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Minimization of Molecular Potential Energy Function Using newly developed Real Coded Genetic Algorithms

Kusum DEEP [a], Shashi [b], Vinod K. KATIYAR [c] and Atulya K. NAGAR [d]

[a b c] Department of Mathematics, Indian Institute of Technology Roorkee - India
Email: kusumfma@iitr.ernet.in, shashibarak@gmail.com, vktmafma@iitr.ernet.in
[d] Centre for Applicable Mathematics and Systems Science (CAMSS), Department of Computer and Mathematical Sciences, Liverpool Hope University - U.K.
Email: nagara@hope.ac.uk

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Abstract. The problem of finding the global minimum of molecular potential energy function is very challenging for algorithms which attempt to determine global optimal solution. The principal difficulty in minimizing the molecular potential energy function is that the number of local minima increases exponentially with the size of the molecule. The global minimum of the potential energy of a molecule corresponds to its most stable conformation, which dictates the majority of its properties. In this paper the efficiency of four newly developed real coded genetic algorithms is tested on the molecular potential energy function and their supremacy is established over other existing algorithms. The minimization of the function is performed on an independent set of internal coordinates involving only torsion angles. Computational results with up to 100 degrees of freedom are presented.

Keywords: Global optimization, Molecular conformations, Real coded genetic algorithm, Potential energy function.
AMS Classification: 90C26, 90C59

1. Introduction

Finding the most stable conformation of a molecule is a captivating problem as it is highly complex and its complexity increases with the increase in number of atoms. Amongst many different spatial configurations for a given molecule, the most stable one is of particular importance as it dictates most of its properties. Experimental evidence [1] shows that in the majority of the cases the most stable conformation corresponds to the one involving the global minimum of potential energy. So it can be formulated as a global optimization problem. It is an eminently challenging global optimization problem as the number of local minima increases exponentially with the size of the molecule [2]. These local minimizers correspond to metastable states of the molecule and the global minimizer defines the energetically most favorable molecular conformation. Many optimization methods have already been applied to this problem, such as branch and bound methods, smoothing methods, simulated annealing, and genetic algorithms. References [2-4] provide an overview about these and other methods for molecular conformation problems. Further, a function [5] has been developed to test methods applied to global minimization of potential energy of molecules. In literature, many researchers for example [6-9] have applied computational intelligence methods for minimizing the potential energy function.

The aim of the present paper is to investigate the effect of newly developed RCGAs on a highly complex molecular potential energy problem and to check the efficiency of the new operators of RCGAs and to look for the their contribution in the success of an algorithm. In this paper the potential energy problem with up to 100 degrees of freedom is solved using four newly developed real coded genetic algorithms: WX-PM, WX-LLM, LX-LLM (Communicated to Applied Mathematics and Computation) and LX-PM [10].

Corresponding Author. Email: kusumfma@iitr.ernet.in

This paper is organized as follows: Section 2 describes the molecular potential energy function mathematically; Section 3 describes the real coded genetic algorithms applied for solving the problem; and Section 4 presents the performance evaluation criteria used in this paper for evaluating the performance of all algorithms used. Computational results and discussions are presented in Section 5 and conclusions in Section 6.

2. Problem Discussion

In a simplified molecular model consists of a linear chain of n beads centered at $x_1,...,x_n$ in a 3-dimensional space for every pair of consecutive beads x_i and x_{i+1}, let $r_{i,i+1}$ be the bond length which is the Euclidean distance between them. For every three consecutive beads x_i, x_{i+1}, x_{i+2}, let $\theta_{i,i+1}$ be the bond angle corresponding to the relative position of the third bead with respect to the line containing the previous two. Likewise, for every four consecutive beads $x_i, x_{i+1}, x_{i+2}, x_{i+3}$, let $\omega_{i,i+3}$ be the angle, called the torsion angle, between the normals through the planes determined by the beads x_i, x_{i+1}, x_{i+2} and $x_{i+1}, x_{i+2}, x_{i+3}$ all of which can be understood from Figure 1.

