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# Accelerating and Optimizing various resource exploration planning sub-processes using Quantum inspired Classical Computing or Vector Annealing on Vector Engine Accelerator (VA on VE)

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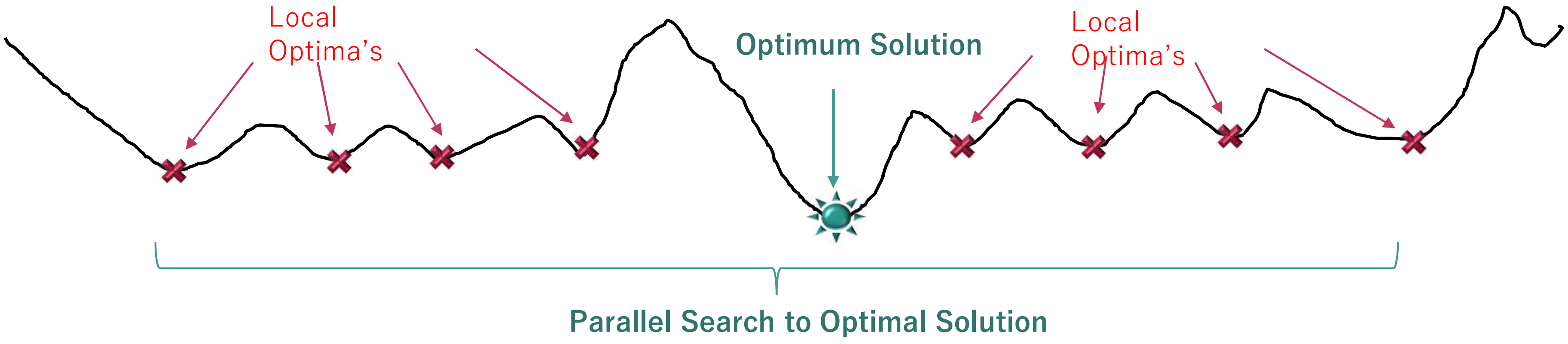
# Combinatorial Optimization Problems

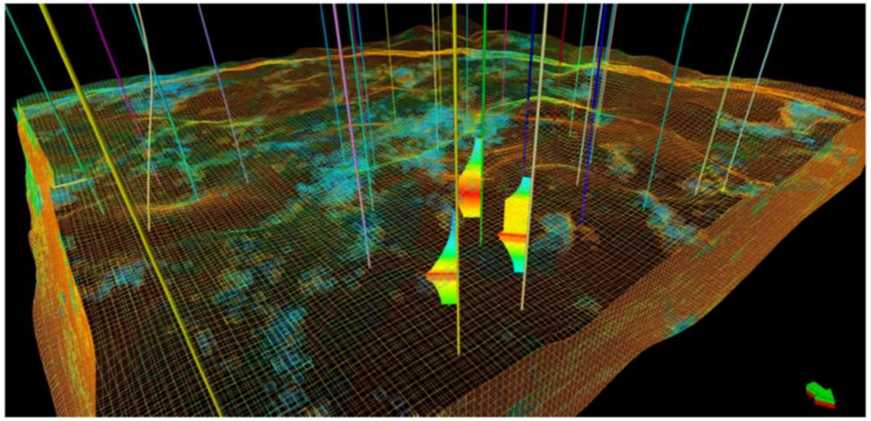



- **Goal:** To find optimal solution or object from a finite set of solutions/space or objects
- **Challenge:** The solution space is typically too large to search exhaustively using brute force or exploring multiple solution or many local minima's.
- **Examples:** Finding shortest/cheapest round trips(TSP), planning/scheduling, Supply Chain Optimization, Circuit design, Protein Structure Prediction etc.
- **A good possible way to solve such problems: Quantum Annealing (QA) or Simulated Annealing (SA) using Vector Engine Accelerators**
- **QA is able to explore the space in parallel using Quantum Effect or energy fluctuations and SA simulates the same by a meta-heuristic way of execution on a classical computer.**

# Combinatorial Optimization Problems Description

- **Combinatorial Problems:**
  - They are characterized by an input, i.e., a general description of conditions and parameters and a question (or task, or objective) defining the properties of a solution.
  - They involve finding a grouping, ordering, or assignment of a discrete, finite set of objects that satisfies given conditions.
  - Candidate solutions are combinations of objects or solution components that need not satisfy all given conditions.
  - Solutions are candidate solutions that satisfy all given conditions.
- **Optimization Problems:**
  - Objective function f measures solution quality (often defined on all candidate solutions)
  - Find solution with optimal quality, i.e., minimize/maximize f
  - Variants of optimization problems:
    - Search variant: Find a solution with optimal objective function value for given problem instance
    - Evaluation variant: Determine optimal objective function value for given problem instance

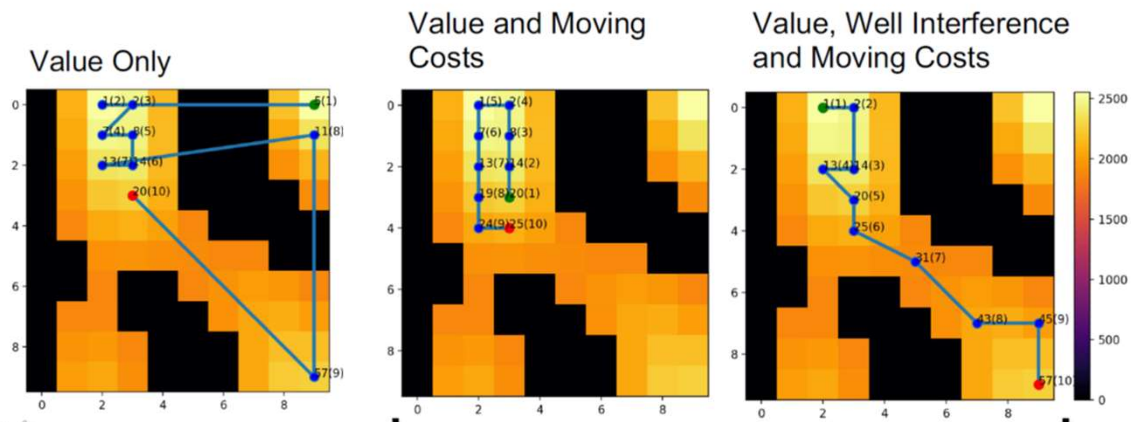
# Oil Field Exploration as a Combinatorial Optimization Problem



Subsurface modeling and characterization are only the beginning of oil field exploration. Given a map of the distribution of oil and a limited number of resources to develop the field, energy companies must plan a drilling sequence that considers:

- The value of placing a well at an optimal location. (**V1**)
- The cost of moving a drilling platform from one location to another. (**V2**)
- The impact on placement of a new well has on production from neighboring wells or well interference. (**V3**)

**V1** **V1+V2** **V1+V2+V3**




Not as complicated

NP-Hard Problem



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NEC is focusing on the quantum annealing method to address society's optimization needs and also promoting research and development toward practical application of the gate-based method.

