### OPTIMAL OPERATION: SCHEDULING, ADVANCED CONTROL AND THEIR INTEGRATION

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### Abstract

This paper discusses the integration of scheduling and advanced control. It gives a brief overview on the challenges for today's production systems, analyses the functional hierarchy for plant operations and discusses similarities and differences between the two domains. Possible benefits of a closer integration are outlined and the realization of a tighter integration is discussed. This is followed by practical integration aspects and before the conclusions the main industrial requirements are highlighted.

#### Keywords

Advanced control, scheduling, online optimization, moving horizon techniques, integration, industrial challenges.

### 1. Introduction

In times when information technologies enable theoretically unlimited possibilities to share and to use data and when optimization and computing technologies have reached the state that many industrial-size problems can be solved within a reasonable times, the question arises how to create added value from these enhanced capabilities? The industries of today are facing merciless global competition and many production plants are under strong pressure to produce cheaper, faster and more flexibly in order to keep up their profitability. More products need to be individually tailored and lead times are shorter in order to reduce the cost and risk of too high inventories, as well as securing profitability in an environment of fluctuating prices of raw-materials and products. All these factors point towards smaller batch sizes and shorter campaigns, which increases the challenge of keeping the production costs low and calls for solutions that can adapt to changing situations.

At the same time as much research effort is devoted to improving existing mathematical algorithms, new business strategies, requirements and models appear, driven by economic, environmental and regulatory factors, challenging traditional approaches and production philosophies. Energy plays a more important role than ever, not only because of its high cost and volatile pricing (spot market prices can vary by a factor of more than 20 depending on the point in time and are even negative occasionally) but also due to the fact that the availability of energy may be restricted in the future. This also calls for agility and flexibility and optimal management in order to make process systems more energy efficient by combining the available information in an intelligent way, as well as identifying and embedding new performance indicators (KPIs) or measures into the decision making processes.

In this paper, the needs and opportunities of advanced process control and production scheduling and their integration are discussed. We stress the common factors of the two domains that result from the solution of optimization problems online, under uncertainties and on a finite, moving horizon.

#### Motivation

The ongoing "software revolution" in industry has resulted in many companies investing in managing the process data in a centralized way, for instance through process information management systems (PIMS). To access, monitor and analyze the relevant data in a useful way, Manufacturing Execution Systems (MES) or Collaborative Production Management (CPM) solutions have recently seen a significant growth and are in fact one of the fastest growing businesses in the process industries. Their mission is to fill the gap between the process control systems and ERP systems. According to ARC (2009) the three main categories of CPM solutions are:

- Plan & Schedule
- Direct & Operate
- Track, Analyze & Inform.

The main task of the first category of tasks "Plan & Schedule" is to determine what products to make, when to make them, and what equipment to use. The segment consists of functions such as short-term production planning, plant simulation and modeling, electronic routing, finite capacity scheduling, etc. The second category "Direct & Operate" focuses on the need to find new and better ways to control process equipment and to operate the plant, and includes, among others, recipe management, dispatching, electronic work instructions, resource management, workflow management. The purpose of the third category "Track, Analyze and Inform" is to gather, store, organize, and communicate data and information, including data collection, performance analysis, enterprise-level reporting, order tracking, messaging, and product genealogy.

In this paper the main focus is on the two first categories. Production scheduling and advanced control are not isolated applications but must work seamlessly together in order to support the operation of a production facility (Fig. 1).



Figure 1. Logical view of a production system (Source: ARC, 2010)

#### 1. The functional hierarchy of process operation

Figure 2 shows a simplified functional hierarchy of the planning, scheduling and control structure of a *batch* production plant. Continuous production can be considered

as being a batch process with a very long duration of the main phase "regular continuous production" but where nonetheless other phases as start-up, change of the operating mode, shut-down are present, so this scheme covers all chemical and biochemical production processes, with different realizations of the functions depicted by the different blocks.



Figure 2: Functional hierarchy of batch production

On the planning layer, the production targets are set, i.e. how much of which product should be produced within a certain period of time. The scheduling layer transforms this plan into planned batches with certain sizes, assigns equipment to the batches and sequences the batches. The execution of the batches is governed by the recipe control system which ideally makes use of production recipes which are generated from general recipes based upon the scheduling decisions. The recipe execution triggers the phases of the recipes and provides the set-points for the process parameters in the phases as well as constraints if a subordinate continuous optimization is implemented. The continuous optimization layer optimizes the trajectories during the phases of the batch. If the production is essentially continuous, this role is taken by the RTO layer that determines an optimal operating point of the plant, using the available information from measurements and state estimators. The advanced control layer implements the optimal trajectory (or set-points in continuous production), typically applying linear model-predictive control (MPC), and provides reference values to the lowlevel (usually single-input-single-output) controllers. Up to the recipe control layer, feedback is provided mostly in the form of continuous measurements or estimates. This information is also used to trigger the transition between the steps in the recipe (including re-work or abnormal termination of a batch). From the recipe control layer upward, only condensed information is provided (endtimes or durations of phases or batches, quality information). Equipment availability has to be transmitted through this functional hierarchy up to the scheduling layer. From scheduling to planning, usually condensed information, e.g. the actual production figures as well as updates on resource requirements (durations of operations, energy consumption) is provided.

