Accelerating the Search for Optimal Solution of Integrated Process-Network Synthesis and Scheduling

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Scheduling is crucial for effective implementations of production, manufacturing, and logistics. With rare exceptions of extremely simple cases, only mathematical programming, e.g., Mixed Integer Linear Programming (MILP), can guarantee the optimal answer to practical scheduling problems. Unfortunately, the applicability of general-purpose MILP solvers is limited by the required computational time. To achieve a sufficiently fast answer in practice by mathematical programming, a highly flexible solution procedure is needed that can be tailored to the problem under investigation. Solution methods utilizing graph theory in parallel with algebraic operations give more room for customization. Process Network Synthesis (PNS) and the P-graph framework were originally developed to design and optimize chemical engineering process structures with continuous operation. Time Constrained Process Network Synthesis (TCPNS) has made it capable to handle batch processes with time constraints and storage strategies. P-graph algorithms extended to TCPNS can solve the precedence-based MILP model formulation of scheduling problems and are highly customizable as well. The aim of the current research is to examine and find the most suitable decision variable selection strategy for P-graph framework's optimization method to gain possible accelerations for different classes of scheduling problems.

1. Introduction

During the last two decades, batch process scheduling showed growing interest. The methods developed present different perspectives and modelling techniques, and they have variant efficiency for solving different problems (Mendez et al., 2006). The main differences come from the various time representations, the way of precedence modelling, and the additional constraints they can handle (Hegyhati et al., 2010). Numerous approaches have been published to solve a wide variety of scheduling problems, party to minimize energy needs or coordinate the production and consumption of renewable energy, including vehicle scheduling (Barany et al., 2010), energy distribution planning (Bertok and Bartos, 2018), and energy generation scheduling (Wu et al., 2020).

To solve real life-problems it is not enough to construct the correct mathematical model, it is also necessary to have such a solution method, which can guarantee to find practical optimal solutions. Methods based on time intervals (Floudas and Lin, 2004) do not necessarily contain the optimal solution, because the required number of the intervals is not known in advance. Precedence based methods do not require a predefined interval number, but it is possible that the optimal solution given by them is not applicable in reality, while graph theoretic methods can guarantee the correct mathematical model (Hegyhati et al., 2009).

Process Network Synthesis (PNS) and the P-graph framework were formally introduced by Friedler et al. (1992) were originally developed to design and optimize chemical engineering process structures with continuous operation (1996). Time Constrained Process Network Synthesis (TCPNS) published by Kalauz et al. (2012) have made it capable to handle batch processes with time constraints and storage strategies. Frits and Bertok (2020) integrated the rigorous model development phase of graph theoretic methods with the precedence-based MILP model formulation and optimization techniques capable of considering logical constraints of practical problems. First the production recipe is defined formally to clarify logical relations of potential tasks and the set of candidate equipment units to perform them. It can be given by a recipe graph for example; see Figure 1.a. Then all the potential assignments and changeovers are represented in a process network by P-graphs; see Figure 1.b. Note that P-graph algorithms can determine not only the optimal order of
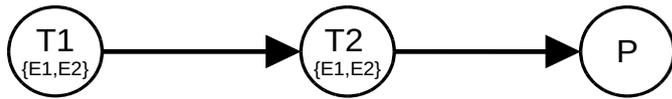
a) *Recipe graph (S-graph) for product P with two consecutive tasks T1 and T2, each of which can be realized by equipment units E1 or E2*
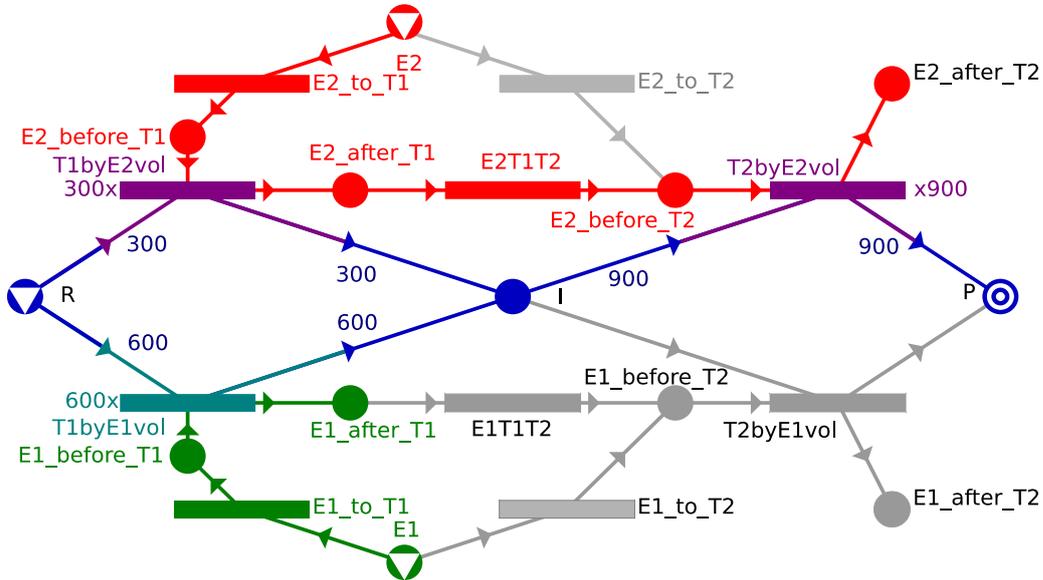
b) *Process graph (P-graph) representing the assignments of equipment units E1 and E2 to task T1, and E2 to T2, with volumes of 600, 300, and 900*
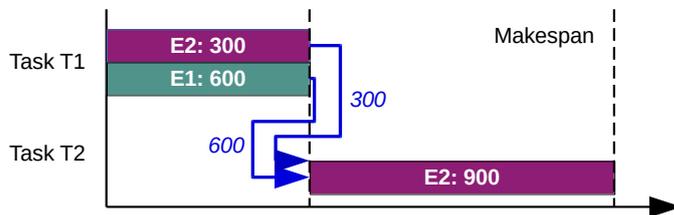
c) *Gannt chart depicting duration of task T1 executed by both equipment unit E1 and E2, and T2 by E2, with volumes of 600, 300, and 900, respectively*

