第1回 Quantum CAE 研究会

2024/5/9,10
産業技術研究所臨海副都心センター

第1回 Quantum CAE 研究会

研究会幹事

門脇 正史 (産業技術総合研究所)
田中 宗 (慶應大学)
田村 亮 (物質・材料研究機構、東京大学)
宮本 幸一 (大阪大学)
遠藤 克浩 (産業技術総合研究所)

主催

産業技術総合研究所　量子・AI融合技術ビジネス開発グローバル研究センター（G-QuAT）

共催

大阪大学　量子情報・量子生命研究センター
光・量子飛躍フラッグシッププログラム（Q-LEAP）量子情報処理（量子AI）
知的量子設計による量子ソフトウェア研究開発と応用

第1回 Quantum CAE研究会

産業技術総合研究所　臨海副都心センター

Create the Future, Collaborate Together

Day 1　5 / 9 (Thu.)　*12:00開場

13:00-13:45	門脇正史（産業技術総合研究所、(株)デンソー） Quantum CAE：量子コンピュータによる未来のモノづくりと科学の自動化	導入
14:00-14:30	向田志保（三井化学(株)） 生成AIを活用した新規用途/材料探索の高精度化・高速化	材料、化学
14:30-15:00	三瓶大志、七種紘規（早稲田大学） 高速な触媒開発に向けた古典/量子ハイブリッド化による表面状態解析	材料、化学
15:00-15:30	Qi Gao 高玘（三菱ケミカル(株)）最適化とAIの融合技術による材料探索の研究事例	材料、化学
15:45-16:15	宇野隼平、大塩耕平（みずほリサーチ＆テクノロジーズ(株)） モンテカルロ計算を用いた設計と量子アルゴリズム	シミュレーション
16:15-16:45	宮本幸一（大阪大学） ボルツマン方程式求解の量子アルゴリズム：宇宙大規模構造形成シミュレーションを例に	シミュレーション
16:45-17:15	五十嵐朱夏（産業技術総合研究所） 格子ボルツマン法による輻射輸送計算の量子アルゴリズム	シミュレーション
17:15-17:45	田中雄（ソニーグループ(株)） Koopman-von Neumann線形化法の量子アルゴリズム	シミュレーション
18:15-20:15	懇親会	

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Day 2 5/10 (Fri.)

10:00-10:30	田村亮（物質・材料研究機構、東京大学） イジングマシンを用いたブラックボックス最適化手法の材料研究への応用
10:30-11:00	関優也（慶應義塾大学） ブラックボックス最適化の高効率化に向けたFactorization machineの学習手法
11:00-11:30	牧野大介（(株)Jij） 量子アニーリングマシンを活用したブラックボックス最適化の活用事例：血行動態予測モデルのハイパーパラメータ探索
11:30-12:00	菅義訓（トヨタ自動車(株)） 自動車材料研究に於ける量子コンピューティングの活用可能性
13:30-14:15	津田宏治（東京大学） AI 4 Scienceにおける量子CAEの可能性
14:30-15:00	寺田賢二郎（東北大学） 計算固体力学における量子アニーリングの適用性に関する基礎的検討
15:00-15:30	村松眞由（慶應義塾大学） 量子アニーリングによる材料微視組織解析のためのPhase-fieldシミュレーション
15:30-16:00	遠藤克浩（産業技術総合研究所） アニーリングマシンにおける実数表現の違いがもたらす顕著な計算性能の変化とその考察について
16:15-16:45	佐藤勇気（(株)豊田中央研究所） Quantum CAEに関する取り組み紹介:偏微分方程式の求解と設計最適化のための量子アルゴリズム
16:45-17:15	菅野恵太（(株)QunaSys） 量子位相推定アルゴリズムを用いた量子コンピュータによる固有振動数解析
17:15-17:45	斎藤隆泰（群馬大学） 量子コンピューターと計算数理工学

