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SYNERGY

Synergy for Smart Multi-Objective Optimisation

D1.3

Potential complex optimisation problems in science and industry

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CONTENTS

1 Introduction

This deliverable results from the European H2020 Twinning project SYNERGY (http://cordis.europa.eu/project/rcn/199104_en.html). It describes potential complex optimisation problems in science and industry. In the document, we report some strategic large-scale applications in different domains where multi-objective optimisation and surrogate-assisted modelling are crucial. The explored domains concern: health, smart factories, smart buildings & homes, smart cities & communications, and smart use of resources.

2 Application domains

Many application domains call for multi-objective optimisation and surrogate-models. This section presents different applications in which the SYNERG partners are involved:

- Scheduling and planning problems
- Logistics and transportation
- Smart factories
- Bio-medical
- Engineering design
- Smart grids, cities and homes – Energy aware systems

2.1 Scheduling and planning problems

Scheduling and planning problems represent a quite complex family of combinatorial optimisation problems. This popular class of problems has many real-life applications in numerous domains such as production and manufacturing systems [4].

In the last two decades, a growing interest arises in multi-objective scheduling and planning. Indeed, solving multi-objective scheduling and planning problems has a great importance in terms of efficiency and effectiveness. Some multi-objective scheduling and planning problems formulated and solved by the project partners are presented in this subsection.

2.1.1 Flow-shop scheduling problems

The Flow Shop scheduling problem has received a great attention since its importance in industrial areas [2]. The adopted methods for its resolution vary from exact methods such as the Branch & Bound to Heuristic search and Metaheuristics [1]. However, the majority of literature deals with the problem in the single-criterion form and aim principally to minimise the makespan (completion time).

The Flow Shop problems is presented as a set of N jobs $\{J_1, J_2, \ldots J_N\}$ to order on M machines. The machines are critical resources: one machine cannot be assigned to two jobs simultaneously. Each job is composed of M consecutive tasks $J_i = \{t_{i1}, t_{i2},.., t_{iM}\}$. t_{ij} represents the j-th task of the job J_i requiring the machine m_j. Subsequently, all the jobs have the same processing sequence on the machines. To each task t_{ij} a processing time d_{ij} is associated, and each job J_i must end, at the latest, at the date l_i.

Scheduling of tasks on different machines must optimise certain regular criteria [2]. These criteria vary regarding the specificity of the treated problem, and generally consist in the minimisation of the following objectives [6]:

C_{max}: makespan time (achievement date of the last planned task);

T_{max} : maximum tardiness;

T : total tardiness;

T_{nb} : number of jobs delayed with regard to their achievement dates l_i;

F_{max}: maximum flow time.

We are interested in the study of permutation flow shop problem F/perm,d_i/(C_{max},T), where the jobs must be ordered in the same order on all the machines. In this work an approach based on multi-objective evolutionary algorithms has been adapted to the multi-criteria case. Several strategies of selection, diversity maintaining and hybridisation have been developed. Moreover, a parallel evolutionary algorithm has been designed. It allows to increase the population size and the limit generation number, and leads to better quality of results [6].

2.1.2 Service deployment in multi-Cloud environments

Public cloud computing is a fast growing technology [8], allowing companies to get computing power without any hardware maintenance cost. Computer resources are rented, with or without upfront fees, and can be scaled to fit company needs at any time [9]. Infrastructure As A Service (IAAS) is the basic bloc in cloud computing, consisting in renting computing resources as services, such as Virtual Machines (VM), disks or network capacity (Figure 1). Changes in offers from IAAS providers often occur [10], and need to be taken into account.

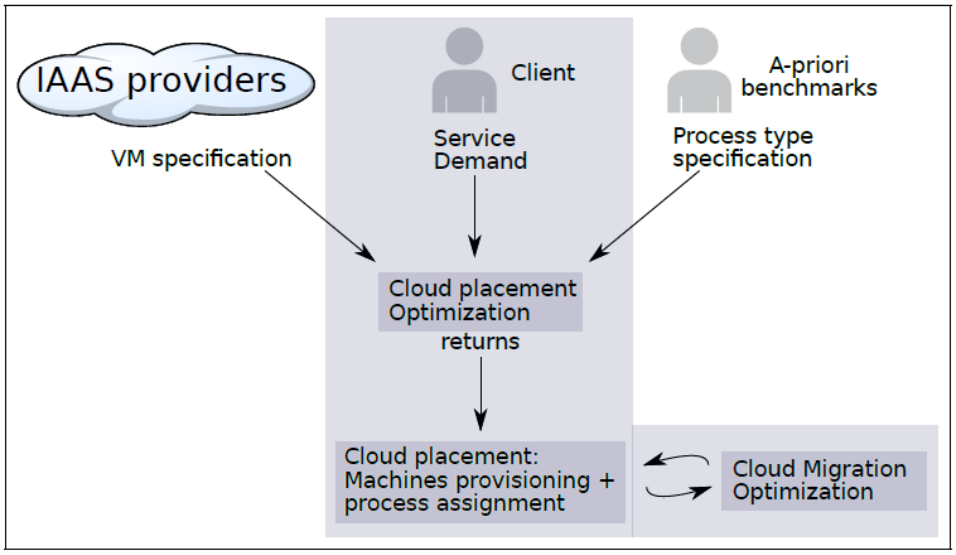

Figure 1: IAAS Clouds: Infrastructure As A Service

One of the major issues in using cloud computing is the optimisation of infrastructure costs. Current research often follows a provider's view of the cloud. The problem consists then to allocate VMs to physical machines with different objectives in mind, such as reducing energy consumption [11], ensuring SLA (Service Level Agreement) [12], or reducing the load of the machines [13].

In this work we consider the client side, and investigate how to efficiently use the VMs bought from IAAS providers. Our purpose is to optimise what we call platform design, an abstraction representing the VM, the processes to be deployed and the placement of those processes. We aim at optimising these three aspects of the platform while keeping enough computing power to maintain sufficient performances.

During the life-cycle of a platform, once the platform has been designed and deployed on VMs, multiple factors can motivate the decision maker to migrate the platform to better meet the needs. New providers can enter the market, or change their offers. A service can evolve and need better performances, or a new service may appear. Such changes can make a new design profitable, or even necessary. If the decision maker uses our previous modelling to optimise his/her costs, doing so ignores the costs related to the migration process itself. Since the platform may be in a production environment, every change must be made carefully, and a complex migration may induce downtime and human costs. Such risks and costs can be hard to predict, but in general the simpler the migration is, the easier it will be applied.

This work introduces several contributions [14]:

1. A new real-life model to optimise the migration of a platform using a multi-objective optimisation approach. The aim is to find Pareto-efficient solutions that offer a good compromise for all objectives. Our approach is based on three objectives optimising the cost of the platform, the simplicity of the solution and the simplicity of the migration.
2. An evolutionary approach to solve the problem. We propose a modified evaluation of solutions and a different comparison operator to find Pareto-efficient solutions.
3. An experimental protocol to assert the pertinence of our approach, using 10 different real industrial datasets. Experiments demonstrate the pertinence of our evolutionary algorithm approach for tackling real-size industrial use-cases.

2.1.3 Hydraulic electricity generation planning

The hydro-scheduling problem (HSP) aims to find a schedule of outflows in a hydro-electric network composed of reservoirs, turbines and pumps that maximises the profit (or minimises the cost). Dynamic programming (DP), an algorithm based on the search of the best path on a graph of states [15] can be used to solve hydro-scheduling problems (Figure 2). But in this case, the size of the graph grows quickly with the number of time periods, the number of reservoirs and their capacities.

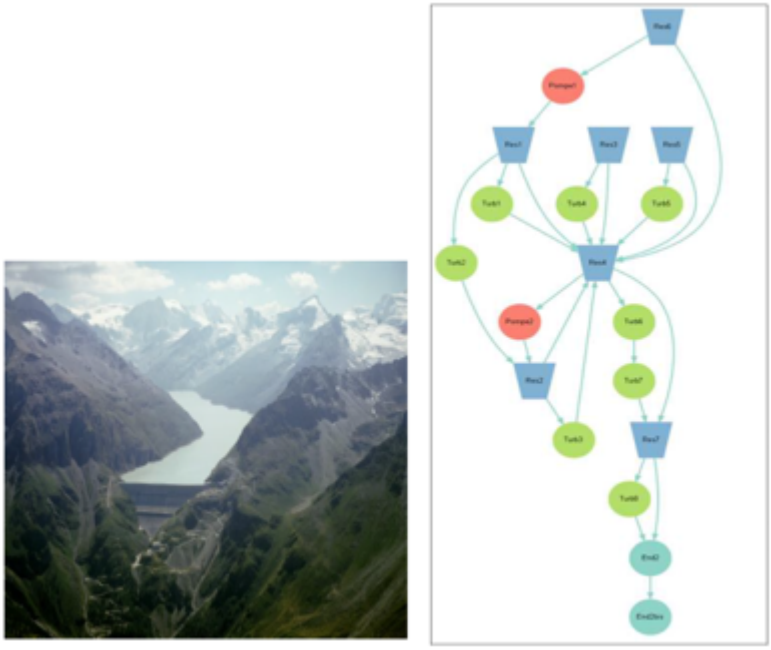

Figure 2: Hydraulic energy generation planning

In practice it is not possible to use the algorithm directly. Nevertheless, some adaptations of dynamic programming have been proposed for this kind of problems [16], but they are very specific to each problem and only allow to deal with problems of relatively small size. Metaheuristic algorithms, such as evolutionary algorithms (EA) could be a solution to overcome the aforementioned difficulties. They have been used to solve hydro-scheduling problems [17]. However evolutionary algorithms tend to converge prematurely and the optimisation process can be stuck at a local optimum. Besides, evolutionary algorithms also take a large number of iterations to reach the global optimal solution. In the case of hydro-scheduling problems, the flaws of this method could be partially explained by the dynamic structure of the problem.

