

## Parallel Strategies for Direct Multisearch

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### ABSTRACT

Direct Multisearch (DMS) is a Derivative-free Optimization class of algorithms suited for computing approximations to the complete Pareto front of a given Multiobjective Optimization problem. It has a well-supported convergence analysis and simple implementations present a good numerical performance, both in academic test sets and in real applications. Recently, this numerical performance was improved with the definition of a search step based on the minimization of quadratic polynomial models, corresponding to the algorithm BoostDMS.

In this work, we propose and numerically evaluate the performance of parallelization strategies for this solver, applied to the search and to the poll steps. The final parallelized version not only considerably decreases the computational time required for solving a Multiobjective Optimization problem, but also increases the quality of the computed approximation to the Pareto front. Extensive numerical results will be reported in an academic test set and in a chemical engineering application.

### KEYWORDS

Multiobjective optimization; derivative-free optimization; direct search methods; parallel algorithms.

### AMS CLASSIFICATION

90C29, 90C56, 68W10, 90C30.

## 1. Introduction

Direct MultiSearch (DMS) [15] is a well-established class of Multiobjective Derivative-free Optimization algorithms, which has been successfully used in real applications from very different scientific areas. Optimization of composite structures [29], economic problems [22], or data science applications [27] are just a few examples of the practical value of DMS. Additionally, the corresponding solver has been considered in benchmark studies, as a reference code for new algorithms [12, 28].

When the algorithmic class of Direct Multisearch was originally proposed, the goal was to generalize directional direct search [5, 13] to Multiobjective Optimization. Surprisingly, the first implementation developed, which did not even comprise a defined search step, showed to be competitive against other state-of-art solvers like evolutionary strategies [17], simulated annealing [8], or direct search algorithms [6]. Recently,

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exceptional good results were also obtained when applying the solver to derivative-based optimization [1].

However, since its first version, in 2010, new releases corresponded to small improvements of the original implementation, with no major changes. Exception occurred in [10], where the definition of a search step based on the minimization of quadratic polynomial models was proposed. This new version of the code was named as BoostDMS.

This paper considers the use of BoostDMS to solve the Multiobjective Derivative-free Optimization problem

$$\begin{aligned} \min \quad & F(x) \equiv (f_1(x), \dots, f_q(x))^\top \\ \text{s.t.} \quad & lb \leq x \leq ub, \end{aligned} \tag{1}$$

where  $q \geq 2$ ,  $lb < ub$  represent bounds on the problem variables, and each  $f_i : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ ,  $i = 1, 2, \dots, q$  denotes a component of the objective function, for which derivatives are not available, neither can be numerically approximated.

When the different components of the objective function are conflicting between each other, it is impossible to find a point that minimizes every function component. Thus, rather than a single point, the solution of a Multiobjective Optimization problem is a set of points, for which it is not possible to improve the value of one component of the objective function without deteriorating the value of at least another. Points with these characteristics are said to be *efficient points* and the corresponding images form the *Pareto front* of the Multiobjective Optimization problem.

Since we are addressing Derivative-free Multiobjective Optimization problems, like in the single objective case, the computational time required for computing a solution is usually large, due to the expensive process of function evaluation. In fact, since the problem solution is no longer a point but a set of points, there is a strong need for strategies that allow to reduce the computational time without deteriorating the quality of the solution computed.

Distributed computing with multiple processors is often considered in the context of single objective optimization, for solving computationally quite demanding problems. Parallelization of Derivative-free Optimization methods for single objective optimization, particularly direct search ones, has been largely studied in the literature. Dennis and Torczon [19] described a first parallel version of a pattern search method which evaluates the function in parallel and synchronizes at each iteration to compare function values and make updates. A first asynchronous parallel version of pattern search was proposed in [26], dynamically initiating actions in response to events. Asynchronous approaches were also followed in [4], where processes solve problems over subsets of variables. Parallel approaches were also adopted for global single objective direct search algorithms [25, 33], often hybridizing metaheuristics with local direct search methods [24, 32].

In Multiobjective Optimization, parallelization appears typically associated to metaheuristics, like is the case of evolutionary strategies [9, 11, 18] or particle swarm approaches [21, 34]. A good overview of different parallel models for Multiobjective Optimization can be found in [30]. However, to the best of our knowledge, parallel approaches have not yet been considered for Multiobjective Directional Direct Search algorithms. Thus, the main goal of this paper will be to develop a parallel version of BoostDMS, which allows a considerable decrease of the computational time required for solving a problem, without deteriorating the quality of the computed approxima-

tion to the Pareto front.

The paper is organized as follows. Section 2 revises the algorithmic structure of BoostDMS algorithm, pointing out possible steps for parallelization. Section 3 details the different parallel strategies considered, evaluating the corresponding numerical performance. Numerical experiments on a chemical engineering problem are reported in Section 4, enhancing the benefits of the selected parallel strategy. Finally, conclusions are drawn in Section 5.

## 2. BoostDMS implementation of Direct Multisearch

BoostDMS [10] is a numerical implementation of a Direct Multisearch [15] algorithm, where the individual or joint minimization of quadratic polynomial models, built for each component of the objective function, is used in the definition of a search step.

The algorithm initializes with a list,  $L_0$ , of feasible, nondominated points, corresponding function values and stepsize parameters. In BoostDMS, following the initialization proposed in [15],  $n$  points are evenly spaced in a line joining the problem bounds. Additionally, the centroid of the feasible region is always considered as initialization. This list represents the current approximation to the Pareto front of the problem and is updated every time that a new feasible nondominated point is found, corresponding to a successful iteration. The new nondominated point is added to the list and all the dominated points are removed from it. Using the strict partial order induced by the cone  $\mathbb{R}_+^q$ , a point  $x$  is said to dominate a point  $y$  if  $F(x) \prec_F F(y)$ , i.e., when  $F(y) - F(x) \in \mathbb{R}_+^q \setminus \{0\}$ .

Each iteration of the algorithm starts by selecting an iterate point,  $(x_k, F(x_k), \alpha_k)$ , from the current list of feasible nondominated points,  $L_k$ , corresponding to the largest gap in the current approximation to the Pareto front, measured using the  $\Gamma$  spread metric:

$$\Gamma = \max_{i \in \{1, \dots, q\}} \left( \max_{j \in \{1, \dots, N-1\}} \{\delta_{i,j}\} \right). \quad (2)$$

Here  $\delta_{i,j} = f_i(y_{j+1}) - f_i(y_j)$ , assuming that for each component  $i$  of the objective function,  $y_1, \dots, y_N$  are the current points in the list  $L_k$ , sorted by increasing order of the corresponding objective function component value. Ties are broken by considering the point with the largest stepsize parameter. This iterate point will be used at the search step, as center of the quadratic polynomial models that will be built for each component,  $f_i$ , of the objective function. In case of failure of the search step in computing a new feasible nondominated point, the poll step will be performed, with the iterate point as poll center.

