Large-scale Multi-objective Optimization for Water Quality in Chesapeake Bay Watershed

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***Abstract*—The careful selection of Best Management Practices (BMPs) to reduce loading, such as nitrogen, phosphorus, and sediments, can substantially improve the water quality of watersheds. This paper introduces the first implementation of a hybrid and customized evolutionary multi-objective (EMO) algorithm to improve the Chesapeake Bay Watershed's (CBW) water quality. To make the algorithm scalable, we inject a few solutions obtained using an integer programming algorithm (IPOPT) in the initial population of EMO. Also, a repair operator is applied to satisfy every equality constraint. Combining these approaches can find a set of non-dominated trade-off solutions from 1,012 variables (Tucker county in West Virginia) to a staggering 153,818 variable problem (the whole state of West Virginia). Furthermore, a preliminary analysis of obtained trade-off solutions finds interesting properties of BMP allocations, providing an optimistic picture of applying the proposed customized optimization algorithm in addressing other bigger states leading to the whole Chesapeake Bay watershed.**

***Index Terms*—Watershed Optimization, Large-scale Optimization, Multi-objective Optimization, Hybrid approach**

I. Introduction

The Chesapeake Bay is the largest estuary in the United States and the third-largest in the world. As a result, the Bay has an enormous historical, social, economic, and ecological importance, with natural benefits estimated at more than \$100 billion per year [1]. With a drainage area of about 166,000 km^2, the Chesapeake Bay Watershed (CBW) includes parts of six states in the Mid-Atlantic region and is home to more than 18 million people. Since the middle of the twentieth century, human activities such as livestock and crop productions, urban development, and stream alteration have resulted in nutrients and sediments excess in waterbodies throughout the watershed, causing water quality impairment, freshwater ecosystems' degradation, and loss of recreational values. In order to address these issues, the Chesapeake Bay Program (CBP) partnership has led the coordination of restoration efforts since 1984. During the last decade, these efforts have been guided by the Chesapeake Bay Total Maximum Daily Load (TMDL), which established limits to nutrients and sediments loadings. Particularly, the TMDL has been used to formulate comprehensive restoration plans known as Watershed Implementation Plans (WIPs) and outline major goals, timelines, and expected outcomes as those established in the Chesapeake Bay Watershed Agreement in 2014 [2].

Due to the complexity of evaluating restoration plans' effectiveness, watershed management in the CBW has been extensively supported by modeling tools [3]. The Chesapeake Assessment Scenario Tool (CAST) is the core modeling tool that reports the impacts of management scenarios on the reduction of point and non-point sources of pollution. Those management scenarios (i.e., portfolios of Best Management Practices, BMPs) have been primarily defined based on expert elicitation. Just recently, single-objective, gradient-based optimization has been used to identify cost-effective BMPs portfolios to improve water quality in the CBW [4], [5]. Since deciding on the implementation of these portfolios involves many stakeholders (e.g., government agencies, commercial entities, nonprofit organizations, academic institutions) at multiple spatial scales (e.g., county, state), a multi-objective optimization approach exploring trade-offs among conflicting objectives is proposed in this study.

One striking aspect of CBW optimization is the large-scale nature of variables and constraints, leading to hundreds of thousands of variables and tens of thousands of constraints. We have customized a base evolutionary multi-objective optimization (EMO) algorithm hybridizing with a point-based mixed-integer programming (IPOPT) algorithm to address this problem. In addition, the optimization problem formulation is exploited to develop a new repair operator to satisfy as many constraints as possible. Moreover, to investigate the performance with increasing problem size, we have considered a mathematical model of the objectives and constraints instead of the CBW's CAST system.

In the remainder of this paper, we provide a brief description of the optimization problem formulation in Section II. The proposed customized EMO approach is described in detail in Section III. Results of this extensive study are presented in Section IV. Finally, conclusions are discussed in Section V.

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II. Problem Statement

We provide a general formulation of the optimization problem. The number of variables and constraints depends on the area of interest (e.g., county, state, watershed) within the CBW.

$$
\begin{aligned}
\text{Min. } & f_1(\mathbf{x}) = \sum_{s\in S} \sum_{h\in H_s} \sum_{u\in U} \sum_{b\in B_u} \tau_b x_{s,h,u,b}, \\
\text{Min. } & f_2(\mathbf{x}) = \sum_{s\in S} \sum_{h\in H_s} \sum_{u\in U} \left[\alpha_{s,h,u} \phi_{s,h,u} \prod_{G^B\in\mathcal{G}^B} \left(1 - \sum_{b\in G^B} \eta^N_{s,h,b} \frac{x_{s,h,u,b}}{\alpha_{s,h,u}} \right) \right], \\
s.t. \quad & \sum_{b\in G^B} x_{s,h,u,b} = \alpha_{s,h,u}, \quad \forall s\in S,\ h\in H_s,\ u\in U_s,\ G^B\in\mathcal{G}^B, \\
& x_{s,h,u,b} \geq 0, \quad \forall s\in S,\ h\in H_s,\ u\in U_s,\ b\in B_u.
\end{aligned} \tag{1}
$$

The variable $x_{s,h,u,b}$ indicates the acres used for implementing a BMP b to reduce a load-source u on an agency h and land-river-segment s. The objective function $f_1(\mathbf{x})$ represents the total cost of implementing all BMPs, while the objective function $f_2(\mathbf{x})$ calculates the Nitrogen load. The parameter τ_b indicates the cost per unit acre of implementing BMP b. $\eta^N_{s,h,b}$ refers to the efficiency of BMP b of removing Nitrogen when applying on agency h and land-river-segment s. α refers to the available acres, and $\mathcal{G}$ contains all the groups of BMPs G that can be applied on a given (s,h,u). All parameter values are chosen from CBW's practice.