Of these layers, the continuous optimization layer and the advanced control layer may not be present. In those cases fixed reference values for the phases of a batch are provided to the low-level controllers and implemented more or less well - by these. The scheduling layer in the majority of the plants is implemented by humans who take the necessary decisions to convert production targets into real operations, with or without computer support. The recipe execution may be simple, using fixed, pre-defined recipes for each product, or more advanced with generic recipes defined for the products from which more detailed ones are generated automatically. Triggering of the transitions between the steps also is often done not automatically but by the operators following operating rules. The execution of the sequences of steps in batch production nowadays is mostly automated. If the plant is essentially continuous, the infrequent shut-down and startup phases usually are not automated and their execution depends crucially on the skills of the operating crew, which therefore are trained using model-driven operator training systems (Schaich and Friedrich, 2004).



Figure 3. Traditional 5-level automation pyramid

In fact, the functional hierarchy shown in Fig. 2 is increasingly implemented by a network of functions that operate partly independently on a joint data-base of measured and computed information A more compact representation of the automation levels is shown in Fig. 3, where the ERP, MES/CPM and control system layers are distinguished. A working integration approach requires, nevertheless, a rich data exchange between all layers.

# 2. Process control and online scheduling – similarities and differences

Both conventional process control and online scheduling are reactive (and partly proactive) activities that have to cope with uncertainties and changes of operating conditions, targets and outcomes, and therefore employ feedback and feed-forward information structures. In (continuous) process control, the focus is on the control of qualitative properties of streams by changing the operating conditions of the plant. The mass flows of the raw materials or of the products are usually prescribed externally. The challenge is to keep the quality parameters constant or to track time-varying set-points for these parameters, possibly for changing throughputs. The implementation of the desired mass flows as well as the control of the inventories are usually taken care of by lowlevel controls. Continuous feedback control is mainly needed to handle the uncertainties involved, i.e. the uncertainty on the dependence of the process outcomes on the degrees of freedom that can be manipulated (inputs) lack of models or *plant-model mismatch* - and the existence of external influences that influence the quality parameters and the economics of the process summarized under the term *disturbances*. Process control is concerned with meeting the constraints on quality indicators, internal states (e.g. maximum pressures or temperature variations), and flows in the presence of these uncertainties. The effect of the discrepancy between the assumed models and the actual plant behavior on the control performance has been extensively discussed in the control literature under the term robust control.

Advanced control, mostly in the form of modelpredictive control continues to gain ground across the industries. Especially in chemicals production where the volumes are lower than in petrochemicals and therefore the expected gain of advanced control projects is usually lower, in recent years big advances could be observed, including nonlinear model-predictive control (NMPC) applications to batch processes. Advanced control is meanwhile recognized in all major companies as a key factor in energy saving, throughput maximization and cost-efficient production.

An exciting trend in advanced control in the recent years is to adopt a different view on the task of the control layer (Engell and Toumi, 2004, Rolandi and Romagnoli, 2005, Engell 2007): to ensure and increase the efficiency and the profitability of the plant directly rather than to obtain good regulatory or tracking performance as a goal in itself. This can be achieved by a clever choice of the regulated variables (Skogestad, 2000, Engell et al., 2005) but also directly by reformulating MPC as an optimization of an economics-related cost function over the prediction horizon rather than as a tracking problem. In such a formulation, constraints e.g. on product purities or due to the limitations of the equipment can be expressed directly rather than indirectly as targets for regulatory control, which always necessitates a safety margin. Thus the control task is formulated in a manner which can be

discussed and agreed upon with the plant operators and managers: There is an economic target, there are constraints, measured variables and degrees of freedom, and the degrees of freedom are utilized such that the target is optimized over the prediction horizon while respecting This the constraints. also enables to solve "unconventional" control problems with many degrees of freedom and few targets and constraints. By using rigorous nonlinear process models, the tasks of real-time optimization (usually based upon a stationary nonlinear process model) and model-predictive control (usually based upon approximate linear time-invariant dynamic models) can be integrated and unified, leading to a more transparent formulation, less inconsistencies, and a much faster dynamic reaction. The potential of this concept has been demonstrated in several studies (Toumi and Engell, 2004, Ochoa et al., 2010, Würth et al., 2011).

