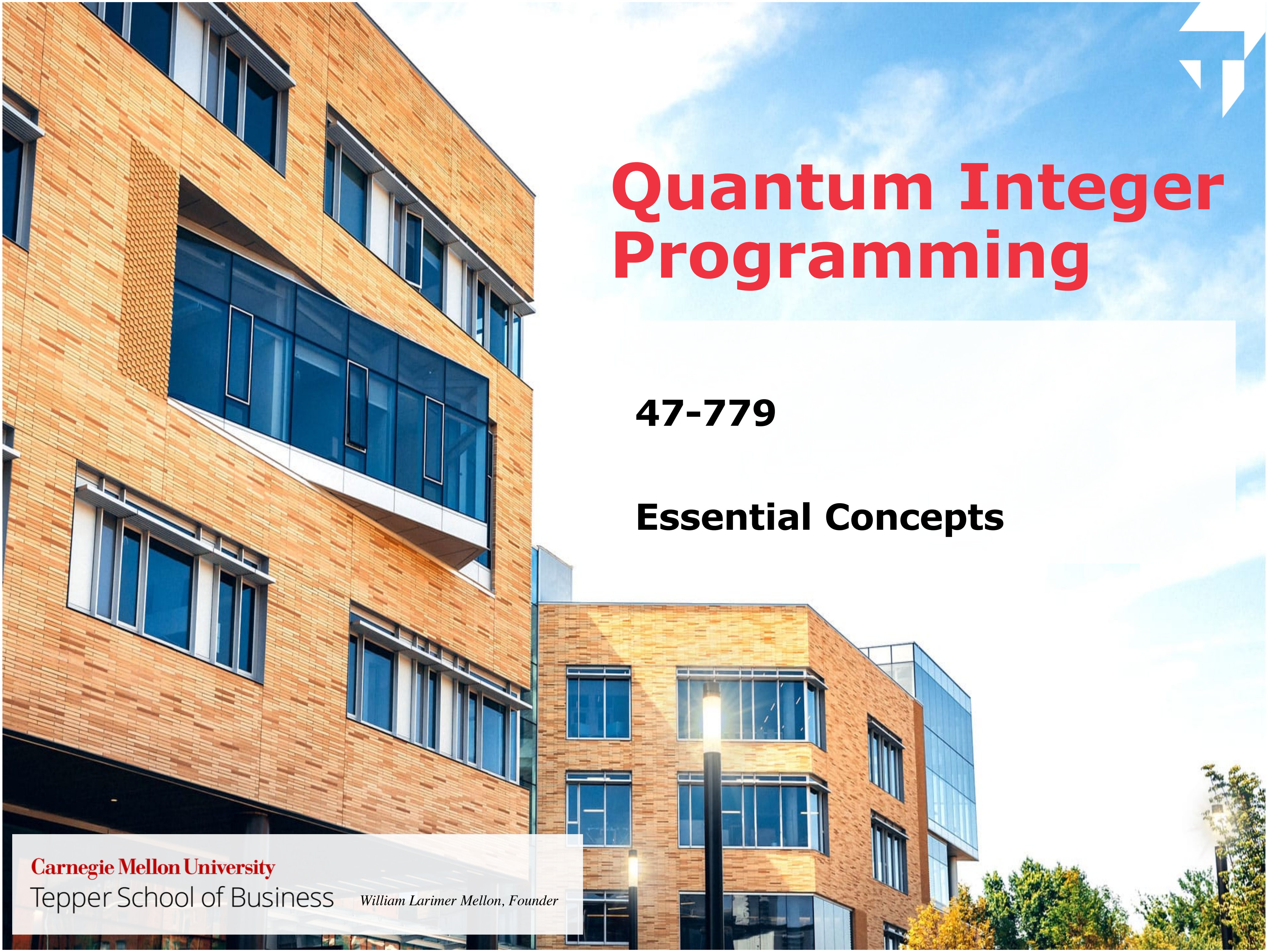


Quantum Integer Programming

47-779

Essential Concepts

Carnegie Mellon University
Tepper School of Business
William Larimer Mellon, Founder

Agenda

- Motivating Applications and Focus
- History of 20th Century Computing, Vocabulary
- Test-Sets, Graver Basis
- Ising Model, QUBO
- GAMA
- Quantum Computing v2.0
- Closing Remarks

Quantum Integer Programming (QuIP)

What can quantum computing do for non-linear integer optimization?