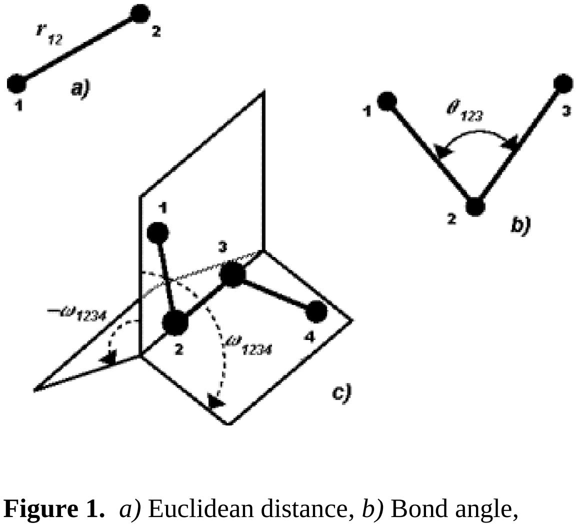

Figure 1. *a)* Euclidean distance, *b)* Bond angle, *c)* Torsion angle of Coordinate Set of Atomic Chain

The potential energy of a system of atoms is explained through force field potentials, where a force field is a mathematical function which returns the energy of a system as a function of the conformation of the system. Now the forces can be written in terms of potential energy functions of various structural features such as bond lengths, bond angle, non bonded interactions etc.

Here the force field potentials corresponding to bond lengths, bond angles and torsion angles will be defined respectively as

$$E_1 = \sum_{(i,j)\in M_1} c_{ij}^1 (r_{ij} - r_{ij}^0)^2,$$

$$E_2 = \sum_{(i,j)\in M_2} c_{ij}^2 (\theta_{ij} - \theta_{ij}^0)^2, \qquad (1)$$

$$E_3 = \sum_{(i,j)\in M_3} c_{ij}^3 (1 + \cos(3\omega_{ij} - \omega_{ij}^0)),$$

where c_{ij}^1 is bond stretching force constant, c_{ij}^2 is angle bending force constant and c_{ij}^3 is the torsion force constant. The constants r_{ij}^0 and θ_{ij}^0 represent the "preferred" bond length and bond angle respectively and ω_{ij}^0 is the phase angle that defines the position of the minima. $M_k, k = 1,2,3$ represents the set of pair of atoms separated by k covalent bonds. In addition to the above, there is also a potential E_4 which characterizes the 2-body interactions between every pair of beads separated by more than two covalent bonds along the chain. We use the following function to represent E_4:

$$E_4 = \sum_{(i,j)\in M_3} \left(\frac{(-1)^i}{r_{ij}} \right), \qquad (2)$$

where r_{ij} is the Euclidean distance between the beads x_i and x_j. The general problem is to minimize the total molecular potential energy $E = E_1 + E_2 + E_3 + E_4$, leading to the optimal spatial position of the beads. Using the parameters defined in [5] potential energy function takes the following form

$$E = \sum_i \left(1 + \cos(3\omega_{i,i+3})\right) + \sum_i \left(\frac{(-1)^i}{\sqrt{10.60099896 - 4.141720682\cos(3\omega_{i,i+3})}} \right), \qquad (3)$$

where $i = 1,...,n-3$ and n is the number of beads in the given system. The problem is thus reduced to find $\omega_{i,i+3}$, $i=1,...,n-3$. As E is a nonconvex function it involves numerous local minimizers even for small value of *n*. These local minimizers correspond to a state which is not truly stationary but is almost stationary called the metastable state of the molecule. Lavour and Maculan [5] have shown that the number of local minimizers of the function (3) is 2^N, where $N=n-3,\ n$ is the total number of beads in a molecule. The global minimum of *E* is the alternate sequence of torsion angles <a, b, a, b, a, b, a, b, …> independent of the number of variables, where a=1.039195303 and b= 3.141592654. And by restricting $\omega_{i,j}$; $0 \le \omega_{i,j} \le 5$ the existence of only one global minimum is guaranteed. As given in [6] it can also be shown that for all value of *n* the difference between the global minimum value E^* and second best value of (3) i.e. E_2 always satisfies the following relation

$$\left| E^* - E_2 \right| = 0.0816608225 \qquad (4)$$

Although many simplifications have been done in the function E despite these, the problem remains very difficult because of the large diversity of local minimizers possible. It can be seen from the fact that corresponding to 20 beads, the number of local minimizers will be $2^{17}=131072$.