In CAST, the CBW is spatially discretized into land-river segments (LRSs) to quantify the total nitrogen, total phosphorus, and sediment loads that are ultimately delivered to the Bay. LRSs result from the intersection of land segments (i.e., counties) and river segments (i.e., drainage areas for river reaches/reservoirs yielding at least 2.8 m^3/s average flow). Thus, multiple LRSs can form an individual county up to the entire CBW. Each LRS contains multiple load sources. A load-source is a type of land, land use, or artificial construct that generates loads (i.e., nitrogen, phosphorus, and sediment) that can be potentially delivered to the Bay. BMPs can be assigned to a specific load source within an LRS to reduce nutrient and/or sediment loadings. It is worth noting that the available BMPs depend on the geographical location of the LRS and the jurisdiction (i.e., agency zone of influence) in which the load source falls (e.g., federal, non-federal). This study only considers "efficiency" BMPs, which are land BMPs modeled as a constant multiplying factor representing pollutant removal effectiveness.

For optimization purposes, the decision variables are represented as the vector of all possible combinations of LRSs within the area of interest, load sources, jurisdictions, and efficiency BMPs. The value of each element in the vector is the area percentage of the corresponding BMP. This percentage is obtained with respect to the total area given by an LRS, load-source, and jurisdictions combination. It is important to note that, in general, when the area of interest is large, the number of decision variables increases as the number of LRSs does. The constraints ensure that all BMPs allocated to each combination of LRS, load source, and jurisdictions adds up to 100% of the available area when the BMPs cannot be overlaid.

Decision-makers might be leaned to consider a fraction of the BMPs, as their knowledge acquired over time gives them an educated guess of what BMPs can be better used on a given LRS. However, not considering all BMPs may lead to unexplored search spaces where innovative solutions might be hidden. Therefore, we decided to include all the possible combinations of variables in our experiment, so besides gaining knowledge of the specificities of the problem, we give the approach to find solutions that would be impossible to find otherwise.

In this paper, we restrict our study to West Virginia. One county, on average, constitutes 13,983 variables arising from 113 LRSs, up to 46 load sources, up to 6 agencies, and up to 119 BMPs in a single group. However, there can be different groups simultaneously. When an entire state is considered, variables can rise to 153,818. These numbers are considered large for any optimization algorithm.

Since we are dealing only with efficiency BMPs, the cost function is linear, but load functions are not linear; in this case, we will adopt only the Nitrogen load as our second function. In addition, we have a problem-dependent set of linear constraints (there is one constraint for each non-overlapping group of BMPs). Nevertheless, the presence of a large number of variables in the overall problem formulation is a difficulty faced by any optimization algorithm. The other obstacle arises from the multi-objective nature of the problem, a matter that we will discuss more in the following subsection.

A. Need for Multiple Objectives

As it is clear from the above description that the CBW management involves simultaneous minimization of two conflicting objectives: (i) minimizing the costs of BMP implementation and (ii) minimizing nitrogen loading to the environment. A multi-objective optimization problem gives rise to a set of trade-off Pareto-optimal solutions in contrast to a single optimal solution [6], [7]. Instead of finding a single Pareto-optimal solution at a time using a point-based method [8], here, we apply an evolutionary multi-objective optimization method – NSGA-III [9] – to find multiple Pareto-optimal solutions in a single run. Although many metaheuristics have been used to solve other watershed problems, the multi-objective nature of this formulation suggests the use of a proven multi-objective approach.

B. Past Studies on Watershed Optimization

Previous works on watershed optimization are mainly focused on agricultural management [10]–[12], urban watershed restoration [13], [14], stormwater management [15], [16], and model calibration [17], [18]. Studies involving BMPs allocation have typically involved a watershed model, a cost evaluation model, and an optimization algorithm, targeting pollutant loading reduction and implementation costs [11]. Optimization algorithms previously used for BMP allocation include gradient-based approaches [4], Tabu search [19], and evolutionary approaches such as NSGA-II, NSGA-III, and C-TAEA [20]–[22].

III. Proposed Customized EMO Approach

In solving large-scale practical problems, the vanilla optimization algorithms with generic procedures (such as a random initialization, a penalty-based constraint handling approach, standard recombination and mutation operators for evolutionary algorithms, etc.) do not work efficiently [23]. This calls for customizing an optimization algorithm for a problem class. CBOP caters to an optimization problem class involving many problem instances over different counties, states, and a cluster of states that involve similar LRSs, similar BMPs for implementation, and similar methods to compute the objective and constraint functions (cost, nitrogen, phosphorous and sediment loads). It is expected to believe that an optimization algorithm developed for the CBOP class will be efficient for most problem instances arising from counties, states, and the watershed level. The difficulty for an optimization algorithm will arise from the increase in problem size (mostly variables and constraints). This paper plans to develop an efficient optimization methodology that works well in various versions of the problem class, whether the CBOP is formulated for a single county, multiple counties, and the state level.

In order to customize an optimization algorithm for a problem class, first, the algorithm must be amenable to customization. For example, there is probably not much sense to customize the conjugate gradient optimization method, as the algorithm already requires that the conjugate directions are to be found, and a line search has to be executed along each conjugate direction. Even if certain key problem knowledge is available, the basic algorithm may not be easy to change.

This paper uses an evolutionary algorithm (EA), which is flexible and amenable to customization. An EA can be customized using problem information in its following features in creating (i) an effective representation scheme, (ii) a reduced and computationally fast evaluation procedure, (iii) a biased initial population, (iv) customized genetic operators, and (v) customized termination criterion. Here, we utilize the first four features in developing our proposed optimization algorithm.

