

# An Overview of Pair-Potential Functions for Multi-Objective Optimization<sup>\*</sup>

Jesús Guillermo Falcón-Cardona<sup>1</sup>[0000–0003–1131–098X], Edgar Covantes Osuna<sup>2</sup>[0000–0001–5991–6927], and Carlos A. Coello Coello<sup>1</sup>[0000–0002–8435–680X]

<sup>1</sup> CINVESTAV-IPN, Computer Science Department, Mexico City, Mexico 07300  
jfalcon@computacion.cs.cinvestav.mx, ccoello@cs.cinvestav.mx

<sup>2</sup> Tecnológico de Monterrey, School of Engineering and Sciences, Monterrey, Nuevo León, Mexico 64849  
edgar.covantes@tec.mx

**Abstract.** Recently, an increasing number of state-of-the-art Multi-objective Evolutionary Algorithms (MOEAs) have incorporated the so-called pair-potential functions (commonly used to discretize a manifold) to improve the diversity within their population. A remarkable example is the Riesz  $s$ -energy function that has been recently used to improve the diversity of solutions either as part of a selection mechanism as well as to generate reference sets. In this paper, we perform an extensive empirical study with respect to the usage of the Riesz  $s$ -energy function and other 6 pair-potential functions adopted as a backbone of a selection mechanism used to update an external archive which is integrated into MOEA/D. Our results show that these pair-potential-based archives are able to store solutions with high diversity discarded by the MOEA/D's main population. Our experimental results indicate that the utilization of the pair-potential-based archives helps to circumvent the known MOEA/D's performance dependence on the Pareto front shapes without meddling with the original definition of the algorithm.

**Keywords:** Pair-potential functions · diversity · manifold discretization · selection mechanism.

## 1 Introduction

The area of Evolutionary Multi-objective Optimization (EMO) involves the design of population-based Multi-objective Evolutionary Algorithms (MOEAs). Given that evolutionary algorithms use a population which is a set of solutions to a given problem, MOEAs are suited in a natural way for solving Multi-objective Optimization Problems (MOPs) since they can generate multiple trade-offs among the (conflicting) objective functions (i. e., solutions in which an objective cannot be improved without worsening another) in a single run [1]. MOPs with

---

<sup>\*</sup> The first author acknowledges support from CINVESTAV-IPN and CONACyT to pursue graduate studies. The third author acknowledges support from CONACyT grant no. 1920 and from SEP-Cinvestav grant. (application no. 4).

four or more objective functions are commonly named Many-objective Optimization Problems (MaOPs) [1].

Well established MOEAs have two basic principles driven by selection. First of all, the goal is to push the current population close to the “true” *Pareto front*. The second goal is to “spread” the population along the front such that it is well covered. The first goal is usually achieved by using selection mechanisms based on the Pareto dominance relation<sup>3</sup>, decomposition techniques, or indicator-based selection [1]. The second goal involves the use of diversity mechanisms to promote the spread of the different solutions along the Pareto front.

In general, providing an adequate balance between selection pressure and diversity is one of the main challenges when designing state-of-the-art MOEAs. These efforts have provided many methodologies, algorithms and techniques whose main goal is to improve the performance of MOEAs on MOPs [1]. On the one hand, the selection pressure of Pareto-dominant MOEAs dilutes when tackling MaOPs. This is due to the increasing number of non-dominated solutions found during the evolutionary process that yields to an inefficient random selection process [1]. On the other hand, due to the inherent methods embedded in MOEAs (mutation, crossover, selection, diversity mechanisms, etc.), the search may be biased into choosing a population with a specific distribution, which may favor a certain geometrical shape on the Pareto front.

In this paper, we focus our attention into the latter problem by introducing the usage of the so-called *pair-potential functions* as density estimators in an external population (archive). These functions are commonly used to distribute points on a manifold (or discretizing a manifold) [2]. Given a  $d$ -dimensional manifold  $\mathcal{A}$  in the search space  $\mathbb{R}^m$  ( $d \leq m$ ) with a given distribution  $X$  and described by some geometric property or by some parametrization, the goal is to generate a large number of  $N$  points in  $\mathcal{A}$  such that they are well-separated and have (nearly) distribution  $X$ . In other words, the aim is to generate the smallest population possible that describes the distribution of the full set of elements in  $\mathcal{A}$ .

One example of such pair-potential functions used in EMO is the Riesz  $s$ -energy function, which has been recently used to improve the diversity of solutions [3,4,5]. We contribute to this line of work by performing an extensive empirical study on the usage of not just the Riesz  $s$ -energy function, but also 6 other pair-potential functions on an external population as an updating rule.

Our goal is twofold. Firstly, we want to show that even if a MOEA by itself is not able to maintain a well-distributed set of points during its execution (e. g., due to constraints of its selection mechanism or population size constraints, among others), the pair-potential functions will maintain solutions in the archive with high diversity. This implies that the total energy value of the system (the Pareto front approximation) is minimized. Consequently, the diversity will be improved for a longer period of time compared to the regular execution of the MOEA, and without meddling with its original definition. Second, we would

<sup>3</sup> Given  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^m$ ,  $\mathbf{x}$  is said to Pareto dominate  $\mathbf{y}$  (denoted as  $\mathbf{x} \prec \mathbf{y}$ ) if and only if  $x_i \leq y_i$  for all  $i = 1, \dots, m$  and  $\exists j \in \{1, \dots, m\}$  such that  $x_j < y_j$ .

like to explore the usage of several pair-potential functions in isolation as an alternative to improve the distribution of the solutions provided by MOEAs. We would like to observe the difference of the diversity achieved between a MOEA and the Pareto front approximation stored in the pair-potential-based archive. This study should provide insights into the performance dependence of a MOEA and the pair-potential functions with respect to the shape of the Pareto front on different MOPs.

The remainder of this paper is organized as follows. In Section 2, we introduce the problems of our interest and the definitions of the *pair-potential functions* analyzed in this paper. Sections 3 and 4 establish the algorithmic framework used throughout our experimental analysis and the results obtained from the such experiments, respectively. Finally, we finish with some discussion and concluding remarks in Section 5.

## 2 Preliminaries

In this paper, we consider, without loss of generality, the minimization of functions  $\mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_m(\mathbf{x}))$ , where  $\mathbf{x}$  is the vector of decision variables that belongs to  $\Omega \subseteq \mathbb{R}^n$ , which is the decision space.  $\mathbf{F}(\mathbf{x})$  is the vector of  $m \geq 2$  objective functions such that  $f_i : \Omega \rightarrow \mathbb{R}$  for  $i \in \{1, 2, \dots, m\}$ . As there is no single point that minimizes all functions simultaneously, the goal is to find a set of so-called Pareto-optimal solutions that represent the best possible trade-offs among the objective functions. A decision vector  $x \in \Omega$  is Pareto optimal if there is no other  $y \in \Omega$  such that  $\mathbf{F}(\mathbf{y}) \prec \mathbf{F}(\mathbf{x})$ . The set of all Pareto-optimal decision vectors  $P^*$  is called Pareto set and its image in the objective space, given by  $PF^* = \mathbf{F}(P^*)$ , is known as the Pareto front.

### 2.1 Pair-Potential Functions

Used to distribute points on a manifold (or discretizing a manifold), the *pair-potential functions* [2] are of the form  $\mathcal{K} : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}$  that model the interaction between two given particles. The total energy  $U$  of a system with  $N$  particles is given as follows:

$$U(\mathcal{A}) = \sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N \mathcal{K}(\mathbf{a}_i, \mathbf{a}_j), \quad (1)$$

where  $\mathcal{A} = \{\mathbf{a}_1, \dots, \mathbf{a}_N\}$  is an approximation set, and  $\mathbf{a}_j \in \mathbb{R}^m, j = 1, \dots, N$ .

In the following, we describe the pair-potential functions which are of interest in this paper. For all cases,  $\mathbf{u} = \mathbf{F}(\mathbf{x}), \mathbf{v} = \mathbf{F}(\mathbf{y}) \in \mathbb{R}^m$  and  $\|\cdot\|$  represents the Euclidean distance.