A relatively easily implementable variant of online optimizing control is to determine the necessary conditions of optimality (Srinivasan et al., 2002a, b) and to track these using conventional control. For instance, in many semi-batch processes, the batch time is minimized by maximizing the feed rate, taking into account constraints on the heat transfer and the accumulation of reactants. This can be implemented either in a two-layer fashion where the optimal trajectories are computed before the batch is started (possibly with a batch-to-batch or intra-batch correction) and implemented by simple controllers (cf. Gesthuisen et al.. 2004) or the optimization can be performed by setting fictitious (very high) targets of the feed rate (cf. Arora and Engell, 2007).

Batch-to-batch improvement of the operational strategy (e.g. Gao and Engell, 2005) and tracking of the best recorded batches ("golden batch") are other relevant techniques to optimize operations by feedback control.

Clearly, optimizing control cannot and should not take care of all possible manipulated variables in a larger unit simultaneously, but only of those that are critical to the economic success. Below the optimizing control layer there will always be a regulatory layer, usually of classical SISO-controllers to stabilize the plant and to control inventories and to implement the higher-level decisions (e.g. control of the temperature of a cooling fluid).

The proposal to re-think control as not being mostly about stabilization and tracking of set-point trajectories and nice transients but about performance optimization where good dynamic responses may be helpful but are not mandatory still sounds strange to most of the automatic control community outside process control. It gives control a much broader and more central role in all applications where tracking of references is not the primary and natural goal. Note that this view has already been also reflected in the ISA-95 (ANSI/ISA, 2005) standard where a control system has the central and coordinating functional role.

#### Similarities of Scheduling and Control

In contrast to the situation in continuous control, the complexity of scheduling problems does not admit a monolithic single-layer formulation for real-world problems. Uncertainties in online scheduling are related to the availability of resources (breakdowns, lack of personnel), uncertain yields or unsuccessful production steps, uncertain durations of operations, and, often most importantly, dynamically changing demands or targets.

Scheduling and control are both real-time decision making functions that have to take into account new information at a regular or irregular frequency. In modelbased control and in model-based scheduling, the decisions are optimized over a forecast horizon in order to take longer term effects due to the inertia of the controlled system into account, but only a subset of "next" decisions or optimized variables have to be fixed and implemented based upon the available information on the new state of the system and new requirements. While the design of such moving horizon schemes has been extensively discussed in the control literature, this topic has so far received limited attention in the scientific literature on scheduling (Sand et al., 2000; Engell et al., 2001; van den Heever and Grossmann, 2003; Mendes and Cerda, 2003; Kelly and Zyngier, 2008; Puigjaner and Lainez, 2008; Shaik et al., 2008; Engell and Cui, 2010).

Secondly, scheduling and control have to deal with uncertainties and therefore act in a feedback structure. This makes continuous control interesting and challenging beyond the computation of optimal inputs or trajectories (cf. all the work on stability of closed-loop systems) but has much less been addressed in scheduling. Scheduling has only rarely been seen as an activity that leads to a dynamic system with feedback, but it is in fact not fundamentally different to optimizing control on a finite horizon.

Feedback can assume different forms, in particular direct feedback in regulatory structures, state updates in model-based control and model (parameter) updates. Scheduling also takes place in a nested feedback structure (see Fig. 4.). The information that is fed back can be the state of the plant (production capability in ISA-95 terms) and an update of the parameters that are assumed in the computation of future schedules.



# Figure 4: Scheduling in a feedback structure (from Engell, 2009)

The state of the production process in scheduling is defined by the amounts of material stored, by the states of the resources (binary: operational or not, discrete: last operation was A, B, C, or continuous (rarely)) and by the progress of the running operations (discrete or continuous). From the scheduling point of view, the state (in the sense of process control) of the continuous parameters of the material and of the equipment only matters as far as it influences the availability of resources, the durations of the operations and the amounts of material delivered upon termination. Consequently, the intra-phase information obtained from the running processes in a feedback structure should be an accurate prediction of the expected finishing times and of the yields of the running batches.

Both in process control and in online scheduling, the difficulty arises from the "inertia" of the processes - the energies and masses stored in the plant in the case of continuous control and the inventories and the irreversible allocations of resources to processing steps in batch plants. The lower this inertia, the faster the production process can be adapted to changing market conditions. Agility roughly is determined by the available range of the degrees of freedom relative to the inertia of the system. The smaller the inertia and the larger the range of the inputs, the faster transitions can be implemented. Translating this into online scheduling, the inertia is determined by the available resources relative to the work in progress and the associated blocking of resources, plus the inertia of the procurement of raw materials. The inertia of the plant and of the procurement of raw materials and other resources causes the need for planning on longer horizons. Planning can be understood as the generation of the reference trajectories for the plant and for the procurement of material, similar to the computation of the optimal operating conditions in process control.

Both in continuous control and in online production scheduling, model abstractions and hierarchy are employed to improve the tractability of the problems. What degrees of freedom are assigned to which layer, how the targets and the target satisfaction are communicated between the layers, and how much autonomy is assigned to the different "players" requires a careful analysis.

