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# PhD Thesis Review Report

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| Faculty: | **Institute of Theoretical and Applied Informatics,<br>Polish Academy of Sciences** |
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| Supervisor: | **dr hab. Bartłomiej Gardas** |
| Co-supervisor: | **dr hab. inż. Łukasz Pawela** |
| Title: | **Validation and benchmarking of quantum annealing technology** |
| Reviewer: | **dr Łukasz Cincio** |

The thesis is based on six published articles. Mgr Konrad Jałowiecki is the first author on four of them. Those papers are published in journals of good standing, including Scientific Reports (impact factor 4.6), Computer Physics Communications (impact factor 3.6) as well as SoftwareX (impact factor 3.4). The papers have been well-received by scientific community as evidenced by the number of citations that they received since their publication. This is a very encouraging sign for Konrad's long-term professional success.

The thesis discusses the problem of benchmarking and validating quantum annealers. The author proposes two algorithms to achieve this goal. The first one is a general quantum dynamics solver. The second one is more practical and deals with railway dispatching problems. Those two algorithms are benchmarked on D-Wave quantum annealers against classical algorithms, which are also developed in the thesis. The author demonstrates that current D-Wave annealers show capability for solving specific tasks, including accurately describing two-level quantum systems and finding high-quality solutions for certain railway conflict management problems. Limitation of D-Wave annealers are also studied in the thesis. The author identifies cases in which the quantum annealer under consideration failed to find sufficiently accurate solution. In several cases, the material included in the theses goes beyond what has been published previously by the author. For example, the original brute-force algorithm in [3] now contains new optimization methods to further increase the system size that can be solved and decrease the time to solution. It is likely that (at the time of publishing) it was the fastest brute-force Ising solver. The benchmarks presented in Chapter 7 also extend the version that has been published. The author includes results from newer generation of quantum annealers and added a discussion on penalty terms.

Chapter 2 is a well-written introduction to Ising models and their various QUBO formulations. It focuses on computational aspects of those problems leaving their physical interpretation aside. This is totally justifiable given the scope of the thesis. The author also gives very pedagogical introduction to big-$\mathcal{O}$ notation and complexity classes. The text can be easily followed by a nonspecialist. The choice and organization of the material presented in this chapter show that the author knows the field very well, is aware of relevant literature and understands the subject sufficiently well, so he can explain it in a concise and easily approachable way.

The introduction is continued in Chapter 3. Here, the author covers adiabatic quantum computation, quantum annealing and describes D-Wave quantum computers that he later uses. D-Wave devices, including their typologies are discussed in great detail. An important aspect of quantum annealers, which is embedding, is also discussed. The discussion is accompanied by easy-to-follow, illustrative examples that clearly help the reader grasp the most important concepts. The chapter includes extended section on Nvidia CUDA, its history, processing flow, architecture and programming environment among other subjects. While I enjoyed reading those sections, it was not immediately obvious to me why such a great detail is necessary. In my opinion, the thesis's completeness would not suffer if most of those low level details were left out. That is not a criticism of the work that the author did, however. Once again, the introductory material shows that the author thoroughly reviewed the literature and understands the subject very well.

Chapter 4 discusses ways of simulating quantum dynamics on quantum annealers. Currently available quantum annealers are not capable of direct simulation of quantum propagator $e^{-iHt}$ for arbitrary Hamiltonian $H$. The only dynamics that they can "naturally" perform is that described in Eq. (3.2). Chapter 4 starts with a description of a method that formulates the simulation problem as an optimization that can be solved on a quantum annealer. The method uses an approach based on Feynman clock and requires discretization of the variables. The approach has significant overhead and therefore the applications are currently limited. As a result, only simplest problems can be studied this way. The author concentrates on a physical system that consists of a single qubit. The results obtained with D-Wave computers are correct only in certain, limited cases. This is not surprising, given how noisy and limited those computers currently are. The chapter contains a section that discusses possible sources of errors. The analysis there is very valuable but I will mention as a minor comment that this part of the thesis might benefit from including a scaling analysis. The author does not discuss resource requirements needed for solving more complicated problems, like those defined on larger number of qubits or those that require higher precision. It would be interesting to know at what scale (number and quality of qubits) the method can compete with gate-based quantum computers on simulating dynamics. My expectation is that those requirements are not realistic and the usage of quantum annealers described in this chapter, while relevant for benchmarking, will probably not find practical implementations.

