borealis — A generalized global update algorithm for Boolean optimization problems

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Abstract

Optimization problems with Boolean variables that fall into the nondeterministic polynomial (NP) class are of fundamental importance in computer science, mathematics, physics and industrial applications. Most notably, solving constraint-satisfaction problems, which are related to spin-glass-like Hamiltonians in physics, remains a difficult numerical task. As such, there has been great interest in designing efficient heuristics to solve these computationally difficult problems. Inspired by parallel tempering Monte Carlo in conjunction with the rejection-free isoenergetic cluster algorithm developed for Ising spin glasses, we present a generalized global update optimization heuristic that can be applied to different NP-complete problems with Boolean variables. The global cluster updates allow for a wide-spread sampling of phase space, thus considerably speeding up optimization. By carefully tuning the pseudo-temperature (needed to randomize the configurations) of the problem, we show that the method can efficiently tackle optimization problems with over-constraints or on topologies with a large site-percolation threshold. We illustrate the efficiency of the heuristic on paradigmatic optimization problems, such as the maximum satisfiability problem and the vertex cover problem.

KEYWORDS: Optimization, Satisfiability, Vertex cover, Monte Carlo, Cluster algorithm

1. Introduction

In computational complexity theory, the complexity class of nondeterministic polynomial — also known as NP — [44, 33, 17, 45] is one of the most fundamental ones. The class consists of decision problems that are *verifiable* in polynomial time, however, no statement is made about the worst-case complexity. Typically, the worst-case complexity scales in a superpolynomial manner. The NP class includes a variety of notoriously hard yet important optimization problems such as Ising spin glasses [10, 37], the Boolean satisfiability problem [17, 33, 31], minimum vertex covers [41, 33], as well as the travelling salesman problem [8, 9]. The aforementioned problems, as well as many others in the NP class, have complex energy (cost function) landscapes with many local minima and are typically only solvable in super-polynomial (e.g., exponential or stretched exponential) times. While at the moment efficient optimization algorithms cannot change the worst-case (or even typical) complexity

to a polynomial in the size of the input, one can hope to at least have algorithms that have smaller prefactors in the time complexity or stretched exponentials with smaller exponents [45, 18, 48]. This could result in substantial speedup and allow for the study of problems with a considerably larger number of variables. In fact, despite Moore's law [52] hopefully still holding for the next few decades, large advances can only be achieved by better algorithms and not raw computing power.

Many optimization problems in the NP complexity class can be solved by local search (LS) heuristics. This type of algorithm starts from a candidate solution and then iteratively moves to a neighboring solution with random or greedy moves of single Boolean variables. However, either the greedy single-variable dynamics is quickly trapped in local minima of the cost function, or exhaustively explores plateaus in the landscape where no local moves can decrease the cost in a reasonable amount of time. To escape this single-move traps, randomizing moves can be performed at the cost of additional computational time. Paradigmatic examples of (stochastic) local search algorithms have evolved from algorithms such as GSAT and WalkSAT [61] for the maximum satisfiability problem, NuMVC [14] for minimum vertex covers, as well as simulated annealing and 2-opt algorithms [38, 32] for the traveling salesman problem. For spin glasses, methods such as extremal optimization [11], local genetic algorithms [55] or the cluster-exact approximation method [25, 26] have been successful in tackling problems with up to approximately 2^{12} variables. In contrast to these local search algorithms that rely on updating one variable at a time and, when trapped in a local minimum are restarted from a new initial configuration, global update algorithms flip multiple variables simultaneously in one iteration. This could, in principle, lead to a large rearrangement of the variables and therefore the ability to escape a local minimum. Notable examples include the building-block wise crossover in genetic algorithms [66] that facilitates inheritance of characteristics by an offspring from its parents and global Swendsen-Wang [62] and Wolff cluster algorithms [67] for the simulation of ferromagnetic Ising models in physics. The latter are typically used to improve thermalization for finite-temperature measurements and greatly reduce autocorrelation times, thus massively speeding up the simulation and allowing for a study of considerably larger system sizes. Therefore, combining LS algorithms with carefully-designed nonlocal cluster updates could allow for a wide-spread sampling of the phase space, and hitherto speeding up the optimization of NP optimization problems.