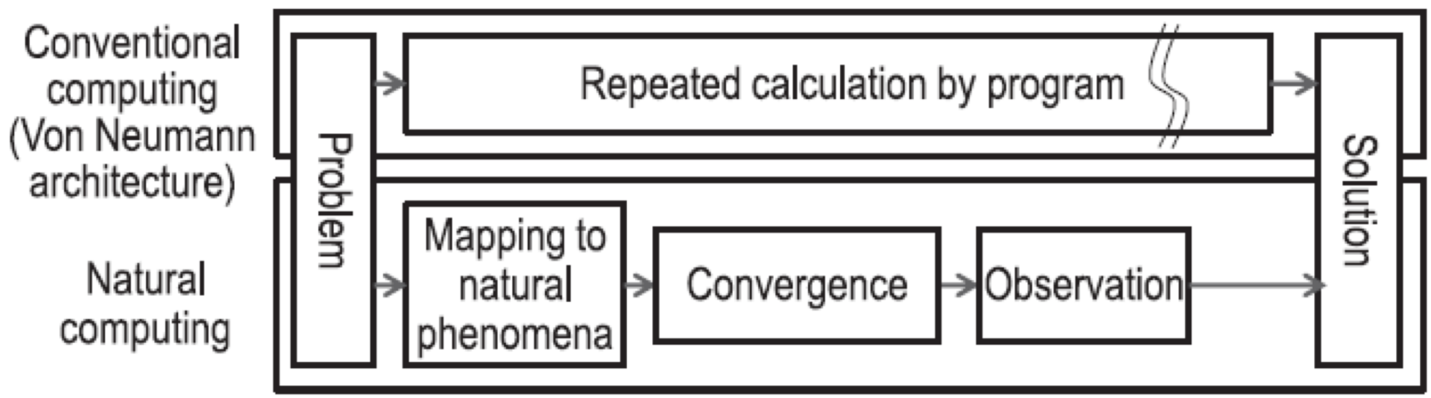
Motivating Applications

- Supply Chain Management
- Computational Biology
- Portfolio Optimization
- Track Reconstruction

Focus

Physics-based algorithms and computing machines that provide a novel approach to solving difficult optimization problems.

Conventional (Digital) v Natural (Analog) Computing



History of 20th Century Computing

- 1900-1929: Quantum Mechanics
- 1925: Ising Model (Lenz)
- 1926-1947: PNP Junction, Transistor
- 1936: Theory of Computing (Turing)
- 1947-1957: Integrated Circuit (“Chip”)
- 1954-1956: Oscillation Based Computing (von Neumann)
- 1939-1968: HP and birth of Silicon Valley; Intel
- 1911-1998: IBM, Microsoft, Apple, Amazon, Google
- 1981: Quantum Computing (Feynman)

Vocabulary

- Bits, Turing Machine, Logic gates
- Sequential State Computing
- Qubits, Spin, Superposition, Entanglement
- Gate/Circuit model, Quantum Logic
- Adiabatic Quantum Computing, Quantum annealing
- Ising Machine
- Collective State Computing

Points of Departure

- **Adiabatic Quantum Computing** *v* Gate/Circuit
- **Test sets** **v** LP Relaxation/B&B/Sub-gradients
- **Computational Performance** **v** Worst Case Complexity Analysis
- **Supply Chain/Finance/Genomics** **v** Cryptography/Quantum Chemistry

Ising Problem
(Combinatorial Optimization Version)

Problem Statement: Given couplings between a set of spins, find the configuration that minimizes the energy function:

$$H(\vec{\sigma}) = -\sum_{1 \leq i < j \leq N} J_{ij}\sigma_i\sigma_j$$

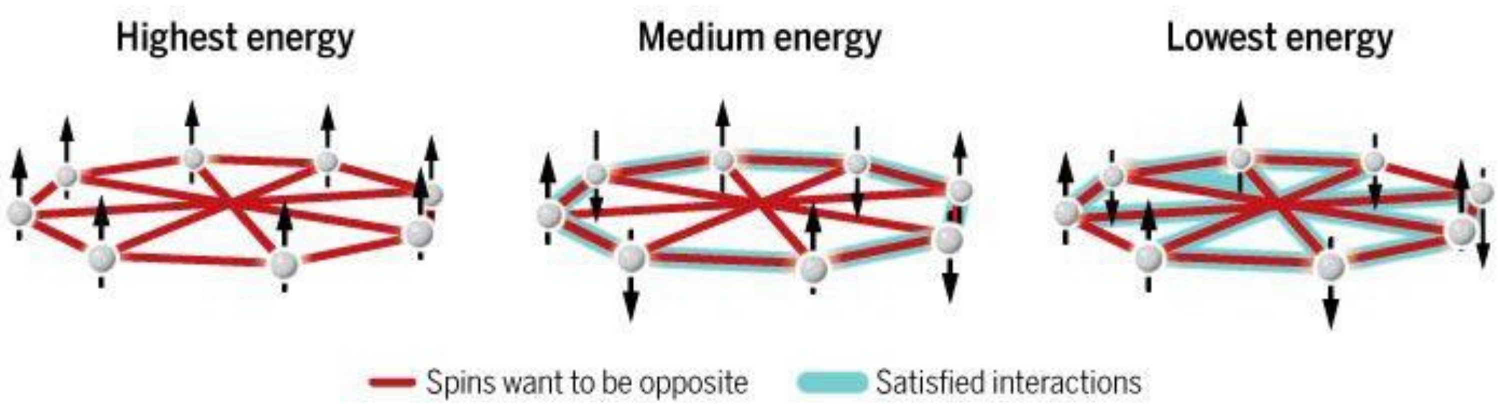


Figure credit: *Science* doi:10.1126/science.354.6310.269

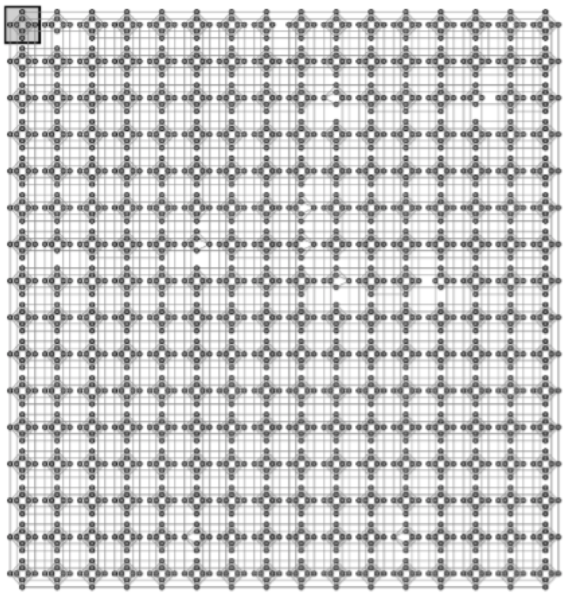
AQC finds the ground state through adiabatic quantum evolution that slowly evolves the ground state of the initial known system into the sought ground state of the problem:

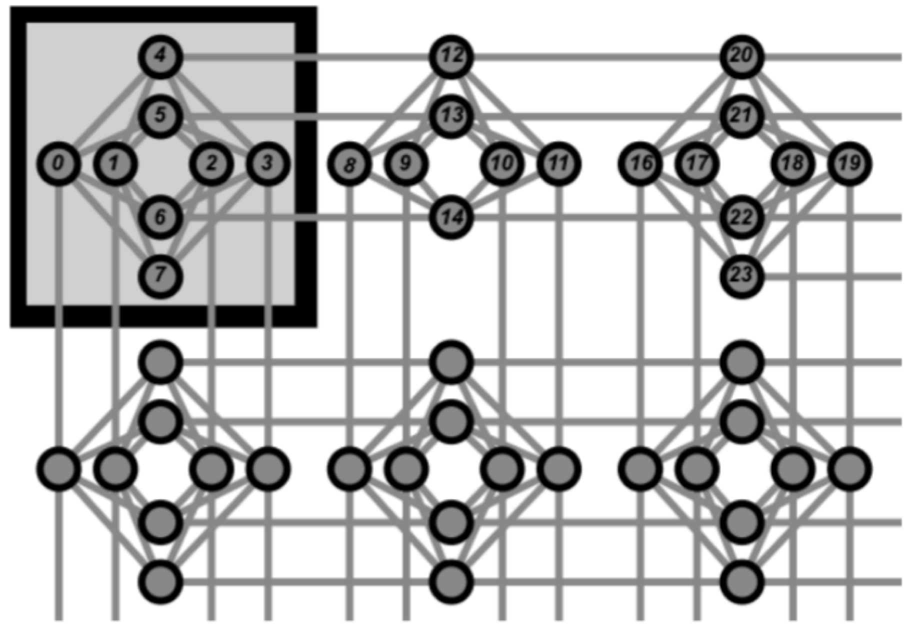
$$H(s) = (1-s)H_{initial} + sH_{problem}.$$

The **slow time** $s = t/T$ goes from 0 to 1 (where T is the effective total time of the adiabatic evolution).