# Quantum Computing

(Broadly defined to include quantum behavior)

## Annealing method, etc.

Solves combinatorial optimization problems by means of the Ising model or other statistical physics model

- Quantum Annealing Superconducting Circuits
  - D-Wave
  - NEC (R&D)
  - AIST
- Digital Circuits
  - NEC (product)
  - Hitachi
  - Fujitsu
  - Toshiba
- Optical Parametric Oscillator
  - NTT

## Quantum gate method

Performs calculations by replacing classical computer bits with qubits

- NEC (R&D)
- RIKEN UTokyo
- IBM
- Google
- Rigetti
- Intel

*Based on NEC's survey. (Due to limited space, not all institutions are covered.)

# Annealing

- Heating material to a critical temperature level resulting in property/structural change. Then cooling the same to retain the change.

- Simulated Annealing (SA) is a probabilistic and metaheuristic technique inspired from process of annealing metals for solving optimization problems.

- The goal is to achieve minimum energy (entropy) or temperature and it results high probability of success in achieving a speedy as well as accurate solutions

# Why Simulated Annealing (SA)?

- SA can solve combinatorial optimization problem or NP-Hard on a classical computer as a Quantum inspired Classical Computing solution.

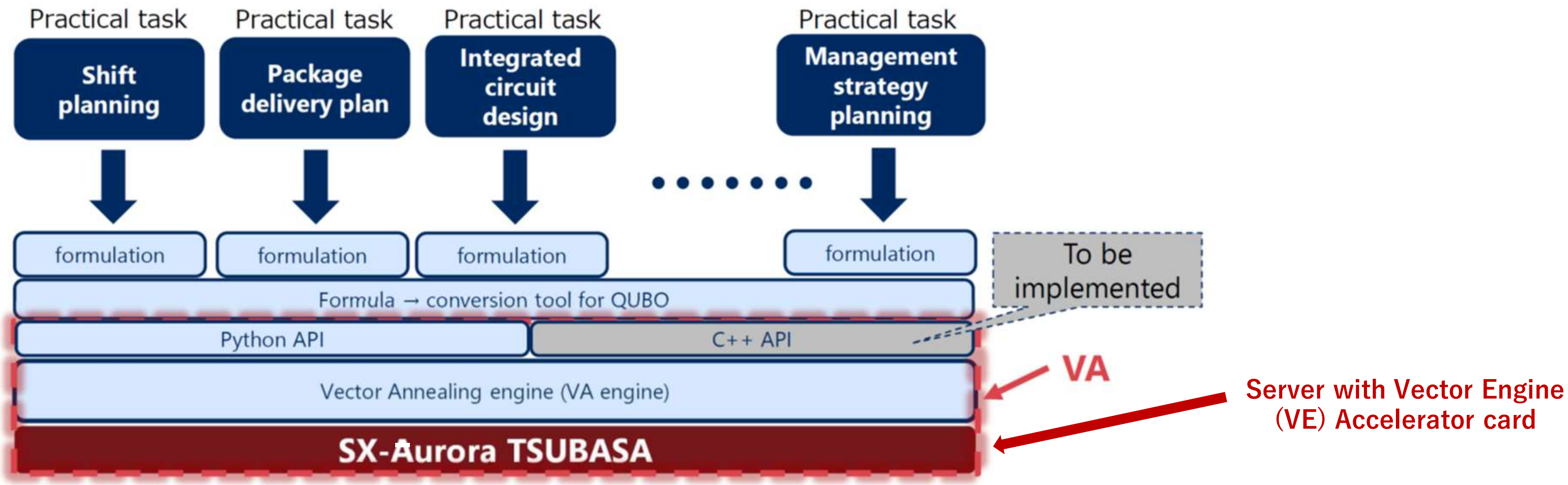
- SA is probabilistic and metaheuristic method for solving huge and complex optimization problems:
  - Faster solution in comparison to typical brute force methods used in classical computers even with complexity of constraints.
  - The output can easily be made predictable and accurate within less time by providing constraints.

- SA software along with hardware solutions like vector engine accelerator provides:
  - Capability of applying existing constraints for even better results.
  - Choice between exploration and exploitation or “Speed” vs “Accuracy”’
  - Capability of solving real-world problems by simulating 100K fully connected qubits per accelerator card.
  - Create re-usable source codes which can be put on an actual quantum annealing system.

# Simulated/Vector Annealing Solution Stack

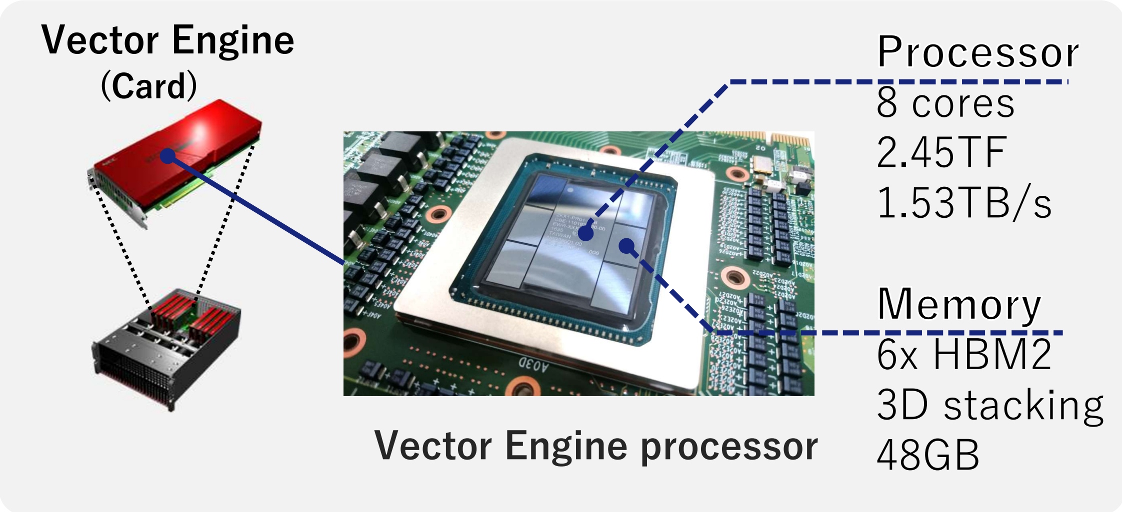
NEC has developed Vector Engine optimized Simulated Annealing(SA) Engine for solving combinatorial problems.

| | |
|---|---|
| **Input** | QUBO format |
| **Problem Size** | Up to 300K Qubit/Variables<br>8 x Vector Engine cards |
| **Connection** | 32-bit floating point, full connection |
| **Algorithm** | Includes our extension to improve result |



# Speeding up solving combinatorial optimization with simulated annealing machine on Vector Engine (VE) Accelerator

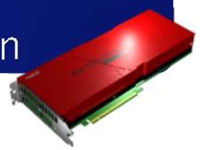
- By utilizing, **large/fast memory and high computation performance** realize **full connection 100K Qubits Simulation per card**
- Can support **further large scale problem with scale-up technology of supercomputer**
- Speeding up by **limiting search space** based on the constraints of the problem
- **Tuned perfectly** for SX-Aurora TSUBASA (VE)