A. Ad-hoc Representation Scheme

As stated earlier, BMPs can only be implemented on a specific triplet of land-river-segment (LRS) agency and load-source serving as a locator. Thus, we added the BMP to such a triplet to make a 4-tuple (LRS, agency, load-source, BMP) data structure representation to hold each variable. The entry for each variable represents the proportion of the triplet that the BMP will be applied. Consequently, our variables are naturally real-valued, lying within $[0, 1]$. In addition, the Chesapeake Bay Program Office (CBPO) has grouped sets of BMPs that can be applied to each triplet of the CBW territory. The BMPs inside each set are non-overlapping among themselves, so they share the whole location; however, BMP sets overlap between them. Hence, one can superpose them without interfering with one group with another. The cardinality of each BMP set can vary significantly, and the number of sets associated with each triplet makes the problem grow exponentially.

B. Reduced Evaluation Time Approach

In a real scenario of optimizing the CBW, the optimization algorithm must use the CAST system to evaluate a solution. Nevertheless, this study uses mathematical models obtained from the available data as objective and constraint functions. This drastically reduces the computational time for completing an optimization run.

C. Biased Initialization

To make the overall search quicker and more efficient, we use a hybrid optimization strategy, in which a point-based interior-point optimization (IPOPT) method is used to seed the initial population of the multi-objective evolutionary algorithm. An ϵ-constraint method [6], [7] with different values of ϵ_k is applied multiple times to find a collection of good solutions. The following single-objective optimization problem (P_k) is solved:

$$\begin{array}{rl} \text{Minimize} & f_1(\mathbf{x}), \\ \text{Subject to} & f_2(\mathbf{x}) \leq \epsilon_k f_2^{\text{base}}, \\ \mathbf{x} \in \mathbf{X}, & \end{array} \tag{2}$$

where f_2^{base} is the nitrogen loading associated with current practice and $\mathbf{X}$ denotes the feasible variable set associated with any other constraints of the original formulation. For different values of ϵ_k, respective solution $\mathbf{x}^{(k)}$ is found and added to the initial population. For our study, we have used 11 values of ϵ_k from 1.0 to 0.70 in decreasing steps of 0.03.

The use of ϵ_k restates our original single-objective problem to a single-point multi-objective approach that needs to be executed k times to achieve a Pareto front with k elements. Independent executions to reach a single point make this approach time-consuming and thus inefficient for a large k. Selecting a small k would make the data-analytics process difficult to gain helpful knowledge from just a few points.

D. Repair Operator

As seen from the problem formulation (in Equation 1), there is an equality constraint with respect to each LRS: all BMP proportions must add up to $\alpha_{s,h,u}$. If the variables x_{ij} (an element of the variable matrix) are randomly chosen in $[0, 1]$, it is very unlikely that their sum across each row will be equal or even close to $\alpha_{s,h,u}$. However, we use a customization trick here in which every variable $x_{s,h,u,b}$ is replaced with $\alpha_{s,h,u}\left(x_{s,h,u,b}/\sum_{b=1}^{B_u} x_{s,h,u,b}\right)$ for every equality constraint. This modification of every element of the matrix will automatically satisfy the respective equality constraint and allow the EC framework to efficiently focus on the feasible search space.

In order to evaluate the contribution of the repair operator to the approach, we fixed all the parameters (including the maximum number of generations, which in this case is 100). We use a pre-specified maximum number of generations in this study. However, we use a hypervolume-based termination concept described in the next section for comparison purposes among different approaches.

IV. RESULTS

For our study, we consider all 11 counties of West Virginia within the Chesapeake Bay Watershed, that is: Berkeley, Grant, Hampshire, Hardy, Jefferson, Mineral, Monroe, Morgan, Pendleton, Preston, and Tucker. Table I shows the variables and constraints of each county. The minimum number of variables involved in any of the counties is 1,012, which is considered a large-scale problem in the context of any optimization algorithm, including evolutionary algorithms. In this paper, we shall demonstrate the results of our proposed algorithm involving the whole state resulting in 153,818 real-parameter variables to be optimized. Furthermore, the base nitrogen values in the table are obtained without any BMP usage to each individual county and the state.

TABLE I
NUMBER OF VARIABLES AND CONSTRAINTS OF THE COUNTIES.

County	#Variables	#Constraints	Base N_2 (f_2^{base})
Berkeley	14,090	1,813	977,896
Grant	25,228	3,448	1,049,450
Hampshire	12,783	1,700	1,012,797
Hardy	18,607	2,491	1,344,295
Jefferson	12,303	1,606	1,018,012
Mineral	20,260	2,698	763,864
Monroe	3,102	399	48,655
Morgan	11,880	1,665	271,134
Pendleton	33,083	4,352	1,133,327
Preston	1,470	193	4,683
Tucker	1,012	144	1,702
Total	153,818	20,509	7,625,818

We perform four experiments focused on gathering insightful information about the problem:

- **Experiment 1**: Knowledge incorporation through solution injection by IPOPT.
- **Experiment 2**: Reduction of constraints with a repair approach.
- **Experiment 3**: Scale-up study.
- **Experiment 4**: Deciphering common patterns of BMP allocation in final trade-off solutions.

Detailed experimental settings are discussed below.

- **Injecting Points**: We computed 11 points using independent executions of the ϵ-constraint approach. The approach increases the ϵ from 0% to 30% nitrogen reduction (inclusive), using 3% of step size. The search method uses the IPOPT, an interior-point-based optimization method that has been found to be effective on many real-world applications.
- **Large-run front**: We generate a non-dominated reference set by injecting solutions (mentioned in the previous item) to the NSGA-III. The NSGA-III is executed during 1,000 generations using a population size of 1,000, and 600 reference points. We adopted standard values for the remaining parameters and performed the same procedure for each of the counties and the merged counties we computed.
- **Performance measure**: We calculated the ratio of the Hypervolume (HV), which refers to obtaining the HV of each execution and dividing it by the PF's HV. To have a fair comparison across all problems, we computed the maximum and minimum value of each produced Pareto front. We used such values to normalize the NSGA-III's output. The adopted reference point was $(1.1, 1.1)$.

