

#### A Julia ecosystem for Quadratic Unconstrained Binary Optimization

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TITLE

What has to be done to incorporate Quantum & other Physics-inspired Technologies in Optimization Workflows?







What has to be done to incorporate Quantum & other Physics-inspired Technologies in Optimization Workflows?



Access Solvers





What has to be done to incorporate Quantum & other Physics-inspired Technologies in Optimization Workflows?



Access Solvers

How to deal with the many different APIs across services?





## Summary What has to be done to incorporate Quantum **Reformulate Models** & other Physics-inspired Technologies in **Optimization Workflows? Access Solvers** How to deal with the many different APIs across services? **A Common Interface**

🔯 🔏 JUMP

QUBO.jl: A Julia ecosystem for Quadratic Unconstrained Binary Optimization JuMP-dev | July 19-21, 2024 | HEC Montréal, Canada



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A Common Interface

A Compiler for Mathematical Programming



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**JUMP** 

A Continuous Benchmarking Library

**A Common Interface** 













#### **Solution Overview**

**A Common Interface** 



$\min_{\mathbf{s} \neq -\mathbf{a}(\mathbf{y}; \mathbf{z})} f(\mathbf{y}; \mathbf{z}) \le 0$	MINLP	
$egin{aligned} & \mathbf{h}(m{y};m{z}) \leq 0 \ & m{h}(m{y};m{z}) = 0 \ & m{y} \in \mathbb{Z}^m; m{z} \in \mathbb{R}^n \end{aligned}$	$ \begin{array}{l} \min \ f(\boldsymbol{y}; \boldsymbol{z}) \\ \text{s.t.} \ \boldsymbol{g}(\boldsymbol{y}; \boldsymbol{z}) \leq 0 \\ \boldsymbol{h}(\boldsymbol{y}; \boldsymbol{z}) = 0 \\ \boldsymbol{y} \in \mathbb{Z}^m; \boldsymbol{z} \in \mathbb{R}^n \end{array} $	7





#### **Solution Overview**





#### **Solution Overview**

JUMP

**A Common Interface** 



#### Integrating an heterogeneous Solver Landscape



**D-Wave** 



Fujitsu



IBM



P. L. McMahon et al., 2016



**Microsoft Research** 



Toshiba, Goto et al., 2019

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



Hitachi, Yamaoka et al.



#### Integrating an heterogeneous Solver Landscape



D-Wave



Fujitsu



IBM



P. L. McMahon et al., 2016



Microsoft Research



Toshiba, Goto et al., 2019



Julia Mathematical Programming



Hitachi, Yamaoka et al.



## **A Common Solver Interface**



•••			
using JuMP using QiskitOpt # IBM Qiskit Optimizati	•••	ing JuMP ing PySA # NASA Parallel Tempering	
<pre>model = Model(QiskitOpt.QAOA.Optimizer)</pre>	using JuMP using DWave # DWave Quantum Annealing	del = Model(PySA.Optimizer)	
<pre>@variable(model, x[1:n], Bin) @objective(    model,    Min,    x' * Q * x + l' * x + c )</pre>	<pre>model = Model(DWave.Optimizer) @variable(model, x[1:n], Bin) @objective(    model,</pre>	<pre>variable(model, x[1:n], Bin) bjective( model, Min, x' * Q * x + ℓ' * x + c</pre>	
optimize!(model)	MIN, x' * Q * x + ℓ' * x + c )	timize!(model)	
@show objective_value(model) @show value.(x)	optimize!(model)	<pre>show objective_value(model) show value.(x)</pre>	
	@show objective_value(model) @show value.(x)		

#### **Testing and Benchmarking Solvers**

A Continuous Benchmarking Library





### **Testing and Benchmarking Solvers**

A Continuous Benchmarking Library



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**

A Continuous Benchmarking Library



#### •••

QUB0Lib.load\_index() do index db = QUB0Lib.database(index) df = DBInterface.execute( db, SELECT instance FROM Instances WHERE dimension < 100 AND guadratic\_density < 0.5; ) |> DataFrame codes = collect(Int, df[!, :instance]) @info "Running DWave Neal" OUBOLib.run!( index, DWave.Neal.Optimizer, codes; solver = "dwave-neal" @info "Running DWave (Quantum)" OUBOLib.run!( index, DWave.Optimizer, codes; solver = "dwave" end







**Z JUMP** 

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



















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

AMPL, JuMP, Pyomo...











