

# Optimizing the Production of Test Vehicles: Classical Solutions Today and Hybrid Quantum/Classical Solutions Tomorrow

Robert M. Parrish<sup>1,\*</sup> and Rachael Al-Saadon<sup>1</sup>

<sup>1</sup> *QC Ware Corporation, Palo Alto, CA 94301, USA*

A complete and completely classical solution of the industrial challenge problem is presented. Additional quantum/classical algorithmic gains are potentially possible for harder future versions of this problem experiencing geometric frustration - we propose a specific research direction along these lines using a QC Ware specialty of quantum number preserving gate fabric circuits to solve a key part of such a hybrid solution.

## I. RESULTS

The problem statements variously ask for optimization of the constituents of a set or “constellation” of  $n_C$  test vehicles, with each test vehicle taken from a state space of  $\sim 469$  binary dimensions called “features” (this and other dimensions quoted below to vary in future problem sizes), and with each test vehicle satisfying hard “feature-group” and “type-build rule” constraints corresponding to  $\sim 25$  basic test vehicle types. The problem statements, predicated by the hard constraints, specifically ask for (1) **SAT**: For a given  $n_C$ , does there exist, for a given set of  $n_{\text{test}} \sim 644$  tests depending through binary expressions on the state space of each test vehicle, a set of  $n_C$  test cars for which the  $n_{\text{test}}$  tests can be separately evaluated, with the caveat that there need be a “multiplicity” of  $K_I \sim 1 - 5$  distinct test vehicles required to satisfy test  $I$  for  $I \in [0, n_{\text{test}}]$ ? (2) **Weighted MAX-SAT**: For a given  $n_C$ , what is the optimal constellation of test vehicles such that the weighted sum of satisfied  $n_{\text{test}}$  tests, each requiring  $K_I$  distinct test vehicles, is maximized? and (3) **Scheduling (not precisely specified)**: For a given set of  $n_{\text{test}}$  tests and corresponding set of  $n_C$  test vehicles satisfying said tests including  $\{K_I\}$  multiplicity constraints in a MAX-SAT formalism of (2), what is the optimal scheduling of said vehicles into a test sequence with at most  $n_{\text{slot}} \sim 10$  tests performed on distinct cars in each timeslot and with tests assigned to integer test groups with definite sorting of test groups within each car?

A specific instance of the problem class described above was provided by BMW. Taken naively, this problem instance involves binary optimization over a state space of  $\sim 469 \times 60 = 28140$  binary variables (plus additional state space variables for scheduling), i.e., a state space of  $2^{28140} \sim 10^{6574}$  dimensions, with hard constraints and fairly generic logical expressions needed to specify constraints and objective function values. As stated by BMW (quotes from the problem statement in italics): “*The provided description is based on the actual numbers and constraints formulated for this model. It, thus, represents the real complexity arising in a productive setting.*”

Within the problem statement document, solutions to the above problems were attempted using existing industry-standard SAT solvers and constraint satisfaction solvers. The SAT problem of (1) was easily solved: “*For 100 cars, the problem can be solved in a few seconds. A linear search counting down from 100 revealed the solution that at least 60 cars are needed to perform all the specified 750 tests.*” However the weighted MAX-SAT problem of (2) was not solvable: “*On the other hand, the MAX-SAT problem was not solvable in a reasonable time with the chosen approach.*” Additionally, the scheduling problem of (3) was not solvable: “*[O]n the test laptop, the full problem with 700 tests wasn’t solvable in less than 24 hours.*”

We provide what we believe under the rules of the problem statement represents a complete and tangible classical solution to all three specified problem variants. The characteristics of our solution are presented in Figure 1 and the specific solution data and corresponding code are present in our publicly-available repository at <https://github.com/qcware/bmw>. Specifically, we developed a custom C++/Python code library to represent the details of the problem in a natural format. The combination of customized classical solution environment and high performance implementation allows for very rapid exploration of the hard-constraint-satisfying parameter space unique to this problem class. Within this environment, we developed a powerful and simple set of heuristics to approximately solve the MAX-SAT variant of the problem. This heuristic MAX-SAT solver produces nested constellations of test cars with increasing  $n_C$  and concomitant increasing MAX-SAT scores. The MAX-SAT solutions coming from this heuristic achieve saturation of all specified 644 tests (including multiplicity considerations) at the same  $n_C = 60$  bound determined by standard SAT solvers for problem (1) in the problem statement document. Thus our MAX-SAT solution provides a tight bound solution for problem (1) in the process of providing approximate solutions for (2). For values of  $n_C \ll 60$ , we believe our heuristic MAX-SAT solutions are within a few percent of the global optimum. For the scheduling problem of (3) we develop additional heuristics to schedule the test sequence from the MAX-SAT optimized constellation of  $n_C = 60$  cars while respecting the hard constraints of distinct cars within each time slot, strict ordering of