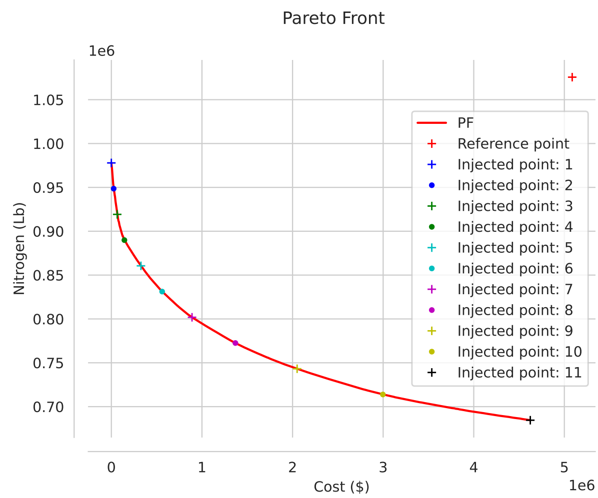

Fig. 1. Berkeley county: Injected points obtained using the interior-point-based ϵ-constraint method

- **Experiment 1**: This experiment aims to find whether the NSGA-III improves its performance if we incorporate knowledge into it. For that sake, we selected different sets of the points generated with our ϵ-constraint approach and injected them into the NSGA-III. The selection of points of each set attempts to find a subset maximizing the diversity of injecting points. Figure 1 shows the performance resulting from the injecting of a different number of points in Berkeley, WV. The points for this and each of the remaining counties are selected as given below:
  - 0 points: No point is injected to NSGA-III.
  - 1 point: Point 1 (best for cost objective) is injected to NSGA-III.
  - 2 points: Points 1 and 11 (best for cost and nitrogen objectives) are injected to NSGA-III.
  - 3 points: Points 1, 6 (a near 50%-50% compromise point) and 11 are injected.
  - 4 points: Points 1, 4, 8, and 11 are injected.
  - 5 points: Points 1, 3, 6, 9, and 11 are injected.
  - 6 points: Points 1 3, 5, 7, 9, and 11 are injected.
  - 11 points: All 11 points are injected.

We modified the termination criterion of the NSGA-III, to get an idea of the performance with different injected-point sets. For this sake, we normalized each Pareto front and computed its Hypervolume (using $(1.1, 1.1)$ as a reference point). Then in each generation, we normalize the current population using the lower and upper bound of the Pareto front and remove solutions exceeding the HV's reference point in any dimension. Finally, we compute the HV of the filtered population.The algorithm is terminated

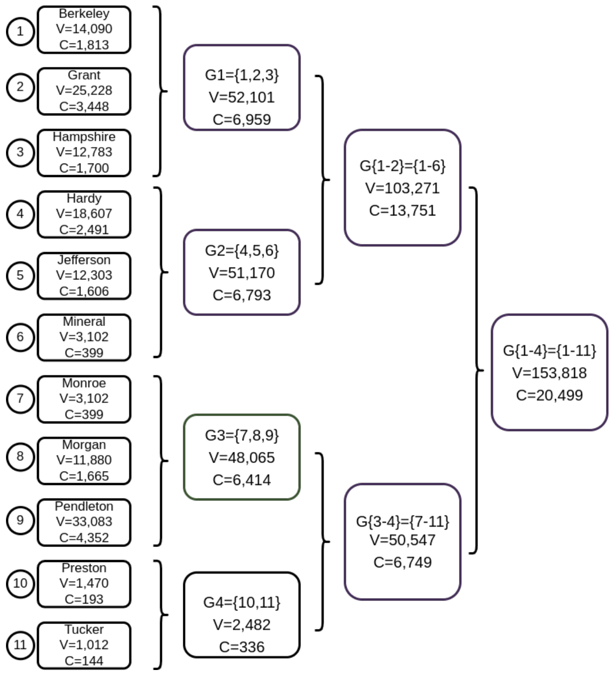

Fig. 2. Strategy to build scaled problems for the scale-up study.

either when (i) the maximum number of generations 1,000 is reached or (ii) a trade-off solution set with 90% of the Large-front- run's HV is obtained. Results are presented in Table II.

We perform 31 runs using different initial populations in all our experiments.

- **Experiment 2:** We adopt a different number of injecting points, similar to our previous experiment. We follow the same selection procedure as presented previously. However, we only explore three options. Having all points (11), selecting 5, and selecting 1 point. This experiment differs from the previous one in that we want to evaluate the effect of our repair approach. For this regard, we compute both the NSGA-III using the original formulation, which we refer to as no-repair (NR), and the NSGA-III using our efficient yet straightforward repair method, which we denote as R in our graphics.
- **Experiment 3:** We investigate the performance of the proposed customized NSGA-III with an increase of variables arising from a single county to the whole state. Therefore, we modify the NSGA-III termination criteria: The algorithm is terminated either when (i) the maximum number of generations 1,000 is reached, or (ii) a trade-off solution set with 97% of the Large-front-run's HV is obtained. The design of this experiment is as follows: First, we execute each county independently, then we gather different counties together, as it is shown in Figure 2. Then, as seen in the mentioned figure, we group a maximum of three counties and continue grouping counties until we finally solve one problem with all the counties together. As shown in Table I, the number of variables varies from 1,012 to a staggering 153,818.
- **Experiment 4:** Finally, we analyze the obtained non-dominated solutions to find if there is any pattern of BMP allocations common to them. We are particularly interested in finding if all prescribed BMPs are necessary to form efficient solutions.

A. Injection of IPOPT Points in Initial Population

Figure 3 shows a boxplot presenting the information regarding the generation where the NSGA-III stopped when optimizing the Berkeley county. This plot demonstrates the importance of injecting solutions to NSGA-III. On the one hand, when zero or one solution was injected, NSGA-III failed to reach 90% of the PF's HV. On the other hand, providing 11 solutions almost automatically fulfilled the 90% goal. When we analyze Figure 3 we can state that NSGA-III starts benefiting from the injection of points when two or more points are injected.