In this work we design a stochastic search algorithm (*borealis*) that can efficiently overcome local minima, as well as globally sample the cost function landscape by large rearrangements of the variables. To overcome energy barriers efficiently, we combine the isoenergetic cluster moves [69] with parallel tempering Monte Carlo.

Parallel tempering (PT) Monte Carlo [22, 29, 34] (also known as replica exchange Markov chain Monte Carlo sampling) is a global update algorithm aimed at improving the dynamic properties of Monte Carlo simulations of physical systems. Although in this algorithm no clusters are generated to perform large-scale variable rearrangements, in PT multiple copies of the system with different initial conditions (i.e., independent Markov chains) are simulated at different temperatures. Then, based on the Metropolis update criterion, one exchanges configurations at different temperatures. This means that different copies of the system perform a random walk in temperature space (in addition to the random walk in cost function space from the single-variable Monte Carlo updates) thus allowing trapped configurations to be "heated" and then "cooled" with the goal of overcoming energy bar-

riers and therefore escaping local minima. PT Monte Carlo has proven to be a versatile "workhorse" in many research fields [19], such as physics, biology and chemistry. Most importantly, by setting the lowest temperature of the simulation to be close to zero, PT can used as an efficient optimizer for any problem that can be cast into Boolean variables [53].

The isoenergetic cluster move (ICM) algorithm [69], related to Houdayer's cluster updates [28], requires two copies of the Boolean system to be studied. Using information from the variables in both systems, clusters are built in the dot-product space of the variables. This cluster "mask" is then applied to both systems. As shown in Ref. [28], the algorithm is rejection free, which means that every update is accepted with probability 1. Furthermore, the value of the cost function (energy) of the combined system does not change in the cluster move, which means that the two systems are "teleported" across phase space at a fixed value of the cost. Typically, the cluster moves are combined with another host algorithm (e.g., PT). The added large global rearrangements vastly improve the overall performance of the host algorithm. This method has been used extremely successfully in recent studies of spin-glass systems. See, for example, Refs. [35, 68, 48].

Fortunately, there is a close relationship between the statistical physics of Ising spin glasses and a wide variety of Boolean NP problems [45]. Mathematically, because the decision form of the Ising spin glass model is NP-complete [10], there exists a polynomial time mapping to any other NP-complete problem with Boolean variables [33]. Here we demonstrate that borealis — a combination of PT with ICM — can be efficiently applied to a variety of NP optimization problems, provided the cost function (Hamiltonian) can be written as a polynomial function of a set of N Boolean variables x_i , i.e.,

$$-\mathcal{H}(x_1,\ldots,x_N) = \sum_i h_i x_i + \sum_{ij} J_{ij} x_i x_j + \sum_{ijk} T_{ijk} x_i x_j x_k + \ldots$$
 (1)

We demonstrate the efficiency of the heuristic *borealis* on the maximum satisfiability and minimum vertex cover problems. Furthermore, we compare the heuristic to current state-of-the-art heuristics, such as CCLS [46], DistUP [1], Dist1 [13] and NuMVC [14].

The paper is organized as follows. In Sec. 2 we introduce the optimization problems used to illustrate *borealis*, followed by a detailed description of *borealis*, parallel tempering Monte Carlo and the isoenergetic cluster move algorithm in Sec. 3. Section 4 shows results on the Boolean satisfiability problem, as well as minimum vertex covers, followed by concluding remarks.

2. Studied benchmarks

In this section we briefly outline the benchmark optimization problems used to illustrate the performance of the *borealis* algorithm. Note that the method can be applied to other difficult optimization problems, such as spin glasses [48].

