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SIMULATION-OPTIMIZATION FOR STOCHASTIC MODELLING TO GENERATE ALTERNATIVES

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ABSTRACT
In solving practical optimization applications, it is generally preferable to formulate several quantifiably good alternatives that provide distinct approaches to the particular problem. This is because decision-making typically involves complex problems that are riddled with incompatible performance objectives and possess competing design requirements which are very difficult − if not impossible − to quantify and capture at the time that the supporting decision models are constructed. There are invariably unmodelled design issues, not apparent at the time of model construction, which can greatly impact the acceptability of the model's solutions. Consequently, it is preferable to generate several alternatives that provide multiple, disparate perspectives to the problem. These alternatives should possess near-optimal objective measures with respect to all known modelled objective(s), but be fundamentally different from each other in terms of the system structures characterized by their decision variables. This solution approach is referred to as modelling to generate-alternatives (MGA). This paper provides a simulation-optimization MGA approach that efficiently creates multiple solution alternatives to stochastic problems that satisfy required system performance criteria and yet remain maximally different in their decision spaces. The efficacy of this stochastic MGA method is demonstrated using a waste facility expansion case study.

INTRODUCTION
"Real world" decision-making typically involves multifaceted stochastic problems that possess design components which are very difficult to incorporate into corresponding mathematical programming models and tend to be riddled with unquantifiable design specifications [1]-[4]. While mathematically optimal solutions provide the best answers to these modelled problems, they are generally not the best solutions to the fundamental "real" problems as there are invariably unquantified issues and unmodelled objectives not apparent during model construction [1][2][5]. Hence, it is generally considered desirable to generate a judicious number of dissimilar alternatives that supply multiple distinct perspectives to the formulated problem [6][7]. These alternatives should possess near-optimal objective measures with respect to the known modelled objective(s), but be as different as possible from each other in terms of the structures characterized by their decision variables. Several approaches collectively referred to as modelling-to-generate-alternatives (MGA) have been developed [5][7] in response to this multi-solution creation requirement. The primary motive behind MGA is to produce a manageably small set of alternatives that are good with respect to the modelled objective(s) yet are as far apart as possible from each other within the decision space. This set of maximally different alternatives provides solutions that perform similarly with respect to the known objectives, yet very differently with respect to any unmodelled issues [4].

In this paper, it is shown how to efficiently construct a set of maximally different solution alternatives by integrating a modified version of the computationally efficient Firefly Algorithm (FA) of Yang [8][9] into a new stochastic MGA approach that employs simulation-optimization (SO). The MGA procedure provided in this study extends the earlier approaches of Imanirad et al. [10][11] by employing an SO-based FA approach to concurrently generate the desired number of solutions in a one-pass algorithm. Hence, this stochastic FA procedure is very computationally efficient from an MGA perspective. The procedure is demonstrated on a municipal waste management (MSW) facilities expansion case study taken from Yeomans [12].

FIREFLY ALGORITHM FOR FUNCTION OPTIMIZATION
While this section provides a brief outline of the FA procedure, more specific details can be found in [8][9][10][11]. The FA is a nature-inspired, population-based metaheuristic. Each firefly in the population represents one potential solution to the problem. The initial firefly population is distributed randomly and uniformly throughout the solution space. The solution procedure employs the following three idealized rules: (i) All fireflies within a population are unisex, so that one firefly will be attracted to other fireflies irrespective of

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their sex; (ii) Attractiveness between fireflies is proportional to their brightness, implying that for any two flashing fireflies, the less bright one will move towards the brighter one. Attractiveness and brightness both decrease as the distance between fireflies increases. If there is no brighter firefly within its visible vicinity, then a particular firefly will move randomly; and (iii) The brightness of a firefly is determined by the landscape of the objective function. Namely, for a maximization problem, the brightness can simply be considered proportional to the value of the objective function. Based upon these three rules, the basic operational steps of the FA are summarized within the following pseudo-code [9].

