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Water Evaporation Optimization: A novel physically inspired optimization algorithm

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ABSTRACT

In this paper a novel physically inspired non-gradient algorithm is developed for solution of global optimization problems. The algorithm being called Water Evaporation Optimization (WEO) mimics the evaporation of a tiny amount of water molecules on the solid surface with different wettability which can be studied by molecular dynamics simulations. WEO is tested and analyzed in comparison to other existing methods on three sets of continuous test problems, a set of 17 benchmark unconstrained functions (consisting of three types of functions: unimodal, multimodal, and shifted and rotated functions), a set of 13 classical benchmark constraint functions, and three benchmark constraint engineering problems, reported in the specialized literature. The results obtained indicate that the proposed technique is highly competitive with other efficient well-known metaheuristics. The features used in WEO are analyzed and its potential implications for real size constrained engineering optimization problems are discussed in details.

1. Introduction

Metaheuristic algorithms are a widely studied field in artificial intelligence in terms of: applying to a wide variety of combinatorial optimization problems, improving the current algorithms, and generating novel ones. The primary reason for this is their ability to reach near global optimums in a reasonable time for non-smooth problems in which gradient information are not available or not reliable.

In the recent decades, many metaheuristics with different philosophy and characteristics are developed and applied to a wide range of fields which can be categorized into three separate classes in terms of how they have been inspired [1]:

(i) Evolutionary algorithms. These methods use techniques that imitate natural evolution. Of these, John Holland's Genetic Algorithm (GA) [2], and Rechenberg and Schwefel's Evolutionary strategies (ES) [3] enjoyed more attention.
(ii) Physical algorithms. These methods inspired by the physical laws. Of these, Simulated Annealing (SA) algorithm of Kirkpatrick et al. [4] mimics the annealing process used in materials science, Tabu Search (TS) method of Glover [5] utilizes a short term memory of the specific changes of recent moves within the search space and preventing future moves from undoing those changes, and Harmony Search (HS) algorithm of Geem et al. [6] that mimics the evolution of a harmony relationship between several sound waves of differing frequencies when played simultaneously, have been accepted as most prevalent algorithms.
(iii) Swarm algorithms. These methods imitate the processes of decentralized, self-organized systems, which can be either natural or artificial in nature. Of these, Ant Colony Optimization (ACO) algorithm of Dorigo et al. [7] which follows the processes of an ant colony searching for food, Kennedy and Eberhart's Particle Swarm Optimization (PSO) algorithm [8] that mimics animal flocking behaviors, and Karaboga's Artificial Bee Colony (ABC) algorithm [9] that is inspired by the food foraging behavior of honey bee swarms, considered as prevalent swarm algorithms.

In recent years many novel algorithms are developed and applied to different multidisciplinary optimization problems which can be categorized in one of the three classes mentioned in the previous paragraph. Some of these methods are listed at the following: Glowworm Swarm Optimization (GSO) [10], Firefly Algorithm (FA) [11], Monkey Search (MS) [12], Cuckoo Search (CS) [11], Bat Algorithm (BA) [11], Krill Herd (KH) Algorithm [13], Grey Wolf Optimizer (GWO) [14], Bird Mating Optimizer (BMO) [15], and Social Spider Optimization (SSO-C) [16] which can be

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considered as swarm algorithms. Intelligent Water Drops (IWD) algorithm [17], Imperialist Competitive Algorithm (ICA) [18], League Championship Algorithm (LCA) [19], Gravitational Search Algorithm (GSA) [20], Galaxy-based Search Algorithm (GbSA) [21], Spiral Optimization (SO) [22], Teaching–Learning-Based Optimization (TLBO) [23], Big-Bang Big-Crunch (BB-BC) algorithm [24], Water Cycle Algorithm (WCA) [25], Golden Ball (GB) algorithm [26], and Group Counseling Optimizer (GCO) [27] which can be considered as physical algorithms.

In the past decade, the first author and his students developed three novel physical algorithms and one novel swarm based algorithm besides many successful modified and hybridized algorithms [28–30]. These novel studies contain Charged System Search algorithm (CSS) algorithm [31], Ray Optimization algorithm (RO) [31], Dolphin echolocation optimization (DEO) [32] and Colliding Bodies Optimization (CBO) algorithm [33]. A comprehensive review on these methods and their applications can be found in [34,35].

As it is clear generating novel metaheuristic algorithms is an interesting subject in the field of optimization. The main objective of this paper is to develop a new physically based metaheuristic to solve global optimization problems. This new metaheuristic is a multiple population based algorithm, and it is called as Water Evaporation Optimization (WEO).