# EXAMPLE




$$\min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_{t} \mathbf{c}' \mathbf{g}^{(t)} + \mathbf{i}' \mathbf{x}$$
s.a. 
$$\sum_{j} g_{j}^{(t)} = d^{(t)} \quad \forall t$$

$$g_{j}^{(t)} \leq u_{j}^{(t)} G_{j}^{(\max)} \quad \forall j, t$$

$$u_{j}^{(t)} \leq x_{j} \quad \forall j, t$$

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

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

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



**OPERATION**  $\min_{\mathbf{g},\mathbf{u},\mathbf{x}}\sum_{t}\mathbf{c}'\mathbf{g}^{(t)}+\mathbf{i}'\mathbf{x}$ s.a.  $\sum_{j} g_{j}^{(t)} = d^{(t)}$  $\forall t$ BALANCE  $g_i^{(t)} \le u_i^{(t)} G_i^{(\max)} \quad \forall j, t$  $u_i^{(t)} \le x_j \qquad \forall j, t$  $g_j^{(t)} \in [0, G_j^{(\max)}] rac{orall j}{OPERATION} orall j, t$  $u_i^{(t)} \in \{0, 1\} \qquad \forall j, t$  $x_i \in \{0, 1\}$  $\forall j$ 





$$\begin{split} \min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_{t} \mathbf{c}' \mathbf{g}^{(t)} + \mathbf{i}' \mathbf{x} \\ \text{s.a.} \sum_{j} g_{j}^{(t)} = d^{(t)} \qquad \forall t \\ g_{j}^{(t)} \leq u_{j}^{(t)} G_{j}^{(\max)} \quad \forall j, t \\ u_{j}^{(t)} \leq x_{j} \qquad \forall j, t \\ g_{j}^{(t)} \in [0, G_{j}^{(\max)}] \quad \forall j, t \\ u_{j}^{(t)} \in \{0, 1\} \qquad \forall j, t \\ u_{j}^{(t)} \in \{0, 1\} \qquad \forall j, t \\ x_{j} \in \{0, 1\} \qquad \forall j \end{split}$$



INVESTMENT

$$\begin{split} \min_{\mathbf{g},\mathbf{u},\mathbf{x}} \sum_{t} \mathbf{c}' \mathbf{g}^{(t)} + \mathbf{i}' \mathbf{x} \\ \text{s.a.} \sum_{j} g_{j}^{(t)} = d^{(t)} \qquad \forall t \\ g_{j}^{(t)} \leq u_{j}^{(t)} G_{j}^{(\max)} \quad \forall j, t \\ u_{j}^{(t)} \leq x_{j} \qquad \forall j, t \\ g_{j}^{(t)} \in [0, G_{j}^{(\max)}] \quad \forall j, t \\ u_{j}^{(t)} \in \{0, 1\} \qquad \forall j, t \\ u_{j}^{(t)} \in \{0, 1\} \qquad \forall j \\ \text{INVESTMENT} \end{split}$$





















•	•									
1 2 3	using JuMP using PySA									
4	<pre>model = Model(PySA.Optimizer)</pre>									
6 7 8 9	@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)									
10 11	<pre>@objective(model, Min, sum(c'g[t,:] for t=1:T) + i'x)</pre>									
12 13 14 15	<pre>@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])</pre>									
16 17	<pre>optimize!(model)</pre>									
18 19	<pre>@show objective_value(model) @show value.(x) snappily.com</pre>									



	OPERATION	INVEST	IENT
$\min_{\mathbf{g},\mathbf{u},\mathbf{x}}$	$\sum_t \mathbf{c}' \mathbf{g}^{(t)}$	$+ \mathbf{i}' \mathbf{x}$	
s.a.	$\sum g_i^{(t)} =$	$d^{(t)}$	$\forall t$
	$\sum_{j}^{j}$	I	BALANCE
	$g_j^{(t)} \le u_j^{(t)}$	$G_j^{(\max)}$	$\forall j, t$
	(t)	UNIT COM	MITMENT
	$u_j^{(i)} \leq x_j$		$\forall j,t$
	(t) -		ESTMENT
	$g_j^{(\iota)} \in [0, C]$	$\begin{bmatrix} \gamma(\max) \\ z_j \end{bmatrix}$	$\forall j, t$
	(t)		LINATION
	$u_j^{(\iota)} \in \{0, 1\}$	1	$\forall j, t$
	-(0, 1)		
	$x_j \in \{0, 1\}$	}	$\forall j$
		INV	ESTMENT

