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GPU-based Ising computing for solving max-cut combinatorial optimization problems[☆]



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ABSTRACT

In VLSI physical design, many algorithms require the solution of difficult combinatorial optimization problems such as max/min-cut, max-flow problems etc. Due to the vast number of elements typically found in this problem domain, these problems are computationally intractable leading to the use of approximate solutions. In this work, we explore the Ising spin glass model as a solution methodology for hard combinatorial optimization problems using the general purpose GPU (GPGPU). The Ising model is a mathematical model of ferromagnetism in statistical mechanics. Ising computing finds a minimum energy state for the Ising model which essentially corresponds to the expected optimal solution of the original problem. Many combinatorial optimization problems can be mapped into the Ising model. In our work, we focus on the max-cut problem as it is relevant to many VLSI design automation problems. Our method is inspired by the observation that Ising annealing process is very amenable to fine-grain massive parallel GPU computing. We will illustrate how the natural randomness of GPU thread scheduling can be exploited during the annealing process to create random update patterns and allow better GPU resource utilization. Furthermore, the proposed GPU-based Ising computing can handle any general Ising graph with arbitrary connections, which was shown to be difficult for existing FPGA and other hardware based implementation methods. Numerical results show that the proposed GPU Ising max-cut solver can deliver more than 2000X speedup over the CPU version of the algorithm on some large examples, which shows huge performance improvement for addressing many hard optimization algorithms for solving practical VLSI design automation problems.

1. Introduction

There are many hard combinatorial optimization problems such as max-flow, max-cut, graph partitioning, satisfiability, and tree based problems, which are important for many scientific and engineering applications. With respect to VLSI design automation, these problems translate to finding optimal solutions for cell placement, wire routing, logic minimization, via minimization, and many others. The vast complexity of modern integrated circuits (ICs), some having millions or even billions of integrated devices, means that these problems are almost always computationally intractable and require heuristic and analytical methods to find approximate solutions. It is well-known that traditional von Neumann based computing can not deterministically find polynomial time solutions to these hard problems [1].

To mitigate this problem, a new computing paradigm utilizing the *Ising spin glass model* or *Ising model* has been proposed [2]. The Ising model is a mathematical model describing interactions between magnetic spins in a 2D lattice [3]. The model consists of *spins*, each taking one of two values $\{+1,-1\}$ (to represent up and down states of a spin

along a preferred axis) and are generally arranged in a 2D lattice. The spin's value is determined so that its energy is minimized based on interactions with its neighbor spins. Such local spin updates will lead to the ground state (globally lowest energy configuration) of the Ising model. It was shown that many computationally intractable problems (such as those in class NP complete or NP hard) can be converted into Ising models [4]. Some natural processes, such as quantum annealing process, were proposed as an effective way for finding such a ground state [5,6]. D-Wave [7] is one such quantum annealing (also called adiabatic quantum computation) solver based on the Ising model and it shows 108 speedup over simulated annealing on the weak-string cluster pair problem [8]. However, existing quantum annealing requires close to absolute zero temperature operating on superconductive devices, which are very complicated and expensive. Furthermore, these machines currently are very limited on the size and complexity of the problems they can solve.

While quantum computing has yet to reach maturity, there exists a number of other hardware-based annealing solutions which have been proposed to exploit the highly parallel nature of the annealing pro-

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^{*} This work is partially supported by NSF grant under No. CCF-1527324, and in part by NSF grant under No. CCF-1816361.

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cess used to solve the Ising model. In Ref. [9], a novel CMOS based annealing solver was proposed in which an SRAM cell is used to represent each spin and thermal annealing process was emulated to find the ground state. In Refs. [10,11], the FPGA-based Ising computing solver has been proposed to implement the simulated annealing process. However, those hardware based Ising model annealing solvers suffer several problems as detailed in Section 2.

In this article, we propose a GPU-based Ising model solver, using a modified simulated annealing heuristic, that can handle any combinatorial problem that is mapped to the Ising model as well as any general problem case associated with it. We focus on the max-cut problem as it is relevant to many VLSI design automation problems. Furthermore, max-cut is a relatively difficult problem to solve without highly efficient heuristic solvers. We show that Ising computing by the simulated annealing process is very amenable to fine-grain GPU-based parallel computing. We further propose an update method that utilizes the GPU scheduler to achieve a random update pattern enabling independent parallel spin updates. This allows us to maximize thread utilization while also avoiding sequential and deterministic update patterns for a more natural annealing process.

Furthermore, unlike other hardware accelerated solvers for the Ising model (e.g. FPGA and ASIC implementations), the proposed method does not require solving the NP-hard graph embedding problem which would drastically increase the computational complexity of the solver.

In summary, our methodology uses an annealing based algorithm to find the ground state of the Ising model. It minimizes the local spin energy of each spin glass in parallel by utilizing the fine-grain parallelism in the GPU. We then use a random flip generator with a decaying flip probability based on the annealing schedule of the solver. By minimizing the local spin energies we also minimize the global model energy which will converge close to the ground state corresponding to the solution of the max-cut problem. Our numerical results show that the proposed GPU Ising solver for the max-cut problem can deliver more than 2000X speedup over the CPU version of the algorithm on some large examples, which shows huge performance improvement.