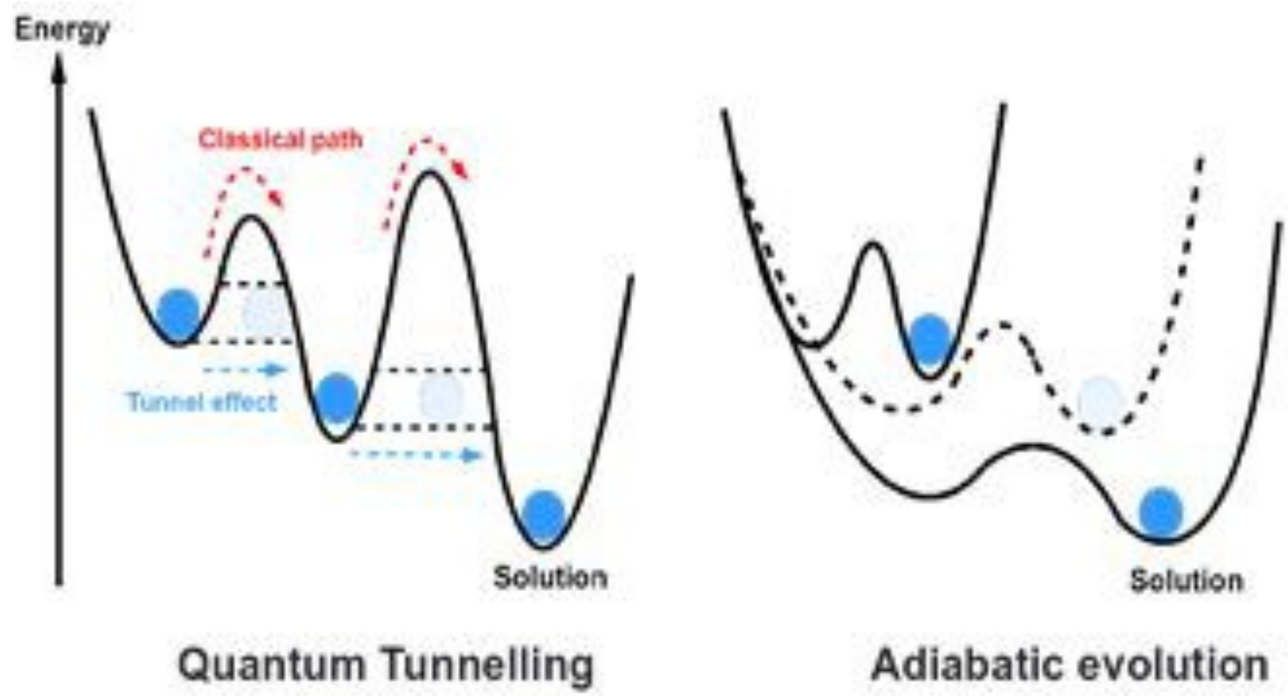
In practice, s could be replaced by a good $g(s)$, for improved performance as it affects the minimum spectral gap of the resulting $H(g(s))$.

D-Wave 2000Q

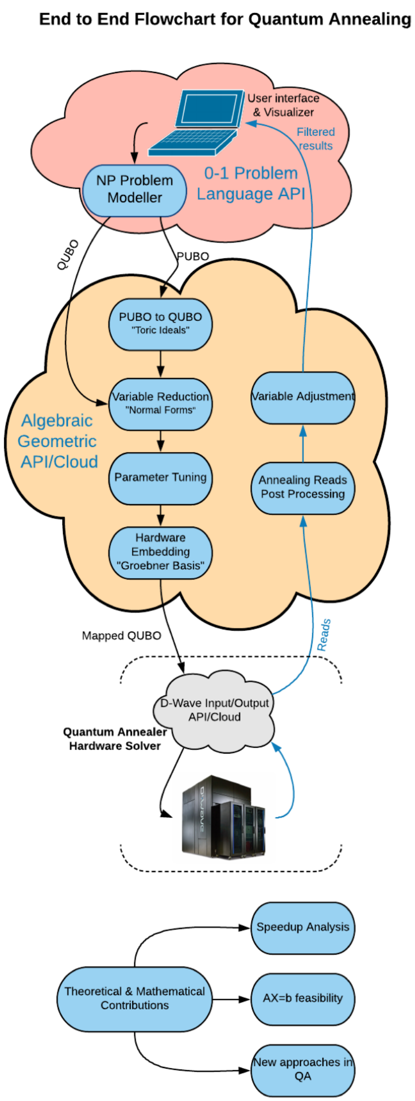




Quantum v Classical



Cloud Quantum Computing (Amazon Braket)



What can we do now?