2.1 Boolean satisfiability problem (SAT)

The maximum satisfiability problem (MAX-SAT) is the combinatorial optimization problem of determining a set of Boolean variables $\{x_1, \ldots, x_N\}$ that maximize the number of satisfied

clauses $\{C_1, \ldots, C_M\}$ in a conjunctive normal form $\Psi = C_1 \wedge C_2 \cdots \wedge C_M$, where

$$C_i = x_{i_1} \lor \dots \lor x_{i_k}, \qquad 1 \le i \le M. \tag{2}$$

The variables x_{i_1}, \ldots, x_{i_k} in Eq. (2) are selected from another set of Boolean variables, $x_1, \ldots, x_N, \overline{x}_1, \ldots, \overline{x}_N$ with the goal of satisfying the Boolean formula. The weighted partial MAX-SAT problem is a generalization of the maximum satisfiability problem in which each clause C_i is assigned a positive weight w_i . The objective of this problem is to maximize the sum of weights of satisfied clauses by any variable assignment. Note, also, that the partial MAX-SAT problem tries to find an optimal assignment to the variables which satisfies all the hard clauses and maximizes the number of soft clauses. The combination of both variations is called the weighted partial MAX-SAT problem. Weighted partial MAX-SAT problems are crucial elements of a broad range in application areas such as telecommunications [42], scheduling [15], combinatorial online auctions [21], as well as circuit design [49], to name a few.

Not-All-Equal Maximum Satisfiability (NAE-MAX-SAT) is one of the central problems in theoretical computer science and is similar to MAX-SAT, except for the additional requirement that at least one of the literals in each clause be true and one be false. NAE-MAX-SAT is symmetric with respect to switching the Boolean variables [43]. This means that a representation of the form presented in Eq. (1) only has term with even powers of x_i . The average Hamming distance of the set of solutions is approximately 50% of the total number of variables and all solutions are statistically uncorrelated [16]. This feature can be exploited to efficiently construct probabilistic membership filters [65] based on SAT formulas [20]. A special case of NAE-MAX-SAT is the weighted XOR-MAX-SAT problem where each clause contains XOR (exclusive or) rather than an OR operators. Generally speaking, local search algorithms take exponential time on random XOR-SAT formulas because flipping any variable will dissatisfy all the currently satisfied clauses [60, 30].

A Hamiltonian \mathcal{H} (cost function) to describe MAX-SAT, NAE-MAX-SAT, or weighted XOR-MAX-SAT may be written such that the Hamiltonian is a measure of the number of unsatisfied clauses, i.e., $\mathcal{H} = \sum_i w_i \overline{C}_i$. The ground state(s) of this Hamiltonian correspond to those assignments with all Boolean variables that violate the minimum number of clauses.

2.2 Minimum vertex cover problem

A minimum vertex cover (MVC) is a vertex covering of a graph G using the smallest possible number of vertices. A graph G = (V, E) is a set of vertices V and a set of edges E. A vertex cover of a graph G can simply be thought of as a set S of vertices of G such that every edge of G has at least one of member of S as an endpoint. Finding a minimum vertex cover of a general graph is an NP-complete problem, the complement of the maximum independent set problem [41]. The MVC problem has many real-world applications such as network security, scheduling and industrial machine assignment [23].

Let x_i be a Boolean variable on each vertex, which is 1 if it is colored, and 0 if it is not colored. The Hamiltonian (cost function) for MVC is given by $\mathcal{H} = \mathcal{H}_A + \mathcal{H}_B$. The penalty term \mathcal{H}_A imposes the constraint that every edge has at least one colored vertex, i.e.,

$$\mathcal{H}_A = A \sum_{ij \in E} (1 - x_i)(1 - x_j). \tag{3}$$

Minimizing the number of colored vertices can be done by setting

$$\mathcal{H}_B = B \sum_i x_i. \tag{4}$$

Choosing the coefficient B < A with A large ensures that it is never favorable to violate the constraints imposed by \mathcal{H}_A .

3. Outline of the *borealis* algorithm

Based on the ideas of reweighting hard constraints, parallel tempering updates and isoenergetic cluster updates, we develop an efficient global update algorithm *borealis* for solving NP problems, which is outlined as follows:

Algorithm 1 borealis

Input: MAX-SAT instance, maxMCS

- 1: Re-weight hard clauses;
- 2: Initialize systems with random truth assignments;
- 3: for MCS = 1 to maxMCS do
- 4: Metropolis update;
- 5: Parallel tempering update;
- 6: **if** site percolation-threshold p_c is high **then**
- 7: Isoenergetic cluster update;
- 8: Keep track of lowest energy E_{min} of all systems;
- 9: return E_{min}

We now describe the different updates performed in the *borealis* algorithm in detail.

