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Three decades of the Shuffled Complex Evolution (SCE-UA) optimization algorithm: Review and applications

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Abstract. The Shuffled Complex Evolution (SCE-UA) method developed at the University of Arizona is a global optimization algorithm, initially developed by Duan et al. [Duan, Q., Sorooshian, S., and Gupta, V. "Effective and efficient global optimization for conceptual rainfall-runoff models", *Water Resources Research*, **28**(4), pp. 1015-1031 (1992)]. for the calibration of Conceptual Rainfall-Runoff (CRR) models. SCE-UA searches for the global optimum of a function by evolving clusters of samples drawn from the parameter space, via a systematic competitive evolutionary process. Being a general-purpose global optimization algorithm, it has found widespread applications across a diverse range of science and engineering fields. Here, we recount the history of the development of the SCE-UA algorithm and its later advancements. We also present a survey of illustrative applications of the SCE-UA algorithm and discuss its extensions to multi-objective problems and to uncertainty assessment. Finally, we suggest potential directions for future investigation.

1. Introduction

The performance of Conceptual Rainfall-Runoff (CRR) models when representing the physical flow of water through the land phase of the earth system depends on the adequacy of the parameter estimation (calibration) of these models [1]. A conceptual rainfall-runoff model f can be "parametrically" expressed as:

$$\mathbf{Y} = f(\mathbf{X}, \boldsymbol{\theta}) + \epsilon, \tag{1}$$

where $\mathbf{Y}$ is the model output, ϵ represents the modeling error, $\mathbf{X}$ represents the system inputs, and $\boldsymbol{\theta}$ represents the tunable parameters of the model. In general, model calibration is carried out by searching for a set of parameters $\boldsymbol{\theta}$ that optimize the value(s) of some metric(s) that quantify the performance of the model [2]. Due to the difficulties of performing such calibration manually, in the 1960s and 1970s, researchers began investigating the possibility of developing automated approaches [2]. Before the 1990s, a number of "local-type" direct search methods were tested [3], due mainly to the fact that such methods do not require explicit information about the gradient of the response surface [4], but instead rely upon function information systematically collected

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from the parameter space during the search procedure [5]. However, such local-type methods were found to be unsuitable for tuning the parameters of highly complex and nonlinear models due, in part, to the multimodal nature of their function response surface, which are theoretically hard or nearly impossible to analyze their equations [5,6].

One of the more successful (in a relative sense) local-type methods was the Downhill Simplex Method (DSM) [3] and a natural suggestion for dealing with multimodality was to implement a multi-start version (multi-start simplex or MSX), which ran several trials of the DSM method staring at multiple independent randomly selected starting points [6]. However, the independence of such DSM runs is inefficient and a large number of restarts is required for high dimensional problems [6]. This inefficiency stems from the lack of communication among the independent DSM searches. As explained by Duan et al. [6], this is similar to asking multiple people to solve the same difficult problem without sharing information and the inefficiency can be resolved by allowing them to alternate between working independently for some period of time and working together to share their findings. The Shuffled Complex Evolution (SCE-UA) method developed at the University of Arizona [1,6] is based on this idea.

The SCE-UA method integrates the strengths of several effective global optimization concepts. It employs both deterministic search strategies and random elements to enable the algorithm to simultaneously benefit from topological response surface information collected during the search. Further, it employs a clustering strategy to focus the search towards regions that tend to be more favorable, while using a version of the DSM search strategy to evolve the population towards the global solution [1]. Since its development, the SCE-UA algorithm has attracted a great deal of attention from scientists and practitioners in various fields of study, especially in water resources management and hydrology [7].

In this paper, we recount the history of development and application of the SCE-UA algorithm over the past three decades. The rest of this paper is organized as follows. In Section 2 we detail the SCE-UA algorithm and summarize some of its extensions and developments. Section 2 also reviews multi-objective and parameter uncertainty assessment tools that were further developed based on SCE-UA concept. Section 3 summarizes the application of the SCE-UA and its extensions to various optimization and calibration problems. Section 4 outlines the potential directions for further investigations. Section 5 concludes the paper.

2. Development

2.1. Single-objective optimization

The SCE-UA method is a general-purpose [2] direct search population-based global optimization algorithm that combines the concepts of complex shuffling [6] with the strengths of DSM [8], controlled random search [9], and competitive evolution [10] to solve a broad class of optimization problems [1]. The algorithm has a simple structure and only few parameters that need to be tuned by the user. Optimization begins by sampling a population of points $\boldsymbol{\theta}_i = [\theta_i^1, ..., \theta_i^n]$ uniformly from the feasible parameter region $\Theta \subset \mathbb{R}^n$. These points are clustered into κ complexes each having m members. An iterative evolution procedure is carried out by sampling q points from each complex to form a sub-complex that is then evolved α times using the DSM strategy. This evolutionary process is repeated β times for each complex, after which the complexes are shuffled to share the information obtained by each during the evolution process. The pseudo code of these steps is outlined in Algorithm 1. As mentioned above, the performance of SCE-UA depends on a small number of algorithm parameters that need to be specified by the user, for which [11] recommended using the default values: $\alpha = 1$, $\beta = 2n+1$, $m = 2n+1$, and $q = n+1$ with n being the dimension of the problem.