An interesting way to solve such problems is to hybridise dynamic programming and metaheuristics. In the proposed approach to solve the hydro-scheduling problem, called DYNAMOP for DYNAmic programming using Metaheuristic for Optimisations Problems, a genetic algorithm based on a representation taking into account the dynamic structure of HSP is used. [18] This representation models a solution as a path in the graph of states (the same as in dynamic programming), each gene will then be a state traversed by the path. This representation allows a greater separability of the fitness function in terms of genes. The fitness is the sum of the edge values and a change on a gene only modifies two edges. This could result in a better locality in the recombination and mutation of the genotypes. In addition, this partial separability allows to apply an iterative evaluation and hence to speed up the computation time of the fitness. Another great advantage of this representation is that it allows to build hybridisation with DP easily.

This approach has many advantages and allows to overcome the drawbacks of DP and classical GA. Firstly, due to the use of a path representation of a solution, the hybridisation with dynamic programming is easy to realise and allows to significantly improve the obtained results. This hybrid approach shows its efficiency and effectiveness in solving real instances associated to the problem (Figure 3).

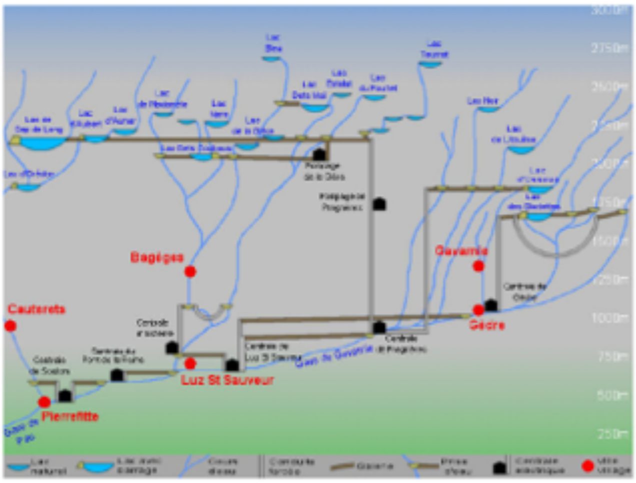

Figure 3: Real-life instance of hydraulic energy generation planning

Such an algorithm offers great potential to solve a large set of other combinatorial problems. Actually this methodology could be generalised to any problem which holds the Bellman property. It involves many different cases of applications, such as graph routing problems, sequencing problems, selection problems, partitioning problems, distribution problems, production or inventory problems or string processing problems. Therefore, we believe that extending DYNAMOP methodology to solve problems with dynamic structure could be a new and interesting line of research. This approach has also been generalised to multi-objective optimisation problems.

2.1.4 Optimisation of manufacturing planning

ETA Cerkno d. o. o. produces components for domestic appliances (e.g., cooking plates, thermostats, and heating elements). One of the main concerns of the manufacturing planning is to assure efficient planning process.

To this end a simulation tool for evaluation of production process was designed, where the production process was simulated based on the data acquired from the company. With the simulation tool available, we were able to develop a customised multi-objective optimisation algorithm for efficient problem solving which considered all the production specifics. To make it friendlier to use, an effective frontend (shown in Figure 4) which allows for easy monitoring of scheduled production plan was implemented.

Figure 4: Simulation tool for evaluation of production cycles

With this tool, we were able to replace locally optimal production schedules (one week time-span) prepared by an expert with global optimal schedules (covering all orders to the finest detail). The production schedule considers the deadline and quantity constraints for all orders. It enables quick and efficient adaptation to the new incoming orders. With some optimisation objectives being conflicting, an efficient manufacturing planning according to many objectives was also enabled. The results are published in [26].

2.1.5 Predictive maintenance

Technical system require maintenance to ensure secure and robust operation. This applies to systems such as buildings, aerospace structures, heating systems, medical equipment, and many more. Often, maintenances follows preset schedules, which may not always be ideal for a certain system. Either, periodic maintenance is performed too often, thus wasting costs due to unnecessary work hours or replacement parts that are implemented earlier than necessary. Or else, certain parts may fail in between scheduled maintenance operations.

One way to deal with both of these issues is to implement a predictive maintenance approach. That is, based on observed data features of the technical system, machine learning techniques are used to predict the need of maintenance, thus avoiding unnecessary maintenance visits or down times due to failures. One important application of predictive maintenance are motors. Here, data that is correlated to the motors health can be collected, such as voltages / currents, vibrations or timings. Since modern motors are usually tightly connected to electronic control systems these data features are readily available for evaluation.

The challenge here is twofold: firstly, to select a good technique of predicting failures, and secondly, to adapt it to a specific appliance,e.g., a specific car (Figure 5), or a specific use case. Hence, this not only involves a challenging machine learning task but also a multi-objective optimisation problem. These objectives are 1) to schedule as few maintenance visits as possible and 2) to avoid as many motor failures as possible. Additional objectives could be involved, such as maintenance costs based on required maintenance time and replacement parts. Furthermore, the derived methods should be fast to evaluate, robust against change in operation conditions and easy to interpret by maintenance personnel. This is especially challenging due to the potentially large data set sizes (due to frequent measurements, and due to being collected at many appliances simultaneously).

Figure 5: Predictive maintenance

To solve these challenges, the main idea is to evaluate and tune potentially applicable machine learning algorithms (Figure 6). Recent work [29] compared (different configurations of) decision tree-based algorithms used to classify the health of the monitored motors. Tree-based algorithms are a promising choice due to a) being able to produce human readable rules b) being robust against noise c) being able to incorporate numeric as well as categorical variables. The tree-based algorithms were compared to standard learning techniques.

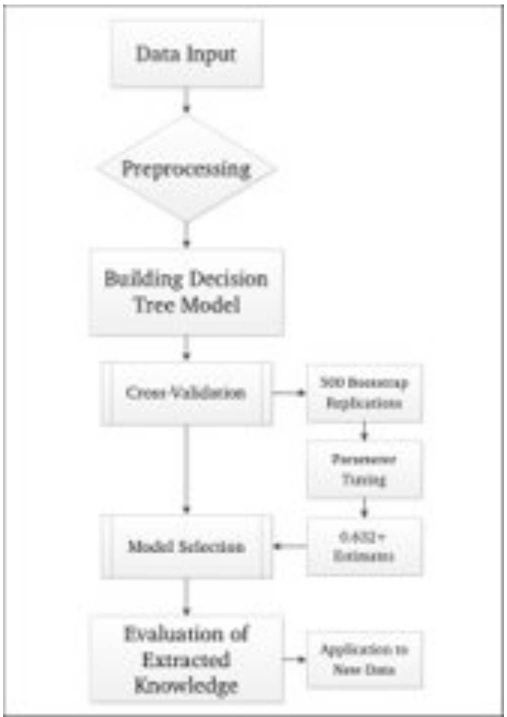

Figure 6: Machine learning for predictive maintenance

The resulting algorithms have been shown to be robust, easy to visualise and interpret and to be capable of effectively handling additional issues such as missing data or redundant / irrelevant data. Ensemble based methods (random forest, Figure 7) provided the best accuracies. Single models based on conditional inference trees proved less accurate, yet faster to train and easier to interpret. First results are published in [29].

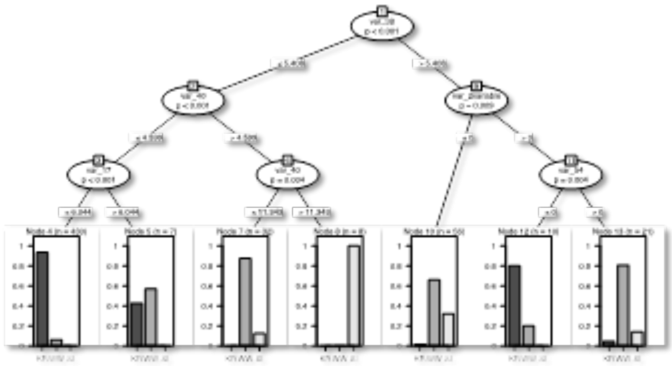

Figure 7: Random forest

2.2 Logistics and transportation

Logistic and transportation problems arise in various applications domains and industries.

2.2.1 Routing problems

By routing problems we mean any problem that involves generating a tour, or a collection of tours, on a network, or a subset of a network, given a set of constraints and the need to optimise one or several fixed objective(s) (Figure 8). Together, routing problems form a highly-studied family of problems that includes the well-known traveling salesman problem. Although such problems are frequently used to model real cases, they are often set up with the single objective of minimising the cost of the solution, despite the fact that the majority of the problems encountered in industry, particularly in logistics, are multi-objective in nature. In real-life, for instance, there may be several costs associated with a single tour. Moreover, the objectives may not always be limited to cost. In fact, numerous other aspects, such as balancing of workloads (time, distance, etc.), can be taken into account simply by adding new objectives.

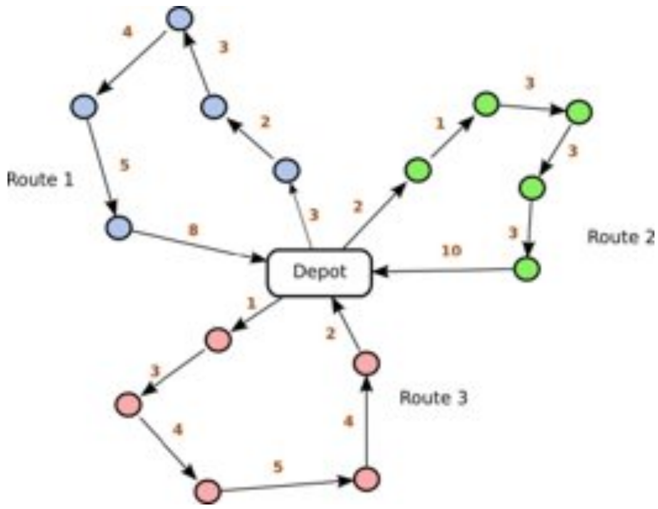

Figure 8: The vehicle routing problem

A routing problem can be defined in terms of the following components: the network, the demand(s), the fleet, the cost(s), and the objective(s) [19].