Figure 1: Illustrations of a) recipe b) P-graph model for optimization, and c) feasible process schedule

task-equipment unit assignments, but optimal load distribution and storage loading and unloading as well. Either a P-graph or a Gannt diagram can represent each feasible schedule together with the material flows, as illustrated in Figures 1.b and 1.c.

After an adequate formulation of the scheduling problem, the solution method has to be efficient as well to get the optimum within a reasonable time, which highly depends on the treatment of integer variables (Floudas and Lin, 2005). Silori and Khanam (2018) reviewed the difficulties of MILP software in solving scheduling problems. Bartos and Bertok (2019) presented how the P-graph algorithms can be tuned to be faster than general purpose MILP solvers searching for optimal and alternative N-best solutions of PNS problems executed on computers with multiple processor cores. The aim of the actual research is to find the most effective search strategy, which can drastically reduce the search space, i.e., the number of subproblems visited on the way leading to the optimal schedule regardless the computational architecture.

2. Problem Statement

The major difficulty of solving a scheduling problem is managing the decisions on assignments and the order of tasks to be performed by the candidate equipment units. In case of integrated process design, the incorporation and scaling of alternative process steps leading to the desired products have to be decided as well. Decisions are represented by including nodes in graph theoretic, and by setting the values of binary variables in MILP approaches; see (Bertok and Bartos, 2018) for formal definitions and more details. For example, if potential activities have minimal feasible volumes $lb(o_i)$, minimal execution times $tf(o_i)$, or fixed minimal costs $tc(o_i)$, then linear relaxations (where $y_i \in [0,1]$ instead of $y_i \in \{0,1\}$) of costs (Equation 2) and execution times (Equation 3) can be far from the real values; see the distance between blue and red lines in Figures 2.a and 2.b.

$$lb(o_i)y_i \leq x_i \leq ub(o_i)y_i \tag{1}$$

$$cost = cf(o_i)y_i + cp(o_i)x_i \tag{2}$$

$$duration \geq \big(time\_bound + tf(o_i)\big)y_i + tp(o_i)x_i - time\_bound \tag{3}$$