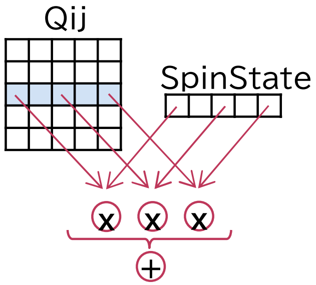


# Vector Annealing (VA) on Vector Engine Accelerator (VE)

**VA Performance is provided by:**
**Matrix operation acceleration by VE, large and fast memory, and optimized algorithm for VE**

## Vector operation on VE
Energy calculation is matrix operation



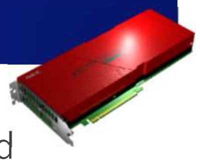



```
for(i=0; i<numSpins; i++)
  DeltaEnergy +=
       Qij[FlipSpin][i] x SpinState[i]
```

Effect from neighbor spin

0 or 1

## Full connect 100k qubits/VE and high memory bandwidth

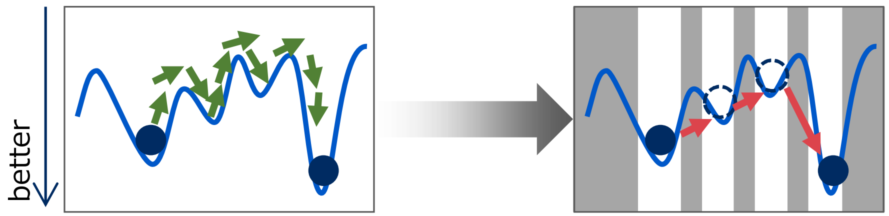


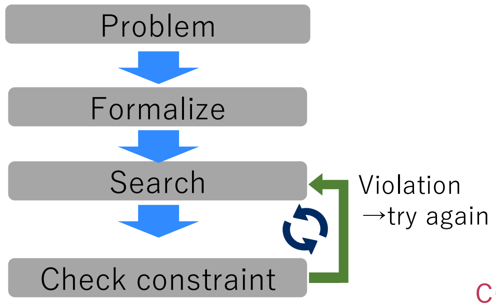
- 48GB memory capacity and 1.5TB/s memory bandwidth
- Multi card supports larger number of qbits (100k qbits x n)$^{1/2}$

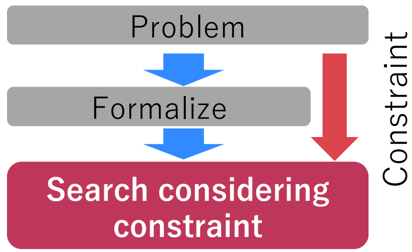
## Avoiding Redundant Search and Optimized algorithm for VE

**Existing search**
Including constraint violations

**VA search**
skip constraint violations

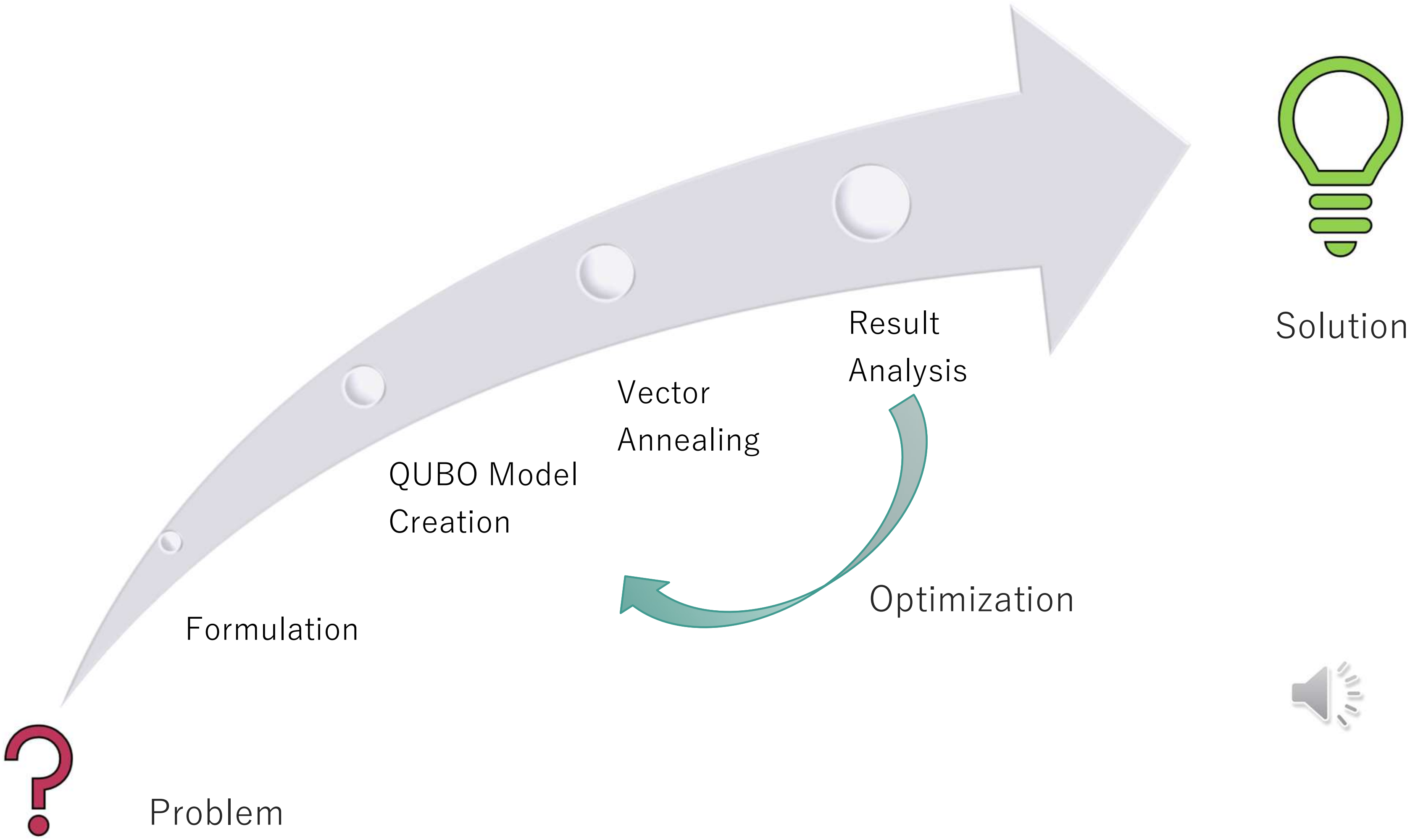



computational complexity reduction

# How to solve problems using Simulated/Vector Annealing?



# Defining a Problem and QUBO Formulation

- Define a problem which can be expressed in as a binary/spin format or Objective function to minimize:
  - Minimize the distance between a pair of locations.
- Define Constraints: The rules and guidelines SA should follow
  - Not to visit the same location more than twice.
  - Not to visit more than two locations at the same time.
- A QUBO problem is defined using an upper-diagonal matrix Q, which is an N x N upper triangular matrix of real weights, and x, is a vector of binary variables, as minimizing the function
- QUBO is created as a Hamiltonian Expression. +,-,*,/ and square **2 are arithmetic expressions can be used in forming the expressions combining objective function and constraints.
- "**Pyqubo**", is a Python library takes the expression as input, and we can generate required QUBO Matrix