The article is organized into five main sections as detailed in the following:

- Section 2 reviews existing works on Ising Computing, primarily those that use hardware acceleration techniques.
- Section 3 presents the Ising model. In Section 3.1 the Ising model is presented in detail. In Section 3.2 the annealing based solution to the Ising model is given.
- Section 4 introduces the max-cut problem and shows how this problem can be mapped to the Ising model.
- Section 5 is split into two parts. It firstly details the GPU architecture
 and programming model in Section 5.1 and secondly presents the
 GPU-based annealing algorithm for finding the ground state of the
 Ising model in Section 5.2.
- Section 6 presents the numerical results of our GPU-based Ising solver for the max-cut problem on the G-set benchmark graphs [12] in addition to some very large custom generated graphs. Section 6.1 compares the quality of the cut results generated by our proposed solver to the best known G-set cut results and also compares it to solutions generated by IBM's CPLEX solver [13]. In Section 6.2, performance results are compared to the traditional CPU-based simulated annealing heuristic showing 1000× speed-up.

2. Review of existing work

There have been several works previously proposed to utilize hardware acceleration techniques, other than quantum computers, as a solver for the Ising model to solve combinatorial optimization problems. The previous works have utilized accelerators such as GPUs [14–16], FPGAs [10,11], and even ASIC implementations [9].

The Ising model for many practical problems can lead to very large connections among Ising spins or cells. Furthermore, embedding those connections into the 2-dimensional fixed degree spin arrays in VLSI chips is not a trivial problem. Doing so requires mitigation techniques such as cell cloning and splitting using graph minor embedding (another NP-hard problem) as proposed in Refs. [10,11,17]. This stems from the fact that these hardware based methods must convert every problem to a nearest-neighbor model to ensure that their regularly arranged hardware spins can accommodate any graph problem. The solution to this NP-hard problem will drastically increase preprocessing time for the Ising solver. Additionally, graph embedding requires the cloning and splitting of nodes in the graph which means the number of spins in the model will also greatly increase. Furthermore, after the solution has been obtained, post-processing must be done to extract the real solution from the solver by deconstructing the graph embedding. This leads to another problem, that being hardware utilization since the number of spins increases when a graph is embedded into the nearest neighbor model which will make it more difficult to fit larger problems on an FPGA or require more area in an ASIC implementation. Alternatively, hardware designs would require drastic increases in routing and connectivity hardware, however, even then it would not be guaranteed to handle every problem. In essence, ASIC implementations are not flexible and can only handle a specific problems or utilize graph embedding due to the fixed topology among spins, and FPGA implementations require architectural redesign, and thus recompilation, for each different problem if graph embedding is not utilized. Lastly, one has to design hardware for the random number generator for each spin cell and simulate the temperature changes, which occupies significant chip area resulting in scalability degradation.

Based on the above observations and the highly parallel nature of the Ising model, in this work, we explore the General Purpose Graphics Processing Unit (GPGPU or simply GPU) as the Ising model annealing computing platform. The GPU is a general computing platform, which can provide much more flexibility over VLSI hardware based annealing solutions as a GPU can be programmed in a more general way, enabling it to handle any problem that can be mapped to the Ising model. That is, it is not restricted by the topology or complex connections that some problems may have. At the same time, it provides massive parallelisms compared to existing CPUs. The GPU is an architecture that utilizes large amounts of compute cores to achieve high throughput performance. This allows for very good performance when computing algorithms that are amenable to parallel computation while also having very large data sets which can occupy the computational resources of the GPU [18,19]. The problem sizes in the design automation domain can easily accomplish this and heuristic methods can solve the Ising model in a parallel manner which makes the GPU ideal for this application. We remark that extensive work for Ising computing on GPUs have been proposed already [14-16], however; they still focus on physics problems which assume a nearest neighbor model only. This model is highly amenable to the GPU computing as it is easily load balanced across threads but is not general enough to handle problems such as max-cut without extensive pre-processing, again through graph embedding. Furthermore, many GPU-based methods use a checkerboard update scheme to ensure spin updates are uncorrelated, but this is still only practical for the nearest neighbor model.

3. Ising model and Ising computing

3.1. Ising model overview

The Ising model consists of a set of spins interconnected with each other by a weighted edge. For the general Ising model, spin connections can take on any topology. One of the connection topologies is the 2D lattice, referred to as the nearest neighbor model, shown in Fig. 1, which describes the ferromagnetic interactions between so-called spin

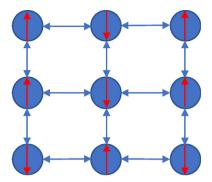


Fig. 1. The 2D nearest neighbor Ising model.

glasses. Many computationally intractable problems can be mapped to this Ising model. It was shown that finding the ground state in the 2D lattice Ising model is an NP-hard problem [20]. However, it has certain characteristics that make it more amenable to the annealing process as each local update results in energy minimization and spin glass updates can be performed in a highly parallel manner.

Specifically, each spin σ_i , has two discrete spin values $\sigma_i \in \{-1,1\}$ and some interaction with adjacent spins in the form of a weighted edge. Then the local energy or Hamiltonian of the spin is described by (1):

$$\mathcal{H}_i(\sigma_i) = -\sum_j J_{i,j}\sigma_i\sigma_j - h_i\sigma_i \tag{1}$$

In this equation, $J_{i,j}$ is the interaction weight between σ_i and σ_j , and h_i is a bias or external force acting on σ_i .