3.1 Weighting scheme in partial MAX-SAT and weighted partial MAX-SAT

Typically hard clauses have to be satisfied and satisfaction of soft clauses is desirable but not mandatory. The simplest way to represent the relative importance of hard clauses is to set their weights to the number of soft clauses plus 1. However, large weights on hard clauses create large energy barriers and significantly slow down the search in configuration space. An optimum weighting strategy adds weights to constraints without distorting the solution space. In principle, one could set the weights of all hard clauses to the number of soft clauses left unsatisfied in an optimal solution (unfortunately, this not known). Cha et al. [15] set weights to a hand-tuned optimal level and Thornton & Sattar [64] later introduced two dynamic constraint weighting schemes according to feedback received during the search. Here, for the simplicity, for each hard clause we set the weights to the maximum sum of the number of literals appearing in soft clauses.

3.2 Parallel tempering update

Parallel tempering (PT) [29] is a simulation method aimed at improving the dynamic properties of simple Markov chain Monte Carlo simulations of physical systems. Essentially,

 N_T copies of the system, each with different initial conditions, are simulated at a range of temperatures $\{T_1, T_2, ..., T_{N_T}\}$. After a simple Monte Carlo sweep of each variable of each copy of the system, configurations at adjacent different temperatures are exchanged based on a Metropolis criterion

$$p(E_i, T_i \to E_{i+1}, T_{i+1}) = \min\{1, \exp(\Delta E \Delta \beta)\},\tag{5}$$

where $\Delta\beta = 1/T_{i+1} - 1/T_i$ is the difference between the inverse temperatures and $\Delta E = E_{i+1} - E_i$ is the difference in the energy of the two neighboring copies at different temperatures. The idea behind this method is to make configurations at high temperatures available to the simulation at low temperatures, and vice versa. This results in a very robust ensemble that is able to sample both low- and high-energy configurations and easily overcomes energy barriers.

One important aspect of PT is that optimal temperature intervals must be carefully chosen [34]. When the temperatures are too far apart, the energy distributions at the individual temperatures do not overlap enough and many moves are rejected. If the temperatures are too close, CPU time is wasted. Although there are a wide variety of "optimal" approaches to determine the location of the individual temperatures [57, 39, 40, 58, 59, 19, 36, 34, 47, 24], usually the most accurate data for a fixed amount of computation are obtained if we ensure that the acceptance probabilities for the individual swaps between neighboring temperatures are approximately independent of the temperature and roughly between 20% - 80% [59]. Any additional optimization of the temperatures constitutes wasted efforts.

PT is an extremely powerful algorithm in the study of spin glasses. For example, the speedup over conventional simple Monte Carlo for a cubic spin glass with N=64 variables at low temperatures is approximately four orders of magnitude. This speedup grows with decreasing temperature and an increasing number of variables N.

3.3 Isoenergetic cluster moves

We begin by simulating two copies of the system at multiple temperatures. The cluster moves alone are not ergodic, as such, these must be combined with simple Monte Carlo updates. One simulation step using isoenergetic cluster moves (ICM) consists of the following steps:

- 1. Identify a cluster in overlap space: Two independent configurations (copies) are simulated at the same temperature. The site overlap between copies (1) and (2), $q_i = x_i^{(1)} \oplus x_i^{(2)}$, is calculated. This creates two domains in q-space: Sites with $q_i = 0$ and $q_i = 1$. Clusters are defined as the connected parts of these domains in q-space [2]. One then randomly chooses one site with $q_i = 1$ and builds the cluster by adding all the connected variables with $q_i = 1$ in the domain with probability 1. When no more variables can be added to the cluster in q-space, the variables in both replicas that correspond to cluster members in q-space are flipped with probability 1, irrespective of their value.
- 2. Perform one isoenergetic cluster move for all temperatures $T \lesssim J$. Note that, in most cases, the characteristic energy scale of the problem in Eq. (1) is J=1. This means that we perform the cluster moves typically for $T \lesssim 1$.

