QUBO.jl

A tale of implementation and benchmarking of a Quantum Optimization Ecosystem in Julia

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ISMP 2024 ❑ July 22, 2024 ❑ Montreal, Canada

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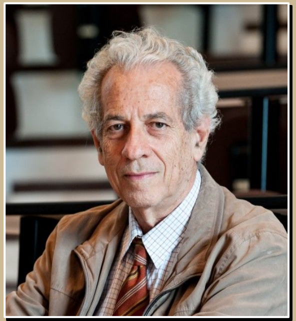

Nelson Maculan
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USRA
NASA Quantum AI Lab

QUBO: Quadratic Unconstrained Binary Optimization

$$\min \; \mathbf{x}'\mathbf{Q}\,\mathbf{x} + \boldsymbol{\ell}'\mathbf{x} + c$$

OBJECTIVE FUNCTION

$$\text{s.t.} \; \mathbf{x} \in \{0, 1\}^n$$

BINARY VARIABLES

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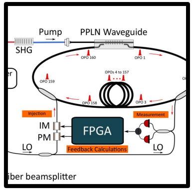
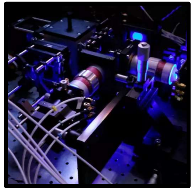
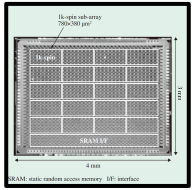


P. L. McMahon et al., 2016


Microsoft Research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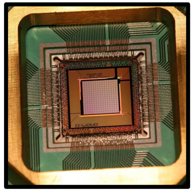
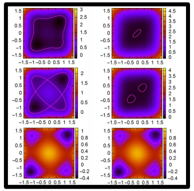
Quantum Annealing, Digital Annealing, Variational Quantum Eigensolver, Quantum Alternating Optimization Ansatz, Coherent Ising Machine, Analog Iterative Machine, Simulated Bifurcation Machine, CMOS Annealing…


D-Wave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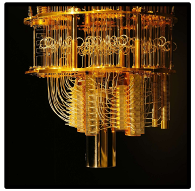
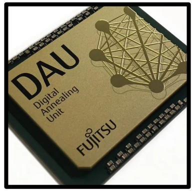
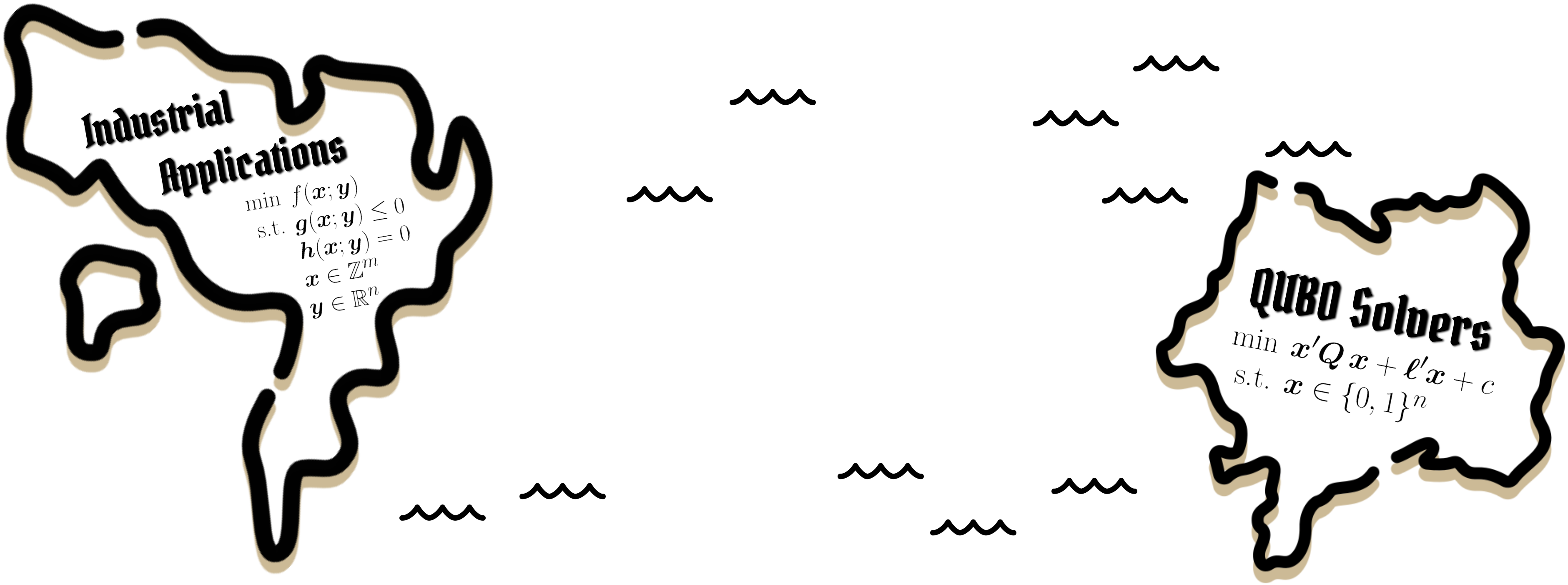