3. Real Coded Genetic Algorithm

Genetic algorithms are population based heuristics which are used to determine solution of non-linear optimization problems. GAs mimics the Darwin's principal of survival of fittest. GA uses three basic operations: selection, crossover and mutation in moving from one generation to another. GAs which make use of the real-encoding of chromosomes are termed as Real Coded GAs (RCGAs). Four different RCGAs are used in this paper, which use two real coded crossover operators WX and LX [11] and two mutation operators LLM and PM [10]. The schema of RCGAs is given in Figure 2.

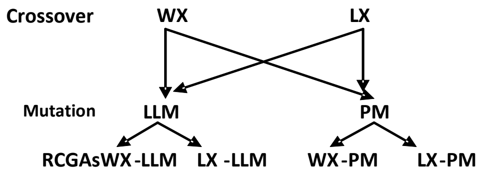

Figure 2. Schema of all RCGAs used

More details of operators used in all the algorithms used here are defined in the following subsections:

3.1. Crossover

Two offsprings O_1 and O_2 are generated from a pair of parents P_1 and P_2 obtained after selection, in the following manner:
Generate a random number $u \in [0,1]$,
Check if $u \le \frac{1}{2}$; then

$$\begin{aligned} O_1 &= P_1 + \beta \times d \\ O_2 &= P_2 + \beta \times d \end{aligned} \qquad (5)$$

otherwise if $u > \frac{1}{2}$, then

$$\begin{aligned} O_1 &= P_1 - \beta \times d \\ O_2 &= P_2 - \beta \times d \end{aligned} \qquad (6)$$

where $d = P_1 - P_2$ is the distance between the parents and β is a random number following Laplace distribution in case of LX and Weibull distribution in case of WX.

3.2. Mutation

A mutated solution M is created in the vicinity of the solution P as follows:
Generate a random number $r \in [0,1]$,
Check if $r < T$; then

$$M = P - \lambda(P - L) \qquad (7)$$

Otherwise, if $r \ge T$, then

$$M = P + \lambda(U - P) \qquad (8)$$

where L and U are the lower and upper bounds of decision variable, $T = \frac{P-L}{U-P}$ and λ is a random number following Power distribution in case of PM and Log Logistic distribution in case of LLM.

3.3. Selection Technique

A selection technique in a GA is simply a process that favors the selection of better individuals in the population for the mating pool. All RCGAs used in this paper uses tournament selection.

3.4. Computational Steps

Computational steps of algorithms used are as follows:

1. *Generate a suitably large initial set of random points within the domain*

prescribed only by the bounds on variable i.e. points satisfying $L \le x \le U$.

2. *Check the stopping criteria, if satisfied stop; else go to 3.*
3. *Apply tournament selection procedure on initial (old) population to make mating pool.*
4. *Apply crossover and mutation to all individuals in mating pool, with probability of crossover* p_c *and probability of mutation* p_m *respectively, to make new population.*
5. *Increase generation ; replace old population by new population; go to 2.*

4. Performance Evaluation Criteria

For evaluating the performance of each method the following are recorded:

1)SuccessRate(SR) $= \frac{Number\ of\ successful\ runs}{Total\ number\ of\ runs} \times 100$

2) Average computational time of successful runs (in seconds).

3) Average number of function evaluations of successful runs (AFE).

4) Minimum number of function evaluations of successful runs (MNFE).

5) Maximum number of function evaluations of successful runs (MXFE).

6) Standard Deviation of function evaluations of successful runs (SDFE).