#### Advances in Scheduling

Due to the high complexity and the wide range of different scheduling problems, there exists no common modeling framework for scheduling. Also, scheduling technologies are being developed by several communities (operations research, computer science, mathematics, economics and engineering), which does not always contribute to success, as the communities are surprisingly isolated. The essential challenge in scheduling is the exponentially growing search space, theoretically quickly leading to unacceptable computing times for any problems of practical interest. However, there are also many real problems for which the needed computing times are well acceptable. Different methodologies to handle the combinatorial complexity have been developed, e.g. mathematical programming, expert systems, simulated annealing, genetic algorithms, neural networks, constraint programming, various heuristics and recently more and more hybrid methods combining some of the above (Mendez et al., 2006; Akyol and Bayhan, 2007; Li and Ierapetritou, 2008; Verderame et al., 2010).

Major advances in the field of scheduling are:

- Availability of more efficient mathematical solvers. Owing to the continuously increasing solution performance, larger problems can today be solved to proven optimality. Commercial solvers such as CPLEX, XPRESS, and GUROBI have successfully embedded elements from constraint programming and heuristics to boost the performance and are also able to use parallel CPUs to reduce the solution time.
- The scope of scheduling problems have increased and many formulations today (Kondili et al., 1993; Pantelides, 1994; Maravelias and Grossmann, 2003) are able to take into account inventory levels and other resource constraints. Most methods are using a discrete time representation, where the solution exactness is always somewhat limited. Event point concepts (Ierapetritou and Floudas, 1998; Castro et al., 2004; Sundamoorthy and Karimi, 2005) formulate resource constraints using a continuous time concept and have shown superior performance on several types of problems. Recently, scheduling problems have also been extended by other resource constraints, e.g. consumption of utilities (Castro et al., 2011).
- Integration with the surrounding layers of the hierarchy in Figs. 2&3. Integration of scheduling and production planning (Van den Heever and Grossmann, 2003, Stephanson et al., 2006, Wu and Ierapetritou, 2007, Verderame and Floudas, 2008, Goebelt et al., 2008, Maravelias and Sung, 2009, Engell, 2009) can expand the long-term awareness and thus lead to more economical solutions. Even if no major breakthroughs have been seen yet in the integration towards control (Harjunkoski et al., 2009), this activity also contribute to more open models where various types of information sources are being integrated to the scheduling context.

Another important topic, re-scheduling, has not been discussed sufficiently in the literature and it can be expected that related aspects become more critical with increasing interaction with the control layer and demands for more dynamic scheduling solutions.

#### 3. Integration of Scheduling and Control

From the point of view of scheduling, control is just a necessary means to implement the planned schedules. The better the control of the process is, the less deviations from the assumed production times and volumes are observed, less rework is needed due to better product uniformity, no unplanned shutdowns etc. occur. The better the control layer works and the less you realize its existence, the better. And one becomes less aware of control problems if there is ample room for corrections, i.e. the targets that are set from the scheduling layer are not too tight.

The traditional integration between these two functions is that the scheduling software (or the production planner) computes a schedule and hands it down to the shop floor where it is implemented more or less well. Deviations are fed back only when they are large enough to really upset the schedule. To implement e.g. reporting on the true batch times still is somewhat a challenge, as this information may not be available electronically and automatically.

From the point of view of control, the schedule provides targets that may be more or less easy to realize. The looser and more flexible the schedule is, the larger the range for corrections if the real evolution of the production differs from the nominal case. So the life is best for both sides if the schedules are loose and include only few transitions, grade and product changeovers etc. Clearly this may not be the most profitable way of operation.

Similar to the integration of continuous optimization of the operation and advanced control into online optimizing control, the scheduling layer and the continuous optimization layer may be integrated to simultaneously optimize all major continuous and discrete degrees of freedom, which then are executed via recipe execution control and advanced process control.

There are several reasons for such an integration of advanced process control and scheduling:

- Plan sequences that avoid costly set-ups and changeovers and reduce the time and the lost product during transitions.
- Reduce maintenance needs and improve equipment life-time.
- Avoid schedules that lead to operational problems.
- Consider continuous degrees of freedom in the scheduling decisions.
- Use more precise and timely information in scheduling.

Below some examples are given where benefits of such an integration can be expected.

#### Grade transitions in polymer plants

Here the main target is to minimize the amount of offspec material during the transitions for given production targets for the different grades within a certain period of time. The amount of off-spec product in each transition is minimized by solving a dynamic optimization problem and simultaneously the due date violations and the overall production costs are optimized through scheduling aspects. Approaches comprise among others decomposition into master and primal problems (Nyström et al., 2005), an MINLP approach (Terrazas-Moreno et al., 2007) and the formulation of a MIDO problem (Prata et al., 2008). Agent-based approaches have also been reported, e.g. in Cao et al. (2008).

