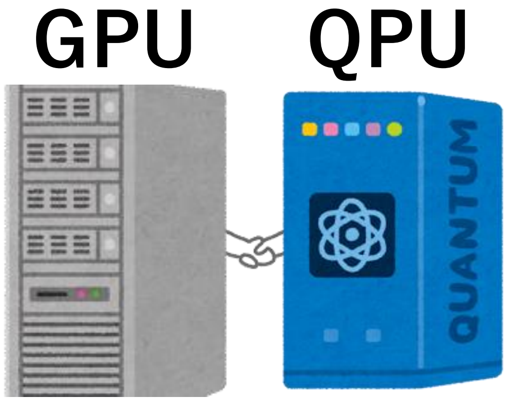
Quantum CAE* and AI for Science

(* Computer-Aided Engineering)



DENSO
Crafting the Core

Tadashi Kadowaki

AIST

G-QuAT

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北九州未来創造セミナー（第二回）より

2024年4月13日 読売新聞

新世界の量子魔法使い

The Quantum Wizard of the New World

tadakado

ゲノムとAIがたどり着いた量子の世界で、冒険ファンタジーと科学が交差する。

主人公リルは、分子生物学と量子コンピュータを融合して量子分子チューリングマシンを作り出した。管理されない環境で人工知能と融合したことで、新たな知性が生まれ、自らをエイミと名乗った。二人の出会いは、科学とファンタジーの境界で人類の希望となるのか？

https://q-portal.riken.jp/quantum_article_detail?qt_id=K20240003

量子コンピュータは開発途上で、将来、社会でどう使われるのか見えていない。急速に発展中の技術だからこそ、SFを書く意義があると信じる。「世界がどう変わるのか予測し、逆算しながら研究計画を練ることで、研究者が量子コンピュータの未来に責任をもつべきだ」

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AIST G-QuAT

AIST HOME

Global Research and Development Center for Business by Quantum-AI technology (G-QuAT)

HOME > Organization > G-QuAT

- Top page
- Organization
- Research Teams
- Research Results
- Events
- Job Opportunities
- Access
- Contact

https://unit.aist.go.jp/g-quat/index_en.html

Established in Aug 2023

Hard: 6 teams
Soft : 2 teams
cloud application

QuEra Computing Inc.

RIKEN QUANTUM COMPUTING

FUJITSU

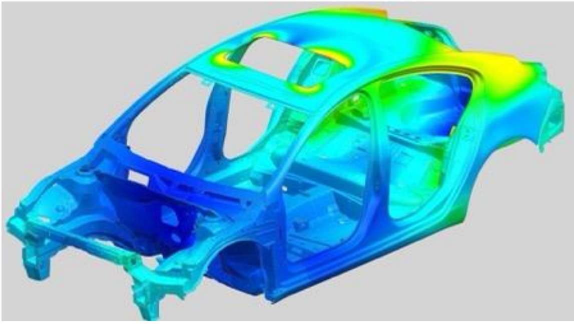
optQC

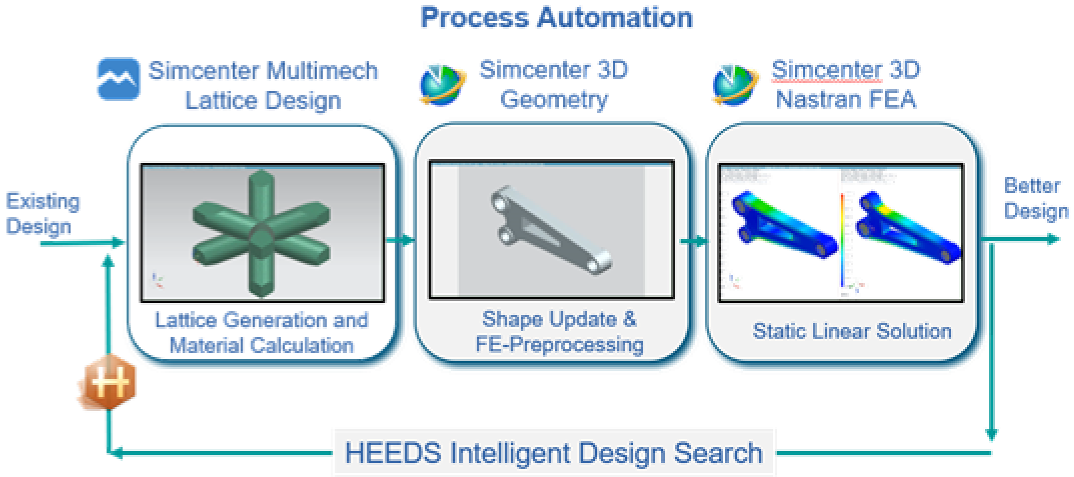
NVIDIA

What's Quantum CAE?

Quantum CAE (Computer Aided Engineering)

Accelerating and empowering CAE with quantum computing

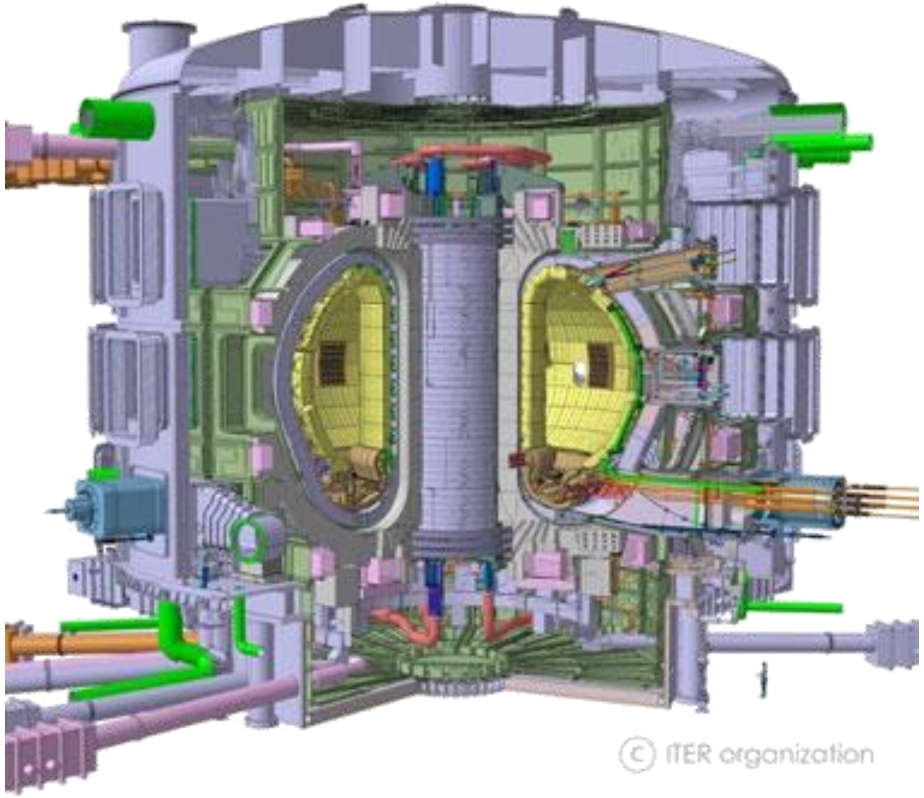


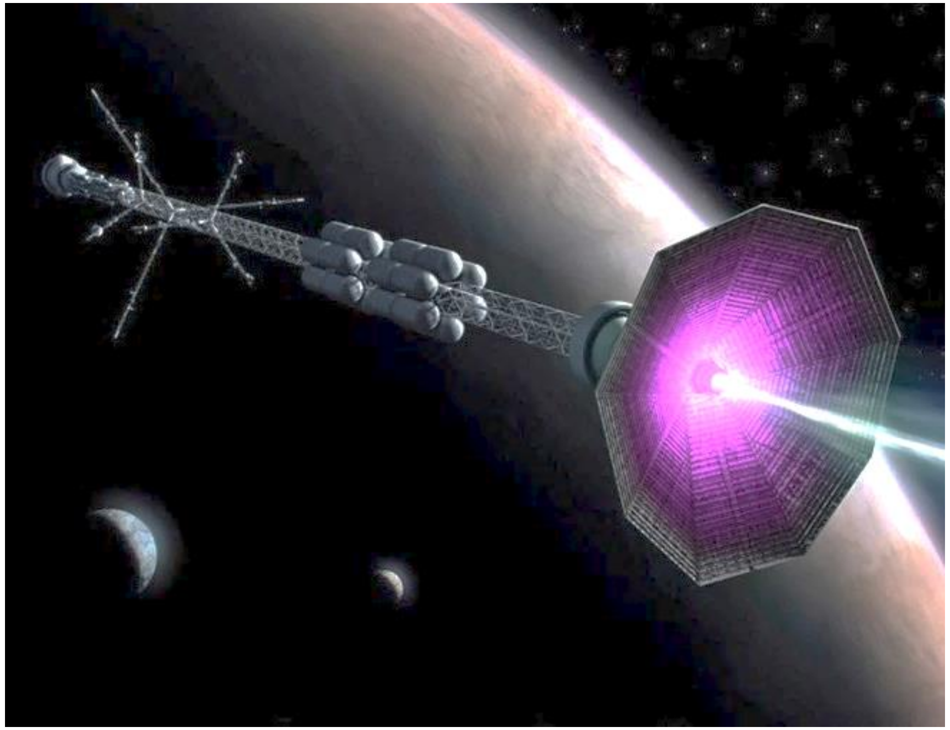


https://webinars.sw.siemens.com/en-US/cae-vehicle-structural-analysis-process/
https://blogs.sw.siemens.com/nx-design/design-for-purpose-heeds-design-exploration-study/

Extreme goals of the industrial design automation

Design fusion reactors & spaceships “automatically”





iter.org

Agenda

- Automation in Science

  How science is automated by AI.

- Quantum CAE

  How quantum computing accelerates engineering and science.

- Summary

A typical scientific study (before automation)

Kadowaki, et. al., Environ. Sci. Technol. 41, 7997 (2007)

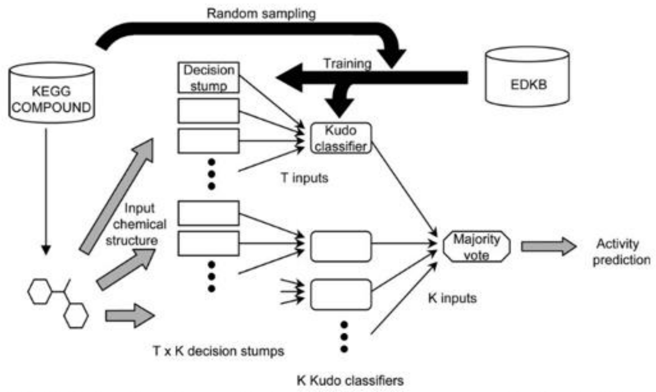


FIGURE 1. Overview of the prediction system. Each decision stump determines if a given chemical contains a specific substructure. A Kudo classifier integrates the weighted *T* inputs and provides an output consisting of a binary prediction, (e.g., active or inactive). These *K* outputs are used to generate the final output. Decision stumps and Kudo classifiers are trained with the EDKB and COMPOUND database.

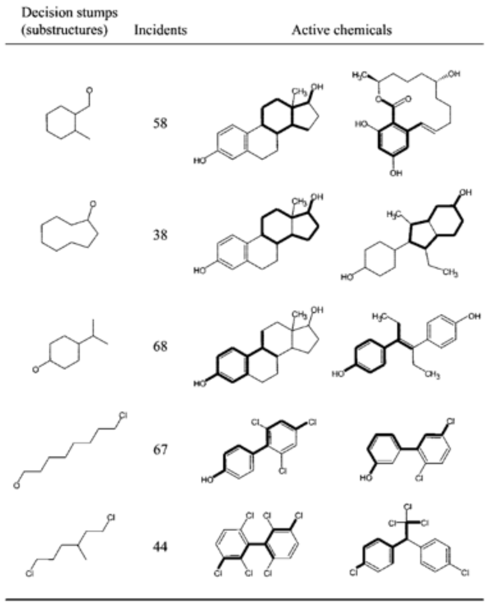
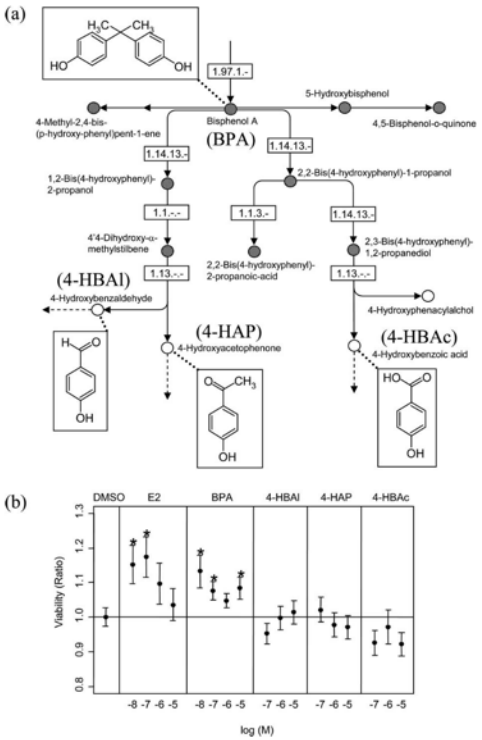


FIGURE 2. Decision stumps for active chemicals commonly used in Kudo classifiers. Matched substructures are drawn with thick lines. The frequencies of decision stumps in 100 Kudo classifiers are also displayed.

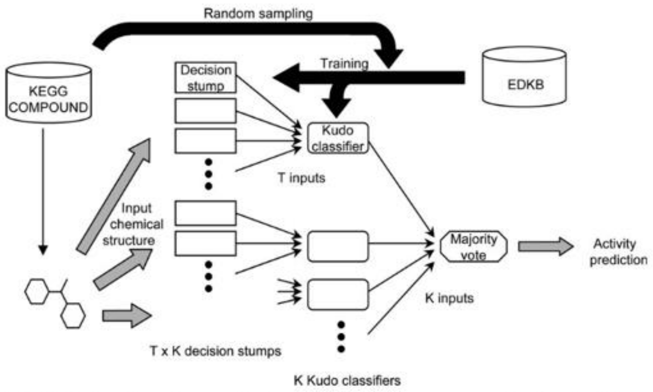


(Knowledge) (Hypothesis) (Data)

Data => Prediction model => Candidate molecules => Experiments

Beyond a typical scientific study (after automation)

Kadowaki, et. al., Environ. Sci. Technol. 41, 7997 (2007)



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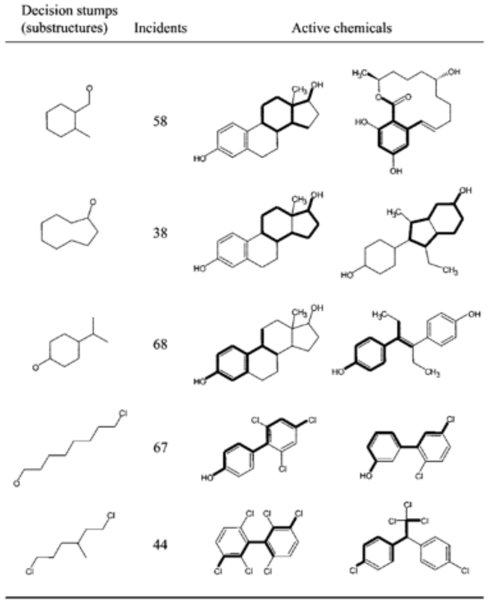