Table II shows the average and standard deviation of the generation in which NSGA-III reached 90% of the PF's HV. A value of 1,000 means that the algorithm could not achieve the 90% goal, while a value close to zero means that it could easily reach such a goal. The results show the importance of injecting points to the NSGA-III for this problem. Table III provides the average and standard deviation of Hypervolume of NSGA-III's last population. Both tables indicate that Tucker and Monroe were the easiest counties to solve because NSGA-III could reach the Pareto Front in some degree. Besides these two counties, NSGA-III required the injection of points to solve the problems. It is notable that it started producing good results with only two points. However, it benefits if more points are provided.

The results might mislead us to believe that this problem is easy, as NSGA-III requires only two generations on many counties to reach 90% of HV when we injected 11 points. Thus, it shall be interesting to see how much NSGA-III can improve when run for some more iterations. Table IV shows the results of running the NSGA-III during 100 generations when injecting 2, 5, and 11 points. Please check 2 (R), 5 (R), and 11 (R). One can observe that running NSGA-III for more iterations continues to improve solutions.

Here, we can again observe that it gets better results with more injected solutions, but this effect seems negligible on some occasions.

B. Effect of Repair Operator

Table IV lists the results for the HV metric using the original constrained formulation versus using the proposed repair operator. We can see that the constraints add an extra burden to the optimization process. When we eliminate the constraints and let the NSGA-III work on a feasible search space, it can produce significantly better results. Figure 6 shows the obtained non-dominated sets of Berkeley county with and without the repair operator [23]. We can easily see that the repair operator improves the NSGA-III performance. In addition, Figure 5 graphically shows through boxplots that the repair operator outperforms the same approach without it.

TABLE II

NSGA-III'S EXIT GENERATION FOR ALL COUNTIES IN WEST VIRGINIA, INJECTING DIFFERENT NUMBER OF POINTS

County	0		1		2		3		4		5		6		11	
	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD
Berkeley	1000	0.0e+00	1000	0.0e+00	76	9.0e+00	40	5.6e+00	31	5.9e+00	25	6.7e+00	19	7.3e+00	2	0.0e+00
Grant	1000	0.0e+00	1000	0.0e+00	66	6.4e+00	40	5.4e+00	30	5.8e+00	24	6.2e+00	18	8.3e+00	2	0.0e+00
Hampshire	1000	0.0e+00	1000	0.0e+00	973	1.4e+02	571	4.4e+02	78	1.5e+02	34	1.0e+01	26	8.3e+00	2	0.0e+00
Hardy	1000	0.0e+00	1000	0.0e+00	76	7.0e+00	40	6.5e+00	32	5.1e+00	24	6.1e+00	18	7.4e+00	2	0.0e+00
Jefferson	1000	0.0e+00	1000	0.0e+00	647	3.5e+02	83	2.7e+01	43	9.9e+00	26	8.4e+00	18	9.3e+00	2	0.0e+00
Mineral	1000	0.0e+00	1000	0.0e+00	981	1.0e+02	710	4.0e+02	103	1.7e+02	34	1.1e+01	22	1.3e+01	10	7.6e+00
Monroe	1000	0.0e+00	1000	0.0e+00	969	1.7e+02	119	7.9e+01	63	5.6e+01	51	1.8e+01	38	1.4e+01	2	1.6e+00
Morgan	1000	0.0e+00	1000	0.0e+00	824	3.6e+02	694	4.4e+02	636	4.4e+02	28	8.6e+00	20	1.1e+01	2	3.5e-01
Pendleton	1000	0.0e+00	1000	0.0e+00	66	7.5e+00	37	7.0e+00	31	4.9e+00	25	4.3e+00	15	8.4e+00	2	0.0e+00
Preston	1000	0.0e+00	1000	0.0e+00	663	3.6e+02	97	9.6e+01	43	6.8e+00	28	6.1e+00	24	4.7e+00	2	1.8e+00
Tucker	1000	0.0e+00	1000	0.0e+00	931	2.0e+02	540	2.6e+02	68	5.5e+01	89	4.4e+01	41	2.3e+01	17	5.8e+00

TABLE III

NSGA-III'S HYPERVOLUME ON THE EXIT GENERATION FOR ALL COUNTIES IN WEST VIRGINIA, INJECTING DIFFERENT NUMBER OF POINTS.

County	0		1		2		3		4		5		6		11	
	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD
Berkeley	0.0000	0.0e+00	0.3842	8.0e-02	0.9013	8.7e-04	0.9045	2.4e-03	0.9067	5.7e-03	0.9082	6.4e-03	0.9078	5.3e-03	0.9355	5.3e-03
Grant	0.0000	0.0e+00	0.5118	5.0e-02	0.9019	1.3e-03	0.9053	4.0e-03	0.9073	5.9e-03	0.9103	6.4e-03	0.9101	5.9e-03	0.9364	2.3e-03
Hampshire	0.0000	0.0e+00	0.5259	6.6e-02	0.5520	9.5e-02	0.8896	1.8e-02	0.9037	3.2e-03	0.9039	3.7e-03	0.9037	3.7e-03	0.9345	8.5e-03
Hardy	0.0000	0.0e+00	0.4532	9.5e-02	0.9011	8.5e-04	0.9041	2.8e-03	0.9066	4.1e-03	0.9105	7.4e-03	0.9098	7.5e-03	0.9346	5.0e-03
Jefferson	0.0000	0.0e+00	0.5750	1.2e-01	0.8753	4.8e-02	0.9015	1.5e-03	0.9046	3.8e-03	0.9069	5.5e-03	0.9072	8.1e-03	0.9259	4.3e-03
Mineral	0.0000	0.0e+00	0.4345	8.3e-02	0.5577	1.5e-01	0.8712	3.5e-02	0.9015	7.6e-03	0.9044	3.0e-03	0.9042	3.9e-03	0.9092	9.4e-03
Monroe	0.0000	0.0e+00	0.7350	4.0e-02	0.7491	5.0e-02	0.9018	2.5e-03	0.9029	2.7e-03	0.9030	4.3e-03	0.9034	3.2e-03	0.9138	4.9e-03
Morgan	0.0000	0.0e+00	0.4219	6.9e-02	0.5446	2.1e-01	0.8426	4.8e-02	0.8719	3.1e-02	0.9049	4.2e-03	0.9073	6.3e-03	0.9164	4.4e-03
Pendleton	0.0000	0.0e+00	0.4830	2.9e-02	0.9011	7.1e-04	0.9056	3.3e-03	0.9072	5.2e-03	0.9097	6.9e-03	0.9112	8.5e-03	0.9459	4.5e-03
Preston	0.0000	0.0e+00	0.7889	3.5e-02	0.8773	3.4e-02	0.9021	2.0e-03	0.9025	1.9e-03	0.9055	4.6e-03	0.9059	3.2e-03	0.9324	5.0e-03
Tucker	0.0000	0.0e+00	0.8144	3.9e-02	0.8355	4.3e-02	0.8994	5.8e-03	0.9054	7.0e-03	0.9012	1.5e-03	0.9047	4.7e-03	0.9084	6.5e-03