#### Optimizing control of wastewater treatment plants

Wastewater treatment plants are a representative of a class of plants where different operational strategies and therefore different control policies with different optimization targets are adequate in different situations, e.g. minimization of the consumption of energy, minimization of the concentrations in the outflow, or maximization of the capacity in anticipation of future large wastewater flow rates due to heavy rain. The scheduling of the different strategies has to consider the possibility of the controller to implement the required transients. Busch et al. (2007) demonstrated that this problem can be tackled by an integrated optimization of the stages.

#### Dynamically shifting control targets in batch production

It has been studied a lot in the control literature to optimize batch trajectories (for the main phase or the main phases of a batch run). Usually the minimization of the batch time has been considered as the natural target of the optimization. If this is embedded into the planning and scheduling context of the overall plant where pre- and post-processing steps have to be performed, and other resources as manpower or transport may be limiting, this may however not contribute to the economic success at all. Depending on whether the step considered is executed on a bottleneck or not, other targets may be more important. This obviously calls for an integrated approach where the economic implications of the strategy on the control layer are communicated explicitly and different control policies are used in different situations.

#### Flexible recipes

Going one step further, flexibility of the batch recipes can be integrated with schedule optimization. (Romero et al., 2003, Mishra et al., 2005, Ferrer-Nadal et al. 2008). For instance, Capon-Garcia et al. (2011) propose to consider variations of the reaction temperatures relative to the optimum temperature with respect to the consumption of energy to reduce the batch times and thereby improve the overall profitability. The modifications of the recipes also lead to different schedules. By adapting the recipes, bottlenecks can be avoided or alleviated. This integration requires that the flexibility in the recipes and the influence of possibly several recipe parameters on all relevant cost values and production targets are modeled explicitly and that this model is taken into account on the scheduling layer.

A variant of recipe flexibility is to adapt the transition condition between the phases of a batch production in order to influence the resource utilization favorably. When batch production processes require constrained resources as e.g. cooling power or electric energy, these constraints should also be taken into account in scheduling. Beyond choosing suitable starting times of the steps of the recipes, the required consumption of utilities can be influenced by the control policies within the batches, e.g. the required cooling power can be traded against the duration of a phase of a batch run. This calls for a fully integrated mixed-integer dynamic optimization.

An example for such a situation is the production of sugar. Here, first the syrup is produced from the raw materials from which the sugar is then crystallized in a number of stages with recycles. The batch crystallizers and the continuous stage are coupled by the consumption of steam, and the temporal uniformity of the steam consumption is crucial for the energy efficiency of the plant. The steam consumption can be influenced both by the scheduling of the start times of the runs of the crystallizers and by the operating policies both in the continuous and the batch stages. Scheduling and control should therefore be considered in an integrated fashion (de Prada et al., 2008).

#### Metals

There are a large number of control challenges in e.g. steel and aluminum production, for instance in hot rolling where typically preset models are used. Due to the presence of disturbances, the process should be monitored and controlled closely. At the same time, scheduling a steel plant is far from trivial and often requires nested decision steps (Harjunkoski and Grossmann, 2001). Practically, this calls for an integration of control and scheduling systems, and an information exchange between scheduling and control is more realistic than a fully integrated mathematical modeling approach. The main information from the process should capture equipment conditions and start and end times of batches. This calls for an MPC-type of scheduling approach, where new schedules must always be linked to actual production situation, taking into account the "inertia" discussed above. In many steel plants there are still no advanced control systems (level 2 systems) implemented to enable this integration but as it provides obvious economical benefits, in most modern plants integrated data acquisition systems have been implemented. How to make use of this enormous amount of data is still a research issue. The dynamics of the availability and the pricing and of electricity is also a pressing issue for energy intensive industries (Paulus and Borggrefe, 2011).

#### **Power Generation**

In power generation there are several aspects to consider that ask for integration of various layers. With the increasing generation from sources of renewable energy, unit commitment problems become more dynamic and scheduling together with optimal control should derive the most economical strategies for power production, taking into account the partly stochastic consumer behavior and the resulting stress for the equipment (Cossent et al. 2011).

In conventional coal power plants, scheduling plans load changes, which are implemented by sophisticated control solutions that minimize the consumption of "lifetime", through e.g. thermal stress. The information about "lifetime cost" can be provided from the control layer to the scheduling as an option to improve the overall economics, also fulfilling asset optimization targets (Antoine et al, 2008)

## 4. Approaches to the integration of scheduling and control

How can scheduling and control be brought closer together? It is natural that the stakeholders in both areas try to push their capabilities and expand their applicability to cover a larger problem scope, i.e. advance in the adjacent territory.

The control community is trying to reach upwards towards scheduling within an MPC framework (Busch et al., 2007, de Prada et al., 2011). There are fewer approaches known to us where the scheduling community has tried to reach down to the APC level using the typical scheduling type of models and approaches. Possibly the main reason for this is that considering APC also requires to take into account more detailed representations of continuous dynamics which are represented by a completely different type of models. The scheduling community rather is looking upwards in the hierarchy towards the integration of planning and scheduling and supply chain optimization.