**Hd: For all pairs of points, the distance d is set only when moving from point p1 to point p2, and the others are set to 0**

$$Hd = \Sigma_{i=0}(\Sigma_{p1=0,p2\neq p1} d_{p1p2} x_{i,p1} x_{(i+1),p2})$$

**Constraints:**

**Ha: Not to visit the same location more than twice**

$$Ha = strength * \Sigma_{i=0}(\Sigma_{j=0} x_{i,j} - 1)^2$$

**Hb: Not to visit more than two locations at the same time**

$$Hb = strength * \Sigma_{j=0}(\Sigma_{i=0} x_{i,j} - 1)^2$$

**QUBO:** $H = Hd + Ha + Hb$

$$f(x) = \sum_i Q_{i,i} x_i + \sum_{i<j} Q_{i,j} x_i x_j$$

$$\min_{x \in \{0,1\}^n} x^T Q x.$$

# Vector Annealing

- Provide the QUBO model to the annealing solver as input

- Provide following basic parameters:
  - Number of reads: Number of initial samples per annealing
  - Number of sweeps: Number of sets of iterations to run over the variables of a problem. More sweeps will usually improve the solution (unless it is already at the global min).
  - Beta or temperature range

- Simulated Annealing External Constraints (Specific to SA software running on Vector Engine):
  - Vector mode: SPEED and ACCURACY
  - Flip options
    - Initialization spin options
    - One-hot options
    - Fixed spin options etc.

**QUBO Generation using Pyqubo:**

```
model = H.compile()
qubo, offset = model.to_qubo(feed_dict={'num_a’: strength})
```

**SA with Additional External Constraints:**

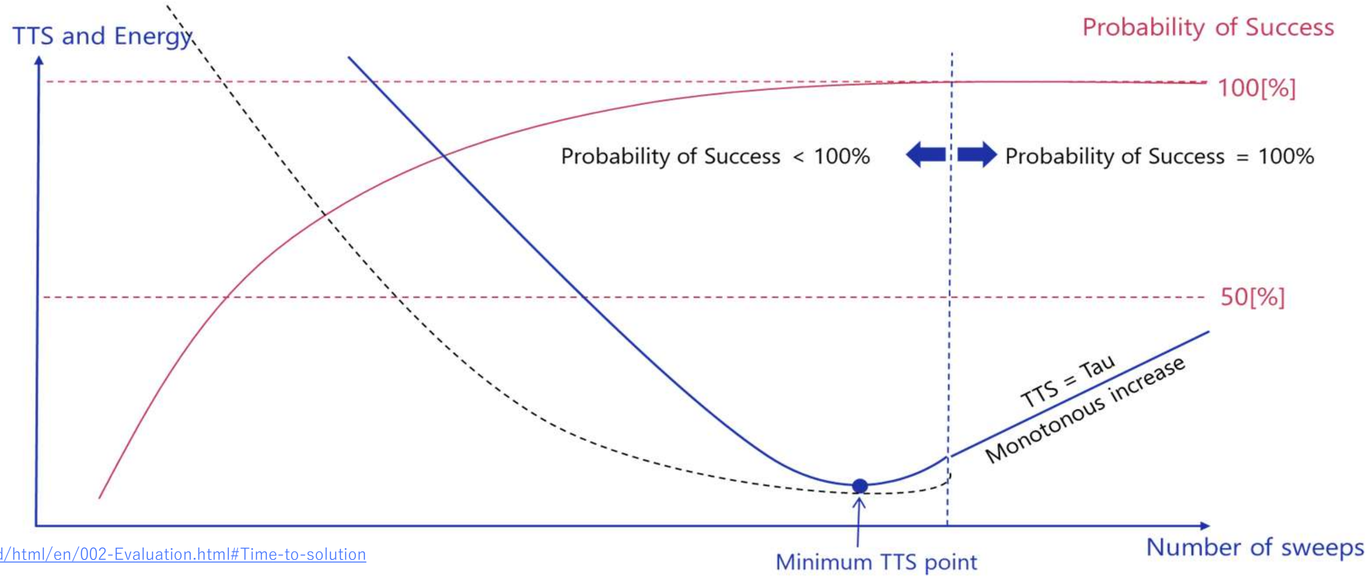
```
va_model = VectorAnnealing.model(qubo, offset, onehot=onehot, fixed=fixed)
sa       = VectorAnnealing.sampler()
results = sa.sample(va_model, num_reads=1, num_sweeps=1000, vector_mode="SPEED")
```

# Result Analysis

- We analyze the following as output:
  - Spin: Output of the annealing
  - Energy: Energy value per solution
  - TTS (Time to Solution): The time required to reach an optimum solution with high probability of success by running multiple annealing processes.

$$\mathrm{TTS}(\tau, p_R) = \tau R = \tau \frac{\ln(1-p_R)}{\ln\{1-p_s(\tau)\}} \quad *$$

- Solution value against minimum energy with highest probability of success (by performing multiple iterations) is the ideal result.




* https://openjij.github.io/OpenJijTutorial/build/html/en/002-Evaluation.html#Time-to-solution