**Riesz  $s$ -energy** [2]: Given a parameter  $s > 0$ , it is defined as follows:

$$\mathcal{K}^{\text{RSE}}(\mathbf{u}, \mathbf{v}) = \frac{1}{\|\mathbf{u} - \mathbf{v}\|^s}. \quad (2)$$

**Gaussian  $\alpha$ -energy** [2]: Given a parameter  $\alpha > 0$ , this pair-potential is defined in the following:

$$\mathcal{K}^{\text{GAE}}(\mathbf{u}, \mathbf{v}) = e^{-\alpha \|\mathbf{u} - \mathbf{v}\|^2}. \quad (3)$$

**Coulomb's law** [6]: it is given by:

$$\mathcal{K}^{\text{COU}}(\mathbf{u}, \mathbf{v}) = \frac{q_1 q_2}{4\pi\epsilon_0} \cdot \frac{1}{\|\mathbf{u} - \mathbf{v}\|}, \quad (4)$$

where we set  $q_1 = \|\mathbf{u}\|$  and  $q_2 = \|\mathbf{v}\|$ , and  $\frac{1}{4\pi\epsilon_0}$  is the Coulomb's constant.

**P3schl-Teller Potential** [7,8]: Given  $V_1, V_2, \alpha > 0$ , it is given by:

$$\mathcal{K}^{\text{PT}}(\mathbf{u}, \mathbf{v}) = \frac{V_1}{\sin^2(\alpha \|\mathbf{u} - \mathbf{v}\|)} - \frac{V_2}{\cos^2(\alpha \|\mathbf{u} - \mathbf{v}\|)}. \quad (5)$$

**Modified P3schl-Teller Potential** [7,8]: Given  $D, \alpha > 0$ , this function is as follows:

$$\mathcal{K}^{\text{MPT}}(\mathbf{u}, \mathbf{v}) = -\frac{D}{\cosh^2(\alpha \|\mathbf{u} - \mathbf{v}\|)}. \quad (6)$$

**General form of P3schl-Teller Potentials** [7,8]: Given  $A, B > 0$ , it is given by:

$$\mathcal{K}^{\text{GPT}}(\mathbf{u}, \mathbf{v}) = \frac{A}{1 + \cos(\|\mathbf{u} - \mathbf{v}\|)} + \frac{B}{1 - \cos(\|\mathbf{u} - \mathbf{v}\|)} \quad (7)$$

**Kratzer Potential** [8,9]: Given  $V_1, V_2, \alpha > 0$ , the Kratzer potential is given as follows:

$$\mathcal{K}^{\text{KRA}}(\mathbf{u}, \mathbf{v}) = V_1 \left( \frac{\|\mathbf{u} - \mathbf{v}\| - 1/\alpha}{\|\mathbf{u} - \mathbf{v}\|} \right)^2 + V_2. \quad (8)$$

### 3 Pair-Potential-based Archives

Following the approaches described in [3,4], we use an iterative selection mechanism based on the calculation of individual contributions to the total energy of a system of  $N$  particles (see Eq. (1)). Hence, given an approximation set  $\mathcal{A} = \{\mathbf{a}_1, \dots, \mathbf{a}_N, \mathbf{a}_{N+1}\}$ , the individual contribution  $C$  of any  $\mathbf{a} \in \mathcal{A}$  is calculated as follows:

$$C(\mathbf{a}, \mathcal{A}) = \frac{1}{2}[U(\mathcal{A}) - U(\mathcal{A} \setminus \{\mathbf{a}\})], \quad (9)$$

where the term  $1/2$  is used since for the adopted pair-potential functions in Eqs. (2) to (8),  $\mathcal{K}(\mathbf{u}, \mathbf{v}) = \mathcal{K}(\mathbf{v}, \mathbf{u})$ . Since  $U$  is to be minimized, the solution to be deleted from  $\mathcal{A}$  such that  $|\mathcal{A}| = N$  is the one with the maximum contribution value, i. e.,  $\mathbf{a}_{\text{worst}} = \arg \max_{\mathbf{a} \in \mathcal{A}} C(\mathbf{a}, \mathcal{A})$ . Using this selection mechanism, we can iteratively reduce the cardinality of a given approximation set  $\mathcal{A}$ .

In this paper, we aim to show that the incorporation of an external population (or archive) based on a pair-potential function to a given MOEA, improves its diversity of solutions. Consequently, we selected the MOEA based on decomposition (MOEA/D) [10] as our baseline algorithm since it is known that its performance depends on the Pareto front shape [11]. The underlying idea is to employ the original MOEA/D algorithm (see Algorithm 1) and every time a new solution  $\mathbf{y}$  is generated, it should be inserted in the archive  $\mathcal{A}$  (which is initialized in Line 4) as shown in Lines 9 and 10, respectively. It is worth noting that the archive is only utilized to store solutions, which implies a unidirectional communication from MOEA/D to it. The use of the archive allows MOEA/D to keep solutions that would be possibly deleted due to its design principles. Once the algorithm reaches its stopping criterion, the main population and the archive are returned as two Pareto front approximations.

---

**Algorithm 1** MOEA/D with external archive

---

**Require:**  $N$ : population size;  $T$ : neighborhood size;  $\mathcal{K}$ : pair-potential function;  
 $A_{\max}$ : maximum archive size  
**Ensure:** Main population and archive as Pareto front approximations  
1: Initialize  $N$  weight vectors  $\lambda^1, \dots, \lambda^N$   
2: Determine the  $T$  nearest neighbors of each  $\lambda^j$   
3: Initialize the main Population  $P = \{\mathbf{x}^1, \dots, \mathbf{x}^N\}$   
4: Initialize archive  $\mathcal{A}$  equals to  $P$ .  
5: Initialize the reference point  $z^*$   
6: **while** Stopping criterion is not satisfied **do**  
7:   **for**  $j = 1$  to  $N$  **do**  
8:     Select mating parents from the neighborhood of  $\mathbf{x}^j$   
9:     Generate a new solution  $\mathbf{y}$  by using variation operators.  
10:    Insert( $\mathcal{A}, \mathbf{y}, \mathcal{K}, A_{\max}$ ).  
11:    Update the reference point  $z^*$   
12:    Evaluate new solutions via scalarizing function  
13:    Update main population  $P$   
14: **return**  $\{P, \mathcal{A}\}$

---

Algorithm 2 describes the process used to insert a new solution  $\mathbf{y}$  in  $\mathcal{A}$ . First,  $\mathbf{y}$  is compared with all the elements in the archive, using the Pareto dominance relation. If  $\mathbf{y}$  Pareto dominates any  $\mathbf{a} \in \mathcal{A}$ , the latter is deleted from  $\mathcal{A}$ . However, if any element in the archive weakly Pareto dominates  $\mathbf{y}$ , then  $\mathbf{y}$  is not inserted and  $\mathcal{A}$  is returned. In case that  $\mathbf{y}$  survives the Pareto-based criterion, it is inserted in the archive. If the maximum archive size  $A_{\max}$  is exceeded, we execute the steady-state selection (prior normalization of the archive) where the solution with the worst contribution to the total energy  $U$ , using  $\mathcal{K}$  as pair-potential function, is iteratively deleted until the desired  $A_{\max}$  size is reached.

Regarding the computational complexity of Algorithm 2, it is  $\Theta(m|A|^2)$  due to the usage of the fast computation of individual contributions proposed in [4].

Smaller terms consist of the for-loop of Lines 1 to 5 and the normalization procedure in Line 7 with complexity  $\Theta(m|A|)$ .

