ABSTRACT

In this work, the focus of the studies is on the dendrimers known as PAMAM, whose applications range from drug elution to molecular encapsulation and gene therapy, and from building blocks for nanostructures to micelles as decontamination agents. This work develops some methods that replace those originally used in the PyPolyBuilder program, aiming to decrease the execution time and improve the molecules generated at the end of the program, making them larger and with a more spherical shape. To develop the methods, the simulations were performed using PAMAM. First, the method that generates the Z-matrix has been improved. This method was the computational bottleneck of the program and because it was one of the early stages of the program, it caused great difficulty in carrying out tests in the following stages. Following, a new fitness function was developed for global optimization. It allows greater control of the shape of the dendrimer that is generated at this stage of the program. And finally, with the intention of improving the individuals generated by global optimization, some of the main evolutionary computation algorithms were tested and adjusted in the PAMAM zero generation, namely: Genetic Algorithm (GA), Differential Evolution (DE), Particle Swarm Optimization (PSO) and Covariance Matrix Adaptation Evolution Strategy (CMA-ES). Each of the algorithms has its own variety of methods and parameters to be adjusted. To avoid the problem known as " the curse of dimensionality ", a random methodology was used in the adjustments, as it does not demand an unreasonably large number of executions and, even so, it guarantees the diversity of individuals in the observed search space. After the algorithms have their parameters and methods adjusted, the top ten are selected and simulated for generations one, two, three, four, five, seven, and ten of PAMAM, so that the best parameters and methods are defined for each algorithm. Thus, the algorithms are compared with each other using the best methods and parameters chosen. GA-based algorithms have the worst results among those observed. The CMA-ES presents the best results for the smaller generations, but it presents memory error in the 10th generation. With the CMA-ES being excluded from the analysis, the DE presents the best results for the younger generations and the PSO presents the best results for the older generations of PAMAM.

Keywords: Dendrimers; PAMAM; Evolutionary Computing; GA; DE; PSO; CMA-ES.