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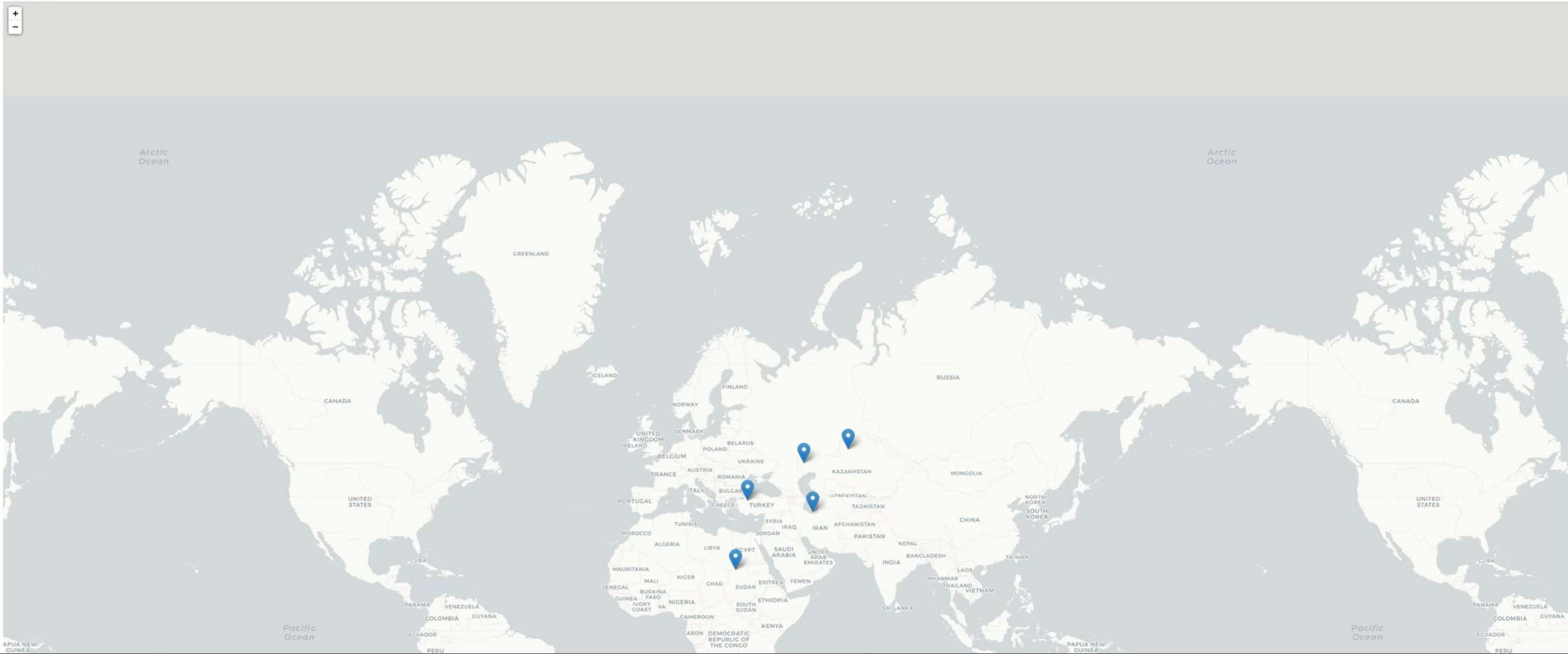
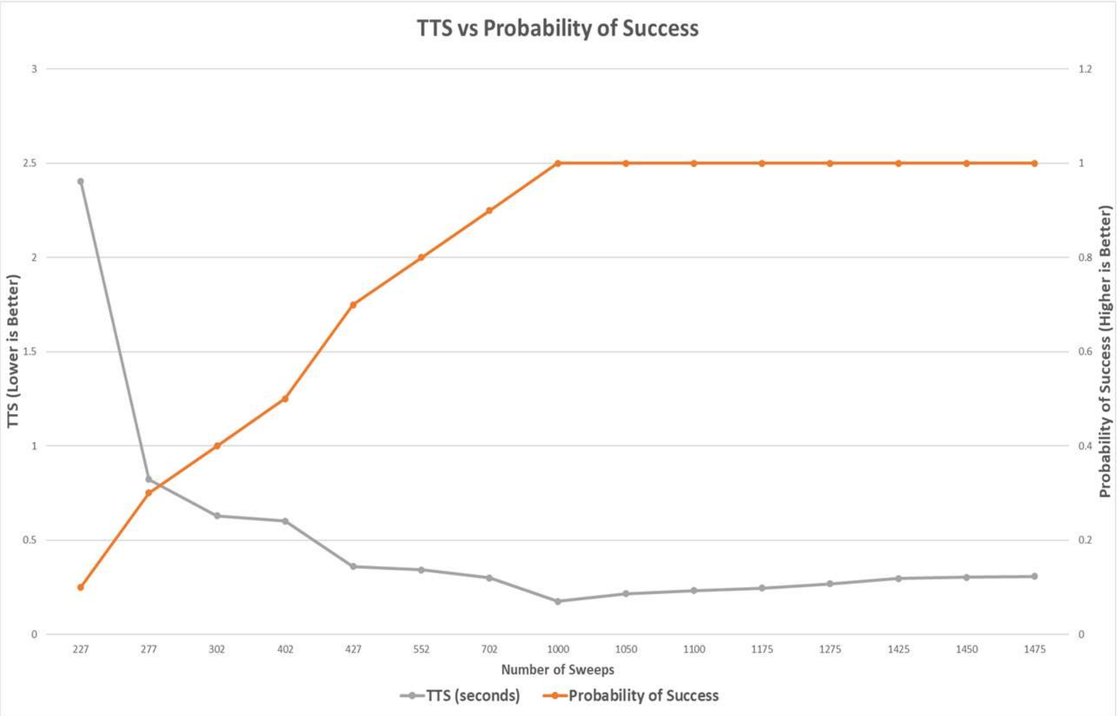
## Drill Plan Optimization using Vector Annealing on Vector Engine

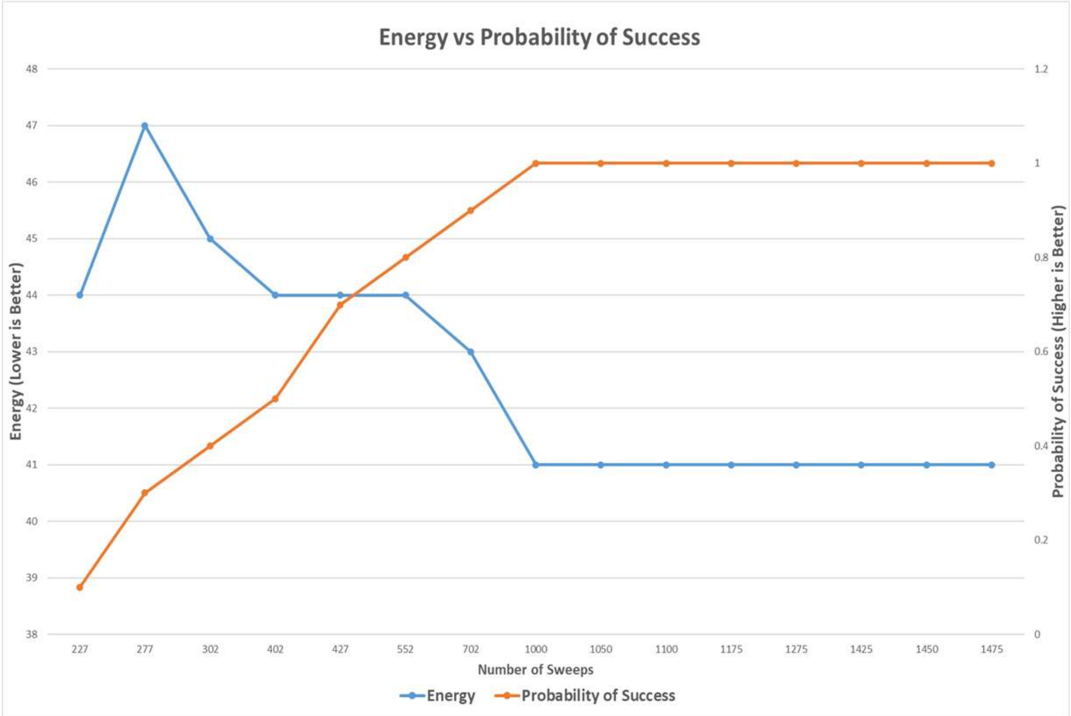
Locations 5



# Oil Field Exploration Demo Result Analysis

- As observed, the increase in the number of sweeps, results in the reduction of the TTS, Energy and increase in the probability of success showing the ideal convergence to the optimum solution.