7) Performance Index (PI).

A run in which the algorithm finds a solution satisfying $f_{\min} - f_{opt} \le 0.01$, where $f_{\min}$ is the best solution found when the algorithm terminates and f_{opt} is the known global minimum of the problem is considered to be successful. For each problem size, MNFE represents minimum and MXFE represents the maximum number of function evaluations needed to achieve the threshold in the 100 runs performed. Also, AFE represents the average number of function evaluations and SDFE represents the standard deviation of the successful runs out of all the 100 runs performed.

The Performance Index (PI) given by Bharti [12] and used in [11] is utilized to compare the relative performance of all the four RCGAs simultaneously. This index gives prescribed weighted importance to SR, AFE and computational time. For each of the algorithms the value of PI is computed as follows:

$$PI = \frac{1}{N}\sum_{i=1}^{N}(k_1\alpha_1^i + k_2\alpha_2^i + k_3\alpha_3^i), \quad (9)$$

where

$$\alpha_1^i = \frac{Sr^i}{Tr^i}, \quad \alpha_2^i = \begin{cases} \frac{Mt^i}{At^i}, & if\ Sr^i > 0 \\ 0, & if\ Sr^i = 0 \end{cases}, \quad \alpha_3^i = \begin{cases} \frac{Mf^i}{Af^i}, & if\ Sr^i > 0 \\ 0, & if\ Sr^i = 0 \end{cases}$$

$i = 1, 2, \ldots N$

and

Sr^i = number of successful runs of ith problem.

Tr^i = total number of runs of ith problem.

At^i = average time used by an algorithm in obtaining the solution of ith problem.

Mt^i = minimum of average time used by all the algorithms in obtaining the solution of ith problem.

Af^i = average number of function evaluations of successful runs used by an algorithm in obtaining the solution of ith problem

Mf^i = minimum of average number of function evaluations of successful runs used all algorithms in obtaining the solution of ith problem

N = total number of problems considered.

Further, $k_1, k_2\ and\ k_3\ (k_1 + k_2 + k_3 = 1 and\ 0 \le k_1, k_2, k_3 \le 1)$ are the weights assigned by the user to the average execution time, average number of function evaluations and the percentage of success respectively. The same methodology is adopted as given in [13] by assigning equal weights to two of these terms ($k_1, k_2\ and\ k_3$) at a time so that, PI become function of a single variable. The resulting cases are as follows:

$a)\ k_1 = w, k_2 = k_3 = \frac{1-w}{2}, 0 \le w \le 1$

$b)\ k_2 = w, k_1 = k_3 = \frac{1-w}{2}, 0 \le w \le 1$

$c)\ k_3 = w, k_1 = k_2 = \frac{1-w}{2}, 0 \le w \le 1.$

All the RCGAs have the same termination criteria i.e. if either the maximum number of generation (5000) is reached or known global minimum is attained.

5. Computational Results and Discussion

In this section we present numerical results obtained for the energy function E. The program is coded in C++ and executed on a Pentium IV with 1.66GHz speed and 512 MB of RAM. The potential energy function *E* is minimized in the specified search space $[0, 5]^n$, where *n* is the total number of beads in a system. Table 1 reproduces the global minimum values of [6] attained for the function *E* corresponding to different chain sizes i.e. corresponding to *n* equal to 20, 40, 60, 80 and 100. top edge indicated.

Table 1. Global minimum value for chains of different sizes (for *n=20 to 100*)

n	20	40	60	80	100
E	-0.822366	-1.644732	-2.467098	-3.289464	-4.111830

Since we are using a probabilistic technique, 100 independent runs are performed, each time using a different seed for the generation of random number. The parameter setting for all algorithms is given in Table 2.

Table 2. Parameter setting of all RCGAs used for finding the Global minimum of E

Parameter	WX-PM	LX-PM	WX-LLM	LX-LLM
Pop size	5*n*	10*n*	5*n*	5*n*
p_c	0.7	0.65	0.75	0.7
p_m	0.08	0.05	0.04	0.06

Computational results are presented in Table 3 in terms of function evaluations: average, minimum, maximum, and standard deviations of successful runs as well as the computational time of all new RCGAs. These are compared with the existing results of Bansal et al. [14] and Barobosa et al. [6].