The search step reuses previously feasible evaluated points (not necessarily nondominated), kept in a cache, thus with no additional cost in terms of objective function values required for model computation. Points are selected in a neighborhood of the iterate point  $x_k$ , i.e., in  $B(x_k; \Delta_k)$ , where  $\Delta_k$  is proportional to the stepsize parameter  $\alpha_k$ . Models are built once that  $n+2$  points have been evaluated in this region. Depending on the number of points available, minimum Frobenius norm models, determined interpolation models or regression approaches can be considered [13].

Let  $m_i$  define the quadratic polynomial model centered at  $x_k$ , corresponding to the

objective function component  $f_i$ ,

$$m_i(x) = f_i(x_k) + g_k^i{}^\top (x - x_k) + \frac{1}{2}(x - x_k)^\top H_k^i (x - x_k), \quad i = 1, 2, \dots, q \quad (3)$$

where the gradient vector  $g_k^i$  and the symmetric Hessian matrix  $H_k^i$  are computed by solving the linear system corresponding to the interpolation conditions

$$m_i(y_j) = f_i(y_j), \quad j = 1, \dots, p, \quad (4)$$

with  $y_j$  representing a feasible point for which the objective function has been previously evaluated, and  $p$  denoting the number of points inside  $B(x_k; \Delta_k)$  that can be used in the computation.

Models can be minimized individually inside  $B(x_k; \Delta_k)$ , in an attempt to improve the ability of the algorithm in generating approximations to the extreme points of the Pareto front. However, the joint minimization of models is also considered, using a weighted Chebyshev norm scalarization, by solving the following problem:

$$\begin{aligned} \min \quad & \zeta \\ \text{s.t.} \quad & m_i(x) \leq \zeta, \quad i \in I \\ & \|x - x_k\| \leq \Delta_k \\ & lb \leq x \leq ub, \end{aligned} \quad (5)$$

where  $I \subseteq \{1, 2, \dots, q\}$ . For each cardinality  $1 \leq l \leq q$  of a subset  $I$  there are  $C_l^q$  possibilities to jointly minimize the models corresponding to the different components of the objective function. The algorithm starts by the individual minimization of each model ( $l = 1$ ). If it fails in finding a new feasible nondominated point for the objective function, combinations of two models are considered ( $l = 2$ ). The process is iteratively repeated, increasing the level  $l$  of model combinations until the joint minimization of all models is considered ( $l = q$ ). If no new feasible nondominated point is found for the objective function, the poll step will be performed.

The poll step corresponds to a local search around the selected iterate point (the poll center), testing a set of directions with an adequate geometry, scaled by the stepsize parameter. Typically, positive spanning sets are considered [16] that conform to the geometry of the feasible region around the poll center. For bound constraints, BoostDMS considers coordinate directions, which are evaluated in a complete polling approach.

At the end of each iteration the stepsize is updated, keeping it constant for successful iterations and halving the stepsize of the poll center for unsuccessful ones.

A simplified description of BoostDMS is provided in Algorithm 1. For a detailed description see [10, 15].

The convergence analysis of Direct Multisearch algorithmic class relies on the behavior of the method at unsuccessful poll steps [15], holding independently of the initialization, of the strategy considered for the selection of the iterate point, of the definition of a search step, or of the type of polling strategy considered (opportunistic variants are allowed, in which polling is interrupted once that a new feasible nondominated point is found). Recently, worst-case complexity bounds were also derived for some variants of Direct Multisearch [14]. BoostDMS, as an algorithmic instance of DMS, inherits the convergence properties of this general class of Multiobjective

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**Algorithm 1:** A simplified description of BoostDMS.

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**Initialization**

Choose a set of feasible points  $\{lb \leq x_{ini}^j \leq ub, j \in \Upsilon\}$  with  $f_i(x_{ini}^j) < +\infty, \forall i \in \{1, \dots, q\}, \forall j \in \Upsilon$ , and  $\alpha_{ini}^j > 0, j \in \Upsilon$  initial stepsizes. Let  $\mathcal{D}$  be a set of positive spanning sets. Initialize the cache of previously feasible evaluated points and corresponding function values

$$L_{cache} = \{(x_{ini}^j, F(x_{ini}^j)), j \in \Upsilon\}.$$

Retrieve all nondominated points from  $L_{cache}$  and initialize the list of feasible nondominated points, corresponding function values and stepsize parameters

$$L_0 = \{(x_{ini}^j, F(x_{ini}^j), \alpha_{ini}^j), j \in \tilde{\Upsilon} \subseteq \Upsilon\}.$$

**For**  $k = 0, 1, 2, \dots$

1. **Selection of an iterate point:** Order the list  $L_k$  according to the largest gap measured with the  $\Gamma$  metric and select the first item  $(x, F(x), \alpha) \in L_k$  as the current iterate, function value, and stepsize parameter (thus setting  $(x_k, F(x_k), \alpha_k) = (x, F(x), \alpha)$ ).
2. **Search step:**  
Select a subset of points in  $L_{cache} \cap B(x_k; \Delta_k)$  to build the quadratic polynomial models. If the cardinality of the subset is smaller than  $n + 2$  go to the poll step.  
**For**  $i = 1, 2, \dots, q$   
Build the quadratic polynomial model  $m_i$ , corresponding to the objective function component  $f_i$ .  
**Endfor**  
Set  $l = 0$ .  
**While**  $l < m$   
Set  $l := l + 1$ , define  $J$  the set of all combinations of  $l$  quadratic polynomial models taken from the total set of  $q$  models and set  $S = \emptyset$ .  
**For**  $j = 1, 2, \dots, |J|$   
Compute the point  $s_j$ , solution of problem (5) considering  $I$  as the set composed by the polynomial models corresponding to combination  $j$ .  
Update  $S = S \cup \{s_j\}$ .  
**Endfor**  
**Check for success**  
Evaluate  $F$  at each point in  $S$  and update  $L_{cache}$ . Compute  $L_{trial}$  by removing all dominated points from  $L_k \cup \{(x_s, F(x_s), \alpha_k) : x_s \in S\}$ . If  $L_{trial} \neq L_k$ , set  $L_{k+1} = L_{trial}$ , stop the cycle loop **while**, declare the iteration as successful and skip the poll step.  
**Endwhile**
3. **Poll step:** Choose a positive spanning set  $D_k$  from the set  $\mathcal{D}$ . Evaluate  $F$  at the feasible poll points belonging to  $\{x_k + \alpha_k d : d \in D_k\}$  and update  $L_{cache}$ . Compute  $L_{trial}$  by removing all dominated points from  $L_k \cup \{(x_k + \alpha_k d, F(x_k + \alpha_k d), \alpha_k) : d \in D_k \wedge lb \leq x_k + \alpha_k d \leq ub\}$ . If  $L_{trial} \neq L_k$ , declare the iteration as successful and set  $L_{k+1} = L_{trial}$ . Otherwise, declare the iteration unsuccessful and set  $L_{k+1} = L_k$ .
4. **Stepsize parameter update:** If the iteration was unsuccessful halve the stepsize parameter corresponding to the poll center, replacing  $(x_k, F(x_k), \alpha_k) \in L_{k+1}$  by  $(x_k, F(x_k), \frac{\alpha_k}{2})$ .