IBM

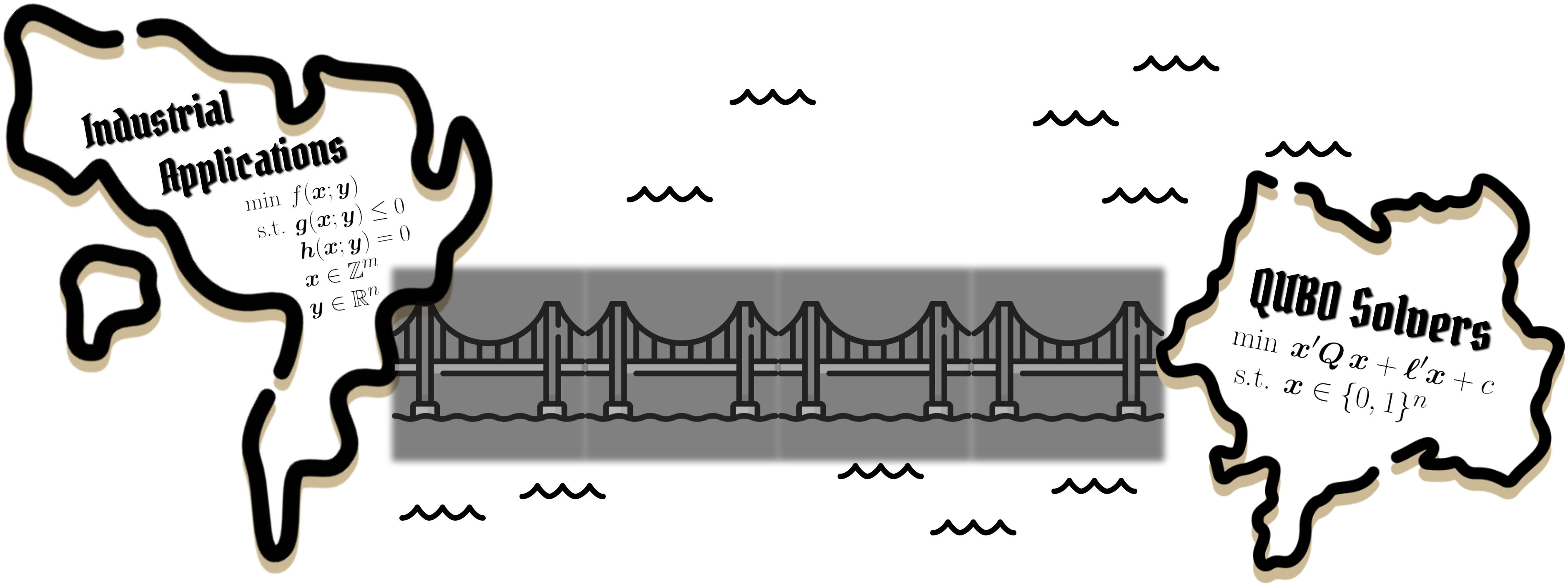


Fujitsu

Our Goal


Industrial Applications
$$\begin{aligned} \min \quad & f(\boldsymbol{x};\boldsymbol{y}) \\ \text{s.t.} \quad & \boldsymbol{g}(\boldsymbol{x};\boldsymbol{y}) \leq 0 \\ & \boldsymbol{h}(\boldsymbol{x};\boldsymbol{y}) = 0 \\ & \boldsymbol{x} \in \mathbb{Z}^m \\ & \boldsymbol{y} \in \mathbb{R}^n \end{aligned}$$
QUBO Solvers
$$\begin{aligned} \min \quad & \boldsymbol{x}'\boldsymbol{Q}\,\boldsymbol{x} + \boldsymbol{\ell}'\boldsymbol{x} + c \\ \text{s.t.} \quad & \boldsymbol{x} \in \{0,1\}^n \end{aligned}$$

Our Goal



Industrial Applications
$\min \; f(\boldsymbol{x};\boldsymbol{y})$
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Tasks

Tasks

Access Solvers

➢ **Common software Interface**

Tasks

Access Solvers

- Common software Interface

Reformulate Models

- Mathematical Programming Compiler

Solution Overview

$$
\begin{aligned}
\min\ & f(\boldsymbol{y};\boldsymbol{z}) \\
\text{s.t. } & \boldsymbol{g}(\boldsymbol{y};\boldsymbol{z}) \leq 0 \\
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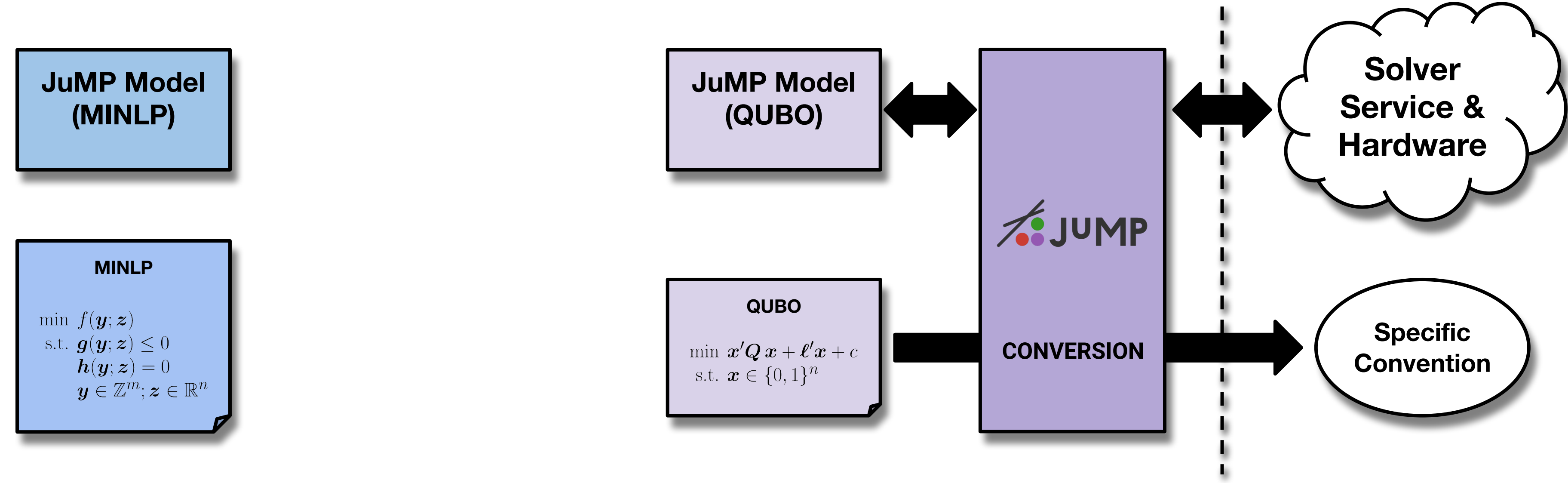
$$

