Optimization by thermal cycling

A. Möbius

Leibniz Institute for Solid State and Materials Research Dresden,
PF 270116, D-01171 Dresden, Germany
E-mail: a.moebius@ifw-dresden.de

K.H. Hoffmann

TU Chemnitz, Institute of Physics, D-09107 Chemnitz, Germany
E-mail: hoffmann@physik.tu-chemnitz.de

C. Schön

Max Planck Institute for Solid State Research,
D-70569 Stuttgart, Germany
E-mail: schoen@fkf.mpg.de

Abstract

Thermal cycling is an heuristic optimization algorithm which consists of cyclically heating and quenching by Metropolis and local search procedures, respectively, where the amplitude slowly decreases. In recent years, it has been successfully applied to two combinatorial optimization tasks, the traveling salesman problem and the search for low-energy states of the Coulomb glass. In these cases, the algorithm is far more efficient than usual simulated annealing. In its original form the algorithm was designed only for the case of discrete variables. Its basic ideas are applicable also to a problem with continuous variables, the search for low-energy states of Lennard-Jones clusters.
I. INTRODUCTION

Optimization problems with large numbers of local minima occur in many fields of physics, engineering, and economics. They are closely related to statistical physics, see e.g. Ref. [1]. In the case of discrete variables, such problems often arise from combinatorial optimization tasks. Many of them are difficult to solve since they are NP-hard, i.e., there is no algorithm known which finds the exact solution with an effort proportional to any power of the problem size. One of the most popular such tasks is the traveling salesman problem: how to find the shortest roundtrip through a given set of cities [2].

Many combinatorial optimization problems are of considerable practical importance. Thus, algorithms are needed which yield good approximations of the exact solution within a reasonable computing time, and which require only a modest effort in programming. Various deterministic and probabilistic approaches, so-called search heuristics, have been proposed to construct such approximation algorithms. A considerable part of them borrows ideas from physics and biology. Thus simulated annealing [3] and relatives such as threshold accepting as well as various genetic algorithms [4] have successfully been applied to many problems. Particularly effective seem to be genetic algorithms in which the individuals are local minima [5, 6]. For recent physically motivated heuristic approaches we refer to thermal cycling [7], optimization by renormalization [8], and extremal optimization [9]. For problems with continuous variables, approaches which combine Monte-Carlo procedures for global search with deterministic local search by standard numerical methods, for example the basin-hopping algorithm, have proved to be particularly efficient [10, 11]. They can be considered as relatives of the genetic local search approaches for the case of discrete variables. Here we focus on the thermal cycling algorithm and illuminate the reasons for its efficiency.

II. THERMAL CYCLING ALGORITHM

Simulated annealing [3] can be understood as a random journey of the sample (i.e. the approximate solution) through a hilly landscape formed by the states of its configuration space. The altitude, in the sense of a potential energy, corresponds to the quantity to be optimized. In the course of the journey, the altitude region accessible with a certain probability within a given number of steps shrinks gradually due to the decrease of the temperature in the
Metropolis simulation involved. The accessible area, i.e., the corresponding configuration space volume, thus shrinks until the sample gets trapped in one of the local minima.

Deep valleys attract the sample mainly by their area. However, it is tempting to make use of their depth. For that, we substitute the slow cooling down by a cyclic process: First, starting from the lowest state obtained so far, we randomly deposit energy into the sample by means of a Metropolis process with a certain temperature $T$, which is terminated, however, after a small number of steps. This part is referred to as heating. Then we quench the sample by means of a local search algorithm. Heating and quenching are cyclically repeated where the amount of energy deposited in a cycle decreases gradually, see Fig. 1. This process continues until, within a ‘reasonable’ CPU time, no further improvement can be found.

It is an essential feature of the thermal cycling algorithm that two contradicting demands are met in heating: the gains of the previous cycles have to be retained, but the modifications must be sufficiently large, so that another valley can be reached. Thus the heating process has to be terminated in an early stage of the equilibration. An effective method is to stop it after a fixed number of successful Metropolis steps.

The efficiency of the proposed algorithm depends to a large extent on the move class considered in the local search procedure. For discrete optimization problems, it is a great advantage of our approach that far more complex moves can be taken into account than in simulated annealing so that the number of local minima is considerably reduced. The local search concerning complex moves can be enormously sped up by use of branch-and-bound type algorithms. Their basic idea is to construct new trial states following a decision tree: At each branching point, a lower bound of the energy of the trial state is calculated. The search within the current branch is terminated as soon as this bound exceeds the energy of the initial state.

The basic thermal cycling procedure can be easily accelerated in three ways: (i) partition of the computational effort into several search processes in order to minimize the failure risk [14], (ii) restricting the moves in heating to the ‘sensible sample regions’ by analyzing previous cycles, or by comparing with samples considered in parallel, and (iii) combining parts of different states [7, 12].
III. APPLICATIONS

The thermal cycling algorithm was first tested on the traveling salesman problem \[7\]. For that, we considered problems of various size from the TSPLIB95 \[15\] for which the exact solutions, or at least related bounds, are known. Fig. 2 gives a comparison of thermal cycling data with results from simulated annealing and from repeated local searches starting from random states. For a meaningful characterization of the algorithms, it relates mean deviations from the optimum tour length to the CPU-time effort for various parameter values. The diagram includes data for two move classes: (a) cutting a roundtrip twice, reversing the direction of one of its parts, and connecting the parts then again, or shifting a city from one to another position in the roundtrip; (b) same as (a) and additionally rearrangements by up to four simultaneous cuts as well as Lin-Kernighan realignments \[16\].