Local spin update: by finding the minimum value of $\mathcal{H}_i(\sigma_i)$, we can determine the local spin value σ_i . Specifically (1) can be written as

$$\mathcal{H}_{i}(\sigma_{i}) = \left(-\sum_{i} J_{i,j}\sigma_{j} - h_{i}\right)\sigma_{i} = -S \times \sigma_{i} \tag{2}$$

From (2), we can see that σ_i can be determined just from the sign of the S value. If S>0, $\sigma_i=1$, otherwise, $\sigma_i=-1$. If S=0, it can take any value of $\{-1,1\}$. This is called a **local spin update or update**, in Ising computing. We note that such an update for obtaining the minimum value of $\mathcal{H}_i(\sigma_i)$ only depends on its neighbors. That is, each individual spin only needs to know the energy of the spins that are directly connected to it for it to determine its next spin value. By ensuring that spin updates are not correlated, then all the spin updates can be done *independently* and thus *in parallel* [9–11,14,15].

The global energy of the model is simply the summation of the local energies. It is apparent then that minimizing the local energies will lead to the ground state of the model. The global energy of the whole Ising model is given by the following (3):

$$\mathcal{H}(\sigma_1, \sigma_2, \dots, \sigma_n) = -\sum_{\langle i, i \rangle} J_{i,j} \sigma_i \sigma_j - \sum_i h_i \sigma_i$$
(3)

Note that $\langle i,j \rangle$ indicates the combination of all spin interactions, and thus the energy of the whole model. Minimizing the energy of this equation essentially requires finding the optimal spin configurations given the interaction of each individual spin with their neighbors. While (2) describes the energy of a single spin, this new equation in (3) describes the total summation of off spins and their interactions.

In general, we refer the problem of finding the minimum energy of the Ising Model, or equivalently the ground state of Ising Hamiltonian, as the Ising problem. It can be shown that the Ising problem shown is equivalent to the problem of quadratic unconstrained Boolean optimization (QUBO) [21]. It was shown that many computationally intractable problems (such as those in class NP-complete or NP-hard) can be converted into Ising models [4].

Previous methods have focused on solving the nearest neighbor Ising model [9–11]. However, this model has the drawback of not being able

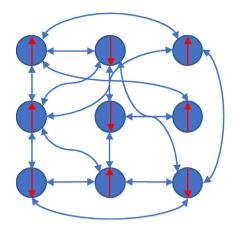


Fig. 2. An example of a generally connected Ising model.

to handle any general problem which may have arbitrary and complex connections. To do so, another NP-hard problem, the graph embedding problem, must be solved first to convert a generally connected graph to the nearest neighbor model which will be very computationally intensive and even resource prohibitive for certain hardware implementations. Therefore, in this work, we assume that a spin glass's connections, or edges, are able to connect to any other spin glass in the model, an example of which is shown in Fig. 2. Using this more general model removes the nearest neighbor restriction on the Ising model and allows us to handle more complex problems.

From the Hamiltonians presented in this section, we can see that if we minimize the local energy of each spin, we also minimize the global energy of the entire system which leads to the ground state of the model. We can then map a combinatorial optimization problem to this Ising model such that the ground state of the Ising model corresponds to the global solution of the corresponding optimization problem. In this way, finding the local energy of each spin, which leads to finding the ground state of the Ising model, is the same as finding the optimal solution to the problem in question.

3.2. Annealing method for Ising model solution

A classical and well known heuristic for combinatorial optimization is Simulated Annealing (SA) [22]. This heuristic mimics the behavior of thermal annealing, found in metallurgy. Essentially, it works by setting the environment to a high "temperature," giving the model high energy and allowing for higher probability of changing states, and then gradually decreases the temperature as the simulation runs. More precisely, it iteratively calculates and evaluates the global solution quality of neigh-

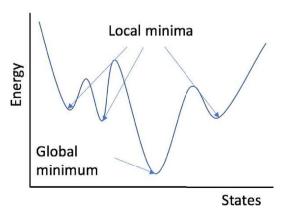


Fig. 3. Depiction of the local minima and global minimum in the energy minimization problem.

bor states of a model and probabilistically allows the acceptance of a new state even if its solution quality is worse than the previous state by utilizing the Metropolis criteria. The probability of accepting a worse state is dependent on the temperature of the system which gradually decays over time. This allows the heuristic to avoid local minima as depicted in Fig. 3.

In this proposed work, we use a simplified/modified Metropolis annealing algorithm to find the ground state as shown in Algorithm 1 that better exploits the features of the Ising model while also allowing us to avoid local minima. In our proposed method, we allow each spin update to minimize its own local energy and do not compute a global solution quality (which would add a large computational penalty). In order to avoid local minima we add energy to our Ising model by utilizing random flip probabilities that decay over time.

```
Algorithm 1 Modified Ising annealing algorithm. 1: input: (M, N, S) 2: initialize all \sigma_i in S 3: for sweep-id in \{1, 2, \ldots, M\} do 4: for \sigma_i in S do 5: \sigma_i \leftarrow \operatorname{argmin}(H(\sigma_i)) based on (2) 6: end for 7: randomly choose and flip N spin glasses in S 8: decrease N 9: end for
```

In Algorithm 1, M is the maximum number of sweeps, N is the number of spins to randomly flip, and S is the set of all spin glasses. Once the spin glasses are initialized, all spin glasses are updated iteratively to propagate the interactions between each spin (a process we will call a "sweep"). When a spin glass updates based on (2), it computes and chooses the spin value that will minimize its local Hamiltonian. At the end of a sweep, N glasses are randomly flipped and N is decreased according to an annealing schedule. After this, the process is repeated for M sweeps or until convergence is achieved.

