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Solving PDE-constrained combinatorial optimization problems with AQO

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Introduction and Motivation

Partial differential equation-constrained combinatorial optimization (PDECCO) problems are NP-hard. They have the following characteristics:

- A partial differential equation (PDE) governs the flow of information across the domain
- One set of boundary conditions is discrete (e.g. on/off controls)
- Design conditions on another boundary may be continuous
- This class of problems is important for optimizing transport problems, e.g. gas network control, microchip cooling, and traffic optimization.
- We have developed a mapping that converts PDECCO problems with linear PDEs as constraints to QUBO problems that can be solved through adiabatic quantum optimization (AQO). On a classical computer, two common approaches for solving such problems are genetic algorithms or simulated annealing. While these algorithms can be modified for a particular type of PDECCO, they fail to provide a solution for any general problem in polynomial time. If an adiabatic quantum computer can speed up the time required to solve QUBO problems, this would be an improvement over existing classical algorithms to solve such problems. Solving PDECCO problems successfully on a quantum computer also guarantees that the solution we find would be the global minimum of the problem, and not a local minimum as may be obtained with a heuristic algorithm. The mapping presented holds only for PDECCO problems constrained by a linear PDE.

Problem Formulation

Formulation of a general PDECCO problem, with linear PDE constraints:

$$\text{minimize } J = \int_{\mathrm{B}} \mathrm{d}^d \boldsymbol{\lambda} |u(\boldsymbol{\lambda}) - u_{\mathrm{d}}(\boldsymbol{\lambda})|^2$$

B **= design boundary**

u_{d} **= design conditions**

Subject to a *linear* PDE:

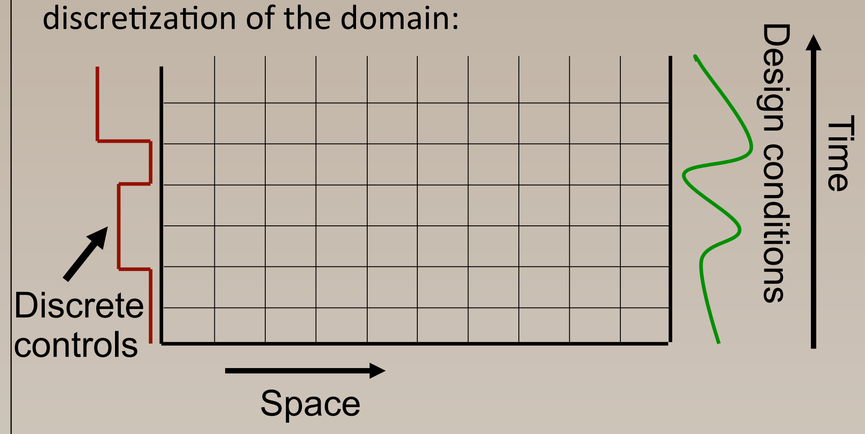
$$F(\boldsymbol{\lambda}, u, \frac{\partial u}{\partial \lambda_1}, \cdots, \frac{\partial^2 u}{\partial \lambda_1 \partial \lambda_2}, \cdots) = 0$$

with boundary conditions

$$u(\lambda_1, 0, 0, \ldots) = f_1(\lambda_1, \lambda_2, \ldots)$$
$$u(0, \lambda_2, 0, \ldots) = f_2(\lambda_1, \lambda_2, \ldots)$$
$$\vdots$$
$$u(0, \ldots, \lambda_c, 0, \ldots) = c,\ c \in C$$

C **= discrete set of control values**

The first step for mapping such problems to QUBO problems is to implicitly discretize the PDE to get a linear system of equations, **Au = b**. **A** is a constant matrix, dependent only on the type of linear PDE, wave speed, for example, and the spatial and temporal discretization. The vector **b** is a function of the controls. The following figure sketches the discretization of the domain:



Solving for **u** and replacing those values in the objective function gives the following QUBO problem, which may be implemented on an AQO:

$$J = \vec{c}^T B \vec{c} + \vec{c}^T \vec{w} + \sum c_i \quad \longleftarrow \text{objective function}$$

$$B = \left(\frac{a}{\Delta s}\right)^2 \left[\left(I_d^T \otimes \vec{e_m}^T\right) A^{-1T} M^T M A^{-1} \left(I_d \otimes \vec{e_m}\right)\right]$$

$$\vec{w} = \left(\frac{2a}{\Delta s}\right) \left[\left(I_d^T \otimes \vec{e_m}^T\right) A^{-1T} M^T\right] \left[\frac{1}{\Delta t} M A^{-1} Q \vec{u_s} - \vec{u_d}\right]$$

The matrix **B** gives the qubit-qubit couplings and **w** the weight-one terms. Matrices **I**, $\mathbf{e_m}$, **M**, **Q** and $\mathbf{A^{-1}}$ are constants and depend on the specific problem details and the PDE constraint. $\mathbf{u_s}$ is a vector containing the boundary conditions. Generally **B** is a dense matrix, so a fully-connected coupling graph is required. Overhead will be incurred when embedding the problem into a physically-realizable coupling graph.

Example results

As an application, we have investigated a version of the gas network optimization problem using a brute-force search. This problem involves minimizing the time compressors are turned on at substations while maintaining a desired supply of gas. As the governing PDE, we consider the advection equation as a proof of concept. The table shows the convergence of the minimum solution with respect to the coarseness of the mesh.

Time steps between two control points	Best Control Sequence	Optimal J value
1	01100000	2.954e-5
4	11111000	5.77e-04
8	11111000	9.71e-04
16	00001000	1.97e-03
24	00001000	2.50e-03

(optimum converges for finer mesh discretization)

Discussion

Scaling of qubits with problem size:

- Since **B** is a dense matrix, in general a fully connected coupling graph is required
- Number of qubits required **does not** scale with mesh size
- Number of qubits required depends **only** on the number of control points desired at one boundary

Time scaling with problem size:

- The main calculation that has to be performed on the classical computer is the matrix inversion process, which scales polynomially with matrix size.
- Scaling of the annealing time required as a function of the dimension of the space of controls is an open problem.

Precision/Error propagation:

- The nominal values of the matrix **B** (coupler strengths) and **w** (qubit weights) are assumed to be continuous.
- Precision errors in **B** affect values of $\mathbf{A^{-1}}$, which in turn changes the nature of the original control PDE.
- Precision errors in $\mathbf{A^{-1}}$ and **w** can then be used to calculate the errors in the initial conditions, $\mathbf{u_s}$.

Limitations and future work:

- The mapping works **only** for linear PDEs.
- Non-linear PDEs cannot be solved with this procedure as we do not obtain a linear system of equations after discretizing the PDEs.
- Local linear approximations of non-linearity might be a way to map non-linear PDECCO problems onto a QUBO form (steady-state problems?).
- Would like to characterize the lowest acceptable precision of coupling strengths that give the correct optimal solution for the original problem.

References

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