Dauzère-Pérès, S., Hassoun, M., & Sendon, A. (2019). A Lagrangian heuristic for minimising risk using multiple heterogeneous metrology tools. *International Journal of Production Research*, 1-17.

https://doi.org/10.1080/00207543.2019.1614693

To appear in the *International Journal of Production Research*
Vol. 00, No. 00, 00 Month 20XX, 1–24

A Lagrangian Heuristic for Minimizing Risk Using Multiple Heterogeneous Metrology Tools

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(Received 4 July 2018; Accepted 07 April 2019; Published online 21 May 2019)

Motivated by the high investment and operational metrology cost, and subsequently the limited metrology capacity, in modern semiconductor manufacturing facilities, we model and solve the problem of optimally assigning the capacity of several imperfect metrology tools to minimize the risk in terms of expected product loss on heterogeneous production machines. In this paper, metrology tools can differ in terms of reliability and speed. The resulting problem can be reduced to a variant of the Generalized Assignment Problem (GAP), the Multiple Choice, Multiple Knapsack Problem (MCMKP). A Lagrangian heuristic, including multiple feasibility heuristics, is proposed to solve the problem that are tested on randomly generated instances.

Keywords: Semiconductor Manufacturing, Metrology, Integer Linear Programming, Lagrangian Heuristic, Multilevel Generalized Assignment Problem, Multiple Choice Multiple Knapsack Problem

1. Introduction

For more than four decades, Lithography machines, bearing the highest price tag of all, have been the traditional bottlenecks in semiconductor fabrication plants (fabs). Metrology tools were relatively cheap, small, and drew very little attention. Any critical congestion at one of the numerous in-line quality control steps would be solved by the acquisition of an additional tool. This is no longer the case since metrology tool prices have skyrocketed. As

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a result, the level of monitoring wished by quality engineers is often no longer practicable. Tightening the control of one production machine often means reducing the control level on another. By working in tandem with a variety of production machines in the line, the congestion of metrology tools has a special effect on the line. Many aspects of the metrology policy in semiconductor manufacturing plants (fabs) have been studied both by practitioners and researchers (Colledani and Tolio (2011), Bettayeb et al. (2012), Gilenson, Hassoun, and Yedidsion (2015), Nduhura-Munga et al. (2012), Nduhura-Munga et al. (2013), Lee et al. (2003), Dauzere-Péres et al. (2010), Rodriguez-Verjan et al. (2013), Shanoun et al. (2011))

In a former publication (Dauzère-Pérès, Hassoun, and Sendon (2016a)), we proposed an approach to optimize the sampling periods of several production machines competing for the capacity of a unique and perfectly reliable metrology tool. We characterized the production machines by their failure propensity, their throughput rate, and their consumption of the metrology capacity. We formulated the resulting problem as an optimization problem where the objective is to minimize the risk in terms of expected product loss happening between the machine failure and its detection, subject to the constraint of metrology capacity, the decision variable being the sampling period applied to each production machine. The problem was reformulated as a Multiple Choice Knapsack Problem (MCKP), for which we proposed and analyzed several heuristics based on the work of Sinha and Zoltners (1979) and Pisinger (1995). Later, in Dauzère-Pérès, Hassoun, and Sendon (2016b), we generalized the problem by considering multiple identical and reliable metrology tools. In this case, decision variables include both the assignment of production machines to metrology tools and the sampling periods of production machines. Heuristics were proposed and validated through computational experiments.

To better fit the industrial reality, this previous research is extended in two ways in this paper. First, more often than not, the inspection is not perfectly reliable since it usually samples only part of the surface of the selected wafers. Second, the same metrology operation can usually be performed on metrology tools that differ from one another in terms of inspection rates, reliability, or even qualification (i.e. the ability to perform a given metrology operation). Hence, in Section 2, we formalize several extensions prompted by multiple heterogeneous and unreliable metrology tools and propose an Integer Linear Program (ILP). Then, in Section 3, the Lagrangian Dual Problem (LDP) obtained by relaxing the capacity constraints in (ILP) is derived. Although the set of feasible solutions of (LDP) satisfies the integrality property, a Lagrangian heuristic based on subgradient search is proposed to solve the problem. This heuristic relies on seven feasibility heuristics that are also presented in Section 3. Computational experiments on the instances of Dauzère-Pérès, Hassoun, and Sendon (2016b) for the case with identical metrology tools, and new instances for the most general case are discussed in Section 4. Finally, some conclusions and perspectives are provided in Section 5, where the use of the Lagrangian heuristic in a Decision Support System is discussed.

2. Problem modeling

2.1 *Problem description*

Several metrology tools $t = 1, \ldots, T$ inspect the products (wafers) of production machines $r = 1, \ldots, R$. Production machines are modeled as Bernoulli experiments, and differentiated by their probability of failure p_r. Let us denote by TP_r the throughput rate of production machine r, and by SP_r the sampling period, i.e. the number of production cycles on machine r between two consecutive inspections. For each production machine r, a certain proportion of the inspection effort is assigned to a given metrology tool t. Differently than in Dauzère-Pérès, Hassoun, and Sendon (2016b), metrology tools are considered to be not identical and not reliable. Hence, let TM_r^t be the throughput rate of metrology tool t when inspecting products processed on machine r. Also, inspection is imperfect and returns with probability α_r^t a false negative, i.e. the results of metrology tool t are good while machine r does not work properly. Note that imperfect inspection may also yield a false positive, i.e. the product inspection returns an out-of-control answer although machine r works properly. However, it is customary to immediately confirm (or deny) any positive control on a product by immediately performing an advanced inspection, often on other metrology tools (two-stage quality control). This advanced inspection is usually highly reliable. Thus, although regular inspection can potentially return a false positive, this does not trigger any additional products to be scrapped or reworked. Therefore false positives have no impact on the objective function. We further assume that false positives have no significant impact on the consumption of the metrology capacity itself, either because the advanced inspection is performed on different metrology tools, or because false positive occurrences are rare enough as to allow neglecting the additional consumed metrology time.

The decision variables are the sampling periods SP_r, $r = 1, \ldots, R$, and the inspection effort sharing of production machines on metrology tools. We assume that one and only one metrology tool t is assigned to the inspection of the totality of the production of machine r. Setting these variables determine both the risk in terms of expected throughput of bad products from production machine r, and its share in the consumption of the capacity of metrology tools. Let us denote by $g_r^t(SP)$ this consumption when metrology tool t is assigned to the inspection of products from machine r for a given sampling period SP:

$$g_r^t(SP) = \frac{TP_r}{SP \cdot TM_r^t} \tag{1}$$

We assume a maximum value SP^{max} over which the quality control is unacceptable. Following a decision to inspect products from production machine r with sampling period SP and to direct wafers to metrology tool t, wafers are reworked or scrapped at a certain expected rate $WL_r^t(SP)$, which are detailed in the following section. This expected rate measures the risk in our problem. A reasonable assumption is that the production of a machine in good condition is perfect, while the production of a defective machine is fully reworked or scrapped. This classical worst-case assumption can be relaxed in our approach by assuming that only a given percentage of the production is reworked or scrapped. There is no difference between the value of products on the different machines. As a consequence, we strive to minimize the expected overall production rate of defective products.