In what follows we prove that ICMs leave the total energy of the combined system of copies (1) and (2) intact. Assume we randomly pick a cluster O^{α} and the interaction matrices (or tensors) associated with Boolean variables in O^{α} are represented as $T^{\alpha}_{ijk...}$. $T^{\alpha}_{ijk...}$ are comprised of two different categories. The ones whose endpoints are all in the cluster O^{α} and rest with only some endpoints in the cluster. Flipping all the Boolean variables in the cluster O^{α} does not change the total energy associated with interaction matrices in the first category because

$$-\sum_{ijk...} T^{\alpha}_{ijk...}(x_i^{\alpha_1} x_j^{\alpha_1} x_k^{\alpha_1} \dots + x_i^{\alpha_2} x_j^{\alpha_2} x_k^{\alpha_2} \dots)$$
 (6)

remains the same if we merely swap Boolean variables $x_i^{\alpha_1}, x_j^{\alpha_1}, x_k^{\alpha_1}$ with $x_i^{\alpha_2}, x_j^{\alpha_2}, x_k^{\alpha_2}$. For the interaction matrices in the second category, the energy associated with these matrices is

$$-\sum_{ijk...} T^{\alpha}_{ijk...}(x^{\alpha_1}_i x^{\alpha_1}_j x^{\alpha_1}_k \dots + x^{\alpha_2}_i x^{\alpha_2}_j x^{\alpha_2}_k \dots) = -\sum_{ijk...} T^{\alpha}_{ijk...} x^{\alpha}_i (x^{\alpha_1}_j x^{\alpha_1}_k \dots + x^{\alpha_2}_j x^{\alpha_2}_k \dots), (7)$$

where the Boolean variables x_j, x_k are included in the cluster O^{α} whereas x_i is not. Therefore, flipping Boolean variables in the cluster only swap $x_j^{\alpha_1}, x_k^{\alpha_1}$ with $x_j^{\alpha_2}, x_k^{\alpha_2}$ and leave the energy unchanged. Note that if the clusters in q-space percolate (i.e., extend the whole size of the problem) a cluster update merely exchanges both configurations and thus represent numerical overhead. Generally speaking, the performance of isoenergetic cluster moves is limited by the site-percolation threshold p_c of the topology of the underlying problems [3], the amount of frustration present in the system (that slows cluster growth as a function of temperature), as well as the performance of vanilla parallel tempering. For cases where p_c is very small ($p_c \to 0$), the cluster updated can be removed from the algorithm because they constitute unnecessary overhead. In this case, it is more efficient to simply run borealis without the cluster updates. In the next section we demonstrate how borealis outperforms, for example, CCLS on planar NAE-MAX-3SAT problems, random weighted XOR-MAX-2SAT, as well as NuMVC on minimum vertex covers with cluster moves included.

4. Experiments

4.1 Benchmark problems studied

For our empirical studies, we evaluate borealis on a broad range of benchmarks, including unweighted MAX-SAT, partial MAX-SAT, weighted partial MAX-SAT, NAE-MAX-SAT, weighted XOR-MAX-SAT and MVC. The MAX-SAT instances comprise the most wide-spread benchmark, including random instances from the Tenth Max-SAT Evaluation in 2015 [4]. To perform a scaling analysis we use the makewff generator [5] with minor modifications to generate random MAX-k-SAT (M/N=30) instances and weighted XOR-MAX-2SAT instances (M/N=1) with certain clause-to-variable ratios. The MAX-NAE-SAT and MVC instances used for our experiments are derived from triangular lattices and random graphs with a ratio of edges to vertices equal to 1.5 (randomly selected). For planar NAE-MAX-3SAT instances, literals in each clause are selected from variables with random signs in a random triangle; the triangular lattice is known to have a site percolation-threshold of $p_c=0.5$ which is optimal for borealis. For MVC, given a random graph of N vertices

and M edges, there exists a site percolation-threshold $p_c = N/2M = 0.33$ [12] below which the network becomes fragmented while above p_c a giant connected component exists. Coefficients A and B in the MVC problem are chosen to be 1.3 and 1, respectively, such that it is never favorable to violate the constraints imposed by the penalty term \mathcal{H}_A .