- Classical Solvers
- Simulated Annealing
- “Brute Force” QUBO
- GAMA: Test-Sets, Graver Basis

Test Sets in Optimization

- Nonlinear integer program:

$$(IP)_{A,b,l,u,f}: \quad \min\left\{ \mathrm{f}(x) \; : \; Ax = b, \;\; x \in \mathbb{Z}^n \;, \;\; l \le x \le u \right\}$$

$$A \in \mathbb{Z}^{m\times n} \;, \;\; b \in \mathbb{Z}^m \;, \;\; l, u \in \mathbb{Z}^n, \;\; f : \mathbb{R}^n \to \mathbb{R}$$

- Can be solved via *augmentation procedure*:

1. Start from a feasible solution
2. Search for augmentation direction to improve
3. If none exists, we are at an optimal solution.

Graver Basis of Matrix A

- Graver Basis is the finite set of conformal minimal elements of:

$$\mathcal{L}^*(A) = \left\{ x \,\middle|\, Ax = \mathbf{0}, \quad x \in \mathbb{Z}^n \quad , \quad A \in \mathbb{Z}^{m \times n} \right\} \setminus \{\mathbf{0}\}$$

- Partial order:

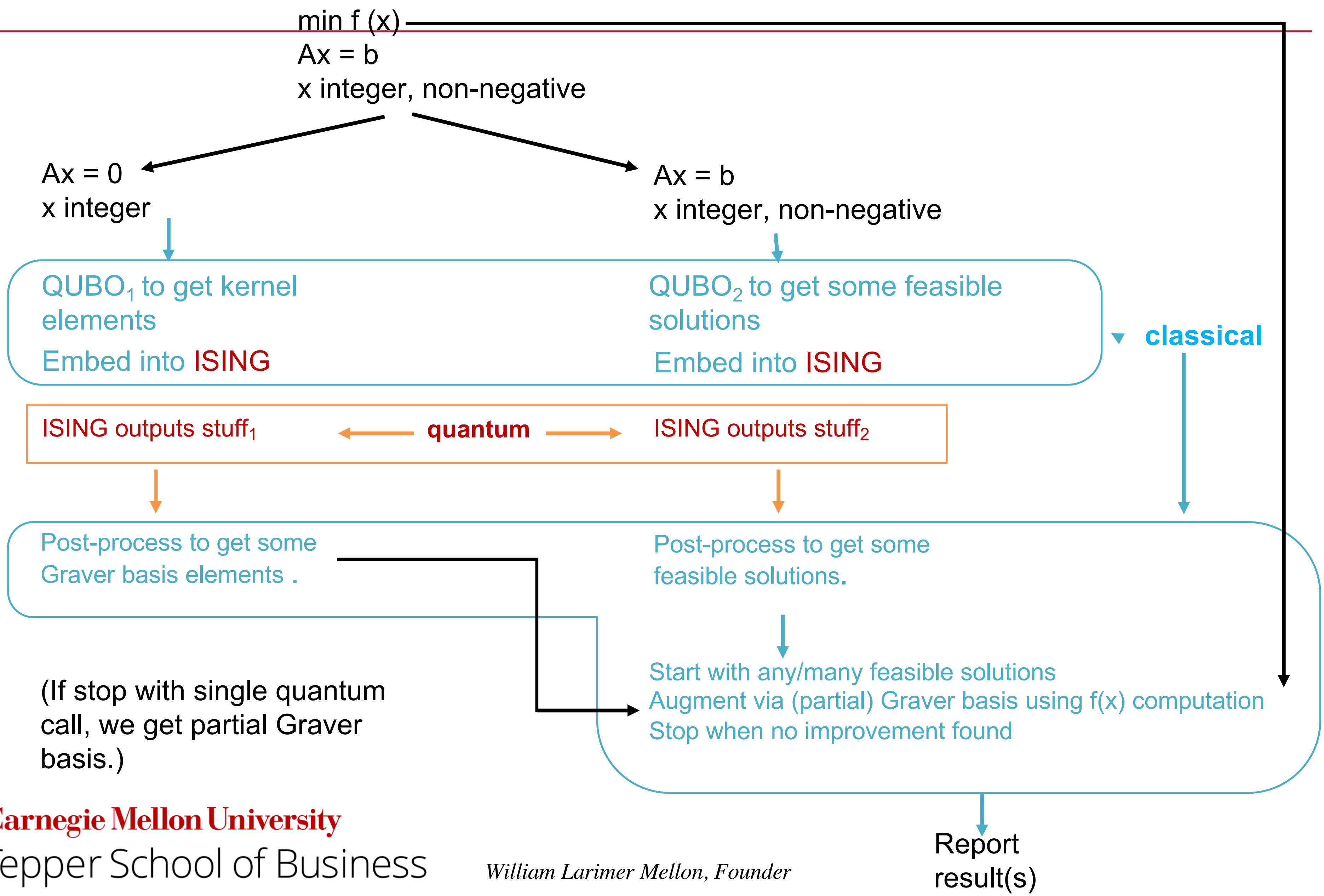
$$\forall x, y \in \mathbb{R}^n \quad x \sqsubseteq y \quad s.t. \quad x_i y_i \geq 0 \quad \& \quad |x_i| \leq |y_i| \quad \forall \quad i = 1, \ldots, n$$