---

**Algorithm 2** Insert

---

**Require:**  $\mathcal{A}$ : archive;  $\mathbf{y}$ : solution to be inserted;  $\mathcal{K}$ : pair-potential function;  $A_{\max}$ : maximum archive size

**Ensure:** Updated archive  $\mathcal{A}$

```

1: for all  $\mathbf{a} \in \mathcal{A}$  do
2:   if  $\mathbf{y} \prec \mathbf{a}$  then
3:      $\mathcal{A} = \mathcal{A} \setminus \{\mathbf{a}\}$ 
4:   else if  $\mathbf{a} \preceq \mathbf{y}$  then
5:     return  $\mathcal{A}$ 
6:  $\mathcal{A} = \mathcal{A} \cup \{\mathbf{y}\}$ 
7: Normalize  $\mathcal{A}$ 
8: while  $|\mathcal{A}| > A_{\max}$  do
9:    $\mathbf{a}_{\text{worst}} = \arg \max_{\mathbf{a} \in \mathcal{A}} C_{\mathcal{K}}(\mathbf{a}, \mathcal{A})$ 
10:   $\mathcal{A} = \mathcal{A} \setminus \{\mathbf{a}_{\text{worst}}\}$ 
11: return  $\mathcal{A}$ 

```

---

## 4 Experimental Results

This section is devoted to comparing the convergence and diversity properties of the main population returned by MOEA/D and the content of the archive based on the seven selected pair-potential functions<sup>4</sup> which gives rise to MOEA/D<sub>RSE</sub>, MOEA/D<sub>GAE</sub>, MOEA/D<sub>COU</sub>, MOEA/D<sub>PT</sub>, MOEA/D<sub>MPT</sub>, MOEA/D<sub>GPT</sub>, and MOEA/D<sub>KRA</sub>. MOEA/D with each external archive is tested on several MOPs from the DTLZ, WFG, DTLZ<sup>-1</sup>, and WFG<sup>-1</sup> test suites with two and three objective functions. Regarding the DTLZ and DTLZ<sup>-1</sup> test problems, the number of variables was set to  $n = m + K - 1$ , where  $m$  is the number of objective functions, and  $K = 5$  for DTLZ1,  $K = 10$  for DTLZ2 and DTLZ5, and  $K = 20$  for DTLZ7. Their inverted counterparts have the same value of  $K$ . Concerning the WFG and WFG<sup>-1</sup> problems,  $n$  was set to 24 and 26, with the position-related parameters equal to 2 and 4 for two and three objective functions, respectively. For a fair comparison, the population size and the maximum archive size are set to  $N = C_{m-1}^{m+H-1} = 120$ , where  $H = 119$  and 14 for MOPs with two and three objective functions, respectively.  $N$  corresponds to the cardinality of the set of weight vectors (constructed by the Das and Dennis method employed by the MOEA/D [10]). For all cases, the stopping criterion was set to 49,920 function evaluations which corresponds to 416 generations. We set the neighborhood size  $T$  of MOEA/D equal to 20 and we employed the achievement scalarizing

---

<sup>4</sup> The source code is available at <http://computacion.cs.cinvestav.mx/~jfalcon/PairPotentials/>.

function for all the test instances. For each test instance, we performed 30 independent executions and the MOEA/D variants used the same random seeds. We selected the Inverted Generational Distance (IGD) [12] and the Pure Diversity (PD) [13] indicators to assess convergence-diversity and diversity, respectively. In order to have statistical confidence of our results, we adopted the one-tailed Wilcoxon rank-sum test, with a significance level of  $\alpha = 0.05$  with null hypothesis as follows: “*is MOEA<sub>A</sub> statistically different than MOEA<sub>B</sub>?*”. Where MOEA<sub>A</sub> is the one having the best indicator value and MOEA<sub>B</sub> is each one of the remaining algorithms. This selection was used for all the tables in this paper with the exception of Table 1 because the latter is a summary of results. In Tables 3 and 4, a symbol # is placed when the best algorithm performs significantly better than the others.

Table 1: Average ranking values obtained by all the Pair-Potential-based selection mechanisms for the IGD and PD indicators.

QI	MOP	Dim.	$\kappa^{\text{RSE}}$	$\kappa^{\text{GAE}}$	$\kappa^{\text{COU}}$	$\kappa^{\text{PT}}$	$\kappa^{\text{MPT}}$	$\kappa^{\text{GPT}}$	$\kappa^{\text{KRA}}$
IGD	DTLZ1	2	4.286 <sup>4</sup>	5.429 <sup>6</sup>	5.000 <sup>5</sup>	1.429 <sup>1</sup>	7.000 <sup>7</sup>	2.143 <sup>2</sup>	2.714 <sup>3</sup>
		3	3.571 <sup>3</sup>	2.143 <sup>2</sup>	2.000 <sup>1</sup>	4.571 <sup>4</sup>	5.571 <sup>7</sup>	5.000 <sup>6</sup>	5.143 <sup>5</sup>
	DTLZ2	2	3.857 <sup>4</sup>	6.000 <sup>6</sup>	1.286 <sup>1</sup>	2.286 <sup>2</sup>	7.000 <sup>7</sup>	3.286 <sup>3</sup>	4.286 <sup>5</sup>
		3	3.286 <sup>2</sup>	1.571 <sup>1</sup>	4.286 <sup>4</sup>	5.286 <sup>7</sup>	5.000 <sup>6</sup>	4.429 <sup>5</sup>	4.143 <sup>3</sup>
	DTLZ5	2	4.000 <sup>4</sup>	5.857 <sup>6</sup>	1.286 <sup>1</sup>	2.286 <sup>2</sup>	7.000 <sup>7</sup>	3.286 <sup>3</sup>	4.286 <sup>5</sup>
		3	1.571 <sup>1</sup>	5.286 <sup>6</sup>	5.286 <sup>6</sup>	2.571 <sup>2</sup>	6.857 <sup>7</sup>	3.571 <sup>4</sup>	2.857 <sup>3</sup>
	DTLZ7	2	4.143 <sup>4</sup>	6.000 <sup>6</sup>	4.571 <sup>5</sup>	1.429 <sup>1</sup>	7.000 <sup>7</sup>	2.429 <sup>2</sup>	2.429 <sup>3</sup>
		3	2.714 <sup>2</sup>	4.000 <sup>5</sup>	5.429 <sup>6</sup>	3.714 <sup>4</sup>	6.286 <sup>7</sup>	3.286 <sup>3</sup>	2.571 <sup>1</sup>
	WFG1	2	5.286 <sup>6</sup>	5.286 <sup>6</sup>	2.429 <sup>2</sup>	1.857 <sup>1</sup>	6.429 <sup>7</sup>	2.857 <sup>3</sup>	3.857 <sup>4</sup>
		3	3.571 <sup>3</sup>	3.143 <sup>2</sup>	1.000 <sup>1</sup>	4.571 <sup>4</sup>	6.143 <sup>7</sup>	5.000 <sup>6</sup>	4.571 <sup>5</sup>
	WFG2	2	3.429 <sup>3</sup>	5.571 <sup>6</sup>	4.286 <sup>5</sup>	1.571 <sup>1</sup>	7.000 <sup>7</sup>	2.571 <sup>2</sup>	3.571 <sup>4</sup>
		3	3.857 <sup>4</sup>	3.429 <sup>2</sup>	1.286 <sup>1</sup>	3.714 <sup>3</sup>	6.429 <sup>7</sup>	4.571 <sup>5</sup>	4.714 <sup>6</sup>
	WFG3	2	4.286 <sup>4</sup>	5.571 <sup>6</sup>	5.000 <sup>5</sup>	2.143 <sup>2</sup>	7.000 <sup>7</sup>	2.143 <sup>3</sup>	1.857 <sup>1</sup>
		3	2.286 <sup>2</sup>	5.714 <sup>6</sup>	5.143 <sup>5</sup>	2.143 <sup>1</sup>	7.000 <sup>7</sup>	2.286 <sup>3</sup>	3.429 <sup>4</sup>
PD	DTLZ1	2	3.857 <sup>4</sup>	5.143 <sup>6</sup>	3.571 <sup>2</sup>	4.286 <sup>5</sup>	5.714 <sup>7</sup>	3.571 <sup>3</sup>	1.857 <sup>1</sup>
		3	3.429 <sup>2</sup>	4.429 <sup>6</sup>	2.286 <sup>1</sup>	3.857 <sup>4</sup>	6.286 <sup>7</sup>	4.286 <sup>5</sup>	3.429 <sup>3</sup>
	DTLZ2	2	4.286 <sup>5</sup>	2.857 <sup>1</sup>	3.714 <sup>3</sup>	3.714 <sup>4</sup>	3.000 <sup>2</sup>	4.714 <sup>6</sup>	5.714 <sup>7</sup>
		3	4.429 <sup>5</sup>	1.000 <sup>1</sup>	5.429 <sup>7</sup>	4.000 <sup>3</sup>	5.143 <sup>6</sup>	3.857 <sup>2</sup>	4.143 <sup>4</sup>
	DTLZ5	2	4.286 <sup>5</sup>	2.571 <sup>2</sup>	4.000 <sup>3</sup>	4.000 <sup>4</sup>	2.143 <sup>1</sup>	5.000 <sup>6</sup>	6.000 <sup>7</sup>
		3	3.571 <sup>3</sup>	3.857 <sup>4</sup>	2.000 <sup>1</sup>	4.571 <sup>5</sup>	3.000 <sup>2</sup>	5.571 <sup>7</sup>	5.429 <sup>6</sup>
	DTLZ7	2	3.571 <sup>3</sup>	5.714 <sup>6</sup>	3.571 <sup>4</sup>	2.571 <sup>1</sup>	6.000 <sup>7</sup>	3.571 <sup>5</sup>	3.000 <sup>2</sup>
		3	2.143 <sup>1</sup>	4.429 <sup>5</sup>	4.857 <sup>6</sup>	3.143 <sup>3</sup>	6.143 <sup>7</sup>	3.000 <sup>2</sup>	4.286 <sup>4</sup>
	WFG1	2	2.857 <sup>2</sup>	3.857 <sup>5</sup>	3.143 <sup>3</sup>	2.714 <sup>1</sup>	7.000 <sup>7</sup>	3.714 <sup>4</sup>	4.714 <sup>6</sup>
		3	2.429 <sup>2</sup>	4.571 <sup>4</sup>	2.143 <sup>1</sup>	3.429 <sup>3</sup>	6.143 <sup>7</sup>	4.714 <sup>6</sup>	4.571 <sup>5</sup>
	WFG2	2	3.286 <sup>3</sup>	6.714 <sup>7</sup>	4.000 <sup>5</sup>	1.857 <sup>1</sup>	5.429 <sup>6</sup>	2.857 <sup>2</sup>	3.857 <sup>4</sup>
		3	3.429 <sup>2</sup>	3.429 <sup>3</sup>	2.571 <sup>1</sup>	4.286 <sup>5</sup>	6.429 <sup>7</sup>	4.429 <sup>6</sup>	3.429 <sup>4</sup>
	WFG3	2	3.286 <sup>3</sup>	5.857 <sup>6</sup>	3.286 <sup>4</sup>	3.857 <sup>5</sup>	6.143 <sup>7</sup>	2.571 <sup>1</sup>	3.000 <sup>2</sup>
		3	3.714 <sup>3</sup>	3.714 <sup>4</sup>	3.286 <sup>2</sup>	4.857 <sup>6</sup>	4.857 <sup>7</sup>	4.714 <sup>5</sup>	2.857 <sup>1</sup>