- The network can be symmetrical, asymmetrical or mixed. It is represented as a graph on which the nodes stand for towns, customers and/or depots, while arcs stand for real links (e.g., roads, pipelines) or symbolic connections. On valuated graphs, a value generally represents the cost of traversing an arc. Time windows associated with nodes or arcs may also be defined in some problems.
- The demands can be fixed or stochastic, can be associated with both nodes and arcs, and can be given for one or several product(s). Generally, demands appear in distribution problems, in which a certain amount of a given product must be delivered to certain nodes (i.e., customers) or must travel along a certain arc (i.e., delivery route). Demands are also a part of pick-up and delivery problems, in which demanded goods must first be picked up at a specific location and then be delivered elsewhere.
- The fleet generates constraints that affect the tours. A fleet can be heterogeneous or homogeneous. It can be composed of a single vehicle or several vehicles, whose use may, or may not, be limited by capacity, time or distance, for example. In addition, there may be dependencies between vehicles, drivers, products, nodes, and/or arcs. The

term fleet does not always refer to a group of vehicles. In fact, in some problems, there are no vehicles at all.

- The costs are generally fixed for the vehicle and variable for its use, in terms of distance travelled or time used. Costs can also include the service penalties incurred when a customer receives a late or incomplete delivery. Related to costs, profit can also be associated to given nodes and/or arcs with the profit being collected when the node is visited and/or the arc is chosen.
- The objectives can be multiple and diverse. The objective function can be computed for a single period or for several periods, though in the latter case, both vehicles and visits must be assigned to the different periods. The most common objectives include minimising the total distance travelled, the total time required, the total tour cost, and/or the fleet size, and maximising the quality of the service and/or the profit collected. However, when multiple objectives are identified, the different objectives frequently conflict. For this reason adopting a multi-objective point of view can be advantageous.

In [20], we address a bi-objective vehicle routing problem in which the total length of routes is minimised as well as the balance of routes, i.e., the difference between the maximal route length and the minimal route length (Figure 9). We propose a meta-heuristic method based on an evolutionary algorithm involving classical multi-objective operators. To improve its efficiency, two mechanisms, which favor the diversification of the search, have been added. First, an elitist diversification mechanism is used in cooperation with classical diversification methodologies. Second, a parallel model designed to take into account the elitist diversification is proposed. Our method is tested on standard benchmarks for the vehicle routing problem. The contribution of the introduced mechanisms is evaluated by different performance metrics. All the experimentations indicate a strict improvement of the generated Pareto set.

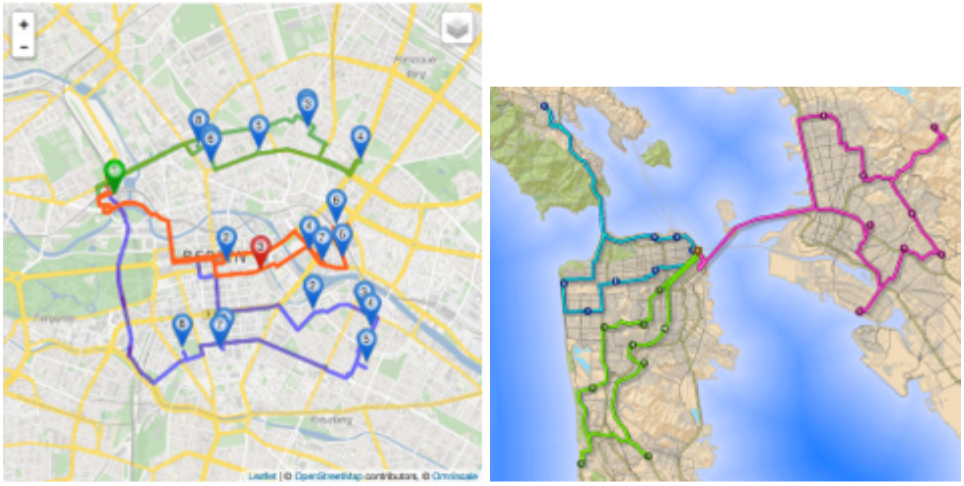

Figure 9: Results for some real-life instances

2.2.2 Packing and cutting problems

In logistic and transportation fields, packing problems may be a major issue in the delivery process. They arise when one wants to minimise the size of a warehouse or a cargo, the number of boxes, or the number of vehicles used to deliver a batch of items. These problems have been the subjects of many papers, but only few of them study multi-objective cases, and to our knowledge, never from an exact point of view. Such a case occurs for example when some pairs of items cannot be packed in the same bin. We have studied the problem in its one-dimensional version. Then we generalise our approach to two- and three-dimensional problems (Figure 10), and to more other conflict constraints, with the notion of distance between items.

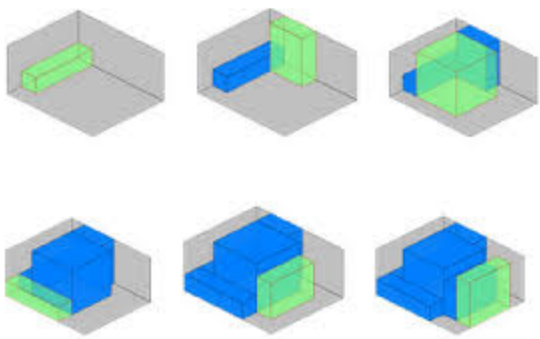

Figure 10: An example of 3D packing problem

Cutting problems occur when pieces of wire, steel, wood, or paper have to be cut from larger pieces. The objective is to minimise the quantity of lost material. Most of these problems derive from the classical one-dimensional cutting-stock problem, which has been studied by many researchers. The problem studied is a two-dimensional bi-objective problem, where rotating a rectangular piece has an impact on the visual quality of the cutting pattern. First we have to study the structure of the cutting-stock problem when rotation is allowed, then we will develop a method dedicated to the bi-objective version of the problem.

In another work, we address a bi-objective two-dimensional vector packing problem (Mo2-DBPP) that calls for packing a set of items, each having two sizes in two independent dimensions, say, a weight and a height, into the minimum number of bins [21]. The width corresponds to a “hard” constraint that cannot be violated while the height is a “soft” constraint. The objective is to find a trade-off between the number of bins and the maximum height of a bin. This problem has various real-world applications (computer science, production planning and logistics). Based on the special structure of its Pareto front, we propose two iterative resolution approaches for solving the Mo2-DBPP. In each approach, we use several lower bounds, heuristics and metaheuristics. Computational experiments are performed on benchmarks inspired from the literature to compare the effectiveness of the two approaches.

2.3 Smart factories

Due to globalisation and increased market and competition aspects on the one hand and the demands of customers on the other hand, products have become more complex and simultaneously the production systems have become more complex as well. A large proportion of the increased complexity falls into the software and algorithm development part and burdens the system engineers, system manufacturers and automation engineers more and more.

Smart factories can be a solution for that. The core idea is to transfer the human expert knowledge into the automation by developing intelligent, resilient and self-adaptive machines [30]. To realise this, appropriate software services and automation technology is needed. This covers machine learning methods, condition-monitoring and diagnostic algorithms and optimisation methods.

Smart factories can be seen as a compound of cyber-physical systems covering the fields of manufacturing processes and logistics. Cyber-physical systems integrate physical processes and embedded software and their communication based on the Internet of things, a network of physical devices embedded with software, sensors and actuators [31].

Smart factories require the fusion of production, information and communication technology. In such highly integrated autonomous systems, new challenges arise to process big data and the requirements for the process to be optimised in real-time [32, 33, 34, 35].

Examples of manufacturing processes that can be optimised in a smart factory follow below.

2.3.1 Optimisation of steel production

Contemporary material production strongly depends on numerical methods and computer support. An example of a material production process to which modern computational approaches are being intensively applied is continuous casting of steel (Figure 11). Here molten steel is cooled and shaped into various semi-finished products. To produce high-quality steel, it is crucial to properly control the metal flow and heat extraction during the process execution. They depend on several process parameters, such as the casting temperature, speed and coolant flows. However, finding the optimal values of process parameters is hard since the number of possible parameter settings grows exponentially with the number of considered parameters, the criteria are conflicting, and on-site parameter tuning is infeasible. Simulation-based optimisation is therefore a reasonable approach to this problem.

Figure 11: Steel production via continuous casting

We dealt with multi-objective optimisation of process parameters on a steel casting machine where the task is to find parameter settings that maximise the quality of the cast steel given the empirically defined quality indicators [50]. We developed an optimisation system consisting of a numerical process simulator and an evolutionary-algorithm-based optimiser, equipped with result visualisation capability (Figure 12). The optimisation is performed with respect to three indicators of the product quality, and trade-off parameter settings are returned as a result.

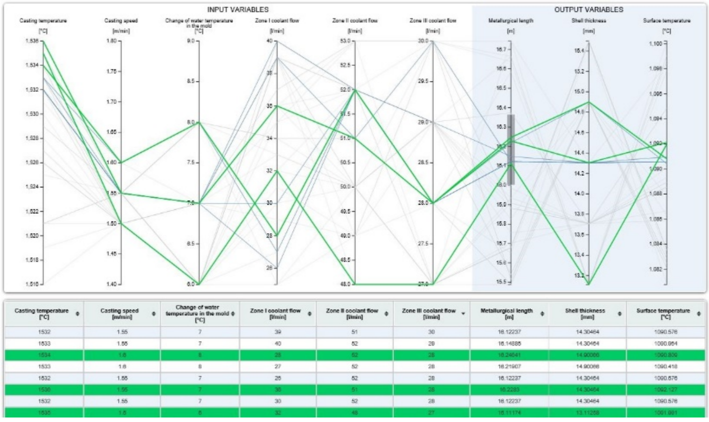

Figure 12: Visualisation of optimised parameter settings for steel casting

The system was installed at a steel plant where it allows for iterative improvement of process parameter settings. The results offer an informative insight into process properties and support decision making on parameter settings with respect to the user preferences. Overall, the system is becoming a key tool for increasing the production flexibility as it supports parameter tuning for various steel grades, product geometries, and preferences among criteria that typically change from one order to another.