Following this process, the local energy of each spin glass, and thus the global energy of the model, is gradually decreased. Furthermore, we avoid the local minima by introducing energy to the model by using uncorrelated random flips which slowly decrease over time.

We want to remark that the modified Ising annealing process can be viewed as a simplified Metropolis Monte Carlo method as we essentially accept the positive energy changes of a spin flip based on a temperature dependent probability [23]. As a result, we should have the convergence properties of the Metropolis method [24], which means that the objective function will be minimized in a statistical way for a sufficient time. We notice that similar Ising annealing processes have been used for FPGA and ASIC based Ising computing [9,10,17].

4. Ising model for the max-cut problem

The Ising model and the method introduced in this paper can be applied to many NP class problems, however, we use the max-cut problem as a practical example. The max-cut problem, in practice, can help find solutions to several EDA and VLSI design problems. For example, the general via minimization problem, the act of assigning wire segments to layers of metallization such that the number of vias is minimized, can be modeled as a max-cut problem [25–27]. The max-cut problem is highly amenable to the Ising model, making it an ideal candidate to introduce the proposed methodology. Furthermore, we also note that the Ising spin model and max-cut have been used as a solution technique for the via-minimization problem in the past [25].

The max-cut problem is defined as partitioning a graph into two subsets S and \overline{S} such that the weighted edges between the vertices of one subset and the other subset are maximized. This is mathematically

formulated by (4) assuming a graph G = (V, E) has a variable x_i assigned to each vertex:

$$\max \frac{1}{2} \sum_{i,j \in V, i < j} w_{i,j} (1 - x_i x_j)$$
(4)

s.t. $x_i \in \{1, -1\}$

In this equation, V is the set of vertices in the graph G, $w_{i,j}$ is the edge weights in E between the ith and jth elements in V, and x_i is an indication of which subset the vertex belongs to and can take the values $\{-1,1\}$.

Intuitively, looking as the Ising spin glass problem in (3), we can see how the max-cut problem should map to the Ising model by associating the spin of a spin glass σ_i with a subset of the graph in the max-cut problem. That is, we can say that if a spin is 1 then the spin glass is in S and if a spin is -1 then it is in \overline{S} , which is analogous to x_i . Furthermore, the weights between vertices $w_{i,j}$ is the same as the interaction weights between spin glasses $J_{i,j}$ and, in this case, there is no bias or external force so the h term in the Ising model is simply zero. The global energy minimization of the Ising model for the max-cut problem is shown below in (5):

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{i,j} \sigma_i \sigma_j \tag{5}$$

Once mapped to the Ising model, the max-cut problem can then be solved by finding the ground state of the model using the methods proposed in this paper. While there are other ways to solve this problem, the method we propose is highly amenable to parallel computation and large problem sets have great performance when implemented on the GPU, thus, giving our method an advantage in scalability.

5. GPU implementation

5.1. GPU architecture

The general purpose GPU is an architecture designed for highly parallel workloads which is leveraged by Nvidia's CUDA, Compute Unified Device Architecture, programming model [18]. GPUs offer massive parallelism favoring throughput oriented computing in contrast to traditional CPUs which focus primarily on latency optimized computation. This gives the GPU an advantage in scalability so long as a problem does not contain large amounts of sequential operations. The Nvidia GPU architecture is comprised of several Symmetric Multiprocessors (SMs), each containing a number of "CUDA" cores, and a very large amount of DRAM global memory [19]. The Kepler architecture based Tesla K40c GPU, for example, has 15 SMs for a total of 2880 CUDA cores (192 cores per SM), and 12 GB DRAM global memory. Additionally, each SM has several special function units, shared memory, and its own cache.

The CUDA programming model, shown in Fig. 4, extends the C language adding support for thread and memory allocation and also the essential functions for driving the GPU [28]. The model makes a distinction between the host and device or the CPU and GPU respectively. The model uses an offloading methodology in which the host can launch a device kernel (the actual GPU program) and also prepare the device for the coming computation, e.g., the host will create the thread organization, allocate memory, and copy data to the device. In practice, a programmer must launch many threads which will be used to execute the GPU kernel. Thread organization is therefore extremely important in GPU programming. Threads are organized into blocks which are organized into grids. Each block of threads also has its own shared memory which is accessible to all the threads in that block. Additionally, the threads in the block can also access a global memory on the GPU which is available to all threads across all blocks.

The GPU fundamentally focuses on throughput over speed. This throughput is achieved through the massive compute resources able

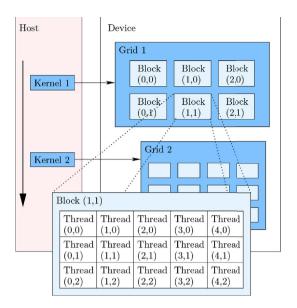


Fig. 4. The Nvidia CUDA programming model showing the Host (CPU) and Device (GPU) and the relation between threads, blocks, and grids.

to be run in parallel. Because of this, it is important to realize that the GPU is not meant for small data sets or extremely complicated operations that may be better suited for a powerful CPU. Instead, the GPU is meant to execute relatively simple instructions on massive data in parallel that can occupy the GPU resources for an extended period of time. This computing paradigm gives the GPU a huge advantage in scalability so long as it has sufficient hardware resources for the problem being solved. So long as this is the case, and there is no significant sequential operations in the GPU kernel, the GPU computation time for a problem will not grow significantly.