---

\*Electronic address: [rob.parrish@qcware.com](mailto:rob.parrish@qcware.com)

(A) SAT and MAX-SAT Solutions:

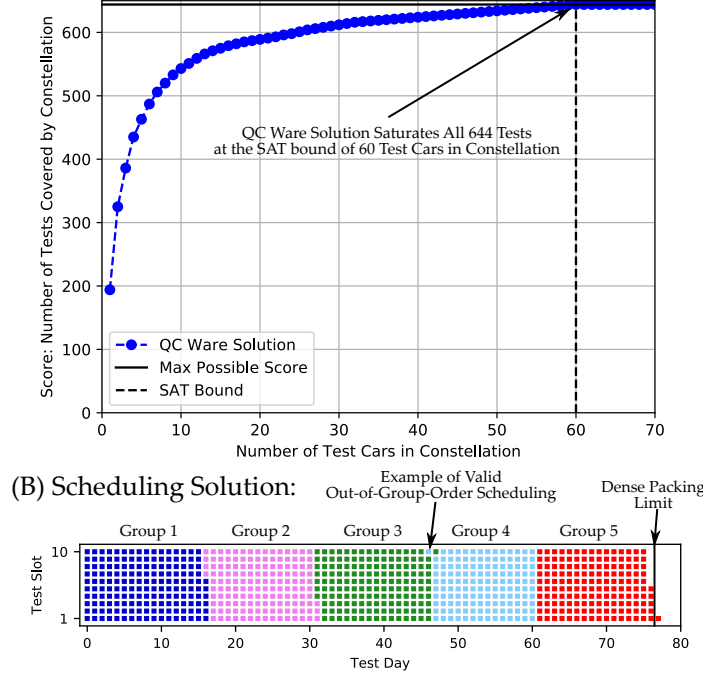


FIG. 1: Characteristics of QC Ware solutions to the “optimizing the production of test vehicles” BMW quantum computing challenge problem. (A) Solutions to the MAX-SAT, and by corollary, SAT variants of problem variants (2) and (1), respectively. (B) Solution to the scheduling problem variant (3).

randomly-specified test groups within cars, and separate cars used within the multiplicity considerations of each test. With the multiplicity considerations included, there are 766 separate test-car pairs required, mandating a theoretical floor of 77 test slots. Our heuristic solution provides a nearly dense scheduling with 78 test slots required, i.e., within 1.3% of dense scheduling. In aggregate, the classical steps required to reach the MAX-SAT/SAT/Scheduling solutions sum to roughly 5 – 10 min total of wall time on a 72-core AWS EC2 `c5n.metal` instance, representing  $\sim \$0.30$  worth of classical computing resources at present prices.

## II. METHODS

### A. C++/Python Environment

To facilitate rapid exploration of the state space for this problem class, we developed a custom C++11/Python3 library API linked by PyBind11. No additional dependencies beyond standard C++11, Python3, and the header-only PyBind11 linker layer are needed - i.e., we do not rely on third-party SAT solvers. This library contains simple classes enumerating the natural representation of the problem contents.

For instance, a `SimpleBinaryExpression` class is implemented to represent the concept of simple all/any binary expressions containing arbitrary not predicates as encountered throughout the type build rules and the test rules. Instances of this class store the state of, e.g., a given build rule predicate or implication expression, and can efficiently check whether this expression is satisfied for a given proposed vehicle configuration. Two `SimpleBinaryExpression` objects are further stacked in a `SimpleBinaryImplication` object to represent the predicate and implication of each type build rule. Multiple `SimpleBinaryExpression` objects are chained together in a `FirstOrderAllBinaryExpression` object to represent the parenthesized binary expressions present in each test rule. Additional data structures are constructed to uniquely represent the type feature groups, the type-specific build rules, the full set of test rules and corresponding multiplicities, eventually yielding a complete C++ representation of the full problem. The critical configuration state space of each test vehicle is efficiently represented by the `std::vector<bool>` concept, i.e., each proposed test vehicle is represented by a `std::vector<bool>` containing the states of the  $\sim 469$  features of each vehicle. The entire library is reflexively exposed to Python3 through PyBind11 to merge the effortless development of Python (i.e., regex for data pars-

ing, short python scripts to manage various experiments, compile-free debugging through python printing) with the speed of compiled C++ for rate-limiting operations. The use of C++ also facilitates the use of single-node parallelism through OpenMP threading.