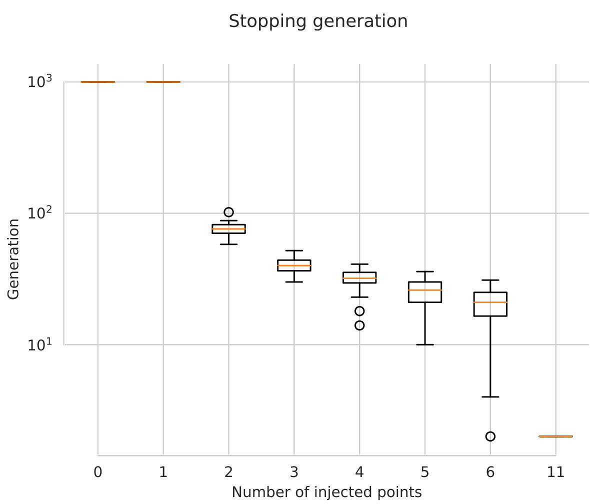

Fig. 3. Berkeley county: Boxplots indicating the generation where the NSGA-III reached 90% of the large run's hypervolume. More injected points produce a faster achievement of the desired hypervolume.

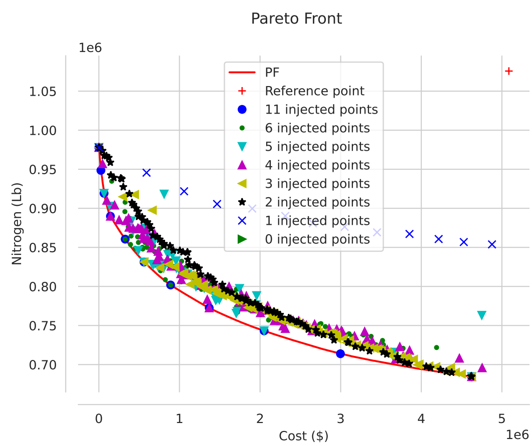

Fig. 4. Berkeley county: NSGA-II non-dominated points obtained from different number of injected IPOPT points in the initial population. Larger the number of injected points, better is the performance of NSGA-III. The line marked with 'PF' corresponds to the large-run NSGA-III.

In this case, the repair operator significantly helped the NSGA-III reach the non-dominated set.

C. Scale-up Study

Next, we perform a scale-up study by increasing the problem size. We use the agglomerating approach shown in Figure 2 for the scaling. Four groups of scaling are considered. The "individual" group contains each individual county, "Small-size" group contains groups of three counties, "Medium-size" group contains groups of five or six counties, and the "Big-size" group contains all 11 counties having 153,818 variables and 20,509 constraints.

We terminate a run when the NSGA-III achieves 97% of the large-size run's HV. Figure 7 shows the number of generations needed to achieve this target. It is remarkable that with an increase in variables from 1,012 to 153,818 from left to right of x-axis, the computational effort does

TABLE IV
RESULTS OF USING THE ORIGINAL CONSTRAINED FORMULATION (NOT REPAIR, DENOTED WITH NR) VS USING A VIOLATION REPAIR APPROACH (REPAIR, DENOTE WITH R).

County	2 (NR)		2 (R)		5 (NR)		5 (R)		11 (NR)		11 (R)	
	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD	Avg.	SD
Berkeley	0.5377	1.1e-01	0.9299	7.0e-03	0.5421	8.2e-02	0.9815	8.9e-04	0.5003	5.0e-02	0.9882	7.0e-04
Grant	0.4767	1.1e-01	0.9412	5.3e-03	0.4952	9.4e-02	0.9843	7.4e-04	0.4143	6.1e-02	0.9888	8.3e-04
Hampshire	0.5967	1.3e-01	0.3997	1.5e-01	0.5786	1.1e-01	0.9500	1.8e-02	0.5510	6.6e-02	0.9527	4.0e-02
Hardy	0.5183	1.2e-01	0.9292	7.0e-03	0.6266	6.4e-02	0.9825	1.1e-03	0.6435	5.3e-02	0.9882	6.4e-04
Jefferson	0.7088	1.2e-01	0.6246	1.4e-01	0.7836	7.5e-02	0.9455	2.6e-02	0.7374	8.2e-02	0.9540	4.2e-02
Mineral	0.4988	9.9e-02	0.3877	1.9e-01	0.5427	8.2e-02	0.9492	2.1e-02	0.5347	6.1e-02	0.9603	2.2e-02
Monroe	0.8445	5.8e-02	0.5690	7.2e-02	0.8408	6.4e-02	0.9327	3.1e-02	0.8486	4.9e-02	0.9728	1.2e-02
Morgan	0.5865	1.4e-01	0.4059	2.4e-01	0.6566	9.8e-02	0.9435	3.4e-02	0.6156	1.0e-01	0.9635	2.4e-02
Pendleton	0.4451	1.4e-01	0.9370	4.6e-03	0.4472	9.0e-02	0.9850	1.0e-03	0.4003	8.8e-02	0.9898	6.1e-04
Preston	0.8599	2.5e-02	0.7490	8.1e-02	0.9442	9.6e-03	0.9584	1.2e-02	0.9498	1.2e-02	0.9776	6.6e-03
Tucker	0.9011	3.7e-02	0.5806	1.5e-01	0.9044	3.2e-02	0.9254	3.9e-02	0.9278	2.4e-02	0.9743	8.9e-03