5.2. Ising model implementation

The GPU, while lacking the massive scaling of a quantum computer, has much larger scaling capabilities than CPUs, allowing it to handle very large problem sizes. Indeed, smaller problems that are unable to fully utilize the GPU resources may achieve worse performance than a CPU.

In order to ensure the best utilization of GPU resources, it is necessary to devise a spin glass update scheme more amenable to parallel computation. Algorithm 1 relies on sequential updates to propagate the interactions between the spin glasses. However, this would be highly inefficient on the GPU as it would mean each thread would have to wait for previous threads to update.

In previous works that have addressed the nearest neighbor Ising model, a checkerboard update scheme is implemented which allows for many spin glasses to be updated in parallel [16]. While the spin glass updates are independent of their neighbors, they are not truly independent since the update pattern is deterministic and can introduce autocorrelation between spin updates but this autocorrelation generally does not affect the global balance of the model [16]. For the problem addressed in this work, however; interactions are not confined to nearest neighbors nor are they restricted to regular patterns. This results in very complex interactions in which spins can be dependent on many other spins across the entire model. Consequently, a different update scheme must be developed for such a general solver to ensure the independence of parallel updates.

To address the above mentioned issues, we modify the original algorithm in Algorithm 1. Firstly, we assign each thread to a single spin glass, and make it responsible for updating that glass. One may notice

that since each spin glass may have a different number of neighbors. then the threads will not be perfectly load balanced. However, the alternative is to use graph minor embedding, another NP-hard problem [29], to create clone nodes such that every thread will have an equal number of updates [10]. However, this means that we need to have the CPU do some intensive pre-processing on the model, and it also means that after each update sweep, a reduction must be performed on each spin glass's clones so that the true spin value can be determined. For these reasons, it is much better to allow for some load imbalance and suffer some computational penalty on the GPU, instead of increasing the complexity of the algorithm. Furthermore, while each update sweep is synchronized, we do not synchronize the updates of each spin which makes them uncorrelated. In practice, this means that threads will update their assigned spin glass as soon as they are scheduled and will use whatever spin status their respective neighbors have at the time of data access. Therefore, there is no guarantee that a spin's neighbors will contain the spin value from the current sweep or from the previous sweep. This naturally propagates the updates of each spin glass in a non-deterministic pattern which ensures that each spin update can be done in independently of its neighbor and in

Another major change to the algorithm is the implementation of the random flips. Instead of randomly selecting a number of spin glasses to be flipped at the end of an update sweep, we let each thread independently decide if it should flip or not. A global variable, visible to all threads, gives the flip probability in the form of a floating point number between 0.0 and 1.0. Each thread then independently generates a random number between 0.0 and 1.0, generated by the CUDA cuRAND library for efficient random number generation, and flips if the number is below the global flip probability. The cuRAND library used for the random number generations allows us to create a random number generator for each thread at the very beginning of the program. Each thread is then responsible for calling its own generator when it requires a random number. The advantage of using the cuRAND library is that the random numbers can be generated completely in parallel and independent of each other by allowing the GPU threads to do their own random number generation work. This also is amenable to our asynchronous update scheme since each thread is responsible for its own flipping and can decide to flip or not as soon as it finishes its update without waiting for other threads which may still be updating. Consequently, a thread may not only update using an already updated neighbor, it may actually update using a neighbor that has been randomly flipped also. The flip probability is then reduced as update sweeps are completed.

In Algorithm 2, the parallel simulated annealing solver for the Ising model is presented. While mostly similar to the Algorithm 1, There are some differences. We replace the number of random flips input with a variable F_p which represents the flip probability mentioned above. Next, we have each thread generate a random number, using the cuRAND library, between 0.0 and 1.0 and compare this to F_p . If it is less, then the thread will flip the spin value. While these changes are subtle, the effect is large as it allows the parallel computation of an entire update sweep.

```
\begin{array}{ll} \textbf{Algorithm 2} & \textbf{GPU Simulated Annealing method for Ising model.} \\ \textbf{input:} & (F_p, \mathbf{S}) \\ \textbf{initialize ALL } \sigma_i \textbf{ in S} \\ \textbf{While } F_p > 0 \textbf{ do} \\ \textbf{for all } \sigma_i \in \textbf{S in parallel do} \\ \sigma_i \leftarrow \text{argmin}(H(\sigma_i)) \\ \textbf{flip } \sigma_i \textbf{ with probability } F_p \\ \textbf{end for} \\ \textbf{reduce } F_p \\ \textbf{end While} \end{array}
```

With respect to GPU programming optimizations, the typical best practices were followed or considered during implementation. We observe that thread divergence is not an issue in our algorithm due to the fact that each thread performs the exact same operations. This means that when a group of threads are running in parallel, they will not be serialized at anytime. Furthermore, while memory coalescing is a standard method of enhancing memory access speeds, we recognize that memory accesses in the Ising model are not regular. This means implementing memory coalescing would result in unnecessary storage complexity.