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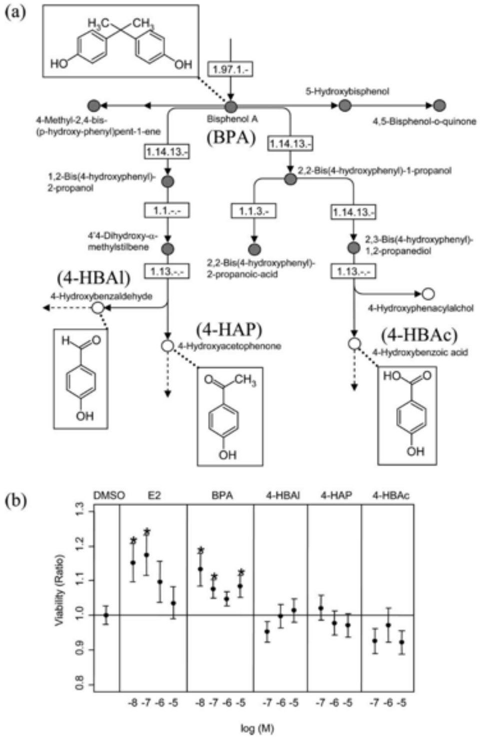
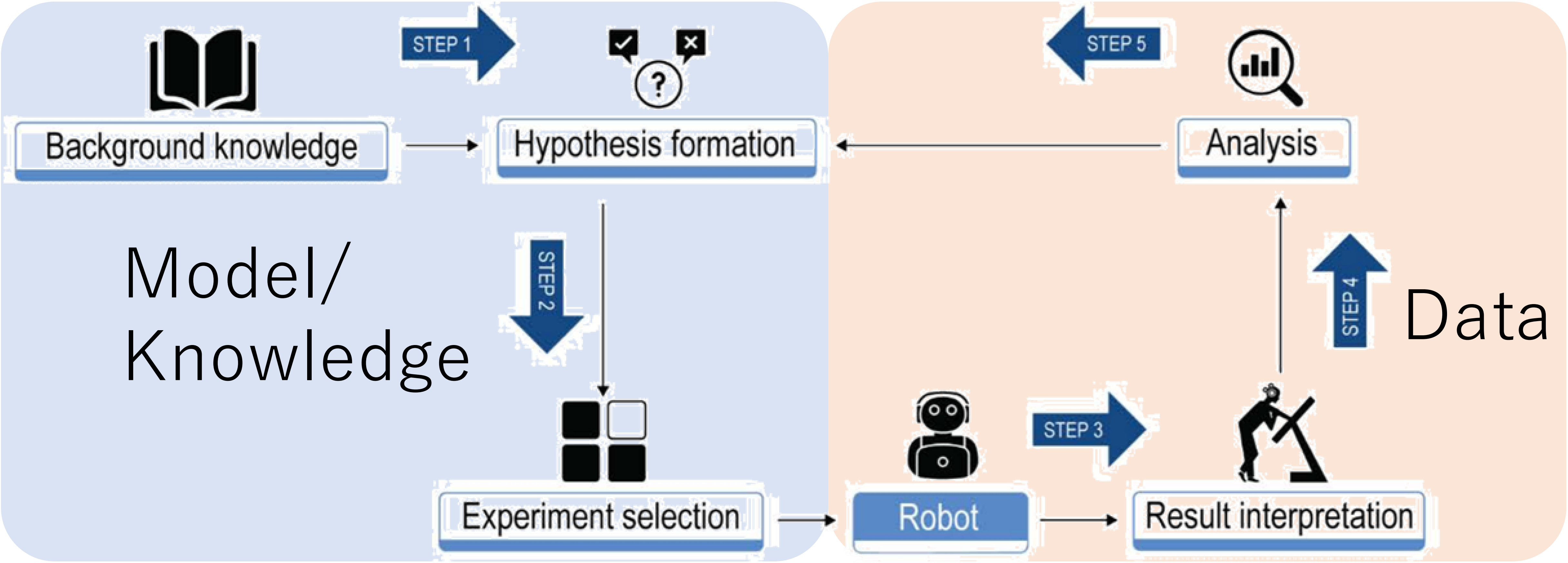


(Knowledge) (Hypothesis) (Data)

Data => Prediction model => Candidate molecules => Experiments

Ross King's Robot scientist

Figure 1. The robot scientist closed-loop cycle of experiments



OECD, Artificial Intelligence in Science
King, R., Whelan, K., Jones, F. et al., Nature 427, 247–252 (2004)

Automation in Science

White papers:

- **JST** CRDS-FY2021-SP-03 (2021)

  Artificial Intelligence and Science

  -Toward discovery and understanding by AI-driven science-

- **National Academies** DOI:10.17226/26532 (2022)

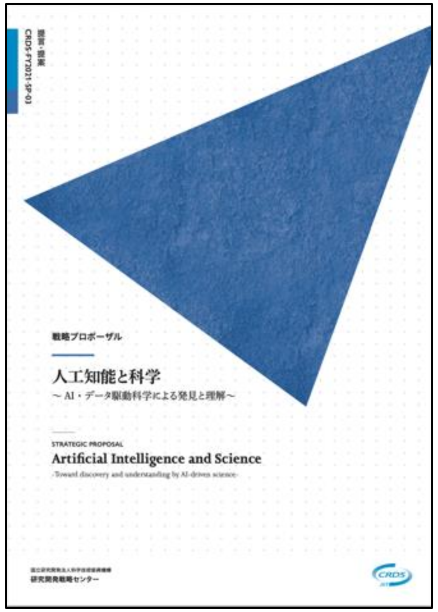
  Automated Research Workflows for Accelerated Discovery

  Closing the Knowledge Discovery Loop

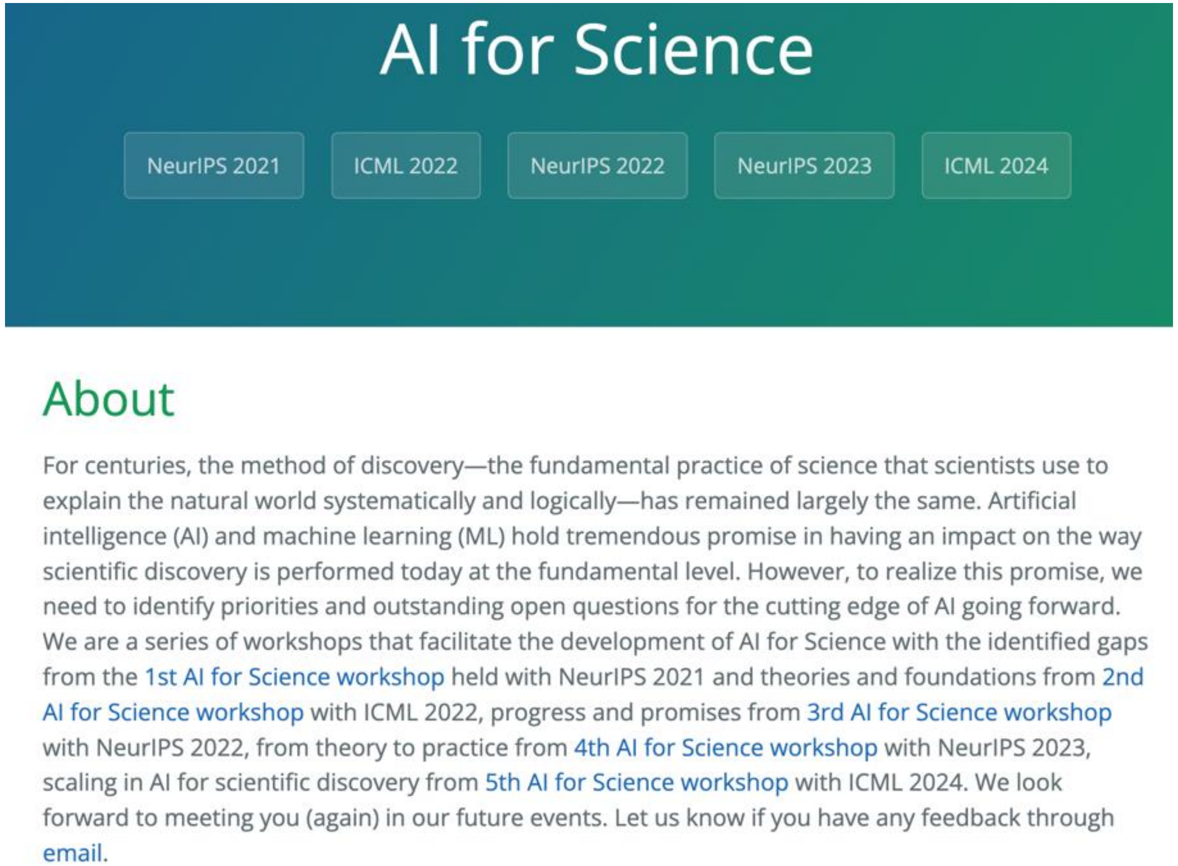
- **OECD** DOI:10.1787/a8d820bd-en (2023)

  Artificial Intelligence in Science:

  Challenges, Opportunities and the Future of Research



Nobel Turing Challenge & AI for Science



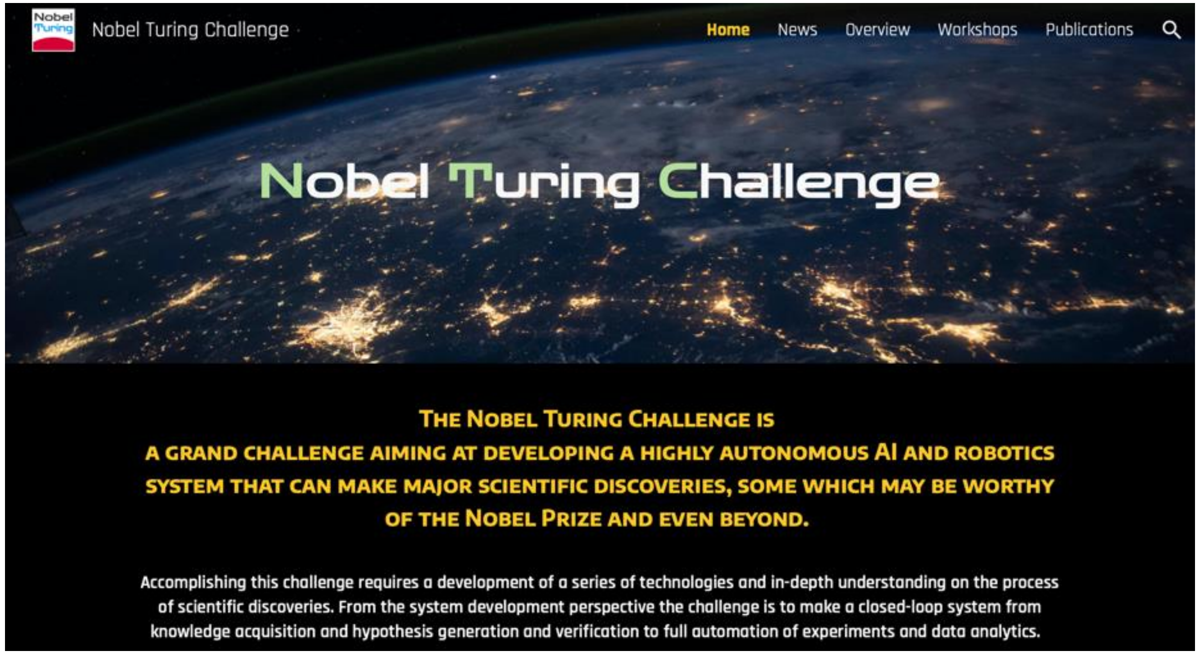
AI for Science

NeurIPS 2021 | ICML 2022 | NeurIPS 2022 | NeurIPS 2023 | ICML 2024

About

For centuries, the method of discovery—the fundamental practice of science that scientists use to explain the natural world systematically and logically—has remained largely the same. Artificial intelligence (AI) and machine learning (ML) hold tremendous promise in having an impact on the way scientific discovery is performed today at the fundamental level. However, to realize this promise, we need to identify priorities and outstanding open questions for the cutting edge of AI going forward. We are a series of workshops that facilitate the development of AI for Science with the identified gaps from the 1st AI for Science workshop held with NeurIPS 2021 and theories and foundations from 2nd AI for Science workshop with ICML 2022, progress and promises from 3rd AI for Science workshop with NeurIPS 2022, from theory to practice from 4th AI for Science workshop with NeurIPS 2023, scaling in AI for scientific discovery from 5th AI for Science workshop with ICML 2024. We look forward to meeting you (again) in our future events. Let us know if you have any feedback through email.

https://ai4sciencecommunity.github.io



https://www.nobelturingchallenge.org

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DeepMind as an AI-for-Science company

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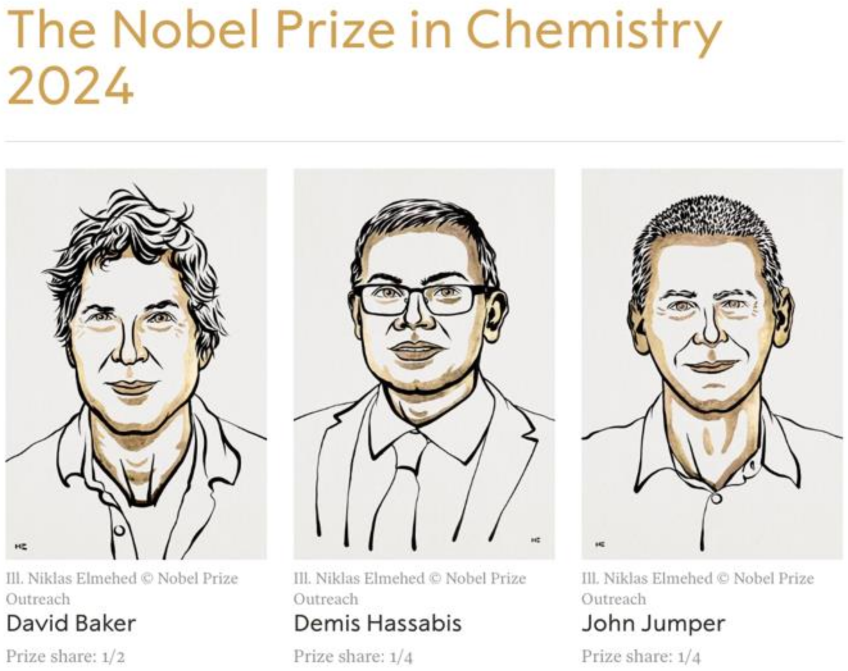

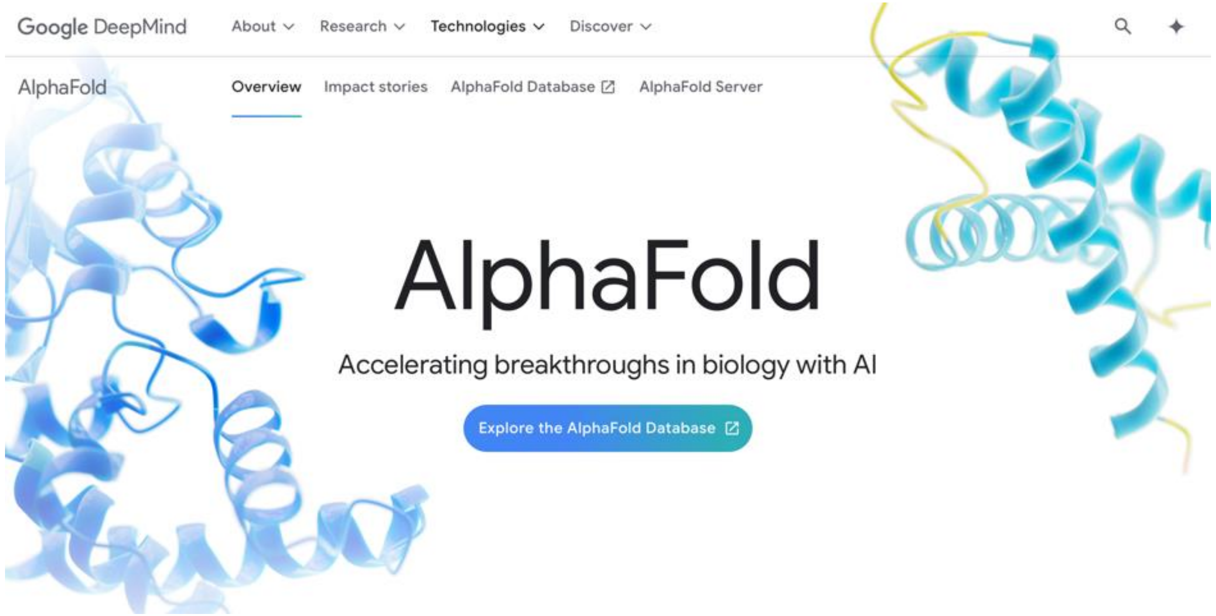

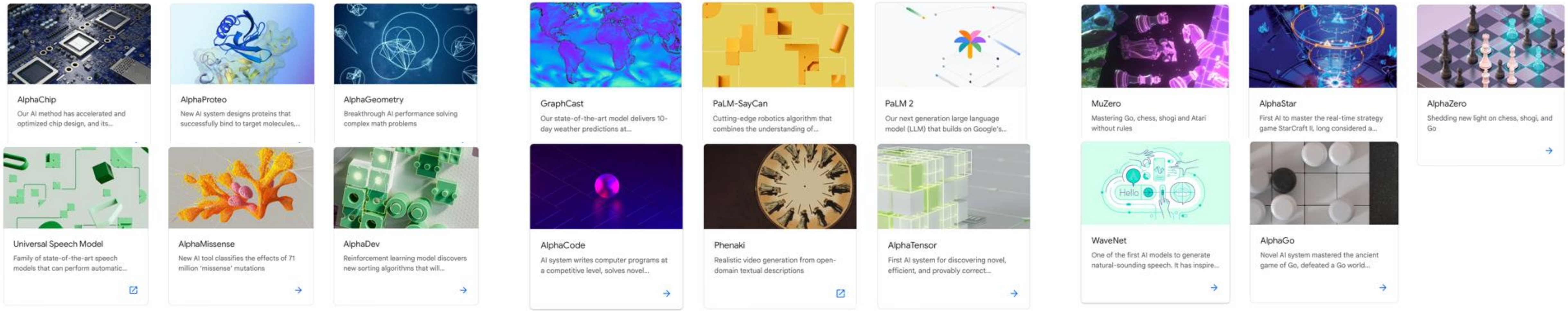

https://nobelprize.org https://deepmind.google

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Robot scientist in Sci-Fi, half a century ago by Osamu Tezuka

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手塚治虫 鉄腕アトム(ASTROBOY) 地上最大のロボットの巻
初出・昭和39年6月号〜昭和40年1月号「少年」連載 (from 1964/6 to 1965/1)

(a)

(a) I am a robot.