In Table 3 rHYB [2] denotes the staged hybrid GA with a reduced simplex and a fixed limit for simplex iterations and qPSO [14] is a hybrid PSO in which quadratic approximation operator is hybridized with PSO. In case of qPSO, no run is found to be successful, i.e. the difference between the best solution found by the algorithm and the known global minima is always greater than 0.01.

It is quite clear from the Table 3 that the newly developed RCGAs have outperformed both rHYB and qPSO.

Table 3. Computational results for simplified molecular model for *n=20 to 100* using WX-PM, LX-PM, WX-LLM, LX-LLM, rHYB [6] and qPSO [14].

n	Algorithm	AFE	MNFE	MXFE	SDFE	Time (sec)
20	WX-PM	15574	8412	24051	3675	0.45
	LX-PM	23257	29313	37096	5523	0.53
	WX-LLM	28969	17643	44867	7117	0.59
	LX-LLM	**14586**	10351	21532	3021	0.34
	rHYB*	35836	31415	41653	2530	27.27
	qPSO**	-	-	-	-	-
40	WX-PM	59999	37863	95335	13015	2.46
	LX-PM	71336	45544	99370	15184	2.57
	WX-LLM	89478	61765	120042	18059	3.34
	LX-LLM	**39366**	34202	53370	4342	1.47
	rHYB*	129611	120967	143940	5350	246.05
	qPSO**	-	-	-	-	-
60	WX-PM	175865	136429	195119	14635	10.39
	LX-PM	280131	203618	329337	35492	15.65
	WX-LLM	225008	195462	300197	25165	12.15
	LX-LLM	**105892**	83272	155530	14865	5.54
	rHYB*	249963	238867	271393	7431	784.93
	qPSO**	-	-	-	-	-
80	WX-PM	302011	281755	323296	21684	20.71
	LX-PM	326287	281876	369451	27841	25.12
	WX-LLM	372836	322095	398969	20432	31.28
	LX-LLM	**237621**	263097	291265	19032	18.03
	rHYB*	387787	370534	405025	8901	3234.59
	qPSO**	-	-	-	-	-
100	WX-PM	369376	324621	412876	30276	30.62
	LX-PM	379998	310432	467427	36848	31.98
	WX-LLM	443786	399601	498352	28659	39.91
	LX-LLM	**320146**	268764	356729	32412	26.48
	rHYB*	554026	534697	581879	11182	4176.03
	qPSO**	-	-	-	-	-

* Barbosa et al., [6], ** Bansal et al., [14]

To further analyze the relative performance of all RCGAs in terms of average function evaluations, a graphical representation in the form of box plot is shown in Figure 3, where the best performer is marked with star. The average function evaluation is directly proportional to the computational cost of the method. It is clear that LX-LLM is the best performing algorithm and so in terms of computational time (see Figure 4).

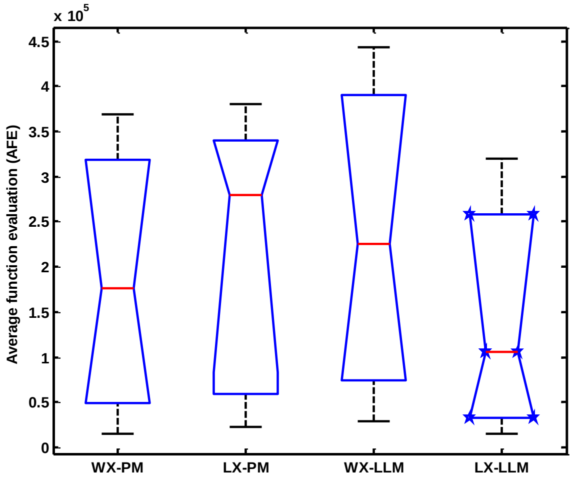

Figure 3. Box plot of Average function evaluations (AFE) for simplified molecular model.

