Abstract—This paper proposes the Fitness Diversity based Adaptive Memetic Algorithm (FIDAMA) for solving the problem of inverse type consisting of retrieving chemical kinetics reaction rate coefficients in the generalised Arrhenius form based on the observed concentrations in a given range of temperatures of a limited set of species which describe the reaction mechanism. FIDAMA consists of the Evolutionary Framework and three Local Searchers adaptively governed by a novel fitness diversity based measure. Moreover, a certain simplification of the decision space was carried out without any deterioration in the result obtained. The numerical results presented show the superiority of FIDAMA compared to the other published computational intelligence methods.

I. INTRODUCTION

Concern on the impact of combustion processes on the environment has led to intensive research on the subject, with chemical modelling becoming an increasingly important tool in the analysis of combustion systems. One of the least understood aspects of combustion is the underlying chemical reaction mechanism, even for simple fuels. In part this is due to the restrictions on experimental methods imposed by the harsh conditions under which combustion proceeds, and in part it is caused by the inherent chemical complexity of the combustion. [1]

To meet the ever increasing demand for more refined predictions to control toxic emissions, and because of the large size of the mechanisms, continuous effort is needed in the construction of thermodynamic and kinetic data bases. A popular method for constructing reaction mechanisms is to use reactions whose rate parameters are known to be within some physical realistic boundaries. These boundaries may then be used to define a search domain for each rate parameter. Such an approach is referred to as the inverse problem of chemical kinetics. Inverse problems for differential equations are difficult to solve and require special techniques to be employed. Apart from these difficulties associated with the large numbers of parameters and relatively large search intervals for the rate parameters, additional problems arise from the ill-posedness typical of such inverse problems [1]. In chemical modelling problems, the level of complexity of the reaction mechanism combined with the uncertainty about many of the rate coefficient parameter makes the optimisation of these systems exceedingly difficult.

It is worth mentioning that the difficulty of the problem under study consists also of the time-consuming derivation of the single candidate solution since a large number of evaluations are involved in it. For example, for the rather simple case (from the point of view of the chemistry) which is considered in this work, each evaluation takes about 0.6 seconds on average. This time increases significantly when working with mechanisms with larger number of reaction. This fact prohibits the use of a large class of algorithms.

Since the objective function in these cases is usually highly structured and multimodal, both traditional optimisation methods and methods based on the linearisation are likely to fail. Response surface methods would introduce too large approximation errors which would strongly effect the resulting solution [2]. These limitations resulted in proposing a genetic algorithm technique [3] which optimises the rate coefficients through matching the heat-release and production rates of the species.

A similar problem to the one under investigation in this paper was solved using several versions of Genetic Algorithms (GAs) but with slightly different decision space (for several parameters) for binary and real representation, in [4], [5], [2]. However these algorithms suffer from a slow convergence rate since they spend too much time detecting regions with promising directions of search. Moreover, the algorithms proposed in [5] and [2], which use a real representation of the parameters, spend too much computational effort in refining the solutions to a degree which is not meaningful because of the physical limitations of modern measurement techniques. In addition, due to their structure, Genetic Algorithms are known to fail in the fine-tuning of the solution [6].

A rather recent trend consists of applying Memetic Algorithms (MAs) which are the hybrids of an Evolutionary Framework with one or several Local Searchers (LSs). More precisely, memetic algorithms are population based metaheuristic search approaches, inspired by Neo-Darwinian’s principles of natural evolution and Dawkin’s notion of a meme defined as a unit of cultural evolution that is capable of local refinements [7]. Hence, a memetic model of adaptation exhibits the plasticity of the individuals that genetic algorithms fail to capture [8].