2.2 *Objective function*

Let j denote the number of inspections on metrology tool t of products from machine r until a reliable inspection takes place. We have $j = 1$ with probability $(1 - \alpha_r^t)$, $j = 2$ with probability $\alpha_r^t(1 - \alpha_r^t)$, etc. A sampling cycle on production machine r is a series of $j \cdot SP$ Bernoulli experiments, each of which corresponds to the production of a product. Therefore, if a failure occurs in the first production cycle, all the following $j \cdot SP$ products (the number of products produced until the next reliable inspection takes place) are reworked or scrapped. Similarly, if a failure occurs in the second production cycle, $j \cdot SP - 1$ products will be reworked or scrapped, and so on. A failure occurring in the last production cycle before the next reliable inspection will yield only one bad product. The expected number of bad products from r with sampling period SP until the first reliable inspection, denoted WLC_r^t (for Wafer Loss Count), is therefore given by:

$$WLC_r(SP, j) = jSPp_r + (jSP - 1)(1 - p_r)p_r + \cdots + 1(1 - p_r)^{jSP-1}p_r$$

$$= p_r \sum_{i=0}^{jSP-1} (jSP - i)(1 - p_r)^i$$

which, when considering the probability of an inspection to be reliable, allows the total expected Wafer Loss for machine r to be computed:

$$WL_r^t(SP) = (1-\alpha_r^t)WLC_r(SP, 1)+\alpha_r^t(1-\alpha_r^t)WLC_r(SP, 2)+(\alpha_r^t)^2(1-\alpha_r^t)WLC_r(SP, 3)+\ldots$$

$$+(\alpha_r^t)^{j-1}(1 - \alpha_r^t)WLC_r(SP, j) + \ldots = (1 - \alpha_r^t) \sum_{j=1}^{\infty} (\alpha_r^t)^{j-1} WLC_r(SP, j)$$

$$= (1 - \alpha_r^t)p_r \sum_{j=1}^{\infty} \left[(\alpha_r^t)^{j-1} \sum_{i=0}^{jSP-1} (jSP - i)(1 - p_r)^i \right] \tag{2}$$

Because of the new parameter α_r^t, the analysis and the expression above are more complex than the ones in Dauzère-Pérès, Hassoun, and Sendon (2016b) and Dauzère-Pérès, Hassoun, and Sendon (2016a).

2.3 *Integer Linear Programming (ILP) model*

For each machine r, SP_r must be chosen in the set of all possible sampling periods $\{1, \ldots, SP_{max}\}$. Let us define the binary variable $w_r^{s,t} \in \{0, 1\}$, where $w_r^{s,t} = 1$ if production machine r is assigned to metrology tool t with a sampling period of s, and $w_r^{s,t} = 0$ otherwise.

Hence, as in Dauzère-Pérès, Hassoun, and Sendon (2016a) but with parameters $WL_r^t(s)$ and $g_r^t(s)$ that are metrology tool dependent, our problem can be formulated as the Integer

Linear Program below, denoted by (ILP):

$$\min \sum_{t=1}^{T} \sum_{r=1}^{R} \sum_{s=1}^{SP^{max}} WL_r^t(s) w_r^{s,t} \tag{3}$$

s.t.

$$\sum_{r=1}^{R} \sum_{s=1}^{SP^{max}} g_r^t(s) w_r^{s,t} \leq 1, \quad t = 1, \ldots, T \tag{4}$$

$$\sum_{t=1}^{T} \sum_{s=1}^{SP^{max}} w_r^{s,t} = 1, \qquad r = 1, \ldots, R \tag{5}$$

$$w_r^{s,t} \in \{0, 1\}, \qquad r = 1, \ldots, R; \ t = 1, \ldots, T; \ s = 1, \ldots, SP^{max} \tag{6}$$

Constraint (4) ensures that the metrology capacity is satisfied, and Constraint (5) that one and only one sampling period and one and only one metrology tool is chosen for each production machine.

Defined as such, (ILP) corresponds to a Multilevel Generalized Assignment Problem (see Ceselli and Righini (2006) or Park, Lim, and Lee (1998)). A special instance of this problem occurs when the metrology tools are all identical, i.e. when both α_r^t and TM_r^t are independent of t. In this case, neither the objective function nor the constraints are dependent of the metrology tool, and the problem is in fact a Multiple Choice Multiple Knapsack Problem (MCMKP) (Dauzère-Pérès, Hassoun, and Sendon (2016b)). If, in addition, we replace condition (6) by $w_r^{s,t} \in [0, 1]$, the problem reduces to a Multiple Choice Knapsack Problem with capacity T, which is discussed in Dauzère-Pérès, Hassoun, and Sendon (2016a).

3. Problem resolution

In this section, we introduce a Lagrangian Relaxation Heuristic, denoted by LRH, because it was important for us to have an efficient approach independent of a standard solver (1) to avoid the cost of the license of a commercial standard solver and (2) to ensure the robustness of computational times in relation to the problem complexity or size. We first derive and analyze the Lagrangian Dual Problem, denoted by (LDP), resulting from relaxing the capacity constraints in (ILP). Although the optimal objective function of (LDP) can be obtained by solving the linear relaxation of (ILP) and because we want to determine an upper bound for (ILP), the Lagrangian Relaxation Heuristic LRH is proposed. This heuristic exploits seven construction heuristics to build feasible solutions from the usually unfeasible solution of the relaxed problem.

3.1 *General scheme*

The Lagrangian Dual Problem (LDP) is defined as follows, where λ_t are the Lagrangian multipliers associated to relaxing Constraints (4) (capacity constraints) in (ILP):

$$\max_{\lambda_t \geq 0;\ t=1,\ldots,T} \min \sum_{t=1}^{T} \sum_{r=1}^{R} \sum_{s=1}^{SP^{max}} (WL_r^t(s) + g_r^t(s)\lambda_t) w_r^{s,t} - \sum_{t=1}^{T} \lambda_t \tag{7}$$

s.t.

$$\sum_{t=1}^{T} \sum_{s=1}^{SP^{max}} w_r^{s,t} = 1, \quad r = 1, \ldots, R \tag{5}$$

$$w_r^{s,t} \in \{0, 1\}, \qquad r = 1, \ldots, R;\ t = 1, \ldots, T;\ s = 1, \ldots, SP^{max} \tag{6}$$

For given Lagrangian multipliers λ_t, $t = 1, \ldots, T$, the Lagrangian Relaxed Problem (LRP(λ_t)) is relatively easy to solve. It is possible to independently solve a sub-problem for each process machine r by selecting the metrology tool t^*, $t^* = 1, \ldots, T$, and the sampling period s^*, $s^* = 1, \ldots, SP^{max}$, such that $(WL_r^{t^*}(s^*) + g_r^{t^*}(s^*)\lambda_{t^*})$ is the smallest, i.e. $(WL_r^{t^*}(s^*) + g_r^{t^*}(s^*)\lambda_{t^*}) = \min_{t=1,\ldots,T;\ s=1,\ldots,SP^{max}}(WL_r^t(s) + g_r^t(s)\lambda_t)$. Then, $w_r^{s^*,t^*} = 1$, and $w_r^{s,t} = 0$ for $t = 1, \ldots, T$ and $s = 1, \ldots, SP^{max}$ such that both $t \neq t^*$ and $s \neq s^*$.

Because (LRP(λ_t)) is actually a simple assignment problem, the set of its solutions satisfies the integrality property for any values of λ_t, $t = 1, \ldots, T$, i.e. (LRP(λ_t)) can always be solved by solving its linear relaxation. In this case, as shown in (Parker and Rardin 1988) and (Guignard 2003), the optimal objective function of (LDP), which is a lower bound of (ILP), is actually equal to the linear relaxation of (ILP), i.e. when Constraints (6) are replaced by $w_r^{s,t} \in [0, 1]$. However, since we mainly want to solve (ILP), i.e. to find upper bounds, we propose to use a subgradient search algorithm to determine both an optimal solution for (LDP) and an upper bound for (ILP), as shown in (Fisher 1981). This approach, known as Lagrangian Relaxation Heuristic, has been successfully applied to many problems such as general assignment problems (e.g. (Jörnsten and Näsberg 1986)), facility locations problems (e.g. (Klincewicz and Luss 1986)), lot-sizing problems (e.g. (Trigeiro, Thomas, and McClain 1989)) and scheduling problems (e.g. (Dauzère-Pérès and Sevaux 2003)).

The idea behind a Lagrangian Relaxation Heuristic is that, at each iteration of the subgradient search in which the Lagrangian multipliers are updated to converge towards the Lagrangian dual, one or more feasible solutions are also determined using the current values of the Lagrangian multipliers. The general scheme of our Lagrangian Relaxation Heuristic (see e.g. Parker and Rardin (1988)), denoted *LRH* in this paper, is presented in Algorithm 1, where seven feasibility heuristics described in Section 3.2 are used in Step 4. In the remainder of this paper, let us denote by $LRH(H_i)$ the lagrangian relaxation heuristic in which only feasibility heuristic H_i is used in Step 4 of *LRH*.