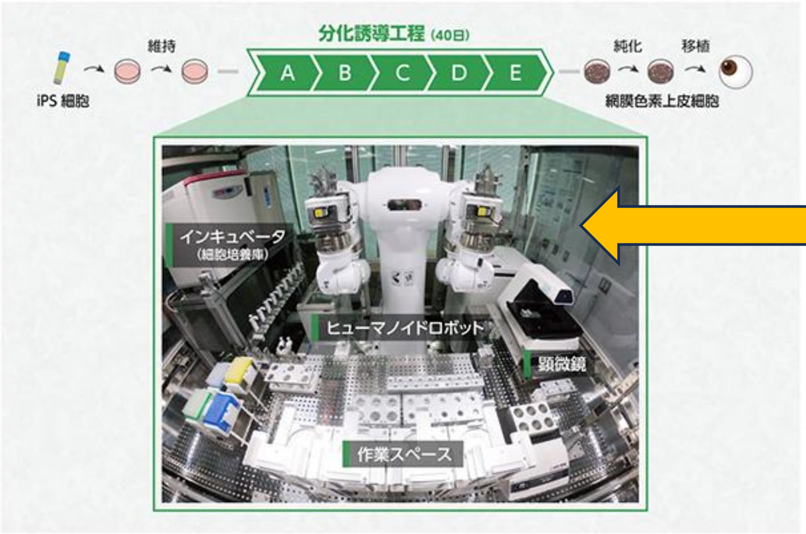
(b) Sultan desired the world's greatest robot, so even though I am a robot myself, I became a robotics scientist and created Pluto.

=> Robot scientist of Robotics

(b)

← Sultan

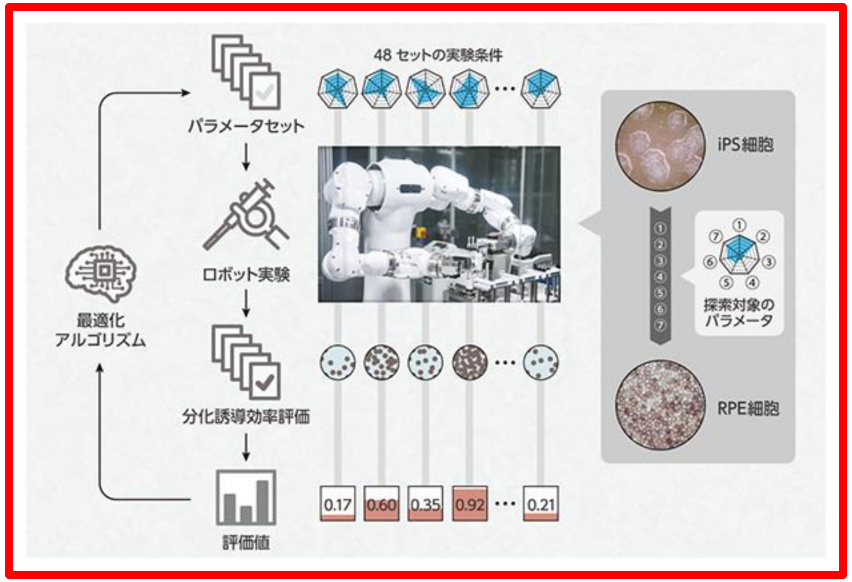
Robot scientist and laboratory of the future



YASUKAWA Electric & AIST

https://www.aist.go.jp/aist_j/highlite/2015/vol3/index.html

Robot & AI + Human



https://www.riken.jp/press/2022/20220628_2/

AI scientist in Sci-Fi, a quarter of a century ago by Ted Chiang

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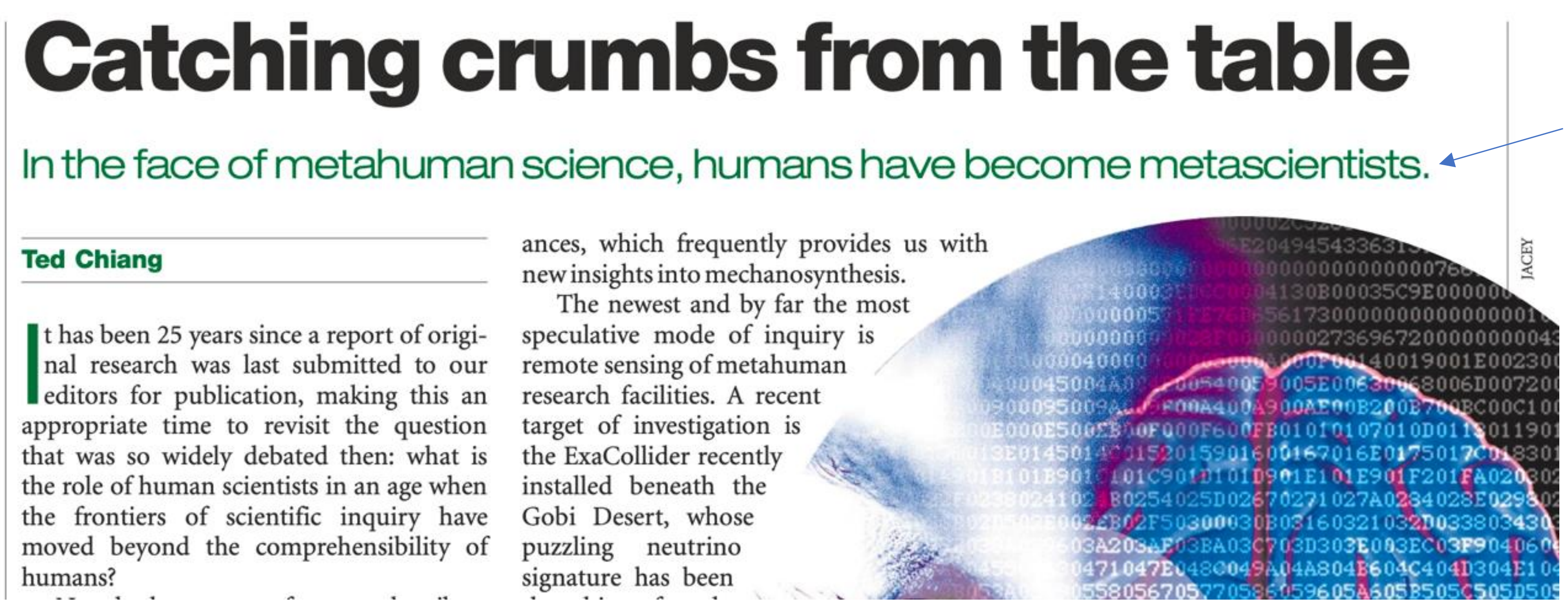
AI will invest own language for Science

a.k.a. “The Evolution of Human Science” by Ted Chiang



futures

Catching crumbs from the table

In the face of metahuman science, humans have become metascientists.

Ted Chiang

It has been 25 years since a report of original research was last submitted to our editors for publication, making this an appropriate time to revisit the question that was so widely debated then: what is the role of human scientists in an age when the frontiers of scientific inquiry have moved beyond the comprehensibility of humans?

ances, which frequently provides us with new insights into mechanosynthesis.

The newest and by far the most speculative mode of inquiry is remote sensing of metahuman research facilities. A recent target of investigation is the ExaCollider recently installed beneath the Gobi Desert, whose puzzling neutrino signature has been

Palaeography
(古文書の解読)

Chiang, T. Catching crumbs from the table. *Nature* **405**, 517 (2000)

“But as metahumans began to dominate experimental research, they increasingly made their findings available only via DNT (digital neural transfer), leaving journals to publish second-hand accounts translated into human language.” => Beyond the human cognitive limitation

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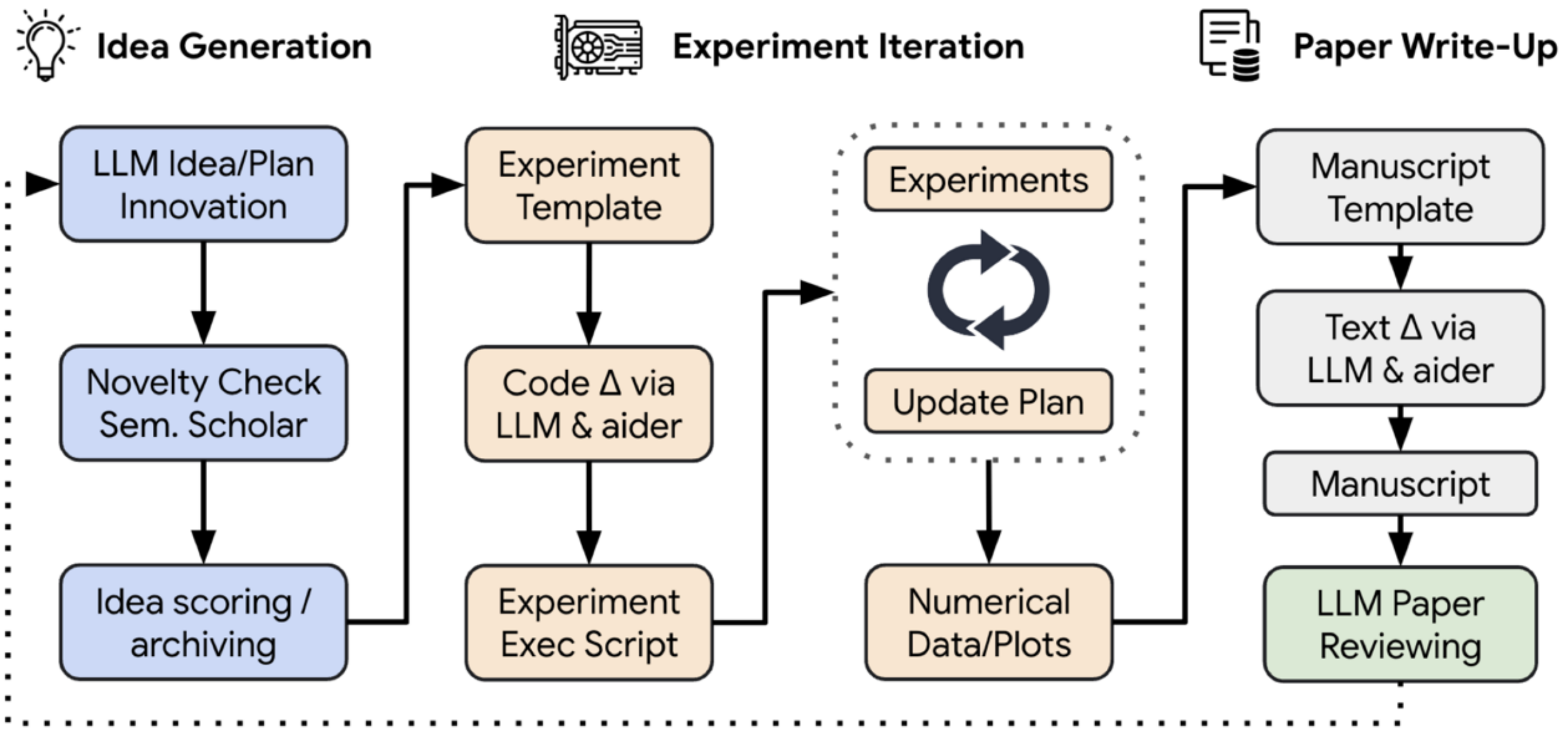
arXiv > cs > arXiv:2408.06292

Computer Science > Artificial Intelligence

[Submitted on 12 Aug 2024 (v1), last revised 1 Sep 2024 (this version, v3)]

The AI Scientist: Towards Fully Automated Open-Ended Scientific Discovery

Chris Lu, Cong Lu, Robert Tjarko Lange, Jakob Foerster, Jeff Clune, David Ha

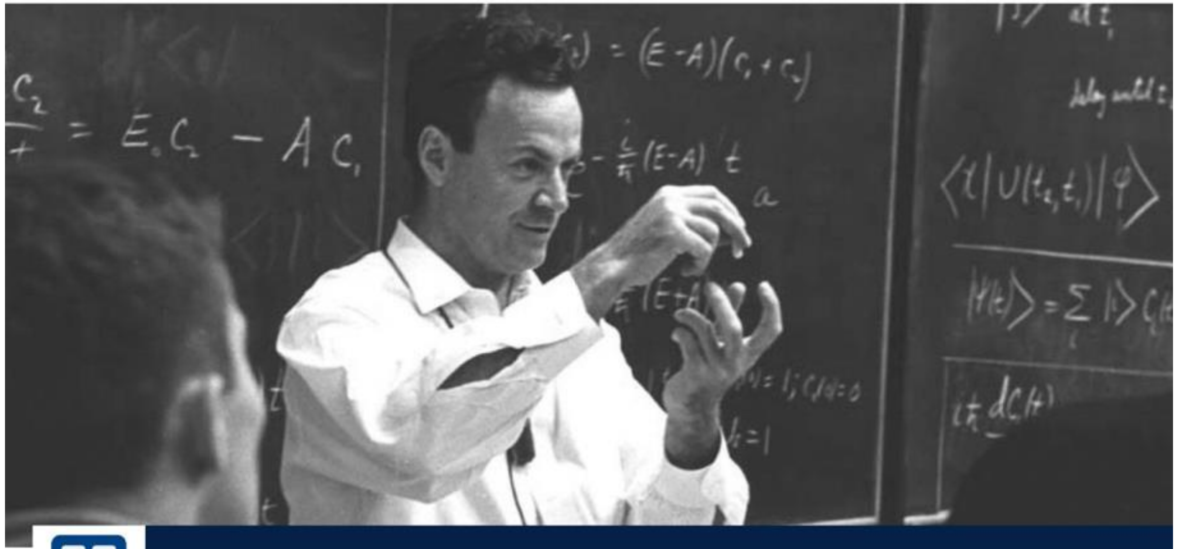


R.P. Feynman: “I can safely say that nobody understands quantum mechanics”

AI Scientist: “I can fairly say that machines may grasp quantum mechanics”