The SCE-UA algorithm employs a process called Competitive Complex Evolution (CCE) as its search engine. CCE evolves each complex C^j, $j = 1, ..., \kappa$, through β steps, with its reflection and contraction steps being based on the DSM method [8]. If these

1: Initialize κ, m and $s = \kappa m$
2: Sample $\{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_s\}$, where $\boldsymbol{\theta}_i \in \Theta$
3: Calculate function values $f_i = f(\mathbf{X}, \boldsymbol{\theta}_i) \quad i = 1, \ldots, s$
4: Sort f_i s.t. $k \leftarrow i$ and $f_1 \leq f_2 \leq f_k \leq f_{k+1} \cdots$
5: $\mathbf{D}^0 = \{(\boldsymbol{\theta}_k, f_k), k = 1, \ldots, s\}$
6: Construct complexes $C^j, j = 1, \ldots, \kappa$ s.t. $C^j = \{(\boldsymbol{\theta}_k, f_k) \in \mathbf{D}^0 | k = (j-1)m+1, \ldots, jm\}$
7: **While** Convergence Criteria **do**
8:     **For** $j = 1 : \kappa$ **do**
9:         Evolve C^j using CCE (Algorithm 2)
10:     **End for**
11:     $\mathbf{D}^l \leftarrow \mathbf{D}^{l+1}$
12:     Go to 6
13: End While

Algorithm 1. Shuffled Complex Evolution (SCE-UA).

Initialization: $2 \leq q \leq m$, $\alpha \geq 1$ and $\beta \geq 1$
For $b = 1 : \beta$ **do**
Assign probability $p_k = \frac{2(m+1-k)}{m(m+1)}$ to each component k in the complex C^j
Randomly select q individuals as *parents* according to p_k
Sub-complex $B^j := \{(u_{\underline{k}}, v_{\underline{k}}) | \underline{k} = 1, \dots, q\}$
Location index set $L^j := \{\underline{l} \in [(j-1)m+1, jm] | (u_{\underline{k}}, v_{\underline{k}}) = (\boldsymbol{\theta}_{\underline{l}}, f_{\underline{l}})\}$
For $a = 1 : \alpha$ **do**
Sort B^j s.t. $v_{\underline{k}}$ are in ascending order
Compute the centroid g:

$$g = \frac{1}{q-1} \sum_{\underline{k}=1}^{q-1} u_{\underline{k}}$$

Compute *reflection* step $\mathrm{r} = 2g - \mathrm{u}_q$
If $\mathrm{r} \in \Theta$ **then**
Compute $f(\mathrm{r})$ and go to 18
Else
Compute the smallest hypercube $H \subset \mathbb{R}^n$ s.t. $C^j \in H$
Randomly sample $\mathrm{z} \in H$
Compute $f(\mathrm{z})$
$\mathrm{r} \leftarrow \mathrm{z}$ and $f(\mathrm{r}) \leftarrow f(\mathrm{z})$
If $f(\mathrm{r}) < f(\mathrm{u}_q)$ **then**
$\mathrm{u}_q \leftarrow \mathrm{r}$ and go to 29
Else Compute *contraction* step $\mathrm{c} = \frac{g+\mathrm{u}_q}{2}$ and $f(c)$
If $f(\mathrm{c}) < f(\mathrm{u}_q)$ **then**
$\mathrm{u}_q \leftarrow \mathrm{c}$ and go to 29
Else
Randomly sample $\mathrm{z} \in H$
Compute $f(\mathrm{z})$
$\mathrm{u}_q \leftarrow \mathrm{z}$
End if
End if
End if
End for
End for

Algorithm 2. Competitive Complex Evolution (CCE).

steps fail to improve the worst point in the sub-complex, the algorithm randomly generates a new location within the smallest hypercube $H \subset \mathbb{R}^n$ that contains all the individuals within the complex C^j. The pseudo code of the CCE process is presented in Algorithm 2.

The SCE-UA algorithm has been successfully applied to a broad range of optimization problems. Its success has spawned a number of extensions to further enhance its performance and extend its applicability. Examples include the Shuffled Frog Leaping (SFL) algorithm, introduced to solve discrete optimization problems [12], that employs a local search method similar to Particle Swarm Optimization (PSO) [13] as the search core. Other studies have replaced or adapted the DSM search strategy with other search methods such as Differential Evolution (DE) [14].