> Objective Function $F(X)$, $X = (x_1, x_2, \dots x_d)$
> Generate the initial population of n fireflies, X_i, $i = 1, 2, \dots, n$
> Light intensity I_i at X_i is determined by $F(X_i)$
> Define the light absorption coefficient γ
> **while** (t < MaxGeneration)
> > **for** $i = 1$: n, all n fireflies
> > > **for** $j = 1$: n, all n fireflies (inner loop)
> > > > **if** ($I_i < I_j$), Move firefly i towards j; **end if**
> > > > Vary attractiveness with distance r via $e^{-\gamma r}$
> > > **endfor** j
> > **end for** i
> > Rank the fireflies and find the current global best solution G^*
> **end while**
> Postprocess the results

In the FA, there are two important issues to resolve: the variation of light intensity and the formulation of attractiveness. For simplicity, it can always be assumed that the attractiveness of a firefly is determined by its brightness which in turn is associated with the encoded objective function. In the simplest case, the brightness of a firefly at a particular location X would be its calculated objective value $F(X)$. However, the attractiveness, β, between fireflies is relative and will vary with the distance r_{ij} between firefly i and firefly j. In addition, light intensity decreases with the distance from its source, and light is also absorbed in the media, so the attractiveness should be allowed to vary with the degree of absorption. Consequently, the overall attractiveness of a firefly can be defined as

$$\beta = \beta_0 \exp(-\gamma r^2)$$

where β_0 is the attractiveness at distance $r = 0$ and γ is the fixed light absorption coefficient for a specific medium. If the distance r_{ij} between any two fireflies i and j located at X_i and X_j, respectively, is calculated using the Euclidean norm, then the movement of a firefly i that is attracted to another more attractive (i.e. brighter) firefly j is determined by

$$X_i = X_i + \beta_0 \exp(-\gamma (r_{ij})^2)(X_i - X_j) + \alpha \varepsilon_i$$

In this expression of movement, the second term is due to the relative attraction and the third term is a randomization component. Yang [9] indicates that α is a randomization parameter normally selected within the range [0,1] and ε_i is a vector of random numbers drawn from either a Gaussian or uniform (generally [-0.5,0.5]) distribution. It should be pointed out that this expression is a random walk biased toward brighter fireflies and if $\beta_0 = 0$, it becomes a simple random walk. The parameter γ characterizes the variation of the attractiveness and its value determines the speed of the algorithm's convergence. For most applications, γ is typically set between 0.1 to 10 [9]. In any given optimization problem, for a very large number of fireflies $n \gg k$ where k is the number of local optima, the initial locations of the n fireflies should be distributed relatively uniformly throughout the entire search space. As the FA proceeds, the fireflies would converge into all of these local optima (including the global ones). By comparing the best solutions among all these optima, the global optima can easily be determined. Yang [9] demonstrates that the FA will approach the global optima when n $\rightarrow \infty$ and the number of iterations t, is set so that $t \gg 1$. In reality, the FA has been shown to converge extremely quickly into both local and global optima [8][10][11].

MODELLING TO GENERATE ALTERNATIVES WITH THE FIREFLY ALGORITHM

Notwithstanding their fundamental limitations, most mathematical programming approaches have focused almost exclusively upon producing optimal solutions to single-objective problem formulations or generating noninferior solutions to multi-objective problem instances. While such algorithms may determine solutions to

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the derived complex mathematical models, whether their results actually establish "best" approaches for providing appropriate decisions to the underlying real problems is certainly questionable. In most "real world" decision problems, there are numerous system objectives and requirements that are never explicitly apparent or included at the decision formulation stage [1][4]. Furthermore, it may never be possible to explicitly express all of the subjective considerations because there are frequently numerous incompatible, competing, design requirements and, perhaps, adversarial stakeholder groups. Therefore, most subjective aspects of a problem remain unquantified and unmodelled in the construction of the resultant decision models. This is a common occurrence in situations where the final decisions are constructed based not only upon clearly stated and modelled objectives, but also upon fundamentally subjective, political and socio-economic goals and stakeholder preferences [7]. Numerous "real world" examples of this type of incongruent modelling duality are described in [5] and [13]-[15].

