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Quantum Computing for HPC Problems

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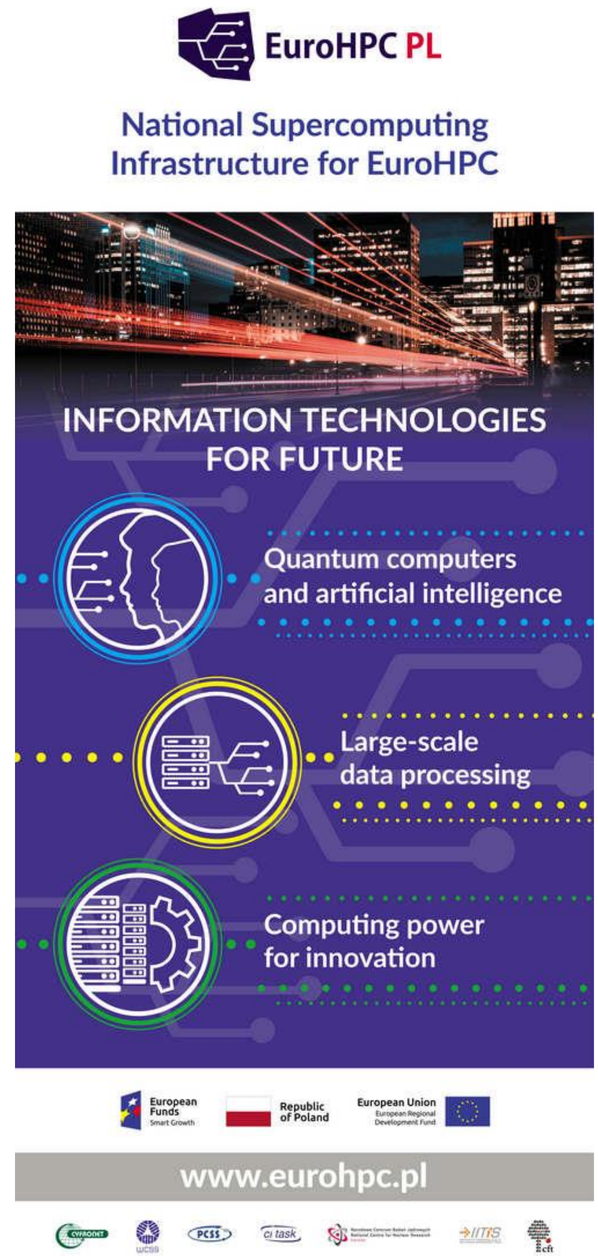
EuroHPC PL

- To provide a hybrid computing infrastructure: supercomputers, **quantum** and neuromorphic accelerators as well as dedicated services,
- Take advantage from the latest HPC technologies under the EuroHPC Joint Undertaking (EuroHPC JU),
- Support for large-scale application (simulations, analyzes of large scientific data sets and advanced visualizations).
- Adjusting research problems and software to the capabilities of exascale supercomputers and modern computing architectures.



http://www.eurohpc.pl

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Workflows

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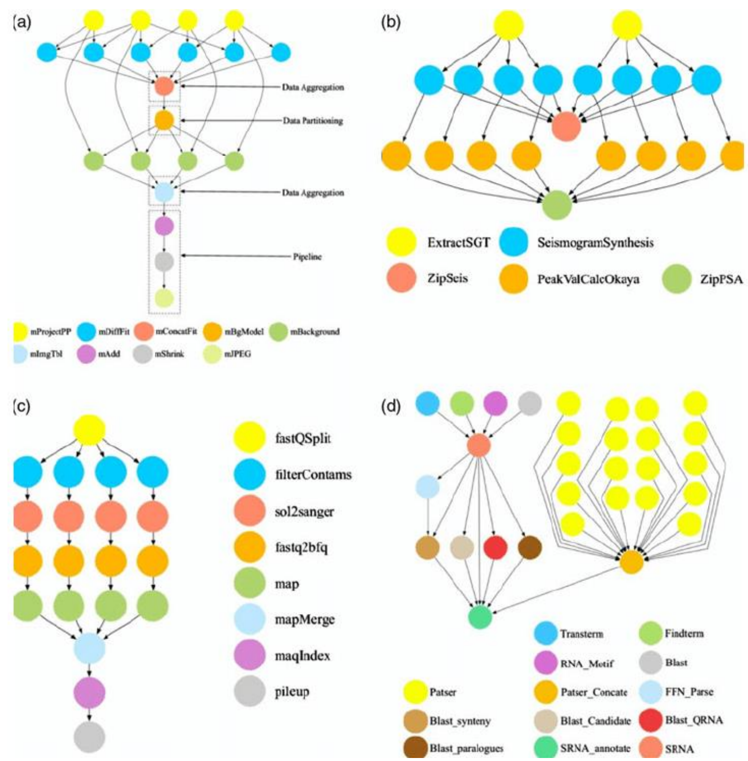
- A paradigm commonly used for describing complex scientific processes and applications.
- Usually represented as DAGs (Directed Acyclic Graphs)
- Example applications: Montage - construction human perceptible images from multiple telescope images, calculating seismic hazard maps



- Examples of scientific workflows: (a) Montage workflow, (b) CyberShake workflow, (c) Epigenomics workflow and (d) Sipht workflow
- Source: Ghafarian, Toktam & Javadi, Bahman & Buyya, Rajkumar. (2014). Decentralised workflow scheduling in volunteer computing systems. International Journal of Parallel Emergent and Distributed Systems.