Extensions of SCE-UA have not been limited only to the hybrid algorithms mentioned above. Several investigations have shed light on the potential for further developments to the performance and structure of SCE-UA. The shuffled complex with principal components analysis (SP-UCI) method, developed at the University of California, Irvine, was proposed to overcome the problem of *population degeneration* in high-dimensional problems, which occurs when the search population spans only a subspace of the search domain and cannot effectively search the whole problem space [15]. To address this issue, the SP-UCI algorithm monitors the dimensions of the population using principal component analysis and restores the missing ones [15]. Further, it uses a Modified Competitive Complex Evolution (MCCE) module that follows all the steps of the DSM method except the *shrink* [15], and replaces the mutation step with multi-normal sampling within the sub-complex. SP-UCI also performs multi-normal resampling after the complexes are shuffled to overcome local roughness.

Recently, Naeini et al. [7] proposed a new version of SCE-UA, titled Shuffled Complex Self Adaptive Hybrid Evolution (SC-SAHEL), which extended the competitive evolution concept to incorporate several search strategies. This approach includes a number of different evolutionary algorithms as search cores and follows an *award and punishment* concept to allocate the complexes to different search methods, thereby adaptively updating itself during the course of the search to find the search method most suitable for the problem at hand [7]. The SC-SAHEL algorithm increases methodological flexibility by using different evolutionary algorithms as search cores and provides an arsenal of tools for initial sampling and boundary handling. Developments and extensions of the SCE-UA algorithm are not limited to the single-objective methods. In the next two subsections, we review the tools which were developed on the basis of SCE-

UA architecture in order to tackle multi-objective optimization problems and to address parameter uncertainty.

2.2. Multi-objective optimization

The original SCE-UA algorithm was developed to address single-objective optimization problems. Later, Yapo et al. [16] extended the method to address multi-objective optimization problems by developing the Multi-Objective Complex Evolution (MOCOM-UA) algorithm at the University of Arizona. MOCOM-UA was introduced to solve the so-called a posteriori optimization problems, in which prior information about the decision making process in the form of weighting preferences among a set of the problem-specific performance metrics, was not available [17]. In such problems, the solution is not unique and improving any one of the performance metrics can be achieved only at the expense of the deterioration of one or more metrics [16]. The goal of multi-objective optimization is, therefore, to converge to the set of solutions known as the *Pareto optimal* set [16], in which none of the solutions can be deemed superior to any other without bringing additional information to bear [18]. The Pareto optimal set is found based on the Pareto dominance concept [17]. The search for the Pareto optimal set ρ^* for a multi-objective minimization problem ($\min_\theta \mathbf{F}(\mathbf{X},\boldsymbol{\theta}) = \{f_1(\mathbf{X},\boldsymbol{\theta}), ..., f_M(\mathbf{X},\boldsymbol{\theta})\}$) depends on the concept of Pareto dominance [16,17]:

$$\rho^* = \{\boldsymbol{\theta}^* \in \Theta |\ \nexists\ \boldsymbol{\theta} \in \Theta,\ \mathbf{F}(\mathbf{X},\boldsymbol{\theta}) \prec \mathbf{F}(\mathbf{X},\boldsymbol{\theta}^*)\}, \tag{2}$$

where dominance ($\prec$) is defined as:

$$\mathbf{F}(\mathbf{X},\boldsymbol{\theta}) \prec \mathbf{F}(\mathbf{X},\boldsymbol{\theta}^*) \longleftrightarrow \forall\ i = 1,\dots,M$$

$$f_i(\mathbf{X},\boldsymbol{\theta}) \leq f_i(\mathbf{X},\boldsymbol{\theta}^*)\ \&\ \exists\ j\ f_j(\mathbf{X},\boldsymbol{\theta}) < f_j(\mathbf{X},\boldsymbol{\theta}^*). \tag{3}$$

Subsequently, *Pareto front*, $\mathcal{F}\rho^*$, can be expressed as:

$$\mathcal{F}\rho^* = \{\mathbf{F}(\mathbf{X},\boldsymbol{\theta})\ |\ \boldsymbol{\theta} \in \rho^*\}. \tag{4}$$

The MOCOM method modifies the SCE-UA algorithm to employ a *Pareto ranking* concept [19], which starts by identifying all the non-dominated individuals within a population and ranks these individuals as *one*. These points are then removed from the population and the process is repeated to find the second group of non-dominated points, which are ranked as *two*. The process is repeated until all the points in the population have been ranked. Hence, the points with the smallest rank are those (within the population) that are closest to the Pareto optimal set [16]. Competitive evolution is then carried out based on the rank of the individuals; in other words, MOCOM effectively converts the multi-objective problem to a single-objective one by replacing the set of multi-objective performance criteria by a rank ordering criterion to determine the improvement direction(s).