After some extensive calibration, the following characteristics for *LRH* have been used in all the numerical experiments of Section 4. In Step 1, α is initialized to 400 and, in Step 7, α is multiplied by 0.9 ($\alpha := 0.9 \cdot \alpha$) if $LB^k < LB^{k-1}$, i.e. if the lower bound has not improved from iteration $k-1$ to iteration k, otherwise α does not change. In Step 5, each Lagrangian

Algorithm 1 Lagrangian Relaxation Heuristic (LRH)

Step 1: **Initialization.**
  a. Initialize all multipliers to 0, i.e. $\lambda_t = 0$, $t = 1, \ldots, T$.
  b. Set iteration number $k = 1$.
  c. Initialize step length α.
  d. Initialize lower bound $LB = -\infty$.
  e. Initialize upper bound $UB = +\infty$.
Step 2: **Solving the relaxed problem.** Solve Lagrangian relaxed problem (LRP(λ_t)) for current values of multipliers λ_t and calculate current lower bound LB^k.
Step 3: **Incumbent saving.** If $LB < LB^k$, then $LB := LB^k$.
Step 4: **Feasibility heuristics.** Use the values of $w_r^{s,t}$ obtained in *Step 2* to find feasible solutions using the feasibility heuristics proposed in Section 3.2, and keep the best upper bound UB^k. If $UB > UB^k$, then $UB := UB^k$.
Step 5: **Updating multipliers.** Lagrangian multipliers λ_t, $t = 1, \ldots, T$, are updated using the subgradient optimization method.
Step 6: **Stopping conditions.** If any stopping condition is met, then stop.
Step 7: **Update step length.** Update α.
Step 8: Increment k and go to Step 2.

multiplier λ_t is updated using the following formula:

$$\lambda_t := \max\left(0, \lambda_t + \alpha \frac{\sum_{r=1}^{R}\sum_{s=1}^{SP^{max}} g_r^t(s) w_r^{s,t} - 1}{\sqrt{\sum_{t'=1}^{T}\left(\sum_{r=1}^{R}\sum_{s=1}^{SP^{max}} g_r^{t'}(s) w_r^{s,t'} - 1\right)^2}}\right).$$

The stopping criteria are (1) the maximum number of iterations which is set to 200 and (2) the minimum step size which is set to 0.1% of $\sum_{t=1}^{T} \lambda_t$, the sum of the Lagrangian multipliers. The latter means that LRH is stopped in Step 6 if $\alpha \leq 0.001 \cdot \sum_{t=1}^{T} \lambda_t$.

3.2 *Feasibility heuristics*

Seven feasibility heuristics are proposed, whose impact in LRH will be analyzed in Section 4 based on computational results.

3.2.1 Straightforward heuristic H_1

The first feasibility heuristic, detailed in Algorithm 2, is the most straightforward. The metrology tool t^* assigned to process machine r is the one assigned when solving the Lagrangian relaxed problem, i.e. $\exists s = 1, \ldots, SP^{max}$ such that $w_r^{s,t^*} = 1$. Only the sampling periods are adjusted to satisfy the capacity constraints of metrology tools, that are considered one at a time. For a given metrology tool t, the selection of the production machine and the sampling period to increase to reduce capacity consumption is based on the ratio between the risk increase and the capacity decrease. The process is repeated until the metrology capacity of t is satisfied.

Algorithm 2 Heuristic H_1

Let $\mathcal{F}(t)$ be the set of fixed pairs (machine, sampling period) for metrology tool t.
Initialize $\mathcal{F}(t)$ by using the optimal solution of the Lagrangian relaxed problem, i.e. $(r, s) \in \mathcal{F}(t)$ if $w_r^{s,t} = 1$.
Let $Capa_t$ be the capacity used on metrology tool t.
Initialize $Capa_t = \displaystyle\sum_{r=1}^{R} \sum_{s=1;(r,s)\in\mathcal{F}(t)}^{SP^{max}} g_r^t(s)$, $t \in 1, \dots, T$.
for $t = 1, \dots, T$ **do**
  while $Capa_t > 1$ and $s \leq SP^{max}$ **do**
    Find the process machine r^* and sampling period t^* with the minimal ratio $\frac{WL_{r*}^t(s+1)-WL_{r*}^t(s^*)}{g_{r*}^t(s^*)-g_{r*}^t(s^*+1)}$ such that $(r^*, s^*) \in \mathcal{F}(t)$, i.e. $\frac{WL_{r*}^t(s^*+1)-WL_{r*}^t(s^*)}{g_{r*}^t(s^*)-g_{r*}^t(s^*+1)} = \min_{(r,s)\in\mathcal{F}(t)} \frac{WL_r^t(s+1)-WL_r^t(s)}{g_r^t(s)-g_r^t(s+1)}$.
    Change sampling period of r^* from s^* to $s^* + 1$, i.e. $\mathcal{F}(t) \leftarrow \mathcal{F}(t) - \{(r^*, s^*)\} \cup \{(r^*, s^* + 1)\}$ and $Capa_t = Capa_t - g_{r^*}(s^*) + g_{r^*}(s^* + 1)$.
  end while
end for

Note that, in Heuristic H_1, the assignment of production machines to metrology tools is fixed from the Lagrangian relaxed problem, and the sampling periods are used as inputs. Also, in LRH, the Lagrangian multipliers λ_t only depend on the metrology tools. Hence, if all metrology tools are identical, then all parameters in the objective function of the Lagrangian relaxed problem are the same for all metrology tools except for the Lagrangian multipliers. Hence, when solving the Lagrangian relaxed problem in Step 2 of LRH, all production machines will be assigned to only one metrology tool, i.e. the metrology tool t with the smallest multiplier λ_t. This is confirmed in the numerical results of Section 4.2 which show that $LRH(H_1)$ performs poorly when metrology tools are identical.

To overcome the limitations of Heuristic H_1, additional feasibility heuristics are proposed that use as inputs either the sampling periods (Heuristics H_2 to H_4 in Section 3.2.3) or the assignment to metrology tools (Heuristics H_5 to H_7 in Section 3.2.4), but not both information. Moreover, in all heuristics, the assignment of production machines to metrology tools can be changed.

3.2.2 Common phases of heuristics H_2 to H_7

All the six remaining feasibility heuristics include two phases, an **assignment phase** and an **improvement phase**, that are detailed below.

In the assignment phase, the metrology tool selected for the production machine can change from the one assigned when solving the Lagrangian relaxed problem. In Algorithm 3, production machine r is assigned to metrology tool t with a sampling period s, and the metrology capacity is updated. If the capacity of t is exceeded, then SP is increased until either the capacity of t is enough or $SP = SP^{max}$. In the latter case, the solution is not feasible.

Algorithm 3 Assignment phase $(r^*, t^*, s^*, Capa_{t^*}, \mathcal{G})$

if $Capa_{t^*} + g_{r^*}^{t^*}(s^*) \leq 1$ **then**
  Assign r^* to t^* with sampling period s^*, i.e. $\mathcal{G} \leftarrow \mathcal{G} \cup \{(r^*, s^*, t^*)\}$.
  $Capa_{t^*} = Capa_{t^*} + g_{r^*}^{t^*}(s^*)$.
else
  while $Capa_{t^*} + g_{r^*}^{t^*}(s^*) > 1$ and $s^* \leq SP^{max}$ **do**
    $s^* = s^* + 1$.
  end while
  if $Capa_{t^*} + g_{r^*}^{t^*}(s^*) \leq 1$ **then**
    Assign r^* to t^* with sampling period s^*, i.e. $\mathcal{G} \leftarrow \mathcal{G} \cup \{(r^*, s^*, t^*)\}$.
    $Capa_{t^*} = Capa_{t^*} + g_{r^*}^{t^*}(s^*)$.
  else
    Assign r^* to t^* with sampling period $s^* = SP^{max}$, i.e. $\mathcal{G} \leftarrow \mathcal{G} \cup \{(r^*, SP^{max}, t^*)\}$.
    $Capa_{t^*} = Capa_{t^*} + g_{r^*}^{t^*}(SP^{max})$ and problem is unfeasible.
  end if
end if

As a final stage of each feasibility heuristic, an **improvement phase** is performed, which is detailed in Algorithm 4. A Multi-Choice Knapsack Problem is solved for each metrology tool with its assigned production machines. This is done using Heuristic $H2/3$ proposed in Dauzère-Pérès, Hassoun, and Sendon (2016a). The new solution for each metrology tool is only kept if it improves the current solution.

