models, reuse of results and their exchange among different models, and repeatability of optimization procedures.

While the primary meaning of the optimization software is in its use with physics based numerical models, it will be possible to replace these models by ANN-based models. One motivation for this effort is in providing faster and thus practicable alternative for use as decision support in process design (while still based on rigorous physics based models, but with CPU intensive computations performed in advance). Another motivation is in providing practically applicable alternative where physics based models are not enough elaborated to produce accurate results, or are too computationally expensive for practical use. Combination of physics based numerical modeling and numerical optimization is generally perceived as superior type of numerical support to making decisions related to process design. However, complexity of steel manufacturing procedures is the reason that ANN based models may be considered as an acceptable shortcut to provide useful results in reasonable time.

The desired ultimate goal for ANN modeling is to model the dependence of the obtained process outcomes (described by a set of output quantities such as tensile strength, hardness, elongation and necking) on process parameters of the production chain in a steel plant, which includes casting, hydrogen removal, reheating, multiple stage rolling, and cooling. ANN models should be coupled with parametric studies, sensitivity analysis and optimization in order to provide a true value as a decision support tool useful in practice.

It is currently impossible to state to what extent this goal is achievable in practice, especially with models based merely on the industrial data acquired in past realizations of the process. One part of research will be directed towards providing answers to this question, or at least providing a clear idea of what is necessary to answer the question. In order to obtain valid answers, it is necessary to develop a model case where we can produce adequate and consistent data in desirable quantities and according to chosen designs of experiments. We will strive to obtain a model with response characteristics as similar as possible to those encountered in the model of the complete process. In this way, we can produce scenarios similar to those appearing in practice and make rough estimates of feasibility of any conceived approach.

We need model cases where we are able to compute relation between input parameters and outcomes, have complete control over sampling the data, the computed relation must recapitulate some relation that is actually present in the industrial practice, and preferably the complexity of the response must be comparable to that of the finally targeted process. Currently, we are capable of producing a useful model case based on the mesh-less simulation of continuous casting, by taking into account only process parameters (without chemical composition). This should be extended, if possible, to include variation of chemical composition in the model. Dr. Vertnik's continuous casting simulator is already coupled with the JMatPro software for calculating material properties of steel with particular chemical composition, which is necessary as input for casting simulator. Currently, the coupling enables manual generation of material parameters for given chemical composition. In order to use this in out model case, generation of material parameters and subsequent run of the simulator on these parameters must be automated, i.e. the whole process must be run noninteractively in a loop where chemical composition for each run is specified programmatically. We are currently not sure whether this is technically feasible, due to the interactive-only interface of JMatPro. Alternative solution could be to employ labor force to manually prepare data, which is in this case completely impractical due to slow, labor intensive and error prone data generation process. In order to include such a model in the project, we must also ensure the access to the JMatPro software.

In parallel, development will be directed towards immediate applicability of the ANN models in industrial practice. Different areas are envisaged, the first one being substitution of the physics-based numerical model for acceptable speed of computation, e.g. for real-time response computations in decision support systems, or at least to achieve computational time short enough to include modeling in validation or optimization of process designs in the industrial practice.

The next area is generation of ANN models based on industrial data rather than data generated by numerical models. This may be possible for individual processes such as heat treatment, but feasibility must be critically assessed, either experimentally (which is expensive) or by numerical models. Conditions are adequacy & sufficiency of data, controlled and constant conditions, controllable scatter in properties of input material and possibility of measuring outputs. We can identify a suitable process for this kind of modeling during the project and leave open replacing the measured data by numerical model-generated data in the case that we don't find an adequate case where conditions are met.

The next possible area is the use of the ANN models for interpolation of given data over a range of independent parameter values for use with numerical models. In this case, ANN models can be used as replacement for phenomenological models, which makes sense when closed-form models adequate over finite ranges of parameters do not exist. This is the case with dependence of material properties on chemical composition of steel, which is currently handled by using the JMatPro software that is based on extensive experimental material database. This is adequate in numerical models where uniform chemical composition can be assumed, but if the model should account for non-uniform concentrations (e.g. in micro modeling of segregation), generation of ANN interpolated models in advance (based on series of JMatPro results) would be sensible due to vast speedups. Another possibility is to use ANN models as replacement for physics-based models, especially where multi-scale models (micro-macro) would otherwise be used. In this approach, a series of micro models can be generated and run in advance with different distribution parameters or boundary/initial conditions, upon which a surrogate ANN model is prepared from the calculated responses acting as a semi-phenomenological model. Such approaches must be used very carefully because they can easily fail due to excessive number of degrees of freedom in the surrogate model. If there is intention to use ANN in this area, applications must be clearly defined at proposal level.

3 Proposed Resources at CO BIK:

3.1 Human Resources

- Optimization: 2 PY[1] (covered by Igor Grešovnik)
- Neural networks: 2 PY (covered by Tadej Kodelja)
- Other (auxiliary algrithms, integration, interfaces): 1 PY (hire by contract)

3.2 Other Expenditure:

- Offices
- Small material (office material, etc.)
- Hardware
  - 3x laptop (mobile workstation), 6000 €
  - Workstation for demanding computations: 12000 €
  - UPS (1500 €), network equipment (1200 €), disks (700 €) – total 3400 €
- Software: 10.000 € (VM OS, Mathematica, Commercial libraries, IDEs, MS Office, etc.)
- Literature (books, etc.): 2500 €
- Travel
  - Project meetings (4x2 pers.): 12000
  - Working meetings with partners (2 or multiparty; 5x) 8000

[1] Person-year.

- 5 international conferences (for dissemination of work and gaining key knowledge of state-of-the-art): 9000
- 4 local conferences (to promote interest of local industry and academia for collaboration): 3200
- Visits of interesting parties, dissemination workshops: 6000

3.3 Contingency

Risks to be accounted for:

- Key person's quit
- Partner's exit
- Underestimated amount of work
- Overestimated industrial partner's capabilities to support numerical procedures
- Overestimated simulation capabilities

4 Administrative data:

4.1 Partner information (Optimization & ANN WPs)

Full name: Centre of Excellence for Biosensors, Instrumentation and Process Control
Acronym: COBIK

Mailing address:
Center odličnosti za biosenzoriko, instrumentacijo in procesno kontrolo
Mednarodni prehod 6, Vrtojba
SI – 5290 Šempeter pri Gorici
Slovenia, Europe

PIC (Participant identification code): 968321901. PIC: 968321901
VAT No. (Tax number): 83212353
ID number: 3660460000
Type: a private found research institution
Approx. No. of employees: 90

Directress (CEO): Rebeka Koncilja (rebeka.koncilja@cobik.si, phone: +386-5-39-32-542)

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Official address (**do not send mail to this address!**):

Velika pot 22
SI-5250 Solkan
Slovenia, Europe

Mailing address:
CO BIK
Tovarniška cesta 26
SI – 5270 Ajdovščina

Laboratory: Laboratory for Advanced Materials Systems (In Slovene: Laboratorij za sisteme z naprednimi materiali)

5 Proposal Related Activities:

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