Solving a combinatorial or mixed integer problem by a Branch & Bound or Cutting Plane method, in each step first the linear relaxation is solved fast to orient the search, and then the necessary decisions are made to correct process volumes, cost, and execution time estimations by fixing the values of the binary variable to be exactly 0 or 1. Our aim is to find the most effective decision variable selection rule that leads to a predefined number of best feasible schedules in the fastest possible way.
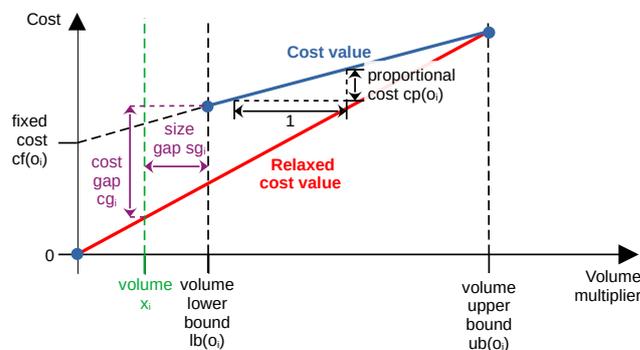
a) Parameters for a cost function with cf(o_i) fixed and cp(o_i) proportional parts and its linear relaxation for an operation oi with lb(o_i) lower and upper ub(o_i) bounds on its volume x_i
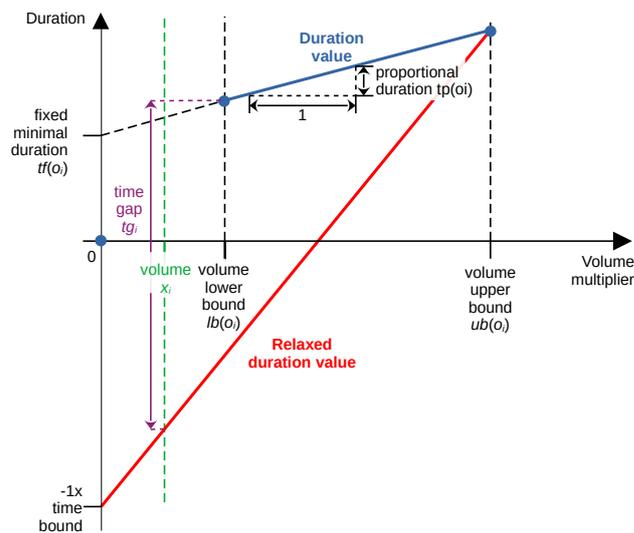
b) Parameters for a duration function with tf(o_i) fixed and tp(o_i) volume proportional parts and its linear relaxation for an operation oi with with lb(o_i) lower and upper ub(o_i) bounds on its volume x_i

Figure 2: Illustrations of a) cost function and b) duration function for any operation o_i with a fixed part and the one depending on the actual volume x_i of operation o_i

3. Methodology

To measure the error of the linear relaxation, three kinds of error values are introduced here for each of the potential activities to be included to or excluded from the process under development. These are called size gaps, cost gaps, and time gaps as illustrated in Figure 2. If the calculated optimal volume x_i of an activity o_i is not zero but smaller than the predefined minimum $l(o_i)$, then size gap sg_i is the difference between $l(o_i)$ and x_i, i.e., how much the volume of an activity is smaller than required. Cost gap cg_i is the difference between the fix charged cost function and its linear relaxation caused by either the size gap or the fixed minimal cost taken into account only partially in the relaxed cost function. The potential error called time gap tg_i of the relaxed linear estimation of the execution time is even higher than the error in cost estimation since without making decisions on the order of the execution of tasks potentially performed by the same equipment unit, the one at the end of a potential changeover can be earlier than the one at the beginning of the potential changeover, otherwise the initial model including changeovers in both direction would be infeasible. Based on the relaxed model of TCPNS (Frits and Bertok, 2020), the relaxed estimation function in Equation 3 may even result in a negative duration for an operation if the optimal volume x_i of the activity o_i is small compared to its potential maximal volume $u(o_i)$, where the relaxed linear duration estimation meets the real execution time value required to perform activity o_i; see Figure 2.