This paper proposes the Fitness Diversity based Adaptive Memetic Algorithm (FIDAMA) for retrieving chemical kinetics reaction rate coefficients in the generalised Arrhenius form based on the observed concentrations in a given range for temperature of a limited set of species which describe the reaction mechanism.
II. PROBLEM DESCRIPTION

The generalised Arrhenius form expresses the dependency of the reaction rate coefficient \( k_i \) on temperature \( T \) with 3 parameters in the following way:

\[
k_i = A_i \exp\left(-\frac{E_i}{RT}\right)T^{b_i}
\]

where the parameters are the pre-exponential factor \( A_i \), the shape parameter \( b_i \), the reaction activation energy \( E_i \), and \( R \) is the gas constant. Boundaries for each particular reaction derived from an assessment of published work can be obtained from the National Institute of Standards and Technology (NIST) chemical kinetics database and Evaluated Kinetic Data for Combustion Modeling [9]. Nevertheless, due to experimental uncertainty, these boundaries are not necessary fixed.

A. Construction of Decision Space

In this study the Authors consider the problem of retrieving rate coefficients for the process of combustion of a hydrogen/nitrogen/oxygen mixture. The mechanism of this process [10] can be described by means of 19 chemical reactions involving 9 species. Therefore using a straightforward representation for each of 3 · 19 parameters leads to consideration of a continuous optimisation problem in 57 dimensions which is computationally time consuming. However, the permissible interval for the values of each dimension can be discretised, since two very close values cannot be distinguished thanks to the physical limitations of the measurement techniques. Due to the different nature of each type of parameter, different discretising steps are assigned to them. More precisely, these steps are a factor of 10 lower than the lower bound for the pre-exponential factors, 0.1 for the shape parameters and 100 for the activation energies.

Moreover, since for six of the reactions involved in the mechanism under investigation the activation energy was zero in [10], an arbitrary interval of \([-1000, 1000]\) was imposed artificially to account for the uncertainty involved in assessing the activation energy to be zero. All initial intervals were adjusted prior to the discretisation in a way to encompass the values on the edges of the intervals.

In (1) the shape parameter \( b_i \) is introduced for the generalised Arrhenius form in order to reproduce the curvature found in experimental data when plotted as \( \log(k_i) \) vs \( 1/T \). Meanwhile there is a strong experimental indication that, in practice, 9 reactions of the considered scheme do not have curvature and therefore for them \( b_i = 0 \). This excludes these 9 parameters from the search and reduces further the dimensionality of the problem under investigation.

The details on the NIST boundaries for the considered reaction mechanism can be found in Table 1. Moreover, for each reaction \( \frac{N_s}{FIDAMA} \) \( \frac{N_i}{FIDAMA} \) and \( \frac{N_s}{FIDAMA} \), presented in the Table, are the numbers of points considered in FIMADA for each \( A_i \), \( b_i \), and \( E_i \) respectively.

The discretisation procedure described above clearly leads to significant simplifications of the problem in terms of computation through the reduction of the cardinality of the decision space and changing the nature of problem parameters from continuous into combinatorial. The new decision space has the following features: each parameter takes values from a finite set, i.e. the set is countable and the overall cardinality of the decision space is of order of \( 10^{57} \). Numerical results obtained indicate that this simplification due to the algorithmic features of the novel method proposed by the Authors does not lead to any loss in the optimal/suboptimal solutions compared to the results obtained in [2].

B. Problem Formulation

To estimate the goodness of the approximation of the observed concentrations, the following objective (fitness) function is used [2]:

\[
f(X) = \left\{ 10^{-8} + \sum_{j=1}^{N_s} \sum_{k=1}^{K} \frac{|X_{jk}^{calc} - X_{jk}^{orig}|}{X_{jk}^{orig}} \right\}^{-1}
\]

where \( X \) is the vector consisting of the parameters of the rate reaction coefficients to be evaluated, \( X_{jk}^{calc} \) is calculated according to \( X \) mole concentrations of the \( j^{th} \) species in the \( k^{th} \) set of operating conditions, \( X_{jk}^{orig} \) are the corresponding original (observed) mole concentrations which were measured or simulated (benchmarking) using the unknown reaction rate parameters; \( N_s \) is the number of species involved in the considered reaction mechanism, and \( K \) is the number of operating conditions.