### B. Test Vehicle Seeds

One might expect that the guess of  $\vec{0}$  (i.e., all features turned off) would yield an acceptable starting guess for a test vehicle configuration. However, already at  $\vec{0}$  some of the type build rules are violated, meaning that  $\vec{0}$  is outside of the hard constraint space. Moreover, we have empirically found that some of the  $\sim 644$  test rules are rather hard to find without specific direction within the constraint space. Therefore, to seed a starting pool of test vehicles, we adopt the following procedure:

1. For each test rule, we generate a seed test vehicle that satisfies this test rule with a randomly selected type.
2. To generate this vehicle, we first flip the required features on to satisfy the test rule.
3. The active test rule features are then “masked” meaning that they are frozen in current values satisfying the test rule throughout all future steps.
4. In the non-masked features, we then chase constraints until we arrive at a valid car satisfying the type build rules.
5. If this procedure fails for a given randomly selected type, we randomly select another type and repeat ad infinitum.

At the end of this procedure we have a pool of  $\sim 644$  test vehicles which are largely “featureless” meaning that only the minimal number of features have been activated to satisfy the test and chase the constraints into the valid type build rule space. All test rules are present in at least one test vehicle in this starting pool.

### C. MAX-SAT Optimization

We start from the empty constellation  $n_C = 0$ . To update this constellation to  $n_C = 1$ , we adopt the following procedure:

1. For each of the  $\sim 644$  test vehicles in the candidate pool, we perform several tens of thousands of directed Monte Carlo moves designed to improve the number of rules simultaneously satisfied by the test vehicle, while respecting the hard constraints. The Monte Carlo moves are described below.
2. We add to the constellation the single car from the updated candidate pool that maximally increases the number of satisfied tests in the constellation.

3. We update the test set used to direct the Monte Carlo moves in Step 1 to include only those rules which are unsatisfied by the current constellation.
4. We iterate this procedure until all test rules are satisfied, increasing the constellation size  $n_C$  by one test vehicle per iteration.

At the end of this procedure, we have a set of  $n_C$  nested constellations each of which is a local approximant to the MAX-SAT [Problem (2)] solution of corresponding constellation size. Once we obtain a constellation that saturates all tests, we have an upper bound for the SAT solution [Problem (1)] which turns out to be tight for the specifics of this problem instance.

### D. Masked Distance-2 Monte Carlo Moves

One of the particular specialties of our approach lies in the strength of our Monte Carlo moves. We adopt the following procedure:

1. For each test vehicle in the candidate pool, we randomly select two feature groups to vary.
2. For each of these feature groups we move with equal probability to deactivate the feature group or to active a random feature index within the group.
3. We check if the proposed move satisfies the type build rules and return to 1 if not.
4. We check if the proposed move would perturb the masked features discussed in the previous section, and return to 1 if so.
5. At this point, we know that the proposed test vehicle is valid and has not moved a masked feature. If this proposed test vehicle improves the number of satisfied tests in the active test set, we accept the updated vehicle and return to 1. Else we reject the proposed test vehicle and return to 1.
6. We loop some user-specified number of iterations, usually on the order of tens of thousands.

There are several key observations that guided this heuristic choice of Monte Carlo move scheme:

- These moves always remain on the constraint space.
- These moves move by feature group rather than binary variables, and therefore automatically satisfy the feature group constraint. Direct moves in binary variables would have vanishing probability of satisfying the feature group constraints.
- Distance-2 moves are much more likely to be interesting and valid than distance-1 moves. E.g., the activation of a single feature group often implies the activation of another feature group through the

type build rules. Such implications can be satisfied with reasonable probability with distance-2 moves, but are often unreachable with a sequence of distance-1 moves.

- The acceptance of moves based on increased test set scores promotes a compounding improvement of the test vehicle through the iterative procedure.