4.2 State-of-the-art algorithms

We have compared *borealis* to four local search solvers: CCLS, DistUP, Dist1 and NuMVC. CCLS combines a configuration checking strategy with a random walk and has won four categories in the incomplete track of the 2015 Max-SAT Evaluation. Dist is a local search algorithm with a clause weighting scheme and variable selection strategy. It has won the weighted partial random MAX-SAT incomplete track of the 2015 Max-SAT Evaluation. DistUP combines an assigning procedure PrioUP with the solver Dist and has won the partial random Max-SAT incomplete track of the 2015 Max-SAT Evaluation. Finally, NuMVC proposes two-stage exchanges and edge weighting strategies for MVC. It is largely competitive on the DIMACS benchmark [6] and dramatically outperforms other state-of-the-art heuristic solvers on all BHOSLIB instances [7].

4.3 Machine specifications

All experiments are carried out on the compute nodes of the Lonestar-5 high-performance computing cluster at the Texas Advanced Computing Center, using a Xeon E5-2690 v3 (Haswell) 2.6 GHz CPU and 64 GB DDR4-2133 memory. The time limit is set to be 300 seconds for each instance. We have implemented *borealis* in the programming language C and complied it with gcc with -02 optimization.

4.4 Results

We first compare the the performance of *borealis* to CCLS, DistUP and Dist1 from the Tenth Max-SAT Evaluation (2015). Then we illustrate how the inclusion of ICM substantially improves the performance over vanilla PT on planar NAE-MAX-3SAT, random weighted XOR-MAX-2SAT and MVC instances. Simulation parameters used in the experiments with *borealis* are shown in Table 1.

Figures 1, 2, and 3 show the time to solution of borealis and CCLS, DistUP and Dist1 as a function category index for unweighted, partial and weighted partial random MAX-SAT instances in Tenth Max-SAT Evaluation (2015), respectively. borealis (isoenergetic cluster moves are not applied because most instances have a low percolation threshold) finds solutions for all instances and significantly outperforms CCLS, DistUP and Dist1 in most categories. In the partial and weighted partial MAX-SAT benchmark instances, PT greatly benefits from weighting schemes which lower energy barriers without distorting the original solution space. Figure 4 demonstrates that borealis scales better than CCLS with large k and ratio M/N.

Figure 5 shows the time to solution for *borealis* and vanilla PT as a function of system size N for planar NAE-MAX-3SAT instances. Each instance is run with and without isoenergetic cluster moves for 10^6 Monte Carlo sweeps. At the end of the runs we consider solutions to be found if two results from each copy agree. Clearly, the inclusion of clus-

Table 1. Parameters of borealis for the different experiments in unweighted MAX-SAT, partial MAX-SAT, weighted partial MAX-SAT, NAE-MAX-SAT, weighted XOR-MAX-SAT and MVC benchmark problems. For each instance category simulated, we perform maxMCS Monte Carlo sweeps (and isoenergetic cluster moves) for each of the $2N_T$ copies of the system. T_{\min} [T_{\max}] is the lowest [highest] temperature simulated, and N_T is the total number of temperatures used in the parallel tempering Monte Carlo method. At each temperature, two copies of the system are needed for the ICM updates. Note that isoenergetic cluster moves only occur for the lowest $N_{\rm c}$ temperatures simulated. If the column for N_T has no value in parentheses, the simulations were done without the inclusion of ICM updates.

Track	category	T_{\min}	$T_{\rm max}$	$N_T(N_c)$	maxMCS
unweighted	all	0.05	1.23	25	30000
partial	$\min 2sat$	0.10	0.50	80	30000
partial	$\min 3$ sat	0.10	0.50	80	30000
partial	pmax2sat	0.10	2.05	40	30000
partial	pmax3sat	0.10	2.05	40	30000
weighted partial	abrame	0.10	39.00	40	30000
weighted partial	wmax2sat	0.10	39.00	40	30000
weighted partial	wmax3sat	0.10	39.00	40	30000
weighted partial	wpmax2sat	0.10	23.50	40	30000
weighted partial	wpmax3sat	0.10	7.90	40	30000
weighted XOR-MAX-2SAT	all	0.05	0.44	40(40)	2^{20}
NAE-MAX-3SAT	all	0.05	1.23	25(20)	2^{20}
MVC	all	0.05	0.50	40(40)	2^{20}