- x is conformal minimal to y: $x \sqsubseteq y$

Graver Basis is Test Set for:

- $\min cx$, Linear
- $\max f(Wx), W \in \mathbb{Z}^{d\times n}$, f convex on $\mathbb{Z}^d$
- $\min \sum f_i(x_i)$, f_i convex (separable convex)
- $min\ |x - x_0|_p$
- Some other nonlinear costs

GAMA



min f (x)
Ax = b
x integer, non-negative
Ax = 0
x integer
Ax = b
x integer, non-negative
QUBO$_1$ to get kernel elements
Embed into ISING
QUBO$_2$ to get some feasible solutions
Embed into ISING
classical
ISING outputs stuff$_1$
quantum
ISING outputs stuff$_2$
Post-process to get some Graver basis elements .
Post-process to get some feasible solutions.
Start with any/many feasible solutions
Augment via (partial) Graver basis using f(x) computation
Stop when no improvement found
(If stop with single quantum call, we get partial Graver basis.)
Report result(s)

QUBO for Kernel

$$\mathbf{A}\mathbf{x} = \mathbf{0}, \quad \mathbf{x} \in \mathbb{Z}^n \quad , \quad \mathbf{A} \in \mathbb{Z}^{m\times n}$$

$$\min \quad \mathbf{x}^T \mathbf{Q}_\mathbf{I} \mathbf{x} \quad , \quad \mathbf{Q}_\mathbf{I} = \mathbf{A}^T \mathbf{A} \quad , \quad \mathbf{x} \in \mathbb{Z}^n$$

$$\mathbf{x}^T = \begin{bmatrix} x_1 & x_2 & \dots & x_i & \dots & x_n \end{bmatrix}, \quad x_i \in \mathbb{Z}$$

- Integer to binary transformation: $x_i = \mathbf{e}_i^T X_i$

$$X_i^T = \begin{bmatrix} \mathrm{X}_{i,1} & \mathrm{X}_{i,2} & \cdots & \mathrm{X}_{i,k_i} \end{bmatrix} \in \{0,1\}^{k_i}$$

- Binary encoding: $\mathbf{e}_i^T = \begin{bmatrix} 2^0 & 2^1 & \cdots & 2^{k_i} \end{bmatrix}$
- Unary encoding: $\mathbf{e}_i^T = \underbrace{\begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix}}_{k_i}$

QUBO for Kernel….

$$\mathbf{x} = \mathbf{L} + \mathbf{E}\mathbf{X} = \begin{bmatrix} Lx_1 \\ Lx_2 \\ \vdots \\ Lx_n \end{bmatrix} + \begin{bmatrix} \mathbf{e}_1^T & \mathbf{0}^T & \cdots & \mathbf{0}^T \\ \mathbf{0}^T & \mathbf{e}_2^T & \cdots & \mathbf{0}^T \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}^T & \mathbf{0}^T & \cdots & \mathbf{e}_n^T \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{bmatrix}$$

(L is the lower bound vector)

- QUBO:

$$\min \quad \mathbf{X}^T \quad \mathbf{Q}_{\mathbf{B}}\mathbf{X} \quad , \quad \mathbf{Q}_{\mathbf{B}} = \mathbf{E}^T\mathbf{Q}_{\mathbf{I}}\mathbf{E} + diag\left(2\mathbf{L}^T\mathbf{Q}_{\mathbf{I}}\mathbf{E}\right)$$

$$\mathbf{X} \in \{0,1\}^{nk} \quad , \quad \mathbf{Q}_{\mathbf{I}} = \mathbf{A}^T\mathbf{A}$$

QUBO for Feasible Solutions

- $$\mathbf{Ax} = \mathbf{b} \qquad\qquad l \le \mathbf{x} \le u$$

$$\min \quad \mathbf{X}^T \mathbf{Q_B X}, \quad \mathbf{Q_B} = \mathbf{E}^T \mathbf{Q_I E} + 2diag\left[\left(\mathbf{L}^T \mathbf{Q_I} - \mathbf{b}^T \mathbf{A}\right)\mathbf{E}\right]$$

$$\mathbf{X} \in \{0,1\}^{nk}, \quad \mathbf{Q_I} = \mathbf{A}^T \mathbf{A}$$

- Using adaptive centering and encoding width for feasibility bound
- Results in many feasible solutions!

