Proposal: Optimization and Artificial Neural Modeling Tasks within the FP7 Project – CNT sensors

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Contents:

1 Introduction

This document contains proposal of the Artificial neural networks modeling tasks within the CNT sensors project. The proposal was initially prepared for the 1st stage submission in 2012, which did not pass the evaluation. The current document is prepared for eventual re-submission in 2013.

2 Work Package: ANN Modeling – COBIK

WP leader: I. Grešovnik
Work: I. Grešovnik, T. Kodelja

- ANN modeling procedures
    - definition of suitable network architecture
    - training procedures
    - validation procedures
- modeling software

- flexible multilevel interpreter - oriented network
- extensive testing module
- uniform approach for benchmark development, algorithm development and industry-scale ANN modeling
- parallel training with different training settings (including architecture) to obtain optimal results

* modelling of sensor response by artificial neural networks
* building an ANN model on experimental data prepared in laboratory (define the partner to perform the measurements)
    - measurements (e.g. cyclic voltammetry or electrochemical impedance spectroscopy) performed for different controlled concentrations of measured ions and environmental factors (e.g. water hardness)
* back analysis procedure to determine concentrations of ions from field measurements
* inspect different possibilities (milestone - make decision which way to go)
    - work in time domain, include time as parameter
    - work in time domain, use different integrators
    - work in frequency domain, smoothing filters for spectrum comparison
    - eventual other techniques

2.1 Competence possessed by COBIK

COBIK has competence in modeling of industrial processes, especially in steel production. Main competence is in the field of artificial inteligence-originated tools, in particular application of artificial neural networks in modeling of industrial processes. The other competence is in modleling of heat transfer and substance transport mechanisms in the presence of electromagnetical field.

Igor Grešovnik has roughly 15 years of experience in the fields of numerical simulation, products and process optimization, leading development of complex technical and business software (in particular in the fields of numerical modeling and optimization). He has been involved in more than 10 European projects (FP5-FP7) and several national projects and has extensive experience in collaboration in and coordination expressively interdisciplinary R&D tasks. He has good overview of software development and is skilled in management of software projects, having direct developmet experience with about 10 programming languages and several different platforms including intended heterogeneous and homogeneous HPC - intended clusters. He has worked on projects from very different fields such as metal forming, steel production, nanoparticle coloids in pharmaceutics and color production, underground construction, nanosensors for tactile sensorics, advanced polymers for human tissue replacement, development of measuring equipment (class I sound level meters, optical instruments, temperature and humidity measuring), etc.

Tadej Kodelja has 5 years of worldwide experience of process automation in the field of steel production. He si currently working on his Ph.D. thesis related to ANN-based modeling of process chains in steel production.

2.1.1 Analysis of Sensor Response by Artificial Neural Networks (ANN)

Work in the ANN package will be directed towards development of procedure and software for quick analysis of sensor response, which will be applicable possible to integrate in low cost equipment arrangements and will also make possible to obtain preliminary results on the field, without the need to send samples to the laboratory.

We will model sensor response by the artificial neural networks. The related ANN model will be obtained by training procedures based on experimental data prepared in the laboratory measurements of sensor responses obtained with different combinations and concentrations of the measured ions.

In the preparation stage, the software and algorithmic frameworks will be prepared to support production of such models. In parallel, ANN modeling will be synchronized with electrochemical measurement procedures, in order to tailor the structure of the model and procedures to the characteristics of the available data. We will coordinate with partners to consider most suitable measurement techniques to be integrated with ANN modeling (e.g. cyclic voltammetry or electrochemical impedance spectroscopy), based on technical issues as well as on judgment of which combination can produce most satisfactory results. In this stage, suitable data representation will be defined as well.

This will be followed by selection on data sets to work on, analysis of data, preparation of models and their validation. Feedback will be obtained about necessary updates in measurement procedures in order to improve the model building stage. Refinements of measurement processing and interpretation will be considered that can have impact on enhancements in model pretictivity and facilitate technical issues (e.g. band pass filtering, application of transforms such as time to frequency domain, application of smoothing filters, etc.).

In the final stage, models will be prepared for integration with other equipment. ANN models will be packed as modular component with clearly defined input and output, and a separate unit for preparation (training) of the models.

2.1.1.1 State of the art – ANN modeling

The study of neural networks is an expressively interdisciplinary field. Over the last years, neural networks were being successfully applied across an extraordinary range of applications, as well as to a number of problem domains such as data integration, data analysis, approximation, time series, pattern recognition, classification, etc.

ANN is a numerical modeling tool that features an interconnected network of processing units (neurons) whose structure is mimicking the structure of human brain. It is capable of recognizing patterns and classifying data into various categories, and is also capable of updating its modeling abilities through “training.” As such, modeling by ANNs is intrinsically a black box modeling, but a very flexible one that in many cases exhibits superior performance over other black box modeling approaches [1]. In particular, ANNs are capable to accommodate to systems with many variables and with highly nonlinear response. They can therefore be successfully applied as modeling tool in areas where underlying physics is not precisely known or is too complex for the numerical models to produce applicable results. A great advantage for use in systems where real time response is crucial is that time consuming training stage can be separated from evaluation of modeled response, which is consequently very quick. These characteristics have been successfully exploited in modeling of complex industrial systems such as steel production plant [3], [4]. However, there are also some things that one must be careful about when applying ANN modeling, and these have been the subject of active research over the last years [1], [2]. As the ANN models are not directly related to the physical basis, and since the mathematical mechanisms behind the obtained models can not be easily tracked and analyzed, noncritical use can easily result in spurious behavior and poor predictive capabilities.

Recently there have been several attempts to use neural networks in analysis of different various types of sensors [5]- [12]. We can also find some attempts on simulating sensors for heavy metal ions detection in water [10]-[12]. However, the sources in this area are still relatively scarce and techniques applied rely on heavily simplified models, often using simple analytical models to generate the training data for the ANN-based models.

2.2 Proposed Resources at CO BIK:

2.2.1 Human Resources

- Neural networks: 4 PY (Igor Grešovnik, Tadej Kodelja)

3 Administrative data:

3.1 Partner information (ANN & numerical modeling)

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
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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

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

3.2 Call Summary (2012 Call)

3.2.1 Deadlines

For the 1st stage – submitted:
October 23, 2012 is deadline for the first stage proposal (information extracted form mail).

For the second stage:
Around New year – answer about going into 2nd stage.

3.2.2 Finance and Duration

Duration: 4 years.

4 million € foreseen for complete project. roughly 400.000 € proposed for the COBIK.

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