2.3.2 Automated quality control in manufacturing of components for automotive industry

Quality-control requirements in automotive industry are very strict. Typically, the allowed proportion of defective supplied products is 1 ppm (part per million). To ensure the required quality of the supplied products, their quality has to be verified during and at the end of the manufacturing process. However, many quality control steps are even nowadays performed manually, which is time consuming. Moreover, human errors are present, and the results of manual inspection may be subjective.

To overcome the drawbacks of manual product inspection in graphite commutator manufacturing, we designed automated quality-control procedures [51, 52, 53]. A commutator is a component of an electric motor that periodically reverses the current direction between the rotor and the external circuit (see examples in Figure 13). It is, for example, used in fuel pump motors in vehicles.

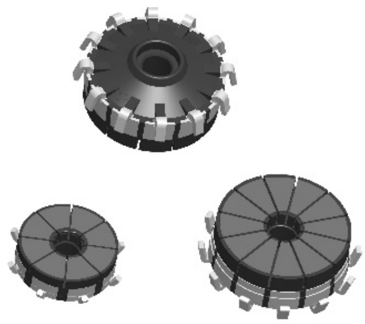

Figure 13: Examples of commutators

In this design process, three methodologies were involved: machine vision, data mining and optimisation. Using machine vision, digital images of products were taken and features extracted from the images. Data mining was applied to construct predictive models to assess the quality of the products from their images. Depending on specific quality control tasks, the models were either decision trees, regression trees or ensembles of both types of trees. Finally, numerous parameters of image processing and data mining were optimised to increase the accuracy and efficiency of the predictive models. It turned out that optimisation was a crucial step to balance between the accuracy of the resulting predictive models and their complexity. The resulting predictive models were implemented on embedded computer platforms and installed on production lines at a plant producing components for automotive industry (Figure 14).

Figure 14: Automated product quality control for automotive industry

In the evaluation period, the automated quality procedures in the form of optimised vision algorithms and predictive models were confirmed reliable and capable of detecting defective products at early production stages. This reflects in the improved product quality which brings a competitive advantage to the manufacturer.

2.3.3 Optimisation of an injection moulding process

Regularly reoccurring optimisation problems arise from the strong plastic industry situated around the campus Gummersbach of the TH Köln. These supply firms focus on producing small plastic parts for the automotive industry and must fulfill strict quality requirements. The utilised injection molding machines can be controlled by a certain number of parameters, such as temperature, pressure and more. Typically, these machines produce a large amount of parts and are adjusted by dedicated experts, which often have a great amount of experience. Even though, these experts sometimes fail to manually optimise a machine to the desired level.

An example is shown in Figure 15. In this particular case, a severe quality issue was present in an injection molding process of small gasket rings. These rings are used in the fuel system of a car and became leaky under certain conditions. Several million of these parts are delivered to an automobile manufacturer every year.

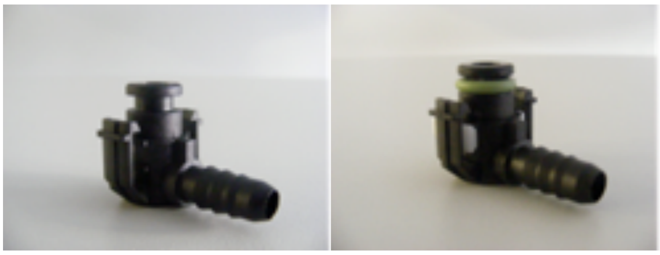

Figure 15: Injection molding process

The optimisation process in this case is particularly complex, as it involves real-world experiments and a large number of potential influencing parameters. These parameters also include not directly visible influences, like open windows, seasonality, employees and more. The process was optimised by means of statistical analysis with help of design of experiments (Figure 16). After identifying the most important parameters and defining a set of real world experiments, a linear regression and tree based analytical model was fit and analysed. Using a response surface methodology to visualise the results, it was identified that only three parameters were needed to explain the behavior of the system.

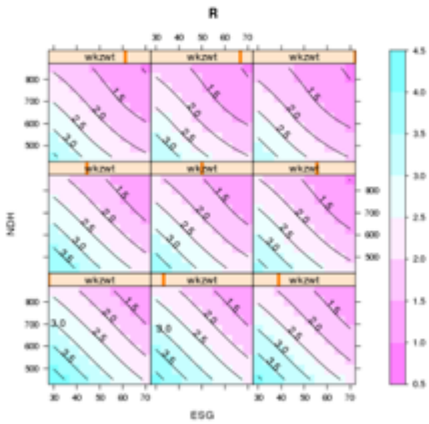

Figure 16: Real-world experiment

The resulting visualisations of the four-dimensional search space assisted in finding an optimal setting for the system (Figure 17). This setting resulted in an improved process quality and a homogenous, smoothened surface of the small gasket rings. The leakage problem wasthus solved.

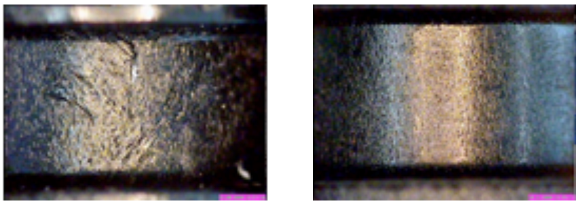

Figure 17: Optimal setting

2.4 Bio-medical

Bio-medical applications represent a great challenge for our society and numerous research entities of different specialities (biology, medical and information technology) are collaborating on specific themes such as genomic and post-genomic and molecular sampling.

2.4.1 Genomic and post-genomic studies

First, genomic studies aim at analysing genetic factors which may explain multi-factorial diseases such as diabetes, obesity or cardiovascular diseases. The scientific goal was to formulate hypotheses describing associations that may have any influence on diseases under study. Secondly, in the context of post-genomic, a very large amount of data are obtained thanks to advanced technologies and have to be analysed. Hence, one of the research issues was to develop analysis methods in order to discover knowledge in data coming from biological experiments. These problems can be modelled as classical multi-objective data mining tasks (association rules, feature selection). As the combinatorial complexity of such problems is very high and the quality criteria not unique, we proposed to model these problems as multi-objective combinatorial optimisation problems. Evolutionary approaches have been applied in order to cope with large scale problems. Nowadays the technology is still going fast and the amount of data increases rapidly.

2.4.2 Molecular sampling and docking in pharmacology

Flexible molecular docking is a very complex combinatorial optimisation problem especially when two components (ligand and protein) involved in the mechanism are both flexible. To deal with such highly combinatorial process in a reasonable time, approximate optimisation methods and massively parallel computing are necessary to use. The focus here is on the flexibility-aware modelling and the design and implementation of near-approached optimisation methods for solving the multi-objective docking problem on large hybrid clusters including Graphics Processing Unit (GPU) accelerators and Many Integrated Core (MIC) coprocessors.

The problem is to predict the optimal complex receptor/ligand according to chemical and geometric properties (Figure 18). Flexible docking is considered in determining which modifications of both molecules are possible.

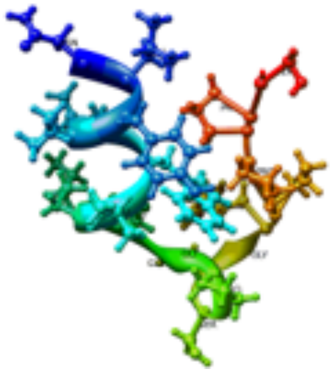

Figure 18: 3D structure of a molecule

Multi-objective mathematical models have been developed for the problem. The tri-objective model combines energetic criteria, surface criterion and a robustness objective. Design of parallel and distributed optimisation algorithms has been carried out for the problem [23]. The parallel algorithm has been deployed on large scale parallel architectures such as Grid'5000. This approach has been included in an open source Docking@Grid software (Figure 19). The developed software is used by many industrial customers such as CEA, Pasteur Lille and Servier.

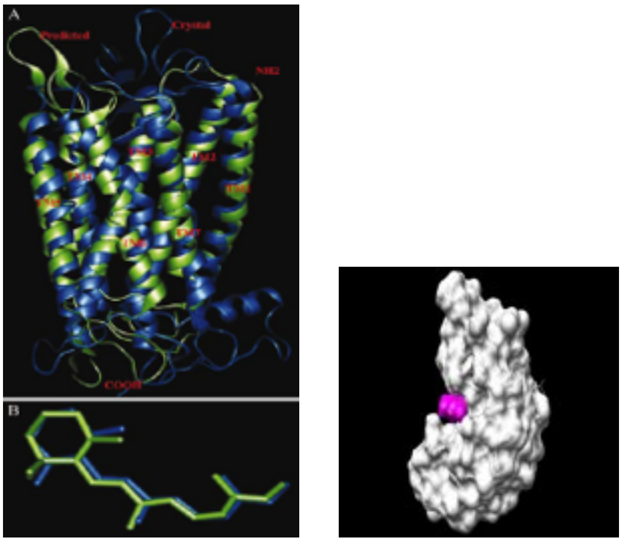

Figure 19: Protein docking problem

2.5 Engineering design

The engineering design process is a methodical series of steps that are used in creating new products and processes. Among the fundamental elements of the design process are the establishment of objectives and criteria, synthesis, analysis, construction, testing and evaluation. The process is highly iterative, where the goal is to acquire optimal result to a predefined objective.

When done manually (engineers repeat parts of the process many times before achieving satisfying results) this is a really time-consuming task. Due to time-consuming nature, it often produces less than optimal results. With the help of computers this process can be improved with regard to the speed and quality of the results. The main requirement that enables this is to have a mean to use the computer to evaluate solutions to the problem.

2.5.1 Lamination and casing optimisation for electric motor

Domel d. o. o. is the leading supplier of electric vacuum motors, DC motors, EC motors and components. In the design of modern electric motors high quality, low cost, long lifespan, and maintenance-free operation need to be achieved. The problem is how to set geometric parameters of an electric motor, as shown in Figure 20, to achieve the desired goals.

Figure 20: An electric motor

To this end, software tools for simulating electric motor power losses and casing rigidity are needed. They were developed and validated on real product with close collaboration of mechanical engineering experts. This was needed in order to develop a tool for optimisation of the independent geometric parameters of the rotor/stator lamination and motor casing as marked in Figure 21.