ter moves results in a significant advantage over vanilla PT for planar NAE-MAX-3SAT instances. borealis benefits from the high site-percolation-threshold ($p_c = 0.5$) of the triangular lattice, as well as the relatively large cluster sizes due to the not-all-equal constraint. Comparisons to the performance of CCLS on planar NAE-MAX-3SAT are not included because CCLS has an extremely low success rate in finding solutions for these instances. Figure 6 shows the time to solution for borealis, vanilla PT and CCLS as a function of system size N for random weighted XOR-MAX-2SAT instances. borealis significantly outperforms CCLS and benefits from the large rearrangement of the variables due to cluster moves and tall energy barriers created by the XOR operators. In addition to planar NAE-MAX-3SAT and weighted XOR-MAX-2SAT problems, we also compare borealis to the state-of-the-art local search algorithm NuMVC on the MVC problems. Figure 7 shows the time to solution of borealis and NuMVC as a function of system size N for the MVC problem. Again, borealis clearly outperforms NuMVC on the scaling, however, its advantage over vanilla PT is less impressive than for planar NAE-MAX-3SAT problems due to the lack of frustrated interactions in MVC problems.

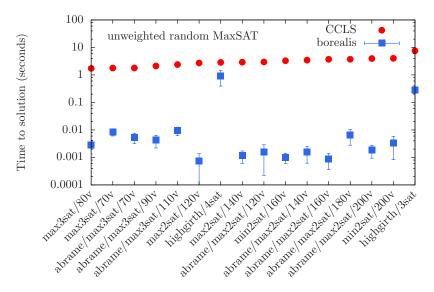


Figure 1. Time to solution (CPU time) in seconds of *borealis* and CCLS. The horizontal axis lists the different categories for the unweighted random MAX-SAT track in the Tenth Max-SAT Evaluation (2015). The time is averaged over all instances in each instance category and error bars for *borealis* are computed via a bootstrap analysis. *borealis* significantly outperforms CCLS in all categories except for the highgirth instances where it is still faster.

5. Conclusions

We have developed a generic global update algorithm for NP optimization problems with Boolean variables, *borealis*, based on a combination of parallel tempering Monte Carlo [29] and isoenergetic cluster moves [69]. The global cluster moves, combined with the tempering scheme allow for a wide-spread sampling of search space and help escaping local minima

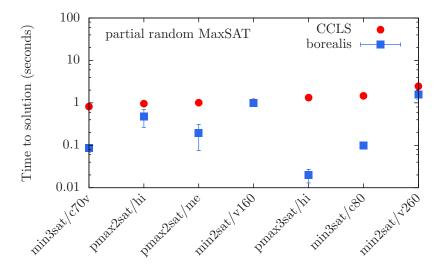


Figure 2. Time to solution (CPU time) in seconds of *borealis* and DistUP. The horizontal axis lists the different categories for the partial random MAX-SAT track in the 2015 Tenth Max-SAT Evaluation. *borealis* significantly outperforms DistUP in all categories except for the Min-2SAT instances where the performance is comparable.

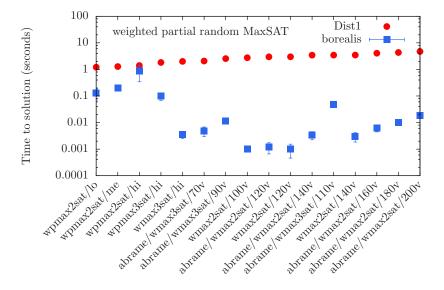


Figure 3. Time to solution (CPU time) in seconds of *borealis* and Dist1. The horizontal axis lists the different categories for the weighted partial random MAX-SAT track in the Tenth Max-SAT Evaluation (2015). *borealis* significantly outperforms Dist1 in all categories except for the weighted partial MAX-2SAT instances with medium clauses to variables ratio where the performance is comparable.

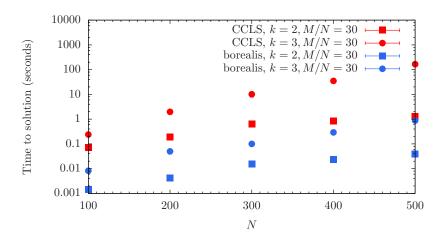


Figure 4. Time to solution (CPU time) in seconds for *borealis* and CCLS as a function of system size N for random unweighted MAX-SAT instances. The time is averaged over 100 instances for a given system size N. Error bars are computed using a bootstrap analysis and are smaller than the symbols. *borealis* outperforms CCLS for all system sizes and scales better with large k and ratio M/N=30.