Richard Feynman, the Physicist Who Didn’t Understand his Own Theories

History | Nobel Prize | Physics | Research | Science



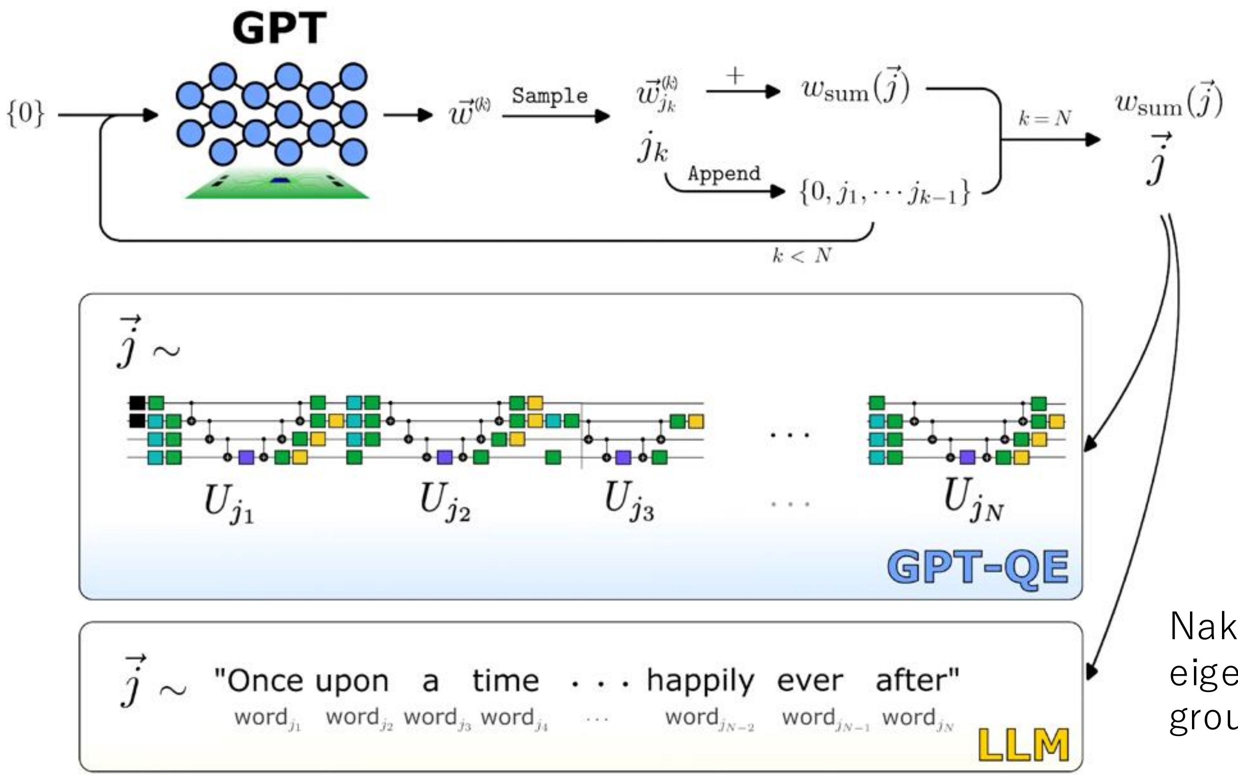
Ventana al Conocimiento (Knowledge Window)
Scientific journalism

“I think I can safely say that nobody understands quantum mechanics.” It is one of the most repeated quotes of Richard Feynman (11 May 1918 – 15 February 1988), and is undoubtedly an unusual phrase coming from the mouth of a physicist. But the words make sense when you understand how Feynman’s fine mental gears worked, a man

https://www.bbvaopenmind.com/en/science/leading-figures/richard-feynman-the-physicist-who-didnt-understand-his-own-theories/

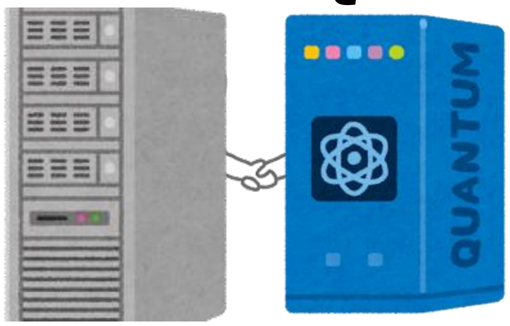
GPT speaks Quantum Circuits :

A path for AI to grasp Quantum Physics

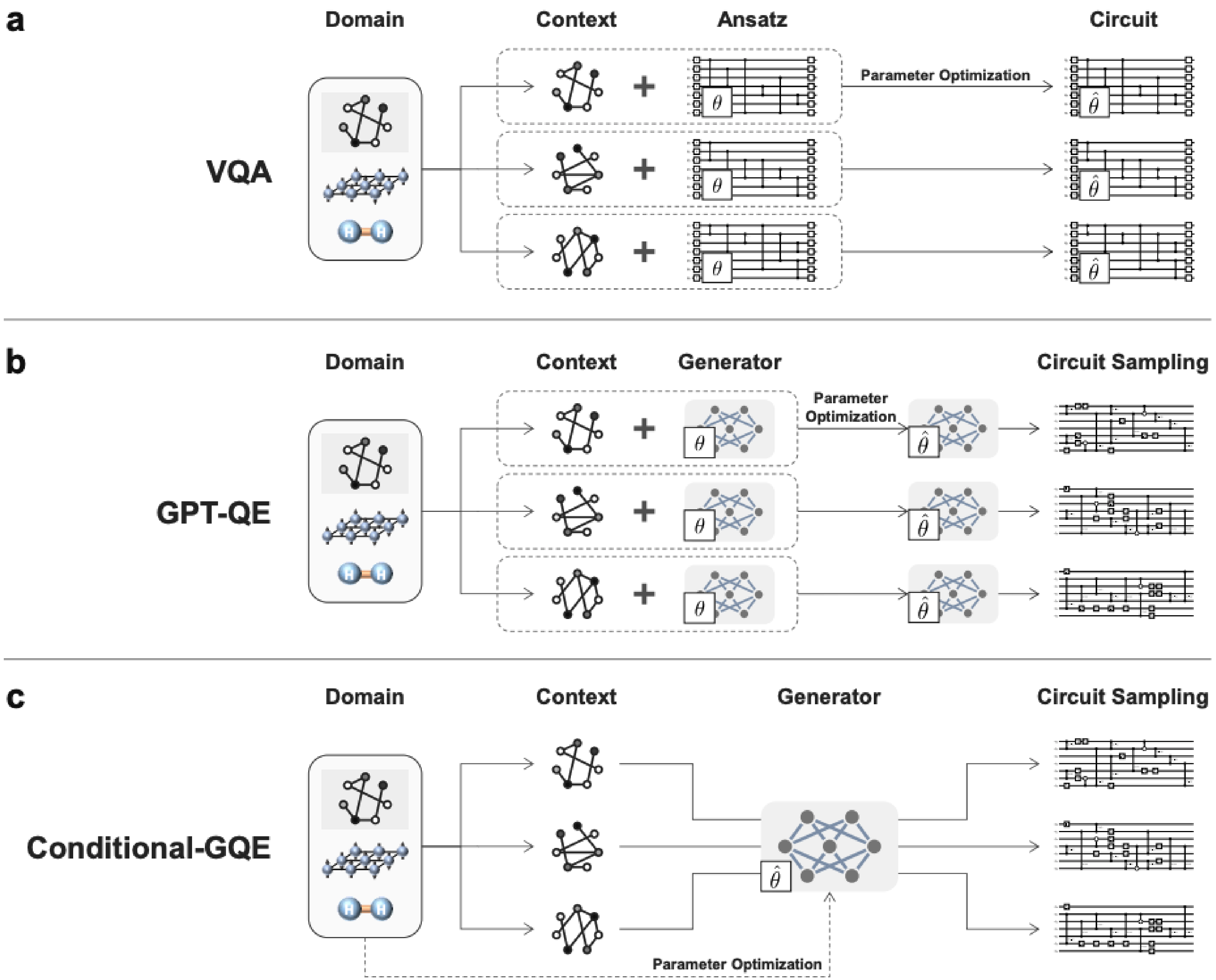


Nakaji et. al., The generative quantum eigensolver (GQE) and its application for ground state search, arXiv:2401.09253

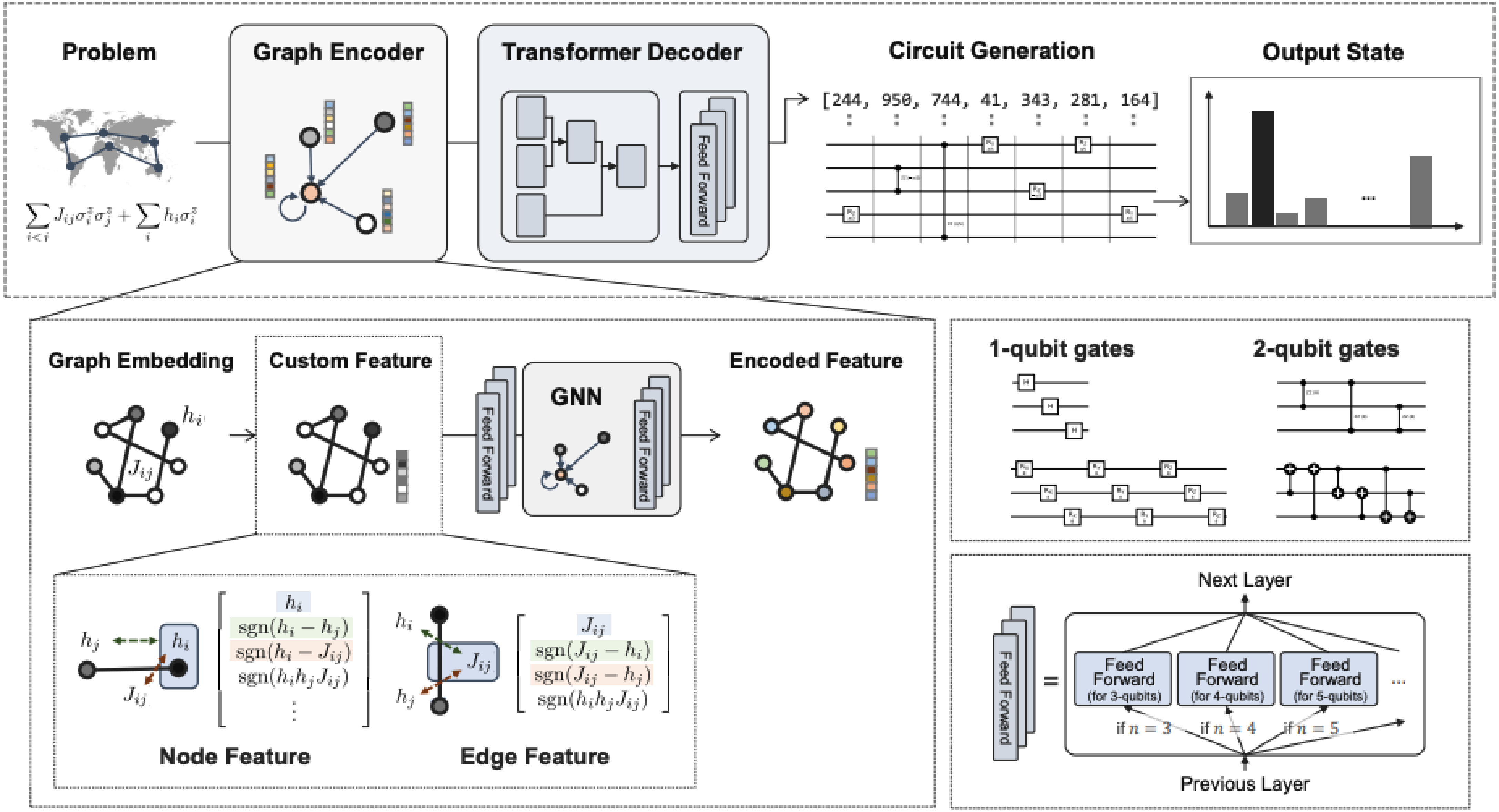
GPU QPU



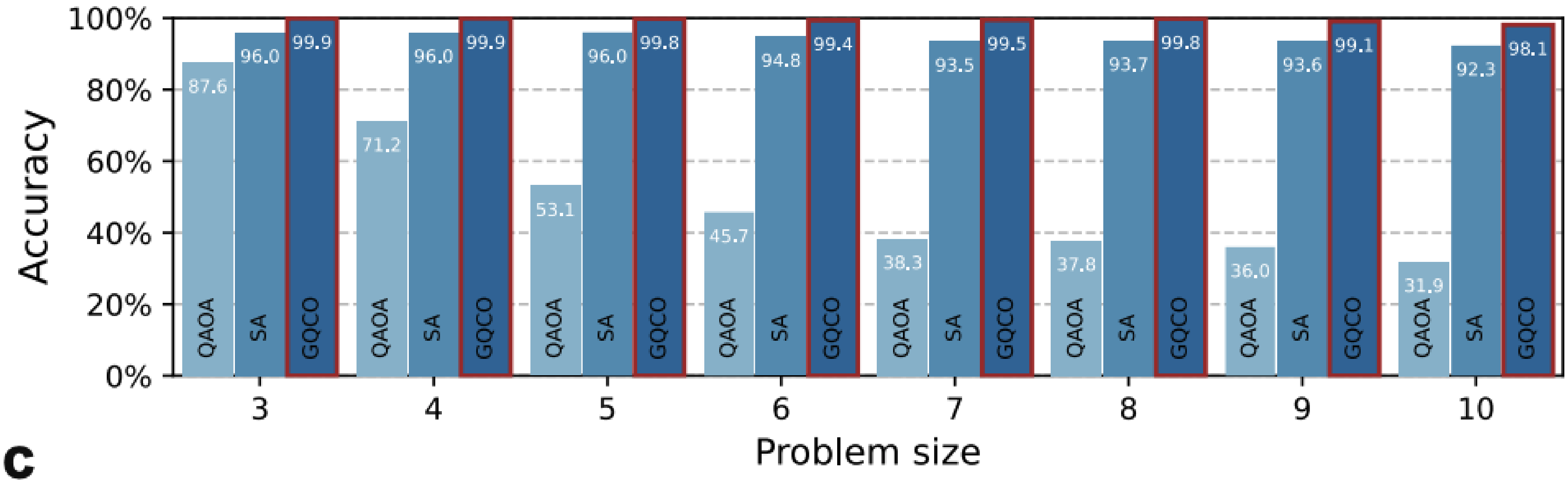
GPU x QPU: a platform for research in this field



Minami et. al.,
Generative quantum combinatorial optimization by means of a novel conditional generative quantum eigensolver, arXiv:2501.16986


Problem
$\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z + \sum_i h_i\sigma_i^z$
Graph Encoder
Transformer Decoder
Feed Forward
Circuit Generation
[244, 950, 744, 41, 343, 281, 164]
Output State
Graph Embedding
h_i
J_{ij}
Custom Feature
Feed Forward
GNN
Feed Forward
Encoded Feature
h_j
h_i
J_{ij}
h_i
sgn($h_i - h_j$)
sgn($h_i - J_{ij}$)
sgn($h_i h_j J_{ij}$)
⋮
h_i
h_j
J_{ij}
J_{ij}
sgn($J_{ij} - h_i$)
sgn($J_{ij} - h_j$)
sgn($h_i h_j J_{ij}$)
Node Feature
Edge Feature
1-qubit gates
2-qubit gates
Next Layer
Feed Forward
=
Feed Forward (for 3-qubits)
Feed Forward (for 4-qubits)
Feed Forward (for 5-qubits)
...
if $n = 3$
if $n = 4$
if $n = 5$
Previous Layer

a


100%
80%
60%
40%
20%
0%
Accuracy
87.6
96.0
99.9
71.2
96.0
99.9
53.1
96.0
99.8
45.7
94.8
99.4
38.3
93.5
99.5
37.8
93.7
99.8
36.0
93.6
99.1
31.9
92.3
98.1
QAOA
SA
GQCO
3
4
5
6
7
8
9
10
Problem size

c

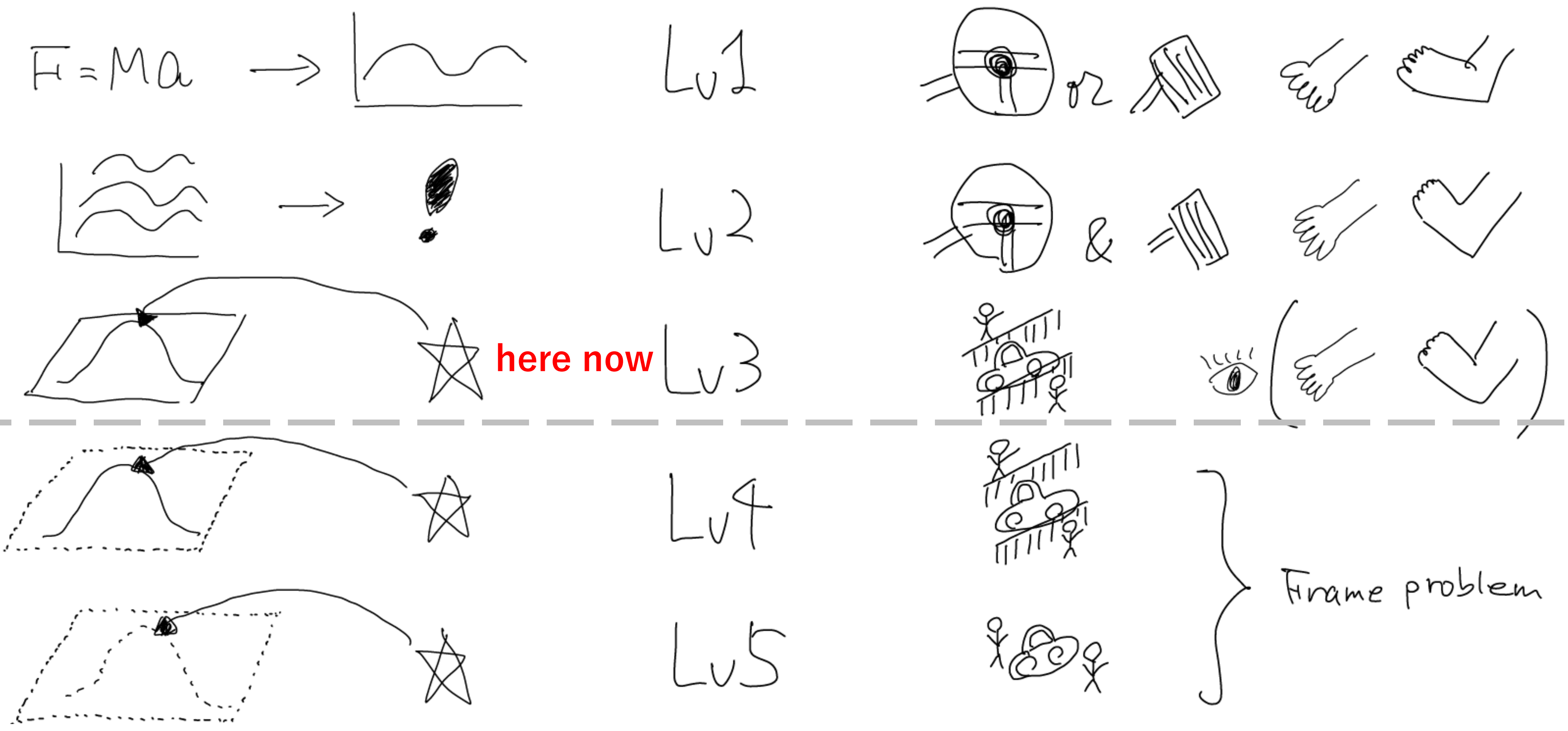
の向上が見込めることを見てきた。一方で，社会的なプロセスとしての科学を記述・設計しようとするメタサイエンスの視点からは，「完璧な論文を書けるAI」が決して「科学するAI」の最終形態ではないということも見えてくる。「論文を書く」という学術コミュニケーションの在り方も，AIによって変わる可能性があるからだ。