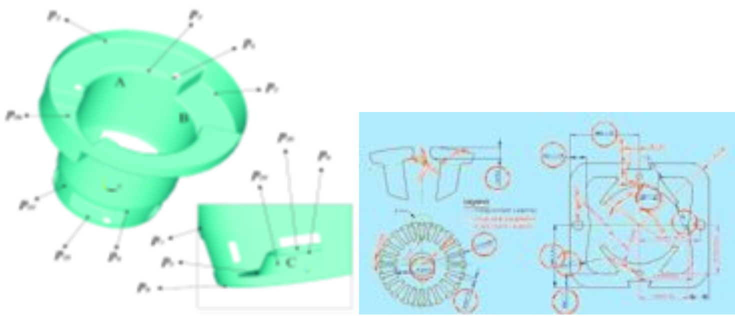

Figure 21: Geometries of casing, stator, and rotor

The final result was a lighter, cheaper, and more powerful electric motor. We were able to decrease the motor power losses up to 40%. Casing thickness of the electric motor was reduced from 1 mm to 0.8 mm, while maintaining all the desired characteristics (stiffness, rigidity, etc.). Due to smaller consumption of material a possibility of substantial reduction of production costs was achieved. The final casing is seen in Figure 22. The results are published in [27].

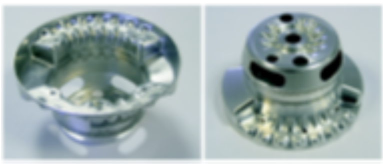

Figure 22: Optimised casing of the electric motor

2.5.2 Multi-objective design of energy supply systems based on renewables

Energy supply systems based on renewable energy sources, such as sunlight and wind, are becoming increasingly popular because of the rapidly changing situation on energy markets and undesirable pollution effects from burning fossil fuels. Nevertheless, designing these systems is a demanding optimisation task because of many decision variables involved, conflicting criteria to be taken into account, and complexity of evaluating candidate designs.

Design of such an energy supply system involves search for optimal system configurations that maximise technical performance measures and minimise the overall costs of the system. Designers typically use stochastic optimisation methods coupled with numerical models of the energy supply systems, and handle multi-objective optimisation problems in a simplified, single-objective manner, either dealing with the weighted sum of objectives, or with the main objective only and transforming the remaining ones into constraints.

We studied the design of an energy supply system for a residential building [54]. A scheme of the system can be seen in Figure 23. Its essential components are photovoltaic modules producing electricity from solar energy, batteries storing electricity and making it available during the periods of low or no solar illumination, and a diesel aggregate to generate electricity in the peak demand periods. Furthermore, the regulator arranges the battery charging in such a way that improper operation states are prevented and appropriate life period of the batteries is ensured. The load can be supplied with electricity either from the batteries via the inverter or from the diesel aggregate. The aggregate can simultaneously supply energy to the load and charge the batteries via the charger if needed.

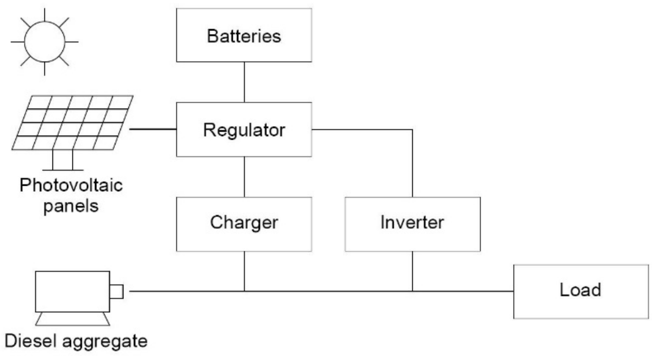

Figure 23: A scheme of the energy supply system

The design variables include the type and the number of photovoltaic modules, the type and the number of batteries, and the diesel aggregate power. There are two conflicting design objectives: to minimise both the proportion of unsupplied energy and the overall system costs consisting of the initial investment, operation costs and maintenance costs.

We created a software tool to assist the designers in finding trade-offs between the system performance and its costs. Its core component is an evolutionary multi-objective optimisation algorithm. It uses a Matlab simulation module to evaluate candidate configurations. An example of a result in the objective space is presented in Figure 24.

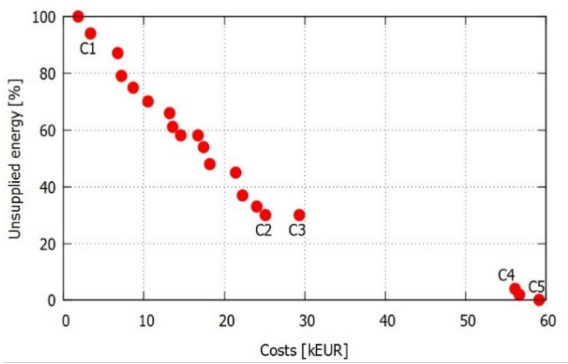

Figure 24: Solutions representing trade-offs between costs and unsupplied energy

The tool is capable of considering technical characteristics and limitations of the system components, their prices and life periods, the yearly solar illumination profile for a given location, and the daily demand profile of the load connected to the supply system. Given these data, it effectively supports feasibility studies and sensitivity analyses that are of interest to potential investors into energy supply systems.

2.5.3 Development of a robust gas sensor

Sensors for in-situ measurements of exhaust gases of large combustion processes are situated in toxic environments and need to be recalibrated to changing conditions of the gases. In these cases, complex multivariate modelling methods are required, which allow a free parametrisation and good interpretability. The results further need to be highly robust, as they are used to control the combustion process (Figure 25). Due the changing conditions and decreasing sensor quality over time, an optimisation process which adapts the model continuously to the changing conditions is needed.

Figure 25: Robust gas sensor

In the carried-out study, several methods were used to tackle this problem. First it was tried to identify the functional relationships between the gases and sensor measurements in an experimental setup. By the use of high quality open source software packages in R, as well as commercial products such as SAS/JMP and Minitab, a process- and data analysis was conducted. The data analysis (Figure 26) was based on mathematical and statistical methods and relies on quantifiable measurement values. Screening design and interactive visualisations helped to identify three relevant process parameters.

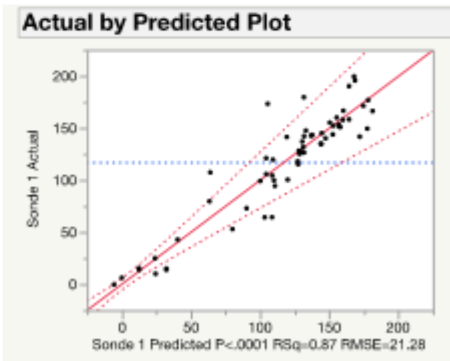

Figure 26: Data analysis

The resulting mathematical model was implemented and verified in a real-world production system (Figure 27). The model showed significant improvements on the system and the results were discussed with project leaders, technical experts, and users to reach a high acceptance rate. Moreover, software tools were introduced to the sensor design process, which allow an individual selection between exactness and robustness of the solution and provided a high amount of understandability, simplicity and interpretability.

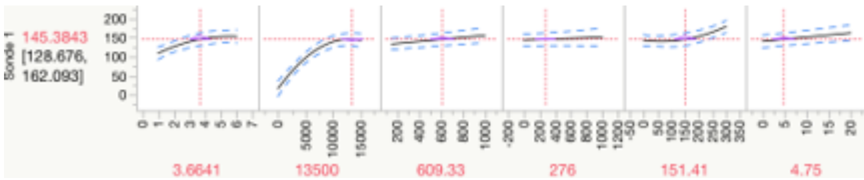

Figure 27: Experiment on real-world production system

2.5.4 Launch vehicle design

The design of launch vehicles involves several disciplines and is customarily decomposed into interacting submodels for propulsion, aerodynamics, trajectory, mass and structure. Each discipline may rely on computing-intensive simulations such as Finite Element analyses for the structure discipline or Computational Fluid Dynamics analyses for the aerodynamics discipline. The launch vehicle performance estimation which results from flight performance, safety, reliability and cost, demands coupled disciplinary analyses (Figure 28). The different disciplines are a primary source of trade-offs due to the antagonist disciplinary effects on launcher performance.

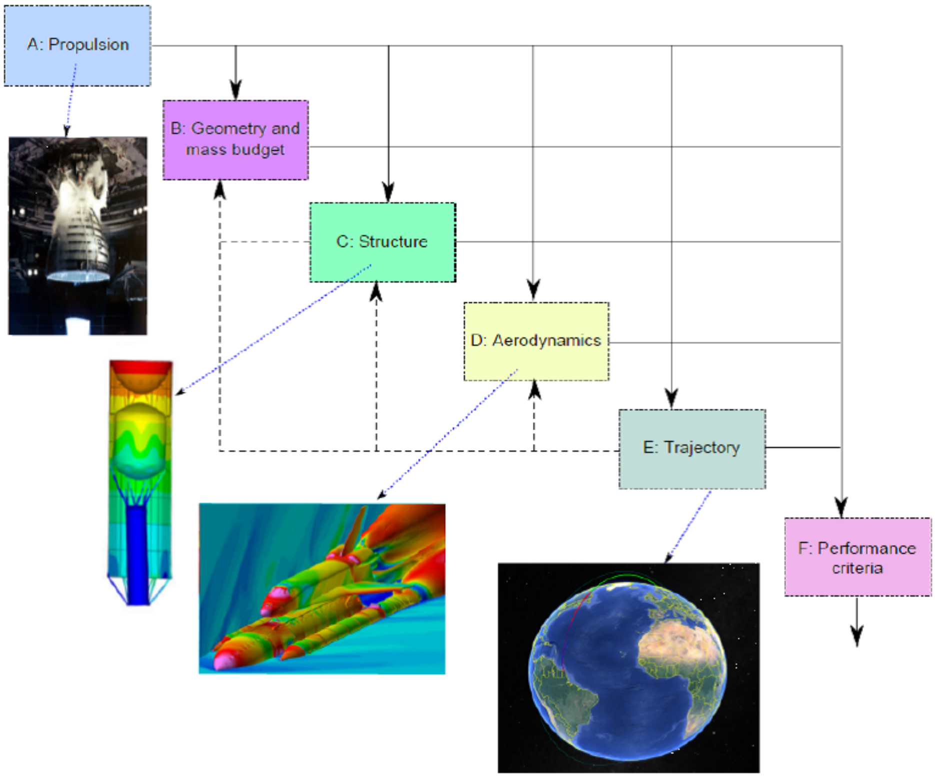

Figure 28: Example of launch vehicle design process

The classical engineering design method consists of loops between different disciplinary optimisations. At each iteration of this loop, every discipline is re-optimised based on the updated data from the previous discipline optimisations. Due to the possible antagonist discipline objectives, a difficult search for a compromise between these conflicting tasks needs to be performed. For instance, the aerodynamics discipline tends to decrease the diameter of the stages in order to decrease the drag during atmospheric flight, whereas the structure discipline tends to increase it for stability reasons. Such design is difficult because the couplings between disciplinary analyses generate large volumes of calculations, many heterogeneous design variables need to be controlled and the compromise between disciplines needs to be formulated. Consequently, the design of space transportation systems needs dedicated methodologies to manage the complexity of the problem to solve. It needs to handle the interdisciplinary couplings between the different disciplines to facilitate the research of compromises and to improve the efficiency of the overall design process.