Workflow scheduling (DAG scheduling, task scheduling)

- Planning of execution with respect to given parameters such as deadline, budget and computing resources.
- An NP-hard problem - strong limitations on the size of practically solvable problems

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Workflow Scheduling @HPC PL

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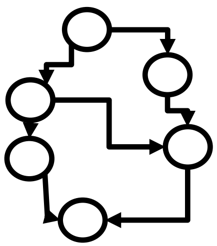


resource 1
resource 2
resource 3
conditions

Test problems

Workflow Management Systems real examples (https://wfcommons.org/)

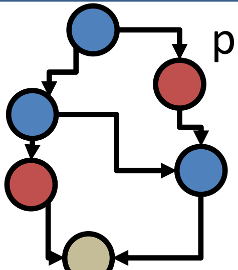
WfCommons

Jupiter Notebook @ supercomputer Prometeus

Classic solvers
- Couenne
- Bonmin
- Pyomo interface

Quantum solvers
- Variational Algorithms (QAOA)
- D-Wave/D-Wave Hybrid
- High level hybrid solver

plan



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Different models of Quantum Computers

- Gate model (e.g. IBM-Q,Rigetti, IonQ)
- different hybrid classical - quantum algorithms examples : QAOA, VQE, Grover Adaptive Search

- Quantum annealer (e.g. D'Wave)
- a metaheuristic for finding the global minimum of a given objective function
- uses quantum tunneling for escaping local minima

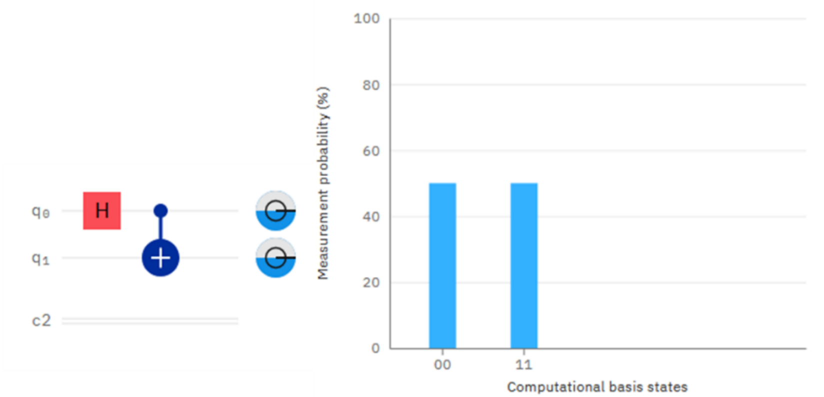

Figure: Sample quantum circuit using gate H and CNOT on IBM-Q

$$\underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2}\left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\text{Final Hamiltonian}}$$

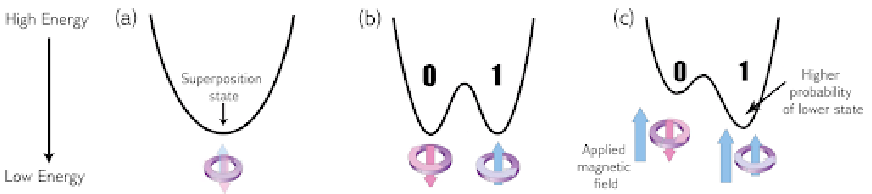

Figure: Energy changes during quantum annealing proces source: https://docs.dwavesys.com/docs/latest/cgs2.html

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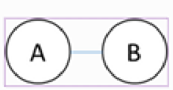
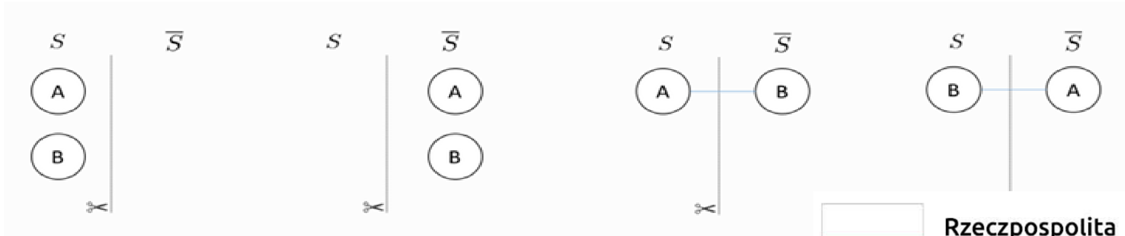
How to use Quantum Computer for optimisation ?