Solution Overview



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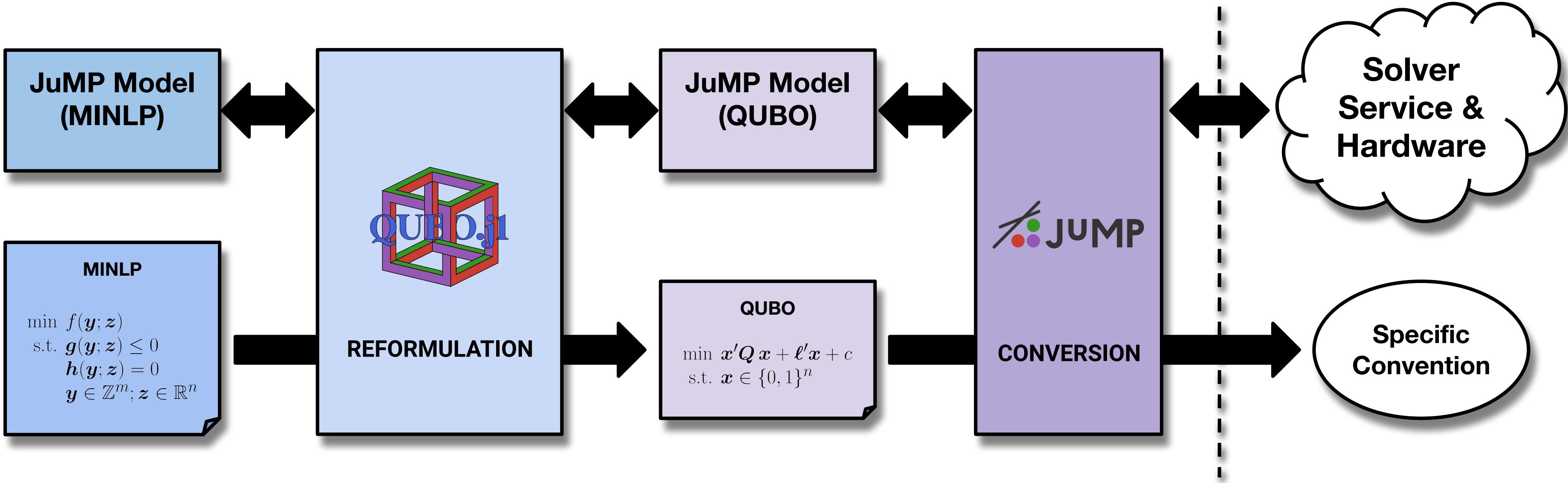
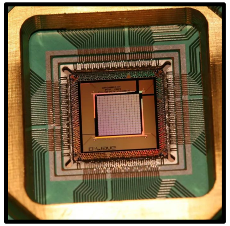


Integrating an heterogeneous Solver Landscape



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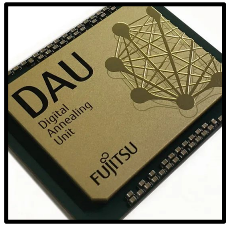

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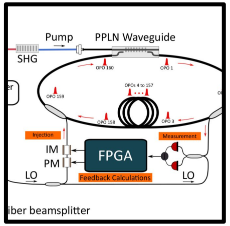

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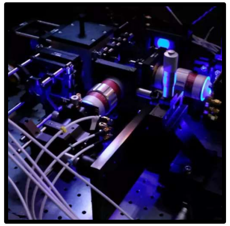

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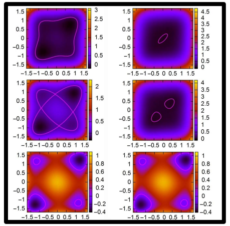

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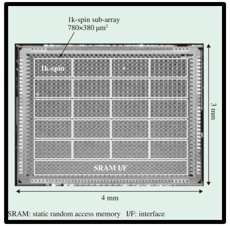

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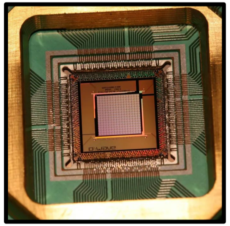

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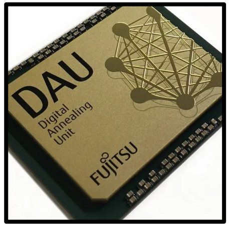

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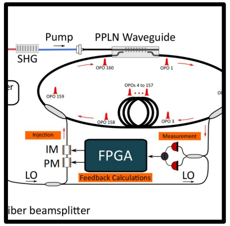

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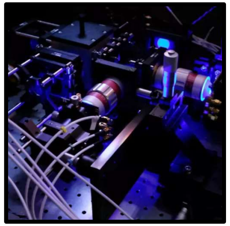

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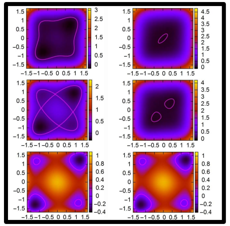

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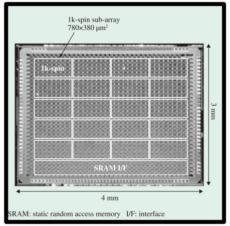


Hitachi, Yamaoka et al.