Hence, the optimisation problem under study is to maximise \( f(X) \) over the set of integer numbers within the given boundaries as described above.

In order to evaluate the obtained approximation \( X \) (i.e. to predict the concentrations of the species after reactions of the considered scheme governed by 19 rate coefficients encoded into \( X \)) a simulation based on the Perfectly Stirred Reactor (PSR) [10] module of CHEMKIN is performed. Certain operating conditions of the original experiment, such as residence time, exact chemical composition of both the fuel and oxidiser, volume of the reaction vessel, are known and are used in the PSR simulations. The PSR module is designed to simulate a heated reaction vessel with an inflow of reactants and an outflow of products. The reactor temperature is defined as its volume, and hence the average residence time for a given inflow rate. The assumption of it being "perfectly mixed" represents the idealised scenario in which mixing within the reaction vessel is sufficiently fast to eliminate species concentration gradients, and thus the behaviour is controlled entirely by the chemical reactions of the species present, with no influence of physical processes related to imperfect mixing.

III. FITNESS DIVERSITY BASED ADAPTIVE MEMETIC ALGORITHM

The Fitness Diversity based Adaptive Memetic Algorithm proposed here is composed of the Evolutionary Framework which evolves the population of candidate solutions, and three Local Searchers, namely Integer Simulate Annealing,
Discretised Hooke-Jeeves algorithms and their combination. It uses an integer representation described in the previous section.

### A. Evolutionary Framework

Following the logic of the Evolutionary Computation methods, FIDAMA evolves the population made up of strings each representing a possible solution of the problem under study. Considering the description of the decision space presented above, these strings are of length 57. Each position in the string is an ordinal number in the list of possible values, returned by the discretisation procedure (i.e. it is an integer number) with respect to the defined boundaries with a certain tolerance added (5%).

In order to speed up the evolution the initial population is over-sampled. A Latin Hypercube sampling technique [11], [12], [13] ensures uniform exploration of the decision space but due to the high cardinality in our case, just dividing each dimension in two parts would require $2^{57} \approx 10^{17}$ fitness evaluations which is not feasible. However, the Authors have selected 9 parameters based on a prior analysis of the decision space presented above, these strings are of length 57. Each position in the string is an ordinal number in the list of possible values, returned by the discretisation procedure (i.e. it is an integer number) with respect to the defined boundaries with a certain tolerance added (5%).