#### Monolithic solution

The ideal solution would in fact be a monolithic solution, where both the scheduling and the control problem characteristics are fully represented (left-hand side of Fig. 5). The main benefits of such an approach are the availability of all information and that available degrees of freedom are fully utilized. It cannot and need not be distinguished anymore which decisions belong to control and which to scheduling. The MPC-based approaches to polymer grade transitions are examples that follow this philosophy.

This type of problems has been tackled also in the context of model predictive control (MPC) by extending it to models with switched dynamics (Bemporad and Morari, 2000, Gallestey et al., 2003; Perea-Lopez et al., 2003, The concept of introducing binary variables for automated selection of a correct controller strategy has been relatively successful in continuous processes, e.g. cement production.

To enable to true integration, also the optimization models should be constructed in a manner, where the two problems to be integrated do not anymore exist separately. This requires a completely new way of thinking, in order not to put the main focus in only one part of the problem, while the other part is only seen as a "complicating factor". It is worthwhile to cite Shobrys and White (2002) highlighting the mental hurdles of integration: "*There exists significant disagreement about the proper organization and integration of these functions, indeed even which decisions are properly considered by the planning, scheduling or control business process.*" So it is a challenge already before starting the actual technical development.



Figure 5. Monolithic and collaborative solution approach

The key challenge for the fully integrated approach is how to solve the resulting extremely challenging mixedinteger dynamic optimization problems, which typically are nonlinear and non-convex. Presently, one type of problems that seem amenable to this approach is where dynamic optimization problems on finite horizons include sequencing decisions with not too many discrete alternatives, as in polymer grade changes or other single unit sequencing problems. Here reformulations by complementarity constraints (Baumrucker and Biegler, 2009, Stein et al., 2004) or multiple-shooting based approaches (Sager, 2009) are very promising. By suitable re-parameterization of the optimization problems, discrete variables can sometimes be avoided and standard NLP techniques can be applied (de Prada et al., 2011). Generally speaking, the resulting problems are hybrid dynamic optimization problems (Engell et al., 2000) for which theoretical characterizations of the optimal solutions exist (Shaikh and Caines, 2007)) but have not yet been transformed into efficient algorithms.

On the other hand, problems which are predominantly classical scheduling problems but are augmented by a small number of degrees of freedom that result from the presence of some adaptable parameters in the recipes seem to be tractable as long as the models for the interaction of the continuous degrees of freedom and the discrete problem are simple, e.g. linear dependencies (Capon-Garcia et al., 2011).

For large numbers of discrete decision variables as they result in even small-sized batch scheduling problems combined with nonlinear continuous dynamics, a bruteforce integrated approach does not seem promising in the near future.

#### Hierarchical approach

A hierarchical solution strategy (right-hand side of Fig. 5) seems to be currently the only realistic approach to tackle industrial size problems, as it leads to sub-problems of reduced complexity.

In the hierarchical approach, three layers have to be considered: 1) The scheduling layer that takes the decisions on batch sizes, assignment to resources, sequencing and possibly timing, 2) the trajectory optimization layer that improves the profitability by computing optimal batch trajectories, and 3) the control layer that implements these trajectories in the presence of uncertainties or directly realizes an economically optimal operation. If the optimality of the operating parameters of the continuous sub-problems can be established by the tracking of necessary conditions of optimality, or an economically optimizing control target is used, the optimization of the continuous operation degrees of freedom can be implicitly performed by the control layer.

#### Classical hierarchical solution

As the scheduling problem encompasses a number of production phases and batches whereas the continuous optimization and control is concerned with single phases or possibly few connected phases and decomposes by pieces of equipment, it is natural that the scheduling system acts as the coordinator in the cooperative approach. One scheduling system may interact with several local controllers for different pieces of equipment. The schedules are computed based on nominal information about the durations of the tasks and their consumption of the most relevant resources. After a schedule has been determined, it is transferred to the optimization and control layer where optimal trajectories during and, if applicable, between the phases are computed and implemented. The real durations of the steps, energy consumptions etc. are fed back to the scheduling layer to update the scheduling model. Ideally, the scheduling layer will only fix resource allocations and sequencing decisions but leave the precise timing of the steps to the control layer which tries to maximize the revenue by making use of variable operating policies. Communication of the economics of the operation is crucial here. As more detailed information is available on the control layer, the revenue function can be more precise than on the scheduling layer.