Fig. 2 shows that, for the traveling salesman problem, thermal cycling is clearly superior to simulated annealing, already if the same move class is considered in both procedures – the simulated annealing code had been carefully tuned too –. However, when taking advantage of the possibility to incorporate more complex moves, thermal cycling beats simulated annealing by orders of magnitude in CPU time. Applied to an archive of samples instead of to a single one, it can compete with leading genetic local search algorithms \[7, 12\].

For several years, we have used thermal cycling as standard approach in numerical investigations of the Coulomb glass, which is basically an Ising model with long-range interactions. Also in this case, thermal cycling proved to be a very efficient tool. Fig. 3 presents data from an investigation comparing several algorithms \[13\]. In simulated annealing, we could efficiently treat only particle exchange with a reservoir and one-particle hops inside the sample, that is occupation changes of one or two sites. However, in the deterministic local search, the simultaneous occupation modification of up to four sites could be considered by means of branch-and-bound approaches. Therefore, the corresponding multistart local search yields significantly better results than simulated annealing. Thermal cycling of the low-energy states proves to be still far more efficient than the local search repeatedly starting from random states.

It is tempting to apply the thermal cycling approach also to problems with continuous variables. Thus we have considered Lennard-Jones cluster of various size because the energy landscapes of this system are known to have large numbers of local minima. The heating
consisted of simultaneously shifting all atoms by small distances a few times according to a thermal rejection rule, and the quench combined the Powell algorithm with a systematic consideration of symmetry positions. The ground states of several clusters of up to 150 atoms could be reproduced within ‘reasonable’ CPU times. Further related investigations should be promising.

[1] Y. Usami and M. Kitaoka, *Int. J. Mod. Phys. B* 11, 1519 (1997).
[2] D. S. Johnson and L. A. McGeoch, in *Local Search in Combinatorial Optimization*, eds. E. Aarts and J. K. Lenstra (Wiley, Chichester, 1997), p. 215.
[3] S. Kirkpatrick, C. D. Gelatt, Jr., and M. P. Vecchi, *Science* 220, 671 (1983).
[4] J. H. Holland, *Adaptation in Natural and Artificial Systems: an Introductory Analysis with Applications to Biology, Control, and Artificial Intelligence*, (University of Michigan Press, Ann Arbor, 1975).
[5] R. M. Brady, *Nature* 317, 804 (1985).
[6] P. Merz and B. Freisleben, in *Proc. 1997 IEEE Int. Conf. on Evolutionary Computation*, Indianapolis, (IEEE Press,1997), p. 159.
[7] A. Möbius, A. Neklioudov, A. Díaz-Sánchez, K.H. Hoffmann, A. Fachat and M. Schreiber, *Phys. Rev. Lett.* 79, 4297 (1997).
[8] J. Houdayer and O. C. Martin, *Phys. Rev. Lett.* 83, 1030 (1999).
[9] S. Boettcher and A. G. Percus, *Phys. Rev. Lett.* 86, 5211 (2001).
[10] D. J. Wales and J. P. K. Doye, *J. Phys. Chem. A* 101 (1997), 5111.
[11] M. Iwamatsu and Y. Okabe, *Chem. Phys. Lett.* 399, 396 (2004).
[12] A. Möbius, B. Freisleben, P. Merz and M. Schreiber, *Phys. Rev. E* 59, 4667 (1999).
[13] A. Díaz-Sánchez, A. Möbius, M. Ortuño, A. Neklioudov and M. Schreiber, *Phys. Rev. B* 62, 8030 (2000).
[14] B. A. Huberman, R. M. Lukose and T. Hogg, *J. Phys. Chem. A* 101 (1997), 5111.
[15] www.iwr.uni-heidelberg.de/groups/comopt/software/TSPLIB95
[16] S. Lin and B. Kernighan, *Operations Research* 21, 498 (1973).
FIG. 1: Time dependence of the energy $E$ (quantity to be optimized) of the sample currently treated in the cyclic process. Gaps in the curve refer to cycles where the final state has a higher energy than the initial state, so that the latter is used as initial state of the next cycle too.

FIG. 2: Relation between CPU time, $\tau_{CPU}$ (in seconds for one PA8000 180 MHz processor of an HP K460), and deviation, $\delta L = L_{\text{mean}} - 27686$, of the obtained mean approximate solution from the optimum tour length for the Padberg-Rinaldi 532 city problem [7]. $\square$: repeated quench to stability with respect to move class (a) defined in the text; $\Delta$: simulated annealing; $\times$ and $\bullet$: thermal cycling with ensembles of various size, and local search concerning move classes (a) and (b), respectively. In all cases, averages were taken from 20 runs. Errors (1$\sigma$-region) are presented if they exceed the symbol size. The lines are guides to the eye only.
FIG. 3: Mean deviation of the energy of the lowest state found from the ground state energy, $\delta E = E_{\text{mean}} - E_{\text{ground state}}$, related to the CPU time $\tau_{\text{CPU}}$ (180 MHz PA8000 processor of HP K460) for one realization of the three-dimensional Coulomb glass lattice model with 1000 sites, half filling, and medium disorder strength [13]. ×: simulated annealing; △: multistart local search considering simultaneous occupation changes of up to four sites; •: thermal cycling. For simulated annealing and multistart local search, averages were taken from 20 runs, for thermal cycling from 100 runs. In thermal cycling, the ground state was always found within 500 seconds.