The MOCOM-UA algorithm employs a concept called the Multi-Objective Simplex (MOSIM) as its search engine to evolve the complexes towards the Pareto optimal set, terminating when all of the individuals in the population become non-dominated, i.e., all are of rank one [16]. The goal of the evolution process is to generate successors that are, on average, better than their corresponding predecessors. Let us denote $R = \{r_i\}_{i=1}^s$ as the set of Pareto ranked individuals and define $R_{max} = \arg\max_{1 \leq i \leq s} r_i$. MOCOM-UA forms the subcomplexes according to the rank of individuals. Algorithm 3 presents the evolutionary strategy of MOCOM-UA.

Weakness of the original MOCOM-UA algorithm, mainly in the MOSIM search engine, have led to the development of several other multi-objective optimization frameworks that use the SCE-UA framework. For example, Yang et al. [20] proposed a multi-objective complex evolution method with PCA and crowding distance operator (MOSPD) to overcome the clustering tendency of non-dominated solutions and premature convergence phenomenon. Also, Guo et al. [21] proposed the Multi-Objective Shuffled Complex Differential Evolution (MOSCDE) method, which employed differential evolution as the search engine. Meanwhile, the SFL algorithm has also been extended to handle multi-objective problems in several other studies [22].

Given n, $\mathbf{D}$ (recall Step 5 Algorithm 1), s, R and R_{max}
Assigning the selection probability:

$$P_i = \frac{R_{max} - r_i + 1}{\left(R_{max}+1\right)s - \sum_{i=1}^s r_i}, \quad i = 1,\dots,s$$

Construct $\mathbf{A} = \{\boldsymbol{\theta}_i \in \mathbf{D}|\ r_i = R_{max}\}$ with $\mathrm{n}_{\mathbf{A}} = |\mathbf{A}|$
While $j < \mathrm{n}_{\mathbf{A}}$ **do**
    $\Delta_j = \{\boldsymbol{\theta}_j \in \mathbf{A}\} \cup \{\boldsymbol{\theta}_1,\dots,\boldsymbol{\theta}_n \in \mathbf{D}|P_i, i = 1,\dots,s\ \&\ P_{(\boldsymbol{\theta}_j)} := 0\}$
end while
$\forall j$, evolve Δ_j independently using MOSIM and update $\boldsymbol{\theta}_j$
$\mathbf{A} \ni \boldsymbol{\theta}_j, j = 1,\dots,\mathrm{n}_{\mathbf{A}}$
$\mathbf{D} \leftarrow \mathbf{A}$

Algorithm 3. Complex evolution strategy in MOCOM-UA.

2.3. Parameters uncertainty assessment tools

While SCE-UA was developed mainly to find (near) optimal solution to global optimization problems, factors such as data errors and model inaccuracies result in parameter estimation errors that necessitate uncertainty assessments associated with the resulting parameter estimates. Because problem complexity in hydrological models cannot be captured using first-order approximations and Gaussian distributions, statistical simulation algorithms such as Markov Chain Monte Carlo (MCMC) have gained popularity as a class of general-purpose methods for problems involving complex inference, search, and optimization [23]. For many applications (including hydrology), the challenge is to employ MCMC samplers that exhibit fast convergence to the global optimum while maintaining adequate representation of the lower posterior probability regions in the parameter space.

Towards this end, Vrugt et al. [24] developed a modified version of the SCE-UA, entitled Shuffled Complex Evolution Metropolis (SCEM-UA), which combined MCMC sampling with shuffled complex evolution to infer the posterior distribution of the parameters. The SCEM-UA algorithm merges the strengths of the Metropolis algorithm, controlled random search, competitive evolution, and complex shuffling to continuously update the proposal distribution and evolve the sampler towards the posterior target distribution [24]. To avoid ignoring parameter regions with lower posterior density, and thereby collapsing into a small region close to the best parameter set, SCEM-UA applies a Bayesian approach in which probabilistic description regarding the unknown parameters $\boldsymbol{\theta}$ is inferred from prior knowledge of $\boldsymbol{\theta}$ and observed information about model output $\mathbf{Y}$. From Eq. (1), and using a Gaussian assumption for the residuals ϵ, the likelihood that the observed data $\mathbf{Y}$ could have been generated by the model conditioned on the parameter set $\boldsymbol{\theta}_i$ is computed as:

$$\mathcal{L}(\boldsymbol{\theta}_i|\mathbf{Y}) = \exp\left[-\frac{1}{2}\sum_{\eta=1}^{N}\left(\frac{\epsilon(\theta_i^\eta)}{\sigma}\right)^2\right]. \tag{5}$$