6. Experimental results

In this section, we present the experimental results showing both the accuracy and speed of our parallel GPU-based Ising model solver for the max-cut problem. The CPU-based solution is done using a Linux server with two Xeon E5-2698v2 2.3 GHz processors, each having 16 cores (2 threads per core for a total of 32 threads per CPU and 64 threads total in the server), and 72 GB of memory. On the same server, we also implement the GPU-based solver using the Nvidia Tesla K40c GPU which has 2880 CUDA cores and 12 GB of memory. Test problems from the G-set benchmark [12] are used for testing as well as some custom made problems to show very large cases. The problems' edge counts are used to represent their size as the size of each problem is typically dominated by the number of edges. However, we remark that this is not always the case for every graph. That is, some graphs may have a very large number of edges but only a few nodes, or vice versa, which may make it easier or harder for a certain algorithm to compute. As such, some graphs with higher numbers of edges may take less time to compute. Furthermore, graphs with large numbers of edges may have more regular connections which will lead to more load balance and thus, quicker computation times. However, the general trend in computation time is that a larger number of edges will take more computation time.

6.1. Accuracy study

To test the accuracy of the method presented in this paper, we compare the max-cut value our method generates with that of the best known solution in the G-set benchmark. In addition to the G-set benchmark comparison, we generated several custom graphs and compared the solution quality of our GPU-based method against IBM's CPLEX mathematical programming solver [13], a state-of-the-art linear programming solver employed to solve combinatorial optimization problems. CPLEX solutions were implemented using a server with a 2.1 GHz Xeon Broadwell processor with 36 threads (18 cores with 2 threads per core) and 128 GB of memory.

For the results in Tables 1 and 2, cut values were obtained by running the GPU solver 10 times per graph and taking the average solution quality. Each time the solver was run we used 1000 annealing steps which is the same number used to generate the performance data in the following performance study section. Additionally, the number of random flips for each solution is set to 200 which decays linearly each sweep by a factor of 0.01. The cut values generated by CPLEX were obtained by running the CPLEX solver for each graph case. The solver time for CPLEX was capped at two days with most cases using all of the allocated time. We also note that we don't compare the solution time to our solver since the CPLEX solution time is on the order of days while the GPU Ising solver's solution time is on the order of seconds. The accuracy% is defined as the ratio of the cut values of the GPU Ising solver over the best known cut (Table 1) or the CPLEX solver cut (Table 2), i.e., the closer to 100% the better the accuracy%. If accuracy% is larger than 100%, then GPU Ising solver obtained a better result than the competing solver.

From the tables, we can see that the GPU consistently performs well with almost all results above 90%. Furthermore, in Table 2 our GPU-based solver is able to consistently beat CPLEX for larger cases which become too large for CPLEX to solve in a reasonable amount of

Table 1
Accuracy comparison of the GPU max-cut value against the best known cut values for the G-set benchmark.

Graph	Best known cut	GPU cut (%accuracy)
G13	580	522(90.0%)
G34	1372	1191(86.8%)
G19	903	844(93.5%)
G21	931	880(94.6%)
G20	941	880(93.6%)
G18	988	938(94.9%)
G51	3846	3754(97.6%)
G53	3846	3756(97.7%)
G54	3846	3756(97.7%)
G50	5880	5803(98.7%)
G47	6656	6619(99.4%)
G40	2387	2267(95.0%)
G39	2395	2269(94.7%)
G42	2469	2325(94.2%)
G41	2398	2284(95.2%)
G9	2048	2004(97.9%)
G31	3288	3227(98.2%)

Table 2Accuracy comparison of the GPU max-cut value against the cut values obtained by CPLEX.

# edges	CPLEX cut	GPU cut (%accuracy)
9999	9473	8884(93.78%)
14999	13357	12776(95.65%)
24998	20206	19981(98.88%)
49995	35248	36228(100.29%)
39998	33605	32914(97.94%)
59997	46371	46510(100.29%)
99995	70566	72009(102.04%)
199990	128448	131930(102.71%)
249995	176556	179391(101.60%)
374993	248505	255078(102.64%)
626988	392912	400540(101.94%)
1249975	741709	751050(101.25%)

time. We also note that in practice, the best result could be picked from a number of GPU simulations and some simulation parameters could be tuned to achieve better results, e.g., annealing schedule and initial flip probability. However, we present average results of a parameter configuration we found to be consistent across many graphs.

In Fig. 5 the region of convergence is shown for the GPU Ising solver and was obtained by running the solver several times for a particular problem. The red line shows the lowest observed accuracy while the green line shows the highest observed accuracy. One example run is also included to show the overall behavior of the convergence. Unlike classic simulated annealing, the solver does not converge to a single state but rather it continues to have minor variations in energy as the solver progresses. This is because of the utilization of the GPU scheduler as the random update pattern which means there will be some oscillations between solution states, even when the number of random flips is small or zero.