When unmodelled objectives and unquantified issues exist, different approaches are required in order to not only search the decision space for the noninferior set of solutions, but also to explore the decision space for *inferior* alternative solutions to the modelled problem. In particular, any search for good alternatives to problems known (or suspected) to contain unmodelled objectives must focus not only on the non-inferior solution set, but also necessarily on an exploration of the problem's inferior region. To illustrate the implications of an unmodelled objective on a decision search, assume that the optimal solution for a quantified, single-objective, maximization decision problem is X^* with corresponding objective value $Z1^*$. Now suppose that there exists a second, unmodelled, maximization objective $Z2$ that subjectively reflects environmental/political acceptability. Let the solution X^a, belonging to the noninferior, 2-objective set, represent a potential best compromise solution if both objectives could somehow have been simultaneously evaluated by the decision-maker. While X^a might be viewed as the best compromise solution to the real problem, it would clearly appear inferior to the solution X^* in the quantified model, since it must be the case that $Z1^a \leq Z1^*$. Consequently, when unmodelled objectives are factored into the decision-making process, mathematically inferior solutions for the modelled problem can be optimal for the real problem. Therefore, when unmodelled objectives and unquantified issues might exist, different approaches are required in order to not only search the decision space for the noninferior set of solutions, but also to simultaneously explore the decision space for inferior alternative solutions to the modelled problem. Population-based procedures such as the FA permit concurrent searches throughout a feasible region and thus prove to be particularly adept methods for searching through a problem's decision space.

The primary motivation behind MGA is to produce a manageably small set of alternatives that are quantifiably good with respect to modelled objectives yet are as different as possible from each other in the decision space. In doing this, the resulting alternative solution set is likely to provide truly different choices that all perform somewhat similarly with respect to the known modelled objective(s) yet very differently with respect to any unmodelled issues. By generating these good-but-different solutions, the decision-makers can explore alternatives that may satisfy the unmodelled objectives to varying degrees of stakeholder acceptability. Obviously the solution-setters must then conduct a subsequent comprehensive comparison of the alternatives to determine which options would most closely satisfy their very specific circumstances. Thus, an MGA approach should necessarily be considered as one of decision support rather than of explicit solution determination.

In order to properly motivate an MGA search procedure, it is necessary to provide a more formal definition of the goals of the MGA process [5][7]. Suppose the optimal solution to an original mathematical model is X^* with objective value $Z^* = F(X^*)$. The following model can then be solved to generate an alternative solution that is maximally different from X^*:

$$\text{Max } \Delta = \sum_i | X_i - X_i^* |$$
$$\text{Subject to: } X \in D$$
$$| F(X) - Z^* | \leq T$$

where Δ represents some difference function (shown as absolute in this instance) and T is a tolerance target specified in relation to the original optimal function value Z^*. T is a user-supplied value that determines how much of the inferior region is to be explored for alternative solutions. The FA-based MGA procedure is designed to generate a small number of good but maximally different alternatives by adjusting the value of T and using the FA to solve the corresponding, new maximal difference problem instance. In this approach, subpopulations within the algorithm's overall population are established as the Fireflies collectively evolve toward different local optima within the solution space. Each desired solution alternative undergoes the common

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search procedure of the FA. The survival of solutions depends upon how well the solutions perform with respect to the modelled objective(s) and by how far away they are from all of the other previously generated alternatives in the decision space.

A SIMULATION-OPTIMIZATION APPROACH FOR STOCHASTIC MGA

In this section, it is shown how the FA-based MGA method can be extended to incorporate stochastic uncertainty using simulation-optimization (SO) in order to efficiently generate sets of maximally different solution alternatives. SO is a family of optimization techniques that incorporates stochastic uncertainties expressed as probability distributions directly into the computational procedure [16][17]. Suppose the mathematical representation of an optimization problem contains n decision variables, X_i, expressed in vector form as $X = [X_1, X_2,…, X_n]$. When stochastic conditions exist, values for the constraints and objective can only be efficiently estimated by simulation. Thus, any solution comparison between two distinct decisions $X1$ and $X2$ necessitates the evaluation of some statistic of F modelled with $X1$ to the same statistic modelled with $X2$ [12][16][17]. SO is a broadly defined set of solution approaches that combine simulation with some type of optimization method for stochastic optimization [16]. In SO, all unknown objective functions, constraints, and parameters are replaced by one or more discrete event simulation models in which the decision variables provide the settings under which the simulation is performed. Since all measures of system performance are stochastic, every potential solution, X, examined would necessarily need to be evaluated via simulation. As simulation is computationally intensive, an optimization component is employed to guide the solution search through the problem's feasible region using as few simulation runs as possible.