This procedure is implemented within C++, which treats the involved logic almost natively. As such, we obtain orders of magnitude improvement over a corresponding Python implementation of this portion of the approach. Additionally, this stage of the procedure is embarrassingly parallel across the  $\sim 644$  test vehicles in the candidate pool. We parallelize this with OpenMP, with dynamic scheduling invoked to attempt to load balance across the anisotropic task sizes encountered.

Note that the efficiency of moves in this scheme relies on the concept that the feature groups of the test vehicles are disjoint. This was not actually the case in the original problem statement, due to a single collision between two feature groups. We adjusted the problem statement to redefine two of the feature group boundaries and to apply additional build constraint rules to yield an entirely equivalent isomorphic representation of the problem. See the Appendix for additional details.

### E. Scheduling

For scheduling, we were initially considering doing some rather exotic work involving global optimization, i.e., building a different constellation of test vehicles that would be more optimized for the scheduling objective function than for the MAX-SAT objective function. However, we started by exploring an extremely simple greedy approach involving attempting to schedule our existing SAT/MAX-SAT constellation of  $n_C = 60$  test vehicles, and found that it produced almost dense packing. Therefore, we will only explain the latter approach here.

The scheduling heuristic approach works as follows:

1. We first sort the test rules by test group (first priority) and by number of required cars for the test (second priority).
2. We traverse the current priority-sorted test set.
3. For each test, we identify and randomly sort the list of cars which satisfy the test.
4. For each car in this list, we attempt to add the car to the current time slot, continuing deeper into the car list if the car already exists in the current time slot, if the car has already been used previously for this test (for multi-car tests), or if the car has already been used for a lower-priority test group. As soon as we find a valid car, we break out of the loop over the car list.

5. If no test-car pair can be added to the current slot, we “nuke” the slot and kick it onto the schedule with no-ops (i.e., empty time/engineer slots) inside.
6. If the addition of a car saturates the number of engineer slots, we kick the slot onto the schedule.
7. We check if the addition of a car saturates a test rule, and update the test rule set to remove this rule if so.
8. We iterate from 2 until all test rules are satisfied, as evidenced by the active test set becoming empty.

There is a small chance that this algorithm will enter an infinite loop where a critical car is greedily used for a lower-priority test, and therefore cannot be used for a higher-priority test. We have encountered this failure case in only about 15% of runs. The existence of even a single successful run producing a dense schedule obviates this concern.

Note that we find the absence of specified test groups in the problem specification to be a major weakness of this part of the challenge. We generated test groups ranging from 1 to 5 from random integers as sketched in the problem statement. We did this exactly once using `numpy.random.randint` and stored the values in our github repository - i.e., we generated what we feel is a fair test and then froze it. Note also that we elected to define the priority order to be sorted from 1 to 5 rather than from 5 to 1 in the problem statement for aesthetic reasons - as these values are isotropically randomly generated this makes no difference in problem structure.

## III. TOWARD HYBRID QUANTUM/CLASSICAL APPROACHES

### A. Motivation

We view the above full solutions as an unexpected *fait accompli* obtained during our formulation of a submission for this challenge. Despite the formidable presentation of this problem [as evidenced by the inability of the BMW working group to provide a solution for problem variants (2) and (3) with conventional techniques], this problem is not so hard as it looks. In particular, there seems to be only a moderate amount of “geometric frustration” between test vehicles. This concept of geometric frustration has many potential manifestations, all stemming from the basic idea that local moves to optimize one subset of the problem could easily have severely penalized the quality of the global solution. For instance, focusing on MAX-SAT, it could well have been the case that feature choices on candidate test vehicles were so tightly correlated through test case satisfaction that attempts to locally maximize the solution quality for each proposed single test vehicle addition to the constellation would severely negatively impact the MAX-SAT score for

larger values of constellation size  $n_C$ . This might manifest as a problem instance where no single test vehicle in the ideal global solution constellation is a “hero” individually satisfying a relatively large number of tests (note that all of our current solution test vehicles are heroes!). Instead each test vehicle in the ideal solution constellation might satisfy only something on the order of  $n_{\text{test}}/n_C$  cars, with the particular test cluster satisfied for by each test vehicle determined by a very brittle set of many-body correlations with the active features sets across all test vehicles in the constellation. Such a case would stymie essentially all heuristic optimization approaches that we can envision.