1. Express your problem as a cost function.
   a. For quantum annealer: QUBO
   b. For gate based devices: QUBO or PUBO (high order)
   Example: $C(x_1, x_2) = x_1 + x_2 - 2x_1x_2 \quad x_1, x_2 \in \{0, 1\}$
2. *(Supported by tools)* Translate your function into a Hamiltonian (energy operator) H such that:
   a. minimal eigenvalue of H (i.e. minimal energy of the system) = optimal value of your cost function C(x)
   b. corresponding eigenstate (i.e. system state in min energy) = the solution to your problem (x)
3. Use QC for finding a solution:
   1. For gate based devices: use variational algorithms (VQE, QAOA)
   2. For Quantum annealer -> use quantum annealing process

Example Max Cut Problem





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Variational Algorithms idea

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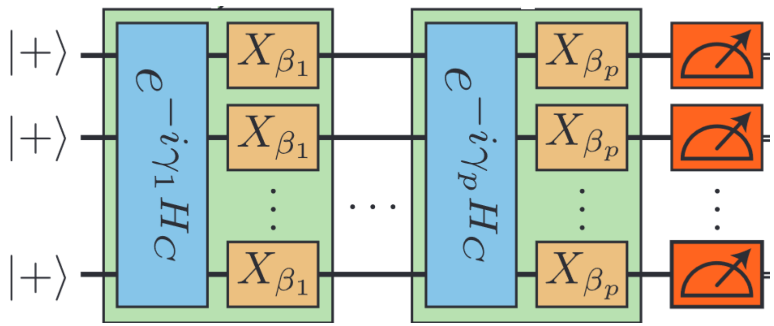
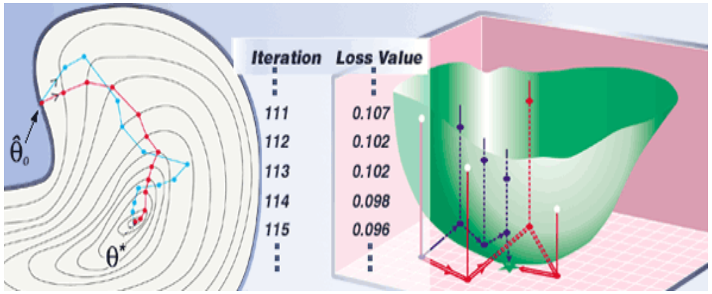
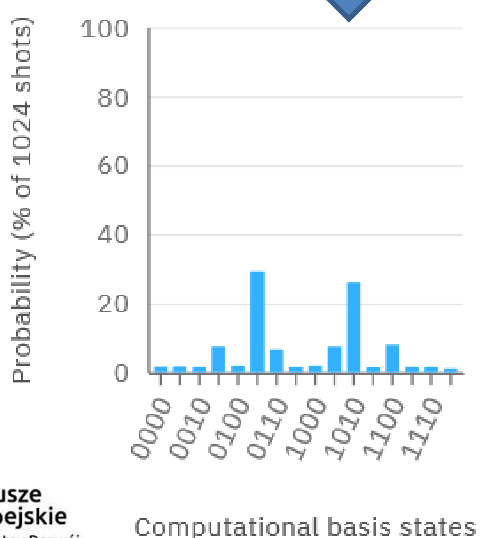
variational parameters

$(\vec{\gamma}, \vec{\beta}) = (\gamma_1, \ldots, \gamma_p, \beta_1, \ldots, \beta_p)$



Classical computer optimisation of **continuous** f $(\vec{\gamma}, \vec{\beta})$





Estimate expectation value <H> seen as f $(\vec{\gamma}, \vec{\beta})$

source of figures: https://www.jhuapl.edu/SPSA/
https://arxiv.org/pdf/1812.01041.pdf

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Variational Algorithms (gate model)