The new FA-driven stochastic MGA procedure extends the earlier approach of Imanirad *et al.* [10][11] by extending FA into SO for stochastic optimization and by exploiting the concept of co-evolution within the FA's solution approach to concurrently generate the desired number of alternatives. FA-directed SO consists of two alternating computational phases; (i) an "evolutionary phase" directed by the FA module and (ii) a simulation module. As described earlier, the FA maintains a population of candidate solutions throughout its execution. The evolutionary phase considers the entire population of solutions during each generation of the search and evolves from a current population to a subsequent one. Because of the system's stochastic components, all performance measures are necessarily statistics calculated from the responses generated in the simulation module. The quality of each solution in the population is found by having its performance criterion, F, evaluated by simulation. After simulating each candidate solution, the respective fitness values are returned to the FA module to be utilized in the creation of the next generation of candidate solutions. One primary principle of an FA is that fitter solutions in the current population possess a greater likelihood for survival and progression into the subsequent generation. The FA module evolves the system toward improved solutions in subsequent populations and ensures that the solution search does not become fixated at some local optima. After generating a new candidate solution set in the FA module, the new population is returned to the simulation module for comparative evaluation. This alternating, two-phase search process terminates when an appropriately stable system state (i.e. an optimal solution) has been attained.

SIMULATION-OPTIMIZATION ALGORITHM FOR STOCHASTIC MGAUSING THE FIREFLY ALGORITHM

An obvious approach to generate alternatives with an FA-directed SO algorithm would be to iteratively solve the maximum difference model by incrementally updating the target T whenever a new alternative must be produced. This approach would be somewhat similar in scope to the original Hop, Skip, and Jump (HSJ) MGA algorithm [13] in which an initial problem formulation is optimized and then supplementary alternatives are generated by systematically adjusting the target constraint to force the creation of suboptimal solutions. While this approach is straightforward, it would require repeated execution of the optimization algorithm, which could prove computationally expensive [7]. The new stochastic MGA procedure is designed to concurrently generate a small number of good but maximally different alternatives in a single pass of the FA procedure (i.e. the same number of runs as if FA were used solely for function optimization purposes) and its efficiency is based upon the concept of co-evolution (see [11]). Namely, the algorithm can simultaneously produce the overall best solution together with n locally optimal, maximally different alternatives to it in a single computational run.

In the co-evolutionary approach, pre-specified stratified subpopulation ranges within the FA algorithm's overall population are established that collectively evolve the search toward the formation of the stipulated number of very different solution alternatives. Each desired solution alternative is represented by each respective

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subpopulation and each subpopulation undergoes the common operations of the FA. This approach can be structured upon any standard FA solution procedure containing appropriate encodings and operators that best correspond to the problem. However, the survival of solutions in each subpopulation depends upon how well the solutions perform with respect to both the modelled objective(s) and by how far away they are from all of the other solutions in the decision space. Thus, the evolution of solutions in each subpopulation is directly influenced by those solutions contained in all of the other subpopulations, which forces the co-evolution of each subpopulation towards good but maximally distant regions of the decision space. This co-evolutionary concept enables the simultaneous production of a set of quantifiably good solutions that are maximally different from each other [7].

By using the co-evolutionary concept, it becomes possible to implement an FA-directed stochastic MGA procedure that concurrently produces alternatives which possess objective function bounds that are somewhat analogous, but superior, to those created by an iterative HSJ-styled approach. Co-evolution is also a much more efficient procedure than HSJ in that it exploits the population-based searches of FA algorithms in order to generate the multiple maximally different solution alternatives concurrently. Namely, while an HSJ-styled approach would be required to run n different times in order to generate n different alternatives, the new algorithm need be run only a single time to produce its entire set of alternatives irrespective of the value of n. Hence, it is a much more computationally efficient process.