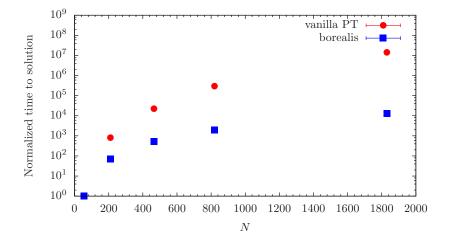


Figure 5. Normalized time to solution (the time to solution for different system sizes is divided by the time to solution for the smallest system size) of *borealis* compared to vanilla PT as a function of system size N for planar NAE-MAX-SAT on a triangular lattice. The time is averaged over 100 instances for a given system size N. Again, *borealis* significantly outperforms vanilla PT and the speedup increases with increasing system size.

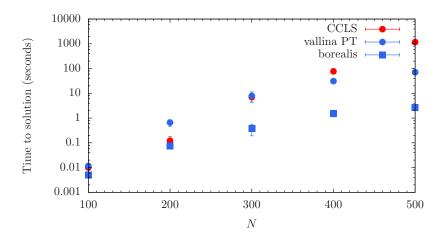


Figure 6. Time to solution (CPU time) in seconds for *borealis* (with/without cluster moves) and CCLS as a function of system size N for random weighted XOR-MAX-2SAT instances (M/N=1). The time is averaged over 100 instances for a given system size N. Error bars are computed using a bootstrap analysis and are smaller than the symbols. *borealis* with cluster updates outperforms CCLS on both CPU time and scaling.

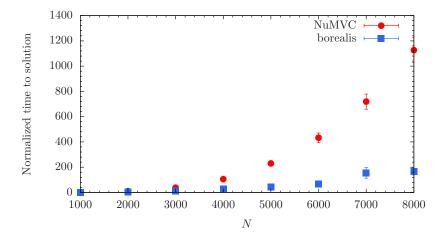


Figure 7. Normalized time to solution (the time to solution for different system sizes is divided by the time to solution for the smallest system size) of *borealis* and NuMVC as a function of system size N for MVC on a random graph with site-percolation threshold $p_c = N/2M = 0.33$. *borealis* scales better than NuMVC and the speedup increases with increasing system size. However, the advantage of *borealis* over NuMVC is less impressive due to the lack of frustrated interactions in MVC problems.

separated by large energy barriers. In addition, by introducing a new weighting scheme in partial and weighted partial MAX-SAT problems, we significantly lower the energy barriers without distorting the solution space and show that *borealis* outperforms state-of-the-art algorithms on all random benchmark instances in the Tenth Max-SAT Evaluation (2015). For optimization problems with relatively high site-percolation threshold, we demonstrate that the inclusion of isoenergetic cluster moves significantly improves the performance over vanilla parallel tempering on planar NAE-MAX-SAT instances, random weighted XOR-MAX-2SAT and minimum vertex cover problems on random graphs.

We intend to apply *borealis* and cluster moves to other optimization problems and algorithms, respectively, in the near future. For instance, cluster moves can be added to speed up the study of fault diagnosis [56] in circuit design and genetic algorithms [26] as a crossover operator to speed up the optimization. In analogy to parallel tempering, we are also exploring the idea of replica exchanges with different constraint strengths for over-constrained NP optimization problems.

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- [2] Connected parts are determined by edges, which is straightforward for the vertex cover problem. For the Boolean satisfiability problem, we assume two different variables in any single clause are connected by an edge.
- [3] In most cases, the determination of the site percolation threshold of the underlying graph relies on numerical approaches [27, 54, 50, 51] (e.g., Monte Carlo simulations combined with a finite-size scaling analysis). Significant algorithmic progress has been made by Newman and Ziff [54] for calculating the cluster size distribution or spanning

probability over the entire range of site or bond occupation probabilities from zero to one in one single run (scaling linearly in the number of sites). In some cases — such as random graphs [12] or triangular lattices [63] — it is even possible to derive the site percolation threshold analytically.

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