Algorithm 4 Improvement phase$(\mathcal{G})$

Set $\mathcal{G}' \leftarrow \mathcal{G}$.
for $t = 1, \dots, T$ **do**
  Solve a Multi-Choice Knapsack Problem with Heuristic $H2/3$ from Dauzère-Pérès, Hassoun, and Sendon (2016a) for the process machines r assigned to metrology tool t, i.e. $\exists s = \{1, \dots, SP^{max}\}$ such that $(r, s, t) \in \mathcal{G}$.
  Update $\mathcal{G}'$ with new sampling periods for metrology tool t.
end for
if $\sum_{t=1}^{T} \sum_{r=1}^{R} \sum_{s=1;(r,s,t)\in\mathcal{G}'}^{SP^{max}} WL_r^t(s) < \sum_{t=1}^{T} \sum_{r=1}^{R} \sum_{s=1;(r,s,t)\in\mathcal{G}}^{SP^{max}} WL_r^t(s)$ **then**
  $\mathcal{G} \leftarrow \mathcal{G}'$.
end if

3.2.3 Sampling period based heuristics H_2 to H_4

For the three heuristics H_2 to H_4, the sampling periods are obtained from the optimal solution of the Lagrangian relaxation problem.

Heuristic H_2, detailed in Algorithm 5, is metrology tool based. At each iteration, the metrology tool t with the largest remaining capacity is selected. Then, the production machine r which provides the larger portion of metrology capacity consumed for t ($g_r^t(s)$) among the production machines not assigned yet is selected. The metrology capacity must be satisfied when assigning r to t.

Algorithm 5 Heuristic H_2

1: Let $\mathcal{R} = \{1, \ldots, R\}$ be the set of process machines.
2: Let $\mathcal{F}$ be the set of fixed pairs (process machine, sampling period). $\mathcal{F} \leftarrow \emptyset$.
3: Initialize $\mathcal{F}$ by using the optimal solution of the Lagrangian relaxation problem.
4: Let $\mathcal{G}$ be the set of fixed triplets (process machine, sampling period, metrology tool). $\mathcal{G} \leftarrow \emptyset$.
5: Let $Capa_t$ be the capacity used on metrology tool t. $Capa_t = 0$, $t = 1, \ldots, T$.
6: **while** $\mathcal{R} \neq \emptyset$ **do**
7: Select t^*, the metrology tool with the lowest current utilization, i.e. such that $Capa_{t^*} = \min_{t=1,\ldots,T} Capa_t$.
8: Determine $\Delta_r = \{g_r^{t^*}(s) - \min_{t'=1,\ldots,T;t' \neq t^* \text{ and } Capa_{t'} + g_r^{t'}(s) \leq 1}(g_r^{t'}(s))\}$, $\forall r \in \mathcal{R}$ and s such that $(r, s) \in \mathcal{F}$.
9: Let $\mathcal{V} = \{r \in \mathcal{R} | \Delta_r = \max_{r' \in \mathcal{R}}(\Delta_{r'})\}$.
10: Select $r^* \in \mathcal{V}$ and s^* such that $(r^*, s^*) \in \mathcal{F}$ and t^* such that $g_{r^*}^{t^*}(s^*) = \max_{r \in \mathcal{V},(r,s) \in \mathcal{F}}(g_r^{t^*}(s))$.
11: **Assignment phase**$(r^*, t^*, s^*, Capa_{t^*}, \mathcal{G})$.
12: $\mathcal{R} \leftarrow \mathcal{R} - \{r^*\}$.
13: **end while**
14: **Improvement phase**$(\mathcal{G})$.

Heuristic H_3, detailed in Algorithm 6, is process machine based. The differences with Heuristic H_2 are shown in blue. The first step is to search the combination of production machine r and metrology tool t such that the portion of metrology capacity consumed $(g_r^t(s))$ is the largest, and to select the production machine r with the largest $g_r^t(s)$. Then, the metrology tool t with the minimum required metrology capacity $g_r^t(s)$ for r and that satisfies the metrology capacity is assigned. If such a metrology tool cannot be found, then the metrology tool t with the lowest utilization is selected.

Algorithm 6 Heuristic H_3

Let $\mathcal{R} = \{1, \ldots, R\}$ be the set of process machines.
Let $\mathcal{F}$ be the set of fixed pairs (process machine, sampling period). $\mathcal{F} \leftarrow \emptyset$.
Initialize $\mathcal{F}$ by using the optimal solution of the Lagrangian relaxation problem.
Let $\mathcal{G}$ be the set of fixed triplets (process machine, sampling period, metrology tool). $\mathcal{G} \leftarrow \emptyset$.
Let $Capa_t$ be the capacity used on metrology tool t. $Capa_t = 0$, $t = 1, \ldots, T$.
while $\mathcal{R} \neq \emptyset$ **do**
  Determine $\Delta_r^t = \{g_r^t(s) - min_{t'=1,\ldots,T;t'\neq t \text{ and } Capa_{t'}+g_r^{t'}(s)\leq 1}(g_r^{t'}(s))\}$ $\forall r \in \mathcal{R}$ and s such that $(r,s) \in \mathcal{F}$, $\forall t \in \mathcal{T}$.
  Let $\mathcal{V} = \left\{(r,t) \in \mathcal{R} \times \mathcal{T} | \Delta_r^t = \max_{r' \in \mathcal{R}, t' \in \mathcal{T}}(\Delta_{r'}^{t'})\right\}$.
  Select $(r^*, t) \in \mathcal{V}$ and s^* such that $(r^*, s^*) \in \mathcal{F}$ and $g_{r^*}^t(s^*) = \max_{(r,t)\in\mathcal{V},(r,s)\in\mathcal{F}}(g_r^t(s))$.
  Select $t^* \in \mathcal{W}$ with the lowest current utilization, i.e. $Capa_{t^*} = \min_{t=1,\ldots,T} Capa_t$.
  Let $\mathcal{W} = \{t \in \mathcal{T} | g_{r^*}^t(s^*) = \min_{t'=1,\ldots,T;t'\neq t \text{ and } Capa_{t'}+g_{r^*}^{t'}(s^*)\leq 1}(g_{r^*}^{t'}(s^*))\}$.
  if $\nexists t \in V^t$ such that $Capa_t + g_{r^*}^t(s) \leq 1$ **then**
    Select $t^* \in \mathcal{T}$ with the lowest current utilization, i.e. $Capa_{t^*} = \min_{t=1,\ldots,T} Capa_t$.
  end if
  Assignment phase$(r^*, t^*, s^*, Capa_{t^*}, \mathcal{G})$.
  $\mathcal{R} \leftarrow \mathcal{R} - \{r^*\}$.
end while
Improvement phase$(\mathcal{G})$.

Heuristic H_4, detailed in Algorithm 7, is a modification of Heuristic H_2. The main difference is that, after choosing the production machine r^* and the sampling period s^*, the initially selected metrology tool t^* can be changed. The selected metrology tool t^* is the one with the smallest and feasible $(Capa_{t^*} + g_{r^*}^{t^*}(s^*) \leq 1)$ remaining capacity once r^* is assigned with sampling period s^* to t^*.