During any search for optimal and best schedules, both infeasible subproblems are to be eliminated, and cost and execution time estimations are to be corrected. The objective can be either makespan minimization with limited cost or cost minimization with limited makespan. The question to be addressed herein is the best way of selecting the next decision to minimize the number of subproblems visited during the search for a given number of best networks, e.g., suggest to make decision on the activity with maximal size gap first, on the one with maximal time gap, or on the one with maximal cost gap. Alternative selection rules have been applied to solve numerous practical production scheduling problems exported from production planning and scheduling software (Frits and Bertok, 2020), and the resultant numbers of subproblems and computational times required to get the optimal schedules have been registered and compared.
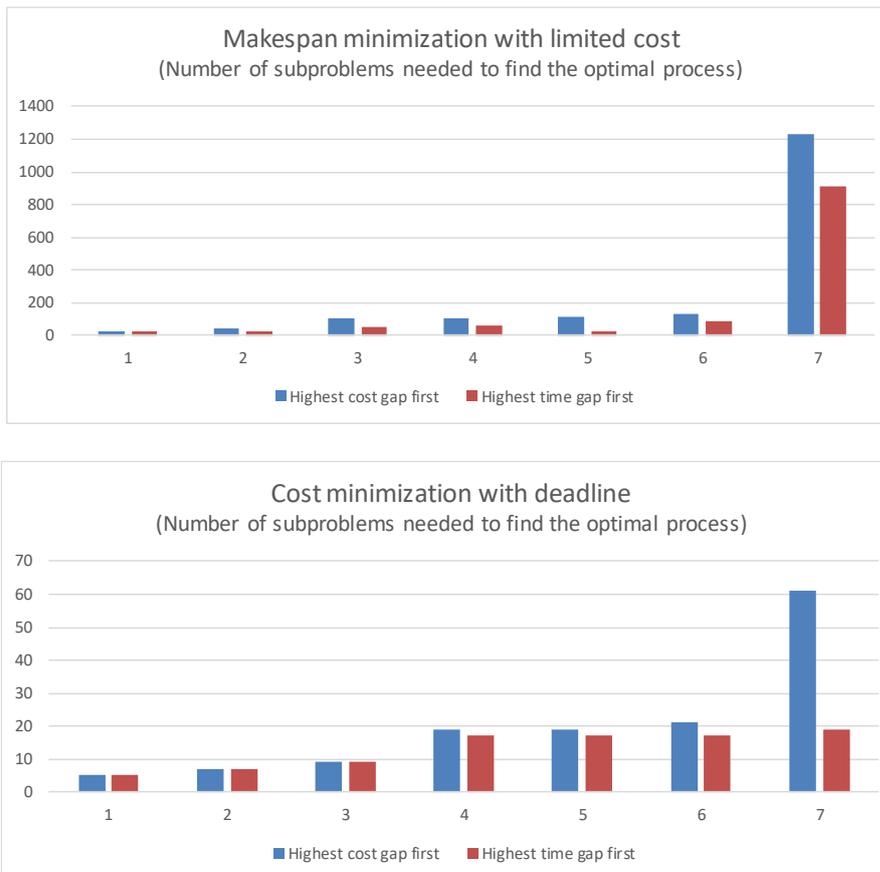

Figure 3: Comparison of the numbers of subproblems required to be examined to find the optimal solutions for problems of different classes due to cost and duration gap based decision variable selections

4. Results

The time-constrained process-network synthesis solver was executed to solve a number of scheduling problems of different difficulties by alternative decision variable selection rules. The best two orders were:

Selection rule #1: Highest cost gap first
- Select the activity o_i with maximum cost gap cg_i first!
- If there exist multiple activities with equal cost gaps, then select the one with maximum sg_i size gap!
- If there exist multiple activities with equal size gaps, then select the one with maximum tg_i time gap!

Selection rule #2: Highest time gap first
- Select the activity o_i with maximum time tg_i gap first!
- If there exist multiple activities with equal time gaps, then select the one with maximum cg_i cost gap!
- If there exist multiple activities with equal cost gaps, then select the one with maximum sg_i size gap!

The test results for the top two selection rules are depicted in Figure 3. The result shows that for problems with time constraints, Selection rule #2, i.e., making decision on the activity with the highest time gap in each step leads to much less subproblems than any other approach, regardless whether the cost is to be minimized or the makespan. The improvement in the computation speed was higher for those problems with shorter deadlines, because short deadlines cause several infeasible schedules, which can be discovered faster if errors in the duration estimations are corrected first.

5. Conclusions

The paper presents three kinds of measures for the error of relaxation applied in solving time-constrained process network synthesis (TCPNS) problems, MILP formulation of scheduling problems, or combinations of the two. As we have demonstrated here, these measures help accelerate the search for optimal and best processes by proposing activity for decision on its inclusion or exclusion, i.e., fixing related binary variable in a MILP model or estimation functions in a graph theoretic method. According to our measurements, making decision on the activity with the highest time gap value leads to 40% acceleration in makespan minimization and 18% acceleration in cost minimization with deadline. The conventional approach, where the cost function is improved as fast as possible, served as the basis for comparison. The potential reason for the improvement identified is the weak relaxation of potential changeovers resulting in negative duration estimations and leading to infeasible schedules while following promising cost values. Note that the results presented herein are equally applicable to vehicle routing problems with time windows formulated by TCPNS, see (Frits and Bertok, 2021).