Vrugt et al. [24] assumed a *non-informative prior* $\mathrm{p}(\boldsymbol{\theta}) \propto \sigma^{-1}$ which followed by the posterior density:

$$\mathrm{p}(\boldsymbol{\theta}_i|\mathbf{Y}) \propto \left[\sum_{\eta=1}^{N}\epsilon(\theta_i^\eta)^2\right]^{-\frac{1}{2}N}. \tag{6}$$

In order to draw the link between Algorithm 1 and Algorithm 4, given prior density $\mathrm{p}(\boldsymbol{\theta})$, s sample points $\{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_s\}$ are generated and their corresponding posterior probabilities $\{\mathrm{p}(\boldsymbol{\theta}_1|\mathbf{Y}), \ldots, \mathrm{p}(\boldsymbol{\theta}_s|\mathbf{Y})\}$ are computed according to Eq. (6). The next step is to sort the points in *decreasing* order of posterior probability and form the set $\mathbf{D}$ (recall step 5 of Algorithm 1). Construction of the complexes follows a procedure similar to Algorithm 1. Referring to steps 7-13 of Algorithm 1, SCEM-UA replaces the evolution step 9 with a Sequence Evolution Metropolis (SEM) strategy as explained in Algorithm 4.

Vrugt et al. [25] subsequently developed a multi-objective extension of the SCEM-UA entitled Multi-Objective Shuffled Complex Evolution Metropolis (MOSCEM) based on the same evolution strategy used

1: Initialization $\mathbf{D}$ and parallel sequence S^j s.t. $S^j := \mathbf{D}_{j,\cdot}$, Likelihood ratio T, β
2: **For** $b = 1 : \beta$ **do**
3: Compute μ_{Cj} and $\sum_{Cj}$ and let $\boldsymbol{\theta}_{(t)}$ be current draw in S^j
4: Compute $\alpha^j = \frac{\mu_{Cj}}{\mu_{Sj}}$
5: **If** $\alpha^j \leq \mathrm{T}$ **then**
6: Sample $\boldsymbol{\theta}_{(t+1)} \sim \mathbf{N}(\theta_{(t+1)}, c_n^2 \sum^j)$
7: **Else** Sample $\boldsymbol{\theta}_{(t+1)} \sim \mathbf{N}(\mu^{(j)}, c_n^2 \sum^j)$
8: **End if**
9: **If** $\boldsymbol{\theta}_{(t+1)} \in \Theta$ **then**
10: Compute $p(\boldsymbol{\theta}_{(t+1)}|\mathbf{Y})$ via (6)
11: **Else** $p(\boldsymbol{\theta}_{(t+1)}|\mathbf{Y}) \leftarrow 0$
12: **End if**
13: Compute $\omega = \mathrm{p}(\boldsymbol{\theta}_{(t+1)}|\mathbf{Y})/\mathrm{p}(\boldsymbol{\theta}_{(t)}|\mathbf{Y})$ and draw $z \sim U[0,1]$
14: **If** $\omega \geq z$ **then**
15: $C_{1,\cdot}^j \leftarrow \boldsymbol{\theta}_{(t+1)}$
16: **Else** $\boldsymbol{\theta}_{(t+1)} \leftarrow \boldsymbol{\theta}_{(t)}$ and $S^j = [S^j; \boldsymbol{\theta}_{(t+1)}]$
17: **End if**
18: Compute $\Gamma^j = \frac{\mu_{C_{1,1}^j}}{\mu_{C_{m,1}^j}}$
19: If $\Gamma^j \leq \mathrm{T}$ & $\mathrm{p}(\boldsymbol{\theta}_{(t+1)}|\mathbf{y}) \leq \mathrm{p}(\mu_{C_{m,1}^j}|\mathbf{y})$ **then** go to 21
20: **Else** $C_{m,\cdot}^j \leftarrow \boldsymbol{\theta}_{(t+1)}$
21: **End if**
22: **End for**

Algorithm 4. Sequence Evolution Metropolis (SEM) strategy in SCEM-UA.

in SCEM-UA. The main difference is the replacement of the single-objective posterior probability with a multi-objective fitness assignment concept [26]. Major reasons for development of this extension were that (i) the MOCOM-UA method failed to represent the tails of Pareto front, as its non-uniform approximation of the Pareto front resulted in a concentrated solution in the compromise region between the objectives, and (ii) the MOCOM-UA evolution strategy failed to converge to the true Pareto optimal set for problems with highly correlated performance criteria and large number of parameters [25]. In a later development, Vrugt et al. [27] developed the Differential Evolution Adaptive Metropolis (DREAM) algorithm to maintain ergodicity and detailed balance, thereby providing better estimation of the posterior distribution [28].