In each hierarchical decision problem, a crucial question is how to handle uncertainties (Engell, 2009). The scheduling decisions must be based on a simplified model of the lower layer, comprising the main factors that influence feasibility and performance, but not all factors. This introduces a mismatch between the model and reality, in addition to the presence of all kinds of disturbances and unforeseen events during the execution of the schedules. This model can be based upon the assumption of the best execution, an average execution, or an average execution with some slacks to avoid infeasibility. In the first case, infeasibility will result in a large fraction of the cases, and mechanisms for repair must be implemented, in the last one the potential may not be realized because there is no incentive to finish faster or produce more than planned. This dilemma can to some extent be overcome by fast feedback, not only of reported results but also of predicted executions, and frequent re-scheduling. An additional improvement can be expected if not fixed plans are communicated and executed but communication is done via a revenue function that indicates e.g. what the economic implications are of a shortening or prolongation of the processing times of some steps or batches or of the delivery times of a product or of additional quantities produced. Then on the optimization and control layer the remaining degrees of freedom can be used to perform as well as possible economically, not only to meet the planned execution.

This issue of on which assumptions the schedules are based is not only relevant for the implementability of the schedules but also for the interaction with the upper layer ("promise to produce"). Neither constantly too optimistic nor constantly too conservative prediction will be helpful here. Therefore, the issue of fast and accurate feedback of the current situation on the optimizing and control layers and of frequent updates of the nominal resource (time, manpower, energy) consumption of the steps or batches is vital for a smooth functioning of the overall production control.

As the schedules cannot be realized as planned all the time, repair mechanisms must be implemented to restore feasibility and to avoid suboptimal behavior, as e.g. waiting for the next operation, although all conditions to start it are already satisfied and no constraints restrict the starting time. Such mechanisms could be implemented either on the scheduling layer or on the control layer. Practically this task is usually delegated to the plant operators.

#### Cooperative solution

What can be imagined as the future way of interaction between scheduling, optimization and control for problems with a high combinatorial complexity? The overall scheduling and optimization problem has a natural primal decomposition: after a schedule has been determined on the basis of a nominal, simplified model of the overall system, the remaining (few) discrete and continuous degrees of freedom can be optimized for this proposed schedule, similar to the optimization which is performed during the execution of the production steps. Often, a decomposition approach according to the different units and hence parallel computations are possible. The results of this optimization can be fed back and be used to evaluate and to "polish" the schedule. This is similar to the algorithmic treatment of two-stage MILPs as proposed in (Till et al., 2007). For the upper level optimization, metaheuristics appear to be promising because they can handle cost functions which are non-convex and can only be evaluated numerically. As discussed in (Tometzki and Engell, 2011), meta-heuristics are efficient in particular when a good initial solution (obtained here from a nominal resource consumption model on the scheduling layer) is available.

Despite the tight interaction of scheduling and continuous optimization in such a scheme, during the realtime execution deviations from the nominal plan will be the rule rather than the exception and appropriate mechanisms for fast re-scheduling must be implemented. (see e.g. Vin and Ierapetritou, 2000, 2001). Scheduling based on timed-automata (Subbiah et al., 2011) may be a promising technique for this task that is somewhat in between rigorous re-optimization and purely heuristic schedule modification and provides good solutions within short computation times. The robustness of the computed solution can be enhanced by taking the uncertainties into account explicitly using a two- or multi-stage representation (Balasubramanian and Grossmann, 2004; Sand and Engell, 2004, Hüfner et al., 2009).

Most reported contributions in the literature have focused on the mathematical formulations of integration problems. This is a very challenging research area and many of the results at hand are unfortunately capable of tackling only laboratory-scale problems, partly because the industry has been unable to provide full-size case studies as the whole area of integration is still quite young.

#### 5. Industrial requirements and state of the art

In the long-term, the industry needs to respond to a number of changes that are driven by economics, scarcity of raw materials, legislations and geo-politics. The reasons for the changes stem from e.g. growing populations and the need to produce according to even higher standards consuming less raw materials and energy, raw-material price increase, demographic changes and global competition and more demanding customers. All this calls for increased operational efficiency and faster adaptation to changing situations. It is expected that the market for CPM/MES is growing faster than that for base automation (Frost & Sullivan, 2010), see Fig. 6. As manufacturing sites become more flexible, complex and interconnected, the role and importance of optimization can be also expected to grow. This also puts more pressure on improving the interfaces and plug-ability of any kind of industrial scheduling, control and production optimization solutions that play an important role in MES. Standards such as ISA-88 and ISA-95 have become common and are often listed as basic functionalities as they can be expected to reduce problems in combining solutions from different MES-vendors.



# Figure 6. MES Market forecast (Frost & Sullivan, 2010)

By using standardized interfaces it is in theory possible to link any two functional IT-components within a plant and modern DCS systems enable to do this. Because of the multitude of options it is very important to carefully investigate and analyze what essentially makes sense and can bring added value to the production process.

The concept of Collaborative Process Automation Systems (CPAS), as discussed e.g. in Hollender (2009) is an attempt to create an application-enabling environment for process control, advanced process control, and operations management applications, plus human empowerment applications such as decision support and advanced analytics. The second generation, CPAS 2.0 (ARC, 2010), expands the vision beyond the traditional distributed control system (DCS) scope, and presents an environment designed for agility and adaptability.