Nomenclature

$cf(o_i)$ – fixed minimum cost of activity o_i

cg_i – error in cost estimation of activity o_i in the relaxed model

$cp(o_i)$ – proportional cost of activity o_i

$l(o_i)$ – lower bound on volume x_i of activity o_i

sg_i – error in volume of activity o_i in the relaxed model

$time\_bound$ – distance between the earliest start and latest end of any activity in the time horizon

$tf(o_i)$ – fixed minimum execution time of activity o_i

tg_i – error in execution time estimation of activity o_i in the relaxed model

$tp(o_i)$ – proportional execution time of activity o_i

$u(o_i)$ – lower bound on volume x_i of activity o_i

x_i – design variable on volume of activity o_i

y_i – binary variable expressing inclusion (y_i =1) or exclusion (y_i = 0) of activity o_i

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References

Barany M., Bertok B., Kovacs Z., Friedler F., Fan L.T., 2010, Optimization Software for Solving Vehicle Assignment Problems to Minimize Costs and Environmental Impacts of Transportation, Chemical Engineering Transactions, 21, 499-504.

Bartos A., Bertok B., 2019, Parameter Tuning for a Cooperative Parallel Implementation of Process-Network Synthesis Algorithms, Central European Journal of Operations Research, 27, 551-572

Bertok B., Bartos A., 2018, Algorithmic Process Synthesis and Optimisation for Multiple Time Periods Including Waste Treatment: Latest Developments in P-graph Studio Software, Chemical Engineering Transactions, 70, 97-102.

Floudas C. A., Lin X., 2004, Continuous-Time Versus Discrete-Time Approaches for Scheduling of Chemical Processes: A Review, Computers and Chemical Engineering, 28, 2109–2129

Floudas C. A., Lin X., 2005, Mixed integer linear programming in process scheduling: Modeling, algorithms, and applications, Annals of Operations Research 139, 131-162.

Friedler F., Tarjan K., Huang Y.W., Fan L.T., 1992, Combinatorial Algorithms for Process Synthesis, Computers & Chemical Engineering, 16, S313-320.

Friedler F., Varga J.B., Feher E., Fan L.T., 1996, Combinatorially accelerated branch-and-bound method for solving the MIP model of process network synthesis, State of the Art in Global Optimization, 609-626

Frits M., Botond B., 2020, Scheduling custom printed napkin manufacturing by P-graphs, Computers & Chemical Engineering, 141, 107017.

Frits M., Botond B., 2021, Routing and scheduling field service operation by P-graph, Computers & Operations Research, 136, 105472.

Garcia-Ojeda J., Bertok B., Friedler F., 2012, Planning Evacuation Routes with the P-graph Framework, Chemical Engineering Transactions, 29, 1531-1536.

Silori G. K., Khanam S., 2018, Performance analyses of LP and MILP solvers based on newly introduced scale: Case studies of water network problems in chemical processes, Chemical Engineering Research and Design, 136, 417-430.

Hegyháti M., Majozi T., Holczinger T., Friedler F., 2009, Practical Infeasibility of Cross-Transfer in Batch Plants With Complex Recipes: S-graph vs MILP methods, Chemical Engineering Science, 64 605-610

Hegyhati M., Friedler F., 2010, Overview of Industrial Batch Process Scheduling, Chemical Engineering Transactions, 21, 895-900.

Kalauz K., Sule Z., Bertok B., Friedler F., Fan L.T., 2012, Extending process-network synthesis algorithms with time bounds for supply network design, Chemical Engineering Transactions, 29, 259-264.

Méndez C.A., Cerdá J., Grossmann I.E., Harjunkoski I., Fahl M., 2006, State-of-the-art review of optimization methods for short-term scheduling of batch processes, Computers & Chemical Engineering, 30, 913-946.

Méndez C.A., Cerdá J., 2007, A Precedence-Based Monolithic Approach to Lotsizing and Scheduling of Multiproduct Batch Plants, Computer Aided Chemical Engineering, 24, 679-684.

Wu L., Xiao S., Hu Y., 2020, Scheduling of the Combined Power and Desalination System, Chemical Engineering Transactions, 81, 1201-1206.