3. Applications of SCE-UA and its descendants

In this section, we look into the diverse applications of the SCE-UA family in different fields. According to the Web of Science (a.k.a web of knowledge), at the time of submitting this manuscript, the original SCE-UA papers [1,6] have been cited by over 2400 documents excluding the self-citations, and MOCOM-UA [16], SCEM-UA [24], and MOSCEM-UA [25] have over 500, 600, and 300 independent citations, respectively. To relatively compare application domains of SCE-UA and its extensions, a sample statistic is calculated and shown in Figure 1. The figure shows the top 10 research fields with the highest contributions to the total number of independent citations for the SCE-UA papers [1,6] by dividing the total number of citing references in that field by the total number of independent citations for each algorithm. As these fields may overlap, the sum of these percentages is larger than 100 percent. Figure 1 reveals that the original SCE-UA papers and its decedents are mostly cited in water resources domain, while engineering and environmental sciences are next in the ranking. Other fields, such as computer science and mathematics, have smaller but still significant contribution to the independent citations of the SCE-UA family. In this section, some of these applications are briefly presented.

3.1. Applications of SCE-UA

The SCE-UA algorithm was initially developed for the automated calibration of CRR models and has since been mostly applied to hydrologic and terrestrial models [29]. Initially, the algorithm was tested on the six-parameter SIXPAR model [6,30], which is a simplified version of the Sacramento Soil Moisture Accounting (SAC-SMA) model [31]. SIXPAR was developed mainly for theoretical and analytical studies of SAC-SMA and was not intended for practical application [32]. The model has been used to test the SCE-UA and its extensions in a number of studies [33]. Following its demonstrated success with the SIXPAR model, the SCE-UA algorithm has been widely used for parameter estimation of several other conceptual models, including the lumped SAC-SMA model [34].

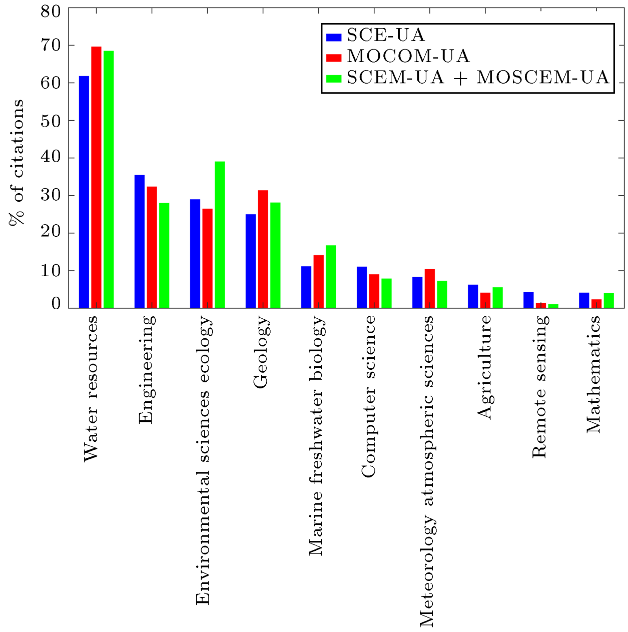

Figure 1. The current top 10 research fields with the highest contribution to the total number of SCE-UA independent citations, and the portion of citation for MOCOM-UA and combined citations for SCEM-UA and MOSCEM-UA for these categories according to the web of science.

Over the past several decades, the SCE-UA has also served as a performance benchmark against which other algorithms such as the Genetic Algorithms (GA) and Simulated Annealing (SA) [35] have been compared. These studies have revealed the robustness and efficiency of the SCE-UA for calibrating a wide class of models [6,36], including lumped models such as Hydrologiska Byrans Vattenavdelning (HBV) [37], HYMOD [38], SIMHYD [39], Xinanjiang [40], and PRMS [41] as well as distributed models such as coupled routing and excess storage Hydrology Laboratory Research Distributed Hydrologic Model (HL-RDHM) [42], coupled routing and excess storage (CREST) [43], Soil & Water Assessment Tool (SWAT) [44], and Variable Infiltration Capacity (VIC) [45] model. Some of these models and their application with the SCE-UA algorithm are listed in Table 1.

Due to its success, the SCE-UA method has been implemented within several optimization tools developed for the calibration of a variety of models. For instance, ParaSoll [46] employs SCE-UA as the core search method used for calibration of the SWAT model [47] and has been coupled with the SWAT Cal-

Table 1. Example of hydrologic models calibrated by SCE-UA.