Julia Mathematical Programming

A Common Solver Interface

```julia
using JuMP
using QiskitOpt # IBM Qiskit Optimizati

model = Model(QiskitOpt.QAOA.Optimizer)

@variable(model, x[1:n], Bin)
@objective(
  model,
  Min,
  x' * Q * x + ℓ' * x + c
)

optimize!(model)

@show objective_value(model)
@show value.(x)
```

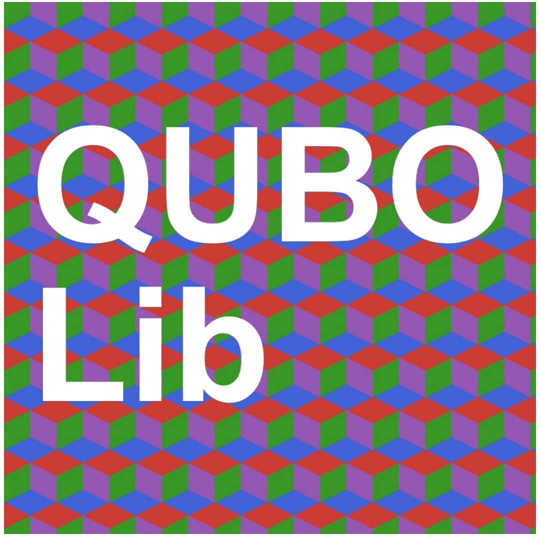
```julia
using JuMP
using DWave # DWave Quantum Annealing

model = Model(DWave.Optimizer)

@variable(model, x[1:n], Bin)
@objective(
  model,
  Min,
  x' * Q * x + ℓ' * x + c
)

optimize!(model)

@show objective_value(model)
@show value.(x)
```

```julia
ing JuMP
ing PySA # NASA Parallel Tempering

del = Model(PySA.Optimizer)

ariable(model, x[1:n], Bin)
bjective(
 model,
 Min,
 x' * Q * x + ℓ' * x + c

timize!(model)

how objective_value(model)
how value.(x)
```

Testing and Benchmarking Solvers

QUBO
Lib

Testing and Benchmarking Solvers



Sources Summary		
Collection	**Instances**	**Size Range**
arXiv:2103.008464 (3R3X)	**2300**	**16 - 4096**
arXiv:1903.100928 (3R3X)	**3200**	**16 - 4096**
arXiv:1903.100928 (5R5X)	**307**	**24 - 24576**
qplib*	**23**	**120 - 1225**

*QPLIB: A Library of Quadratic Programming Instances, Mathematical Programming Computation, 2018

Testing and Benchmarking Solvers

```julia
QUBOLib.load_index() do index
    db = QUBOLib.database(index)
    df = DBInterface.execute(
        db,
        """
        SELECT instance FROM Instances
        WHERE dimension < 100 AND quadratic_density < 0.5;
        """,
    ) |> DataFrame

    codes = collect(Int, df[!, :instance])

    @info "Running DWave Neal"
    QUBOLib.run!(
        index, DWave.Neal.Optimizer, codes; solver = "dwave-neal"
    )

    @info "Running DWave (Quantum)"
    QUBOLib.run!(
        index, DWave.Optimizer, codes; solver = "dwave"
    )
end
```

MINLP $\Longrightarrow$ QUBO

$$
\begin{aligned}
\min\ & f(\boldsymbol{y};\boldsymbol{z}) \\
\text{s.t. } & g_i(\boldsymbol{y};\boldsymbol{z}) \in S_i \\
& \boldsymbol{y} \in \mathbb{Z}^m; \boldsymbol{z} \in \mathbb{R}^n
\end{aligned}
$$

MINLP $\Longrightarrow$ QUBO

VARIABLE ENCODING

$$\begin{aligned} \min \quad & f(\boldsymbol{y};\boldsymbol{z}) \\ \text{s.t.} \quad & g_i(\boldsymbol{y};\boldsymbol{z}) \in S_i \\ & \boldsymbol{y} \in \mathbb{Z}^m; \boldsymbol{z} \in \mathbb{R}^n \end{aligned}$$

$$\begin{aligned} \min \quad & f(\boldsymbol{x}) \\ \text{s.t.} \quad & g_i(\boldsymbol{x}) \in S_i \\ & \boldsymbol{x} \in \{0,1\}^k \end{aligned}$$

MINLP $\Rightarrow$ **QUBO**

$$\begin{aligned} \min\ & f(\boldsymbol{y};\boldsymbol{z}) \\ \text{s.t.}\ & g_i(\boldsymbol{y};\boldsymbol{z}) \in S_i \\ & \boldsymbol{y} \in \mathbb{Z}^m; \boldsymbol{z} \in \mathbb{R}^n \end{aligned}$$

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CONSTRAINT PENALIZATION

$$\begin{aligned} \min\ & f(\boldsymbol{x}) + \textstyle\sum_i \rho_i \left\| g_i(\boldsymbol{x}) - S_i \right\| \\ \text{s.t.}\ & \boldsymbol{x} \in \{0,1\}^k \end{aligned}$$

MINLP → QUBO

$$\begin{aligned} \min\ & f(\boldsymbol{y};\boldsymbol{z}) \\ \text{s.t.}\ & g_i(\boldsymbol{y};\boldsymbol{z}) \in S_i \\ & \boldsymbol{y} \in \mathbb{Z}^m; \boldsymbol{z} \in \mathbb{R}^n \end{aligned}$$

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PSEUDO-BOOLEAN MAPPING

$$\begin{aligned} \min\ & \varphi(\boldsymbol{x}) = \sum_{\omega} c_\omega \prod_{j \in \omega} x_j \\ \text{s.t.}\ & \boldsymbol{x} \in \{0,1\}^k \end{aligned}$$

MINLP → QUBO

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QUADRATIZATION

$$\begin{aligned} \min \quad & \psi(\boldsymbol{x};\boldsymbol{w}) = [\boldsymbol{x};\boldsymbol{w}]' Q [\boldsymbol{x};\boldsymbol{w}] \\ \text{s.t.} \quad & [\boldsymbol{x};\boldsymbol{w}] \in \{0,1\}^{k+p} \end{aligned}$$

A Compiler for Mathematical Programming

C, C++, Julia, Rust...