### TABLE I

<table>
<thead>
<tr>
<th>$i$</th>
<th>Reaction</th>
<th>$A_i$(NIST)</th>
<th>$N_{FIDAMA_i}$</th>
<th>$b_i$(NIST)</th>
<th>$N_{b_i,FIDAMA}$</th>
<th>$E_i$(NIST)</th>
<th>$N_{E_i,FIDAMA}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$H + O_2 = O + OH$</td>
<td>[1.3e+16, 6.3e+16]</td>
<td>22</td>
<td>[0, 0.1]</td>
<td>6</td>
<td>[12000, 20000]</td>
<td>85</td>
</tr>
<tr>
<td>2</td>
<td>$H_2 + O = H + OH$</td>
<td>[1.3e+10, 3.2e+10]</td>
<td>11</td>
<td>[0.7, 1.3]</td>
<td>6</td>
<td>[6600, 11100]</td>
<td>46</td>
</tr>
<tr>
<td>3</td>
<td>$H_2 + OH = H_2O + H$</td>
<td>[9.9e+08, 1.5e+09]</td>
<td>61</td>
<td>[0.9, 1.7]</td>
<td>9</td>
<td>[2700, 4600]</td>
<td>20</td>
</tr>
<tr>
<td>4</td>
<td>$OH + OH = H_2O_2 + O$</td>
<td>[4.3e+08, 7.5e+08]</td>
<td>31</td>
<td>[0.9, 1.7]</td>
<td>9</td>
<td>[-1000, 1000]</td>
<td>21</td>
</tr>
<tr>
<td>5</td>
<td>$H + OH + M = H_2O + M$</td>
<td>[5.6e+23, 9.3e+23]</td>
<td>39</td>
<td>[-3.5, -1.9]</td>
<td>15</td>
<td>[-1000, 1000]</td>
<td>21</td>
</tr>
<tr>
<td>6</td>
<td>$O_2 + M = O + O + M$</td>
<td>[1.3e+11, 2.4e+11]</td>
<td>11</td>
<td>[0.3, 0.7]</td>
<td>5</td>
<td>[71000, 119500]</td>
<td>480</td>
</tr>
<tr>
<td>7</td>
<td>$H_2 + M = H + H + M$</td>
<td>[1.6e+12, 2.8e+12]</td>
<td>13</td>
<td>[0.3, 0.7]</td>
<td>5</td>
<td>[69400, 115800]</td>
<td>465</td>
</tr>
<tr>
<td>8</td>
<td>$H_2 + O_2 = OH + OH$</td>
<td>[1.3e+12, 2.2e+13]</td>
<td>11</td>
<td>[0.0, 0.0]</td>
<td>0</td>
<td>[35800, 59800]</td>
<td>21</td>
</tr>
<tr>
<td>9</td>
<td>$H + O_2 + M = H_2O_2 + M$</td>
<td>[1.5e+18, 2.7e+18]</td>
<td>13</td>
<td>[-1.5, -0.7]</td>
<td>7</td>
<td>[-1000, 1000]</td>
<td>21</td>
</tr>
<tr>
<td>10</td>
<td>$H + O_2 + O_2 = H_2O_2 + O_2$</td>
<td>[8.0e+19, 1.5e+19]</td>
<td>35</td>
<td>[-1.8, -1.0]</td>
<td>9</td>
<td>[-1000, 1000]</td>
<td>21</td>
</tr>
<tr>
<td>11</td>
<td>$OH_2 + H = H_2O + O_2$</td>
<td>[5.0e+19, 8.4e+19]</td>
<td>35</td>
<td>[-1.8, -1.0]</td>
<td>9</td>
<td>[-1000, 1000]</td>
<td>21</td>
</tr>
<tr>
<td>12</td>
<td>$H_2 = H + O_2 + O_2$</td>
<td>[1.6e+13, 2.6e+17]</td>
<td>61</td>
<td>[0.0, 0.0]</td>
<td>0</td>
<td>[34100, 56000]</td>
<td>229</td>
</tr>
<tr>
<td>13</td>
<td>$H_2O_2 + H = H_2O + H_2$</td>
<td>[1.0e+12, 2.2e+12]</td>
<td>11</td>
<td>[0.0, 0.0]</td>
<td>0</td>
<td>[2800, 4700]</td>
<td>20</td>
</tr>
<tr>
<td>14</td>
<td>$H_2O_2 + O = H_2O + O_2$</td>
<td>[3.3e+12, 1.7e+13]</td>
<td>51</td>
<td>[0.0, 0.0]</td>
<td>0</td>
<td>[1300, 2300]</td>
<td>11</td>
</tr>
</tbody>
</table>

### B. Local Searchers

1. **Integer Simulated Annealing (ISA):** is a probabilistic local searcher inspired by the classical Simulated Annealing (SA) [15],[16], which is adopted for the integer representation. Starting from the point randomly selected from the whole population, but the best individual found so far, it samples thoroughly the objective function wandering in the decision space and accepting all uphill moves. However, ISA also accepts downhill moves with non-zero probability. This
probability decreases with fitness evaluations, and also as the difference between fitness values of the current point and a possible point to move to decreases. Therefore, after some time ISA becomes greedy. Thanks to accepting worse solutions in the initial stages, applying an algorithm of SA type facilitates jumping to the basin of the attraction of the fitness function different from the one of the initial point. However, applying this type of algorithms could lead to a deterioration of the solution and the loss of the promising direction of search.