**Endfor**

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Derivative-free Optimization methods.

From the algorithmic description provided, it is clear that parallelization strategies can be applied to both the search and the poll steps, enhancing the numerical performance of the algorithm. Section 3 will detail possible strategies for parallelization, from the simple distribution of objective function evaluations among the different processors to more sophisticated schemes, including the parallel computation of the quadratic polynomial models, or the simultaneous selection of several iterate points.

### 3. Parallelization strategies

BoostDMS is part of a Derivative-free Optimization Toolbox of solvers, suited for local and global single objective and multiobjective problems, implemented in Matlab and freely available for use at <https://docentes.fct.unl.pt/algb/pages/boostdfo>, under a GNU Lesser General Public License. The toolbox provides a GUI, which allows a non-expert user to take advantage of the different solvers options, including parallelization [31]. For running BoostDMS, the Matlab toolboxes of Optimization and Parallel Computing are required for the minimization of the quadratic models at the search step and for distributing tasks to the different processors, respectively.

The expensive cost of function evaluation, associated to Derivative-free Optimization problems, naturally motivates its parallelization. However, additional parallelization strategies can and will be considered, not only with the goal of time reduction but also with the concern of keeping or improving the quality of the computed approximation to the Pareto front.

To assess this quality, typical metrics from the Multiobjective Optimization literature are used: purity and spread, as defined in [15], and the hypervolume indicator [35, 36]. For completeness, we provide a short description of each one of these metrics. A recent revision of Multiobjective Optimization metrics can be found in [3].

Purity measures the capability of a given solver in generating nondominated points. Let  $F_{p,s}$  denote the approximation to the Pareto front computed for problem  $p \in \mathcal{P}$  by solver  $s \in \mathcal{S}$ , and  $F_p$  denote the true Pareto front of problem  $p$ . The purity metric, for problem  $p \in \mathcal{P}$  and solver  $s \in \mathcal{S}$ , is defined by the ratio

$$Pur_{p,s} = \frac{|F_{p,s} \cap F_p|}{|F_{p,s}|},$$

taking values between zero and one. Higher values of  $Pur_{p,s}$  indicate a better Pareto front in terms of percentage of nondominated points generated. In general,  $F_p$  is not known, being considered an approximation to it by joining all the final approximations computed by all the solvers tested and removing all the dominated points from it.

Spread metrics assess the quality of the distribution of nondominated points across the final approximation to the Pareto front generated by the solver. Since we are interested in computing the complete Pareto front, spread metrics need to consider the ‘extreme points’ associated to each objective function component (see [15]). The  $\Gamma$  metric (2), previously used to select the iterate point based on the maximum gap between consecutive points lying on the approximation to the Pareto front, is now computed using a set that includes the ‘extreme points’. Let us assume that solver  $s \in \mathcal{S}$  has computed, for problem  $p \in \mathcal{P}$ , an approximated Pareto front with points  $y_1, y_2, \dots, y_N$ , to which we add the ‘extreme points’ mentioned above ( $y_0$  and  $y_{N+1}$ ).

The metric  $\Gamma_{p,s} > 0$ , for problem  $p \in \mathcal{P}$  and solver  $s \in \mathcal{S}$ , is given by

$$\Gamma_{p,s} = \max_{i \in \{1, \dots, q\}} \left( \max_{j \in \{0, \dots, N\}} \{\delta_{i,j}\} \right), \quad (6)$$

where  $\delta_{i,j} = f_i(y_{j+1}) - f_i(y_j)$  (assuming that the objective function values have been sorted by increasing order for each objective function component  $i$ ).

The second spread metric [17] measures the uniformity of the gap distribution across the computed Pareto front:

$$\Delta_{p,s} = \max_{i \in \{1, \dots, q\}} \left( \frac{\delta_{i,0} + \delta_{i,N} + \sum_{j=1}^{N-1} |\delta_{i,j} - \bar{\delta}_i|}{\delta_{i,0} + \delta_{i,N} + (N-1)\bar{\delta}_i} \right), \quad (7)$$

where  $\bar{\delta}_i$ , for  $i = 1, \dots, q$ , represents the average of the distances  $\delta_{i,j}$ ,  $j = 1, \dots, N-1$ .

The hypervolume indicator is a good compromise between spread and purity, since it measures the volume of the portion of the objective function space that is dominated by the computed approximation to the Pareto front and is limited by an upper corner  $U_p \in \mathbb{R}^q$  (a point that is dominated by all points belonging to the different approximations computed for the Pareto front by all solvers tested). Thus, the hypervolume indicator can be defined as follows:

$$HV_{p,s} = Vol\{y \in \mathbb{R}^q \mid y \leq U_p \wedge \exists x \in F_{p,s} : x \leq y\} = Vol \left( \bigcup_{x \in F_{p,s}} [x, U_p] \right),$$

where  $Vol(\cdot)$  denotes the Lebesgue measure of a  $q$ -dimensional set of points and  $[x, U_p]$  denotes the interval box with lower corner  $x$  and upper corner  $U_p$ . The approach proposed in [23] was used for its computation, after scaling all the hypervolume values to the interval  $[0, 1]$  (see [10] for details).

The final metric considered is the CPU time required for solving a problem. As test set, we considered 99 bound constrained Multiobjective Optimization problems from the collection available at <http://www.mat.uc.pt/dms>, now coded in Matlab, with a number of variables,  $n$ , between 1 and 30, and with 2, 3, or 4 objective function components (problem WFG1 was not considered due to some numerical instabilities of Matlab). Since these are academic problems, the time associated to function evaluation is quite small, of the order of milliseconds, very different from real applications, where function evaluation typically requires seconds or even minutes of computational time. For a fair assessment of the benefits of parallelization strategies, each function was modified with an average computational time of 0.1 seconds (in single objective optimization, computational times of similar magnitude have already allowed benefits from parallelization [31]). Results are reported for average CPU time, considering five runs.

Performance profiles [20] are computed for the different metrics. Let  $t_{p,s}$  be the value of a given metric obtained for problem  $p \in \mathcal{P}$  with solver  $s \in \mathcal{S}$ , assuming that lower values of  $t_{p,s} > 0$  indicate better performance. The cumulative distribution function for solver  $s \in \mathcal{S}$  is given by:

$$\rho_s(\tau) = \frac{1}{|\mathcal{P}|} |\{p \in \mathcal{P} : r_{p,s} \leq \tau\}|,$$

with  $r_{p,s} = t_{p,s} / \min\{t_{p,\bar{s}} : \bar{s} \in \mathcal{S}\}$ . Thus, the value of  $\rho_s(1)$  represents the probability of solver  $s$  winning over the remaining ones. Since for purity and hypervolume larger values indicate better performance, for these metrics the profiles considered  $t_{p,s} := 1/t_{p,s}$ , as proposed in [15].

