QSPIN: A High Level Java API for Quantum Computing Experimentation

Tim Barth

NASA Ames Research Center
Moffett Field, California 94035 USA
(Timothy.J.Barth@nasa.gov)

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Introduction and Outline

- Overview of the D-Wave Quantum Annealer
- QSPIN Java API and benchmark applications
- Hybrid quantum-classical QUBO solvers
- Ising and QUBO model errors
- Looking forward
Overview of the D-Wave Quantum Annealer

The behavior of the D-Wave quantum annealer ground state is closely approximated by Ising spin model objective minimization

**Ising spin model**

\[
s^* = \arg\min_s \sum_{i=1}^{N} h_i s_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} s_i J_{ij} s_j , \quad s_i \in \{-1, +1\}
\]

with \(h_i \in [-2, 2]\) and \(J_{ij} \in [-1, 1]\) which is mathematically equivalent to the Quadratic Unconstrained Binary Optimization function minimization

**QUBO**

\[
x^* = \arg\min_x \sum_{i=1}^{N} \sum_{j=i}^{N} x_i Q_{ij} x_j , \quad \xi_i \in \{0, 1\}
\]

Ising and QUBO problems are NP-hard and thus, if \(P \neq NP\), can not be solved in polynomial time.

The hardware graphs associated with \(J\) and \(Q\) are sparse but this does not change the NP-hardness of the reduced problems.
Adiabatic Quantum Optimization:

The annealing process starts from an initial transverse field Hamiltonian $H_0$ and slowly transitions in normalized time to the desired Ising spin Hamiltonian $H_1$ along the nondecreasing path $f(t) : [0, 1] \mapsto [0, 1]$ with effective Hamiltonian

$$H(t) = (1 - f(t))H_0 + f(t)H_1$$

The transverse field Hamiltonian $H_0$ plays a key role as it is responsible for quantum tunneling through tall narrow peaks in the energy landscape.
Application programmers often encounter two challenges associated with the D-Wave quantum annealer.

1. **Solving large scale Ising/QUBO problems on small scale quantum annealing hardware**
   Ising and QUBO problems with dense coupling graphs require an embedding onto the sparse D-Wave hardware chimera graph. This can be accomplished by the introduction of auxiliary qubits but it significantly decreases the size of problems that can be executed entirely on the D-Wave hardware.

2. **Coping with large Ising/QUBO coefficients and model error**
   The Ising and QUBO mathematical models are only approximately realized by the D-Wave hardware which can negatively impact optimization performance and complicate the selection of software parameters.

These issues are primary research areas for the QSPIN software project that are addressed via the use of hybrid quantum-classical algorithms.
QSPIN API

**QSPIN** is a platform independent Java language API to the D-Wave 2000Q quantum annealer.

1. **QSPIN-SAPI**: a low level Java native interface (JNI) to the D-Wave SAPI library.
2. **QSPIN-CORE**: a pure Java language counterpart of the D-Wave SAPI storage classes and methods.
3. **QSPIN-LEVEL2**: high level Java objects and methods that greatly simplify use of the D-Wave system, provides hybrid quantum-classical solver algorithms and constrained QUBO representations, and tools to support ongoing hybrid quantum-classical algorithm research.
4. **QSPIN-DEMO**: a suite of 18 NP-hard and NP-complete applications (summarized in A. Lucas, 2013) written entirely in Java using QSPIN.

<table>
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<tr>
<th>graph coloring</th>
<th>graph MIS</th>
<th>graph K-way partitioning</th>
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<tr>
<td>Hamiltonian cycles</td>
<td>traveling salesman</td>
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<td>minmax job sequencing</td>
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<td>exact set covering</td>
<td>set packing</td>
</tr>
</tbody>
</table>

**Remark**: Traveling salesman problem using exact $O(n^2 2^n)$ dynamic programming algorithm on exascale classical computer with $n = 100$ cities:

$$100^2 2^{100} \frac{ops}{10^{18} ops} \times \frac{sec}{365 \times 24 \times 60^2 sec} \approx 402 \text{ million years}$$
Hybrid quantum-classical QUBO solvers decompose a large QUBO problem into smaller QUBO subproblems that execute on the D-Wave quantum annealer.

D-Wave has supported the development of \textit{QBSolve}\textsuperscript{2} which uses tabu local search for a QUBO problem combined with D-Wave quantum annealing solves of smaller partitioned QUBO subproblems.