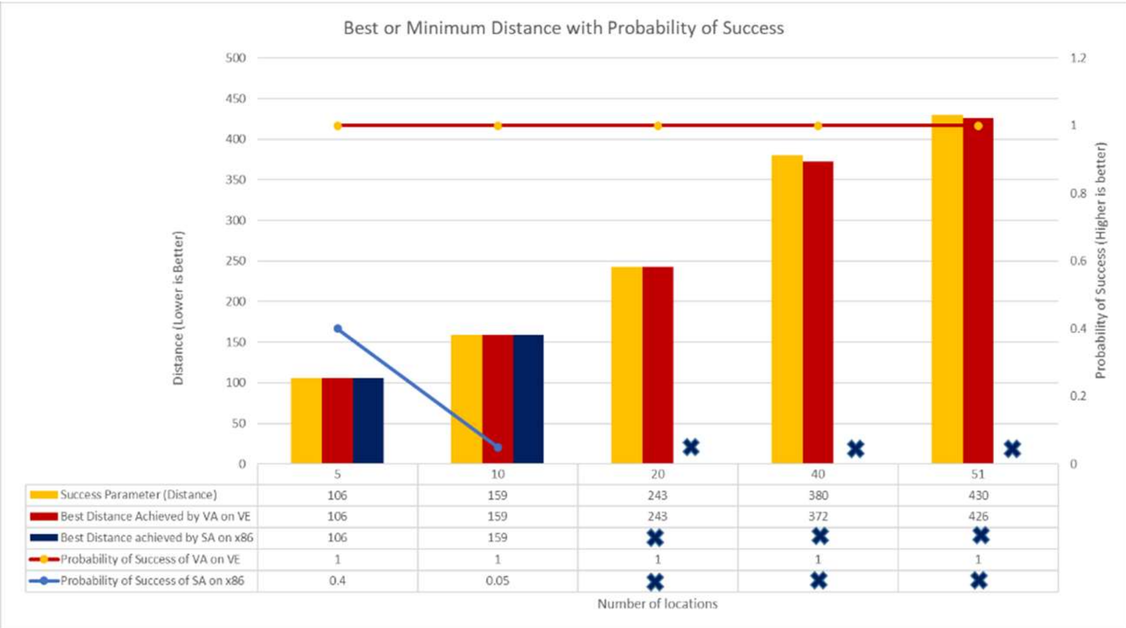


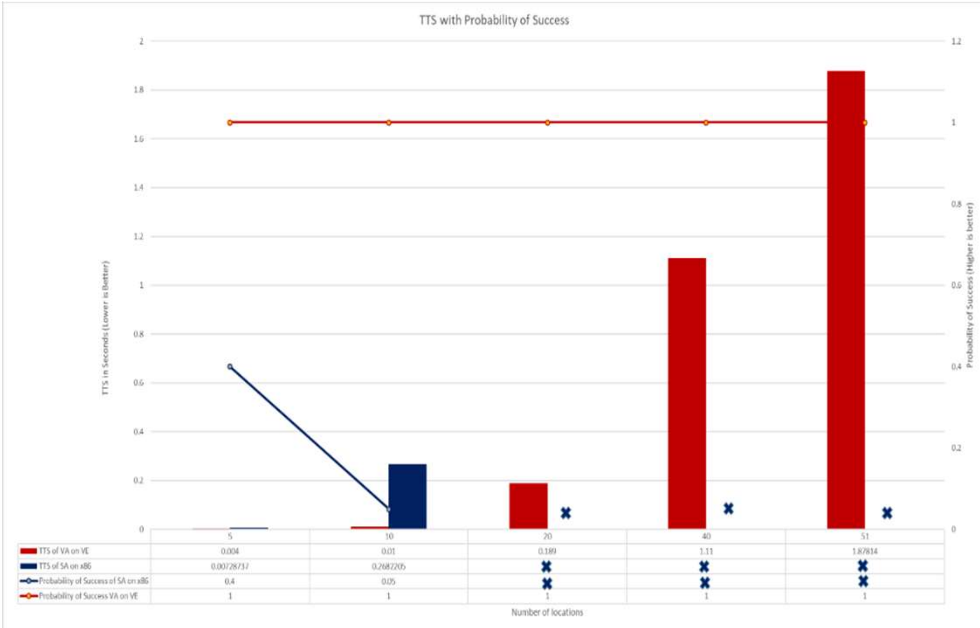




* NEC Internal Evaluations

# Performance Results

- Goal: Achieve minimum TTS with highest probability of Success and highest accuracy.

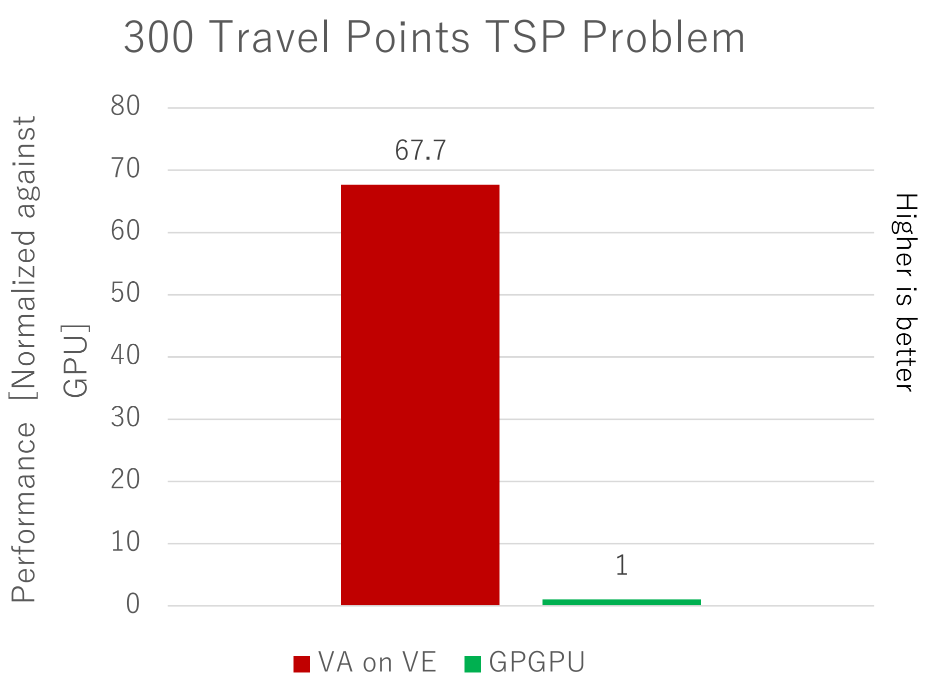



* NEC Internal Evaluations

# Performance Results

- TSP is frequently used to optimize logistics problem.
- For the real-world problem at least 120 to 150 travelling points must be handled.
- For such and even larger cases VA on VE (with flip-options) is much faster than other annealers.
- Number of travel points can be improved by increasing number of variables/bits over multiple cards using MPI such as in VA on VE.