All numerical experiments were performed using Matlab R2020a, on a Xeon Platinum 8171M CPU machine from the Azure cloud, running Linux as operating system. Default options were assumed for BoostDMS [10] and all executions ran using 8 processors. In particular, a maximum of 20 000 function evaluations or a minimum value of  $10^{-3}$  for the stepsize parameter  $\alpha_k$  of each point in the list were used as stopping criteria.

### 3.1. Parallelization of objective function evaluations

Typical Derivative-free Optimization problems are associated to expensive function evaluation. In BoostDMS, parallelization of function evaluations was considered both at the poll and the search steps, as a way of improving the numerical performance of the solver.

In Directional Direct Search, the poll step has a natural structure for parallelization. BoostDMS considers a complete polling approach, allowing to take full advantage of an embarrassingly parallel scheme. The set of points to be evaluated at the poll step is generated and, before function evaluation, infeasible points or points considered identical (within a tolerance equal to the minimum stepsize allowed) to others already included in the cache are discarded. This filtered set of points is now evaluated in parallel.

All evaluated points are included in the cache ( $L_{cache}$ ) and dominance is checked, adding nondominated points to the list  $L_k$ , one by one, in a similar way to what is done in the sequential version. This approach ensures that the approximation generated for the Pareto front is exactly the same than the one generated by the sequential version, keeping the quality of the final computed solution.

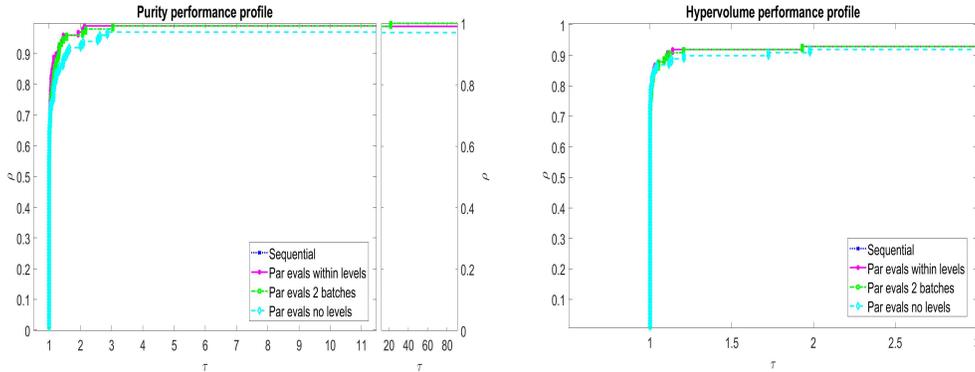
As described in Section 2, the search step considers an approach by levels, when minimizing the quadratic polynomial models. Subproblem (5) may need to be solved for all combinations of  $l$  models. At level  $l = 1$ , the individual minimization of the models is achieved through function `trust.m`, from Matlab, and projecting the resulting points in the feasible region. For levels two and above ( $l \geq 2$ ), the joint minimization of models resources to Matlab's function `fmincon.m`. All solutions of the subproblems at a given level are evaluated and, only in case of failure in finding a new feasible nondominated point, the next level is considered.

Three different approaches have been tested, regarding the parallelization of function evaluations at the search step. The first, *Par evals within levels*, keeps the function evaluation structure by levels of the sequential implementation. A maximum of  $q$  batches of parallel function evaluations can be performed (one associated to each level). In this case, the quality of the solution is identical to the one of the sequential version, although a reduction in computational time is expected. The second variant, denoted by *Par evals 2 batches*, considers function evaluation in two batches, one corresponding to level  $l = 1$  and, in case of failure in finding a new feasible nondominated point, all the remaining levels, corresponding to the joint minimization of two or more models. Finally, the variant denoted by *Par evals no levels* solves all subproblems (5), evaluating the objective function at the corresponding solutions in parallel. In any of the three strategies, subproblems (5) are always solved sequentially. Only function

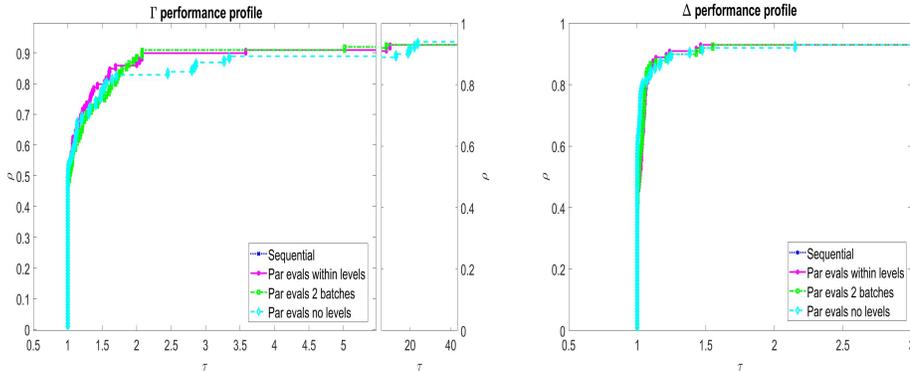
evaluations are parallelized, being the procedure followed identical to the one adopted for the parallelization of the poll step.

A level-by-level approach would be beneficial if success is often found in lower levels, even though it could not take advantage of all the potential of parallelizing function evaluations. However, if success is typically achieved in higher levels or if the search step is often unsuccessful, considering a single batch of parallel function evaluations of points, corresponding to all levels, would be more efficient.

Figures 1, 2, and 3 compare the results obtained with the sequential version to the three parallelization strategies described above, for the five metrics considered.



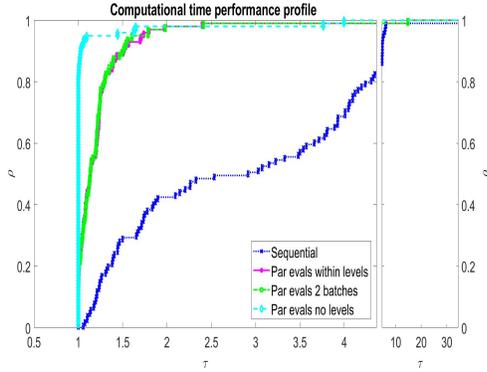
**Figure 1.** Comparison between sequential version of BoostDMS, and parallel versions *Par evals within levels*, *Par evals 2 batches*, and *Par evals no levels*, by means of purity and hypervolume metrics.