\textbf{QSPIN} provides a number of tools for research activities in hybrid quantum-classical solvers

- Suite of graph manipulation tools for graph contraction, restriction, prolongation, and visualization.
- A Java implementation of the \textit{QBSolve} hybrid quantum-classical QUBO solver,
- A Java JNI to the METIS multi-level graph partitioner,
- D-Wave full graph solver with precomputed fixed embedding,
- Java-GPU accelerated simulated annealing solver.

QBSolve is 2-level QUBO solver. An key data structure is a ranked *impact vector* which measures the change in the objective function when a particular bit is flipped.

**Algorithm QBSolve (Booth *et al.*, 2017):**

1. The global QUBO problem is approximated by a local tabu search,
2. Subproblems are selected from the ranked impact vector,
3. QUBO subproblems are solved on the D-Wave quantum annealer with clamped external values,
4. Values of the global problem are updated,
5. If no progress is made after the subproblem update, the bits associated with the subproblem are randomized.
6. Go to (1) until no further progress is obtained.
**Hybrid Quantum-Classical Example: K-way partitioning**

**K-way Graph Partitioning**

\[
\mathbf{x}^* = \arg\min_x \quad \sum_{(v_i,v_j) \in E} \sum_{k=1}^{K} \sum_{l=1}^{K} x_{v_i,k} x_{v_j,l}
\]

\[
\begin{align*}
\text{minimize cut edges} & \\
+ \delta_0 \sum_{i=1}^{|V|} \left( 1 - \sum_{k=1}^{K} x_{v_i,k} \right)^2 & + \delta_1 \sum_{k=1}^{K} \left( \frac{|V|}{K} - \sum_{i=1}^{|V|} x_{v_i,k} \right)^2
\end{align*}
\]

unique vertex partition index

balance partition vertices

5-way graph partitioning (600 vertices)

110 cut edges, 118 cut edges (METIS)

**QBSolve performance**

subproblem dim = 67
Graph 4-Coloring Problem

\[ x^* = \arg\min_x \delta_0 \sum_{i=1}^{|V|} \left( \sum_{k=1}^4 x_{v_i,k} - 1 \right)^2 + \delta_1 \sum_{(v_i,v_j) \in E} \sum_{k=1}^4 x_{v_i,k} x_{v_j,k} \]

- unique vertex color
- distinct adjacent colors

4-colored planar graph (400 vertices)

QBSolve performance
- subproblem dim = 67
The development of hybrid quantum-classical QUBO solvers is just in its infancy. The topic is rapidly gaining interest in the technical community and several variants of \texttt{QBSolve} have already been suggested:

- Alternative approaches to the selection of QUBO subproblems,
- Multi-level strategies for certain problems, e.g. graph partitioning,
- Hybrid simulated annealing-quantum annealing solvers.
Ising and QUBO Model Error

In reality, the D-Wave annealer solves perturbed Ising and QUBO models

**Ising spin model**

\[ s^{\ast}, \delta = \arg\min_{s} \sum_{i=1}^{N} (h_i + \Delta h_i) s_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} s_i (J_{ij} + \Delta J_{ij}) s_j \quad s_i \in \{-1, +1\}, \]

**QUBO**

\[ x^{\ast}, \Delta = \arg\min_{x} \sum_{i=1}^{N} \sum_{j=i}^{N} x_i (Q_{ij} + \Delta Q_{ij}) x_j \quad \xi_i \in \{0, 1\}, \]

with \( \Delta \) perturbations arising from
- weak 3-body qubit interactions and leakage of \( h \) biases,
- low frequency qubit flux noise,
- DAC quantization (perhaps as few as 6-8 bits),
- I/O system signal contamination,
- nonuniformity of qubits.

Unfortunately, these sources of model error can negatively impact optimization performance and complicate the determination of software parameters.
Model Error and Penalty Constraint Imposition

Model problem

\[
\begin{align*}
\text{minimize} & \quad (4x_1 - x_2 - 1)^2 \\
\text{subject to} & \quad x_1 + x_2 = 1
\end{align*}
\]

Penalty formulation, \( \delta \in \mathbb{R} \)

\[
(x_1, x_2)^* = \arg\min_{x} (4x_1 - x_2 - 1)^2 + \delta(x_1 + x_2 - 1)^2
\]

Discrete optimization, \( x_i \in \{0, 1\} \):

\[
(x_1, x_2)^* = (1, 0) \quad \text{for } \delta > 3
\]