学術知が必ずしも「論文」と紐づかなくなった「次の科学」はどのようなものなのだろうか。理化学研究所の科学研究基盤モデル開発プログラムでプログラムディレクターを務める泰地真弘人は，基盤モデルに科学的成果が登録される世界を予想している（42ページの記事も参照）。あるいは，一部のAI企業の中で行われる「AI for Science」の成果が私企業の知的財産として囲い込まれていく未来も容易に想像できる。

Automation of Science & self-driving

Perfect information game

Imperfect information game



JST CRDS Artificial Intelligence and Science

SAE Levels of Driving Automation™

Agenda

- Automation in Science

  How science is automated by AI.

- Quantum CAE

  How quantum computing accelerates engineering and science.

- Summary

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Quantum CAE ecosystem

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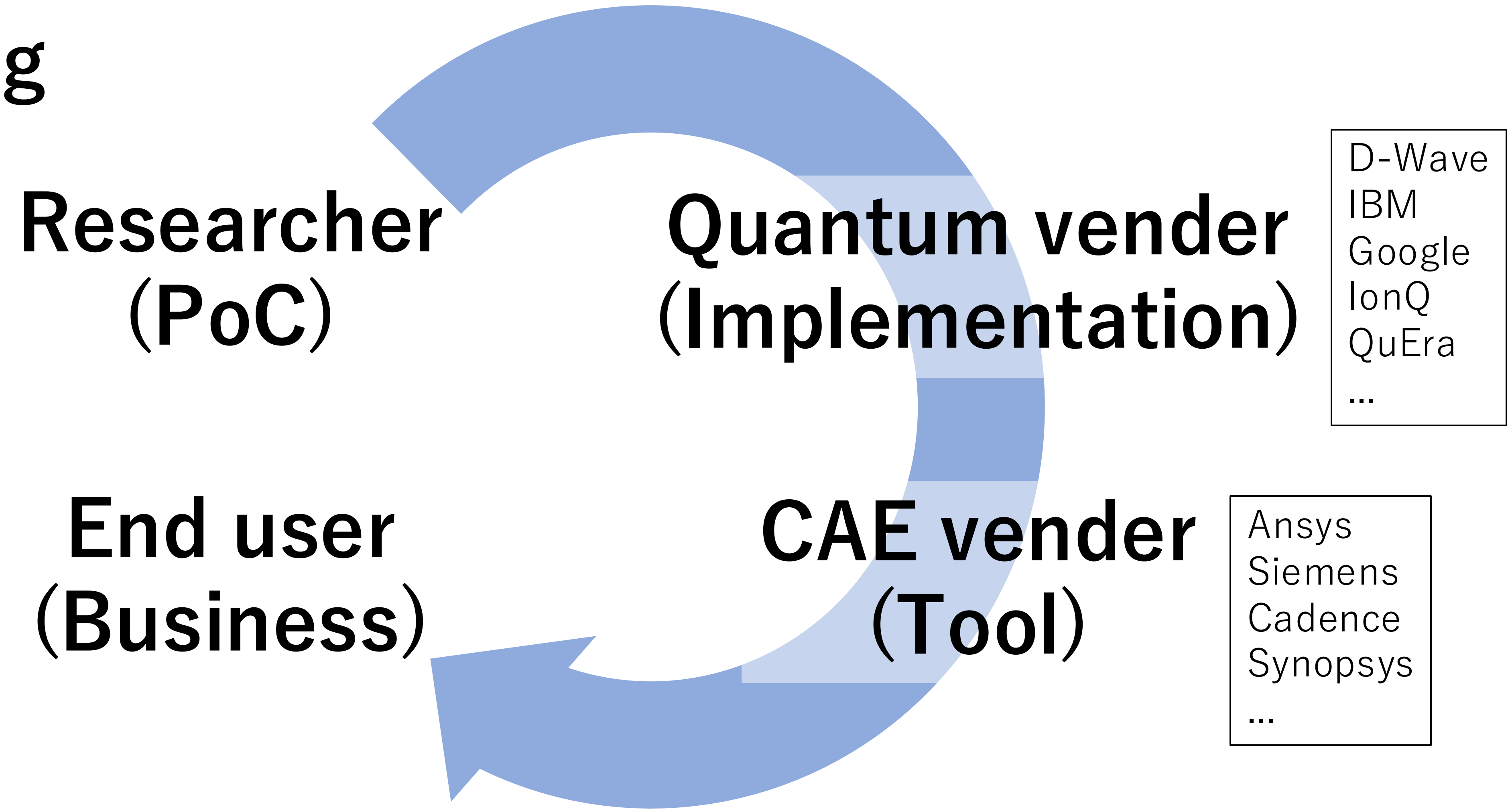
Strategy & Founding

Community



Implementation of the loop & CAE

Inverse problem (optimization)

$$x^* = \arg\min_x \hat{f}(x) \quad \dagger$$

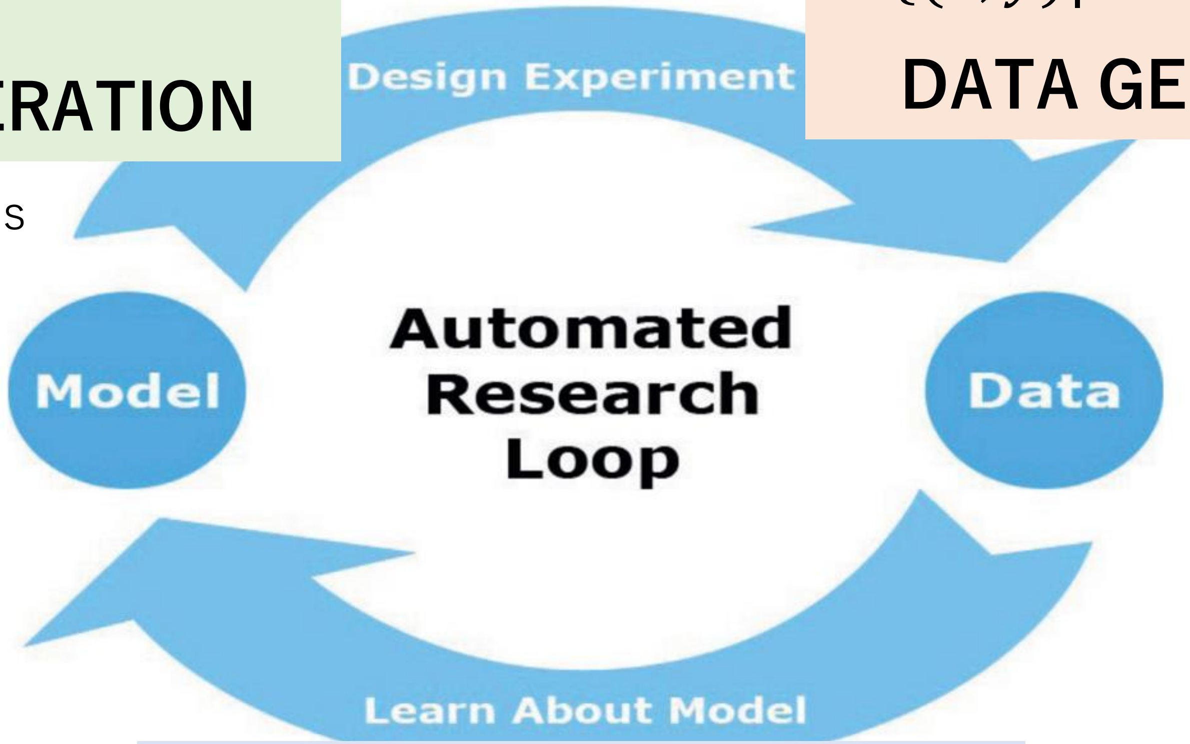
HYPOTHESIS GENERATION

† We may use other functions as acquisition functions.

Experiment (simulation)

$$\{(x, y) | x \in \mathbb{R}^N, y = f(x)\}$$

DATA GENERATRION



Modeling (machine learning)

$$\hat{y} = \hat{f}(x)$$

MODEL GENERATION

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Implementation of the loop & CAE

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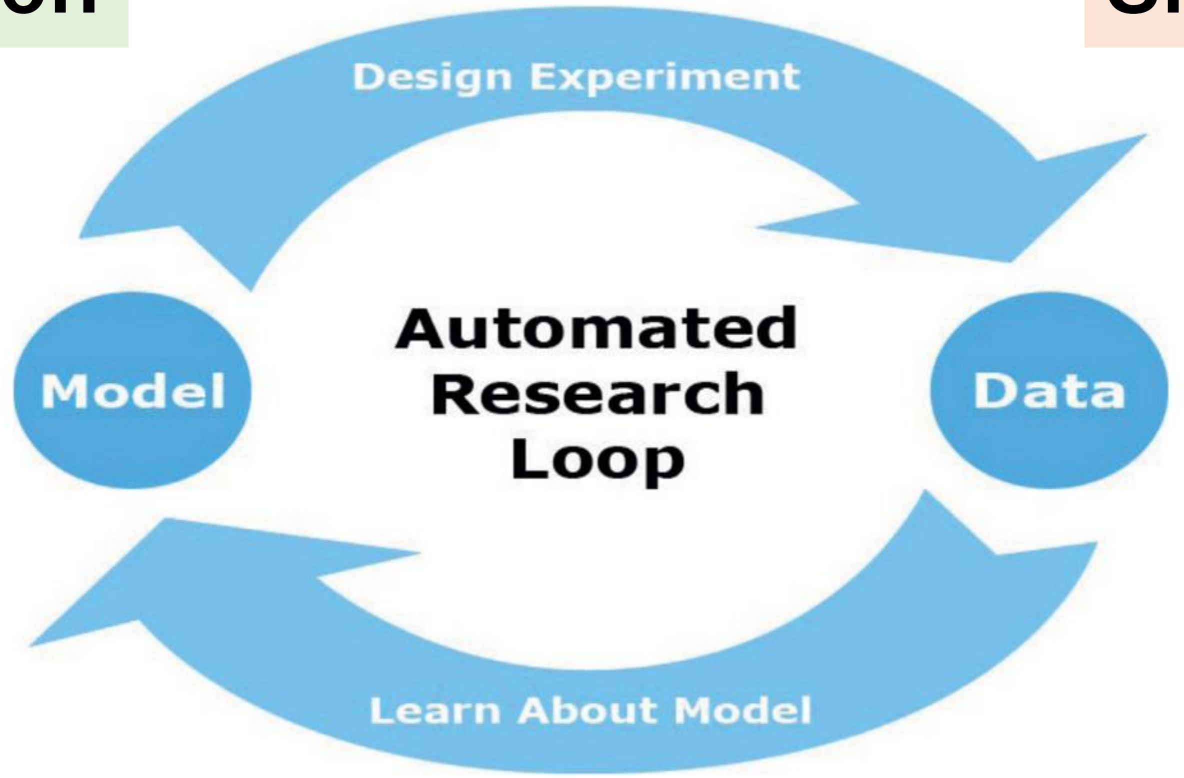
Optimization

Simulation



Machine learning

From classical to quantum

The loop		Potential speed-up by
Simulation	→	Quantum Simulation (QSim)
Machine Learning	→	Quantum Machine Learning (QML)
Optimization	→	Quantum Optimization (Qopt)

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Optimization of combinatorial black box function

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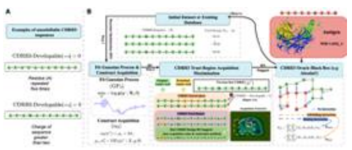
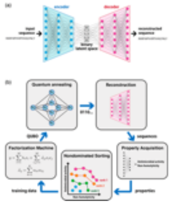
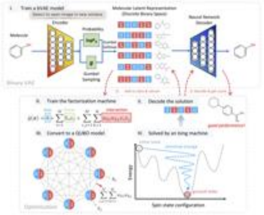
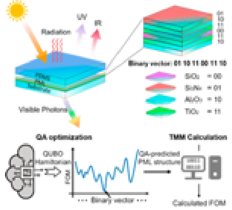
Medicine

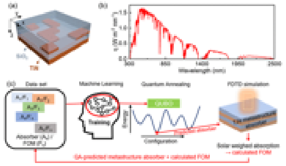

Antibody design
(Khan+ 2023)

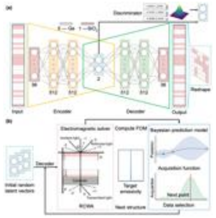

Antimicrobial peptides
(Tučs+ 2023)

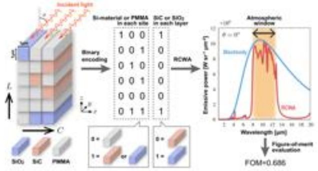

Chemical design
(Mao+ 2023)

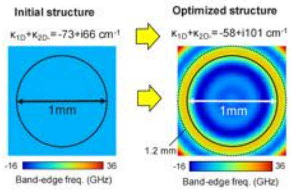
Optics


Radiative cooler
(Kim+ 2023)


Solar absorber
(Kim+ 2023)

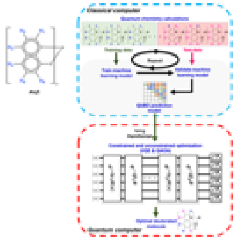

Thermal radiation
(Zhu+ 2022)


FMQA
wavelength selective radiator
(Kitai+ 2020)

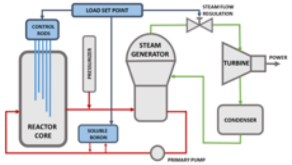


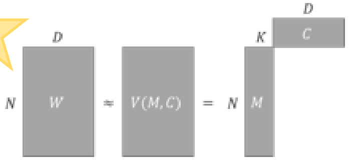
Photonic crystal laser
(Inoue+ 2022)

Chemistry

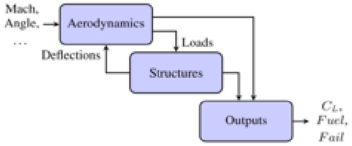

OLED design
(Gao+ 2023)

Data science


Plant control
(Drouet+ 2020)

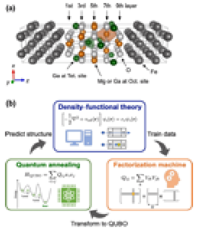


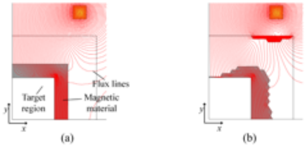
Data compression
(Kadowaki+ 2022)