AMPL, JuMP, Pyomo...

A Compiler for Mathematical Programming

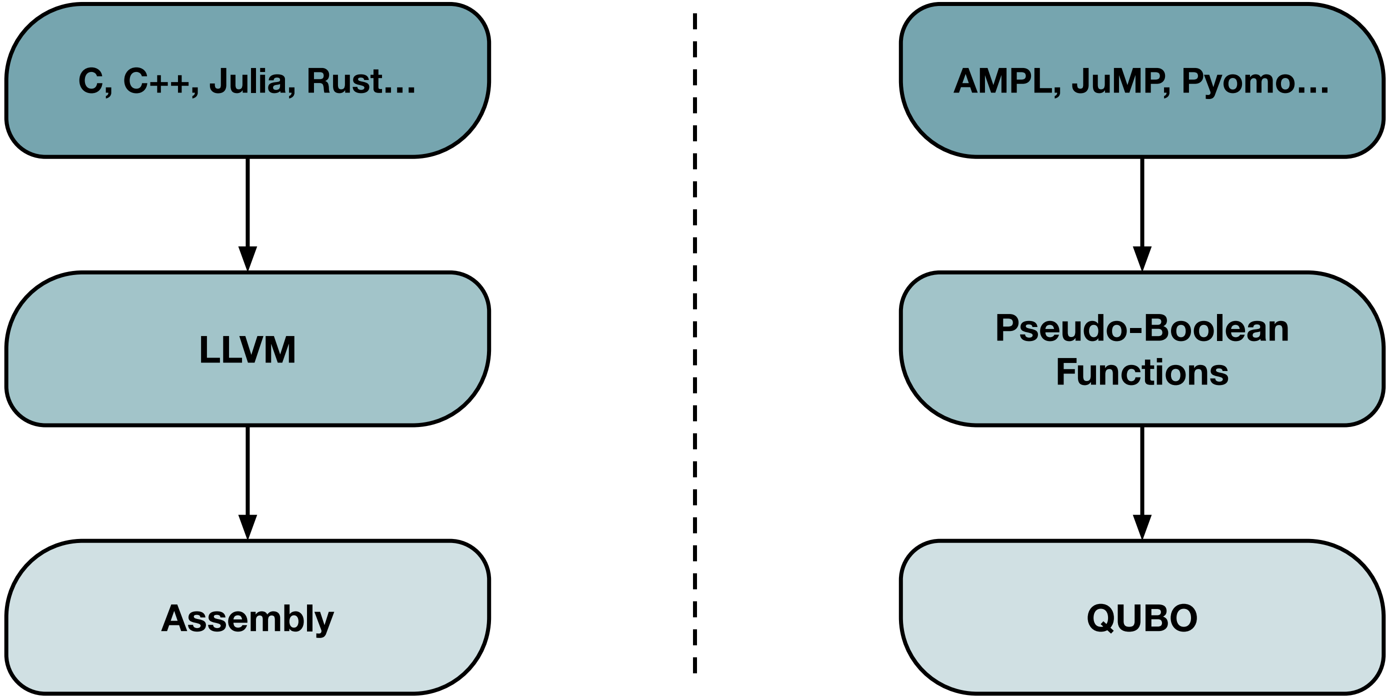
C, C++, Julia, Rust…

Assembly

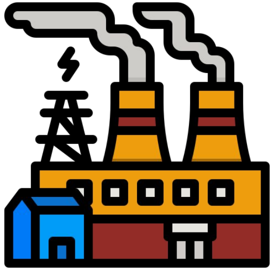
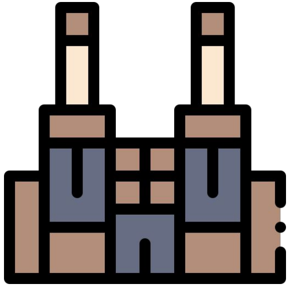
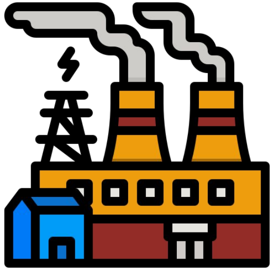
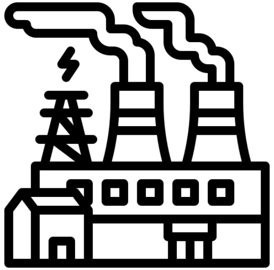
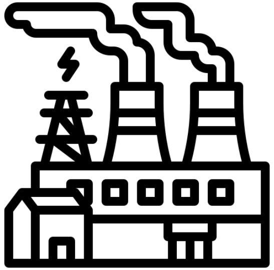
AMPL, JuMP, Pyomo…