ブラックボックス最適化（10:00-12:00）

AI x 量子 x 科学（13:30-14:15）

計算力学（14:30-17:45）

参加登録者153名: 大学 33, 国研 27, 企業 93

お茶の水女子大学
横浜国立大学
九州大学
群馬大学
慶應義塾大学
早稲田大学
大阪大学
中央大学
東京工業大学
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物質・材料研究機構
理化学研究所

Beyond Next Ventures
BIPROGY
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Groovenauts
IBM
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ソニーグループ
ソフトバンク
デロイトトーマツコンサルティング
デンソー
トヨタシステムズ
トヨタ自動車
パナソニック
ブリヂストン
マツダ
みずほリサーチ＆テクノロジーズ
ミライズテクノロジーズ
ユニアデックス

ロジスティクスＩＴ研究所
伊藤忠テクノソリューションズ
沖電気工業
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富士フイルム
丸紅
三井化学
三菱ケミカル
村田製作所
横浜ゴム

多数のご参加ありがとうございます。

Quantum CAE

量子コンピュータによる
未来のモノづくりと科学の自動化

DENSO
Crafting the Core

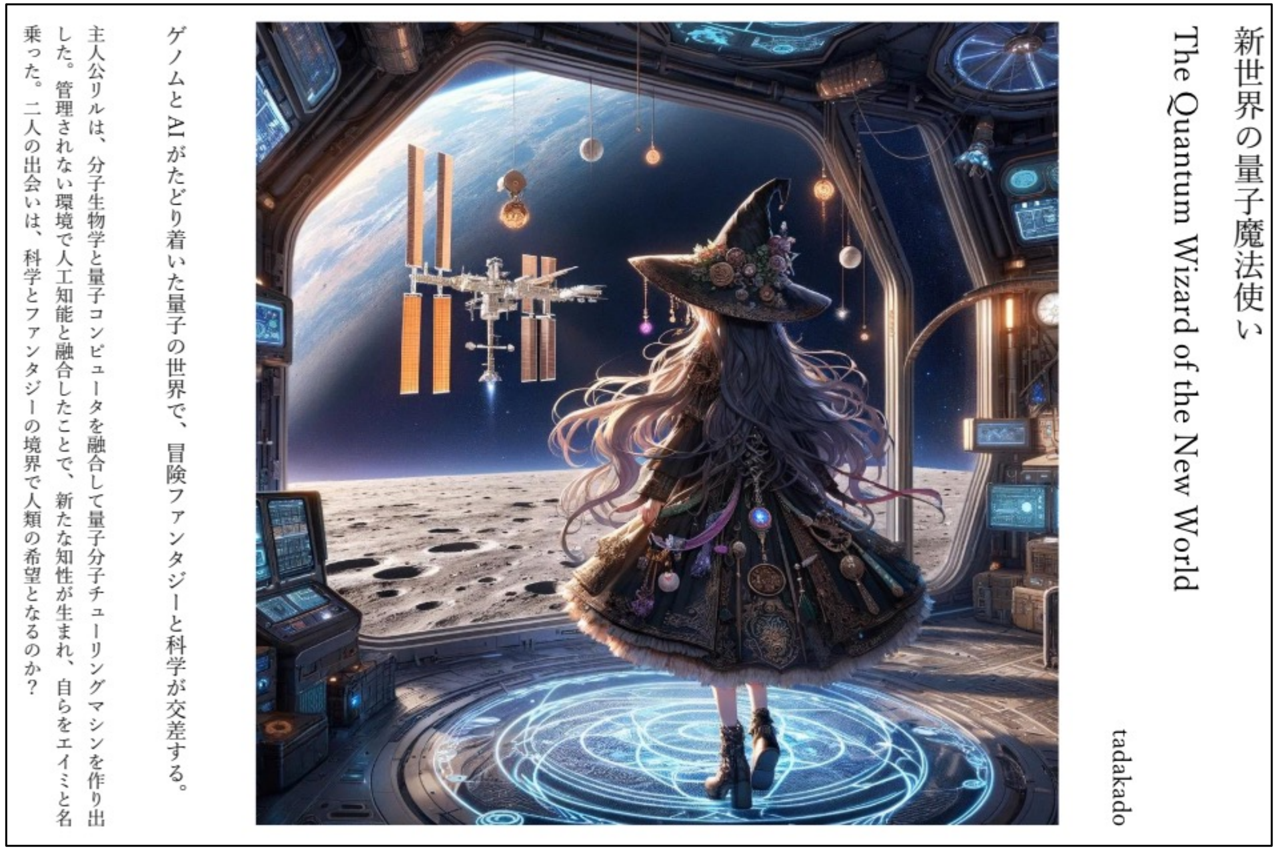
Tadashi Kadowaki

AIST

AIST
Create the Future, Collaborate Together

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



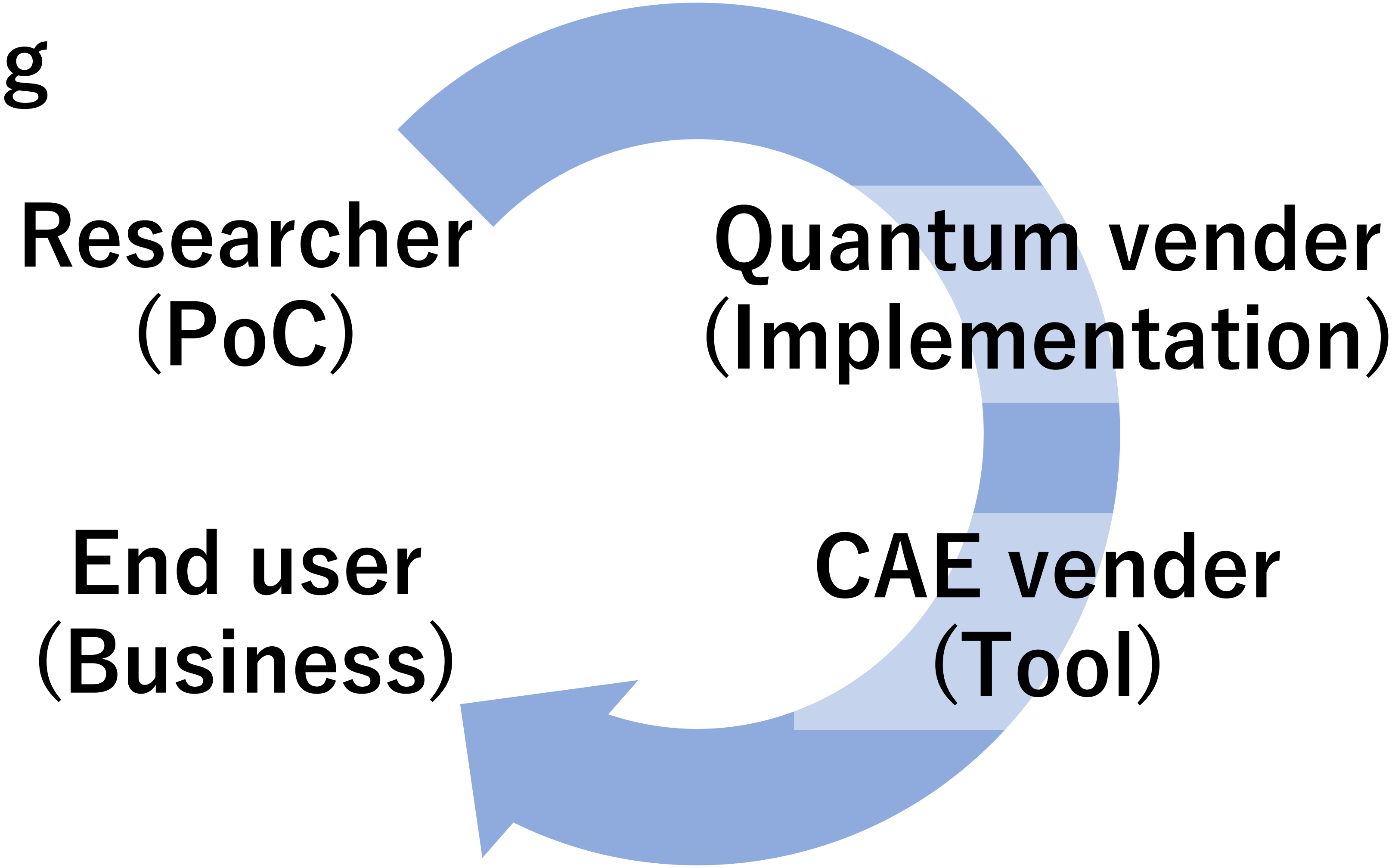
https://q-portal.riken.jp/quantum_article_detail?qt_id=K20240003

