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Multicanonical jump walk annealing assisted by tabu for dynamic optimization of chemical engineering processes

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Abstract

A hybrid methodology, viz., multicanonical jump walk annealing assisted by tabu list (MJWAT) is proposed for solving dynamic optimization problems in chemically reacting systems. This method combines the power of multicanonical sampling with the beneficial features of simulated annealing. Incorporating tabu list further enhances the efficiency of the method. The superior performance of the MJWAT is highlighted with the help of five benchmark case studies.

Keywords: Dynamic optimization; Monte Carlo simulations; Multicanonical algorithms; Metaheuristics; Simulated annealing; Tabu conditions

1. Introduction

Dynamic optimization (i.e. open loop control) problems are encountered in several industrially important applications; for example, chemically reacting systems, optimal control of batch, semi-batch and fed-batch reactors control and scheduling of batch processes, startup, upset, shutdown and transient analysis; safety studies and the evaluation of control schemes etc. have recently received significant interest. Optimal control deals with the problem of finding a control policy for a given system such that a certain optimality criterion is achieved. Dynamic optimization problems (DOP) are challenging due to their highly non-linear nature and the presence of constraints on both the state and control variables. DOP formulations can be solved by deterministic or stochastic approaches (for review and references therein, Srinivasan et al., 2003; Biegler and Grossmann, 2004). This work considers application of stochastic global optimization methods to solve DOP.

Stochastic optimization methods such as, genetic algorithms (Mitchell, 1998; Said, 2005), simulated annealing (Triki et al., 2005), tabu search (Chelouah and Siarry, 2000; Glover and Hanafi, 2002), ant colony optimization (Dréo and Siarry, 2004; Dorigo and Blum, 2005) have recently become very popular as effective methods for handling difficult global optimization problems in different fields. Some of these have also been successfully applied in solving DOP (Kapadi and Gudi, 2004; Faber et al., 2005; Zhang et al., 2005).

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Monte Carlo (MC) simulation methods have found applications in diverse fields, including chemistry, biology, physics, engineering, and economics. Simulated annealing (SA) is perhaps the most popular flavor of MC simulations (Hamam and Hindi, 2000; Naït-Ali and Siarry, 2002; Xambre and Vilarinho, 2003; Hifi et al., 2004; Triki et al., 2005). In statistical physics, MC simulation based global optimization methods are routinely developed to solve molecular dynamics problems, which are known to be NP-complete. Problems involving Lennard-Jones and Morse clusters, protein folding structures, spin glass systems (Sugita and Okamoto, 2000; Frantz, 2001; Newman and Barkema, 2001; Lee and Berne, 2001;Yaşar et al., 2002; Hansmann and Okamoto, 2004; Reynal and Diep, 2005) are some of the examples which have been solved successfully by Monte Carlo methods. Metropolis MC based simulations are most widely used due to the inherent simplicity. The method chooses the new configuration in the neighborhood of a current solution with unit probability if it has a lower energy and if it has higher energy than the current configuration, it will be accepted based on Boltzmann probability. For application to sophisticated systems with multimodal functionality and high-energy barriers between the potential energy minima in a system, several different modifications of the basic Metropolis MC simulations and simulated annealing have been devised (Beichl and Sullivan, 1999; Berg, 2003; Andricioaei and Straub, 1997; Iwamatsu and Okabe, 2000; Frantz, 2001; Ortiz et al., 2003). Most of these modifications incorporate appropriate changes in the basic acceptance probability function. Among the advanced MC algorithms, multicanonical sampling is most frequently used (Gubernatis and Hatano, 2002; Hansmann and Okamoto, 2004; Reynal and Diep, 2005). In multicanonical algorithms (MUCA) the configurations are sampled with a probability inversely proportional to the density of the corresponding energy states. This strategy enables the algorithm to explore the high-energy barriers. Nevertheless, pure multicanonical methods may not efficiently sample low-energy configurations as the weight factor used is derived from the previous iterations, which has no information concerning the unexplored low-energy regions of the landscape (Xu and Berne, 1999). In jump walk MC simulations (Frantz, 2001), a low-temperature simulation is permitted to attempt jumps to configurations that were sampled in a simulation that was run at a higher temperature. A Metropolis criterion is applied while deciding whether or not to accept the move. To implement the jump walk algorithm, one usually performs a high-temperature simulation and subsequently stores a subset of configurations from the high-temperature simulation. Then, a low-temperature simulation reads the stored configurations and randomly picks one for the jump. This approach obviously requires large disk space to save the high-temperature configurations. Many authors proposed combination of ideas from MUCA, Jump walk and annealing process (Zhou and Berne, 1997; Xu and Berne, 1999, 2000; Okamoto, 2001). Xu and Berne (2000) implemented combination of MUCA and Jump walk approaches, called multicanonical jump walk annealing, where, MUCA enhances the weights of relevant rare configurations against high-energy barriers that facilitate SA to adequately search low-energy states.

This work proposes the application of multicanonical jump walk annealing assisted by tabu conditions (MJWAT) to solve dynamic optimization problems. Tabu conditions help the algorithm to selectively choose high-energy states (uphill moves made by the system corresponding to minimization of objective function). Three criteria that are adopted from Ji and Tang (2004) are used to define a move as tabu.

In this work, solution process of DOP is based on parameterization of control variables using piecewise-constant approach. It results into a NLP formulation, which is solved using the proposed algorithm. The performance is tested on five case studies from process engineering literature. The results show the effectiveness of the multicanonical sampling based methods to solve DOP.

The paper is organized as follows: Section 2 describes the multicanonical jump walk annealing method assisted by tabu conditions to solve function optimization problems; Section 3 deals with the definition and formulation of dynamic optimization problems. Results and discussion are given in Section 4 while salient conclusions and possible directions for future work are provided in Section 5.

2. Multicanonical jump walk annealing assisted by tabu conditions (MJWAT)

To make the paper self-contained, a basic overview of simulated annealing, multicanonical sampling and application of tabu list in the tabu search algorithm is given, before describing the proposed algorithm in detail.