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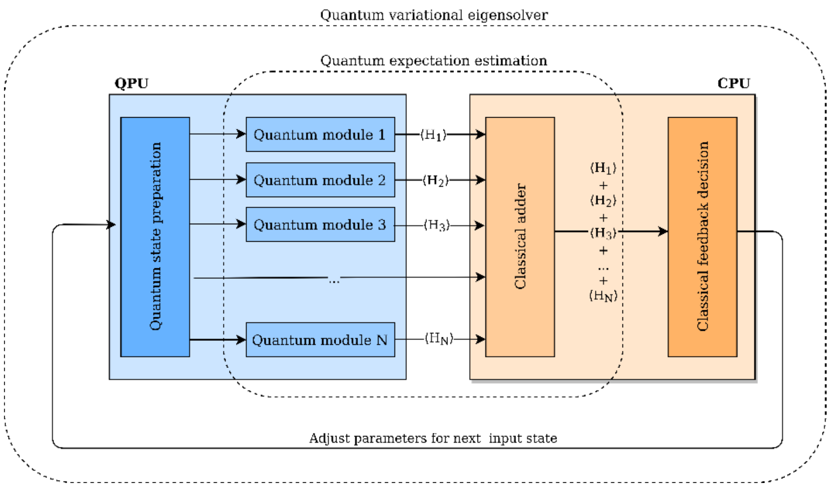
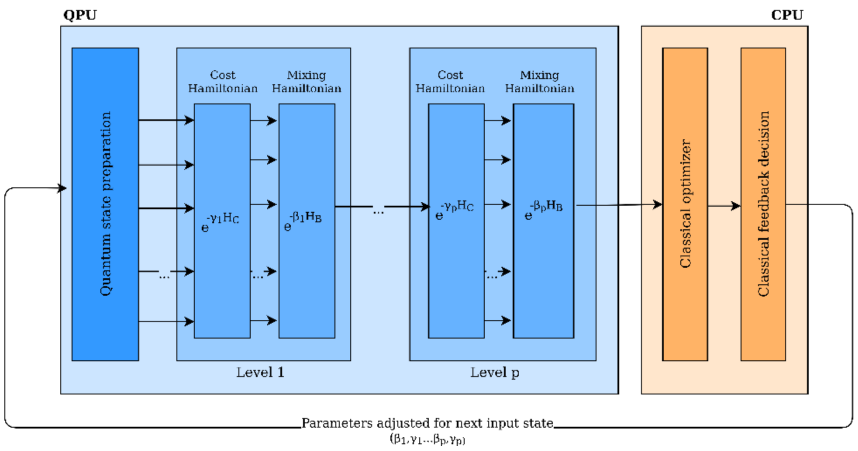
- a hybrid algorithms: a quantum subroutine runs inside of a classical optimization loop
- quantum part is responsible for :
  - preparing a quantum state (ansatz) basing on the parameters got from classical part
  - calculate expectation value of H (energy) for a given state
- the variational principle ensures that this expectation value is always greater than the smallest eigenvalue of H (lower bound)
- classical part uses non-linear optimizer to minimize the expectation value by varying ansatz parameters



Variational Quantum Eigensolver



Quantum Approximate Optimization Algorithm

Hybrid algorithms for workflow scheduling problem in quantum devices based on gate model, Julia Plewa, Joanna Sienko; Master of Science Thesis supervised by Katarzyna Rycerz, AGH University of Science and Technology, Department of Computer Science, Krakow, Poland (2021)

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Variational Algorithms Comparison

	VQE	QAOA
Usual applications	finding grand state of molecules	combinatorial problems
Problem Hamiltonians	general (inluding σ_x, σ_y, σ_z terms)	diagonal (Ising model with σ_z terms)
Ansatz	anything that fits	specific prescription : built from problem and mixer hamiltonian
Ansatz parameters	growing with qbits numer and ansatz repetitions	two per each ansatz level
Measurement	need to add measurement results for different basis (X,Y,Z)	only Z basis

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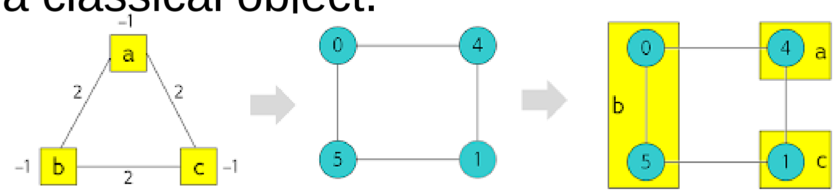
Quantum Annealing

- starts in the lowest-energy eigenstate of the initial Hamiltonian
- slowly changes initial H into final (our problem) H
- this change is done by introducing the couplers (J) and biases (h)
- (Ideally) system stays in the minimum energy state throughout the whole process
- the system ends up in the minimum energy state of the problem Hamiltonian = we have an answer to our problem
- By the end of the anneal, each qubit is a classical object.

$$\underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2}\left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\text{Final Hamiltonian}}$$



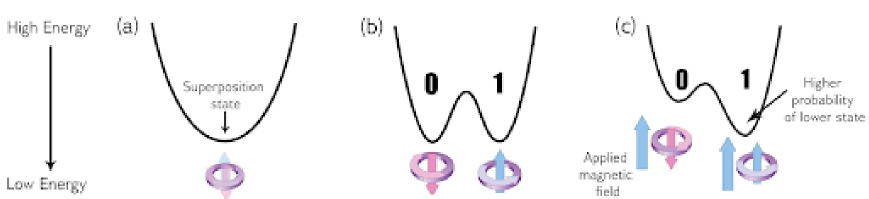
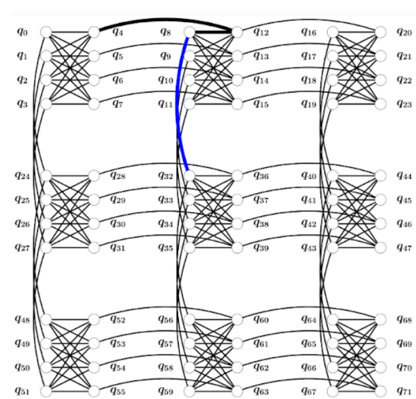