WEO mimics the evaporation of a tiny amount of water molecules adhered on a solid surface with different wettability which can be studied by molecular dynamics simulations. The evaporation of water is very important in biological and environmental science [36,37]. Based on the molecular dynamics simulations [38] it is well-known that, as the surface changed from hydrophobicity to hydrophility, the evaporation speed does not show a monotonically decrease from intuition, but increases first, and then decreases after reaching a maximum value. When the surface wettability of the substrate is not high enough, the water molecules accumulate into the form of a sessile spherical cap. The predominant factor that affects the evaporation speed is the geometry shape of the water congregation. Meanwhile when the surface wettability of the substrate is high enough, the water molecules spread to a monolayer and the geometric factor no longer affects much and the energy barrier provided by the substrate instead geometry shape, affects the evaporation speed.

Based on the previous paragraph the reader can see a fine analogy between this type of water evaporation phenomena and a population based metaheuristic algorithm. Water molecules are considered as algorithm individuals. Solid surface or substrate with variable wettability is reflected as the search space. Decreasing the surface wettability (substrate changed from hydrophility to hydrophobicity) reforms the water aggregation from a monolayer to a sessile droplet. Such a behavior is consistent with how the layout of individuals changes to each other as the algorithm progresses. And the decreasing wettability of the surface can represent the decrease of objective function for a minimizing optimization problem. Evaporation flux rate of the water molecules is considered as the most appropriate measure for updating the individuals which its pattern of change is in good agreement with the local and global search ability of the algorithm and can help us to develop the WEO with significantly well converged behavior and simple algorithmic structure.

WEO is tested and analyzed on three sets of test problems, a set of 17 benchmark unconstrained functions consisting of three types of functions: unimodal, multimodal, and shifted and rotated functions, a 13-fold classical benchmark constraint problems, and three benchmark constraint engineering problems reported in the specialized literature. The most effective available state-of-the-art metaheuristic optimization methods based on the author's knowledge are used here as the basis of the comparisons. The optimization results demonstrate the efficiency and competitive performance of the WEO.

The rest of this paper is organized as follows. Section 2 deals with analogy between WEO and the evaporation of a tiny amount of water on the solid surface with varying wettability which can be inferred by molecular dynamics simulation. Section 3 develops the novel proposed WEO algorithm in detail. Section 4 investigates the parameter settings and the search behavior of the WEO in depth and experimentally validates the WEO and compared to the most effective available state-of-the-art metaheuristic optimization methods on three test cases. Conclusions are derived in Section 5.

2. Analogy between water evaporation and population-based optimization

2.1. Molecular dynamics simulations for water evaporation

The evaporation of water is very important in biological and environmental science. The water evaporation from bulk surface such as a lake or a river is different from evaporation of water restricted on the surface of solid materials. Water evaporation of bulk surface is a classical topic and has been studied for long time [37,39] and is not the topic of this study. Recent works show that the nanoscale confined water and water restricted on the surface of solid materials is ubiquitous in nature [40], and this type of water evaporation is essential in the macroscopic world such as the water loss through the surface of soil [41]. Lee et al. [42] have used scanning electric microscope to study the evaporation efficiency of micro-scaled water droplet from nanoporous micro cantilevers of various hydrophobicity and stated that the dynamics of water evaporation between hydrophobic and hydrophilic conditions are very different. Wang et al. [38] presented Molecular Dynamics (MD) simulations on the evaporation of nanoscale water aggregation on a solid substrate with different surface wettability at room temperature to find out how the surface wettability affects the evaporation of the tiny water aggregation. At the following their simulation result is outlined which is considered as an effective essence to develop the present WEO algorithm.

MD simulations were carried out in a box with predefined dimensions. The substrate contained equal positive and negative charges, and is neutral. By changing the value of charge (q), a substrate with tunable surface wettability can be obtained. Initially, the fixed number of water molecules was piled upon the substrate in a water cube form as shown in Fig. 1(a). In the simulation, q is sampled from 0 to 0.7e with an increment of 0.1e. The simulations show that the water spreads smoothly on the substrate when $q \geqslant 0.4e$ (Fig. 1(c)). When $q < 0.4e$, the water shrinks gradually into a sessile droplet like a spherical cap as q decreases (Fig. 1(b)). In this phase, the contact angle can be affected by the amount of

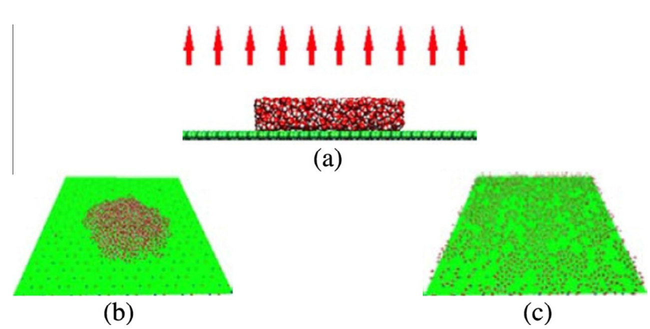

Fig. 1. (a) Side view of the initial system; (b) snapshot of water on the substrate with low wettability (q = 0e); (c) snapshot of water on the substrate with high wettability (q = 0.7e) [38].