QUBO

A Compiler for Mathematical Programming



Example: Generation capacity expansion

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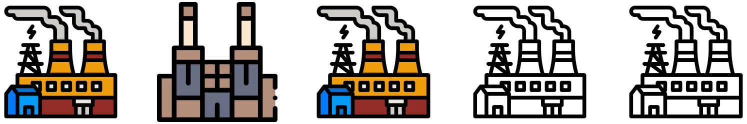

$$
\begin{aligned}
\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_t \mathbf{c}'\mathbf{g}^{(t)} + \mathbf{i}'\mathbf{x} & \\
\text{s.a.} \sum_j g_j^{(t)} = d^{(t)} & \qquad \forall t \\
g_j^{(t)} \leq u_j^{(t)} G_j^{(\max)} & \qquad \forall j,t \\
u_j^{(t)} \leq x_j & \qquad \forall j,t \\
g_j^{(t)} \in [0, G_j^{(\max)}] & \qquad \forall j,t \\
u_j^{(t)} \in \{0,1\} & \qquad \forall j,t \\
x_j \in \{0,1\} & \qquad \forall j
\end{aligned}
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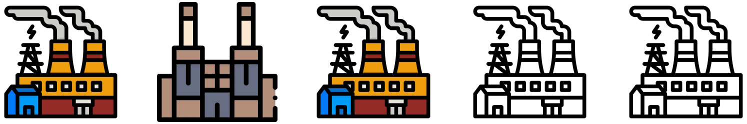

OPERATION

$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_t \mathbf{c}'\mathbf{g}^{(t)} + \mathbf{i}'\mathbf{x}$$

$$\text{s.a.} \sum_j g_j^{(t)} = d^{(t)} \qquad \forall t$$

BALANCE

$$g_j^{(t)} \leq u_j^{(t)} G_j^{(\max)} \qquad \forall j, t$$

$$u_j^{(t)} \leq x_j \qquad \forall j, t$$

$$g_j^{(t)} \in [0, G_j^{(\max)}] \qquad \forall j, t$$

OPERATION

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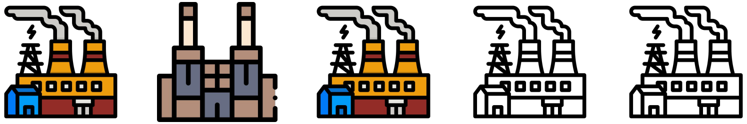

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UNIT COMMITMENT

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Example: Generation capacity expansion

INVESTMENT

$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_t \mathbf{c}'\mathbf{g}^{(t)} + \mathbf{i}'\mathbf{x}$$

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INVESTMENT

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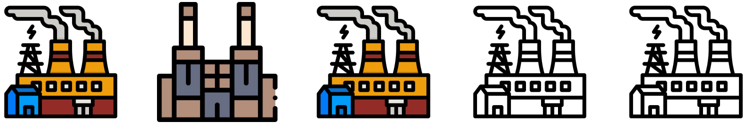
INVESTMENT



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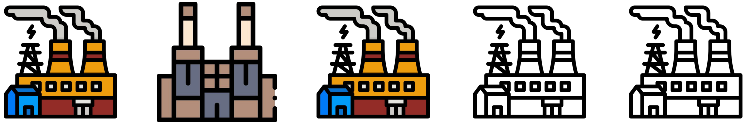


$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \underbrace{\sum_t \mathbf{c}'\mathbf{g}^{(t)}}_{\text{OPERATION}} + \underbrace{\mathbf{i}'\mathbf{x}}_{\text{INVESTMENT}}$$

$$\text{s.a.} \sum_j g_j^{(t)} = d^{(t)} \qquad \forall t$$

BALANCE

$$g_j^{(t)} \leq u_j^{(t)} G_j^{(\max)} \qquad \forall j, t$$

UNIT COMMITMENT

$$u_j^{(t)} \leq x_j \qquad \forall j, t$$

INVESTMENT

$$g_j^{(t)} \in [0, G_j^{(\max)}] \qquad \forall j, t$$

OPERATION

$$u_j^{(t)} \in \{0, 1\} \qquad \forall j, t$$

UNIT COMMITMENT

$$x_j \in \{0, 1\} \qquad \forall j$$

INVESTMENT

Example: Generation capacity expansion

OPERATION INVESTMENT

$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_t \mathbf{c}'\mathbf{g}^{(t)} + \mathbf{i}'\mathbf{x}$$

$$\text{s.a.} \sum_j g_j^{(t)} = d^{(t)} \quad \forall t$$

BALANCE

$$g_j^{(t)} \leq u_j^{(t)} G_j^{(\max)} \quad \forall j,t$$

UNIT COMMITMENT

$$u_j^{(t)} \leq x_j \quad \forall j,t$$

INVESTMENT

$$g_j^{(t)} \in [0, G_j^{(\max)}] \quad \forall j,t$$

OPERATION

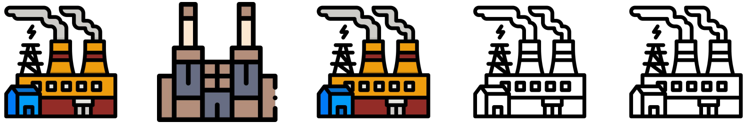
$$u_j^{(t)} \in \{0,1\} \quad \forall j,t$$

UNIT COMMITMENT

$$x_j \in \{0,1\} \quad \forall j$$

INVESTMENT

REFORMULATION →



$$\rho_{balance} \left(\sum_t \left(\sum_j g_j^{(t)} - d^{(t)} \right)^2 \right)$$

$$\rho_{invest} \left(\sum_{j,t} \left(g_j^{(t)} + s_{UB} - x_j G_j^{(max)} \right)^2 \right)$$

$$g_j^{(t)} = \alpha \sum_k 2^k y_{k,j}^{(t)} \ \text{s.t.} \ \ y_{k,j}^{(t)} \in \{0,1\}$$

Example: Generation capacity expansion

OPERATION | INVESTMENT

$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_t \mathbf{c}'\mathbf{g}^{(t)} + \mathbf{i}'\mathbf{x}$$