The steps in the co-evolutionary algorithm are as follows:

1. Create an initial population stratified into P equally-sized subpopulations. The value for P must be established *a priori* by the decision-maker. P represents the desired number of maximally different alternative solutions within a prescribed target deviation from the optimal to be generated. S_p represents the pth subpopulation set of solutions, $p = 1,…,P$ and there are K solutions contained within each S_p.

2. Evaluate all solutions in S_p, $p = 1,…,P$, with respect to the modelled objective using the simulation module of SO. Solutions meeting the target constraint and all other problem constraints are designated as *feasible*, while all other solutions are designated as *infeasible*.

3. Apply an appropriate elitism operator to each S_p to preserve the best individual in each subpopulation. In S_p, $p = 1,…,P$, the best solution is the feasible solution most distant in decision space from all of the other subpopulations (the distance measure is defined in Step 6). Note: Because the best solution to date is always placed into each subpopulation, at least one solution in S_p will always be feasible.

4. Stop the algorithm if the termination criteria (such as maximum number of iterations or some measure of solution convergence) are met. Otherwise, proceed to Step 5.

5. Identify the decision space centroid, C_{ip}, for each of the $K' \le K$ feasible solutions within $k = 1,…,K$ of S_p, for each of the N decision variables X_{ikp}, $i = 1,…,N$. Each centroid represents the N-dimensional centre of mass for the solutions in each of the respective subpopulations, p. As an illustrative example for determining a centroid, calculate $C_{ip} = (1/K') * \sum_k X_{ikp}$. In this calculation, each dimension of each centroid is computed as the straightforward average value of that decision variable over all of the values for that variable within the feasible solutions of the respective subpopulation. Alternatively, a centroid could be calculated as some fitness-weighted average or by some other appropriately defined measure.

6. For each solution $k = 1,…,K$, in each S_q, calculate D_{kq}, a distance measure between that solution and all other subpopulations. As an illustrative example for determining a distance measure, calculate

$$D_{kq} = \text{Min } \{ \sum_i |X_{ikp} - C_{ip}| ; p = 1,…,P, p \ne q \}.$$

This distance represents the minimum distance between solution k in subpopulation q and the centroids of all other subpopulations. Alternatively, the distance measure could be calculated by some other appropriately defined measure.

7. Rank the solutions within each S_p according to the distance measure D_{kq} objective – appropriately adjusted to incorporate any constraint violation penalties. The goal of maximal difference is to force solutions from one subpopulation to be as far apart as possible in the decision space from the solutions of each of the other subpopulations. This step orders the specific solutions in each subpopulation by those solutions which are most distant from the solutions in all of the other subpopulations.

8. In each S_p, apply appropriate FA "change operations" to the solutions and return to Step 2.

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CASE STUDY OF STOCHASTIC MGAFOR THE EXPANSION OF WASTE MANAGEMENT FACILITIES

As mentioned earlier, "real world" decision-makers generally prefer to be able to select from a set of "near-optimal" alternatives that significantly differ from each other in terms of the system structures characterized by their decision variables. The ability of the stochastic co-evolutionary FA-directed MGA procedure to concurrently produce such maximally different alternatives will be illustrated using the municipal waste management (MSW) facilities expansion case study taken from Yeomans [12]. The region in the facility expansion planning problem consists of three separate municipalities whose MSW disposal needs are collectively met by a landfill and two waste-to-energy (WTE) incinerators. The planning horizon consists of three separate time periods with each of the periods covering an interval of five years. The landfill capacity can be expanded only once over the entire 15-year planning horizon. Each of the WTE facilities can be expanded by any one of four possible options in each of the three time periods. The expansion costs escalate over time to reflect anticipated future conditions and are discounted to present value cost terms for use in the objective function. The MSW waste generation rates and the costs for waste transportation and treatment vary both temporally and spatially. The MSW case requires the determination of the preferred facility expansion alternatives during the different time periods and the effective allocation of the relevant waste flows in order to minimize the total system costs over the planning horizon.