Due to the representation of the individuals of the evolutionary framework, an appropriate perturbation operator should be chosen. In ISA it consists of applying, to a selected individual, a random mask with values in each position distributed according to the symmetric Beta distribution, which resembles the creep mutation recommended for this type of representation in [6]. The Authors have chosen this particular distribution because it prefers small values to large ones but at the same time it is bounded, unlike the Gaussian distribution. This causes less jumping off from the permissible interval. To ensure the correctness of an obtained individual, the correction procedure described above is performed. The temperature is decreasing according to the hypergeometric progression. Moreover, a parameter defining the maximum possible random value generated (maximum variance) in percentage of the total amount of points in this dimension, is defined. Details on the parameter setting for the ISA can be found in Table III.

2) Discretised Hooke-Jeeves Algorithm (DHJA): is a direct deterministic search method which takes its logic from the classical Hooke-Jeeves Algorithm [17]. Each iteration of the DHJA consists of exploratory and pattern moves.

The exploratory move starts from a point selected according to the rules described below and explores each dimension with its own step size proportionate to the total number of points in this dimension. According to some heuristic rules, the initial step size is set to 20% of the total number of the points in the dimension. First the algorithm tries to make a move from the initial point in a positive direction separately for each dimension. Then for those dimensions for which no improvement was found, separately it attempts to make a move in the negative direction with the same step size. Choosing the best point among the initial and generated ones concludes the exploratory move. If no improvement, with respect to the fitness value of the initial point, is found then the exploratory move is repeated with the step size halved.

Otherwise, in order to explore better the promising direction found during the exploratory move, the pattern move is performed. This consists of an attempt to move further in this direction. If this attempt is successful then the search procedure is re-centred to the newly found point and the exploratory move is performed for it with the same step size. These moves are repeated until a certain termination condition is met.

The DHJA is designed in order to assist the evolution on average, i.e. to improve gradually every individual in the current population. However, the fitter ones are preferred since those with relatively low fitness values would be eliminated from the population by the selection procedure of the evolutionary framework. For this purpose a flag is introduced for each individual which is reset when the individual is initialised or created (i.e. during initialisation, recombination, mutation stages or ISA). This flag is considered when selecting the individual to undergo the DHJA. The DHJA attempts to find the individual in the population with the highest possible fitness value to which the deterministic search method has not been applied yet. In case it fails to find such an individual, flags of all individuals in the current population are reset since it means that all individuals were already upgraded to a certain level, but new assistance is required for the Evolutionary Framework. Details on the parameter setting for the DHJA can be found in Table III.

3) Consecutive run of ISA and DHJA: is used as the third Local Searcher in FIDAMA. First, for the randomly selected point of the population (excluding the best individual found so far) ISA is launched. Then DHJA is applied to the result of ISA. The advantage of using this combination is high exploration assured by ISA which facilitates the possibility of jumping to another basin of attraction and immediate improvement by means of DHJA. This Local Searcher is designed to be used in the extreme situations of the possible convergence of the algorithm to the local optimum.

C. Online Fitness Diversity Measures

When dealing with Memetic Algorithms (MAs) four major questions should be answered [8]:

1) How often to apply Local Searchers?
2) On which solution should the Local Searcher be applied?
3) How long should the Local Searcher be run?
4) Which Local Searcher should be run?

Every search algorithm introduces a certain bias into its search which defines the efficiency of the method for some classes of problems but not others [18]. Therefore, the choice of the Local Searcher to be employed is crucial.

In order to assign the probability of launching the Local Searcher and its parameters, in [19] each individual of the population is classified into one of three groups depending on its fitness. It is assumed that individuals in different groups should be treated differently by the Local Searcher.