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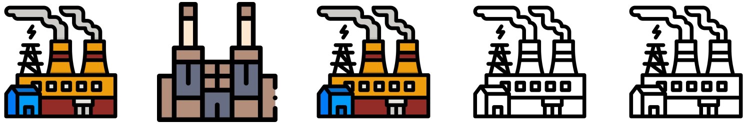

```julia
using JuMP
using PySA

model = Model(PySA.Optimizer)

@variable(model, 0 ≤ g[1:T,j=1:n] ≤ Gmax[j])
@variable(model, u[1:T,1:n], Bin)
@variable(model, x[1:n], Bin)

@objective(model, Min, sum(c'g[t,:] for t=1:T) + i'x)

@constraint(model, [t=1:T], sum(g[t,:]) == d[t])
@constraint(model, [t=1:T,j=1:n], g[t,j] ≤ u[t,j] * Gmax[j])
@constraint(model, [t=1:T,j=1:n], u[t,j] ≤ x[j])

optimize!(model)

@show objective_value(model)
@show value.(x)
```

Example: Generation capacity expansion

OPERATION INVESTMENT

$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_t \mathbf{c}'\mathbf{g}^{(t)} + \mathbf{i}'\mathbf{x}$$

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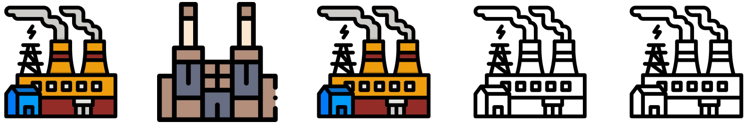

```julia
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using PySA

model = Model(PySA.Optimizer)

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optimize!(model)

@show objective_value(model)
@show value.(x)
```

Example: Generation capacity expansion

$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \underbrace{\sum_t \mathbf{c}'\mathbf{g}^{(t)}}_{\text{OPERATION}} + \underbrace{\mathbf{i}'\mathbf{x}}_{\text{INVESTMENT}}$$

$$\text{s.a.} \sum_j g_j^{(t)} = d^{(t)} \quad \forall t$$

BALANCE

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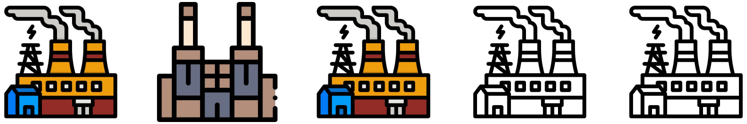

```julia
using JuMP
using PySA

model = Model(PySA.Optimizer)

@variable(model, 0 ≤ g[1:T,j=1:n] ≤ Gmax[j])
@variable(model, u[1:T,1:n], Bin)
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@objective(model, Min, sum(c'g[t,:] for t=1:T) + i'x)

@constraint(model, [t=1:T], sum(g[t,:]) == d[t])
@constraint(model, [t=1:T,j=1:n], g[t,j] ≤ u[t,j] * Gmax[j])
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optimize!(model)

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```

Example: Generation capacity expansion

OPERATION **INVESTMENT**

$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_t \mathbf{c}'\mathbf{g}^{(t)} + \mathbf{i}'\mathbf{x}$$

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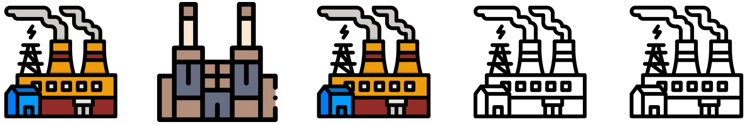
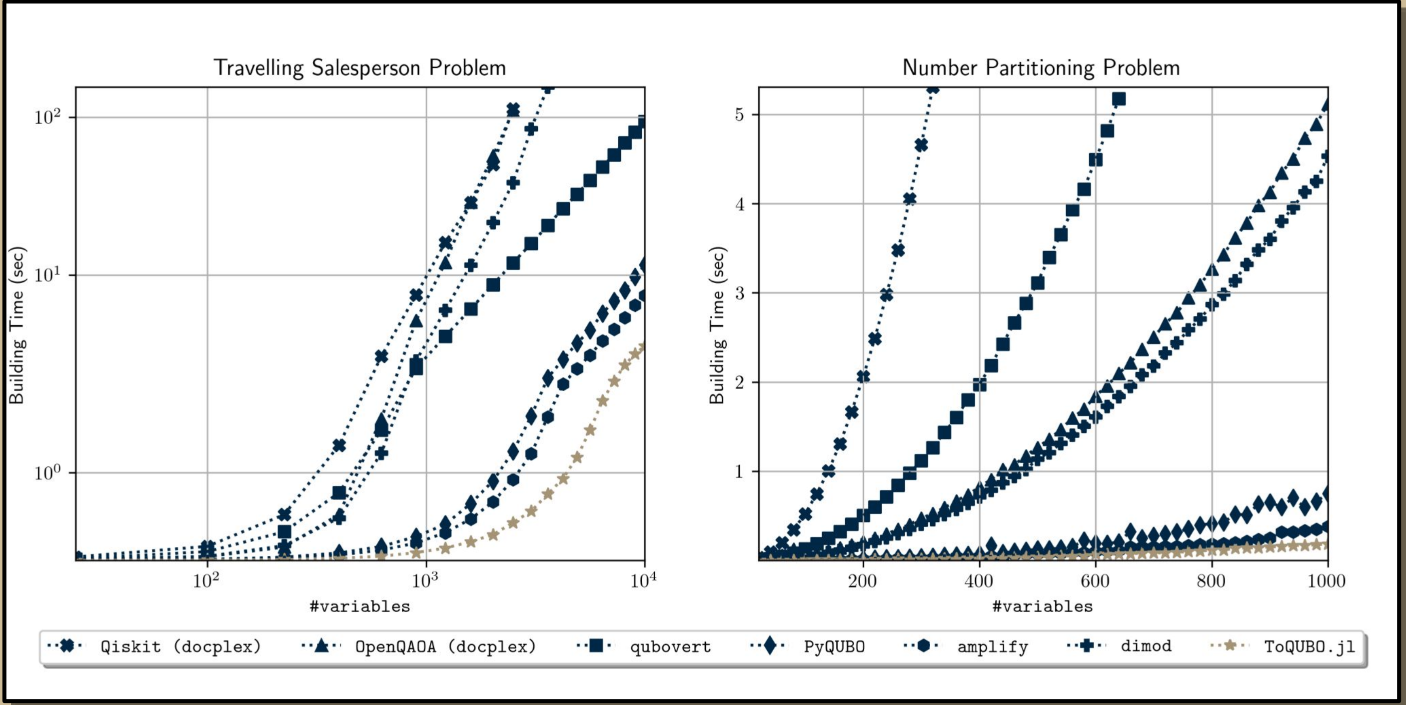