Yeomans [12] produced a single best solution to the expansion problem costing $600.2 million. As outlined earlier, planners generally prefer to be able to select from a set of near-optimal alternatives that differ significantly from each other in terms of the system structures characterized by their decision variables. In order to create three alternative planning options, it would be possible to place extra target constraints into the maximal difference model which would force the generation of solutions that were different from this newly determined, optimal solution by target values of, for example, 2%, 5%, and 8%, respectively. By adding these specific target constraints to the original model, the problem would need to be resolved an additional three times. However, to improve upon the process of running four separate instances of the SO algorithm to determine these solutions, the stochastic FA-directed MGA procedure described in the previous section was run once to produce the objectives for the 4 alternatives shown in Table 1.

Table 1: System Expansion Costs ($ Millions) for the 4 Alternatives.

	Overall "Optimal" Solution	Best 2% Solution	Best 5% Solution	Best 8% Solution
System Expansion Costs	600.21	602.78	612.54	616.38

This example has demonstrated how the stochastic FA-directed MGA modelling approach could be used to efficiently generate a good set of policy alternatives that satisfy required system performance criteria according to prespecified bounds within stochastic environments and yet remain as maximally different from each other as possible in the decision space. Given the performance bounds established for the objective in each problem instance, decision-makers would be reassured by the stated performance bounds for each of these options while also being aware that the perspectives provided by the set of dissimilar decision variable structures are as maximally different from each other as is feasibly possible. Hence, if there are stakeholders with incompatible standpoints holding diametrically opposing viewpoints, the policy-makers could conduct an assessment of these different options without being myopically constrained by a single overriding perspective based solely upon the objective value. In addition to its alternative generating capabilities, the FA component within the MGA algorithm simultaneously performs extremely well with respect to its role in function optimization. It should be explicitly noted that the overall best solution produced by the MGA algorithm for the case is indistinguishable from the optimal solution determined in [12].

In the computational testing of this section, the results from the example highlight several important characteristics with respect to the new stochastic FA-based MGA method: (i) An FA can be employed as the underlying search process for optimization in SO; (ii) By the design of the MGA algorithm, the alternatives

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generated are good for planning purposes since all of their structures will be as mutually and maximally different from each other as possible (i.e. these differences are not just simply different from the overall optimal solution as in the HSJ-style approach to MGA); (iii) The co-evolutionary capabilities within the FA can be exploited to generate more good alternatives than planners would be able to create using other MGA approaches because of the evolving nature of its population-based solution searches; (iv) The approach is very computationally efficient since it need only be run once to generate its entire set of multiple, good solution alternatives (i.e. to generate n solution alternatives, the MGA algorithm needs to run exactly the same number of times that the FA would need to be run for function optimization purposes alone – namely once – irrespective of the value of n); and, (v) The best overall solutions produced by the stochastic MGA procedure will be very similar, if not identical, to the best overall solutions that would be produced by the FA for function optimization alone.

CONCLUSION
"Real world" decision-making problems generally possess multidimensional performance specifications that are compounded by incompatible performance objectives and unquantifiable modelling features. These problems usually contain incongruent design requirements which are very difficult – if not impossible – to capture at the time that supporting decision models are formulated. Consequently, there are invariably unmodelled problem facets, not apparent during the model construction, that can greatly impact the acceptability of the model's solutions. These uncertain and competing dimensions force decision-makers to integrate many conflicting sources into their decision process prior to final solution construction. Faced with such incongruencies, it is unlikely that any single solution could ever be constructed that simultaneously satisfies all of the ambiguous system requirements without some significant counterbalancing involving numerous tradeoffs. Therefore, ancillary modelling techniques used to support decision formulation have to somehow simultaneously account for all of these features while being flexible enough to encapsulate the impacts from the inherent planning uncertainties.

In this paper, a new stochastic FA-directed MGA approach was introduced that demonstrated how the structures of the computationally efficient, population-based FA could be exploited to concurrently generate multiple, maximally different, near-best alternatives via its co-evolutionary solution technique. In this stochastic MGA capacity, the FA-directed approach produces numerous solutions possessing the requisite problem characteristics, with each generated alternative guaranteeing a very different perspective. Since the new FA-directed stochastic technique could be adapted to solve a wide variety of problem types, the practicality of this stochastic MGA approach can clearly be extended into numerous "real world" applications. These extensions will become the focus of future research

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