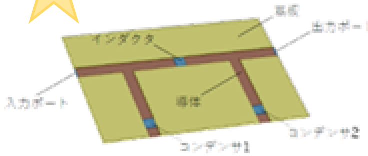
BOCS
Model parameter reduction
(Baptista+ 2018)

Spintronics & Magnetism

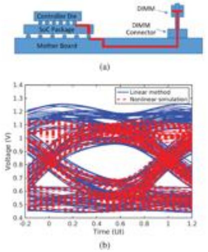

Barrier materials in MTJ
(Nawa+ 2023)

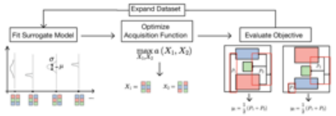

Magnetic shield
(Maruo+ 2022)

Electronics


Noise filter
(Okada+ 2023)


Mounting holes
(Matsumori+ 2022)


Circuit analysis
(Dou+ 2022)


Chip design
(Oh+ 2022)

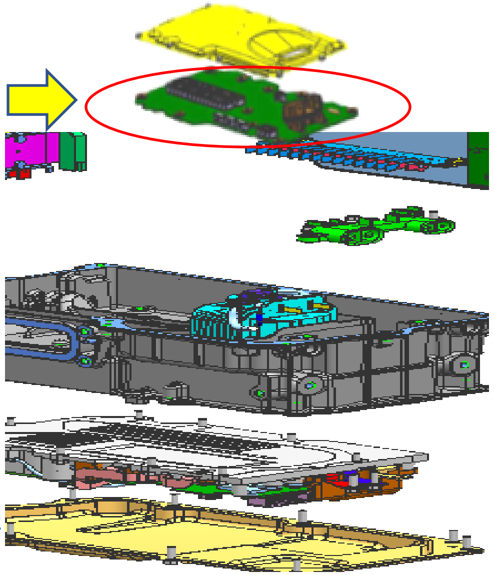
DENSO Crafting the Core

Printed circuit board design to protect from resonant vibration

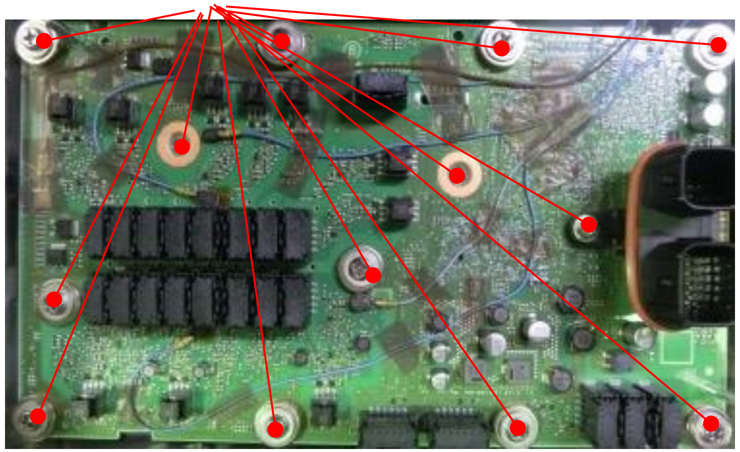
AIST Create the Future, Collaborate Together

Power control unit

https://www.denso.com/jp/ja/news/newsroom/2019/20190522-01/-/media/8c44d0012d0148f893903eb515d52b67.ashx



Mounting holes : number and positions



Printed circuit board

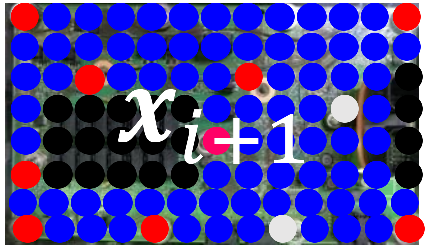
The more mounting holes we place, the higher the natural frequency we achieve, which avoid defects of electric parts by the resonance. On the other hand, mounting holes is costly, we want to reduce them.

Matsumori, et. al. Sci Rep 12, 12143 (2022)

Implementation of the loop & CAE

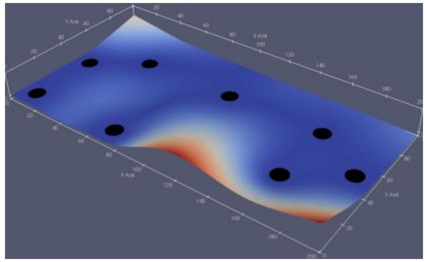
Optimization

$$x_{i+1} = \underset{x \in \{0,1\}^n}{\operatorname{argmin}} \hat{f}(x)$$

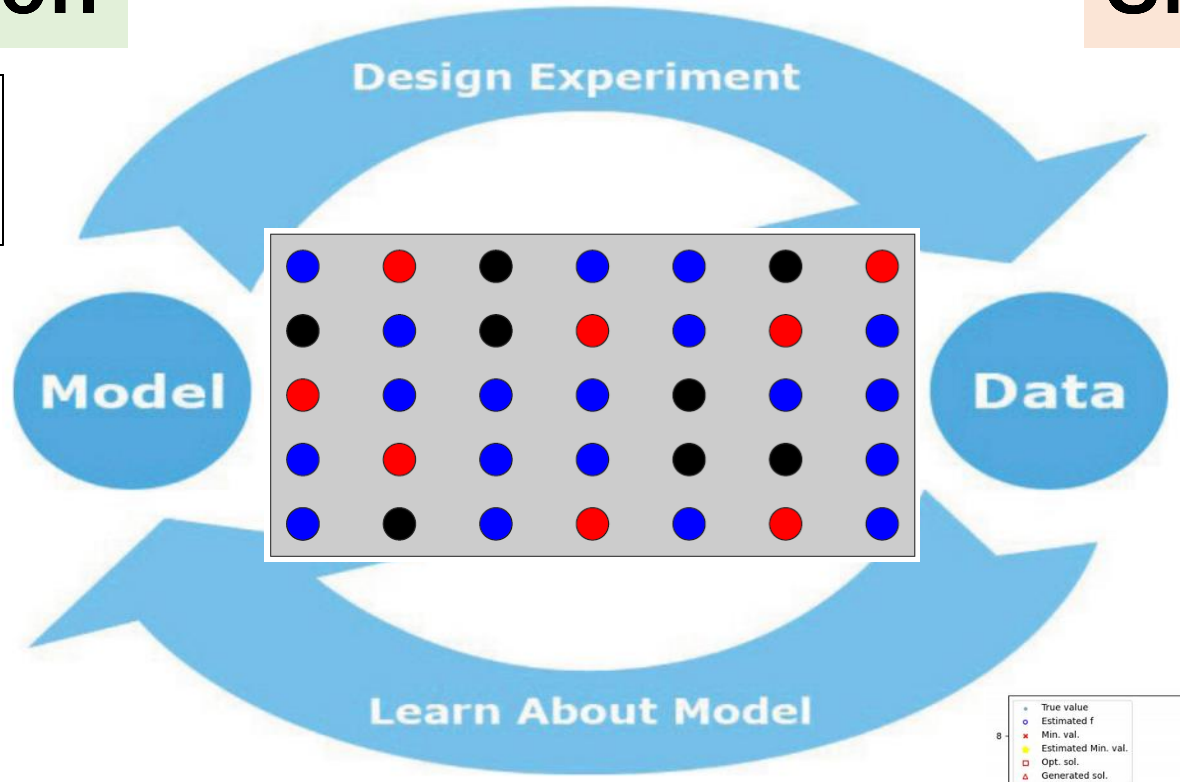


Simulation

$$y_{i+1} = f(x_{i+1})$$



FEM analysis

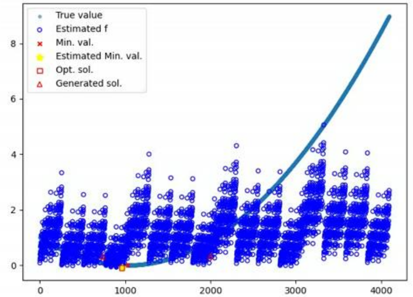


QUBO form

$x^{\mathrm{T}} Q x + b$

$$\hat{y} = \hat{f}(x)$$

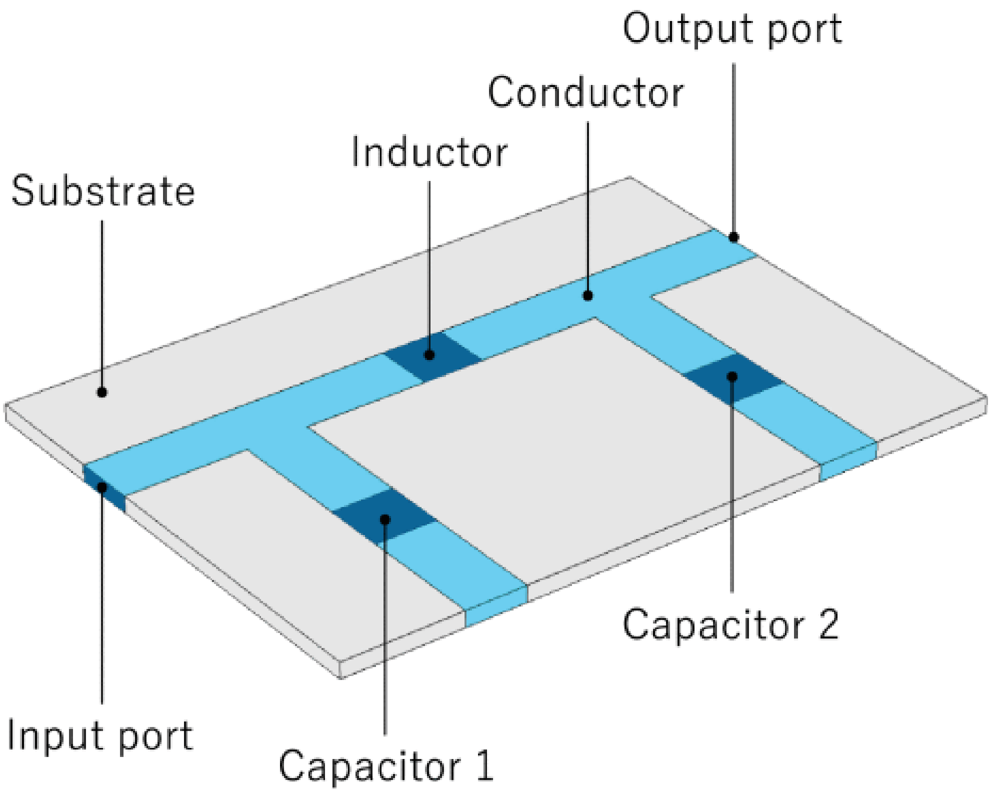
Machine learning

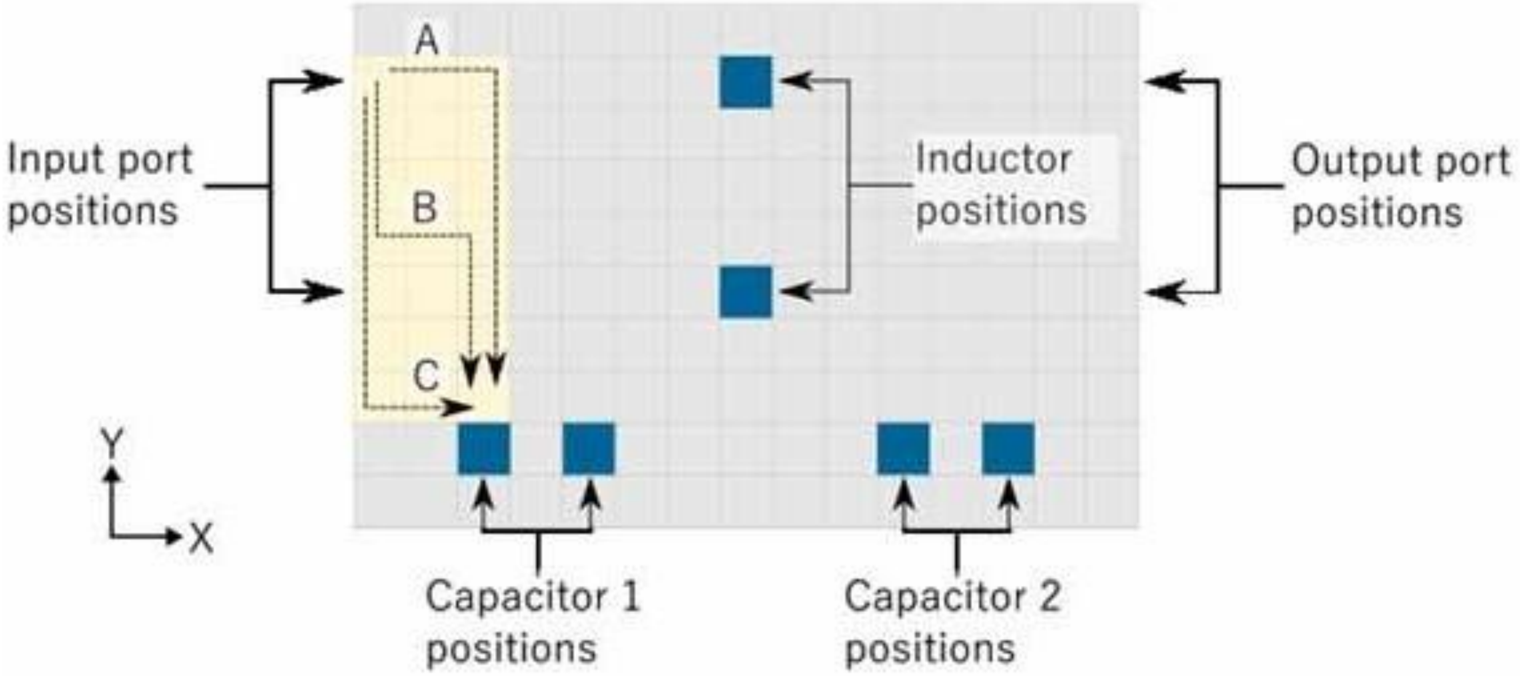


Matsumori, et. al. Sci Rep 12, 12143 (2022)

Noise filter design: component location and conductor pattern optimization in a distributed-element circuit

Printed circuit board

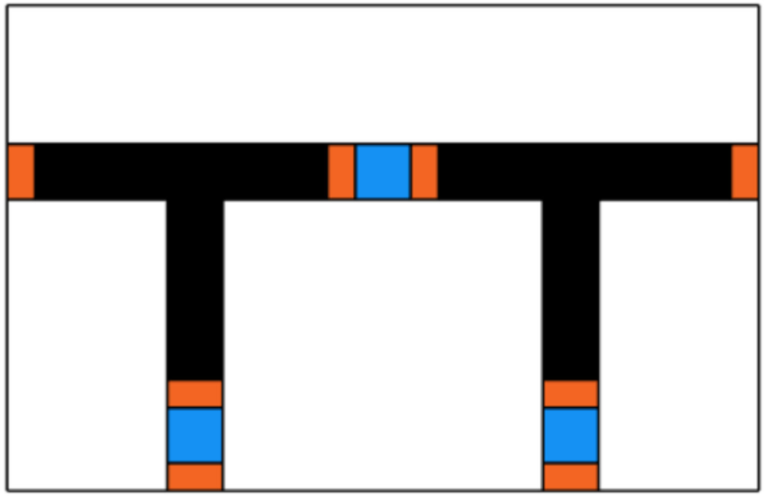




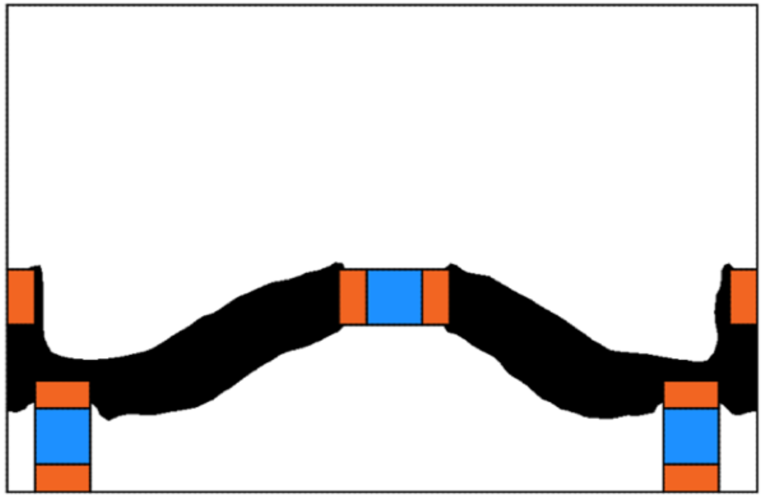
Okada, et. al., IEEE Access, vol. 11, pp. 44343-44349 (2023)