Continuous optimization, \( x_i \in \mathbb{R} \):

\[
(x_1, x_2)^*,\delta = (\delta/(4 + \delta), 0), \quad (x_1, x_2)^* = \lim_{\delta \to \infty} (x_1, x_2)^*,\delta = (1, 0)
\]

The D-Wave system automatically rescales QUBO problems, \( Q_{ij} \in [-1, 1] \),

\[
(x_1, x_2)^* = \arg\min_{x} \frac{1}{\delta} \left(4x_1^2 + x_2^2\right) + (x_1 - 1)^2
\]

**Goldilocks predicament:** Choosing \( \delta \) too small (\(< 4\)) yields an incorrect minimum; choosing \( \delta \) too large can potentially deteriorate the resolution of the objective function relative to model error.
Model Error and Penalty Constraint Imposition

Example: Traveling Salesman Problem

\[ H(x) \equiv \sum_{(v_i, v_j) \in E} \text{dist}(v_i, v_j) \sum_{k=1}^{|V|} (x_{v_i,k} x_{v_j,k+1} + x_{v_i,k+1} x_{v_j,k}) + \delta_0 \sum_{i=1}^{|V|} \left( \sum_{k=1}^{|V|} x_{v_i,k} - 1 \right)^2 + \delta_1 \sum_{k=1}^{|V|} \left( \sum_{i=1}^{|V|} x_{v_i,k} - 1 \right)^2 + \delta_2 \sum_{(v_i, v_j) \not\in E} \sum_{k=1}^{|V|} (x_{v_i,k} x_{v_j,k+1} + x_{v_i,k+1} x_{v_j,k}) . \]

minimize path distance

vertex \( v_i \) visited once

position \( k \) occupied once

exclude path edges not in graph

City sites

\{ (0, 0), (1, 0), (0, 1), (1, 1), (0.5, 0.51) \}

3 tightly clustered (constraint satisfying) QUBO energies

\{ 4.400, 4.412, 4.428 \}

D-Wave 2000Q sensitivity to penalty parameters (# reads = 10000, spin reversal = 10)

<table>
<thead>
<tr>
<th># successes</th>
<th>( \delta_0 = \delta_1 = \delta_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>1</td>
</tr>
<tr>
<td>70</td>
<td>2</td>
</tr>
<tr>
<td>3280</td>
<td>4</td>
</tr>
<tr>
<td>250</td>
<td>6</td>
</tr>
<tr>
<td>65</td>
<td>10</td>
</tr>
<tr>
<td>43</td>
<td>100</td>
</tr>
</tbody>
</table>
Coping with Model Error and Large QUBO Coefficients

Remarks:
- The recently installed D-Wave 2000Q has shown a significant improvement in model error.
- There is a technique for reducing large QUBO coefficients by spreading a large coefficient over auxiliary qubits. For example
  \[
  \text{minimize } 4x_1^2
  \]
  is mathematically equivalent to
  \[
  \text{minimize } (x_1 + x_2)^2 \quad \text{subject to } x_1 - x_2 = 0
  \]
  This technique is used heavily in the D-Wave graph embedding step.
- As an alternative, QSPIN includes a hybrid quantum-classical iterative Lagrange multiplier form of the QUBO problem
  \[
  QUBO^{(n)}(x) = QUBO_0(x) + \lambda^{(n)} QUBO_1(x) + \delta^{(n)} QUBO_2(x)
  \]
  where the coefficients \( \lambda^{(n)} \) and \( \delta^{(n)} \) are updated by the host application during \( QUBO^{(n)}(x) \) iterations. By choosing \( \lambda^{(n)} \) and \( \delta^{(n)} \) correctly, one can reduce or eliminate the dependence on penalties (work in progress).
The **QSPIN-DEMO** provides a suite of NP-hard and NP-complete applications for the D-Wave system that may be solved using the D-Wave QUBO solver for small problems and the hybrid **QBSolve** solver for large problems.
The calculation of Ising spin ground states is a natural target problem for both quantum annealing and quantum logic computers. Consequently, algorithmic developments on the D-Wave system may translate to other quantum architectures.

Hybrid quantum-classical algorithms will undoubtedly play an important role in near term quantum computing devices constrained by relatively low qubit counts.

Most practical problems in discrete optimization contain constraints so advanced techniques for imposing them in quantum annealing and in general quantum models of computation will continue to be an active area of algorithm research.