Another way is to select a proper Local Searcher, which matches the current needs of the population in the online fashion, since the optimal choice of operators can not be only instance specific within a class of problems but also dependent on the state of the evolutionary search [6]. In other words, it must be decided which individuals undergo lifetime learning and from the set of local searchers which one should be used during the different stages of the optimization process [20]. In [8] an interesting approach, based on the entropy of the fitness values of the population, is proposed. Three more online fitness diversity measures are proposed in [21] and [22], [23], [24] which are respectively

\[ \xi = \min \left\{ \frac{f_{\text{best}} - f_{\text{avg}}}{f_{\text{best}}}, 1 \right\}, \]

\[ \psi = 1 - \left| \frac{f_{\text{avg}} - f_{\text{best}}}{f_{\text{worst}} - f_{\text{best}}} \right|, \]

\[ \nu = \min \left\{ \frac{\sigma f}{f_{\text{avg}}}, 1 \right\}. \]

where \( f_{\text{best}}, f_{\text{avg}}, f_{\text{worst}} \) are the best, average and worst fitness values in the current population and \( \sigma f \) is the standard deviation of the fitness values in the population.

Their relative drawbacks are that they consider too few statistical characteristics of the population which can decrease their sensitivity in some cases. The measure proposed in [24] uses mean and standard deviation of the fitness values in the population which contain more information regarding the distribution of values. Nevertheless, all these measures assess the dynamics of the population from different perspectives and prove to be efficient in various cases.

In order to encapsulate more information into the online fitness diversity measure, the Authors have proposed a novel scheme for its construction. The idea behind the new measure is to estimate the balance between the tails of the empirical probability density function (histogram) of the fitness values. More precisely, it is constructed as follows:

1) at the end of each generation \( i \) of the evolutionary framework, the wideness \( d_i \) of the interval of fitness values in the current population is calculated using \( d_i = f_{\text{max}}^i - f_{\text{min}}^i \).

2) the number of points \( n_3^i \) of the current population whose fitness falls within the first third of \( d_i \), i.e. those whose fitness belongs to the subinterval \( \left[ f_{\text{min}}^i, f_{\text{min}}^i + d_i / 3 \right] \), is found,

3) the number of points \( n_3^i \) of the current population whose fitness falls within the last third of \( d_i \), i.e. those whose fitness belongs to the subinterval \( \left[ f_{\text{max}}^i - d_i / 3, f_{\text{max}}^i \right] \), is found,

4) their difference is found, \( \tau_3^* = n_3^i - n_1^i \),

5) for a future convenience \( \tau_3^* \) is rescaled and shifted to be within \([0, 1]\)

\[ \tau_3 = 0.5 + \frac{\tau_3^*}{2 \cdot N_{\text{pop}}}, \]

where \( N_{\text{pop}} \) is the size of the population of the evolutionary framework.

\( \tau_3 \) is designed to be used in the manner proposed in [21] and [22], [23], [24] as a rule to understand the proper necessities of the population of the evolutionary framework.

The setting of \( \tau_3 \) should rely on the experimental observation that the successful evolution process is usually governed by a few superior individuals which "pull" the rest of the population. This means that for the population to evolve successfully by its own means (i.e. by the evolutionary operators) the value of \( \tau_3 \) should lie somewhere within \([0.1, 0.4]\). However, the real optimal value for this interval would depend strongly on the fitness landscape under investigation. The situation when \( \tau_3 \in [0.65, 1] \) looks highly improbable for most fitness landscapes.

Those fitness values of the individuals of the population which fall within the second third, i.e. \( [f_{\text{min}}^i + d_i / 3, f_{\text{max}}^i - d_i / 3] \), do not govern directly the dynamics of the population. They only possess sufficiently good genetic material suitable to produce promising solutions. The Authors have decided to divide the interval \( d_i \) of the fitness values into three subintervals according to some heuristic rules. However, other variants of the proposed scheme can of course be the area of future research.

In practice, \( \tau_3 \) shows circular behaviour compared to the measures proposed before. More precisely, any significant shift in the balance of points on the tails of the fitness values distribution would mean for \( \tau_3 \) tending to either 0 or 1. Meanwhile for the measure described above there are no similarities in population dynamics when they approach 0 and 1 and show behaviour non-circular in this sense.

Nevertheless, direct comparison of \( \xi, \psi, \nu \) and \( \tau_3 \) is complicated and potentially meaningless because these measures are just different characteristics of the population and should be used simultaneously to interpret better the dynamics of the whole population undergoing evolution process.