The challenge to meet all requirements is immense. The connectivity to control refers to a holistic control system with different kinds of process control tools, for example:

- Model predictive control (MPC)
- Statistical process control (SPC)
- Fault detection and classification (FDC)
- Data reconciliation
- Online optimization

There are numerous potential opportunities to innovate new ways of using the available information and defining which exact system components should interact. The approach of optimizing scheduling and control problems completely isolated from each other may lead to suboptimal solutions – or even worse – into two systems that work against each other while merely focusing on increasing their local performance.

In the European project F3 "Flexible Fast Future Factory", a new production concept for medium and smallsize chemical production is investigated: modularized continuous intensified production units which make it possible to adapt the capacity of a plant to the evolution of the market by adding identical parallel production lines, hence reducing the engineering cost for the extension drastically. The project also aims at a future standardization of the modules to reduce the cost of the modules. Compared to traditional batch production, better reproducibility and less consumption of energy and solvents is targeted, leading to a more sustainable production and lower cost. Finally such modularized plants can be deployed in a decentralized manner, close to or on the site of the provider of raw materials or the customer to reduce transportation cost and environmental impact. Also included in this concept is the idea of adapting the larger modules (called process equipment containers, PEC) by exchanging or adding internal modules (process equipment assemblies, PEA) such that different products with different requirements e.g. on residence times or post-processing can be produced in a single train. This concept leads to new challenges for automation (the modules should bring their own automation soft- and hardware that can be seamlessly integrated into the overall automation system) and planning and scheduling because now on a weekly or monthly horizon also rearrangements of the equipment in order to produce a certain product portfolio must be considered.



Figure 7. Future electricity grids (Source: ABB)

Another emerging requirement stems from the smart grid concept and stronger integration of renewable energy forms (Fig. 7). This means that electricity networks become more dynamic. The more renewable and unplannable energy forms (e.g. wind and solar) we use, the more uncertain the power availability also becomes. What is more, not only the availability but also pricing of electricity will fluctuate. This adds another complex dynamic system to take into consideration, with many similarities to a control system of today.

The topic of industrial demand side management, i.e. how flexibly a plant can react to dynamically changing energy price and availability conditions is a direct example of integrating scheduling with a dynamic system (e.g. Palensky and Dietrich, 2011). It is clear than more structured energy management strategies are needed, possible even linking emission control directly to scheduling. This will also be enforced by more strict legislative requirements, e.g. plans within European Union to enforce energy efficiency on the industry.

In general, despite the potential benefits outlined above, the integration between scheduling and advanced control is still more a theoretical issue than practice. There are still only a few success stories that have been applied in industry. These represent however specific problem types that cannot be easily generalized. In the successful cases, mainly a strong contribution from the industry has also been necessary, which indicates that a close academic-industrial collaboration is vital.

The main challenges for the implementation of integrated solutions seem to be the following ones:

- Modeling. Integrated solutions require high-fidelity representations of both the scheduling problem and the dynamics of the plant. The cost of modeling in both domains is still much too high and the process is quite time-consuming and this is a main obstacle to even the exploration of the potential benefits of integrated solutions.
- Optimization algorithms. Here not only the demonstration that the problem can be solved in reasonable computing times is crucial but also the robustness of the solution when implemented online.
- Interaction with the user / human operator. A painful lesson learnt in advanced control is that if solutions are not accepted by the operators, they are not used in the long term, even if a benefit could be demonstrated. If two complex systems are interacting or are integrated, the challenge of providing sufficient insight and interaction to the operators is huge.
- Automation systems and components. The automation of a process plant is provided by a DCS which ideally would come from one vendor, but often large systems contain modules from multiple companies. Integration of different software systems for different functions acting on a joint open data structure will be needed because not every vendor of good MPC solutions is also the best choice for providing a scheduling solution and vice versa.
- Systems engineering. The design of integrated systems is a challenge for which no guidelines are available:
  - What roles do the system components have?
  - How much intelligence is placed on which levels?
  - Who triggers whom in the communication?
  - How to balance individual requirements and the collaboration?
  - How to ensure convergence in case of diverging targets etc.?

### Conclusions

An overview of the main advances and challenges within integration of scheduling and control has been given. It can be concluded that there is still a long way to go until such an integration will become reality, and that the challenges are technical, business-related as well as psychological. It would definitely speed up the development, if industry and academia could commit to collaboration with the target of aiming at systematically tackling at least some of the above challenges. So far, partly due to little interaction, it is hard to prove the business value of the integration, as well as the technical feasibility on a plant scale.

Nevertheless, as can be seen by the recent developments in the energy markets, the world is changing rapidly and new challenges for dynamic optimization may arise quickly.

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