#### 4.1 Pair-Potential Functions Parameters Setting

The pair-potential functions introduced in this paper require the definition of some parameter values. Hence, prior to use the functions in the external archive of MOEA/D, it is mandatory to determine such values. To this aim, we have performed a trial-and-error experimentation to determine good parameter values. Based on the true Pareto fronts of problems DTLZ1, DTLZ2, DTLZ5, DTLZ7, WFG1, WFG2, and WFG3 with two and three objectives, we performed a cardinality reduction, using the seven pair-potential functions, to obtain subsets of

size 20, 50, 100, 200, 300, 400, and 500, following the approach described in [4]. The generated subsets were then assessed using IGD and PD. Table 1 shows the statistical average ranking values obtained by the seven selection mechanisms using the parameter values that we found, where a value closer to one is better. Based on the several comparisons performed, we found out that the parameter values in Table 2 allow to produce approximation sets having good IGD and PD values. In contrast to the quality of Riesz  $s$ -energy-based reference sets in [4], the IGD and PD results of Table 1 show that the utilization of other pair-potential functions led to better diversity results.

Table 2: Parameter values found by trial-and-error.

Pair-potential function	Parameter values
$\mathcal{K}^{\text{RSE}}$	$s = m - 1$
$\mathcal{K}^{\text{GAE}}$	$\alpha = 512$
$\mathcal{K}^{\text{PT}}$	$V_1 = 5.0, V_2 = 3.0, \alpha = 0.02$
$\mathcal{K}^{\text{MPT}}$	$D = 1.0, \alpha = 10.0$
$\mathcal{K}^{\text{GPT}}$	$A = 1.0, B = 1.0$
$\mathcal{K}^{\text{KRA}}$	$V_1 = 5.0, V_2 = 3.0, \alpha = 10.0$

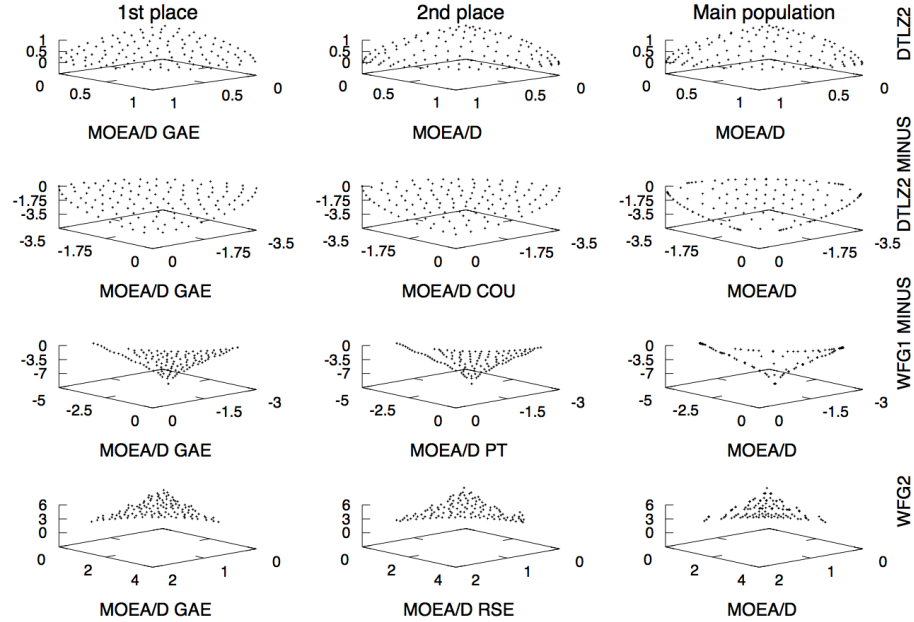


Fig. 1: Comparison of three-objective approximation sets between the 1st and 2nd places in the PD comparison with the resulting main population. The approximation sets correspond to the PD median.



## 4.2 Improving Diversity Results

According to Ishibuchi *et al.* [11], the performance of MOEA/D strongly depends on the Pareto front shape. This is because the weight vectors that MOEA/D uses, cannot completely intersect irregular Pareto front geometries. To overcome this issue, we propose to aggregate a pair-potential-based archive to store solutions found throughout the evolutionary process with a high diversity degree.

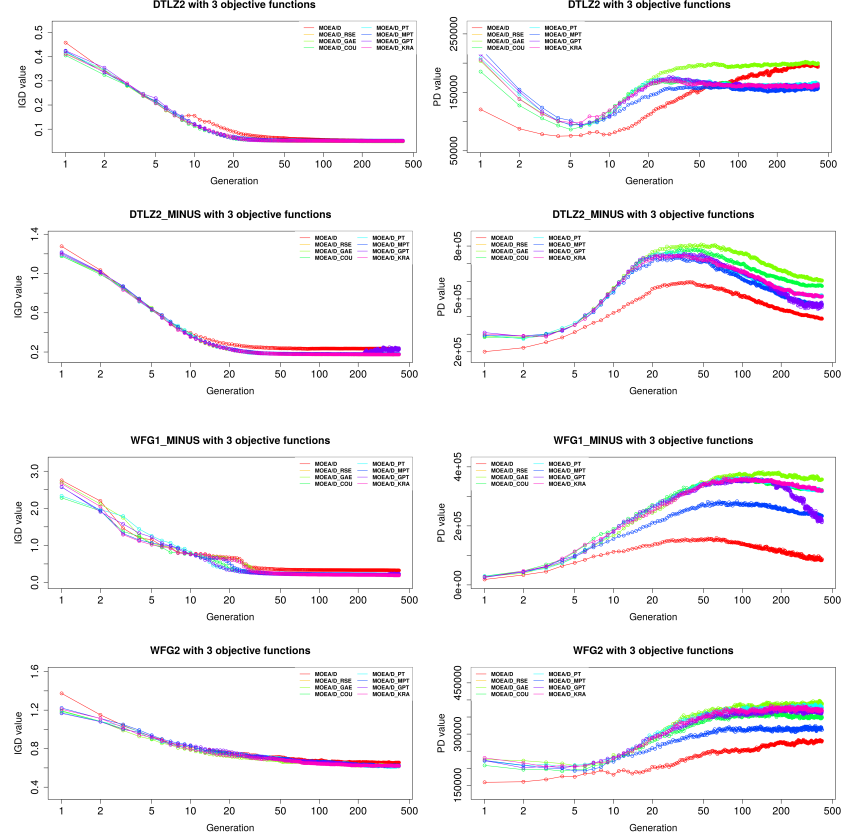


Fig. 2: IGD and PD values of the main population and the Pair Potential-based archives throughout the evolutionary process.