Algorithm 7 Heuristic H_4 (modification of H_2)

Let $\mathcal{R} = \{1, \ldots, R\}$ be the set of process machines.
Let $\mathcal{F}$ be the set of fixed pairs (process machine, sampling period). $\mathcal{F} \leftarrow \emptyset$.
Initialize $\mathcal{F}$ by using the optimal solution of the Lagrangian relaxation problem.
Let $\mathcal{G}$ be the set of fixed triplets (process machine, sampling period, metrology tool). $\mathcal{G} \leftarrow \emptyset$.
Let $Capa_t$ be the capacity used on metrology tool t. $Capa_t = 0$, $t = 1, \ldots, T$.
while $\mathcal{R} \neq \emptyset$ **do**
    Select t^*, the metrology tool with the lowest current utilization, i.e. such that $Capa_{t^*} = \min_{t=1,\ldots,T} Capa_t$.
    Determine $\Delta_r = \{g_r^{t^*}(s) - \min_{t'=1,\ldots,T; t' \neq t^* \text{ and } Capa_{t'} + g_r^{t'}(s) \leq 1} (g_r^{t'}(s))\}$, $\forall r \in \mathcal{R}$ and s such that $(r, s) \in \mathcal{F}$.
    Let $\mathcal{V} = \{r \in \mathcal{R} | \Delta_r = \max_{r' \in \mathcal{R}}(\Delta_{r'})\}$.
    Select $r^* \in \mathcal{V}$ and s^* such that $(r^*, s^*) \in \mathcal{F}$ and t^* such that $g_{r^*}^{t^*}(s^*) = \max_{r \in \mathcal{V}, (r,s) \in \mathcal{F}} (g_r^{t^*}(s))$.
    Assign t^*, the metrology tool with the lowest remaining and feasible capacity when r^* is assigned to t^* with sampling rate s^*, i.e. such that $1 - (Capa_{t^*} + g_{r^*}^{t^*}(s^*)) = \{\min_{t=1,\ldots,T;\ Capa_t + g_{r^*}^{t}(s^*) \leq 1} (1 - (Capa_t + g_{r^*}^{t}(s^*)))\}$.
    Assignment phase$(r^*, t^*, s^*, Capa_{t^*}, \mathcal{G})$.
    $\mathcal{R} \leftarrow \mathcal{R} - \{r^*\}$.
end while
Improvement phase$(\mathcal{G})$.

3.2.4 *Metrology tool based heuristics H_5 to H_7*

In the three remaining feasibility heuristics H_5, H_6 and H_7, the initial assignment of production machines to metrology tools is the one of the optimal solution of the Lagrangian relaxation problem. The sampling periods are then determined by solving the MCKP with Heuristic H_1 of Dauzère-Pérès, Hassoun, and Sendon (2016a) for a unique metrology tool with a metrology capacity of T. Heuristics H_5, H_6 and H_7 are based on heuristics H_2, H_3 and H_4, respectively. The main differences are in red in the algorithms of this section.

Heuristic H_5, detailed in Algorithm 8, is metrology tool based and is a modification of H_2.

Algorithm 8 Heuristic H_5 (based on H_2)

Let $\mathcal{R} = \{1, \ldots, R\}$ be the set of process machines.
Let $\mathcal{F}$ be the set of fixed pairs (process machine, sampling period). $\mathcal{F} \leftarrow \emptyset$.
Let $\mathcal{M}$ be the set of fixed pairs (process machine, metrology tool). $\mathcal{M} \leftarrow \emptyset$.
Initialize $\mathcal{M}$ by using the optimal solution of the Lagrangian relaxation problem.
Determine $\mathcal{F}$ by solving the Multi-Choice Knapsack Problem with Heuristic H_1 presented in Dauzère-Pérès, Hassoun, and Sendon (2016a) for the process machines $r = 1,\ldots, R$ considering a unique metrology tool with capacity $\sum_{t=1}^{T} Capa_t$. Use $g_r^t(s)$ and $WL_r^t(s)$ with the metrology allocation in $\mathcal{M}$.
Let $\mathcal{G}$ be the set of fixed triplets (process machine, sampling period, metrology tool). $\mathcal{G} \leftarrow \emptyset$.
Let $Capa_t$ be the capacity used on metrology tool t. $Capa_t = 0$, $t = 1, \ldots, T$.
while $\mathcal{R} \neq \emptyset$ **do**
  Select t^*, the metrology tool with the lowest current utilization, i.e. $Capa_{t^*} = \min_{t=1,\ldots,T} Capa_t$.
  Determine $\Delta_r = \{g_r^{t^*}(s) - \min_{t'=1,\ldots,T;t'\neq t^* \text{ and } Capa_{t'}+g_r^{t'}(s)\leq 1}(g_r^{t'}(s))\}$ $\forall r \in \mathcal{R}$ and s such that $(r, s) \in \mathcal{F}$.
  Let $\mathcal{V} = \{r \in \mathcal{R} | \Delta_r = \max_{r' \in \mathcal{R}}(\Delta_{r'})\}$.
  Select $r^* \in \mathcal{V}$ and s^* such that $(r^*, s^*) \in \mathcal{F}$ and t^* such that $g_{r^*}^{t^*}(s^*) = \max_{r\in\mathcal{V},(r,s)\in\mathcal{F}}(g_r^{t^*}(s))$.
  Assignment phase$(r^*, t^*, s^*, Capa_{t^*}, \mathcal{G})$.
  $\mathcal{R} \leftarrow \mathcal{R} - \{r^*\}$.
end while
Improvement phase$(\mathcal{G})$.

Heuristic H_6, detailed in Algorithm 9, is process machine based and is a modification of H_3.

Algorithm 9 Heuristic H_6 (based on H_3)

Let $\mathcal{R} = \{1, \ldots, R\}$ be the set of process machines.
Let $\mathcal{F}$ be the set of fixed pairs (process machine, sampling period). $\mathcal{F} \leftarrow \emptyset$.
Let $\mathcal{M}$ be the set of fixed pairs (process machine, metrology tool). $\mathcal{M} \leftarrow \emptyset$.
Initialize $\mathcal{M}$ by using the optimal solution of the Lagrangian relaxation problem.
Determine $\mathcal{F}$ by solving the Multi-Choice Knapsack Problem with Heuristic H_1 presented in Dauzère-Pérès, Hassoun, and Sendon (2016a) for the process machines $r = 1, \ldots, R$ considering a unique metrology tool capacity $\sum_{t=1}^{T} Capa_t$. Use $g_r^t(s)$ and $WL_r^t(s)$ with the metrology allocation in $\mathcal{M}$.
Let $\mathcal{G}$ be the set of fixed triplets (process machine, sampling period, metrology tool). $\mathcal{G} \leftarrow \emptyset$.
Let $Capa_t$ be the capacity used on metrology tool t. $Capa_t = 0$, $t = 1, \ldots, T$.
while $\mathcal{R} \neq \emptyset$ **do**
    Determine $\Delta_r^t = \{g_r^t(s) - min_{t'=1,\ldots,T; t' \neq t \text{ and } Capa_{t'} + g_r^{t'}(s) \leq 1}(g_r^{t'}(s))\}$ $\forall r \in \mathcal{R}$ and s such that $(r, s) \in \mathcal{F}$, $\forall t \in \mathcal{T}$.
    Let $\mathcal{V} = \left\{(r, t) \in \mathcal{R} \times \mathcal{T} | \Delta_r^t = \max_{r' \in \mathcal{R}, t' \in \mathcal{T}}(\Delta_{r'}^{t'})\right\}$.
    Select $(r^*, t) \in \mathcal{V}$and s^* such that $(r^*, s^*) \in \mathcal{F}$ and $g_{r^*}^t(s^*) = \max_{(r,t) \in \mathcal{V}, (r,s) \in \mathcal{F}}(g_r^t(s))$.
    Let $\mathcal{W} = \{t \in \mathcal{T} | g_{r^*}^t(s^*) = \min_{t'=1,\ldots,T; t' \neq t \text{ and } Capa_{t'} + g_{r^*}^{t'}(s^*) \leq 1}(g_{r^*}^{t'}(s^*))\}$.
    Select $t^* \in \mathcal{W}$ with the lowest current utilization, i.e. $Capa_{t^*} = \min_{t=1,\ldots,T} Capa_t$.
    if $\nexists t \in V^t$ such that $Capa_t + g_{r^*}^t(s) \leq 1$ **then**
        Select $t^* \in \mathcal{T}$ with the lowest current utilization, i.e. $Capa_{t^*} = \min_{t=1,\ldots,T} Capa_t$.
    end if
    Assignment phase$(r^*, t^*, s^*, Capa_{t^*}, \mathcal{G})$.
    $\mathcal{R} \leftarrow \mathcal{R} - \{r^*\}$.
end while
Improvement phase$(\mathcal{G})$.

Heuristic H_7, detailed in Algorithm 10, is metrology tool based and is a modification of H_4.