Capital Budgeting

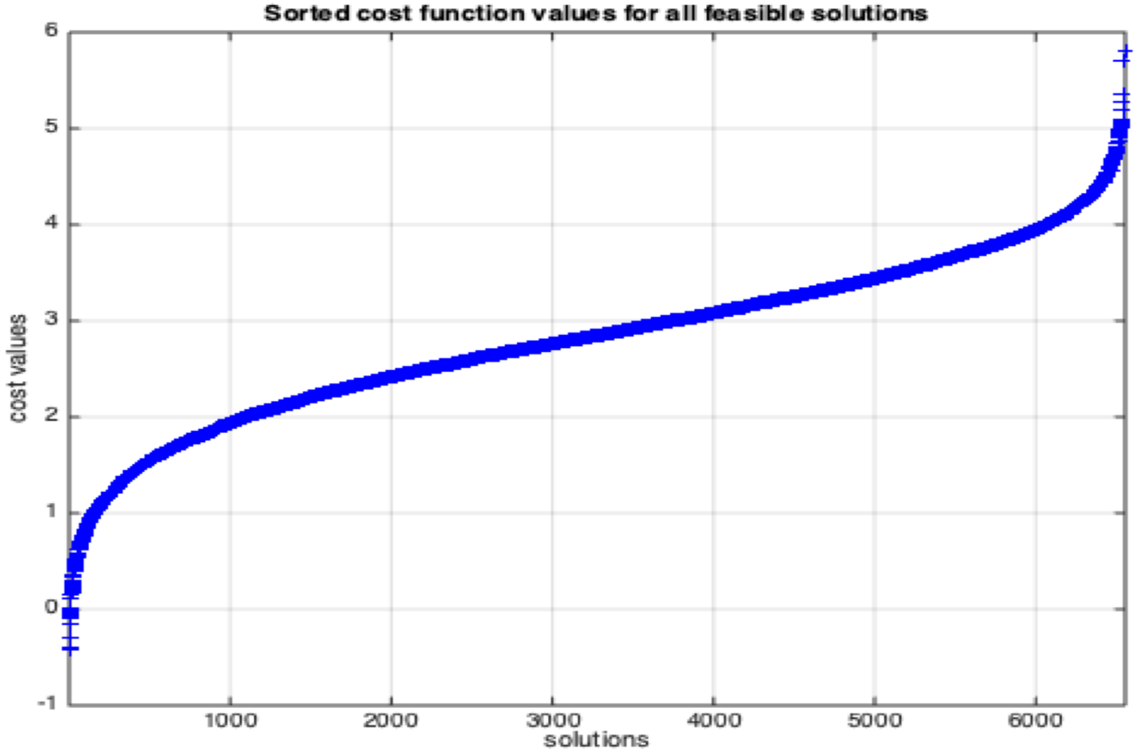
- Important canonical Finance problem
- μ_i expected return
- σ_i variance
- ε risk
- Graver Basis in 1 D-Wave call (1 bit encoding)

$$\begin{cases} \min \quad -\sum_{i=1}^{n} \mu_i x_i + \sqrt{\frac{1-\varepsilon}{\varepsilon} \sum_{i=1}^{n} \sigma_i^2 x_i^2} \\ Ax = b \quad , \quad x \in \{0,1\}^n \end{cases}$$

$$A \in M_{5\times 50}(\{0,\cdots,t\}) \quad \mu \in [0,1]^{50\times 1} \quad \sigma \in [0,\mu_i]^{50\times 1}$$

when t = 1 we have: $\mathcal{G}(A) \in M_{50\times 304}(\{-1,0,+1\})$

~ 6500 Solutions in One Call!