Tables 3 and 4 show IGD and PD comparisons, respectively, between the MOEA/D's main population and the final content of the archives. Regarding IGD, it is clear that the main population had the worst IGD values for almost all the test instances. In contrast, MOEA/D<sub>KRA</sub> and MOEA/D<sub>COU</sub> obtained the best IGD values in 7 problems each. These results are followed by MOEA/D<sub>GAE</sub>, MOEA/D<sub>RSE</sub>, MOEA/D<sub>PT</sub>, MOEA/D<sub>MPT</sub>, and MOEA/D<sub>GPT</sub>. Hence, these re-

Table 3: Mean and, in parentheses, standard deviation of the IGD indicator. The two best values are shown in gray scale, where the darker tone corresponds to the best value.

MOP	Dim.	MOEA/D	MOEA/D <sub>DRSE</sub>	MOEA/D <sub>GAE</sub>	MOEA/D <sub>COU</sub>	MOEA/D <sub>PT</sub>	MOEA/D <sub>MPT</sub>	MOEA/D <sub>GPT</sub>	MOEA/D <sub>KRA</sub>
DTLZ1	2	4.16699e-02 # (2.01977e-02)	1.83832e-03 # (1.80399e-04)	3.42702e-03 # (2.44610e-04)	1.80603e-03 # (1.06879e-04)	1.81171e-03 # (1.02240e-04)	7.11954e-03 # (5.46462e-04)	4.41173e-02 # (2.42189e-02)	1.77681e-03 # (7.14530e-05)
	3	7.99717e-02 # (4.84669e-02)	2.40635e-02 # (8.42281e-03)	2.37463e-02 # (1.12911e-02)	2.44407e-02 # (8.99591e-03)	2.45880e-02 # (8.71192e-03)	3.20072e-02 # (2.11900e-02)	2.49069e-02 # (7.98485e-02)	2.15902e-02 # (4.48457e-03)
DTLZ1 <sup>-1</sup>	2	4.24716e-02 # (4.88277e-03)	4.24717e-02 # (5.13271e-04)	4.24717e-02 # (8.74281e-04)	4.24717e-02 # (9.14437e-04)	4.24717e-02 # (7.48481e-04)	4.24739e-02 # (3.93110e-03)	4.25143e-02 # (9.76065e-01)	4.24717e-02 # (7.47017e-04)
	3	3.68845e-02 # (1.96289e-01)	3.68474e-02 # (2.30345e-02)	3.66553e-02 # (4.11676e-02)	3.66471e-02 # (1.86958e-02)	3.66471e-02 # (2.27840e-02)	3.66550e-02 # (5.82435e-04)	3.66795e-02 # (2.87605e-02)	3.66471e-02 # (2.20036e-02)
DTLZ2	2	6.45514e-03 # (1.80419e-03)	3.96080e-03 # (5.22621e-05)	6.73022e-03 # (2.99141e-04)	3.87465e-03 # (6.39975e-05)	3.86496e-03 # (7.34055e-05)	1.25687e-02 # (5.88095e-04)	3.88312e-03 # (6.72611e-05)	3.84946e-03 # (7.52537e-05)
	3	5.33267e-02 # (9.80607e-03)	5.07144e-02 # (5.33960e-02)	4.93631e-02 # (5.73930e-04)	5.03090e-02 # (9.18912e-04)	5.07144e-02 # (5.83969e-04)	5.24591e-02 # (5.82435e-04)	5.07687e-02 # (4.89447e-04)	5.09328e-02 # (6.52321e-04)
DTLZ2 <sup>-1</sup>	2	5.49282e-02 # (5.18232e-04)	1.36760e-02 # (3.73089e-04)	2.34854e-02 # (1.37504e-03)	1.63947e-02 # (4.92027e-04)	1.37446e-02 # (2.69881e-04)	4.51832e-02 # (2.90508e-03)	1.45337e-02 # (7.63203e-07)	1.45337e-02 # (2.69731e-04)
	3	2.35097e-01 # (5.95203e-04)	1.75365e-01 # (1.82272e-03)	1.73952e-01 # (1.83936e-03)	1.77818e-01 # (2.01012e-03)	1.75370e-01 # (1.83109e-03)	1.79083e-01 # (1.91014e-03)	2.33447e-01 # (2.95072e-02)	1.74815e-01 # (1.76284e-03)
DTLZ5	2	6.45204e-03 # (1.81173e-03)	3.91649e-03 # (6.32125e-05)	6.68597e-03 # (2.84917e-04)	3.86544e-03 # (7.19131e-05)	3.90080e-03 # (6.94532e-05)	1.28969e-02 # (5.81590e-04)	3.88845e-03 # (6.24134e-05)	3.90454e-03 # (8.18740e-05)
	3	1.82299e-02 # (1.89916e-04)	4.41628e-03 # (1.11749e-04)	6.69361e-03 # (3.23475e-04)	4.68129e-03 # (1.37917e-04)	4.38377e-03 # (1.05509e-04)	1.11960e-02 # (7.42902e-04)	1.35193e-02 # (1.69091e-03)	4.39993e-03 # (9.74480e-03)
DTLZ5 <sup>-1</sup>	2	7.50041e-00 # (1.07115e-05)	7.49904e-00 # (5.87607e-06)	7.49998e-00 # (1.38885e-05)	7.49992e-00 # (8.37868e-06)	7.49990e-00 # (6.33767e-06)	7.50028e-00 # (5.10516e-05)	7.50545e-00 # (7.03690e-03)	7.49990e-00 # (6.34822e-06)
	3	8.11421e-01 # (8.74349e-04)	7.98821e-01 # (7.19282e-04)	7.99381e-01 # (1.02276e-03)	7.99097e-01 # (6.88729e-04)	7.98821e-01 # (7.19282e-04)	8.01379e-01 # (1.04017e-03)	8.54652e-01 # (5.33821e-02)	7.98798e-01 # (7.81630e-04)
DTLZ7	2	8.47468e-02 # (2.24229e-01)	1.28470e-01 # (2.80885e-01)	1.57312e-01 # (2.99318e-01)	7.89899e-02 # (2.26125e-01)	7.89232e-02 # (2.26130e-01)	7.00296e-02 # (1.83690e-01)	8.23145e-02 # (2.25078e-01)	7.89461e-02 # (2.26144e-01)
	3	4.50851e-01 # (3.19370e-01)	3.48131e-01 # (3.55093e-01)	4.16920e-01 # (3.72243e-01)	3.51166e-01 # (3.53650e-01)	3.68843e-01 # (3.68220e-01)	4.19440e-01 # (3.47477e-01)	3.05284e-01 # (3.47679e-01)	4.11607e-01 # (3.47679e-01)
DTLZ7 <sup>-1</sup>	2	5.65428e-02 # (2.47240e-02)	1.53021e-02 # (6.81679e-02)	2.84796e-02 # (1.17916e-02)	2.84367e-02 # (1.17916e-02)	2.81541e-02 # (1.17916e-02)	8.69850e-03 # (1.00730e-02)	8.24151e-03 # (1.00730e-02)	2.77438e-03 # (8.78720e-05)
	3	2.07731e-01 # (2.86927e-01)	1.23298e-01 # (2.74663e-01)	9.90051e-02 # (1.96510e-01)	8.22698e-02 # (1.79020e-01)	8.34197e-02 # (1.78763e-01)	1.19062e-01 # (2.05152e-01)	1.60119e-01 # (1.95405e-01)	9.82748e-02 # (1.96831e-01)
WFG1	2	9.40149e-01 # (1.02722e-00)	9.37612e-01 # (1.03206e-00)	9.38672e-01 # (1.02552e-00)	9.35366e-01 # (1.02552e-00)	9.36965e-01 # (1.03206e-00)	9.30754e-01 # (1.03206e-00)	9.39748e-01 # (1.03206e-00)	9.34587e-01 # (1.03206e-00)
	3	1.68240e-02 # (1.68240e-02)	2.04699e-02 # (2.04699e-02)	1.98636e-02 # (1.98636e-02)	2.37691e-02 # (2.37691e-02)	2.04699e-02 # (2.04699e-02)	2.37350e-02 # (2.37350e-02)	2.61922e-02 # (2.61922e-02)	1.77713e-02 # (1.77713e-02)
WFG1 <sup>-1</sup>	2	2.03835e-01 # (1.66623e-01)	9.86575e-02 # (5.92276e-03)	1.02622e-01 # (1.39681e-02)	9.74137e-02 # (6.33247e-03)	1.08114e-01 # (4.01971e-02)	1.09262e-01 # (7.89185e-03)	1.30780e-01 # (4.81363e-02)	1.08113e-01 # (4.01972e-02)
	3	3.26816e-01 # (6.95373e-03)	1.94208e-01 # (9.94318e-03)	1.94692e-01 # (8.63704e-03)	1.94275e-01 # (8.42051e-03)	1.94208e-01 # (8.42051e-03)	2.10987e-01 # (7.48807e-02)	2.37356e-01 # (3.86867e-02)	1.92709e-01 # (7.48698e-03)
WFG2	2	3.55164e-01 # (1.74628e-01)	3.13523e-01 # (1.22246e-01)	3.21753e-01 # (1.34299e-01)	2.93221e-01 # (1.40095e-01)	2.88497e-01 # (1.16692e-01)	3.27417e-01 # (1.21564e-01)	3.28666e-01 # (1.75371e-01)	2.88497e-01 # (1.75371e-01)
	3	6.08625e-01 # (2.40989e-01)	5.41954e-01 # (2.42461e-01)	5.85096e-01 # (2.96169e-01)	5.78210e-01 # (1.79298e-01)	5.41954e-01 # (2.42461e-01)	5.95089e-01 # (2.05041e-01)	5.64424e-01 # (1.51387e-01)	5.51342e-01 # (1.51387e-01)
WFG2 <sup>-1</sup>	2	3.95207e-02 # (3.17820e-02)	1.11329e-02 # (2.22819e-04)	1.58286e-02 # (5.97706e-04)	1.03059e-02 # (1.38876e-04)	1.06089e-02 # (2.03573e-04)	2.09910e-02 # (1.31269e-03)	1.06747e-02 # (1.99930e-04)	1.06226e-02 # (2.01047e-04)
	3	3.08642e-01 # (4.51539e-03)	2.27261e-01 # (3.10810e-03)	2.21860e-01 # (3.16543e-03)	2.30840e-01 # (3.57290e-03)	2.27261e-01 # (3.10810e-03)	2.34587e-01 # (2.90668e-03)	2.28530e-01 # (8.68697e-03)	2.28546e-01 # (2.89074e-03)
WFG3	2	1.88259e-02 # (1.22206e-02)	1.94991e-02 # (1.01781e-02)	2.06792e-02 # (3.83526e-03)	1.56567e-02 # (5.16011e-03)	1.87728e-02 # (1.23040e-02)	3.40757e-02 # (4.36339e-03)	1.59466e-02 # (8.79419e-03)	1.59466e-02 # (1.23056e-02)
	3	2.80790e-01 # (7.10754e-02)	1.35926e-01 # (3.40878e-02)	1.19806e-01 # (2.10583e-02)	1.52502e-01 # (7.14212e-02)	1.35926e-01 # (3.40878e-02)	1.52181e-01 # (4.02817e-02)	1.43240e-01 # (6.51997e-03)	1.52450e-01 # (8.19368e-02)
WFG3 <sup>-1</sup>	2	1.09120e-02 # (1.18155e-04)	1.09771e-02 # (2.08401e-04)	1.85137e-02 # (8.19021e-04)	1.09604e-02 # (2.37950e-04)	1.08521e-02 # (1.49188e-04)	4.00714e-02 # (2.63634e-03)	1.08524e-02 # (1.48345e-04)	1.08524e-02 # (1.48345e-04)
	3	2.47571e-01 # (7.34309e-04)	1.59218e-01 # (4.85961e-03)	1.54469e-01 # (3.26849e-03)	1.57423e-01 # (3.28197e-03)	1.59218e-01 # (4.85961e-03)	1.77135e-01 # (5.02871e-03)	1.63408e-01 # (1.60638e-02)	1.58612e-01 # (3.84477e-03)