A family of adapted techniques, called Multidisciplinary Design Optimisation (MDO), has been developed to help solve this problem. MDO is a set of engineering methods to handle complex design problems. MDO deals with the global design problem as a whole unlike classical engineering design methods (Figure 29). It provides an informed decision framework for system designers. MDO methods take advantage of the inherent synergies and couplings between the disciplines involved in the design process to decrease the computational cost and/or to improve the quality of the global optimal design [25]. Unlike the sequential disciplinary optimisations performed with classical design methods, the interactions between the disciplines are directly incorporated in the MDO methods. However, the complexity of the problem is significantly increased by the simultaneous handling of all the disciplines. To subdue this complexity, various MDO formulations have been developed. In the 90's, several surveys classed MDO formulations into two general types of architectures: single-level methods, and multilevel methods. Multi-level approaches introduce disciplinary level optimisers in addition to the system level optimiser present in single-level methods in order to facilitate the MDO problem convergence.

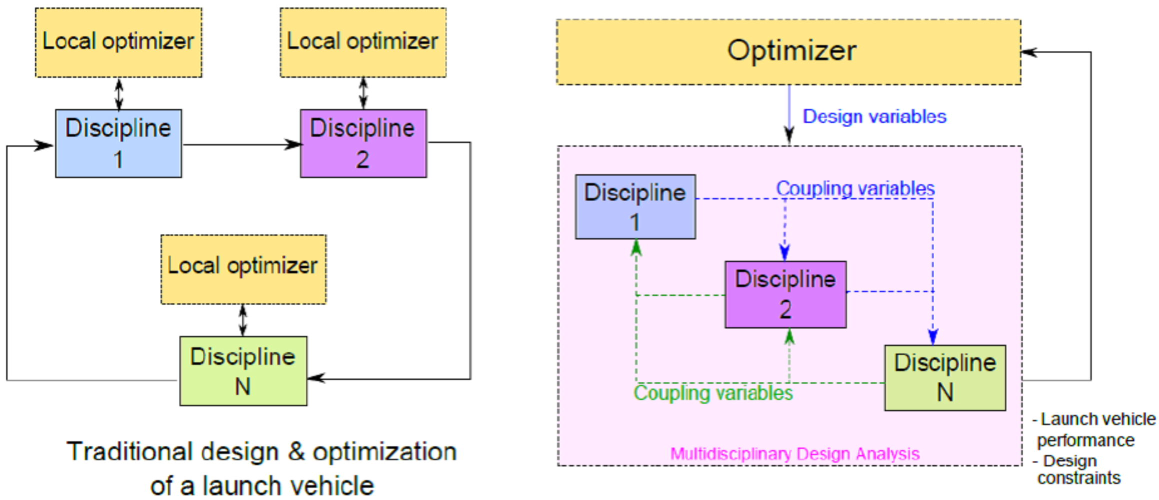

Figure 29: Example of traditional process (left) and MDO process (right)

2.5.5 Network design

With the extraordinary success of mobile telecommunication systems, service providers have been affording huge investments for network design and infrastructure. Mobile network design is of outmost importance, and is thus a major issue in mobile telecommunication systems. In fact, with the continuous and rapid growth of communication traffic, large scale planning becomes more and more difficult. Hence, automatic, interactive and self-adaptive optimisation algorithms and tools would be very useful and helpful. Advances in this area will certainly lead to important improvements in terms of quality of service, network management and cost.

Engineering of mobile telecommunication networks endures two major problems: the design of the network, and the frequency assignment. The network design problem can be formulated as a multi-objective constrained combinatorial optimisation problem. We propose an evolutionary algorithm that approximates the Pareto front of the problem. Advanced techniques have been used such as Pareto ranking, sharing and elitism. The evolutionary algorithm has been implemented in parallel on a network of workstations to speed up the search. To evaluate the algorithm performance, we have introduced two new quantitative indicators: the entropy and the contribution. Encouraging results are obtained on real life problems [24].

2.6 Smart grids, cities and homes – Energy-aware systems

With the smart grid revolution, the whole market of energy production and consumption changes. Various types of renewable energy with changing energy production profiles depending on weather and daytime make the whole system, including the prices, more dynamic. So optimising the energy consumption based on the current prices becomes more and more economically relevant. For these optimisation tasks the development of smart metering devices, home automation systems and other methods for the adaption of production and consumption processes is necessary. These methods make it possible to plan resource intensive processes for best economic results (e.g., lower energy costs) while maintaining the existing quality standards (industrial applications) or comfort (home users).

On the other hand, there are large parts of the energy market which have energy demands that are totally inelastic with respect to the market (i.e., the energy demand does not follow the price of the energy itself). Especially the usage of electricity for light, heating or cooling fall in this category. So, the development of new control methods for more efficient devices is important.

The supply of electricity for this base load is still provided by large coal-fired power plants and this will remain for longer periods of time. Therefore, it is necessary to further improve the capabilities of these power plants to reduce the environmental pollution. Especially improvements regarding the efficiency of dust separators contribute to this aspect.

In the following sections, we describe our research contributing to these topics. Starting with a new optimisation process for faster development of an efficient refrigerator control, continuing with efficiency improvements of dust separators, energy efficient monitoring of drinking water systems and closing with a highly developed home automation system, which incorporates, beside the energy consumption, also the production and storage capabilities of electric cars, batteries and photovoltaic panels.

With the smart grid revolution, house energy consumption will play a significant role in the energy system. Home users are indeed responsible for a significant portion of the world's energy needs, but are totally inelastic with respect to the market (i.e., the energy demand does not follow the price of the energy itself).

2.6.1 Fast temperature simulation and effective control optimisation

Gorenje is one of the leading European manufacturers of household appliances (see Figure 30). Achieving the lowest possible energy consumption of refrigerator/freezer, while the desired temperature is sustained is one of their most important goals.

Figure 30: Refrigerator

Since mathematical modelling is practically impossible, a simulation tool for quick estimation of temperatures inside the refrigerator at different modes of regulation was developed (see Figure 31). Afterwards, an advanced optimisation algorithm with integrated simulation tool for finding the optimal control-setting was developed. This enabled for the appliances to quickly and accurately react to environment changes.

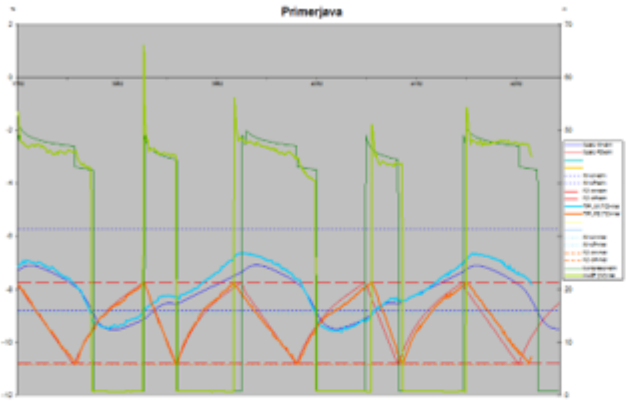

Figure 31: Diagram of estimated temperatures

This enabled optimal regulation of a refrigerator. As a side effect this also enabled easy and quick adaptation to a new product and shortened its development. So, development costs of a refrigerator can be crucially reduced by replacing slow thermal processes within the appliance with validated simulation tool as shown in Figure 32. The results are published in [28].

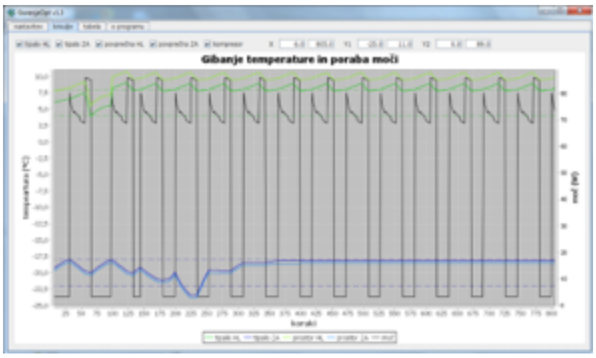

Figure 32: Simulation tool for refrigerator thermal processes

2.6.2 Reduction of emissions from coal-fired power plants

Operators of coal-fired power plants are faced with the increasing demand for the reduction of emissions. A core issue is to reduce the amount of particles in flue gases. Due to their robustness, one frequently used solution are cyclonic dust separators [40]. They are intended to induce a cyclonic type of gas stream via a cylindrical shaped device. Thus, the centrifugal force will push particles to the outer walls of the device, where they can fall down towards a dust collector. The cleaned air typically leaves the cyclone through an exit pipe at the top. The typical geometry of a cyclonic dust separator is shown in Figure 33. The parameters of this geometry influence the separators performance and has to be optimised.