Algorithm 10 Heuristic H_7 (based on H_4)

1: Let $\mathcal{R} = \{1, \ldots, R\}$ be the set of process machines.
2: Let $\mathcal{F}$ be the set of fixed pairs (process machine, sampling period). $\mathcal{F} \leftarrow \emptyset$.
3: Let $\mathcal{M}$ be the set of fixed pairs (process machine, metrology tool). $\mathcal{M} \leftarrow \emptyset$.
4: Initialize $\mathcal{M}$ by using the optimal solution of the Lagrangian relaxation problem.
5: Determine $\mathcal{F}$ by solving the Multi-Choice Knapsack Problem with Heuristic H_1 presented in Dauzère-Pérès, Hassoun, and Sendon (2016a) for the process machines $r = 1, \ldots, R$ considering a unique metrology tool capacity $\sum_{t=1}^{T} Capa_t$. Use $g_r^t(s)$ and $WL_r^t(s)$ with the metrology allocation in $\mathcal{M}$.
6: Let $\mathcal{G}$ be the set of fixed triplets (process machine, sampling period, metrology tool). $\mathcal{G} \leftarrow \emptyset$.
7: Let $Capa_t$ be the capacity used on metrology tool t. $Capa_t = 0$, $t = 1, \ldots, T$.
8: **while** $\mathcal{R} \neq \emptyset$ **do**
9: Select t^*, the metrology tool with the lowest current utilization, i.e. $Capa_{t^*} = \min_{t=1,\ldots,T} Capa_t$.
10: Determine $\Delta_r = \{g_r^{t^*}(s) - \min_{t'=1,\ldots,T; t' \neq t^* \text{ and } Capa_{t'} + g_r^{t'}(s) \leq 1}(g_r^{t'}(s))\}$ $\forall r \in \mathcal{R}$ and s such that $(r, s) \in \mathcal{F}$.
11: Let $\mathcal{V} = \{r \in \mathcal{R} | \Delta_r = \max_{r' \in \mathcal{R}}(\Delta_{r'})\}$.
12: Select $r^* \in \mathcal{V}$ and s^* such that $(r^*, s^*) \in \mathcal{F}$ and t^* such that $g_{r^*}^{t^*}(s^*) = \max_{r \in \mathcal{V}, (r,s) \in \mathcal{F}}(g_r^{t^*}(s))$.
13: Assign t^*, the metrology tool with the lowest remaining and feasible capacity when r^* is assigned to t^* with sampling rate s^*, i.e. such that $1 - (Capa_{t^*} + g_{r^*}^{t^*}(s^*)) = \{\min_{t=1,\ldots,T;\ Capa_t + g_{r^*}^t(s^*) \leq 1}(1 - (Capa_t + g_{r^*}^t(s^*)))\}$.
14: **Assignment phase**$(r^*, t^*, s^*, Capa_{t^*}, \mathcal{G})$.
15: $\mathcal{R} \leftarrow \mathcal{R} - \{r^*\}$.
16: **end while**
17: **Improvement phase**$(\mathcal{G})$.

4. Numerical experiments

In this section, we analyze the performance of the Lagrangian heuristic LRH, and in particular the impact of the feasibility heuristics H_{1-7} in LRH, on numerous randomly generated instances, and compare it with the results obtained with the ILP and the standard solver IBM ILOG CPLEX 12.6. LRH running in less than 1 second for each instance, we decided to limit the standard solver to 60 seconds. Since the optimal solution is not always obtained, we provide the lower bound (LB) and the upper bound (UB) given by IBM ILOG CPLEX after 60 seconds. We first study in Section 4.1 the general problem described in section 2. Then, we study in Section 4.2 the performance of LRH for the special case of reliable identical machines and compare it with the best heuristic introduced in Dauzère-Pérès, Hassoun, and Sendon (2016b). This comparison is important to ensure that LRH is as effective on this special case than a dedicated procedure, in particular because LRH is embedded in a Decision Support System that can be used on problems with identical machines.

4.1 *Results for heterogeneous metrology machines*

4.1.1 Experiment description

The scenarios used to study the general case of heterogeneous and unreliable machines were generated as follows. Note that the scenarios were generated so that the efficiency of LRH could be analyzed in different extreme cases, in particular regarding the variability of parameters and the number of production machines and metrology tools. The number of process machines is chosen in set $\{5, 10, 20, 40\}$ and the characteristics of each process machine r are defined as follows. The probability of failure p_r is generated from a uniform distribution $U[p_{min}; p_{max}]$, where p_{min} is kept constant ($p_{min} = 0.01$) and p_{max} is chosen in the set $\{0.05, 0.2\}$. The throughput rate TP_r is generated from a distribution $U[TP_{min}; TP_{max}]$, where $TP_{max} = 1000$ and TP_{min} is chosen in the set $\{100, 900\}$. The number of metrology tools is in the set $\{3, 5\}$, and their reliability α_r^t is randomly generated from $U[\alpha_{min}; \alpha_{max}]$ with $\alpha_{min} = 0.01$ and α_{max} in the set $\{0.05, 0.1, 0.2\}$.

Three cases are considered to generate the measurement rate TM_r^t for metrology tools values, which is determined using the ratio $\frac{R \cdot \overline{TP_r}}{T \cdot TM_r^t}$. In the first case, all metrology tools are equally fast ($TM_r^t = TM$), and their measurement rate is independent of the different products processed on process machines r. The ratio $\frac{R \cdot \overline{TP_r}}{T \cdot TM_r^t}$ is chosen in the set $\{5, 10, 30\}$, where $\overline{TP_r}$ is the average throughput rate for the considered instance, thus leading to a unique measurement rate for all tools and machines. This case is denoted “Identical Measurement rate” (IM). Note that, contrary to the case presented in section 4.2, the metrology machines remain different from one another since their reliabilities (α_r^t) differ. In the second case, the measurement rate depends on the metrology tool, but remains independent of the production machines ($TM_r^t = TM^t, \forall r$). One value of $\frac{R \cdot \overline{TP_r}}{T \cdot TM_r^t}$ is randomly chosen from a uniform distribution. The distribution range is first set at $U[2.5, 7.5]$, then at $U[5, 15]$ and finally at $U[15, 45]$. These ranges are defined around the values chosen for the fixed case, and allow for the fastest metrology tool to run at most three times faster than the slowest one. This group of instances is denoted “Related Measurement rate” (RM). In the last case, we allow any value for each TM_r^t, regardless of others, based on the ratio $\frac{R \cdot \overline{TP_r}}{T \cdot TM_r^t}$ taken from the same uniform distributions previously mentioned. We denote this last group “Unrelated Measurement rate” (UM).

A maximum sampling rate of $SP^{max} = 500$ is set for all machines. Combining these parameters leads to 864 instances, with 10 instances generated for each fixed set of distribution ranges. Thus, a total of 8640 different experiments were conducted. The calculation of $WL_r^t(SP)$ includes an infinite sum that is calculated iteratively. In order to keep the accuracy level uniform between experiments, the calculations are stopped when the values of two consecutive $WL_r^t(SP)$ differ by less than 0.1%.

4.1.2 Comparing the impact of the feasibility heuristics

We first justify the need for combining the seven feasibility heuristics in LRH by presenting their individual performance. Table 1 first shows for each feasibility heuristic the portion of cases in which it has been the one to provide the best solution. Then, the second and third rows show the portion of cases in which the heuristic reaches a solution within 1% of the best solution, and cases in which not only did it provide the best solution, but no other solution is within 1% of the best solution. Last, the portion of cases in which the heuristic was within 1% of the upper bound is provided. No heuristic seems superfluous. Although $LRH(H_2)$ and $LRH(H_5)$ are exclusively close to the best result in only 0.1% of the cases, they cannot be removed without impeding the solution in some cases. All heuristics provide the best solution, or give an excellent solution (within 1% of the best), in numerous cases.

Table 1.: General performance of Heuristics $LRH(H_{1-7})$ on heterogeneous machines

	H_1	H_2	H_3	H_4	H_5	H_6	H_7
Best	9.2%	23.1%	40%	22.2%	6.6%	28.8%	8.1%
Close to best	28.8%	52.2%	76.2%	54.1%	45.5%	73.8%	46.4%
Exclusive close to best	2.1%	0.1%	1.1%	0.5%	0.1%	2.9%	0.2%
Close to IBM ILOG CPLEX UB	11.2%	30.2%	47.4%	31.3%	23.2%	43.3%	24.2%

Next, Tables 2 and 3 count the number of times each heuristic yields the best and close-to-best solution, respectively, together with any other heuristic. As an example, $LRH(H_2)$ reached a close-to-best solution in 4507 cases, 10 of which exclusively, and in 4284 cases, $LRH(H_3)$ also reaches a close-to-best solution. There is no case in which a heuristic appears to offer a high level of redundancy with another one. This reflects the way the heuristics were developed and gradually added to LRH to cover for other ones' blind spots.

