Molecular Dynamics Optimizer

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Abstract. Molecular system possesses two main characteristics that seem to be applicable for the contrary goals of proximity and diversity in multiobjective optimization, namely the converging pressure in potential fields as dictated by the Maxwell-Boltzmann distribution and the inherent drift to a homogenous and uniform equilibrium with maximum entropy, even without any prior knowledge on the geometry and state of the enclosure. Inspired by this association, this paper explores the notion of exploiting molecular motion to solve multiobjective problems. By adapting the algorithmic structure of molecular dynamics, which essentially represents a technique for the computer simulation of molecular motion, a molecular system that is relevant for multiobjective optimization is proposed, known as molecular dynamics optimizer (MDO). The performance of MDO was subsequently compared with other conventional multiobjective optimizers, specifically EA and PSO, and the experimental results demonstrated that MDO is indeed a viable and practical approach for multiobjective optimization.

Keywords: Multiobjective optimization, molecular dynamics.

1 Introduction

The development of computational techniques for multiobjective optimization (MOO) has significantly grown in the last few years due to their success in satisfying the optimization goals of attaining near-optimal, diverse and uniformly distributed solution sets for various multiobjective problems (MOP). The basic requirement for multiobjective optimizers is to balance between the proximity and diversity goals of MOO, providing sufficient convergence pressure without compromising diversity. Hence, regardless of the configurations of the initial solution, the ultimate solutions generated by the multiobjective optimizer should ideally be well distributed within the optimal region for the MOP.

Many of these optimizers were actually inspired from nature, for instance evolutionary algorithm (EA) from evolutionary biology, ant colony optimization (ACO) from the behavior of real ant colony and particle swarm optimization (PSO) from the swarm behavior of birds. Actually, one could find a resemblance between the evolving solutions generated by evolutionary optimizers and the dynamics of ideal gas molecules in an enclosure. In the presence of unequal potential fields, there will

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be a higher probability for molecules to reside in the lower potential regions. Furthermore, these molecules will always tend to a homogenous and uniform equilibrium with maximum entropy [1], even without any prior knowledge on the geometry and state of the enclosure. The convergence and diversity nature of molecular motions appears to be inherently well suited for MOO. Thus, it might be possible to develop a multiobjective optimizer based on this natural phenomenon.

Actually, the notion of exploiting the dynamics of molecules for MOO is not new. Kita *et al* [2] and Cui *et al* [3] formulated strategies based on the thermodynamic notion of energy and entropy that will prevent premature convergence by maintaining an appropriate level of diversity. Similarly, Sobieski *et al.* [4] designed variation operators that project solutions based on a bell-curve distribution. This idea was realized in [5], where an expansion operator designed based on the thermodynamic behavior of ideal gas expanding in an enclosure was used to complement the crossover and mutation operation. Of more recent issue, a selection strategy and stopping conditions were designed by using the natural principles of a dynamical system approaching its equilibrium state [6]. Closely related to molecular motion is a well established theoretical framework, statistical mechanics, which studies the overall behavior of many molecules in terms of their actual motion and interactions. While statistical mechanics cannot chart out the life history of one molecule in a system, it is able to describe the macro behavior of the molecular system as a whole. Because MOO usually involve manipulating populations of solutions, the value of this framework is obvious. In fact, statistical mechanics had been used on several occasions to analyze the dynamics of EA [7].

Nevertheless, analytical solutions in statistical mechanics are restricted only for simple and ideal cases. For intractable systems, molecular simulation is used instead for more accurate results and has played an important role as a bridge connecting models to theory. Molecular simulation is a general term for the use of computer models to describe physical systems at a molecular level of detail, particularly the individual position and orientation of every molecule and from that, both thermodynamic and kinetic properties of the system could be derived. Molecular simulation is commonly done by employing either Monte Carlo or molecular dynamics [8], with the latter being the research subject in this paper. Molecular dynamics numerically solves Newton's equations of motion on molecular system and update their state properties correspondingly.

Since molecular dynamics is essentially a computer simulation of molecular motion and considering the inherent diverse behavior of molecular system and their converging drift pressure in the presence of unequal potential fields, molecular dynamics appears to be a possible computational platform to apply molecular motion for MOO purposes. As such, this idea will be explored in this paper. By adapting the algorithmic structure of molecular dynamics, a molecular system that is relevant for multiobjective optimization is proposed, known as molecular dynamics optimizer (MDO). It should be highlighted that this paper aims to show that the basic principles derived from the dynamics of molecules can be applied for MOO purposes, instead of modeling exactly any real-life molecular phenomenon. Thus, the model proposed will be as generic as possible and the proof of principle study will focus mainly on the investigation of its feasibility and characteristics.