Figures 2-b, 2-c, 2-d present the description of the population dynamics by means of \( \xi, \psi, \nu \) and \( \tau_3 \) of three different versions of FIDAMA, details on which are described below in section III.E, with adaptation governed by \( \tau_3 \). It can be stated that for this particular kind of fitness landscape \( \psi \) and \( \tau_3 \) are highly correlated which is an unexpected result to be obtained if considering significant differences in the ideas behind constructing both measures. Moreover, \( \xi \) does not look really adequate just by itself, since it is very sensitive and therefore, it normally decreases significantly throughout the evolutionary process when the population is
simply becoming more concentrated towards the promising area of the search space.

Thus, using one of the fitness diversity measures described above gives an answer for the first and the fourth questions listed at the beginning of this subsection. At the current stage of the research the answers to the second and the third questions are considered to be fixed as stated in part III.B.

D. Adaptive Coordination of the Local Searchers

In order to launch a suitable Local Searcher in FIDAMA, the fitness diversity measure \( \tau_3 \) described in the previous section is used. More precisely, at the end of each generation of the Evolutionary Framework a decision is taken based on the value of \( \tau_3 \) for the current population according to the following rule:

1) if \( \tau_3 \in [0, 0.04] \) then ISA+DHJA is launched,
2) if \( \tau_3 \in (0.04, 0.4] \) then DHJA is launched,
3) if \( \tau_3 \in (0.4, 0.6) \) then no Local Searcher is launched,
4) if \( \tau_3 \in [0.6, 1] \) then ISA is launched.

The thresholds for situations 1–4 listed above are set according to the following considerations. The situation when \( \tau_3 \) is inside the interval defined in case 1 means there are too many points with low fitness values which are not able to produce better solutions by means of variation operators of the Evolutionary Framework. Then a combination of ISA and DHJA, performed in the consecutive fashion, could first refresh the genotype of the solution by ISA and then immediately try to improve it by means of DHJA, hopefully immediately introducing a superfit solution to the population. Inside the interval defined in case 2, the evolution is going on rather successfully, but in order to speed it up in general some superfit individuals can be introduced by DHJA. Being inside the interval for case 3 means that no assistance is needed for the evolution process. As stated before the probability of \( \tau_3 \) falling within the subinterval, defined in case 4, is quite low for most types of fitness landscapes. However if it occurs it could mean that the population has got stuck in several local maxima and some highly explorative Local Searcher is required. Since in ISA worsening moves can be accepted with non-zero probability it can assist in an escape from a local optima [6]. In this case the risk of introducing a solution with a worse fitness (compared to the fitness values of the population) is balanced with the possibility of introducing “fresh” genetic information and therefore jumping to another basin of attraction.

The exact values of the threshold are set heuristically. The result returned by the selected Local Searcher is placed into the population of the Evolutionary Framework in order to proceed to its following generation.

E. Local Search Launch Period

In order to investigate the effect of employing the Local Searchers, an additional parameter, the local searcher launch period \( p_{LS} \), was introduced. This parameter is the minimal number of generations of FIDAMA’s evolutionary framework that should elapse since the last launch of the LS before another launch of LS can take place. Figure 1 shows the performance trends for the three versions of FIDAMA with different local searcher launch periods. FIDAMA1, FIDAMA2 and FIDAMA4 are FIDAMAs described in the previous sections with \( p_{LS} = 1 \), \( p_{LS} = 2 \), \( p_{LS} = 4 \) respectively. Moreover, to understand better the dynamics of the populations of FIDAMAs, their fitness diversity is monitored by means of three measures. This information is presented in Figure 2. All trends are averaged over 50 runs.