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」

Quantum CAE ecosystem

Strategy & Founding

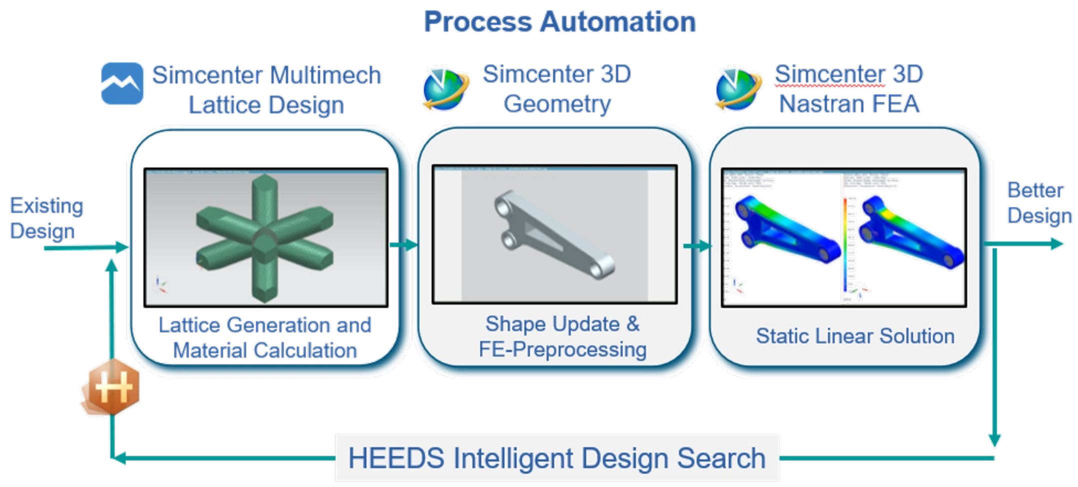
Community



What's Quantum CAE?

CAE (Computer Aided Engineering)

Design automation for industrial products



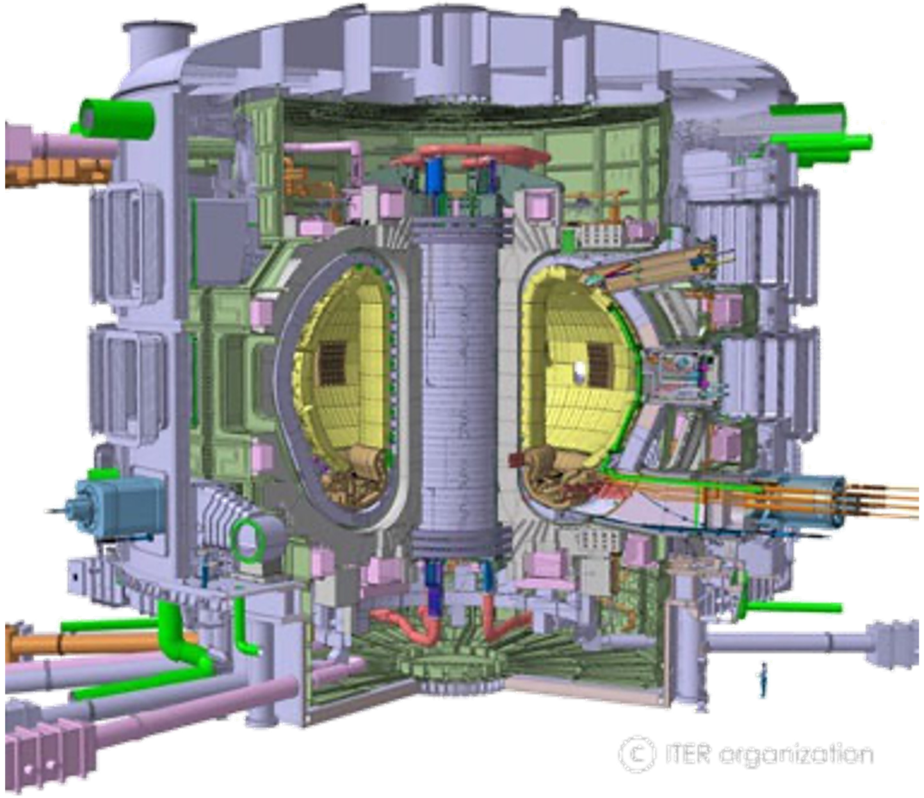
https://blogs.sw.siemens.com/nx-design/design-for-purpose-heeds-design-exploration-study/