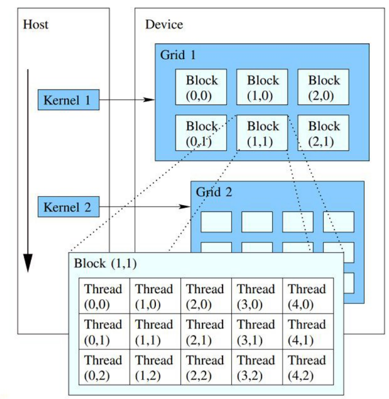
- From any feasible point in ~24-30 augmenting steps reach optimal cost = -3.69

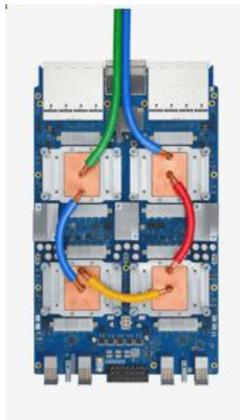
Quantum Computing v2.0

	Quantum Computing v1.0 1981-2017	Quantum Computing v2.0 2017-
Computing Model	Gate/Circuit Model	Ising Model
	Sequential State computation	Collective State computation
Algorithms	Worst-case Performance	Hybrid Quantum-Classical
	Quantum Complexity Theory (QCT)	Quantum Integer Programming (QuIP)

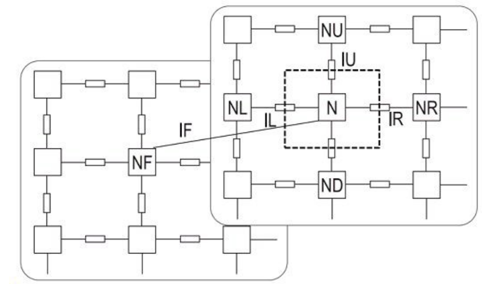
Nvidia, Google, Fujitsu, Hitachi, Toshiba…

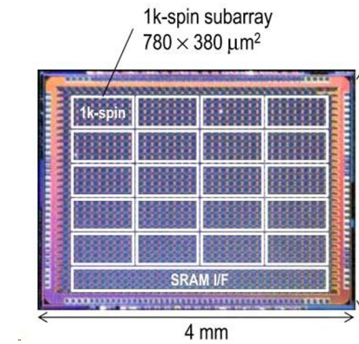
GPUs and TPUs





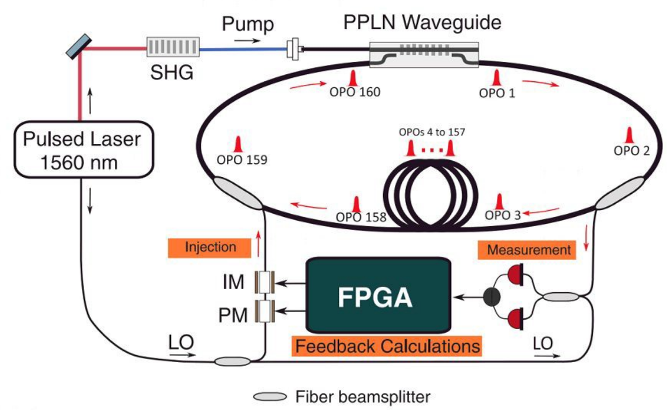
Complementary metal-oxide semiconductors (CMOS)





Digital annealers

Oscillator Based Computing



Available Ising Solvers

	Fixstars Optigan	D-Wave 2000Q	Hitachi CMOS Annealing	Fujitsu Digital Annealer	Toshiba SBM
Calculation method	GPU	Quantum annealing	Digital circuit	Digital circuit	GPU
Maximum number of bits	Over 100,000	2,048 (16x16x8)	61,952 (352x176)	1,024 / 8,192	10,000
Coefficient parameter	Digital (32 / 64bit)	Analog (about 5bit)	Digital (3bit)	Digital (16/64 bit)	Digital (32bit)
Combined graph	Fully combined	Chimera graph	King Graph	Fully combined	Fully combined
Total number of combined conversion bits	65,536	64	176	1,024 / 8,192	1,000
API endpoint	Fixstars	D-Wave Cloud	Annealing Cloud Web	DA Cloud	AWS

2020 Tayur Prize

Hardware Challenge

Cheap

Room-Temperature

Based on available components

Non-classical computation

Coherent Ising Machine (CIM)

Oscillation Based Computing

March 2020: NSF $10M funding to NTT, Stanford, Cornell, NASA consortium for CIM!

Closing Remarks

- Non-linear Integer Programs model a variety of real world problems from many domains
- Solving them classically has limitations
- We explored non-classical approaches based on Ising
- GAMA is a general purpose heuristic that utilizes Test-Sets
- There are a variety of options to solve large scale Ising model, expect more in the future
- What will 21st Century Computing look like?