Figure: Energy changes during quantum annealing proces source: https://docs.dwavesys.com/docs/latest/cgs2.html



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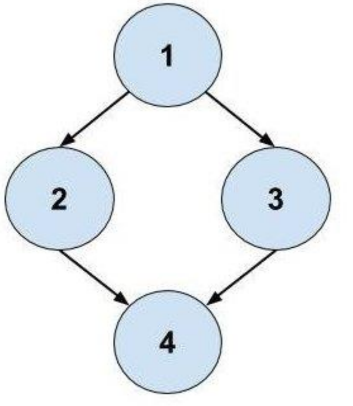
Workflow problem

- given ***t*** tasks, ***m*** machine types
- infinite number of machine types instances
- tasks in a form of DAG (***p*** paths)
- cost matrix, time matrix, deadline
- **goal: to minimize cost**
- **constraint: to fulfill deadline d**



	task 1	task 2	task 3	task 4
machine 0	6	3	12	9
machine 1	8	4	16	12

Cost matrix

	task 1	task 2	task 3	task 4
machine 0	6	3	12	9
machine 1	2	1	4	3

Time Matrix

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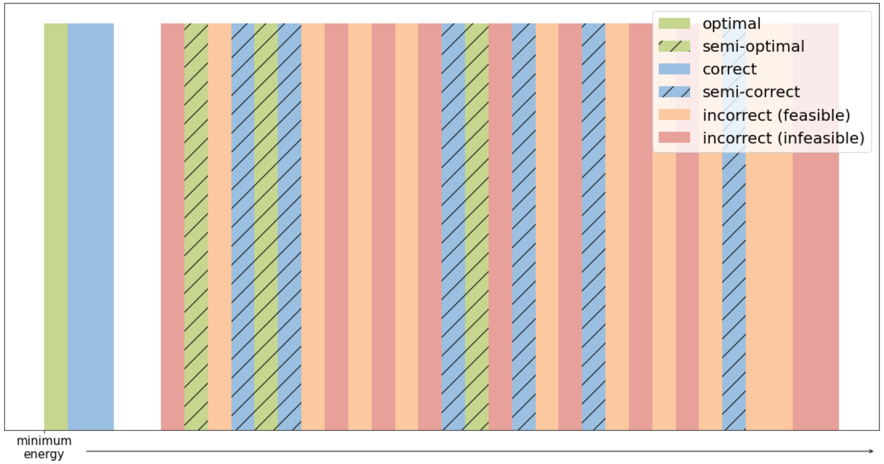
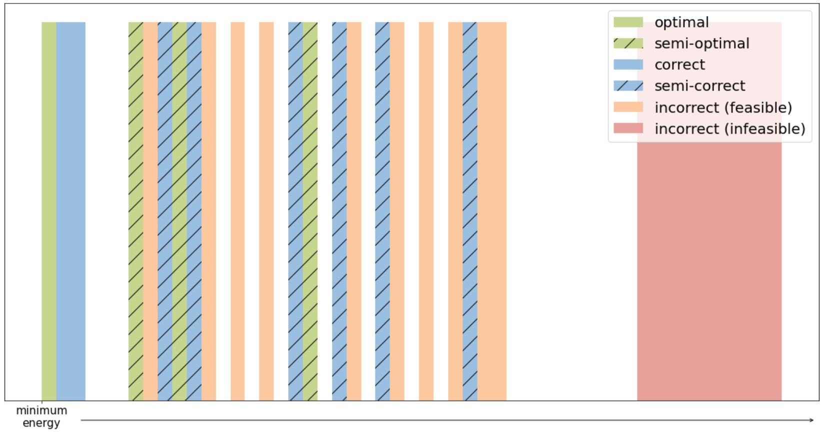
Cost function: Setting weights

$$O(X,Y) = A\sum_i^N \sum_j^M c_{i,j}x_{i,j} + B\cdot\sum_k^R \Big(d - \big(\sum_i^N\sum_j^M p_{i,k}t_{i,j}x_{i,j} + \sum_l^{s_k} 2^l y_{k,l}\big)\Big)^2$$