1 2 3	using JuMP, QUBO using PySA
4 5	<pre>model = Model(()</pre>
6 7 8	<pre>@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)</pre>
9 10 11	<pre>@objective(model, Min, sum(c'g[t,:] for t=1:T) + i'x)</pre>
12 13 14 15	<pre>@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])</pre>
16 17	<pre>optimize!(model)</pre>
18 19	<pre>@show objective_value(model) @show value.(x) snappify.com</pre>



# RESULTS

### **Reformulation Performance**



# Qualitative Analysis

TABLE I: Comparing the support provided by of proposed framework and existing libraries and framework in each step of quantum optimization.

 $\checkmark$  indicates that the corresponding action is performed automatically.

 $\checkmark$  signifies that a proper function is available for implementing the step.

× indicates that the method is not fully supported.

<sup>+</sup> denotes that logarithmic encoding is also compatible with bases different from two.

\* signifies that the encoding techniques can be exploited only for constraints translation.

<sup>†</sup> indicates that the polynomial reduction is implemented by exploiting the corresponding qubovert function.

Summer			Existing	Existing Fra	Proposed					
Supports for each step		pyqubo [31]	qubovert [32]	dimod [33]	Qiskit [34]	fixstars [35]	openQAOA [36]	AutoQUBO [37]	QUBO.jl [38]	Framework
Floati	ng Encoding	×	×	×	×	×	×	×	1	1
	Logarithmic [39]	1	1	1	1	1.	×	×	1	<b>√</b> +
	Unitary [39]	1	1	×	×	¥*	×	×	1	1
Integer Encoding	Dictionary [39]	1	×	×	×	×	×	×	1	1
	Domain-Wall [40]	1	×	×	×	×	×	×	1	1
	Bounded-Coeff [41]	×	×	×	×	×	×	×	1	1
	Arithmetic [42]	×	×	×	×	1.	×	×	1	1
	Equality [22] [21]	×	1	1	1	1	1	×	1	1
Functions	Inequality [22]	×	1	1	1	1	1	×	1	1
	Boolean [22]	1	1	1	×	1	×	×	×	1
Penalty Weight	UB positive [43]	×	×	×	×	×	×	×	×	1
	MQC [43]	×	×	1	×	×	×	×	×	1
	VLM [44]	×	×	×	×	×	×	1	×	1
	MOMC [43]	×	×	×	×	×	×	×	×	1
	MOC [43]	×	×	×	×	×	×	×	×	1
	UB Naive [45], [46]	×	1	×	1	×	×	1	×	1
	UB posiform [45], [46]	×	×	×	×	×	×	1	×	1
Polynomial Reduction		1	1	1	×	1	×	1	1	à
	Dwave QA	1	×	1	×	1	×	1	1	1
	QAOA	×	×	×	1	×	1	×	1	1
Solvers	VQE	×	×	×	1	×	1	×	1	1
	GAS	×	×	×	1	×	×	×	×	1
	SA	1	1	1	1	1	×	1	1	1
Soluti	Solution Decoding		1	1	1	1	1	1	1	1
Check Constraints		1	1	1	×	1	×	1	1	1
Penalty Update	Sequential [47]	×	×	×	×	×	×	×	×	1
	Scaled [47]	×	×	×	×	×	×	×	×	1
	Binary search [47]	×	×	×	×	×	×	×	×	1

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

**CITATION** 

ALERT

# Qualitative Analysis

TABLE I: Comparing the support provided by of proposed framework and existing libra quantum optimization.

 $\checkmark$  indicates that the corresponding action is performed automatically.

- $\checkmark$  signifies that a proper function is available for implementing the step.
- × indicates that the method is not fully supported.
- <sup>+</sup> denotes that logarithmic encoding is also compatible with bases different from two.
- \* signifies that the encoding techniques can be exploited only for constraints translation.
- <sup>†</sup> indicates that the polynomial reduction is implemented by exploiting the corresponding qubovert function