A geometrically frustrated problem instance of this type is not hard to imagine occurring in real engineering practice. In fact, we would argue that such geometric frustration is already present in the current problem instance, albeit to a low enough degree that some halfway clever heuristics and the big hammer of a `c5n.metal` node can defeat such geometric frustration. In particular, as the feature groups, build rules, and test sets all grow in both size and complexity in future practice at BMW, we will likely see cases that are highly resilient to direct solution by local heuristics.

Below, we propose a specific directed research project to develop novel hybrid quantum/classical algorithms to target such frustrated MAX-SAT problems. Key to our approach is the idea that one should use the CPU (or other high-performance classical computing resources) and QPU separately for what each are best at. As such, we propose a two-stage approach where one first uses the CPU to generate a large, diverse, and structured candidate pool of cars (dealing with the hard build constraints on the cars on the CPU) and then selecting the best constellation of  $n_C$  test cars from this pool by using the QPU to solve a variant of MAX-COVER. This variant of MAX-COVER is an interesting and non-trivial extension of standard MAX-COVER that represents a total Hamming-weight-constrained polynomial binary optimization problem (a specific PCBO problem).

Before discussing the proposed approach, we will briefly discuss a red herring approach that will serve to contrast with our selected approach:

### B. A Path to Avoid

It is highly tempting to map the binary state space of the MAX-SAT variant of the problem to the qubits or qudits of a quantum device. This mapping would provide the most direct encapsulation of the problem on the quantum hardware and would retain the conceptually sacred possibility of an exact global optimum. Conceptually, one would create a quantum superposition over all possible binary strings in the state space, and then start applying MAX-SAT-Hamiltonian-aware methods like quantum amplitude amplification (using either traditional deep quantum phase estimation circuits or a

variant of the new short-depth maximum likelihood estimation, Grover zeroing, or Chinese remainder theorem circuit schedules), QAOA, or VQE to boost the observation probability of the global optimum or other local optima. One could immediately improve this idea by either conceptually or physically using qudits to represent each feature group - this would drastically reduce the search space size and simultaneously mitigate issues with the feature group constraints.

We do not recommend pursuing any approach along these lines for exactly one reason: test vehicle build constraints. These constraints severely limit the valid state space of the test vehicles and are posed as generic predicate/implication binary logic statements involving up to dozens of simultaneous variables per expression. Such constraints are completely alien in a quantum computing context, in the same way that mapping a deeply serial code to a GPU is a technical non-starter. Therefore, we see no viable path (even for error-corrected quantum approaches in the  $\geq$ decade timeframe) to develop general purpose quantum circuits that can provide powerful moves within the Hilbert space while simultaneously respecting these generic build rules.

### C. A Path to Take

We instead propose a hybrid quantum/classical approach to the geometrically frustrated MAX-SAT problem. The approach works as follows:

1. Use classical high performance computing resources such as extensions of our existing methodology to build a large, diverse, and highly structured pool of  $\sim 10^2$  to  $\sim 10^6$  candidate test vehicles. This pool generation approach can be tuned for various frustration cases, e.g., providing penalties for “hero” test vehicles, providing repulsive terms between test vehicles with overlapping feature sets, or encouraging small groups of test vehicles to work together to realize tests with high multiplicities.
2. Use novel symmetry-preserving constrained binary optimization optimization approaches on quantum hardware to solve the modified MAX-COVER problem of selecting the optimal constellation of  $n_C$  test vehicles from the candidate pool.
3. Perform additional heuristic refinement on classical resources to further increase the MAX-SAT score.

### D. The Quantum Problem

The modified MAX-COVER problem that represents the basic task of the quantum hardware in our hybrid method has the following two compelling features: (1) the problem maps much more naturally to a qubit device than the approach discarded in the previous section and

(2) the problem has an extremely interesting global Hamming weight constraint structure that merits additional quantum algorithm development, i.e., there is something new, tangible, and valuable to be done here on the quantum algorithms research side.

Specifically, we have a binary state space of  $n_P$  binary variables, where  $n_P \sim 10^2 - 10^6$  is the number of test vehicles in the candidate pool. We are asked to produce a  $n_P$ -dimensional binary string with Hamming weight (total number of 1-state bits)  $n_C$ , where the  $n_C$  1-state bits identify the pivots of the test pool to place into the test constellation. This binary string is to be optimized to maximize the number of satisfied test cases in the constellation, including multiplicity considerations. This last consideration generalizes the problem beyond standard MAX-COVER somewhat, implying some extensions to the Hamiltonian considerations that we will consider in future work.