sults show that it is possible to tackle the MOEA/D's performance dependence on the Pareto front shape by using a pair-potential-based archive. During the evolutionary process, some solutions with high diversity created by MOEA/D are not added to its main population because of its design principles but the pair-potential-based archives could store such deleted solutions to increase the diversity quality. In this light, the PD values in Table 4 indicate that the approximation sets stored in the archive are better than those of the main population in terms of diversity. Concerning PD, MOEA/D<sub>GAE</sub> presents a more dominant performance since it generated the best diversified approximation sets in 15 out of 28 test instances. The second best results are generated by MOEA/D<sub>DRSE</sub>, creating 9 of the best approximation sets. In this case, the main population of MOEA/D was ranked as the worst one. In Figure 1, we compared the main population and the approximation sets having the best and second best PD value. From the figure, it is clear the lack of diversity of MOEA/D's main population when dealing with irregular Pareto front geometries (three-objective DTLZ2<sup>-1</sup>, WFG1<sup>-1</sup>, and WFG2). In contrast, the use of pair-potential-based archives helps

to circumvent such an issue. Additionally, Figure 2<sup>5</sup> indicate that, in general, the use of the pair-potential-based archives help to increase the diversity throughout the evolutionary process. In consequence, this supports the claim that these archives store solutions that were possibly discarded by the main population even though they have a high diversity.

Table 4: Mean and, in parentheses, standard deviation of the PD indicator. The two best values are shown in gray scale, where the darker tone corresponds to the best value.