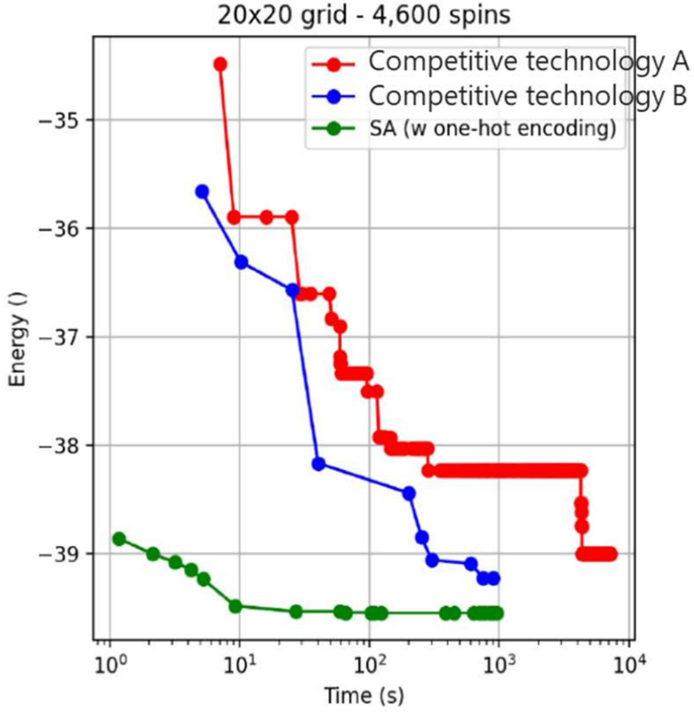



* According to a survey by NEC

# PoC Case History

- Completed PoC with software company in US focusing on energy resource exploration optimization problem.

- VA on Vector Engine Accelerator with external constraints like one-hot encoding provided best results in comparison to other ISV SA software running on classical computers as well as accelerators.




NEC achieved lowest energy with shortest time

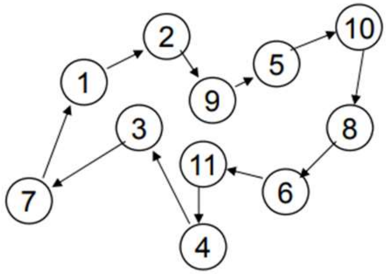
# Expectation for Quantum Annealing

## Faster solving combination optimization problems than mathematical approaches

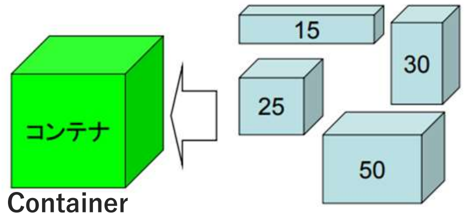
Combination Optimization Problems:
To find a combination which provides max/min value of an evaluation function from huge number of combinations with satisfying constraints

### Typical problems

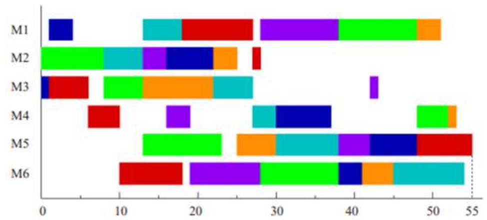
- Travelling Salesman Problem
- Knapsack Problem
- Job Shop Problem
- Work Shift Problem



Travelling Salesman



Knapsack

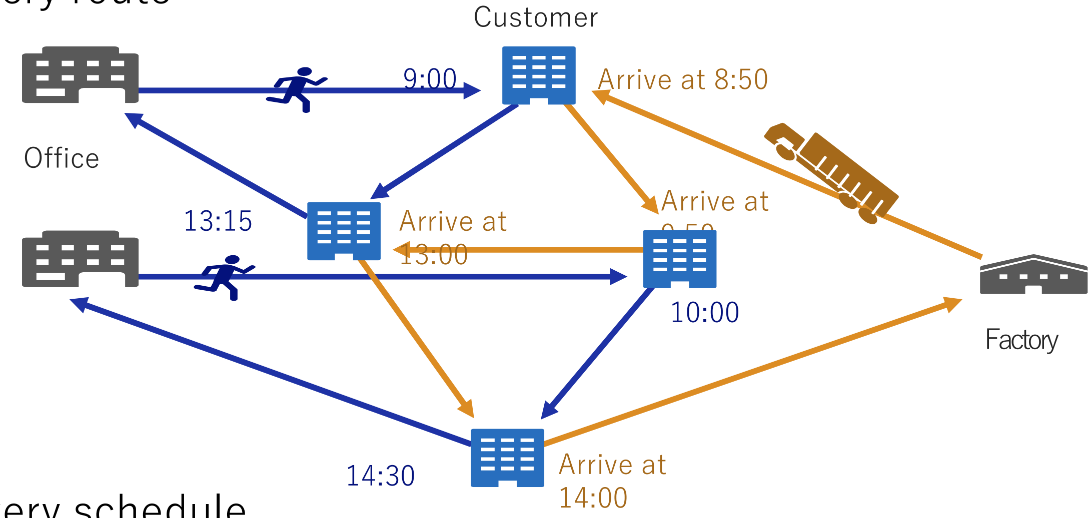


Job Shop

# Delivery Route and Schedule Optimization

## Optimizing Delivery Route and Schedule for costs, time and energy reduction

delivery route

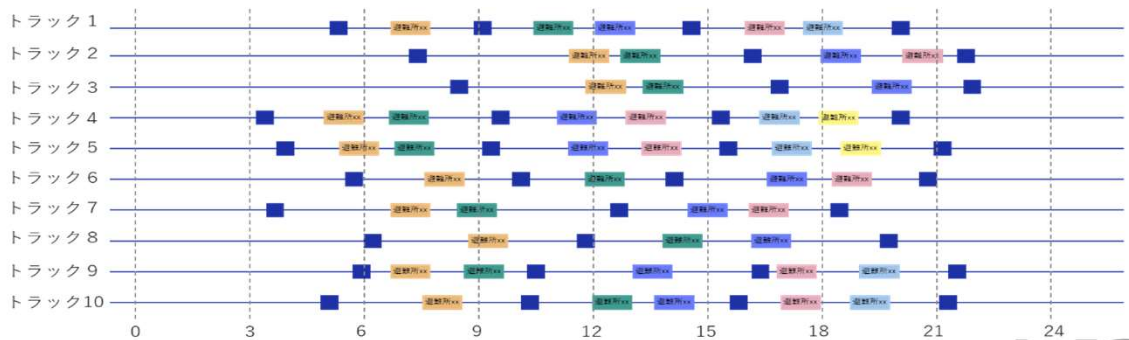



EX.