```julia
using JuMP, QUBO
using PySA

model = Model(() -> ToQUBO.Optimizer(PySA.Optimizer))

@variable(model, 0 <= g[1:T,j=1:n] <= Gmax[j])
@variable(model, u[1:T,1:n], Bin)
@variable(model, x[1:n], Bin)

@objective(model, Min, sum(c'g[t,:] for t=1:T) + i'x)

@constraint(model, [t=1:T], sum(g[t,:]) == d[t])
@constraint(model, [t=1:T,j=1:n], g[t,j] <= u[t,j] * Gmax[j])
@constraint(model, [t=1:T,j=1:n], u[t,j] <= x[j])

optimize!(model)

@show objective_value(model)
@show value.(x)
```

Reformulation Performance



Qualitative Analysis

CITATION ALERT

TABLE I: Comparing the support provided by of proposed framework and existing libraries and framework in each step of quantum optimization.
✔ indicates that the corresponding action is performed automatically.
✓ signifies that a proper function is available for implementing the step.
✗ indicates that the method is not fully supported.
+ denotes that logarithmic encoding is also compatible with bases different from two.
* signifies that the encoding techniques can be exploited only for constraints translation.
† indicates that the polynomial reduction is implemented by exploiting the corresponding qubovert function.

Supports for each step		Existing Libraries						Existing Frameworks		Proposed
		pyqubo [31]	qubovert [32]	dimod [33]	Qiskit [34]	fixstars [35]	openQAOA [36]	AutoQUBO [37]	QUBO.jl [38]	Framework
Floating Encoding		✗	✗	✗	✗	✗	✗	✗	✔	✔
Integer Encoding	Logarithmic [39]	✓	✓	✓	✓	✓*	✗	✗	✔	✔+
	Unitary [39]	✓	✓	✗	✗	✓*	✗	✗	✔	✔
	Dictionary [39]	✓	✗	✗	✗	✗	✗	✗	✔	✔
	Domain-Wall [40]	✓	✗	✗	✗	✗	✗	✗	✔	✔
	Bounded-Coeff [41]	✗	✗	✗	✗	✗	✗	✗	✔	✔
	Arithmetic [42]	✗	✗	✗	✗	✓*	✗	✗	✔	✔
Penalty Functions	Equality [22] [21]	✗	✓	✓	✓	✓	✓	✗	✔	✔
	Inequality [22]	✗	✓	✓	✓	✓	✓	✗	✔	✔
	Boolean [22]	✓	✓	✓	✗	✓	✗	✗	✗	✔
Penalty Weight	UB positive [43]	✗	✗	✗	✗	✗	✗	✗	✗	✔
	MQC [43]	✗	✗	✓	✗	✗	✗	✗	✗	✔
	VLM [44]	✗	✗	✗	✗	✗	✗	✔	✗	✔
	MOMC [43]	✗	✗	✗	✗	✗	✗	✗	✗	✔
	MOC [43]	✗	✗	✗	✗	✗	✗	✗	✗	✔
	UB Naive [45], [46]	✗	✓	✗	✔	✗	✗	✔	✗	✔
	UB posiform [45], [46]	✗	✗	✗	✗	✗	✗	✔	✗	✔
Polynomial Reduction		✓	✓	✓	✗	✓	✗	✔	✔	✔†
Solvers	Dwave QA	✔	✗	✔	✗	✔	✗	✔	✔	✔
	QAOA	✗	✗	✗	✔	✗	✔	✗	✔	✔
	VQE	✗	✗	✗	✔	✗	✔	✗	✔	✔
	GAS	✗	✗	✗	✔	✗	✗	✗	✗	✔
	SA	✔	✔	✔	✔	✔	✗	✔	✔	✔
Solution Decoding		✓	✓	✓	✓	✓	✓	✔	✔	✔
Check Constraints		✓	✓	✓	✗	✓	✗	✔	✔	✔
Penalty Update	Sequential [47]	✗	✗	✗	✗	✗	✗	✗	✗	✔
	Scaled [47]	✗	✗	✗	✗	✗	✗	✗	✗	✔
	Binary search [47]	✗	✗	✗	✗	✗	✗	✗	✗	✔

***Towards an Automatic Framework for Solving Optimization Problems with Quantum Computers*, arXiv:2406.12840, 2024**

Conclusions & Future Work

MAIN TAKEAWAYS

- ❑ ***QUBO.jl gives OR practitioners a smooth experience for accessing advanced hardware***
- ❑ ***Provides tools & infrastructure for benchmarking novel optimization technologies***

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NEXT STEPS

- ❑ ***Set up benchmarking service and use results to guide reformulation***
- ❑ ***Expand Reformulation Library and Solver support***
- ❑ ***Investigate architecture-oriented compilation***

Thanks!

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pedrox@cos.ufrj.br