**Figure 2.** Comparison between sequential version of BoostDMS, and parallel versions *Par evals within levels*, *Par evals 2 batches*, and *Par evals no levels*, by means of spread metrics ( $\Gamma$  and  $\Delta$ ).

All strategies present a similar performance in terms of hypervolume and  $\Delta$  metrics. As expected, there is a clear advantage in computational time for the parallel versions, with the variant *Par evals no levels* performing the best (see Figure 3). A strategy that gathers all the points before evaluation, reduces the number of batches to be parallelized, translating to better computational times.

However, analyzing the plots corresponding to purity and  $\Gamma$  metrics, we conclude that this strategy presents a worse performance than the other parallel versions. In fact, the results for the three remaining strategies are very close, indicating that feasible nondominated points are typically found in the first level, when the individual



**Figure 3.** Comparison between sequential version of BoostDMS, and parallel versions *Par evals within levels*, *Par evals 2 batches*, and *Par evals no levels*, considering the computational time.

minimization of models occurs. Strategy *Par evals no levels* performs a larger number of function evaluations per search step, promoting the exhaustion of the function evaluations budget at early iterations, which could contribute to better computational times, but does not allow to refine the quality of the computed approximation to the Pareto front.

The variant *Par evals within levels*, that keeps the structure of the parallel function evaluations in batches corresponding to levels, allows a good performance in terms of computational time, keeping the quality of the final solution generated by the sequential version. This was the option taken in terms of strategy for function evaluation and will be adopted in the following numerical experiments.

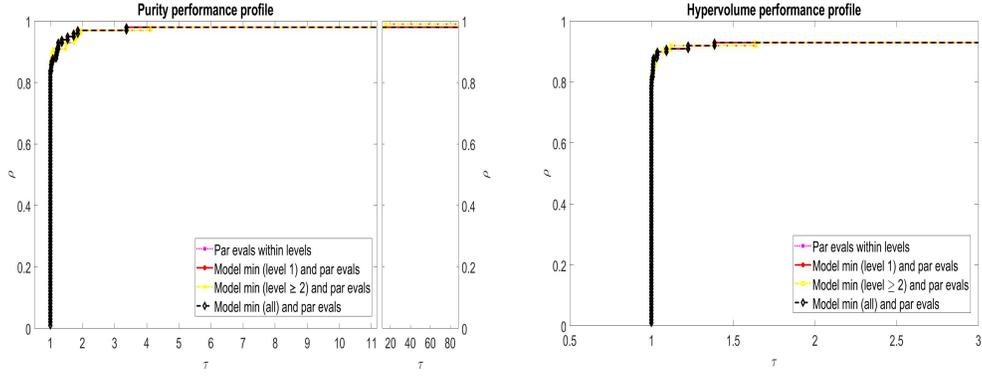
### 3.2. Parallelization of models computation and minimization

The parallelization can obviously be extended to the computation of the quadratic models for each component of the objective function and to the corresponding individual or joint minimization. Thus, three new parallel strategies were developed.

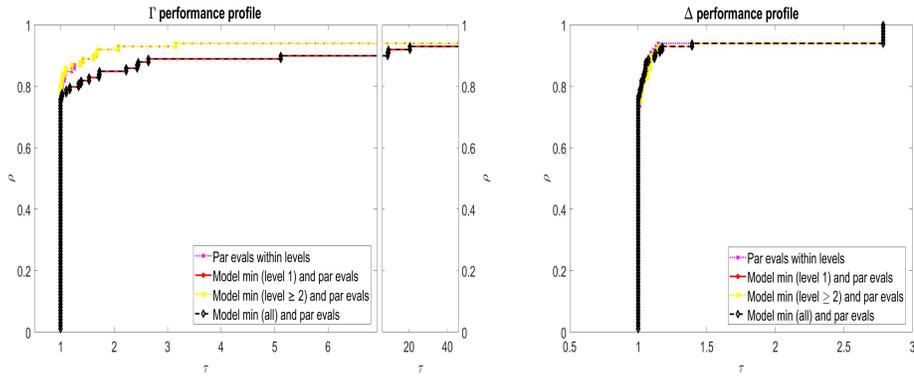
The first, denoted by *Model min (level 1) and par evals*, parallelizes the individual computation and minimization of models, for each objective function component. Strategy *Model min (level  $\geq 2$ ) and par evals* builds models and performs their individual minimization sequentially, only parallelizing the joint minimization of models. Considering the results of Section 3.1, the approach of evaluating batches of points by level is always followed. Since the numerical results of Section 3.1 indicate that the search step is mainly successful at level  $l = 1$ , the number of search steps where levels  $l \geq 2$  will be considered is reduced, thus no major improvement is expected with this second variant. A final strategy, denoted by *Model min (all) and par evals*, parallelizes model building and minimization at all levels.

Figures 4, 5, and 6 report the corresponding performance profiles.

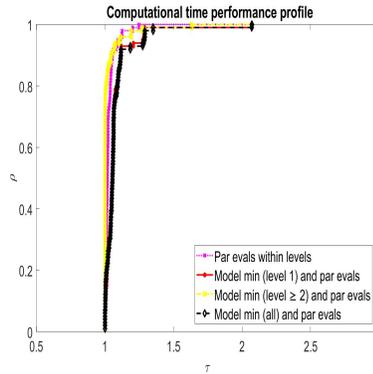
The performance of *Par evals within levels* is very similar to the one of any of these three new strategies in terms of purity, hypervolume, and  $\Delta$  metrics. The two strategies that parallelize the model computation present a slightly worse performance in terms of computational time. This could be explained by the fact that we are addressing problems with a low number of components in the objective function, with a reasonably small dimension ( $n \leq 30$ ), which has implications in the linear systems of equations to be solved for computing the quadratic models. It is also noteworthy



**Figure 4.** Performance profiles corresponding to the parallelization of models building and minimization, by means of purity and hypervolume metrics.



**Figure 5.** Performance profiles corresponding to the parallelization of models building and minimization, by means of spread metrics ( $\Gamma$  and  $\Delta$ ).



**Figure 6.** Performance profiles corresponding to the parallelization of models building and minimization, considering the computational time.

the fact that some of the Matlab’s functions that are used to solve the linear systems of equations are implicitly parallelized in Matlab. In fact, that justifies the differences related to the performance of the  $\Gamma$  metric, since the models obtained are different when built sequentially or in parallel, even when providing exactly the same set of points for computation.

Since the results did not bring advantages, the strategy *Par evals within levels* continues to be the default.

### 3.3. Iterate point selection based on spread

As described in Section 2, each iteration of the algorithm starts with the selection of an iterate point, which will be used as model center, at the search step, or, in case of failure of the search step in finding a new feasible nondominated point, as poll center, at the poll step. The selection is made from the list  $L_k$  of feasible nondominated points, corresponding to the point with the largest value of the  $\Gamma$  metric (2).