6.2. Performance study

Next, we look at the GPU Ising solver's performance. The speed of the GPU Ising solver is judged by measuring how long it takes to perform a number of update sweeps on various sized models. We run both the proposed GPU Ising solver and the sequential CPU implementation of the algorithm for 1000 sweeps (which is the same number of sweeps used to generate the accuracy results above) and compare the computation time. Because the GPU performs best when its resources are fully utilized, and because it is not optimized for small workloads, we expect

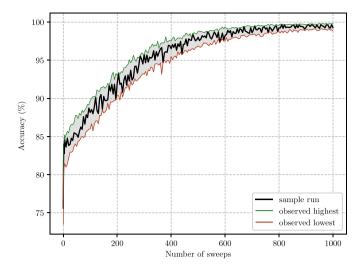


Fig. 5. Convergence region of the GPU-based annealing for the Ising model on the G-set G47 problem.

to see performance gain over the cpu to improve as the problem size increases. We also should not expect a large speed-up over a CPU version for smaller problems.

In Table 3, the time (in seconds) to complete 1000 simulation sweeps is shown for the CPU and GPU for various G-set problems of increasing edge counts. In this table, column torus indicates whether the graph is a torus or not. Columns $t_{CPU}(s)$ and $t_{GPU}(s)$ are the

run times for CPU and GPU based solutions respectively. Column speedup is the speedup of GPU solution over CPU solution defined as speedup = $t_{CPU}(s)/t_{GPU}(s)$. Furthermore, we include several very large custom made and randomly generated non-torus graphs in the table to show the scalability of the proposed method against the CPU-based solution. It should be noted that accuracy results are not included for the custom graphs as there is no data for best known or optimal maximized cut values. Additionally, Fig. 7 graphically shows the speed results in seconds for increasing problem sizes and Fig. 6 shows a bar graph of the results in log scale (the large custom graphs are omitted from the figures). For all simulations, small and large, the GPU outperformed the CPU competition. For the very large custom graphs, the scalability of the GPU can really be seen as the CPU struggles to handle such large problems while the GPU is able to finish them quite quickly and even achieve over 2000X speedup for the largest problems.

The CPU based Ising solution time grew approximately quadratically with the problem size which is expected and is similar to the observations of the reported quantum adiabatic computing on the exact cover problem [30]. We can also see that the GPU solver time seems to remain quite constant until it starts working on the very large random graphs. This seamingly constant computation time trend can be explained by the GPU architecture. The GPU achieves its performance by utilizing a vast number of computational resources which enables high throughput computations. Because of this, we do not expect the computation time to rise dramatically with a rise in problem size so long as the computational resources of the GPU are sufficient to handle the problem size. In contrast, the CPU's computation time will be impacted regardless of the problem size.

Table 3Performance results comparing GPU performance against CPU performance for the G-set benchmark (G prefix) problems and large custom problems (C prefix).

graph	# vertices	# edges	torus	t_{CPU} (s)	$t_{\rm GPU}$ (s)	speedup
G13	800	1600	yes	0.17	0.11	1.5
G34	2000	4000	yes	0.29	0.11	2.6
G19	800	4661	no	0.39	0.17	2.3
G21	800	4667	no	0.39	0.17	2.3
G20	800	4672	no	0.39	0.15	2.6
G18	800	4694	no	0.39	0.16	2.5
G51	1000	5909	no	0.41	0.18	2.3
G53	1000	5914	no	0.41	0.19	2.1
G54	1000	5916	no	0.41	0.20	2.0
G50	3000	6000	yes	0.49	0.15	3.2
G47	1000	9990	no	0.64	0.15	4.3
G70	10000	9999	no	5.34	0.34	15.7
G57	7000	10000	yes	1.44	0.15	9.3
G40	2000	11766	no	0.81	0.24	3.4
G39	2000	11778	no	0.76	0.20	3.7
G42	2000	11779	no	0.76	0.26	2.9
G41	2000	11785	no	0.76	0.25	3.1
G55	5000	12498	no	2.26	0.21	10.8
G62	7000	14000	yes	2.73	0.16	17.5
G65	8000	16000	yes	3.27	0.16	21.0
G61	7000	17148	no	4.36	0.21	20.9
G66	9000	18000	yes	4.19	0.16	27.0
G9	800	19176	no	1.27	0.17	7.6
G31	2000	19990	no	1.16	0.16	7.4
G67	10000	20000	yes	5.06	0.16	32.5
G77	14000	28000	yes	9.64	0.16	61.8
G59	5000	29570	no	4.07	0.34	11.9
G81	20000	40000	yes	19.89	0.16	125.6
G64	7000	41459	no	7.97	0.39	20.6
C1	10000	100E3	no	26.63	0.18	147.9
C2	10000	250E3	no	59.81	0.38	157.39
C3	10000	500E3	no	121.5	0.61	199.5
C4	10000	750E3	no	179.87	0.91	197.65
C5	10000	1E6	no	234.86	1.18	198.69
C6	100E3	5E6	no	1.56E4	7.11	2200.81
C7	100E3	7E6	no	2.05E4	9.99	2254.74

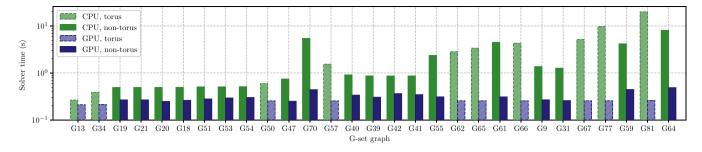


Fig. 6. Speedup results of the GPU against the CPU for the G-set benchmark problems.