Model	Developed by	Application
The Coupled Routing and Excess Storage (CREST)	[43]	[109,110,111,112,113]
Hydrologiska Byrans Vattenavdelning (HBV)	Swedish Meteorlogical and Hydrological Institute [37]	[114,115,116,117,118]
HYdrological MODel(HYMOD)	[38]	[96,97,119,120,121]
Système Hydrologique Européen (MIKE SHE)	DHI water & environment [122]	[123,124,125,126]
abcd	[127]	[128,129,130,131,132]
Sacramento Soil Moisture Accounting (SAC-SMA)	[31]	[84,49,133,134,120]
Six Parameter (SIXPAR)	[30]	[1,135,33]
Soil, Water, Atmosphere and Plant (SWAP)	[136]	[137,138,139,140]
Soil & Water Assessment Tool (SWAT)	[44]	[141,142,143,144,145]
Simplified Hydrology Model (SIMHYD)	[39]	[146,147,148,149,150]
Storm Water Management Model (SWMM)	Environmental protection agency [151]	[152,153,154,155]
TOPMODEL	[156]	[157,158,159,160]
Precipitation-Runoff Modeling System (PRMS)	[41]	[161,162,163,164]
Variable Infiltration Capacity (VIC)	[45]	[165,166,167,168,169]
Xinanjiang	[40]	[170,171,172,173]

ibration and Uncertainty Program (SWAT-CUP) [48]. In addition, the Multi-step Automatic Calibration Scheme (MACS) uses the SCE-UA algorithm as its optimization engine [49].

Beyond its application to hydrologic and land surface models, the SCE-UA method has been applied in other domains such as ground water [50], water quality [51], water demand [52], rating curve [53], radar rainfall [54], and stochastic rainfall models [55].

Further, it has been used to solve other kinds of optimization problems. Ketabchi and Ataie-Ashtiani [56] applied the SCE-UA to groundwater management problems and showed that it provided better solutions than those obtained using other meta-heuristic algorithms such as GA and DE. Moreover, Liong and Atiquzzaman [57] applied the SCE-UA to aid in optimal design of water distribution network and optimization of reservoir operation [58].

Beyond hydrology and water resources management, the SCE-UA framework has found numerous applications in other fields of science and engineering. In the fields of data analysis and machine learning, it has been used to calibrate the parameters of statistical distributions such as the $\mathcal{B}$eta probability distribution [59], copulas [60], Generalized Extreme Value (GEV) [61], and $\mathcal{G}$amma function [62]. It has also been used in conjunction with several machine learning algorithms including Support Vector Regression (SVR) [63], Support Vector Machine (SVM) [64], Random Forest (RF) [65], and fuzzy neural network [66]. The related SP-UCI algorithm has been used for calibrating the parameters of the Artificial Neural Networks (ANNs) [67].

Applications of SCE-UA in other fields include pavement and road design [68], optimal air traffic flow [69], earthquake and structural engineering [70], crop yield analysis [71], fluid mechanics [72], oil spill modelling [73], wireless sensor networks load optimization [74], modeling sorption in polymers [75], dielectric spectra analysis [76], astronomy [77], and many other fields [78]. These studies illustrate the wide utility of the SCE-UA algorithm and its tremendous potential for helping to solve a wide variety of classes of optimization problems.

Finally, the SCE-UA method has been adapted for use with computationally expensive models by incorporating the use of surrogate models [79] to provide lower-cost information about the nature of the objective function response surface. For instance, Wu et al. [80] employed SCE-UA with SVMs for the optimization of groundwater use, Ketabchi and Ataie-Ashtiani [81], used it with ANNs for coastal management, Gan et al. [82] coupled it with Multivariate Adaptive Regression Splines (MARS) for use with hydrologic models, and Wang et al. [83] used it with a general adaptive Gaussian Process (GP) surrogate model for optimization.

3.2. Applications of MOCOM-UA

The MOCOM-UA method has also been widely used for calibrating hydrologic and land surface models including, SAC-SMA [84,85], HYMOD [38], Biosphere-Atmosphere Transfer Scheme (BATS) [86], VIC [87], Alpine Hydrochemical Model (AHM) [88], Ecomag [89], and many other models [90]. Its applicability to multi-objective problems has enabled the investigation of uncertainty bounds of parameters for different CRR models by providing a Pareto optimal set for the parameters [91]. The MOCOM-UA and its extensions have been also used for calibrating other types of models, such as those related to the carbon cycle [92], ecohydrology [93], and the optimization of reservoir discharges [20]. Notably, MOCOM-UA has been used as the core optimization tool within the U.S. Geological Survey Modular Modelling System (MMS) for parameter estimation [94].