$$+C\cdot\sum_i^N \Big(1-\sum_j^M x_{i,j}\Big)^2$$





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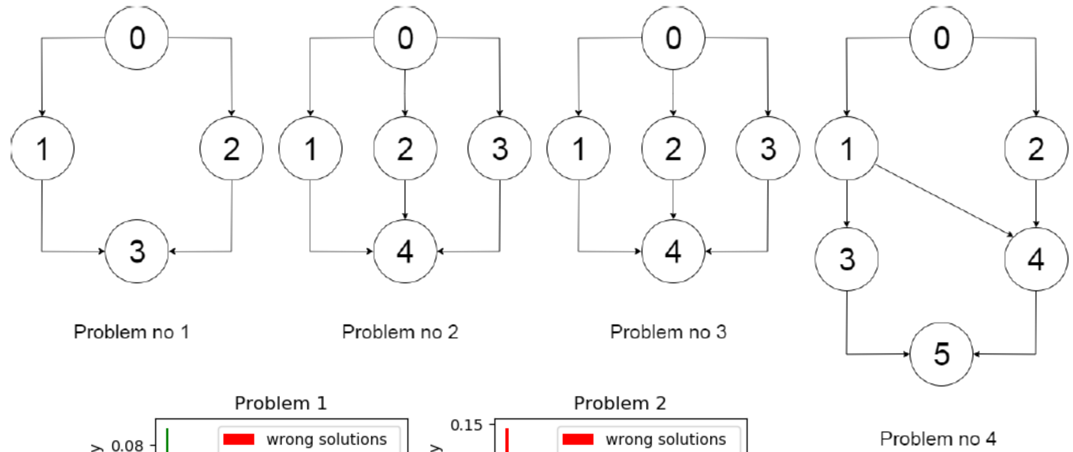
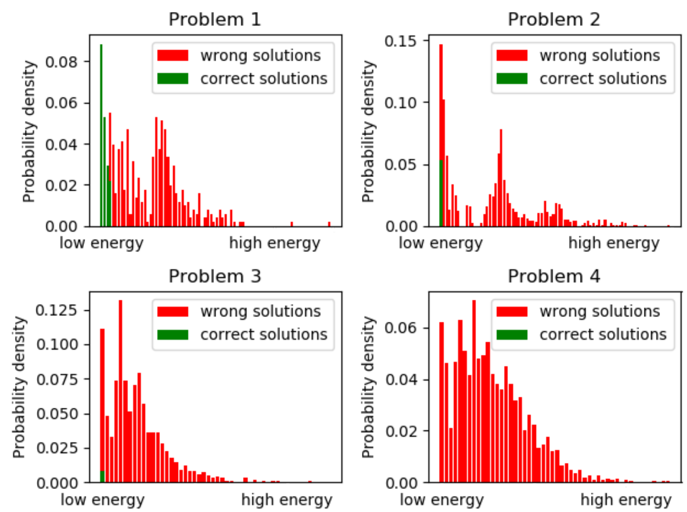
Workflow Scheduling optimisations on D-Wave

- for weights the grid search method was used
- reference Gurobi solver
- manual full graph embedding – additional weight (chain strength)



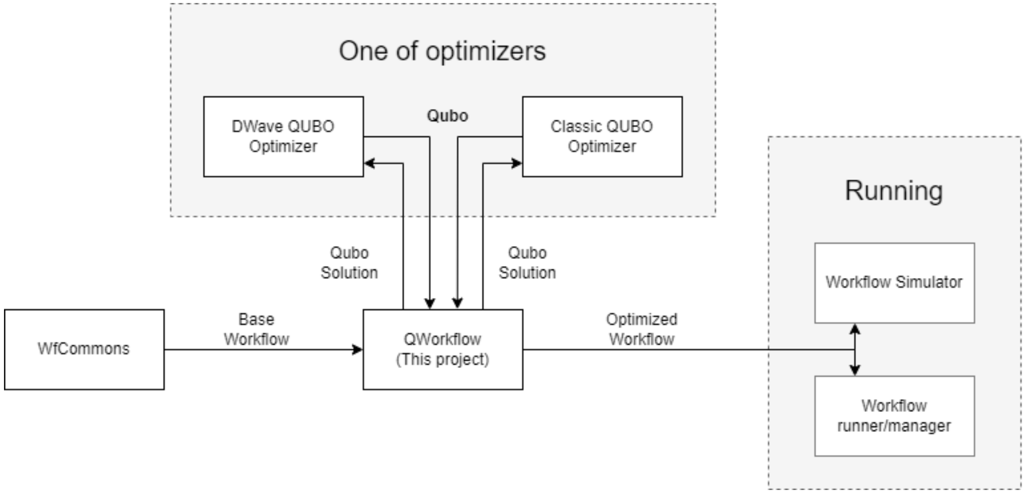


Analysis of D'Wave2000Q Applicability for Job Scheduling Problems, Dawid Tomasiewicz; Master of Science Thesis supervised by Katarzyna Rycerz, AGH University of Science and Technology, Department of Computer Science, Krakow, Poland (2020)

D. Tomasiewicz, M. Pawlik, M. Malawski, K. Rycerz: *Foundations for workflow application scheduling on D-Wave system*. Computational Science - ICCS 2020: 20th International Conference: Amsterdam, The Netherlands, June 3–5, 2020:

Integration with Wfcommons

- Parser of Wfcommons format + QUBO generation
- Integration with synthetic workflow generator
- Possible use of real trace database (Pegasus traces)
- More binary variables - Integration with DWave hybrid solvers:
  - Kerberos always chose the classic path as better solution
  - CQM gives promising results (for around 100 binary variables), but most of the CQM code is hidden



Author: M. Hurbol „Selected aspects of adapting the DWave annealer solutions to Workflow Management Systems"