	6			Existing	Existing Frameworks		Proposed			
Support	pyqubo [31]	qubovert [32]	dimod [33]	Qiskit [34]	fixstars [35]	openQAOA [36]	AutoQUBO [37]	QUBO.jl [38]	Framewor	
Floati	ng Encoding	×	×	×	×	×	×	×	1	1
	Logarithmic [39]	1	1	1	1	4.	×	×	1	<b>√</b> +
	Unitary [39]	1	1	×	×	ו	×	×	1	1
Integer Encoding	Dictionary [39]	1	×	×	×	×	×	×	1	1
	Domain-Wall [40]	1	×	×	×	×	×	×	1	1
	Bounded-Coeff [41]	×	×	×	×	×	×	×	1	1
	Arithmetic [42]	×	×	×	×	1.	×	×	1	1
	Equality [22] [21]	×	1	1	1	1	1	×	1	1
Functions	Inequality [22]	×	1	1	1	1	1	×	1	1
	Boolean [22]	1	1	1	×	1	×	×	×	1
Penalty Weight	UB positive [43]	×	×	×	×	×	×	×	×	1
	MQC [43]	×	×	1	×	×	×	×	×	1
	VLM [44]	×	×	×	×	×	×	1	×	1
	MOMC [43]	×	×	×	×	×	×	×	×	1
	MOC [43]	×	×	×	×	×	×	×	×	1
	UB Naive [45], [46]	×	1	×	1	×	×	1	×	1
	UB posiform [45], [46]	×	×	×	×	×	×	1	×	1
Polynon	nial Reduction	1	1	1	×	1	×	1	1	<b>v</b> †
	Dwave QA	1	×	1	×	1	×	1	1	1
	QAOA	×	×	×	1	×	1	×	1	1
Solvers	VQE	×	×	×	1	×	1	×	1	1
	GAS	×	×	×	1	×	×	×	×	1
	SA	1	1	1	1	1	×	1	1	1
Solutio	Solution Decoding		1	1	1	1	1	1	1	1
Check	Check Constraints		1	1	×	1	×	1	1	1
Penalty Update	Sequential [47]	×	×	×	×	×	×	×	×	1
	Scaled [47]	×	×	×	×	×	×	×	×	1
	Binary search [47]	×	×	×	×	×	×	×	×	1

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

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# What's new?

- Additional attributes to control reformulation
  - e.g. ConstraintPenaltyHint, VariableEncodingMethod
- Reformulation Callbacks
- Architecture-based dispatch
- Disjuctive Programming (DisjunctiveToQUB0.jl)

















#### Integrating an heterogeneous Solver Landscape



D-Wave



Fujitsu



IBM



P. L. McMahon et al., 2016



**Microsoft Research** 



Toshiba, Goto et al., 2019



Julia Mathematical Programming



Hitachi, Yamaoka et al.



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U



Toshiba, Goto et al., 2019





D-Wave

IBM





Toshiba, Goto et al., 2019

P. L. McMahon et al., 2016



Hitachi, Yamaoka et al.

(QUBO) min  $\mathbf{x'Qx} + \boldsymbol{\ell'x} + c$ s.t.  $\mathbf{x} \in \{0, 1\}^n$ 



Microsoft Research AOC

(QUMO) min  $\mathbf{z'Q}\mathbf{z} + \boldsymbol{\ell'z} + c$ s.t.  $\mathbf{z} = [\mathbf{x}; \mathbf{y}]$  $\mathbf{x} \in \{0,1\}^m$  $\mathbf{y} \in [-1, +1]^n$ 













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MOI Bridges: [2002.03447] MathOptInterface: a data structure for mathematical optimization problems (arxiv.org)

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MOI Bridges: [2002.03447] MathOptInterface: a data structure for mathematical optimization problems (arxiv.org)

JUMP



MOI Bridges: [2002.03447] MathOptInterface: a data structure for mathematical optimization problems (arxiv.org)

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MOI Bridges: [2002.03447] MathOptInterface: a data structure for mathematical optimization problems (arxiv.org)

JUMP



MOI Bridges: [2002.03447] MathOptInterface: a data structure for mathematical optimization problems (arxiv.org)

# What about MOI Bridges?

- □ In fact, it is good to use as many MOI Bridges as possible
- □ Some of the operations are too destructive
  - e.g. Penalization, Encoding Continuous Variables
- □ Solver-dependent reformulation path finding
- □ Fine-grained control over reformulation steps



- Generalize the reformulation algorithm
- Expand constraint support
- Set up continuous benchmarking service
- Draw insights from benchmarking to guide reformulation



# Wishlist Food for Thought

- Asynchronous optimize! call
- Communication protocol for client-server apps



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#### THANKS FLATICON.COM FOR THE FIGURES


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**GitHub Repository** 

arXiv Preprint