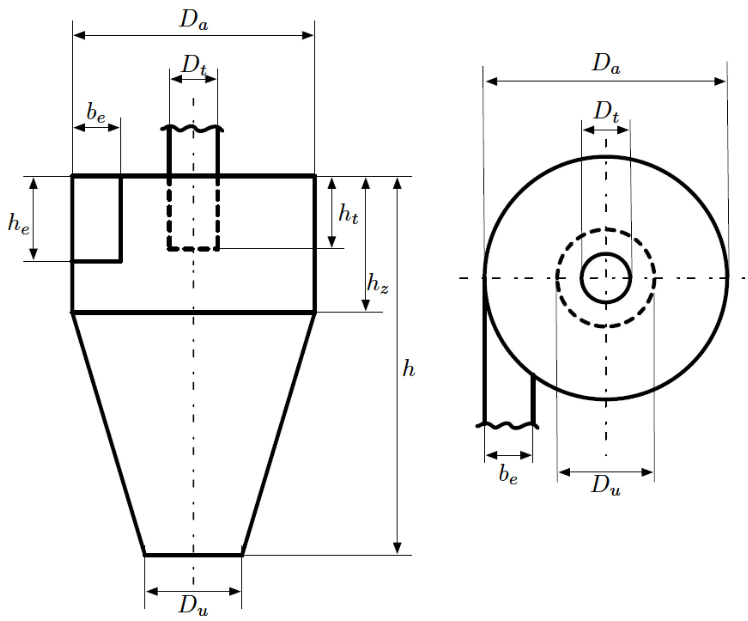

Figure 33: Typical geometry of a cyclonic dust separator

While cyclonic dust separators are conceptually simple and robust with respect to operating conditions (temperatures, pressures), the exact behaviour of flue gases is based on complex, non-linear fluid dynamics. This requires to use either very rough, analytical models (which are fast yet inaccurate) or else complex CFD simulators (which are potentially more accurate but time-consuming) [41, 42]. Evaluations by real-world experimentation is usually infeasible, or strictly restricted to heavily down-scaled experiments, e.g., based on 3D-printing [43]. Furthermore, the performance of cyclonic dust separators depends on their geometry (or shape). The performance is also multi-objective [44]. That is, it can be measured based on separation efficiency, pressure loss or manufacturing and maintenance costs. Finally, operators would like to understand why certain solutions are suggested by an optimisation algorithm. They would like to have a sound reason, such that they are more confident to invest the required computational or material resources for testing the proposed solution. All these issues render the cyclone optimisation problem (COP) a challenging issue.

To deal with the above issues, one core approach is the use of surrogate-based optimisation. To that end, we can employ different types of models: analytical models, CFD models and data-driven surrogate models. One framework that allows to combine these diverse data-sources is Sequential Parameter Optimisation [45]. It enables to use surrogates and ensemble techniques to derive accurate yet cost-efficient models of the COP. A schematic of a typical SPO process for the COP can be found in Figure 34.

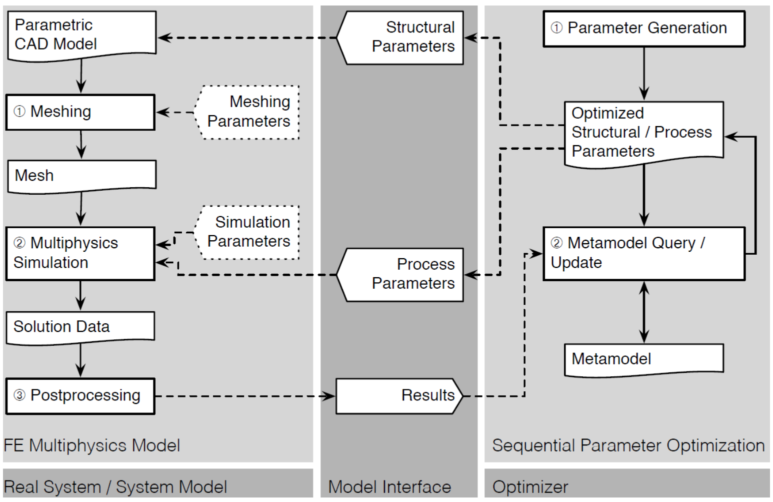

Figure 34: Model based optimisation with SPO for the solution of multi-physics optimisation problems, such as the COP

Recently, an ensemble approach was suggested to combine various data-sources with a hierarchical modelling approach, employing stacked generalisation (stacking) [46, 47]. With the resulting ensemble model, standard optimisers (often based on heuristics such as evolutionary algorithms) can be employed to search for promising candidate solutions. This framework further allows to take a multi-objective approach: Separate models can be trained for to, e.g., capture the influence of geometry parameters on efficiency and pressure loss [48].

Multi-objective optimisers can then search for the Pareto front based on the surrogate models, or else, some set-based infill criterion (e.g., Expected Hypervolume Improvement) can be subject to single-objective optimisation.

While these approaches are potentially very powerful, they do not address the requirement for creating understandable solutions. Some general information (such as variable importance) may be deduced from most standard surrogate models. Further, ensembles based on stacking also provide information on which models contribute how much information for the overall model. But none of the more frequently used models can provide human-readable formulas that can be easily interpreted by users or operators. Genetic Programming can potentially resolve that issue by specifically searching for well-fitting formulas of low complexity [49].

These studies show how the analytical model, CFD simulation, 3D-printing experiments and various data driven surrogates can be combined in a stacking model. As a demonstration, improved geometries are generated via an evolutionary algorithm. The results are heavily affected by the complex nature of the underlying data sources. E.g., 3D-printed cyclones have been tested via laboratory experiments and were subject to considerable noise influences. Analytical models were further problematic, due to a counter-intuitive effect of changing the flue gas exit pipe immersion. CFD models provided more reliable results, which however were sparse due to the computational cost. Still, promising new cyclone geometries could be derived.

As a further result, the stacked generalisation model robust and flexible with regards to integrating additional data into the optimisation process. Interpretability and understandability (via Genetic Programming) as well as an extension to multi-objective problems are still open issues.

Preliminary results have been published in [43]. An updated publication is currently under review.

2.6.3 Water quality management and event detection

The quality of drinking water is a major concern as it directly affects the public health and safety. Hence, highly strict and demanding water quality regulations have been imposed. In addition, the protection of the critical drinking water infrastructure against terrorism is a core requirement. The complexity of ensuring hygienic drinking water is widely influenced by extreme weather fluctuations caused by global warming. A study conducted by the DVGW – German Technical and Scientific Association for Gas and Water clearly showcases the effects of climate change on the drinking water supply [36]. With the current state of knowledge, moderate climate changes are to be expected which directly affect the quality and availability of drinking water. The climate gets hotter and drier in summer while in winter, milder and wetter than the previous years. This will change the expected precipitation pattern [37]. The consumption of drinking water in the Federal Republic of Germany is falling in contrast to the global trend as it is evident in Figure 35. This creates problems that do not exist in other regions. In addition, sedimentation in underused water networks will lead to misleading and unreliable predictions for the future water demands. On the whole, the uncertainties get bigger with the variation in the scale of various climatic factors (temperature, precipitation, evaporation, etc.). It is necessary to timely respond to emerging trends, allowing for long-term operational and investment decisions. Also, any deviations in the water quality if present should be accurately detected as early as possible. This will enable the water suppliers with easy proactive maintenance and there by providing safe drinking water to the public.

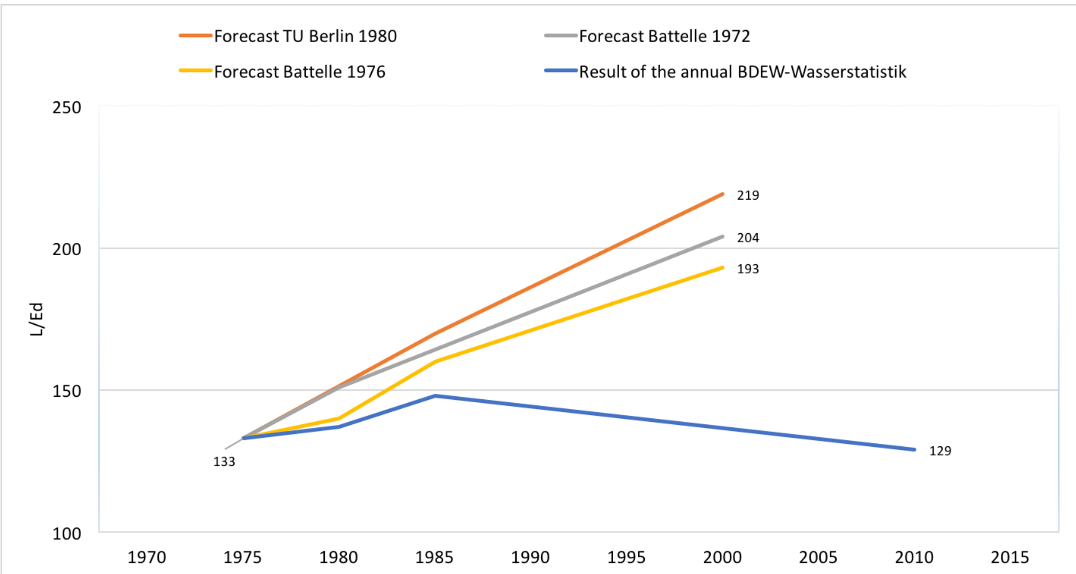

Figure 35: Drinking water consumption in Germany. Forecasts from the 1970s until recent consumption. Due to the wrong forecasts, the drinking water network is now too large and this demands additional flushing of water.

In order to cope up with the challenges, the water suppliers are constantly focusing on the protection of the drinking water supply and distribution systems against accidental or purposive contamination. The current technological advancements have made more and more affordable online sensors available. The recent rapid breakthrough in robust statistical analysis, along with more low cost online sensors have enabled the development of online Contamination Warning System (CWS) widely called as Event Detection Systems (EDS). Such CWS has been developed by the US Environmental Protection Agency (EPA) [38, 39]. It aims to monitor the quality of drinking water in real time. However, there is huge scope for improvement which focuses on various Computational Intelligence (CI) and Machine Learning (ML) techniques which can enhance the performance of the prediction models enormously.