The most interesting feature of the problem is the total Hamming weight constraint. This formally reduces the dimension of the search space from  $2^{n_P}$  to  $\binom{n_P}{n_C}$ , which is still a roughly exponentially large search space. Standard heuristics for MAX-COVER will likely fail in this environment due to the same geometric frustration between choices that motivated our basic consideration of a hybrid quantum/classical algorithm. The challenge at this point is to craft a quantum optimization algorithm that respects the hard Hamming weight constraint while also providing strong optimization power. Some existing approaches have discussed this case, such as a variant of the quantum alternating operator ansatz (QAOA) with ring or complete graph mixers [1], or the mixer-phaser ansatz for QAOA with hard Hamming constraints [2]. Both of these methods share the common traits that they start from Dicke states (essentially the usual  $|+\rangle$  state of equal amplitudes on all state space configurations, but restricted to preserve target Hamming weight), and then use arrays of 2-qubit XY mixer gates (similar to the “reversible beamsplitter or RBS gates” of quantum optics” or the “Givens gates” of quantum chemistry) to provide Hamming-weight-preserving exploration through the Hilbert space during the QAOA optimization process. It might be possible to directly implement one of this existing methods to solve the MAX-COVER problem for our problem instance. However, we note that there exist several potential problems with these proposed ansatzes. Most tangibly (1) it is well known that networks of Givens or similar gates do not provide full entangling power across the Hamming-weight-preserving Hilbert space, and therefore may not be able to provide quantum advantage when used as QAOA elements and (2) some of the most promising variants of the existing approaches, such as the complete graph XY mixers use highly nonlocal pairs of non-adjacent qubits that may be prohibitively difficult to implement on near-term quantum devices with limited qubit connectivity. We propose an avenue of research that goes somewhat beyond these existing methods, and that works to directly con-

front these two major issues: the adoption of universal Hamming-weight-preserving gate fabrics into an extended version of QAOA or VQE that can provide full universality within the Hamming-weight-preserving subspace while simultaneously being amenable to implementation on NISQ-era quantum devices as a simple 3-local nearest-neighbor gate fabric.

These Hamming-weight-preserving quantum number gate fabrics were noticed as an aside during a collaborative effort between QC Ware Corp. and Covestro Deutschland AG to develop universal but simple gate fabric circuits for the simulation of fermions in the context of quantum chemistry [3]. Fermions exhibit numerous symmetry constraints which must be respected during quantum algorithms simulating these fermions, and one of these symmetries in Hamming weight. Therefore, as an intermediate to full the full fermionic gates that were the major finding of Ref. 3, we considered the prerequisite question of the minimal circuit that is universal for total Hamming weight while also preserving a semblance of simplicity and linear locality. As is well-known in the literature, we noted that the two-qubit fabric of Givens gates as in Figure 2 (similar to the XY mixers discussed above) are not universal, but an extension of this concept to a local fabric of three-qubit Hamming-weight-preserving gates as depicted in Figure 3 achieves universality while preserving the global Hamming weight constraint.

A tangible and potentially highly valuable research direction is to build an extension of QAOA or VQE built around these three-qubit quantum number preserving gates to address the MAX-COVER problem needed for our hybrid quantum/classical solution to the geometri-

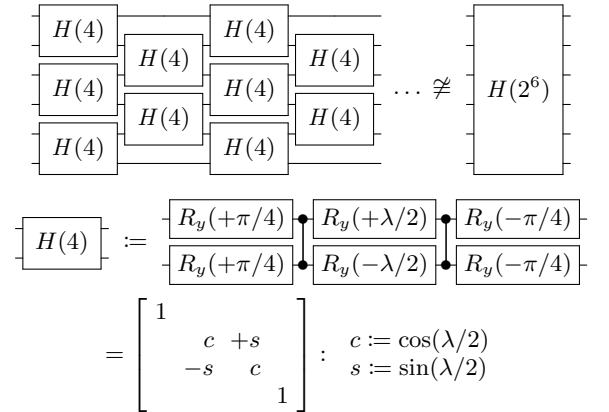
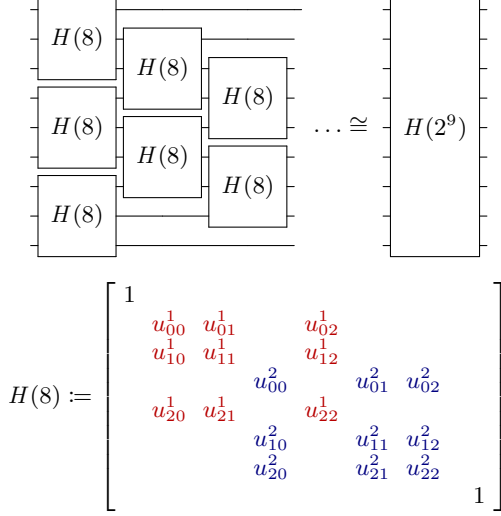