MOP	Dim.	MOEA/D	MOEA/D <sub>RSE</sub>	MOEA/D <sub>GAF</sub>	MOEA/D <sub>COU</sub>	MOEA/D <sub>PT</sub>	MOEA/D <sub>MPT</sub>	MOEA/D <sub>GGT</sub>	MOEA/D <sub>KRA</sub>
DTLZ1	2	5.952986e+02 <sup>#</sup> (1.567214e+02)	9.819786e+02 <sup>#</sup> (1.646415e+02)	9.752486e+02 <sup>#</sup> (1.884763e+02)	8.170121e+02 <sup>#</sup> (5.073579e+01)	9.415797e+02 <sup>#</sup> (1.273846e+02)	8.941377e+02 <sup>#</sup> (1.503196e+02)	8.893690e+02 <sup>#</sup> (5.122440e+02)	8.920211e+02 <sup>#</sup> (1.001645e+02)
	3	3.894113e+04 <sup>#</sup> (1.687247e+04)	7.949559e+04 <sup>#</sup> (1.074164e+04)	8.090461e+04 <sup>#</sup> (1.020899e+04)	7.308939e+04 <sup>#</sup> (1.163954e+04)	7.941942e+04 <sup>#</sup> (7.317877e+03)	5.570146e+04 <sup>#</sup> (1.358686e+04)	2.772268e+04 <sup>#</sup> (6.117830e+04)	7.898577e+04 <sup>#</sup> (6.570989e+03)
DTLZ1-1	2	9.829245e+05 <sup>#</sup> (2.304527e+05)	1.095819e+06 <sup>#</sup> (1.263888e+05)	1.062928e+06 <sup>#</sup> (2.245031e+05)	8.127116e+05 <sup>#</sup> (5.435064e+04)	9.842686e+05 <sup>#</sup> (1.158998e+05)	1.019312e+06 <sup>#</sup> (1.732923e+05)	9.994363e+05 <sup>#</sup> (1.722732e+05)	9.844474e+05 <sup>#</sup> (1.158242e+05)
	3	1.042068e+07 <sup>#</sup> (1.625627e+06)	6.120604e+07 <sup>#</sup> (3.951464e+06)	6.338800e+07 <sup>#</sup> (4.135194e+06)	6.221416e+07 <sup>#</sup> (5.160296e+06)	6.081194e+07 <sup>#</sup> (3.932779e+06)	4.635094e+07 <sup>#</sup> (4.612712e+06)	5.666077e+07 <sup>#</sup> (7.222818e+06)	5.883329e+07 <sup>#</sup> (7.222818e+06)
DTLZ2	2	1.291014e+03 <sup>#</sup> (9.071074e+01)	1.733441e+03 <sup>#</sup> (2.035706e+02)	1.682569e+03 <sup>#</sup> (3.354642e+02)	1.666750e+03 <sup>#</sup> (1.813600e+02)	1.654943e+03 <sup>#</sup> (2.123469e+02)	1.648889e+03 <sup>#</sup> (3.204995e+02)	1.616164e+03 <sup>#</sup> (1.935316e+02)	1.683851e+03 <sup>#</sup> (1.588133e+02)
	3	1.949957e+05 <sup>#</sup> (1.643671e+04)	1.650157e+05 <sup>#</sup> (9.689496e+03)	1.897169e+05 <sup>#</sup> (1.076623e+04)	1.375865e+05 <sup>#</sup> (7.379285e+03)	1.650157e+05 <sup>#</sup> (9.689496e+03)	1.565059e+05 <sup>#</sup> (9.949892e+03)	1.608309e+05 <sup>#</sup> (8.977004e+03)	1.628630e+05 <sup>#</sup> (8.977004e+03)
DTLZ2-1	2	3.460118e+03 <sup>#</sup> (1.447837e+02)	5.677262e+03 <sup>#</sup> (5.377094e+02)	6.295488e+03 <sup>#</sup> (1.501710e+03)	6.623736e+03 <sup>#</sup> (1.405020e+03)	5.668957e+03 <sup>#</sup> (5.186942e+02)	5.682854e+03 <sup>#</sup> (1.350085e+03)	4.242075e+03 <sup>#</sup> (4.710251e+02)	5.669005e+03 <sup>#</sup> (5.187033e+02)
	3	3.860403e+05 <sup>#</sup> (2.221565e+04)	5.177377e+05 <sup>#</sup> (3.150570e+04)	6.040356e+05 <sup>#</sup> (3.450382e+04)	5.720838e+05 <sup>#</sup> (3.754922e+04)	5.177362e+05 <sup>#</sup> (3.150570e+04)	4.650628e+05 <sup>#</sup> (2.956968e+04)	4.706842e+05 <sup>#</sup> (4.209904e+04)	5.139558e+05 <sup>#</sup> (1.392277e+04)
DTLZ5	2	1.291014e+03 <sup>#</sup> (9.071074e+01)	1.733441e+03 <sup>#</sup> (2.035706e+02)	1.682569e+03 <sup>#</sup> (3.354642e+02)	1.666750e+03 <sup>#</sup> (1.813600e+02)	1.654943e+03 <sup>#</sup> (2.123469e+02)	1.648889e+03 <sup>#</sup> (3.204995e+02)	1.616164e+03 <sup>#</sup> (1.935316e+02)	1.683851e+03 <sup>#</sup> (1.588133e+02)
	3	5.881850e+04 <sup>#</sup> (2.292902e+03)	7.711397e+04 <sup>#</sup> (1.114531e+04)	7.251771e+04 <sup>#</sup> (9.428644e+03)	8.303132e+04 <sup>#</sup> (1.131798e+04)	7.661495e+04 <sup>#</sup> (1.050952e+03)	7.322066e+04 <sup>#</sup> (1.224087e+04)	6.869597e+04 <sup>#</sup> (9.700606e+03)	7.501115e+04 <sup>#</sup> (1.152780e+04)
DTLZ5-1	2	3.460118e+03 <sup>#</sup> (1.447837e+02)	5.677262e+03 <sup>#</sup> (5.377094e+02)	6.295488e+03 <sup>#</sup> (1.501710e+03)	6.623736e+03 <sup>#</sup> (1.405020e+03)	5.668957e+03 <sup>#</sup> (5.186942e+02)	5.682854e+03 <sup>#</sup> (1.350085e+03)	4.242075e+03 <sup>#</sup> (4.710251e+02)	5.669005e+03 <sup>#</sup> (5.187033e+02)
	3	5.074749e+05 <sup>#</sup> (1.814572e+04)	6.458456e+05 <sup>#</sup> (3.182224e+04)	7.234121e+05 <sup>#</sup> (2.971116e+04)	7.100611e+05 <sup>#</sup> (3.629466e+04)	6.457661e+05 <sup>#</sup> (3.150492e+04)	6.075672e+05 <sup>#</sup> (2.984732e+04)	5.094598e+05 <sup>#</sup> (4.981328e+04)	6.536891e+05 <sup>#</sup> (3.806488e+04)
DTLZ7	2	1.658939e+03 <sup>#</sup> (4.982475e+02)	1.703469e+03 <sup>#</sup> (6.169178e+02)	1.571216e+03 <sup>#</sup> (5.838278e+02)	1.572009e+03 <sup>#</sup> (4.203846e+02)	1.595144e+03 <sup>#</sup> (4.414085e+02)	1.536629e+03 <sup>#</sup> (3.978827e+02)	1.512220e+03 <sup>#</sup> (4.334773e+02)	1.659590e+03 <sup>#</sup> (4.044080e+02)
	3	6.08615e+04 <sup>#</sup> (1.228435e+04)	1.105173e+05 <sup>#</sup> (3.395800e+04)	1.848888e+05 <sup>#</sup> (3.705969e+04)	1.090111e+05 <sup>#</sup> (3.272136e+04)	1.095923e+05 <sup>#</sup> (3.571369e+04)	7.822746e+04 <sup>#</sup> (1.720248e+04)	7.005433e+04 <sup>#</sup> (2.245271e+04)	9.947844e+04 <sup>#</sup> (3.143508e+04)
DTLZ7-1	2	6.601602e+02 <sup>#</sup> (1.427766e+01)	9.241120e+02 <sup>#</sup> (2.052206e+02)	8.281332e+02 <sup>#</sup> (2.052206e+02)	8.697297e+02 <sup>#</sup> (1.165725e+02)	8.704665e+02 <sup>#</sup> (1.097159e+02)	7.470244e+02 <sup>#</sup> (1.274952e+02)	8.500112e+02 <sup>#</sup> (1.333475e+02)	8.554335e+02 <sup>#</sup> (1.333475e+02)
	3	1.477186e+04 <sup>#</sup> (5.663096e+03)	5.307180e+04 <sup>#</sup> (1.817877e+04)	5.945956e+04 <sup>#</sup> (2.991456e+04)	5.713357e+04 <sup>#</sup> (1.617295e+04)	5.475668e+04 <sup>#</sup> (1.521980e+04)	3.871680e+04 <sup>#</sup> (1.559135e+04)	2.227547e+04 <sup>#</sup> (1.409303e+04)	5.462697e+04 <sup>#</sup> (1.977314e+04)
WFG1	2	1.565536e+03 <sup>#</sup> (6.227043e+02)	4.335804e+03 <sup>#</sup> (6.341935e+02)	4.196410e+03 <sup>#</sup> (6.088311e+02)	4.196410e+03 <sup>#</sup> (5.728016e+02)	4.286319e+03 <sup>#</sup> (4.124380e+02)	4.349743e+03 <sup>#</sup> (7.376629e+02)	4.204975e+03 <sup>#</sup> (4.414066e+02)	4.204975e+03 <sup>#</sup> (4.414066e+02)
	3	4.599818e+05 <sup>#</sup> (3.509304e+04)	5.184674e+05 <sup>#</sup> (1.929072e+04)	5.297481e+05 <sup>#</sup> (2.155747e+04)	5.203680e+05 <sup>#</sup> (2.863031e+04)	5.184674e+05 <sup>#</sup> (1.929072e+04)	4.461624e+05 <sup>#</sup> (3.114678e+04)	5.156971e+05 <sup>#</sup> (1.528391e+04)	5.153043e+05 <sup>#</sup> (2.767038e+04)
WFG1-1	2	4.634857e+03 <sup>#</sup> (4.046707e+03)	4.235804e+03 <sup>#</sup> (8.806378e+02)	4.744780e+03 <sup>#</sup> (8.040138e+02)	4.150133e+03 <sup>#</sup> (4.563455e+02)	4.214520e+03 <sup>#</sup> (4.183232e+02)	4.324686e+03 <sup>#</sup> (7.944825e+02)	4.158365e+03 <sup>#</sup> (4.117834e+02)	4.190205e+03 <sup>#</sup> (4.117834e+02)
	3	7.715876e+04 <sup>#</sup> (8.352894e+03)	3.141305e+05 <sup>#</sup> (2.194826e+04)	3.461392e+05 <sup>#</sup> (1.599973e+04)	3.073141e+05 <sup>#</sup> (1.906281e+04)	3.141413e+05 <sup>#</sup> (2.194225e+04)	2.270112e+05 <sup>#</sup> (1.736704e+04)	2.111477e+05 <sup>#</sup> (5.681661e+04)	3.102097e+05 <sup>#</sup> (1.969159e+04)
WFG2	2	2.476658e+03 <sup>#</sup> (4.968231e+02)	2.790792e+03 <sup>#</sup> (7.035403e+02)	2.843289e+03 <sup>#</sup> (4.917881e+02)	2.701249e+03 <sup>#</sup> (4.563455e+02)	2.828557e+03 <sup>#</sup> (4.748070e+02)	2.600459e+03 <sup>#</sup> (6.143328e+02)	2.828184e+03 <sup>#</sup> (5.581615e+02)	2.831176e+03 <sup>#</sup> (4.774635e+02)
	3	2.800111e+05 <sup>#</sup> (5.723262e+04)	3.777302e+05 <sup>#</sup> (6.475809e+04)	3.883116e+05 <sup>#</sup> (7.671066e+04)	3.485334e+05 <sup>#</sup> (4.423614e+04)	3.777302e+05 <sup>#</sup> (6.475809e+04)	3.127121e+05 <sup>#</sup> (5.093723e+04)	3.676892e+05 <sup>#</sup> (5.223327e+04)	3.680925e+05 <sup>#</sup> (2.674303e+04)
WFG2-1	2	1.766248e+03 <sup>#</sup> (2.638803e+02)	2.333515e+03 <sup>#</sup> (3.177426e+02)	2.337436e+03 <sup>#</sup> (3.515560e+02)	2.353181e+03 <sup>#</sup> (4.519447e+02)	2.254460e+03 <sup>#</sup> (3.640165e+02)	2.306952e+03 <sup>#</sup> (4.353679e+02)	2.331899e+03 <sup>#</sup> (4.145174e+02)	2.331899e+03 <sup>#</sup> (4.145174e+02)
	3	3.810451e+05 <sup>#</sup> (1.557674e+04)	5.127600e+05 <sup>#</sup> (9.150939e+02)	5.715054e+05 <sup>#</sup> (9.062012e+02)	5.192733e+05 <sup>#</sup> (3.908777e+04)	5.127600e+05 <sup>#</sup> (9.150939e+02)	4.945208e+05 <sup>#</sup> (2.548218e+04)	5.163662e+05 <sup>#</sup> (2.452925e+04)	5.131372e+05 <sup>#</sup> (2.160505e+04)
WFG3	2	4.737892e+03 <sup>#</sup> (1.212466e+03)	5.682896e+03 <sup>#</sup> (9.150939e+02)	5.283769e+03 <sup>#</sup> (9.062012e+02)	4.598677e+03 <sup>#</sup> (4.967458e+02)	5.323202e+03 <sup>#</sup> (9.883039e+02)	5.300394e+03 <sup>#</sup> (8.054953e+02)	5.418351e+03 <sup>#</sup> (8.187545e+02)	5.318340e+03 <sup>#</sup> (8.187545e+02)
	3	3.530812e+05 <sup>#</sup> (4.627007e+04)	4.992648e+05 <sup>#</sup> (4.028765e+04)	5.140610e+05 <sup>#</sup> (3.330771e+04)	4.771445e+05 <sup>#</sup> (3.341461e+04)	4.992648e+05 <sup>#</sup> (4.028765e+04)	4.505951e+05 <sup>#</sup> (5.602672e+04)	4.994122e+05 <sup>#</sup> (4.829807e+04)	4.943398e+05 <sup>#</sup> (3.517098e+04)
WFG3-1	2	5.148218e+03 <sup>#</sup> (9.435951e+02)	5.430409e+03 <sup>#</sup> (6.812039e+02)	5.390651e+03 <sup>#</sup> (8.890972e+02)	4.196157e+03 <sup>#</sup> (2.813812e+02)	5.065853e+03 <sup>#</sup> (6.730455e+02)	4.860643e+03 <sup>#</sup> (9.733448e+02)	5.077295e+03 <sup>#</sup> (6.643410e+02)	5.077295e+03 <sup>#</sup> (6.643410e+02)
	3	2.293842e+05 <sup>#</sup> (2.498524e+04)	6.037343e+05 <sup>#</sup> (2.325666e+04)	6.442096e+05 <sup>#</sup> (4.495150e+04)	5.977539e+05 <sup>#</sup> (2.421289e+04)	6.037343e+05 <sup>#</sup> (2.325666e+04)	5.228685e+05 <sup>#</sup> (2.540989e+04)	5.912077e+05 <sup>#</sup> (2.997981e+04)	6.046485e+05 <sup>#</sup> (2.531948e+04)