This spread metric is considered in an attempt to reduce the gap between consecutive points lying in the current approximation to the Pareto front, after projection of each objective function component in the corresponding dimension. Since the range of each objective function component can be in very different scales, this metric could be biased towards one/some of the function components.

Two additional strategies were considered to prevent this fact. The first, denoted by *Par evals within levels (Gamma normalized)*, before computing the largest gap, normalizes the values of each objective function component  $i \in \{1, \dots, q\}$  using the formula:

$$\frac{f_i(y_j) - \min_{j=1, \dots, N} f_i(y_j)}{\max_{j=1, \dots, N} f_i(y_j) - \min_{j=1, \dots, N} f_i(y_j)},$$

where  $y_1, \dots, y_N$  represent the points in the current list of feasible nondominated points  $L_k$ . This way, a fairer selection of the largest gap among all components is expected.

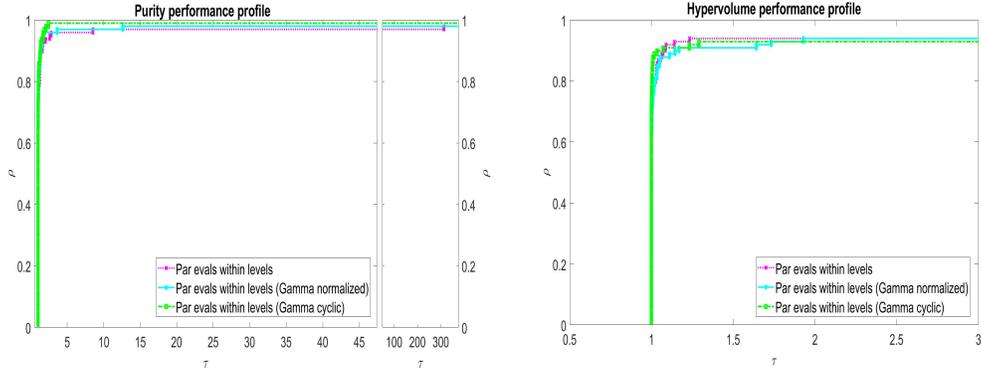
The second strategy, denoted by *Par evals within levels (Gamma cyclic)*, considers a cyclic approach, changing the objective function component for which the largest gap is computed from iteration to iteration in a recurrent way.

Figures 7, 8, and 9 compare these two strategies with *Par evals within levels*. As usual, function evaluation is parallelized both at the search and the poll steps, in the former respecting the levels structure.

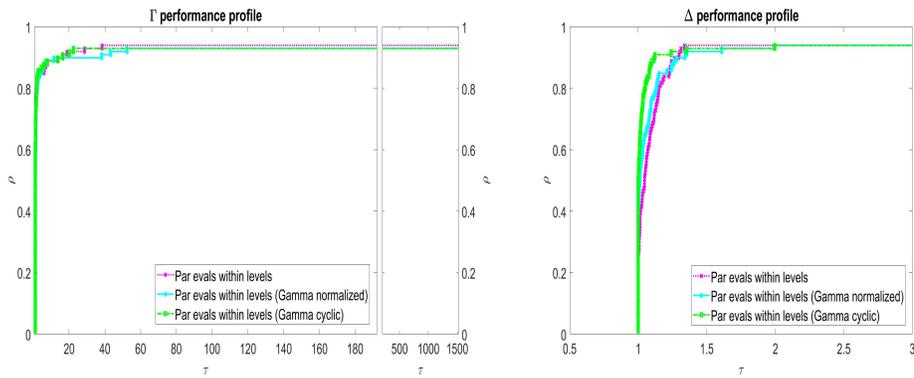
Although the results are very similar for hypervolume and  $\Gamma$  metrics, a slight advantage of *Par evals within levels (Gamma cyclic)* is noticed for purity,  $\Delta$  and computational time, which justifies our option to use it as strategy for the iterate point selection.

### 3.4. Selection of more than one iterate point

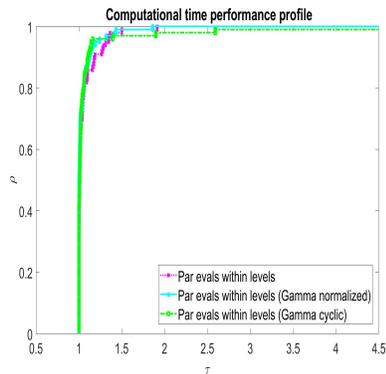
Iterate points are important not only as base points for trying to close gaps in the Pareto front, but can also be a way of expanding the Pareto front, in an attempt of reaching the corresponding extreme points. Several parallel strategies were developed, focusing on these two goals. Variants included the selection of more than one iterate point per iteration, considering the  $\Gamma$  metric applied in a cyclic way, the objective



**Figure 7.** Comparison between strategies *Par evals within levels*, *Par evals within levels (Gamma normalized)*, and *Par evals within levels (Gamma cyclic)*, by means of purity and hypervolume metrics.



**Figure 8.** Comparison between strategies *Par evals within levels*, *Par evals within levels (Gamma normalized)*, and *Par evals within levels (Gamma cyclic)*, by means of spread metrics ( $\Gamma$  and  $\Delta$ ).

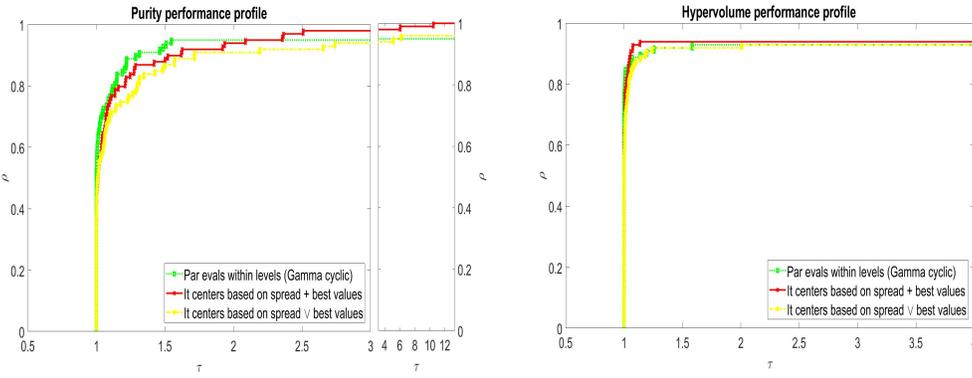


**Figure 9.** Comparison between strategies *Par evals within levels*, *Par evals within levels (Gamma normalized)*, and *Par evals within levels (Gamma cyclic)*, considering the computational time.