Table 2.: Common best solution of Heuristics $LRH(H_{1-7})$ on heterogeneous machines

	Best	H_1	H_2	H_3	H_4	H_5	H_6	H_7
H_1	791		3	27	10	2	27	5
H_2	2000	3		1527	904	236	194	183
H_3	3455	27	1527		910	204	1037	194
H_4	1916	10	904	910		187	214	300
H_5	573	2	236	204	187		320	184
H_6	2484	27	194	1037	214	320		194
H_7	699	5	183	194	300	184	194	

Table 3.: Common performance of Heuristics $LRH(H_{1-7})$ on heterogeneous machines

	Close to best	Exclusive	H_1	H_2	H_3	H_4	H_5	H_6	H_7
H_1	2488	179		1473	2147	1474	1277	2034	1236
H_2	4507	10	1473		4284	4278	3796	3852	3678
H_3	6583	96	2147	4284		4325	3742	5862	3705
H_4	4671	39	1474	4278	4325		3723	3935	3837
H_5	3931	6	1277	3796	3742	3723		3746	3467
H_6	6378	248	2034	3852	5862	3935	3746		3624
H_7	4007	13	1236	3678	3705	3837	3467	3624	

4.1.3 Performance analysis of LRH

The next step is to analyze the performance of LRH. In Table 4(a), the average and maximum gaps between the solutions of LRH and of the standard solver IBM ILOG CPLEX 12.6 are detailed for each combination of the number of production machines and number of metrology tools. Although the maximum gap is above 8% for the instances with 5 production machines, the average gap is always below 1% for instances with 3 metrology tools and below 2% for instances with 5 metrology tools. Table 4(b) shows the Lagrangian gaps. The same behavior than in Table 4(a) can be observed, Lagrangian gaps are reducing when the ratio between the number of production machines and the number of metrology tools is increasing. This is interesting and validate the use of LRH in practical settings, since the number of metrology tools is usually much smaller than the number of production machines when metrology capacity is tight. Table 4(c) shows the average number of iterations in LRH to reach the largest lower LB, i.e. close to the Lagrangian dual, and the average number of iterations in LRH to determine the smallest UB. Note that the first average number is rather stable between 161 and 171. Looking at the second average number, it is interesting to see that the subgradient search helps LRH to reach good solutions with the feasibility heuristics since more than 50 iterations are often required.

Table 4.: General performance of $LRH(H_{1-7})$

(a) vs. IBM ILOG CPLEX

		T	
R		3	5
5	Avg	0.5%	
	Max	6.4%	
10	Avg	0.6%	1.3%
	Max	3.9%	8.5%
20	Avg	0.7%	1.3%
	Max	3.5%	4.8%
40	Avg	0.7%	1.2%
	Max	3.0%	4.4%

(b) Lagrangian gap

		T	
R		3	5
5	Avg	3.8%	
	Max	13.4%	
10	Avg	1.5%	3.6%
	Max	6.1%	14.6%
20	Avg	1.0%	2.3%
	Max	4.5%	9.4%
40	Avg	0.9%	2%
	Max	5.1%	10.0%

(c) Average number of iterations

		T	
R		3	5
5	LB	161.2	
	UB	16.2	
10	LB	162.0	164.8
	UB	41.0	48.8
20	LB	164.5	167.5
	UB	59.5	67.3
40	LB	165.5	171.2
	UB	77.2	89.1

The analysis by parameter provided in Tables 5 and 6 shows that LRH tends to perform better when the variability is lower on parameters α_{max}, Ratio Level and TP_{min}, i.e. when $\alpha_{max} = 0.05$, the Ratio Level is equal to 1 and $TP_{min} = 900$. This is the opposite for p_{max}, since the instances generated with $p_{max} = 0.2$ have lower average gaps than the instances generated with $p_{max} = 0.05$. Finally, there is no significant trend for the average gaps whether the instances are with "Identical", "Related" or "Unrelated" TM types.

4.2 *Special case of reliable identical metrology tools*

In Dauzère-Pérès, Hassoun, and Sendon (2016b), we introduce and solve a special case of the problem presented here, namely with perfectly reliable, identical metrology machines. In this section, the performance of the seven heuristics presented in Section 3.2 is analyzed, and LRH is compared with the best heuristic proposed in Dauzère-Pérès, Hassoun, and Sendon

Table 5.: Break down of LRH performance by parameter (1/2).

(a) By α_{max}

		T					
R		3			5		
α_{max}		0.05	0.1	0.2	0.05	0.1	0.2
5	Avg	0.4%	0.4%	0.6%			
	Max	5.6%	6.4%	4.9%			
10	Avg	0.5%	0.6%	0.8%	1.1%	1.2%	1.7%
	Max	3.4%	3.6%	3.9%	8.5%	7.8%	7.5%
20	Avg	0.4%	0.6%	1%	0.8%	1.2%	1.8%
	Max	1.7%	1.9%	3.5%	4.8%	4%	4.4%
40	Avg	0.4%	0.6%	1%	0.7%	1.1%	1.7%
	Max	1.8%	1.8%	3%	2.7%	2.6%	4.4%

(b) By p_{max}

		T			
R		3		5	
p_{max}		0.05	0.2	0.05	0.2
5	Avg	0.5%	0.4%		
	Max	4.9%	6.4%		
10	Avg	0.7%	0.5%	1.5%	1.2%
	Max	3.9%	3.6%	7.5%	8.5%
20	Avg	0.8%	0.5%	1.5%	1%
	Max	3.5%	2.4%	4.8%	4%
40	Avg	0.8%	0.5%	1.4%	0.9%
	Max	3%	2.3%	4.4%	3.1%

(c) By Ratio Level

		T					
R		3			5		
Ratio Level		1	2	3	1	2	3
5	Avg	0.6%	0.5%	0.3%			
	Max	6.4%	4.9%	3.2%			
10	Avg	0.9%	0.7%	0.3%	1.9%	1.3%	0.8%
	Max	3.5%	3.9%	2.9%	8.5%	6.5%	5.1%
20	Avg	0.9%	0.7%	0.4%	1.7%	1.3%	0.8%
	Max	3.5%	2.8%	2.1%	4.8%	4.3%	3.3%
40	Avg	0.9%	0.7%	0.4%	1.5%	1.2%	0.7%
	Max	3%	2.8%	1.8%	4.4%	3.9%	2.7%

(2016b), and on the same set of 2880 instances.

4.2.1 *Comparing the impact of the feasibility heuristics for reliable identical metrology tools*

Let us first consider the question of possible dominance of heuristics $LRH(H_{1-7})$ among themselves, when solving the special case of identical reliable metrology machines. Table 7

Table 6.: Break down of LRH performance by parameter (2/2).

(a) By TP_{min}

		T			
R		3		5	
TP_{min}		100	900	100	900
5	Avg	0.5%	0.4%		
	Max	6.4%	4.2%		
10	Avg	0.7%	0.6%	1.5%	1.2%
	Max	3.9%	2.8%	8.5%	5.4%
20	Avg	0.7%	0.7%	1.3%	1.3%
	Max	3.5%	2.6%	4.8%	4.4%
40	Avg	0.7%	0.7%	1.2%	1.1%
	Max	3%	3%	4.3%	4.4%

(b) By type of TM values

		T					
R		3			5		
TM values		Identical	Related	Unrelated	Identical	Related	Unrelated
5	Avg	0.7%	0.2%	0.5%			
	Max	4.9%	2.5%	6.4%			
10	Avg	0.8%	0.6%	0.5%	1.2%	1%	1.8%
	Max	3.9%	2.7%	3.6%	7.1%	4%	8.5%
20	Avg	0.8%	0.8%	0.4%	1.3%	1.4%	1.1%
	Max	3.5%	2.8%	2.4%	4.4%	4.3%	4.8%
40	Avg	0.8%	0.8%	0.3%	1.3%	1.2%	1%
	Max	3%	3%	2%	4.4%	4%	2.9%

provides the proportion of cases in which each heuristic reaches the best solution, followed by the proportion of cases in which each heuristic provides a solution close to the best one by less than 1% ("Close to best") and of cases in which no other heuristic solution is close to the best one by less than 1%. Finally the ratio of cases in which each heuristic reaches a solution different by less than 1% than the upper bound found by the standard solver is provided.