## 5 Conclusions and Future Work

In physics, the total potential energy of a system of  $N$  particles plays an important role in macroscopic and in molecular fields. To measure the potential energy due to the interactions of pairs of particles, pair-potential functions are employed.

<sup>5</sup> All the IGD and PD graphs are available at <http://computacion.cs.cinvestav.mx/~jfalcon/PairPotentials/>.

In this paper, we used several pair-potential functions (Riesz  $s$ -energy, Gaussian  $\alpha$ -energy, Coulomb's law, Pöschl-Teller and Kratzer potential) to increase the diversity of MOEAs. To this aim, we adopted the pair-potential functions as the backbone of a selection mechanism to update an external archive which is coupled to MOEA/D. Our experimental results based on the IGD and PD indicators showed that the pair-potential-based archives store solutions with high diversity that otherwise would be discarded by MOEA/D's main population. Hence, the utilization of the pair-potential-based archives helps to circumvent the known MOEA/D's performance dependence on the Pareto front shapes. As part of our future work, we aim to mathematically analyze the selected pair-potential functions in order to design better selection mechanisms and test them on MaOPs.

## References

1. Bingdong Li, Jinlong Li, Ke Tang, and Xin Yao. Many-Objective Evolutionary Algorithms: A Survey. *ACM Comput. Surv.*, 48(1), 2015.
2. Sergiy V. Borodachov, Douglas P. Hardin, and Edward B. Saff. *Discrete Energy on Rectifiable Sets*. Springer Monographs in Mathematics. Springer-Verlag, 1 edition, 2019.
3. Jesús Guillermo Falcón-Cardona, M. T. M. Emmerich, and C. A. Coello Coello. On the cooperation of multiple indicator-based multi-objective evolutionary algorithms. In *In proc. of CEC '19*, pages 2050–2057, 2019.
4. Jesús Guillermo Falcón-Cardona, Hisao Ishibuchi, and Carlos A. Coello Coello. Riesz  $s$ -energy-based reference sets for multi-objective optimization. In *In proc. of CEC '20*, pages 1–8, 2020.
5. J. Blank, K. Deb, Y. Dhebar, S. Bandaru, and H. Seada. Generating Well-Spaced Points on a Unit Simplex for Evolutionary Many-Objective Optimization. *IEEE Transactions on Evolutionary Computation*, pages 1–1, 2020.
6. John David Jackson. *Classical electrodynamics*. Wiley, 3rd edition, 1999.
7. Shi-Hai Dong. *Pöschl-Teller Potential*, pages 95–110. Springer Netherlands, 2007.
8. M. Hamzavi and S.M. Ikhdair. Approximate  $l$ -state solution of the trigonometric pöschl-teller potential. *Molecular Physics*, 110(24):3031–3039, 2012.
9. Gary Simons, Rober G. Parr, and J. Michael Finlan. New alternative to the Dunham potential for diatomic molecules. *The Journal of Chemical Physics*, 59(6):3229–3234, 1973.
10. Qingfu Zhang and Hui Li. MOEA/D: A Multiobjective Evolutionary Algorithm Based on Decomposition. *IEEE Transactions on Evolutionary Computation*, 11(6):712–731, 2007.
11. Hisao Ishibuchi, Yu Setoguchi, Hiroyuki Masuda, and Yusuke Nojima. Performance of Decomposition-Based Many-Objective Algorithms Strongly Depends on Pareto Front Shapes. *IEEE Transactions on Evolutionary Computation*, 21(2):169–190, 2017.
12. Carlos A. Coello Coello and Nareli Cruz Cortés. Solving Multiobjective Optimization Problems using an Artificial Immune System. *Genetic Programming and Evolvable Machines*, 6(2):163–190, 2005.
13. H. Wang, Y. Jin, and X. Yao. Diversity assessment in many-objective optimization. *IEEE Transactions on Cybernetics*, 47(6):1510–1522, 2017.