TABLE V
SCALE-UP STUDY: NSGA-III'S EXIT GENERATION FOR ALL COUNTIES IN WEST VIRGINIA.

County	Berkl.	Grant	Hmpsh.	Hardy	Jefrs.	Minr.	Monr.	Morg.	Pndtl.	Prstn.	Tuck.
Individual	18 ± 3.1	17 ± 2.8	57 ± 110	17 ± 3.4	48 ± 36	162± 290	71 ± 61	168 ± 310	16 ± 2.8	48 ± 15	60 ± 52
Small-size	15 ± 2.4			315 ± 350			139 ± 280			15 ± 2.4	
Medium-size	23 ± 3.5						115 ± 230				
Big-size	21 ± 3.8										

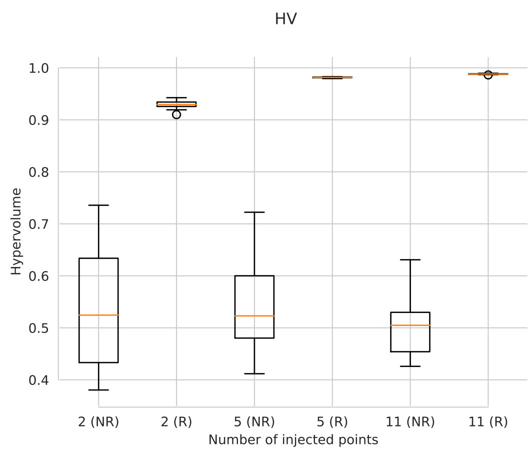

Fig. 5. Berkeley County: Boxplots considering the original constrained approach (no repair, denoted with NR) vs the violation repair operator (R), indicating that NSGA-III with repair works much better than without repair.

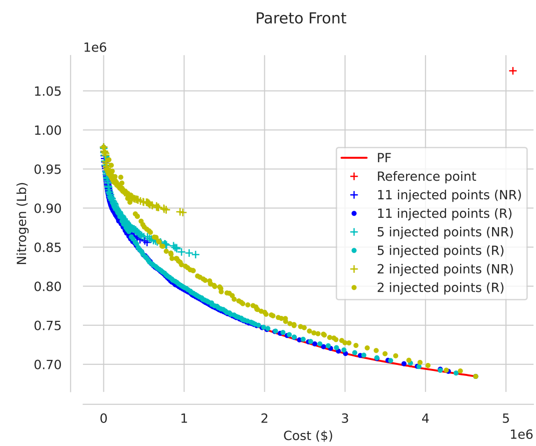

Fig. 6. Berkeley County: Not repair (NR) vs. repair operator (R). Repair operator helps in reaching a more diverse set of points.

not have a monotonic increasing trend. The results clearly show a transition phase. First, it becomes more challenging as the targeting areas are scarce. However, when more counties are added, there is a break-point with enough target areas to apply BMPs, and the problem starts relaxing. Hampshire is difficult to solve, but when Berkeley and Grant are added, the problem becomes more accessible as NSGA-III, requires fewer iterations to solve it. While Hampshire country demography makes the optimization challenging to reduce the nitrogen level with a small cost, the addition of neighboring counties takes the load and helps solve the combined problem faster. Interestingly, we observe this phenomenon in other groups as well. Nevertheless, handling a 153,818 variable problem within an average of 21 generations of our proposed NSGA-III approach is remarkable and shows promise for our approach to be applied to multiple counties to the watershed level.

D. "Innovized" Principles

Table VI shows the results of inspecting the number of non-used variables – BMPs which are assigned a small percentage of usage (10% or less used here) for a triplet. We count all variables across the population and determine the percentage of variables having a small usage in the initial population, the injected set of points, and the final non-dominated population.

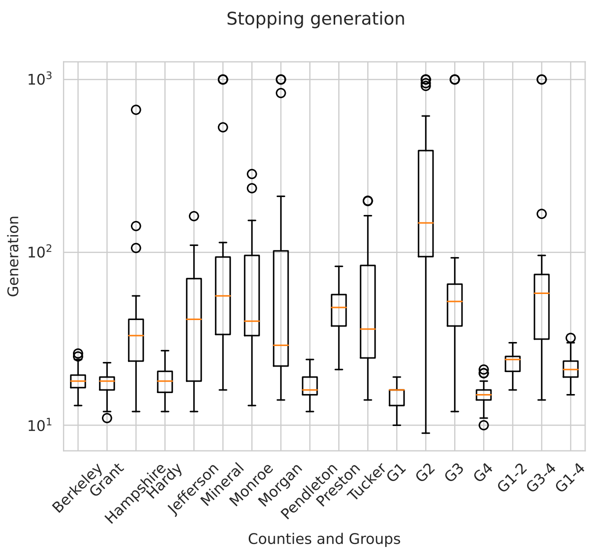

Fig. 7. Scale-up results covering 1,012 to 153,818 variables.