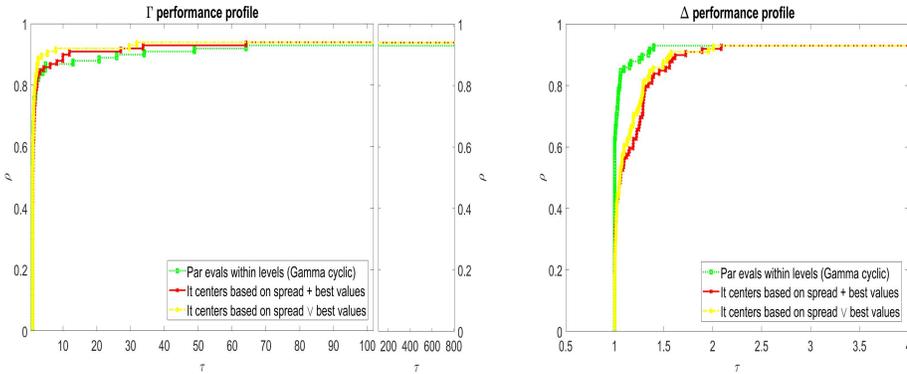
function value (minimum and maximum values at each component), and the stepsize parameter (largest indicating more promising points). We only report results for the two most successful variants.

Both new strategies take into account the two points defining the largest gap for the objective function component corresponding to the current iteration as well as the  $q$  points corresponding to the lowest value for each objective function component. In the first strategy, denoted by *It centers based on spread + best values*, these  $q + 2$  points are used as iterate points. In the second strategy, *It centers based on spread  $\vee$  best values*, iterations alternate between the selection of the two points corresponding to the largest gap and the  $q$  points corresponding to the lowest objective function components values. As usual, function evaluation is performed in parallel, keeping the levels structure at the search step.

Figures 10, 11, and 12 compare these two strategies with *Par evals within levels (Gamma cyclic)* (*Gamma cyclic*).

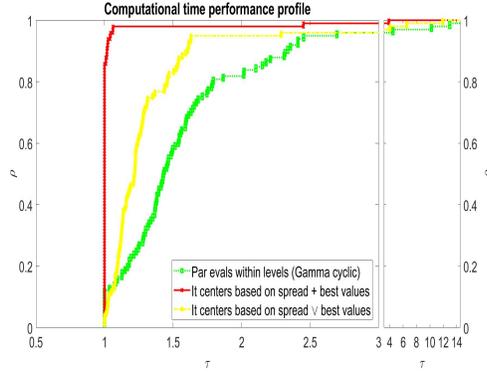


**Figure 10.** Comparison between parallel strategies *Par evals within levels (Gamma cyclic)*, *It centers based on spread + best values*, and *It centers based on spread  $\vee$  best values*, by means of purity and hypervolume metrics.



**Figure 11.** Comparison between parallel strategies *Par evals within levels (Gamma cyclic)*, *It centers based on spread + best values*, and *It centers based on spread  $\vee$  best values*, by means of spread metrics ( $\Gamma$  and  $\Delta$ ).

Although *Par evals within levels (Gamma cyclic)* presents a better performance for purity and  $\Delta$  metrics, strategy *It centers based on spread + best values* clearly outperforms the other strategies in computational time, and presents a slightly better



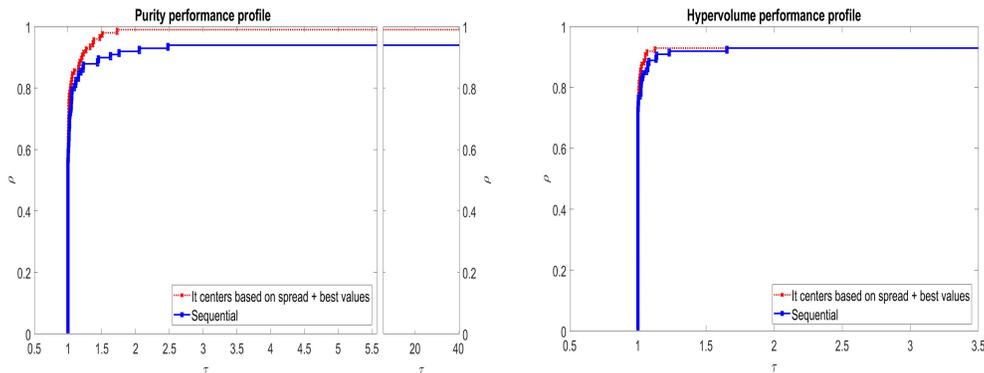
**Figure 12.** Comparison between parallel strategies *Par evals within levels (Gamma cyclic)*, *It centers based on spread + best values*, and *It centers based on spread  $\vee$  best values*, considering the computational time.

performance in what respects to the hypervolume metric, justifying our option for it.

### 3.5. Selected parallelization approach

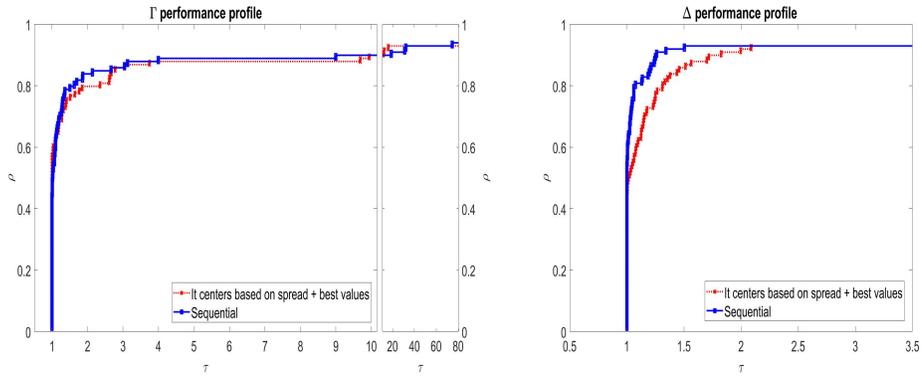
Finally, we compared our selected parallel strategy with the sequential variant of BoostDMS. At each iteration, this strategy considers  $q + 2$  iterate points from the current list  $L_k$ , corresponding to the  $q$  points with the lowest value for each component of the objective function and to the two points defining the largest gap in the component of the objective function associated to the current iteration (which changes in a cyclic way between iterations). These  $q + 2$  points will be used as model centers at the search step and all those that fail in generating a new feasible nondominated point will be used as poll centers. Function evaluations are always performed in parallel, at the search and poll steps. In the former, the levels structure is respected, only evaluating a given level if the previous one was unable to generate a new feasible nondominated point.

Figures 13, 14, and 15 report the performance profiles comparing *It centers based on spread + best values* strategy with the initial sequential version of BoostDMS.