Table 7.: General performance of $LRH(H_{1-7})$ on identical machines

	H_1	H_2	H_3	H_4	H_5	H_6	H_7
Best	0%	57.8%	57.8%	60.1%	30.8%	30.8%	31.3%
Close to best	0%	99.4%	99.4%	99.8%	93.6%	93.6%	93.9%
Exclusive close to best	0%	0%	0%	0.2%	0%	0%	0%
Close to IBM ILOG CPLEX UB	0%	97.1%	97.1%	98%	88.6%	88.6%	89%

As expected, Heuristic $LRH(H_1)$, which is directly based on the Lagrangian relaxation solution, struggles to provide any good solution when the metrology tools are identical. Heuristics $LRH(H_{2-7})$ all prove to be highly efficient in solving the identical machine case. Note that only $LRH(H_4)$ provides, extremely rarely (0.2%), an "exclusive" solution (no other heuristic finds a solution which is within 1% of the best solution). In all other cases, there is always one or more solutions close to the best one, which clearly prompts the question of possible dominance between heuristics. In Table 8, for each feasibility heuristic (rows), the total number of instances in which the heuristic provides the best solution is indicated. Then, out of this number, the number of times the best solution is reached together with each other heuristic is indicated. Note that $LRH(H_2)$ and $LRH(H_3)$ systematically provide the best solution together. The same holds for $LRH(H_5)$ and $LRH(H_6)$. The same analysis is provided for solutions within 1% of the best one, in Table 9, and the same observations can be made. It is then possible to conclude that heuristics $LRH(H_2)$ and $LRH(H_3)$, and heuristics $LRH(H_5)$ and $LRH(H_6)$ are interchangeable and two of them are unnecessary when solving the problem for reliable, identical machines.

Table 8.: Common best solution of$LRH(H_{1-7})$ on identical machines

	Best	H_1	H_2	H_3	H_4	H_5	H_6	H_7
H_1	0		0	0	0	0	0	0
H_2	1664	0		**1664**	994	631	631	589
H_3	1664	0	**1664**		994	631	631	589
H_4	1731	0	994	994		600	600	654
H_5	886	0	631	631	600		**886**	589
H_6	886	0	631	631	600	**886**		589
H_7	902	0	589	589	654	589	589	

Table 9.: Common performance of $LRH(H_{1-7})$ on identical machines

	Close to best	Exclusive	H_1	H_2	H_3	H_4	H_5	H_6	H_7
H_1	0	0		0	0	0	0	0	0
H_2	2862	0	0		**2862**	2858	2691	2691	2693
H_3	2862	0	0	**2862**		2858	2691	2691	2693
H_4	2874	6	0	2858	2858		2690	2690	2700
H_5	2695	0	0	2691	2691	2690		**2695**	2640
H_6	2695	0	0	2691	2691	2690	**2695**		2640
H_7	2704	0	0	2693	2693	2700	2640	2640	

4.2.2 Performance analysis of LRH for reliable identical metrology tools

Let us now compare the performance of LRH to heuristic H_1^+ proposed in Dauzère-Pérès, Hassoun, and Sendon (2016b). The performance of both heuristics is deemed equivalent if their resulting wafer loss figures are within 0.1% of each other, and one of them is considered better if it provides a wafer loss lower than the other by more than 0.1%. Overall, LRH provides strictly better results in 39.6% of the cases (1140 instances). Both heuristics are equivalent in 60.4% of the cases (1232 instances). Hence, LRH strictly dominates H_1^+. Additionally, LRH is so efficient for identical machines that a drill down analysis by factor, as conducted in Dauzère-Pérès, Hassoun, and Sendon (2016b) for cases offering some difficulties for H_1^+, is unnecessary. Table 10 shows that the average gaps between LRH and the best solution obtained by IBM ILOG CPLEX is always lower than 0.6%.

Table 10.: Comparison between $LRH(H_{1-7})$ and IBM ILOG CPLEX

		T			
		3		5	
R		Non-opt.	Opt.	Non-opt.	Opt.
5	Avg.	0%	0.2%		
	Min.	0%	0%		
	Max.	0%	2.3%		
10	Avg.	0.1%	0.3%	0.1%	0.4%
	Min.	0%	0%	0%	0%
	Max.	0.7%	1.2%	0.4%	1.7%
20	Avg.	0.1%	0.2%	0.2%	0.6%
	Min.	0%	0%	-0.1%	0.2%
	Max.	0.3%	0.6%	1.1%	1.1%
40	Avg.	0%	0.1%	0.1%	0.2%
	Min.	0%	0%	-0.1%	0.1%
	Max.	0.1%	0.2%	0.4%	0.4%

5. Conclusions and perspectives

In a previous body of work, we first tackled the problem of assigning a unique metrology tool capacity to minimize the risk in terms of expected product loss of several different production machines. This problem was defined as a Multiple-Choice Knapsack Problem. Later, we solved an extension of this first problem that considers several similar metrology tools, which was defined as a Multiple Choice Multiple Knapsack Problem. In both these works, heuristics were proposed.

In the present paper, we significantly extend the scope of the problem by assuming, first, that the metrology tools are no longer reliable, and second, that they differ in their characteristics (measurement rate, reliability). This problem emerges as a Multiple Choice Generalized Assignment Problem for which greedy or simple heuristics fail to provide an acceptable solution. To avoid using a standard solver and solve the problem in less than one second, we proposed a Lagrangian Relaxation Heuristic (LRH). LRH is based on the mathematical formulation of the problem and combines seven feasibility heuristics, that proved to be efficient both on a large set of scenarios designed to cover various situations, and on the special case of identical machines solved previously with a much simpler heuristic. The feasibility heuristics derive a solution from the resolution of the Lagrangian relaxed problem in a variety of manners, starting from measurement rates or from assignments of production machines to metrology tools. The results, when compared to the optimal solution, show that LRH is efficient over a broad range of scenarios.

The Lagrangian heuristics has been implemented in a Decision Support System (DSS) for the factory of the semiconductor manufacturing company in which one of the co-authors performed his PhD thesis. The primary use of the DSS is to propose optimal sampling rates that users can modify before implementation in the control system of the factory. However, the DSS can also help to evaluate the impact in terms of risk reduction, respectively increase, associated to increasing, respectively reducing, metrology capacity. This is in particular important to justify the acquisition of new metrology tools. From another angle, when new production machines are added, the DSS can also help to analyze the impact in terms of risk increase if the same set of metrology tools is used.

Further directions can be explored based on the results obtained so far. Up to this point, our problem allows the metrology capacity to be fully utilized. The underlying assumption allowing this is that there is a perfect synchronization between the monitoring needs and the metrology availability. In industrial scenarios, this is not always the case. The queue at the metrology tool is expected to induce a delay which could impede quality. Other future research could include additional features of the problem as it presents itself to practitioners in factories. In particular, our model is applicable to cases where a single-stage inspection takes place, i.e. the inspection operation only controls process machines that are right before the metrology tools. Cases where a series of process operations, and therefore a series of process machines, are controlled through a concluding inspection operation add a level of complexity that is far from trivial. Also, we are studying an extension of the current framework that considers the effects of false positives when metrology tools are not only used for ongoing monitoring of the process, but also contributes to the investigation following an out-of-control result.

Acknowledgments

Parts of this research were carried out whilst the second author was visiting the Department of Manufacturing Sciences and Logistics of the Center of Microelectronics in Provence of the Ecole des Mines de Saint-Etienne, Gardanne, France in September and October 2016 and October 2017.
This work has been partially financed by the ANRT (Association Nationale de la Recherche et de la Technologie) through the PhD number 2014/0079 with CIFRE funds and a cooperation contract between STMicroelectronics and Mines Saint-Etienne.

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