Chapter 5 describes classical algorithm based on tensor networks for finding low-energy spectra of Ising spin glasses. The algorithm works by representing the Boltzmann distribution by a tensor network (more precisely, by Projected Entangled Pair States or PEPS). PEPS is contracted line by line, where the edge is described by Matrix Product State (MPS). It is a well-tested algorithm for contracting PEPS but its application to solving binary optimization problems is novel. PEPS is coupled with branch and bound approach and overall, the algorithm performs exceptionally well. The author benchmarks the PEPS algorithm on sets of droplet as well as deceptive cluster loops instances that are designed to be hard for classical solvers. He uses parallel tempering as well as D-Wave machines to compare the results. The PEPS algorithm finds true ground states for all droplet problem instances. Other algorithms fail to find some of the solutions but they generally find the approximate solution faster. The PEPS algorithm performs exceptionally well also on deceptive cluster loops instances. For those cases, it either matches or outperforms previously known approximations. Author's approach also outperforms previous state-of-the-art in terms of capability of describing large ground state degeneracy. The method can easily describe degeneracies exceeding $10^8$ on problem sizes larger than 2000 spins. Overall, this is an impressive algorithm for solving spin glass problems that successfully makes use of modern tensor network techniques.

The author moves to brute-force spin glass solvers in Chapter 6. Here, he makes use of parallel CUDA architecture that was introduced before. The results are equally impressive as those presented in Chapter 5. The author's algorithm is capable of finding ground state of problem instances of size $N = 50$ within an our on standard GPU and within few minutes on server-grade GPU. Those calculations require looping over $2^{50}$ states and computing energy for all of them. The author carefully describes his approach to loop over all configuration while avoiding memory transfer bottlenecks. The algorithm is used to benchmark an MPS solver that is also outlined in the thesis. The algorithm is further improved by more optimal energy evaluation. Instead of computing energy for each configuration from scratch, the author recognizes that if two configurations differ by one bit only, the energy of the second configuration can be obtained from the first one much more cheaply. That approach requires different ordering of the configurations, which is achieved with the Gray Code. This and some other technical improvements allow the author to dramatically reduce computational time and reach very large system sizes.

Finally, in Chapter 7, the author describes an application of previously introduced techniques (quantum annealing, tensor networks and brute-force search) to railway conflict management. The author starts by constructing mathematical framework that describes train delays. This part culminates in derivation of a cost function together with penalty terms written in QUBO. The author's construction allows for a lot of flexibility including different priorities for different trains traveling in various directions. The author optimizes the cost function with suitable penalty terms using D-Wave quantum annealer as well us a suite of classical algorithms including approaches developed by the author as a part of his thesis. The performance of D-Wave computers varies significantly between devices. Not surprisingly, the newer generation computers achieve much better results. The author's findings are corroborated by classical optimization methods. Here, the results are more predictable and indicate that the tools built by the author are of very high quality.

The thesis focuses on building tools for benchmarking and validations of quantum annealers, which is definitely a timely topic. Various companies and intuitions are perfecting their quantum computers and slowly but surely, they become a valid computational devices. It is therefore important to find the best ways of utilizing them as well as build classical tools for benchmark and validation purposes. The presented thesis clearly achieves those goals. The author demonstrated high levels of understanding and technical knowledge, which allowed him to efficiently use D-Wave quantum computers as well as validate the results with his own classical methods. The author set out various, well-designed problems to test quantum annealers. The methodology used in those assessments was correctly identified and applied. The results indicate that quantum annealers are becoming competitive with classical methods, especially when time to solution (not necessarily the overall quality) is the most important factor. The author's classical methods used to benchmark quantum annealers are important in their own right and are likely to find applications outside the initial scope.

There are several novel aspects of the presented research. While there have been many studies focused on benchmarking quantum annealers, the author chose to work on interesting and non-trivial examples, which have not been extensively studied before. In my opinion, the most valuable part of the work is the development of state-of-the-art classical solvers based on tensor networks and GPU exhaustive search. The author clearly maximized the hardware available to him and developed a long list of improvements that allowed him to reach very large problem sizes. There is no doubt that the methods developed by the author will be applied by other researchers in the field. It is evident from the already large number of citations that his work has received over the short period of time.

Significant weaknesses of the presented thesis are not identified and small issues described above are not related to the quality of research or issues in methodology. Instead, my comments focus on presentation aspects in specific chapters and raise follow-up research questions.

In my opinion, the presented material meets all the requirements and in many instances goes well beyond what is expected from an excellent PhD thesis. The author has published several high-quality papers and continues to be scientifically very active. His contribution to the field is significant and is highlighted by high-profile, well-cited publications. For these reasons, I strongly recommend that the presented PhD thesis be awarded a distinction.

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