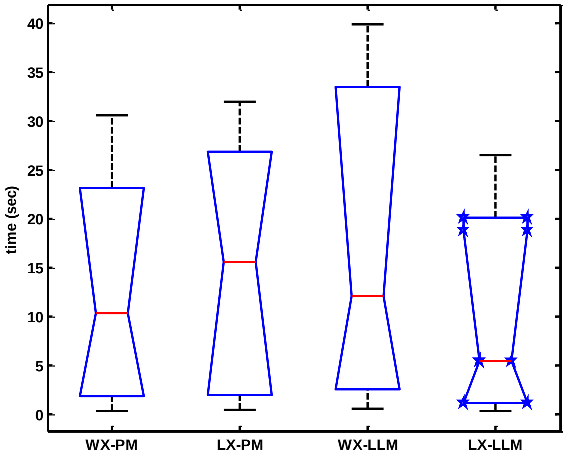

Figure 4. Box plot of computational time (in sec) for simplified molecular model.

Table 4 compares the success rate of all the four RCGAs considered in this paper. The success rate is directly proportional to the reliability of the method. The corresponding box plot is shown in Figure 5. It is clear that in this case also the performance of LX-LLM is the best amongst all.

Table 4. Success Rate (SR) for simplified molecular model for *n=20 to 100* using WX-PM, LX-PM, WX-LLM, LX-LLM.

n	WX-PM	LX-PM	WX-LLM	LX-LLM
20	100	100	100	100
40	100	100	98	100
60	93	91	89	95
80	71	79	78	82
100	89	88	82	86

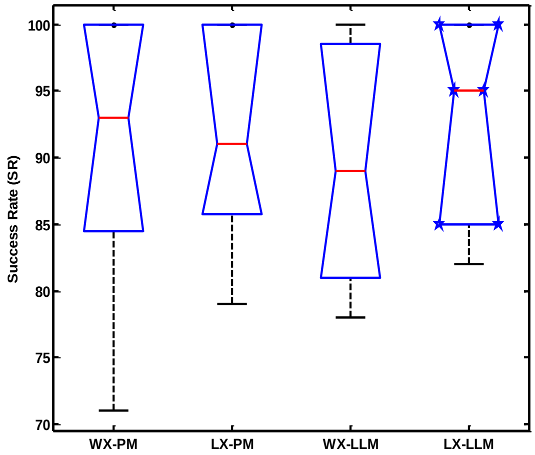

Figure 5. Box plot of Success rate (SR) for simplified molecular model.

To see the consolidated effect of all the factors (AFE, SR and the computation time together), the performance index (PI) is plotted (Figure 6 – Figure 8) for all the three cases (*a*, *b*, *c*) discussed in the previous section. Now the PIs clearly indicate the supremacy of LX-LLM over WX-PM, WX-LLM and LX-PM.

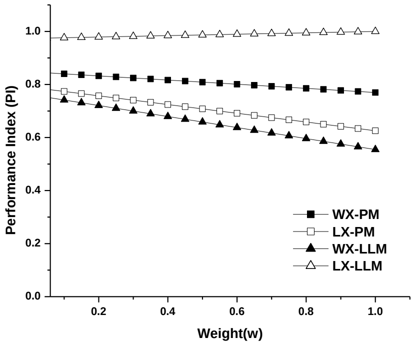

Figure 6. PI for WX-PM, LX-PM, WX-LLM, LX-LLM when $k_1 = w, k_2 = k_3 = (1-w)/2$

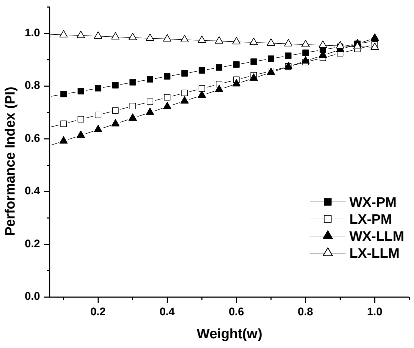

Figure 7. PI for WX-PM, LX-PM, WX-LLM, LX-LLM when $k_2 = w, k_1 = k_3 = (1-w)/2$