### Delivery of parts and dispatch of Engineers

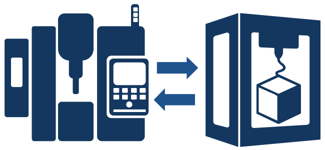
- Parts are delivered by truck
- Engineers move by car/train
- Have to consider skills of each engineer

delivery schedule



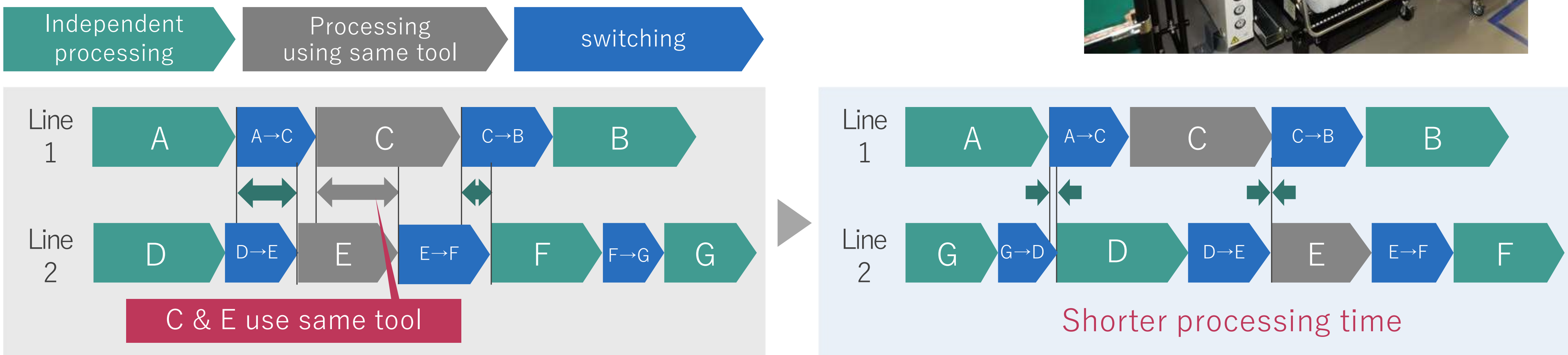
# Production Planning Optimization

## Optimizing complex planning for multi-product production lines



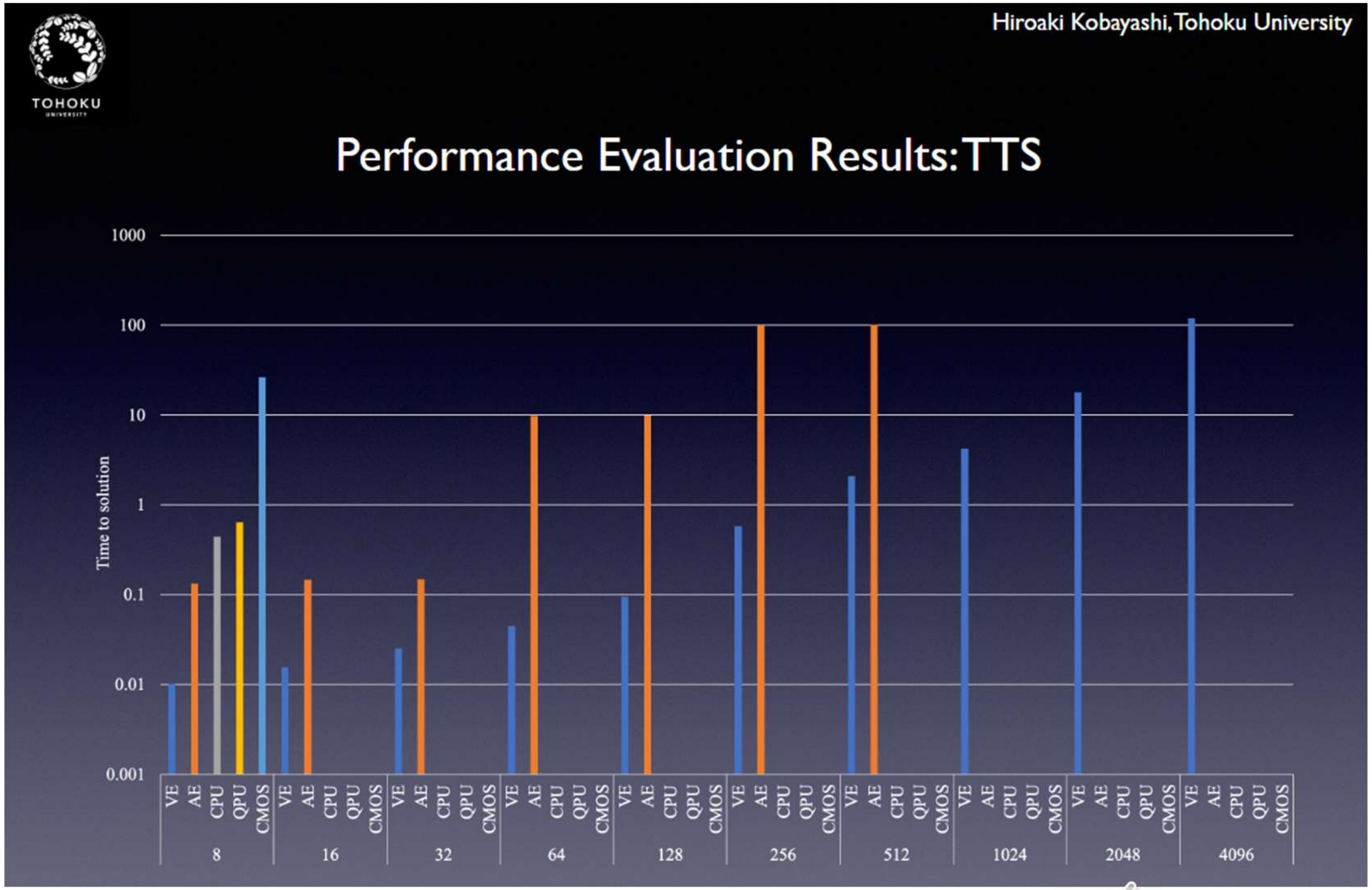
Higher versatile processing equipment needs
highly optimized product planning for higher efficiency

- Switching processed product makes idling time of equipment
- Production planning can reduce the idling time



# Benchmark (Clustering)

Evaluated by Tohoku University
Reference: 33rd WSSP Workshop, May 2022




## Benchmark Program

Clustering of test data (8~4096) into 3 clusters
100 trials

## Platforms

| | | |
|---|---|---|
| ■ | NEC Vector Annealer | (Aurora VE) |
| ■ | Fixstars Amplify AE | (GPGPU) |
| ■ | D-Wave Neal SA | (Xeon Gold 6126) |
| ■ | D-Wave Leap QA | (QPU) |
| ■ | Hitachi CMOS Annealer | (Dedicated device) |

## Results:

**VA provides the highest performance compared to latest annealers**

Small data: VA is the fastest
Medium data: VA > AE on GPU
Large data: Only VA works

# Solving social issues using quantum computing

| Advertisement/ Utilities/ Infrastructure | Manufacturing | Transportation/ Logistics | Financial | Material Development/ Drug Discovery |
|---|---|---|---|---|
| - Matching and recommendation | - Production planning | - Crew scheduling | - Card fraud detection | - Screening |
| - Base station control | - Order planning for parts | - Delivery planning | - Monte Carlo simulation | - Experimental parameter search |
| - Surveillance sensor control | - Sophisticated SI | - Cargo layout | - Risk calculation and data completion | |

* Includes systems in ranges of stages from research to customer demonstration and practical application

NEC Vector Annealing Service

# Summary and Future Work

- VA on VE can be used to solve real-world and complex, multiple optimization problems which would benefit like demonstrated today for oil field or resource exploration optimization planning problem.

- The python codes developed using SA or VA can be re-used/worked together in hybrid for an actual Quantum Annealing system in future.

- VA is supported for using multiple VE accelerator cards.

- NEC will continue to work on solving more combinatorial optimization problems like, knapsack, scheduling, manufacturing process etc. to provide value to the workflow of oil and gas and other verticals.

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