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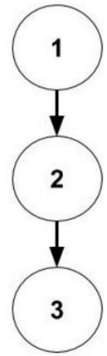
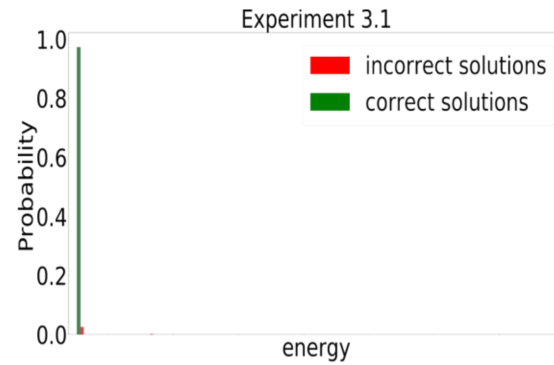
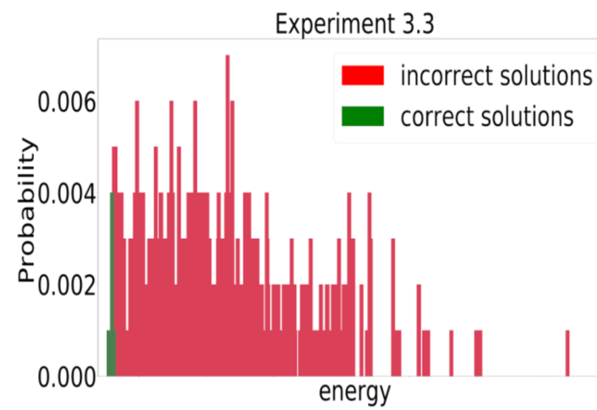
Workflow Scheduling optimisations on IBM-Q (VQE)

- for A, B, C weigths the grid search method was used
- reference direct eigensolver (NumPyEigensolver)
- the best results were achieved when setting parameters A, B, C to 1, 40, 1
- we used RealAplitudes ansatz
- random initial angles selection
- 2 repetitions, full entanglement





simulator



quantum hardware

Configuration	Result vector	Total time	Total cost
$t_{1,1}+t_{2,1}+t_{3,1}$	0001111100	7	28
$t_{1,1}+t_{2,1}+t_{3,0}$	0011100100	15	24
$t_{1,1}+t_{2,0}+t_{3,1}$	0101011010	9	27
$t_{1,1}+t_{2,0}+t_{3,0}$	0111000010	17	23
$t_{1,0}+t_{2,1}+t_{3,1}$	1000111000	11	26
$t_{1,0}+t_{2,1}+t_{3,0}$	1010100000	19	22
$t_{1,0}+t_{2,0}+t_{3,1}$	1100010110	13	25
$t_{1,0}+t_{2,0}+t_{3,0}$	111000xxxxx	21	21

Solving optimisation problems using Qiskit Aqua, Małgorzata Stachoń; Master of Science Thesis supervised by Katarzyna Rycerz, AGH University of Science and Technology, Department of Computer Science, Krakow, Poland (2020)

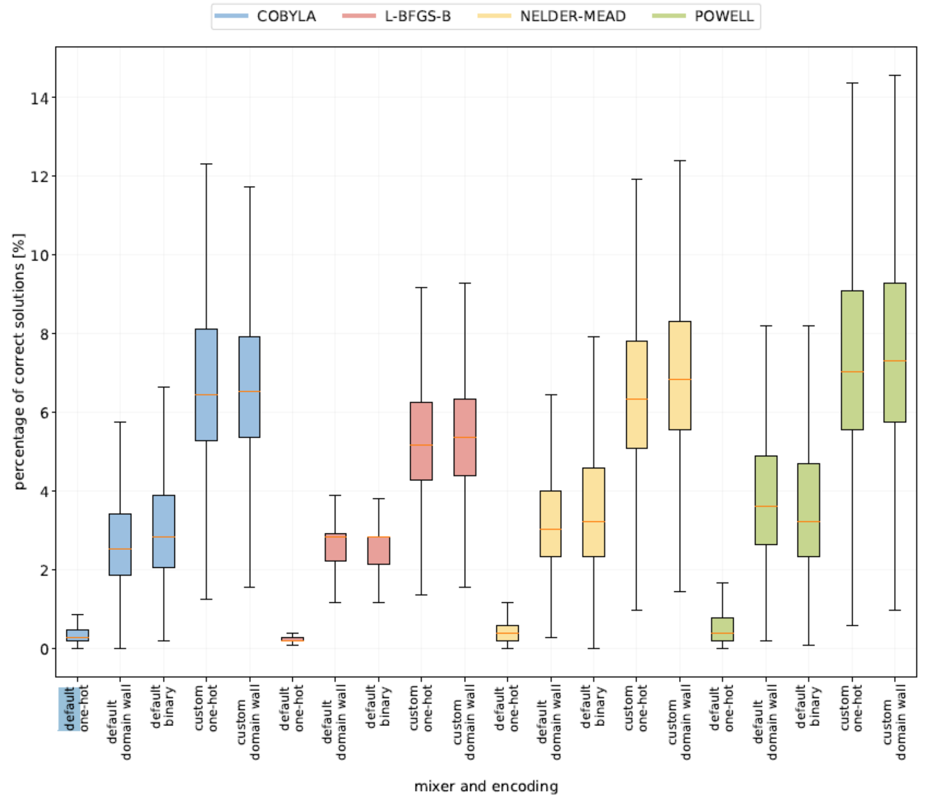
Searching appropriate settings for variational algorithms

