Scientific Report

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Name of the *Host Organisation*	VTT
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Period of the fellowship	02/05/2011 to 30/04/2012

I – SCIENTIFIC ACTIVITY DURING YOUR FELLOWSHIP

My scientific activity during this fellowship has been mainly focused on the integration of simulations and multi-objective optimisation algorithms. More precisely, my work was to study and implement the combination of simulation tools based on the Simantics platform with metaheuristics.

I divided this work into two general tasks:

- Designing software tools to provide the support of optimisation features by the Simantics platform;
- Developing prototypes of simulation-optimisation combinations to assess feasibility and interest.

To complete the first task I created an ontology which matches closely the formal definition of optimisation problems. I then made use of the Simantics platform SDK to design and implement a graphical user interface allowing users to define an optimisation problem corresponding to their simulation model. This GUI permits the selection of optimisation-related concepts such as decision variables, objectives and constraints among all the parameters of all components of the simulated system. I implemented this GUI as an Eclipse RCP (Rich Client Platform) wizard. The Simantics SDK itself is based on Eclipse RCP. Being part of the 10 to 12 people development team of Simantics greatly improve my skills in programming with this framework.

For the second task, I did a bibliographic a bibliographic search focused on:

- the combination of simulation and optimisation methods, in particular the combination of dynamic simulation and evolutionary algorithms, the general purpose of evolutionary algorithms used as optimisers (like other metaheuristics) allows to solve optimisation problems without a priori knowledge such as the linearity or the derivability of the objective functions, thus in my approach the simulation model was considered as a black box receiving some input values (the decision variables and information about the context of execution of the simulation) and providing output values (the objective/constraint values or other auxiliary scalar values or time series allowing to compute the objective/constraint values). But, because they are iterative algorithms working on sets of solutions, evolutionary algorithms usually require a high number of evaluations. In this case, evaluation (the process of calculating the objectives and constraints from the decision variable values) consists in running a simulation, intensively repeating simulation runs is time consuming. I had to distribute the experiments on a computer grid totalising 48 processors and 144 GB of memory;
- the assessment of multi-objective optimisation algorithm performance, because evolutionary algorithms are stochastic by nature, their performance needs to be assessed statistically. I used state-of-the-art comparison methods involving statistical tools such as box plots and Wilcoxon rank tests.

My implementations were based on the Simantics-based application APROS (Advanced

PROcess Simulator), developed by VTT and Fortum and the jMetal (Java Metaheuristics Library), an open source library developed at the University of Málaga. The two simulation models I used as test cases were developed by a research scientist from the System dynamics and optimisation team of VTT. We collaborated to define the most suited corresponding optimisation problems. The first test case was a chemical process design problem. The simulation modeled a system controlling the concentration (of a specific chemical) in a flow (that was supposed to be part of a larger process). The system was composed of a QIC controller and a tank. It was a good test case because it requires a post-treatment of the time series outputted by the simulation runs involving Fourier transforming. The goal was to find the settings of the controller and the best dimensions of the tank that optimise the conflicting objectives of dampening the flow, achieving the targeted concentration and minimising the cost of the system. The second test case was similar to a job-shop scheduling problem. The simulation modelled the two stage separation (filtration) of a flow. The two filters need to be cleaned regularly in order to keep their filtration efficiency. The goal was to find the settings for the pumps feeding and driving the system and the two (one for each filter) cleaning schedules that maximise the total amount of permeate, minimise the amount of impurity in the permeate and minimise the energy consumption. It was a good test case because it features both continuous and discrete decision variables.

During this fellowship, I also took part in the project of combining simulation models with the interactive multi-objective optimisation software NIMBUS from the University of Jyväskylä.

II – PUBLICATION(S) DURING YOUR FELLOWSHIP

Jouni Savolainen, Jean-Laurent Hippolyte, Hannu Niemistö, Christelle Bloch, Pascal Chatonnay and Antonio J. Nebro. *Multi-Objective Optimization of a Two-Stage Membrane Process with Metaheuristics.* Euromembrane 2012, European conference on Membrane science and technology, London, United Kingdom, 2012.

III – ATTENDED SEMINARS, WORKSHOPS, CONFERENCES

APROS Initial Training Course, VTT, Espoo, June 6th-8th, 2011: I have learned the basics of using the APROS modelling and dynamic process simulation tool.

Dynamic millwide process simulation with APROS, University of Jyväskylä, March 21st, 2011: seminar about the specificities of simulating the process of a whole plant and links with optimization, hosted by the Industrial Optimization Group.

IV – RESEARCH EXCHANGE PROGRAMME (REP)

1. University of Málaga, Computer Sciences and Languages Department
   I have been hosted by Pr. Antonio Nebro, one of the main developers of the jMetal library. We discussed improvements and customisation of the library in order to integrate the Simantics platform. I implemented some of these improvements during my stay in Málaga. I also presented the ontology-based Simantics platform to members of the “Data and Knowledge Management for the Semantic Web” and the ”Metaheuristics and Advanced Algorithms” teams of that department.
2. ETH Zürich, MOSAIC (MOdels, Simulations, and Algorithms for Interdisciplinary Computing) group.
   I have been hosted by Pr. Ivo Sbalzarini. His group’s activities include the study of algorithms for black-box optimization and sensitivity analysis. I made a presentation of the simulation- optimisation prototypes I was developing. We discussed tools to analyse the “landscapes” of objective functions of optimisation problems. Many results exist in the literature regarding single-objective optimisation problems. The analysis of multi-objective landscapes is a growing subject of research.