Our research team currently works on this problem by implementing various Computational Intelligence (CI) and Machine Learning (ML) techniques. For this purpose, a testbed is setup on the research facility metabolon shown in Figure 36. The testbed includes a water distribution system connected with various online sensors and servers as in Figure 37. This testbed enables simulation of various kinds of impurities which can be studied exhaustively. The goal is to build a robust online prediction model that identifies true undesirable variations in the water quality. At the same time, false alarm rates have to be very low.

Figure 36: Left - Our research facility: metabolon. Right - Planned water distribution test stand

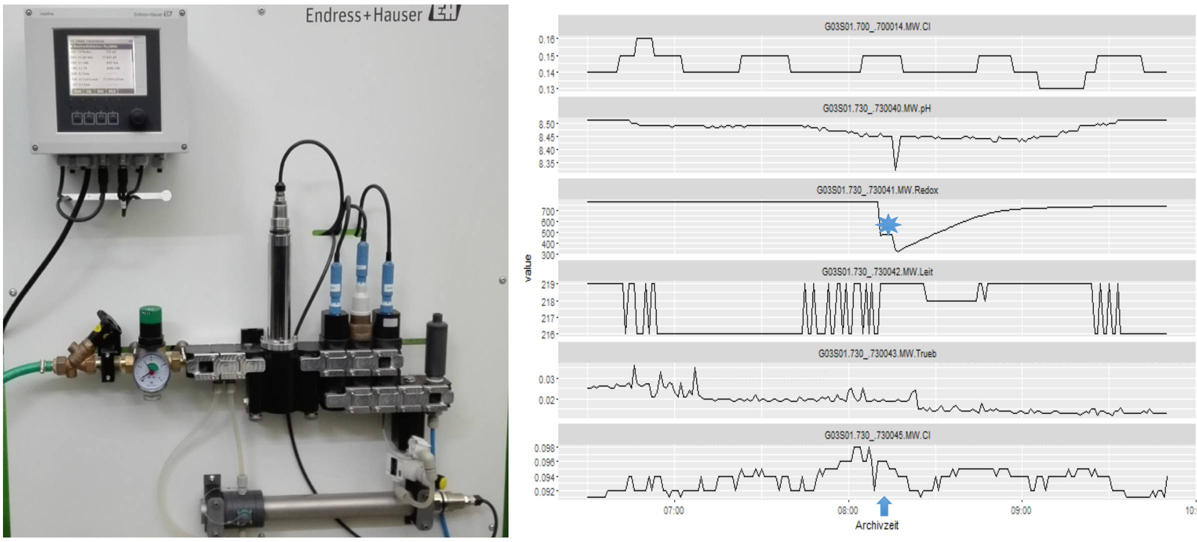

Figure 37: Left - Online measurement of water quality with various sensors. Right - A sample event identification from one of our prediction model

The early studies show promising, reliable and robust results. The ongoing research focuses on the implementation and comparison of the performance of various CI and ML prediction models that takes into account multiple uncertain climatic and environmental factors. In order to improve the reliability aspect of the model prediction, care is taken such that the false alarm rates are very low.

2.7 Demand side management in smart homes

The whole energy generation and distribution system performance can be improved by optimising the house energy management (Figure 38). Those problems are concerned by multiple objectives such as cost and users' comfort, and multiple decision makers such as end-users and energy operators. We propose a home automation system that can monitor appliance scheduling in order to simultaneously optimise the total energy cost and the customer satisfaction. The key challenge is to propose new optimisation models and new hybrid optimisation algorithms to the demand side management of smart grids in a context of uncertainty and in the presence of several conflicting objectives. Those complex optimisation problems are also characterised by the presence of both continuous and discrete variables.

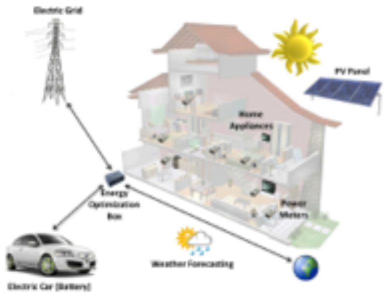

Figure 38: Demand side management in a smart home

In [22], a multi-objective model for the residential DSM is proposed. The smart home is composed of appliances, a battery and a photovoltaic panel. The resolution of this model is a matheuristic based on combining a multi-objective evolutionary algorithm and an exact liner programming solver (CPLEX). Candidate solutions in this hybrid approach are incompletely represented in the representation, and the exact solver is used as a decoder to determine the missing parts in an optimal way. In our case, hybridisation involves solving a Mixed Integer Linear Programming (MILP) sub-problem by CPLEX managing the battery and the photovoltaic panel constraints. Through case studies, it is shown that the coordination between the photovoltaic panel and the battery is effective to reduce the total electricity cost, the discomfort and the standard deviation of power consumed especially in summer conditions.

3 Case study: Cardiology application

The SYNERGY project focuses on enhancing multi-objective optimisation through parallel computation and surrogate modelling. Pursuing this goal, the project partners have, in addition to other activities, selected the electrocardiogram (ECG) simulator tuning as a benchmark problem to exploit the synergistic effects of parallelisation and surrogates in solving multi-objective optimisation problems [55]. This section presents the background on ECG and its simulation, the optimisation task, and the synergistic approach of the partners working on the problem.

3.1 Introduction and motivation

ECG is a non-invasive procedure used to monitor the heart's electrical activity that arises from rhythmical contractions of the heart muscle (myocardium) pumping the blood throughout the body. Electrical currents are generated in myocardium as side effects of the contractions. Since the human body is electrically conductive, electrical currents can be detected on the body surface where they are measured by an ECG machine. ECG readings can be observed for deviations of ECG shape from the typical or normal ECG shape, as some diseases and health conditions cause observable and well known symptoms in the ECG.

Although the normal ECG shape and some typical defects are well known, the transfer function that maps the ECG measured on the body surface to individual cells of myocardium is not known. This function is influenced by the complex heart geometry, the changes of geometry in time (heart contractions), the difference in myocardium cells, the geometry and electrical conductance of the surrounding tissue, and other factors. Gathering additional knowledge on the transfer function would help improve ECG based diagnostics and enable better prediction of health condition, based on the ECG reading.

3.2 ECG simulator

One of the basic tools for studying the transfer function and unveiling additional knowledge on heart activity is a computer simulator of the human heart. We use the simulator [56, 57] that was utilised to gain new insights into possible shapes of action potentials (APs) in myocardium. APs represent voltage as a function of time for an individual cell. Voltage is measured as the potential difference of cell exterior against the cell interior. APs of human heart cells can be modeled as a system of non-linear time-dependent differential equations [58], which is quite time consuming. Therefore, it was approximated by a combination of exponential functions [59] to make the computer simulation of a large number of cells feasible. The combination of exponential functions was further refined [57] after it was discovered it contains a physiologically unrealistic symmetry. The AP function for each layer in the considered 3D model of the heart (Figure 39) is parameterised with nine parameters.

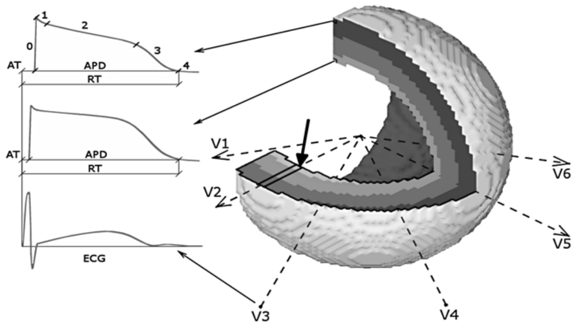

Figure 39: 3D model of the heart

3.3 The optimisation problem

The optimisation goal is to fine-tune the simulator to produce realistic ECGs. Out of nine AP function parameters, two have predefined values, while the remaining seven are subject to optimisation. As three layers of myocardium cells are considered in the model, the total number of optimisation variables is 21.

The simulator output is assessed by comparing the output of the simulation, i.e., two simulated ECGs at different positions on the body surface, with measured ECGs at the same locations on the body surface. The objectives are to maximise the Pearson correlation coefficients between the measured and the simulated ECG signals for the two positions. The simulator is unable to simulate the actual ECG amplitudes as its focus is on the signal shape. Therefore, the objectives were selected to ensure that the difference in ECG amplitudes is not considered, while the features of the simulated ECGs should match the measured ECG features in time.

3.4 Synergistic approach

Joint work on the ECG simulator tuning problem consists of contributions by all SYNERGY partners as follows. JSI provides the simulator and the optimisation algorithm, and performs experimental tuning of the simulator-optimiser environment. USTL focuses on the parallelisation of both the simulator and the optimisation algorithm. CUAS studies the performance of various modelling techniques for solving this problem.

We use an augmented version of the simulator [56, 57] integrated with the AMS-DEMO (Asynchronous master-slave differential evolution for multi-objective optimisation) algorithm

[60]. The initial optimisation results indicate the simulator is still unable to reproduce the ECG signals in their initial part (the first 50ms of the heart beat) with sufficient accuracy. A comparative analysis of various surrogate modelling techniques (Kriging, Support vector regression, Random forest) applicable to this problem also provides beneficial insights into the current performance of the simulator [61]. On the other hand, the two-level parallelisation substantially reduces the execution time of the optimisation runs [55]. We believe that further improvements are possible both at the level of the simulator accuracy and the optimisation algorithm tuning. In particular, the speedup due to parallelisation should allow a refinement of the time and space discretisation in ECG simulation. The ability of performing faster and more accurate simulations can also help building better surrogate models for the fine-tuning of the ECG simulator. These hypotheses will be tested in our future work.

4 Conclusion

This report shows that many application domains can be approached with multi-objective optimisation and surrogate-models. It presents examples of complex optimisation problems in science and industry. The reported strategic large-scale applications belong to different domains where multi-objective optimisation and surrogate-assisted modelling are crucial. The explored domains concern: health, smart factories, smart buildings & homes, smart cities & communications, and smart use of resources. The SYNERGY partners will use the reported use cases in promoting smart multi-objective optimisation among potential academic and industrial users.

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