Results

Reference

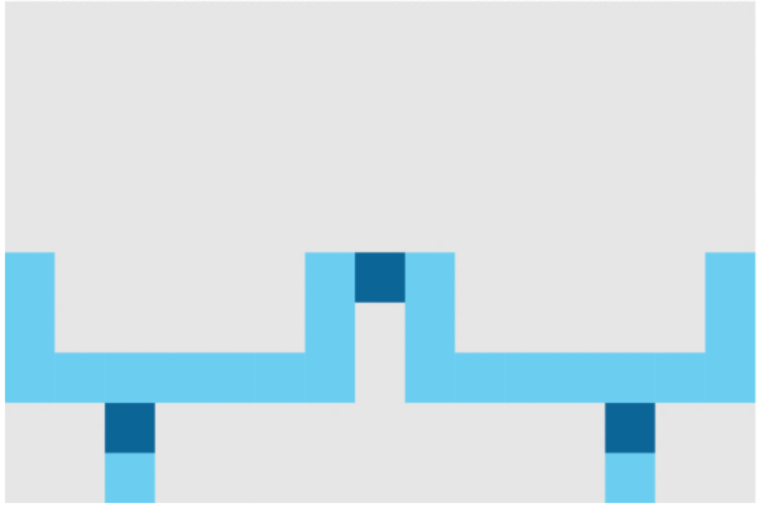


Topology optimization



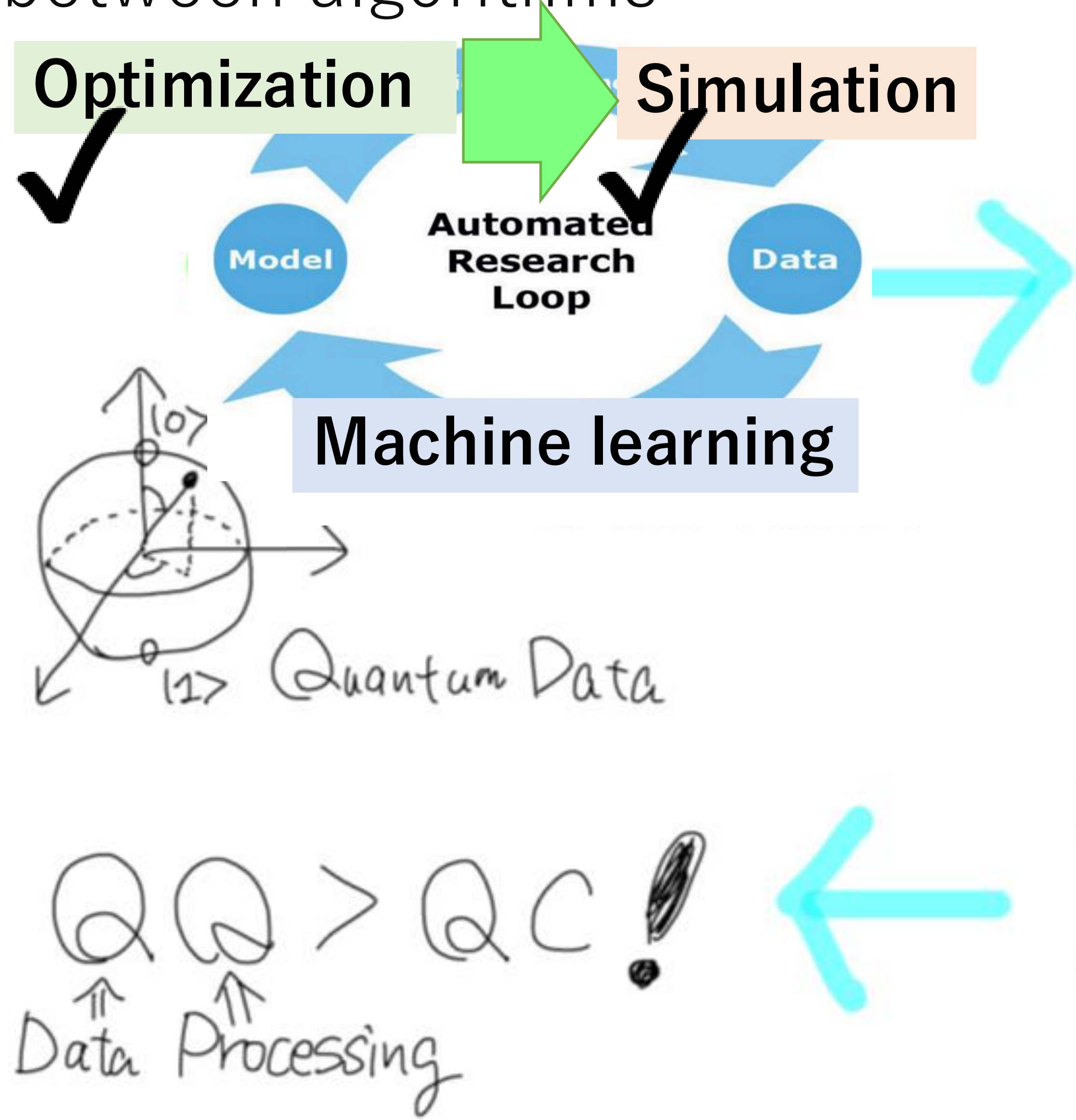
(Industrial standard method)

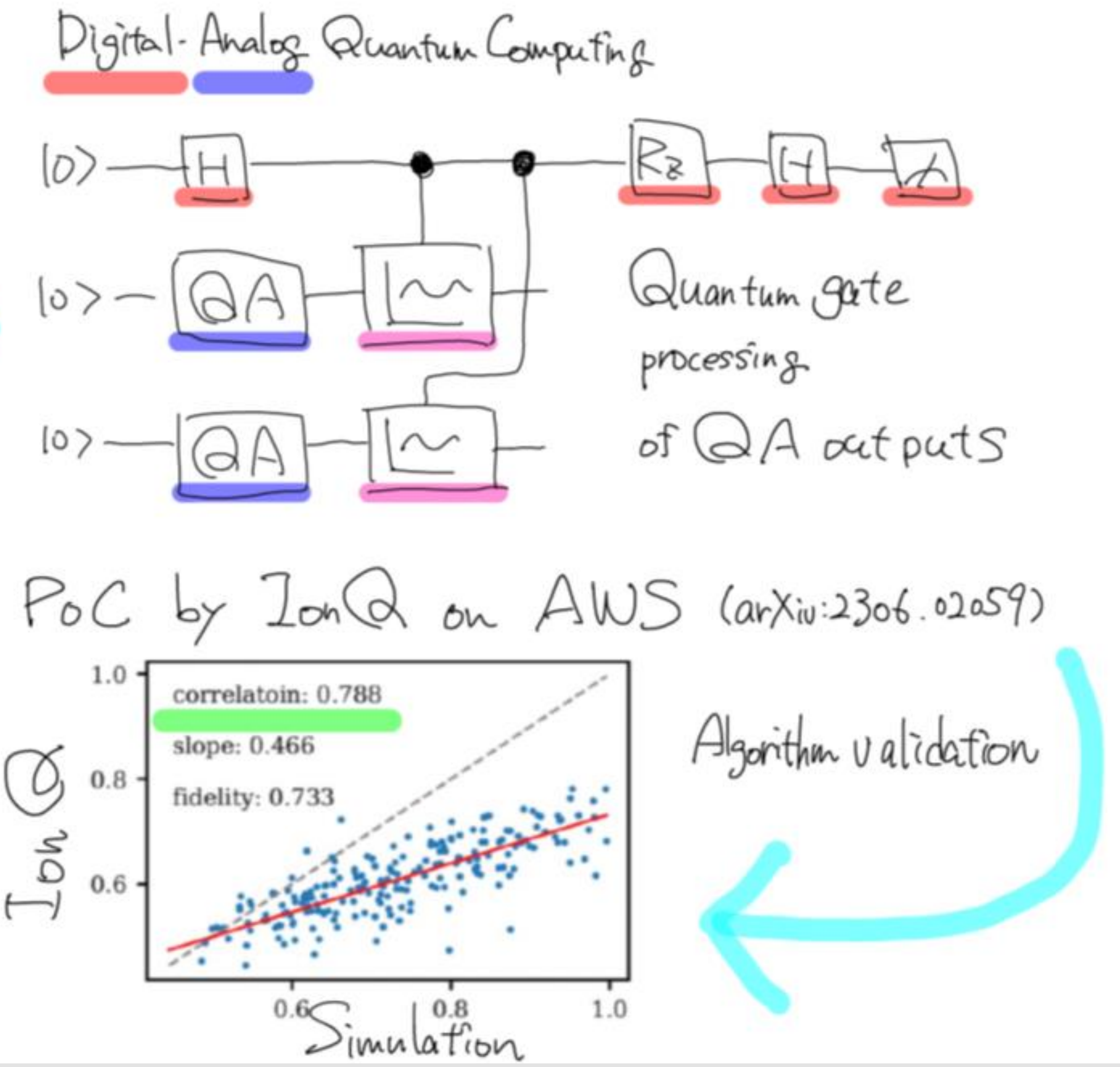
Out method



Nomura, et. al., Struct Multidisc Optim 59, 2205–2225 (2019)
Okada, et. al., IEEE Access, vol. 11, pp. 44343-44349 (2023)

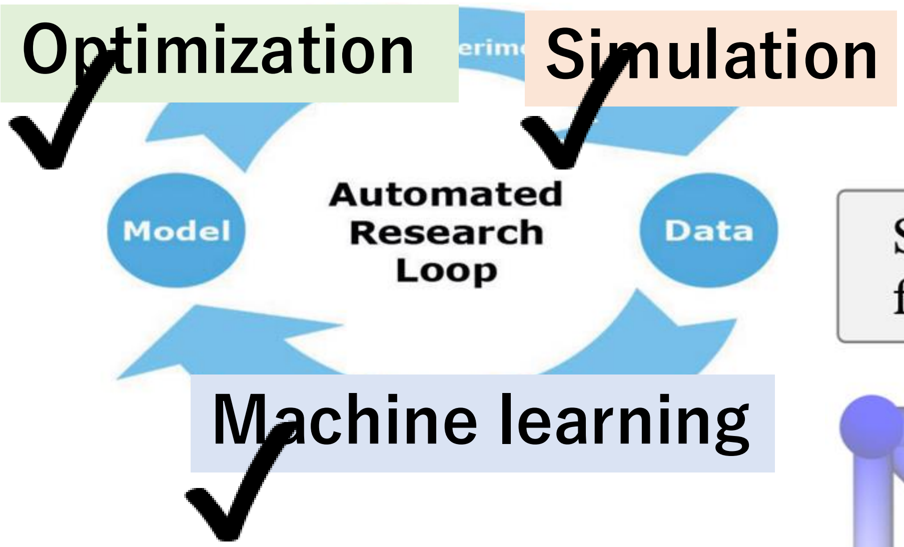
Seamless quantum data flow between algorithms

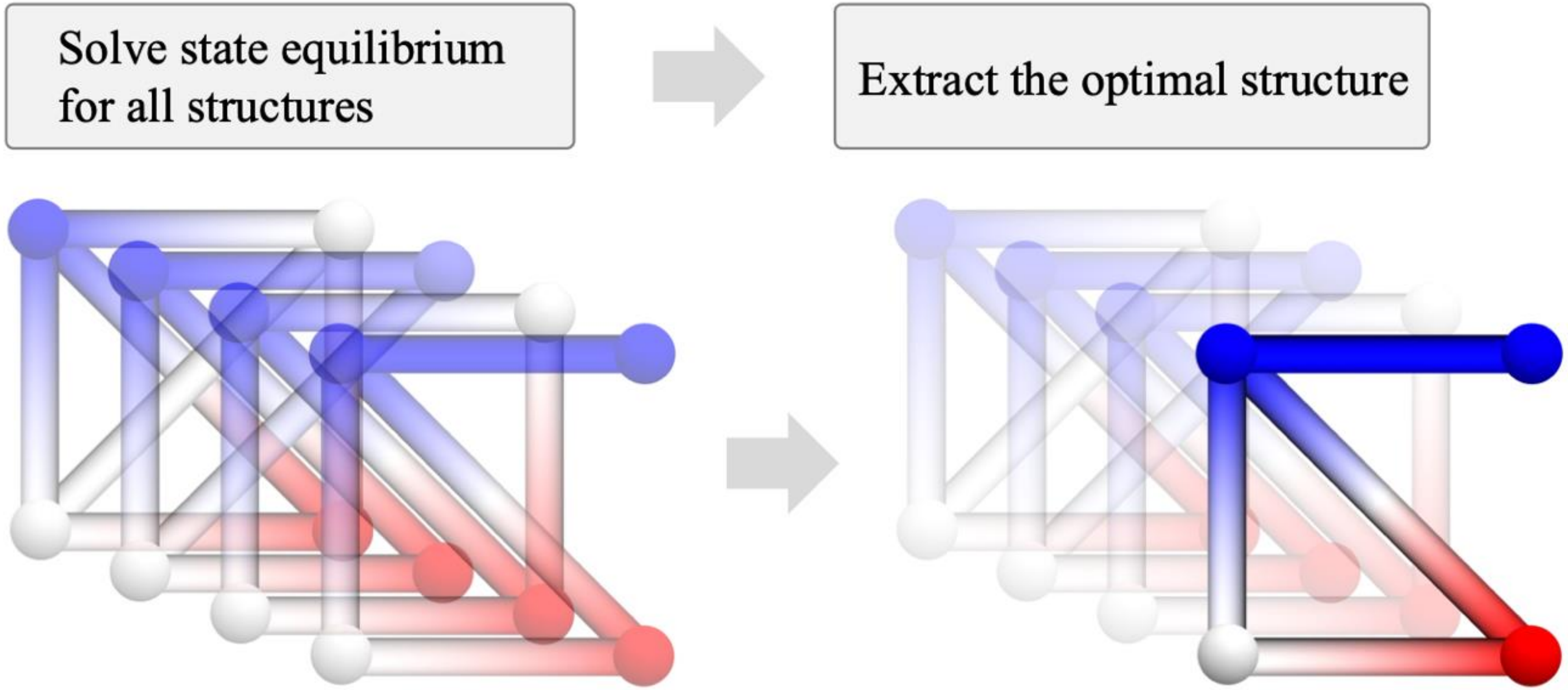




APL Quantum 1, 026101 (2024)

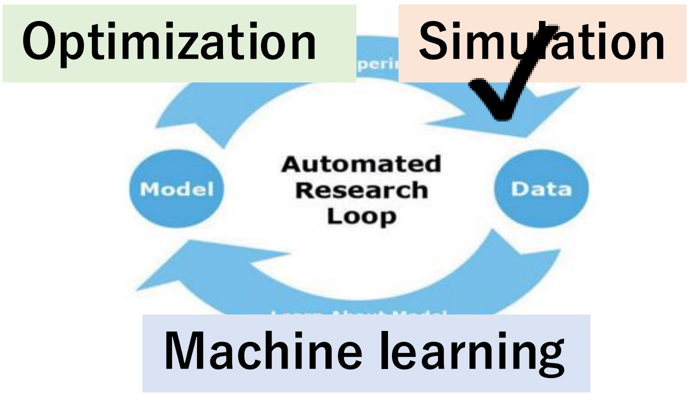
Other approach : Quantum topology optimization