3.3. Applications of SCEM-UA and MOSCEM-UA

The SCEM-UA and MOSCEM-UA methods have been widely used for parameter uncertainty assessment. The SCEM-UA method has been extensively applied to hydrologic models including the SAC-SMA [95], HYMOD [96,97], MOD-HMS [98], LISFLOOD [99], HBV [100], Xinanjiang [101], TopNet [102], and Flex [103] model. Further, Blasone et al. [104] used SCEM-UA to sample the prior distribution of the parameters for Generalized Likelihood Uncertainty Estimation method (GLUE) [105] and demonstrated its superior performance in comparison with other sampling methods. The SCEM-UA enabled GLUE method has also been used for uncertainty assessment of the MIKE-SHE model [106]. In other applications, Haddeland et al. [107] used SCEM-UA to find optimal reservoir releases, while the MOSCEM-UA algorithm has been used for uncertainty assessment of several hydrologic models [25,100].

4. Future directions

As reported above, the SCE-UA algorithm has been extensively studied and applied to a wide variety of optimization problems, and has also spawned a number of descendant methodologies. However, since the time it was first introduced, there has been a rapid increase in problem complexity across all of the scientific domains, and this motivates the need for further improvements. Here, we briefly mention some potential research directions:

- The application of optimization algorithms can be severely limited by computational burden, which is closely linked to the number of model or function evaluations required. Hence, complexity of the models, and the associated function can hinder application of SCE-UA type algorithms to high dimensional problems. The use of surrogate models has been proposed by Wang et al. [83] to address this issue. Further investigations can extend the application of SCE-UA to more complex systems;
- Initial sampling and boundary handling methods can play a significant role in the performance of optimization algorithms. To-date, there have been very few studies on the effects of initial sampling and boundary handling on the performance of the SCE-UA;
- Self-adaptive search mechanisms can extend the application of the SCE-UA to a wider class of optimization problems [7]. The investigation of other adaptive procedures for implementation within SCE-UA is likely to be a productive direction for future research;
- While the SCE-UA algorithm was initially developed for continuous problems, many engineering problems deal with discrete, mixed-integer, and binary problems. Although the SFL algorithm [12] was introduced to tackle this class of problems, there is room to explore mixed-integer and binary optimization problems. The recent development of new hybrid algorithms [7] illustrates the flexibility of the SCE-UA family of methods for employing discrete, mixed-integer, and binary evolutionary methods;
- While MOCOM-UA and its extensions were developed to tackle multi-objective problems, extending the application of SCE-UA to many-objective problems (with 4 or more objective functions) needs further investigation;
- The architecture of SCE-UA makes it suitable for parallel computing. Since the complexes within SCE-UA evolve independently during each evolution loop, each complex can be assigned to a different processing unit [7]. To-date, the prospect of accelerating SCE-UA through parallel computing method has been little studied [108].

5. Conclusion

Since its introduction in 1992, the SCE-UA algorithm has been successfully applied to scientific and engineering problems ranging from water resources management to machine learning and statistics. In this paper, we reviewed the history of its development and application, and its extensions to multi-objective problems and uncertainty assessment. We showed that the methodology had found a wide range of applications to different fields of science and engineering, and explored future directions for further development. It seems clear that the SCE-UA methodology shows great potential to become more prominent in the field of optimization. In summary, its popularity is due to:

- The algorithm is simple to understand and easy to implement. This argument is supported by the widespread implementation of SCE-UA on different platforms and its application to a wide range of problems as referenced above;
- The algorithm has proven to provide more robust and efficient performance than many traditional optimization methods such as GA, DE, and SA [35,57];
- The algorithm has only a few control parameters (e.g., β, m, κ, q) that need to be tune by the user. Duan et al. [11] made suggestions for typical values of β, q, and m and these recommendations have stood the test of time.

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The senior author of this invited paper, "Prof. Sorooshian," wishes to reflect on the immense contributions of Professor Abolhassan Vafai to whom this special issue of the journal is dedicated:

"I had the honor of getting to know Professor Vafai in the early 1990's during his stop at the University of Arizona, Tucson (UAZ). He had one mission and that was to promote educational and scientific interactions between international academic institutions including those in the US. Since that first visit, Dr. Vafai tirelessly continued his mission of promoting these exchanges resulting in a number of bilateral workshops and exchanges on topics of mutual interest between the Iranian and American academics through the US and Iranian National Academies of Sciences. Looking back at this almost 30 years, many of the students in my research group, whether at UAZ or at the University of California, Irvine (UCI) whose dissertation research was related to the topic of our paper, were from Iran. I am certain that their ability to come to the US and contribute to our research in this field would not have come to reality without the selfless efforts of Dr. Vafai, through the National Academies, promoting the idea that students should be granted visas to pursue their educational goals in the US. Lastly, Scientia Iranica Journal, which I have had the honor of serving on its editorial board, owes its prestige to the vision of Professor Vafai as its founding editor in 1991, who saw the need for a high quality, international science and technology journal."

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