![Figure 1](image1.png)  
Fig. 1. Comparison of algorithmic performance of different versions of FIDAMA for \( p_{LS} = 1 \), \( p_{LS} = 2 \), \( p_{LS} = 4 \), respectively

![Figure 2](image2.png)  
Fig. 2. Comparison of fitness diversity measure for different versions of FIDAMA

It can be seen that too frequent launch of the LS (as in FIDAMA1) does not bring to the better results in terms of performance. The reason being that the fitness diversity is rather low and stable throughout the evolution. In this case, the evolutionary operators do not manage to produce
fresh individuals and the population is driven mostly by
the individuals obtained via LS, with a risk to obtain the
prematurely converged population. Compared to FIDAMA1,
the quality and dynamics of the population of FIDAMA2
look more promising. The fluctuations in the fitness diversity
 correspond well to the launches of LSs. The width of
 "window" of the fitness values remains almost the same
 throughout the evolution which is good from the point
 of view of maintaining population diversity and avoiding
 premature convergence. The quality of the solutions in the
 case of FIDAMA4 is sufficiently high. There are several
 peaks in diversity measures which do not correspond to the
 launches of LSs. This means that the population is capable
 of producing fitter individuals by its own means via the
 evolutionary operators. The average diversity is higher
 compared to the cases of FIDAMA1 and FIDAMA2. However,
 the capability of FIDAMA4 in producing better individuals
decreases throughout the evolution. Therefore, when setting
 $p_{LS}$, a certain balance should be found.

### IV. NUMERICAL RESULTS

Using FIDAMA4 as an example, the results were com-
pared against the conventional GA presented in literature
[5]. The Authors considered here two GAs with different
decision spaces, with the original NIST boundaries and with
the boundaries modified in the same way as for FIDAMA.
The parameter settings for both GAs are the same and they
are presented in Table IV. The trends are averaged over 50
runs. The comparison is presented in Figure 3.

![Fig. 3. Algorithmic performance](image)

Fig. 3. Algorithmic performance

Clearly, FIDAMA outperforms both of them in terms of
both quality of the obtained solutions and the velocity it
tracks the optimal search direction.

Figures 4 and 5 show the comparison of the mole fractions
of the three major stable species and the mole fractions
of the three major radical species at different operating
conditions (temperature). In these figures simulations based
on the latest version of the GRI Mechanism [25], widely used

![Fig. 4. Observed and predicted concentrations of stable species](image)

![Fig. 5. Observed and predicted concentrations of radicals](image)

TABLE IV

<table>
<thead>
<tr>
<th>GA PARAMETERS</th>
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<tbody>
<tr>
<td>Parameter</td>
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<td>---------------</td>
</tr>
<tr>
<td>Initial sampling</td>
</tr>
<tr>
<td>Population size</td>
</tr>
<tr>
<td>Number of offsprings</td>
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<tr>
<td>Parent selection</td>
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<td>Tournament probability</td>
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<td>Crossover probability</td>
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<td>Mutation probability</td>
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<td>Mutation</td>
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in engineering applications are presented. This mechanism was produced by assembling a reasonably comprehensive reaction mechanism encompassing hydrogen, oxygen, C₁, C₂ and simple nitrogen based species, and then optimising it against a wide variety of data and placing the data and resulting mechanism on the web, thus facilitating its widespread use. It can be seen that there is excellent agreement between the observed values and the values obtained by FIDAMA. The precision of FIDAMA does not depend on the operating conditions of the original combustion process which is its advantage.

V. CONCLUSIONS

The Fitness Diversity based Adaptive Memetic Algorithm, proposed in this paper, proves to be a more efficient tool in solving the problems of inverse type, compared to the other published computational intelligence methods. This happens because of the algorithmic features and correct complexity reduction performed prior to the optimisation. The novel online fitness diversity measure proves to track well the dynamics of the evolving population.

The use of FIDAMA for chemical modelling purposes enables the efficient optimisation of chemical reaction mechanisms against available experimental data, thus providing improved chemical mechanisms for use in real world engineering applications.

Future work can be performed regarding the reasoning and fine tuning of the scheme proposed for constructing the online fitness diversity measures and integrating them more efficiently into the structure of the Memetic Algorithms.

REFERENCES