The table clearly shows that populations initialized at random do not have coinciding variables less than 0.1, meaning that every initial solution utilizes almost every BMP in every LRS by every agency and every load source. Such a solution is usually not cost-effective and challenging from the implementation point of view. On the other hand, the injected points show a bias, where 90% of the variables have a negligible value across the population. Such a bias helped NSGA-III to start its search in a better way. Finally, the non-dominated population of NSGA-III uses only a few BMPs.

Three counties/scale (Monroe, Tucker, and G1) use more BMPs (less number of negligible BMP usage) in their final solution compared to IPOPT solutions, indicating that intermediate trade-off NSGA-III solutions need a more diverse set of BMPs to have a cost-nitrogen compromise in these counties.

E. Achieved Solutions

Figure 8 shows the graphical representation of three different solutions taken from the non-dominated produced by our approach. To ease the graphical representation of our solutions, we colored the area of each land-river-segment proportionally regarding the BMPs selected to be applied to them. Therefore, if only one single BMP is selected to be applied on a given land-river-segment, then the whole area will be colored with a single color. Similarly, if the proposed approach selects different BMPs to be applied to a given land-river-segment, the total area will be colored proportionally regarding each associated BMP. However, to avoid showing tiny coverage area of a BMP, we gathered few BMPs together and show the cluster with a single color. This developed graphical representation might ease the comprehension of the BMPs and their geographical application.

In the figure, we presented three different efficient solutions. The first two (selected solutions 1 and 2) come from minimal cost region and are very similar regarding the BMPs. For both cases, our approach selected the two BMPs with the best cost/benefit for this area: Off Stream Watering Without Fencing and Nutrient Management Plan High-Risk Lawn. However, for achieving reduced nitrogen level, the third solution uses more efficient BMPs, despite their higher cost. Solution 3 uses 17 different BMPs. A visual comparison of these maps clearly indicate that irrespective of cost-nitrgen trade-off, certain BMPs are always allocated to certain land-river-segments. They are the invariants of the state-wide or watershed-wide BMP allocations, which would stay as vital knowledge about efficient management policies. In addition, the multi-objective approach produces a set of non-dominated solutions that allow the decision-makers to choose a preferred one from a myriad of options.

V. Conclusions

In this extensive study, we have considered a mathematical model of the Chesapeake Bay Watershed management problem and attempted to find Best Management Practice (BMP) allocation to improve water quality by minimizing nitrogen content and minimizing the cost of BMP implementation. We have chosen West Virginia state and provided results at the county, multi-county, and state levels. They have involved 1,012 to 158,818 real-parameter linked variables and 144 to 20,509 constraints, making it as one of the largest practical problems solved using an evolutionary algorithm. The scalability has been achieved due to following modifications to the base NSGA-III procedure: (i) a set of good mixed-integer programming (IPOPT) solutions are injected at the initial population, and (ii) linear constraints are repaired to make population members feasible. The following important conclusions are made: (i) injection of more IPOPT solutions produces faster convergence of NSGA-III procedure, (ii) grouping of certain counties together for optimization help find efficient solutions faster than optimizing for a single county alone, (iii) the proposed customized NSGA-III's time to converge to a specific hypervolume level does not increase with the addition of counties, and (iv) the final solutions use only 10% or less BMP options to produce a cost-nitrogen trade-off for most counties. These initial findings are extremely encouraging for us to launch a more extensive optimization study at the watershed level including phosphorous and sediment objectives and also using a more realistic simulation-based evaluation procedure.

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TABLE VI

PERCENTAGE OF INSIGNIFICANT VARIABLE VALUES IN FINAL SOLUTIONS. A LARGE PERCENTAGE MEANS FEWER DISTINCT BMP USAGE.

County	Berkl.	Grant	Hmpsh.	Hardy	Jefrs.	Minr.	Monr.	Morg.	Pndtl.	Prstn.	Tuck.	G1	G2	G3	G4	G{1-2}	G{3-4}	G{1-4}
Rand Pop.	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Inj. Pts.	90.1	88.2	90.9	94.3	95.4	92.8	92.4	90.7	91.5	95.6	91.9	91.5	95.4	91.7	94.8	92.8	91.9	88.8
Non-dom Pop.	90.7	89.2	91.3	94.6	97.6	94.2	36.5	91.3	92.2	96.9	21.0	39.2	97.6	92.9	94.6	93.5	92.9	91.0

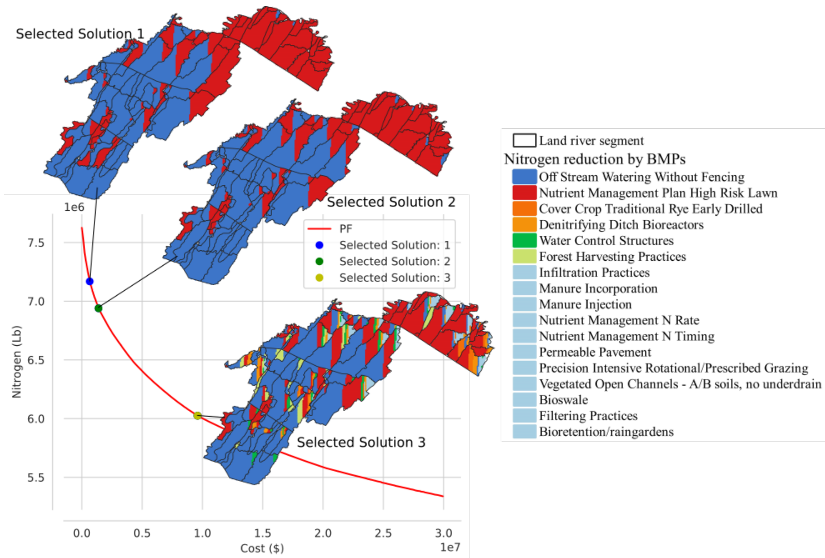

Fig. 8. Example of solutions produced by our proposed approach.

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