Idea: select initial ansatz params with uniform distribution, calculate statistics for chosen metrics (average final energy, percent of correct solutions etc)

- Three different codings: One hot, Domain wall, Integer.
- Comparison of QAOA i VQE
- Different ways of searching solutions space (QAOA mixers)
- Four different optimisation methods

Main conclusions:

- Dense codings allow for fitting larger problems
- Proper QAOA mixer reduces numer of infeasible solutions

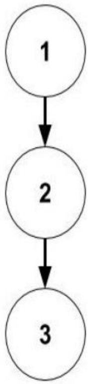


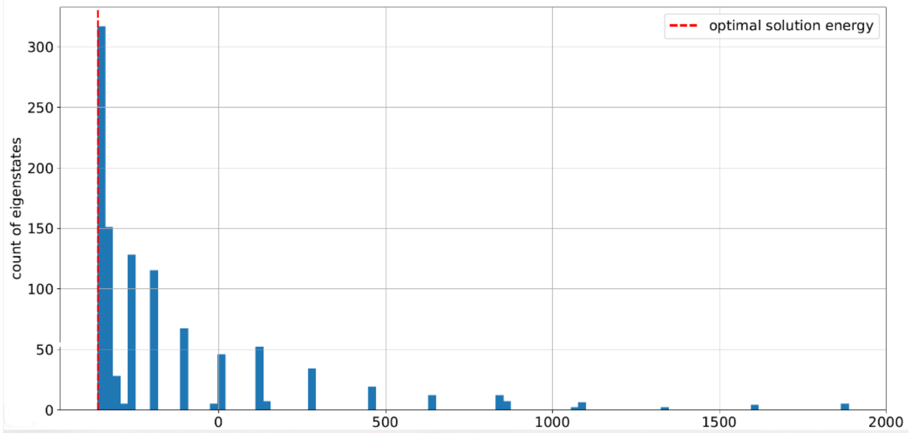
Plewa, J., Sieńko, J., Rycerz, K. (2021). Variational Algorithms for Workflow Scheduling Problem in Gate-Based Quantum Devices. COMPUTING AND INFORMATICS, 40(4), 897–929

Hybrid algorithms for workflow scheduling problem in quantum devices based on gate model, Julia Plewa, Joanna Sienko; Master of Science Thesis supervised by Katarzyna Rycerz, AGH University of Science and Technology, Department of Computer Science, Krakow, Poland (2021)

Sample result (QAOA)

- One of the best samples fror the QAOA algorithm
- domain wall encoding
- 43 optimal solutions and 83 correct (but not optimal) solutions per 1024 shots
- a custom mixer,
- the NELDER-MEAD optimizer
- QAOA levels p=2





Eigenstate histogram (IBM QASM symulator without noise model)

	Machine A	Machine B	Machine C
Task 1	6	8	8
Task 2	3	4	4
Task 3	12	16	16

Table 6.1: Small problem: cost matrix

	Machine A	Machine B	Machine C
Task 1	6	2	8
Task 2	3	1	2
Task 3	12	4	8

Table 6.2: Small problem: time matrix

noise model	optimal	semi-optimal	correct	semi-correct	incorrect	feasible
none	4.2%	17.9%	8.1%	61.9%	7.9%	100.0%
Melbourne	0.2%	2.3%	3.0%	42.7%	51.8%	26.0%
Guadalupe	0.2%	1.7%	2.5%	46.8%	48.8%	28.1%
Mumbai	0.2%	1.8%	2.6%	45.1%	50.3%	27.1%

Table 7.7: A result breakdown for domain-wall-encoded QAOA with different noise models

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Conclusions and future work

- We show how to solve workflow scheduling problem using quantum computers
- There is a lot of research with various optimization problems and QC (quite a hot topic)
- Finding appropriate settings for the algorithms is not trivial and often require advanced methods (AI methods)
- Current architectures allows to run small instances, but various approaches are develloped to overcome this problem:
  - Different codings
  - Hybrid approaches
- Adapt the presented problem to the real workflows word is still a challange

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More information

- QC team @ Cyfronet: Mariusz Sterzel, Justyna Zawalska
- Come to KQIS seminar by Marian Bubak (II AGH, Sano) and Tomasz Stopa (IBM)

https://www.informatyka.agh.edu.pl/pl/badania-i-rozwoj/seminaria-kqi/

- Justyna talk on using Neural Networks for quessing QAOA params:

https://www.youtube.com/watch?v=NfSSqL4Sx0c

- Publications:

http://dice.cyfronet.pl