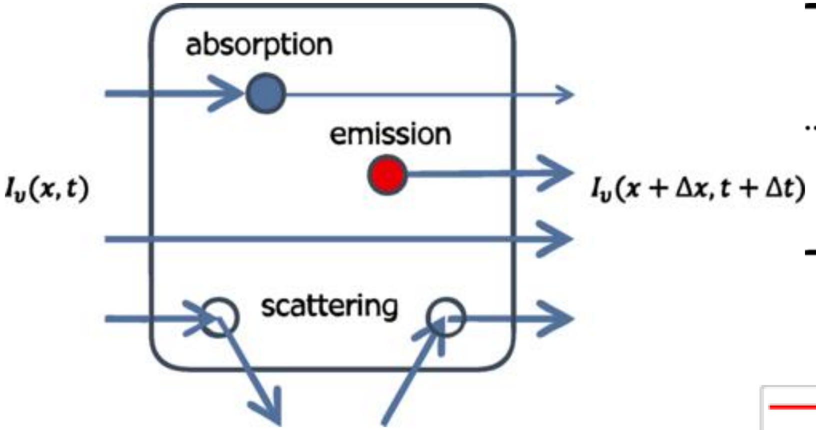


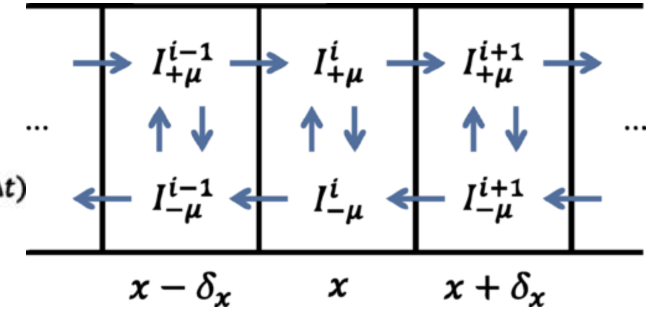


Sato, et. al., arXiv:2207.09181
(IEEE Quantum Week 2023)

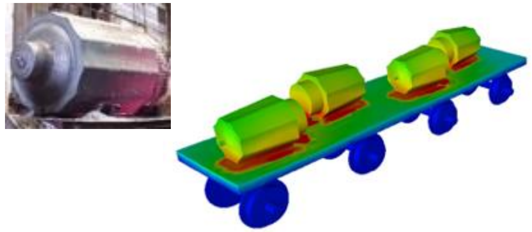
Quantum algorithm for the radiative-transfer equation

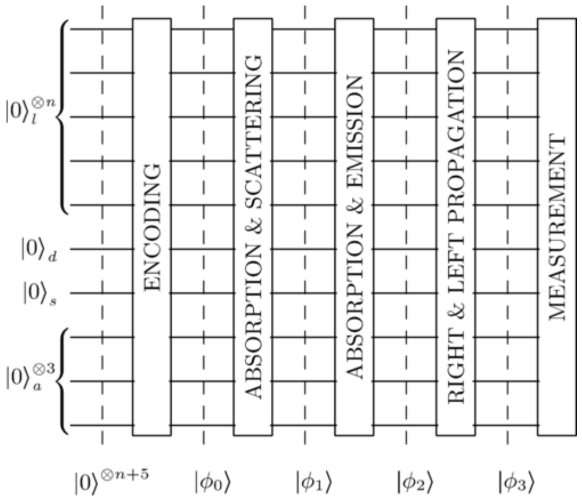


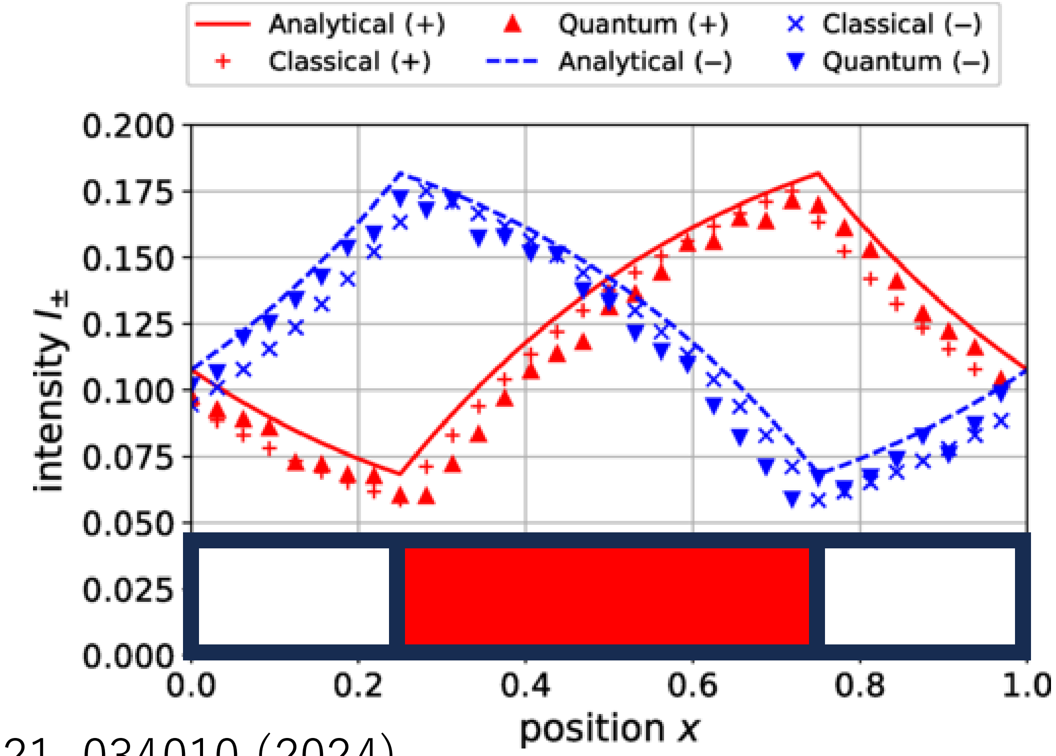




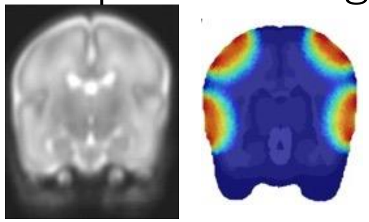
radiative cooling







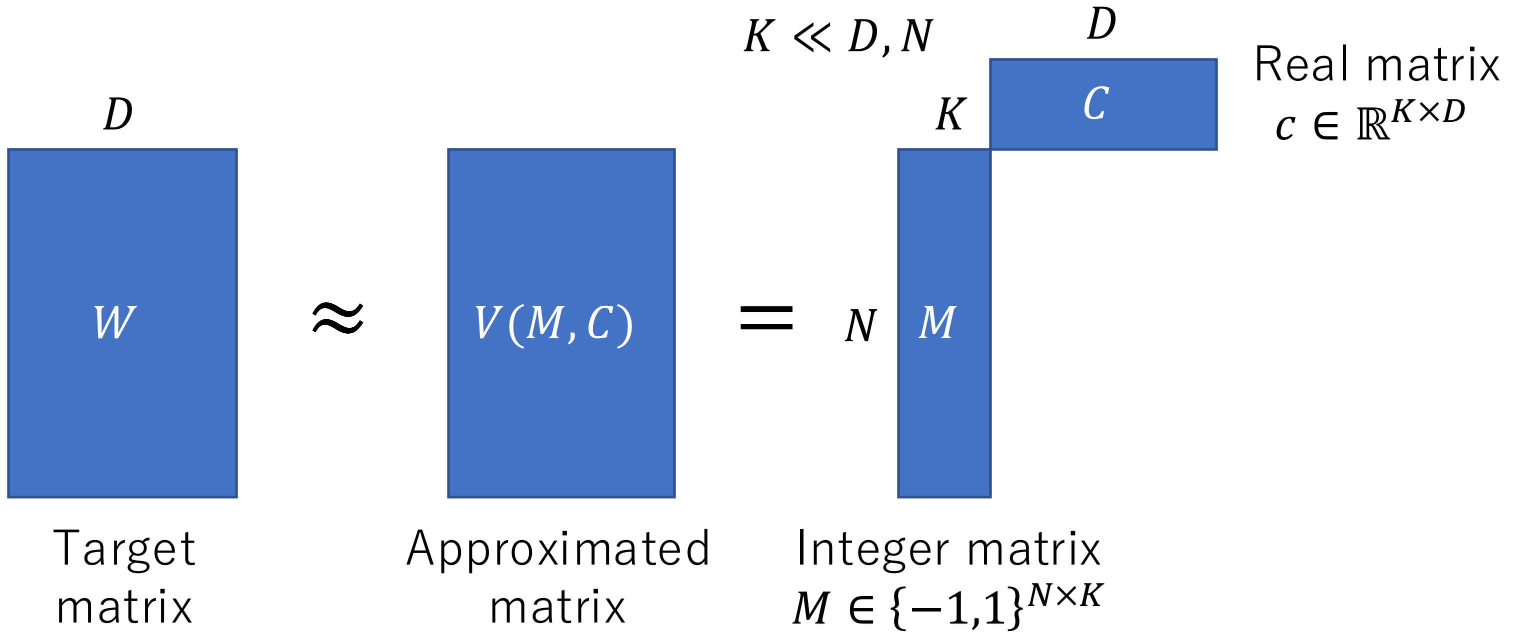
diffuse optical tomography



Igarashi, et.al., Phys Rev Applied 21, 034010 (2024)

Integer decomposition (lossy matrix compression)

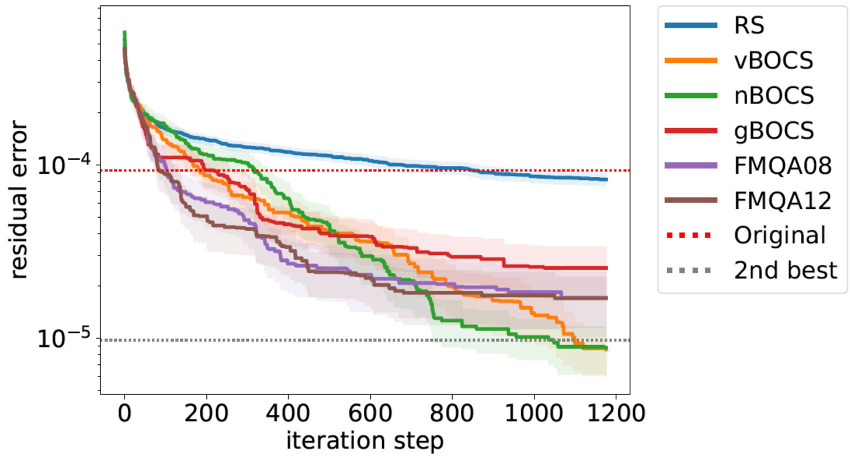
Optimization ✓ | Simulation | Machine learning



$$\underset{\substack{M\in\{-1,1\}^{N\times K} \\ C\in\mathbb{R}^{K\times D}}}{\text{argmin}} |W - V|^2$$

mixed-integer non-linear programming; MINLP This compression problem is NP-hard.

BBO algorithm variations



Ambai and Sato, ECCV2014
Yoon et. al., Sci. Rep. 2022

Automation of Science & self-driving

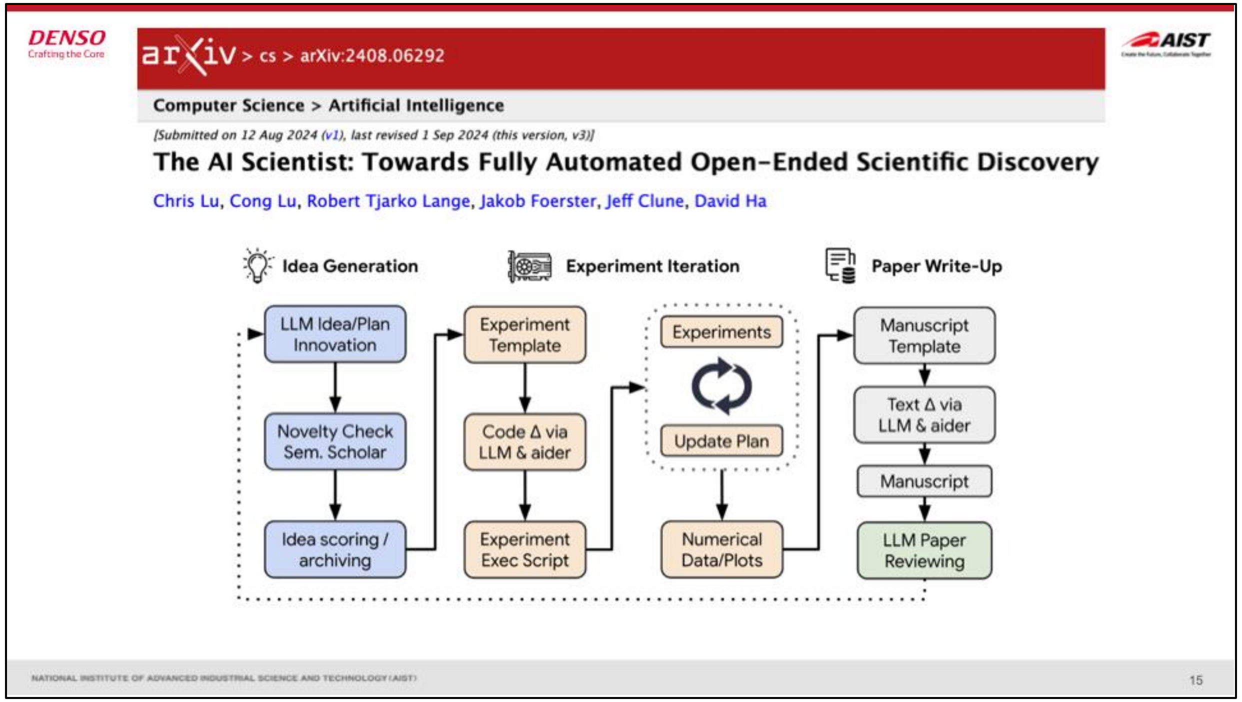
Perfect information game

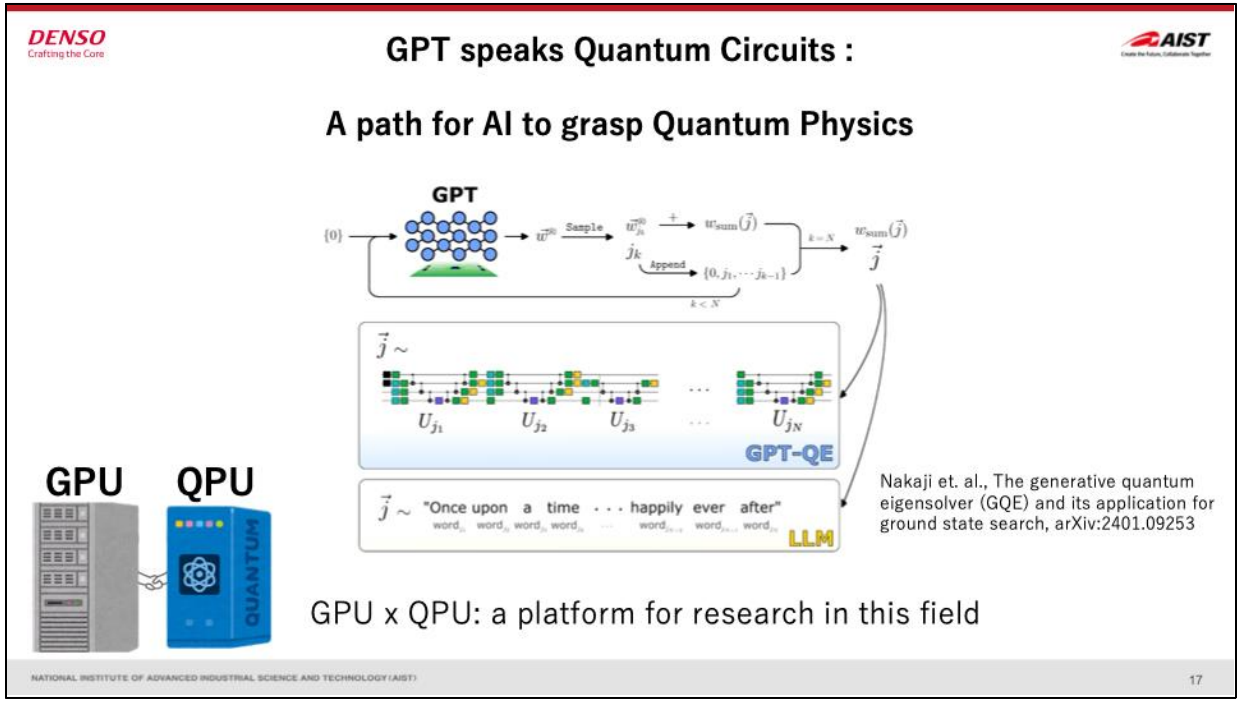
Imperfect information game

JST CRDS Artificial Intelligence and Science

SAE Levels of Driving Automation™

A solution toward level 4 & 5 automation?





DENSO
Crafting the Core

Summary

AIST
Create the Future, Collaborate Together

- CAE aims to automate product design process in Engineering.
- Automation in Science and Engineering follows a similar structure.
- Level 3 automation has been extensively studied and applied across various Scientific and Engineering fields.
- Examples show how quantum computing accelerates complex CAE tasks.
- The combination of AI and QC will accelerate Science and Engineering.