FIG. 2: From Ref. 3: Gate fabric attempt *not* universal for the Hamming-weight-preserving subgroup  $\mathcal{H}(2^N)$  (sketched for  $N = 6$ ). The gate fabric is a 2-local-nearest-neighbor tessellation of alternating even and odd qubit-pair 1-parameter, 2-qubit Hamming-weight-preserving  $\hat{H}(4)$  gates. The gate fabric exactly commutes with the Hamming weight operator  $\hat{P} \equiv \sum_p (\hat{I} - \hat{Z}_p)/2$ , but the gate fabric does not span  $\mathcal{H}(2^N)$  for any depth.



$$\hat{u}^d := \exp(\hat{x}^d) \in \mathcal{SO}(3) : \hat{x}^{d\dagger} = -\hat{x}^d : \hat{x}^d \in \mathbb{R}^3 \times \mathbb{R}^3, d \in [1, 2]$$

FIG. 3: From Ref. 3: Gate fabric universal for the Hamming-weight-preserving subgroup  $\mathcal{H}(2^N)$  (sketched for  $N = 9$ ). The gate fabric is a 3-local-nearest-neighbor tessellation of cascading qubit-triple 6-parameter, 3-qubit Hamming-weight-preserving  $\hat{H}(8)$  gates. Each  $\hat{H}(8)$  gate is composed of a 3-parameter  $\mathcal{SO}(3)$  rotation in the  $d$ -Hamming-weight subspace, where  $d \in [1, 2]$  for a total of 6 parameters. The gate fabric exactly commutes with the Hamming weight operator  $\hat{P} \equiv \sum_p (\hat{I} - \hat{Z}_p)/2$  and spans  $\mathcal{H}(2^N)$  at sufficient depth.

cally frustrated test vehicle production MAX-SAT problem. This is the basis of our research proposal to BMW.

- 
- [1] Jeremy Cook, Stephan Eidenbenz, and Andreas Bärtschi. The quantum alternating operator ansatz on maximum k-vertex cover. In *2020 IEEE International Conference on Quantum Computing and Engineering (QCE)*, pages 83–92. IEEE, 2020. URL: <https://arxiv.org/pdf/1910.13483.pdf>.
  - [2] Ryan LaRose, Eleanor Rieffel, and Davide Venturelli. Mixer-phaser ansatzes for quantum optimization with hard constraints. *arXiv preprint arXiv:2107.06651*, 2021. URL: <https://arxiv.org/pdf/2107.06651.pdf>.
  - [3] Gian-Luca R Anselmetti, David Wierichs, Christian Gogolin, and Robert M Parrish. Local, expressive, quantum-number-preserving vqe ansatzes for fermionic systems. *arXiv preprint arXiv:2104.05695*, 2021. URL: <https://arxiv.org/pdf/2104.05695.pdf>.

## Appendix A: Details of Problem Refinement and Solution Validation

### 1. Feature Groups Collision Issue

The efficient exploration of the state space in terms of moves in feature groups requires that the feature groups be disjoint. We found that this was not the case in the specified problem due to a collision between feature groups 40 and 41. To fix this issue, we modified these two groups and added additional type build rules to produce an isomorphic variant of the problem with disjoint feature groups. Details:

Group 40 (28 elements): [245, 246, 247, 250, 251, 252, 253, 254, 255, 256, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 284]

Group 41 (46 elements): [245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 285, 286, 287, 288, 289, 290, 291, 292, 293]

Union (48 elements): [245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293]

Intersection (26 elements): [245, 246, 247, 250, 251, 252, 253, 254, 255, 256, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282]

In Group 40 but not Group 41 (2 elements): [266, 284]

In Group 41 but not Group 40 (20 elements): [248, 249, 257, 258, 259, 260, 261, 262, 263, 264, 283, 285, 286, 287, 288, 289, 290, 291, 292, 293]

This is hugely vexing for efficient enumeration of group-feature-satisfying vehicle candidates.