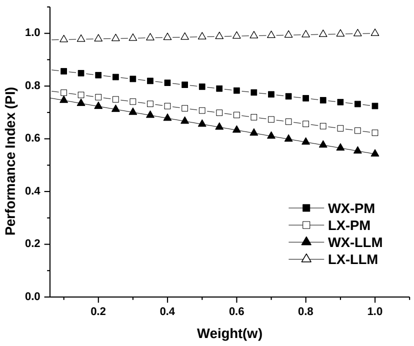

Figure 8. PI for WX-PM, LX-PM, WX-LLM, LX-LLM when $k_3 = w, k_1 = k_2 = (1-w)/2$

6. Conclusions

In this paper, newly developed RCGAs are successfully applied to a scalable simplified energy function. Although the energy function is taken in simplified form yet it keeps the main difficulty that the number of local minima of the function grows exponentially with problem size, making it difficult to find the global minima. Computational tests are performed with degrees of freedom varying from 20 to 100. It is clear that LX-LLM is the best performing algorithm as it is less computationally expensive (in terms of AFE and time) as well as more reliable (in terms of SR) amongst all other RCGAs applied for obtaining the global minimum. Also the consolidated effect of all factors can be seen together in the plots for PI and it is very clear that LX-LLM is performing the best.

Although LX-LLM is the best, from this it can not be concluded that Laplace crossover (LX) is better than Weibull crossover (WX) because in that case LX-PM should have performed better than algorithms which use WX. This fact compels us to notice the importance of mutation operators in the efficiency of a genetic algorithm. Then again, mutation alone can not be credited for the success of an algorithm. It is the appropriate combination of the crossover and mutation operators which guides the search of a genetic algorithm in an effective manner. In other words, exploration of the search space should be backed with appropriate diversity of the population. So here in the case of molecular potential energy function this job is done by LX-LLM.

Finally, LX-LLM has successfully obtained the global minimum of molecular potential energy function, it is observed that LX-LLM is an efficient search algorithm which is it not limited to the cases considered here but can also be applied to some other and more complex functions.

Acknowledgments

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***Kusum Deep** is Associate Professor in the Department of Mathematics, Indian Institute of Technology Roorkee, India. Her research interests are in numerical optimization including evolutionary computations: genetic algorithms, memetic algorithms, particle swarm optimization, etc. She has more than 50 research papers in journals/conferences. She holds a number of national and international awards.*

***Shashi** is currently pursuing her Ph.D. degree in Mathematics at Indian Institute of Technology Roorkee, India. She received her Master of Science in Mathematics from University of Delhi. Her research interests are Real Coded Genetic Algorithms, Particle Swarm Optimization and their applications to the bio-related fields.*

***Vinod K. Katiyar** is a Professor in Department of Mathematics, Indian Institute of Technology Roorkee, India. His research interests are Fluid Mechanics, M.H.D., Biofluid mechanics, Plasma Physics, Industrial Mathematics and Mathematical Modeling etc. He has more than 80 research papers in Journals/ Conferences.*

***Atulya K. Nagar** holds the Foundation Chair of Computer and Mathematical Sciences, and is the Head of the Department of Computer Science, at Liverpool Hope University. He received a prestigious Commonwealth Fellowship for pursuing his Doctorate in Applied Non-Linear Mathematics, which he received from the University of York in 1996. He holds BSc (Hons.), MSc and MPhil (distinction) in Mathematical Sciences from the MDS University of Ajmer, India. Prior to joining Liverpool Hope University, he worked for several years as a Senior Research Scientist at Brunel University. His multidisciplinary research interests include relativistic cosmology, non-linear differential equations, systems engineering, natural computing (membrane computing), computational optimisation and intelligent systems.*