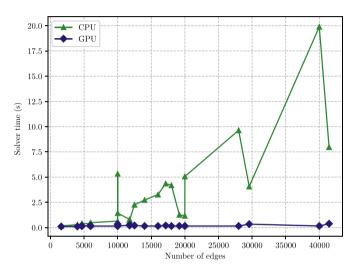


Fig. 7. Graphic of the performance in seconds of the GPU and CPU for increasingly large graphs.

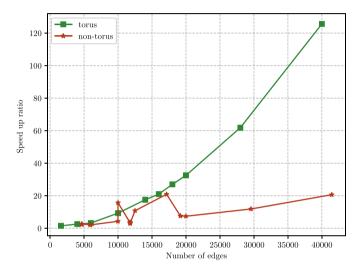


Fig. 8. The performance results for the GPU against the CPU, separated by the graph type, torus and non-torus.

For the most part, as the problem size increased, so did the GPU speedup. However, we note that there were some graphs which the CPU performed quite well and the speedup that the GPU achieved was much smaller than on other graphs. This is primarily seen in the smaller graphs where the large amount of compute resources cannot be fully utilized on the GPU. It is important to note that the GPU performance is achievable due to the large amount of compute resources that can be utilized in parallel. However, if the size of the graph is much larger than the amount of compute resources, then we would expect the performance to degrade but also to still be better than the CPU. Additionally, for very small graphs that don't occupy the GPU resources, we should expect the performance gain compared to a CPU based version to be much smaller after further inspection we identified that the solvers had interesting performance depending on the graph structure which prompted further investigation.

We immediately noticed that the performance of both the GPU and CPU was dependent on whether or not the graph was a 2D torus structure. As seen in Fig. 8, the speedup (GPU solver time over CPU solver time) is separated by the graph type, green for a torus and red for a non-torus. By examining this figure, we see that the speedup of the torus structure, which is highly regular, steadily increases as the problem size increases. However, the non-torus structure, while still showing speedup, is less consistent but generally shows an increase in speedup as the problem size increases.

We further investigate the individual performance of the CPU and GPU by plotting their speed results individually and also separating these results by graph type in Figs. 9 and 10 respectively. From

these graphs we can make a few observations. For both the CPU and GPU versions, we firstly notice that the speed trends when solving the torus structures is highly consistent with the increasing problem sizes while the non-torus structures have erratic behavior. This can be easily explained by the irregularity of the graph structure. Each node will have different numbers of edges in the non-torus structure. Coincidentally, on the CPU, the torus structures take longer to solve than the non-torus structures due to the fact that the torus graphs in the g-set benchmark happen to have many more nodes than the non-torus structures(see 3 for node numbers). More interesting, we see that the GPU performance on the torus structures is highly efficient with almost no noticeable change in computation time between the graph with 6000 edges and the graph with over 40000 edges. This can be explained by the regularity of the graph structures. This regularity will lead to load balance amongst the GPU threads during computation which allows the GPU performance to really shine. We should expect this nearly constant compute complexity so long as the GPU has sufficient compute resources for the problem size. Any growth in computation time then, could be attributed to host to device memory transfers. However, as soon as the resources become insufficient, certain spin updates will need to be serialized, thus, decreasing performance.

We can also make the observation that the torus graphs are graphs that are similar to nearest neighbor models. That is, they result in highly load balanced workloads. In this way, we can also see that the cost of handling generally connected graph is present in these results by looking at the computation time of non-torus graphs compared to the torus graphs. However, we remark that this cost is still much better

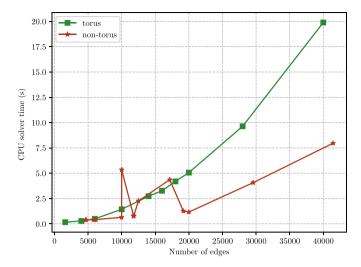


Fig. 9. CPU performance comparing torus and non-torus graphs.

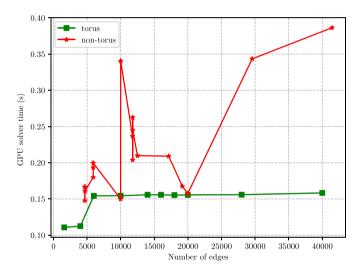


Fig. 10. GPU performance comparing torus and non-torus graphs.

than if we had to pre-process the graph by solving a graph embedding problem which would also increase our node counts and finally require post-processing to extract the actual answer from the embedded graph.

7. Conclusion

In this work, we have proposed the Ising spin model based computing to solve the max-cut combinatorial optimization problem, which is widely used method for VLSI design automation, on the general purpose GPU (GPGPU). Our new algorithm is based on the observation that Ising computing by the simulated annealing process is very amenable to finegrain GPU based parallel computing. GPU-based Ising computing provides clear advantage as a general solver over existing hardware-based Ising computing methods that utilize integrated circuits and FPGAs. We further illustrate how the natural randomness of GPU thread scheduling can be exploited during the annealing process to improve GPU resource utilization. We also showed that GPU-based computing can handle any general Ising graph with arbitrary connections, which was shown to be difficult for FPGA and other hardware based implementation methods. Numerical results show that the proposed GPU Ising max-cut solver can deliver over 2000X speedup over the CPU version of the algorithms over some large examples, which renders this method very appealing for solving many practical VLSI design automation problems.

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