This can be overcome by (1) redefining Group 40 to be [266, 284] and then (2) adding a new global (added for all types) rule to the type build rules:

```
F266 | F284 => !F245 & !F246 & !F247 &
!F250 & !F251 & !F252 & !F253 & !F254 & !F255
& !F256 & !F267 & !F268 & !F269 & !F270 &
!F271 & !F272 & !F273 & !F274 & !F275 & !F276
& !F277 & !F278 & !F279 & !F280 & !F281 &
!F282
```

If the group features are chosen randomly, uniformly, and independently, this rule has a probability of  $2/(1+2)$  to be activated (if 266 xor 284 are true). The probability of the rule being violated is  $\sim 26/(1+46) \sim 0.55$ . Therefore the joint probability of the rule being activated and failing is  $(2/3) * (26/47) \sim 0.37$ . Note that this high success probability is somewhat accidental, and is only due to the fact that the in-40-but-not-in-41 subset is small

relative to the intersection *and* the in-41-but-not-in-40 subset is large relative to the the intersection. In future, it is recommended that collisions between feature groups be avoided at all costs in the formulation of this problem, insofar as is possible.

### 2. Solution Verification

A standalone Python code was used to verify that the solutions reported satisfy both the buildability and test constraints.

The MAX-SAT heuristic produced a constellation of test vehicles with specified active features. The test vehicles must comply with a set of buildability constraints related (1) vehicle type, (2) feature group exclusivity, and (3) configuration rules.

Each vehicle can be one of 25 types, which dictates allowed features. The type rules were sorted in a (*number of types*  $\times$  *number of available features*) boolean array, with allowed features set to True. For each vehicle in the solution constellation, if a feature was True, it was compared to the allowed features for that vehicle type to assert that the vehicle met type rules.

The feature groups constraints consist of 42 feature groups, which contain a set of mutually exclusive features. For each test vehicle, one feature in the group can be true. The feature groups were sorted in a (*number of groups*  $\times$  *number of available features*) boolean array with each feature in the group set to True. For each test vehicle, if a feature was True, the feature group for which that feature was present was found and the bitwise AND was taken between these two arrays, returning one True value if satisfied.

The set of test vehicles must also satisfy the configuration constraints. For a given test vehicle type, a set of features is either forced and/ or forbidden based on the presence and absence of specific features. There are 4032 configuration constraints in the problem. Each configuration rule was separated into an initial condition and a forced implication. Theses were further reduced to 'on' sets, 'off' sets, and sets where 'any' one feature can be true, all of which were stored as True in boolean arrays. For each test vehicle, the configuration rules associated with the vehicle type were evaluated. First the initial condition then forced implication was checked, in the same procedure outlined below. (1) If the rule had a set of 'on' features, the logical AND of the test vehicle features and 'on' features rule was computed. The number of True values in the resultant array should equal those in the 'on' features array if satisfied. (2) If the rule had a set of 'off' features, the array of features for the test vehicle was inverted, so that 'off' features were set to True. Then the logical AND was computed, which should have the same number of True elements as the 'off' features array if satisfied. (3) If the rule had an 'any' set, where one of the features must be true, the AND was taken between the 'any' features array and the



test vehicle features, which should return one True value.

For the scheduling solution, we verified that the results obey the scheduling rules. The scheduling rules stipulate that there are up to 10 tests per day and that each vehicle can undergo one test per day. We check that for each test day, each vehicle index appears once. Next, each test is ranked in a group, and for each test vehicle, it must undergo tests in order according to the test ranking. To test that this condition is satisfied, we sort through the

group rank of each test vehicle. If a group index is out of order, we find which vehicle is in that slot, and trace back all previous tests that the vehicle underwent. If the tests for that specific vehicle are in order of ranking, the test set satisfies the test group rank rules. Finally, each test requires a certain number of test vehicles. For each test, we find and count all occurrences of that specific test and compare it to the number required for that test.