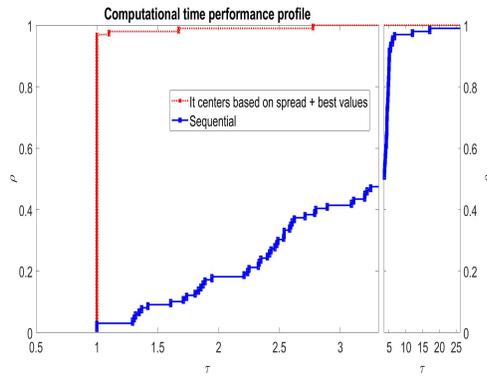


**Figure 13.** Comparison between the selected parallel version and the sequential implementation of BoostDMS, by means of purity and hypervolume metrics.

Although there is a decrease in performance for spread (see Figure 14), the advan-



**Figure 14.** Comparison between the selected parallel version and the sequential implementation of Boost-DMS, by means of spread metrics ( $\Gamma$  and  $\Delta$ ).



**Figure 15.** Comparison between the selected parallel version and the sequential implementation of Boost-DMS, considering computational time.

Solver	Purity	Hypervolume	Gamma	Delta	AvgTime(s)	FuncEvals
DMS	0%	0.002	3.96e+06	1.071	3987	9260
BoostDMS	53%	0.70	3.13e+06	1.173	6970	14978
Parallel BoostDMS	89%	0.78	2.52e+06	1.224	1670	20000

**Table 1.** Metrics associated to the solution of the chemical engineering problem, computed by solvers DMS, BoostDMS, and the selected parallel version of BoostDMS.

tage brought by the parallel strategy selected is clear. Not only it presents a huge increase in performance regarding computational time (Figure 15), but also a better performance for purity and a slight advantage in terms of hypervolume (see Figure 13).

#### 4. A chemical engineering application

Often academic problems, like the ones considered in Section 3, do not reflect all the challenges of real applications. In this section we consider the real chemical engineering problem, related to the production of styrene, as described in [2, 7].

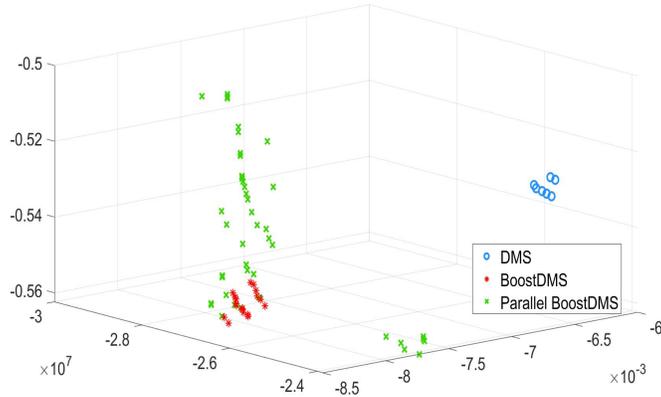
The styrene production process involves four steps: preparation of reactants, catalytic reactions, a first distillation – where styrene is recovered, and a second distillation – where benzene is recovered. During this second distillation, unreacted ethylbenzene is recycled, as an initial reactant on the process. This is a tri-objective problem ( $q = 3$ ), where it is intended to maximize the net present value associated to the process ( $f_1$ ), the purity of the produced styrene ( $f_2$ ) and the overall ethylbenzene conversion into styrene ( $f_3$ ) [7]. The problem has 8 variables, subject to bounds constraints, and 9 other constraints, some process-related (*e.g.* environmental norms regarding excesses) and some economical (*e.g.* investment value). More details can be found in [2].

A C++ numerical simulator has been developed for this chemical engineering process, where each complete simulation corresponds to a function evaluation. Due to the presence of recycling loops, like the one of ethylbenzene, the process must be entirely simulated until a result is provided. The total time associated to the computation of a function value fluctuates, with an average of 1 second, when the code succeeds in evaluating a given point. Additionally, the problem reveals hidden constraints, since feasible points, according to the defined constraints, often fail to produce a finite numerical value for the objective function. In this case, the simulation is generally faster, with an average computational time of 0.001 seconds. Note that these computational times were obtained with the hardware/software configuration described in Section 3.

We used DMS [15], BoostDMS [10] and the selected parallel version of BoostDMS, described in Section 3.5, to solve the problem. All the defaults were considered for the solvers, with exception of the initialization, where line sampling was replaced by a single point, provided in literature [2]. Figure 16 corresponds to the approximations to the Pareto front generated by each one of the three solvers.

The 7 points in the final solution computed by DMS are all dominated by each one of the approximations to the Pareto front computed by BoostDMS or its parallel version (which comprise 19 and 44 nondominated points, respectively). It is also clear the gain in volume of the dominated region obtained with both versions of BoostDMS. Table 1 presents the values of the different multiobjective metrics for the three solvers, as well as the computational time (an average of five runs) and the total number of function evaluations performed.

BoostDMS is considerably slower than DMS, but presents a remarkable improvement in the quality of the solution computed. This quality increases in the solution



**Figure 16.** Final approximations to the Pareto front computed for the chemical engineering problem by solvers DMS, BoostDMS, and the selected parallel version of BoostDMS.

computed by the parallel version of BoostDMS, particularly in what respects to purity. These results corroborate what was observed in the academic test set, with the parallel version of BoostDMS allowing relevant gains in terms of purity, a slight advantage regarding hypervolume, but a worse performance in spread metric  $\Delta$ .

Although the parallel version of BoostDMS performs a larger number of function evaluations than any of the two other solvers, it is considerably faster than any of the two sequential versions. In fact, if we compute the speedup associated to the parallel version, we will get a value of 4.17, corresponding to an efficiency of 52.17% (for the test set of Section 3, the average speedup is in the interval  $[3.22; 4.45]$  and the average efficiency in  $[40.31\%; 55.68\%]$ , in both cases with 95% of confidence). However, considering that the number of function evaluations performed by the sequential version is clearly lower than the one of the parallel version, a crude correction, assuming that a total of 20 000 function evaluations was performed by both variants, would give a speedup of 5.6, corresponding to an efficiency of 70%.

## 5. Conclusions

In this work we have proposed and analyzed the numerical performance of parallelization strategies for BoostDMS, an implementation of a Direct Multisearch method.

Additionally to the obvious parallelization of function evaluation at the poll step, strategies for parallelizing the function evaluation at the search step were also considered, stressing the benefits associated to the evaluation by levels performed in the sequential version of the code. The value of parallel strategies for models computation and minimization at the search step was also assessed. New strategies for the selection of the iterate point were proposed, based on modifications of the  $\Gamma$  spread metric, and considering the possibility of selecting several iterate points at a given iteration.

The best strategy, at each iteration selects  $q + 2$  iterate points from the current approximation to the Pareto front, corresponding to the best value for each component of the objective function and to the two points defining the largest gap in a given component of the objective function, with cyclic changes between iterations. Function evaluation is always performed in parallel, respecting the levels approach of the search

step.

This best version allows a remarkable improvement in computational time, with a significant improvement in purity and a slight improvement in hypervolume metrics. Conclusions hold both in an extensive academic test set and in a real engineering application.

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