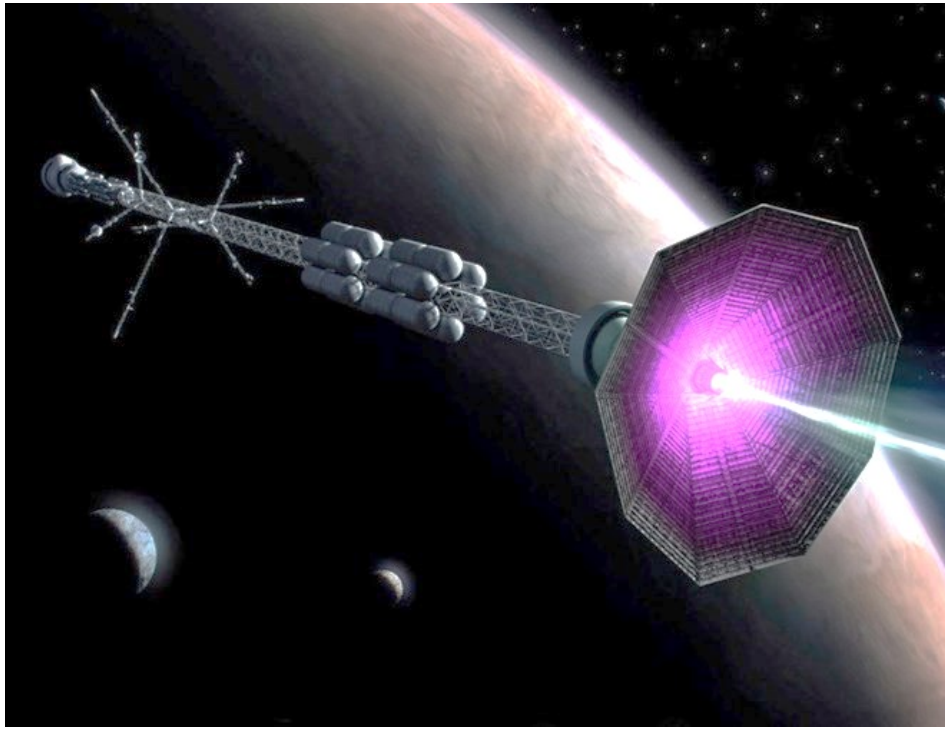
Quantum CAE

Accelerate or empower CAE by quantum computing

Extreme goals of the industrial design automation

Design fusion reactors & spaceships automatically





iter.org

Science & Engineering : Explore "no one has gone before!"

wikipedia

Space: the final frontier. These are the voyages of the starship *Enterprise*. Its continuing mission: to explore strange new worlds; to seek out new life and new civilizations; to boldly go where no one has gone before!

Space: [science] hypothesis space, [engineering] design space, etc.
to explore: "our" daily activities (Lab work)
where no one has gone before : new findings, values, products, etc.

Continuous space: conventional worlds (Earth, Solar system) => efficient algorithms (Linear programming, Bayesian optimization, …)

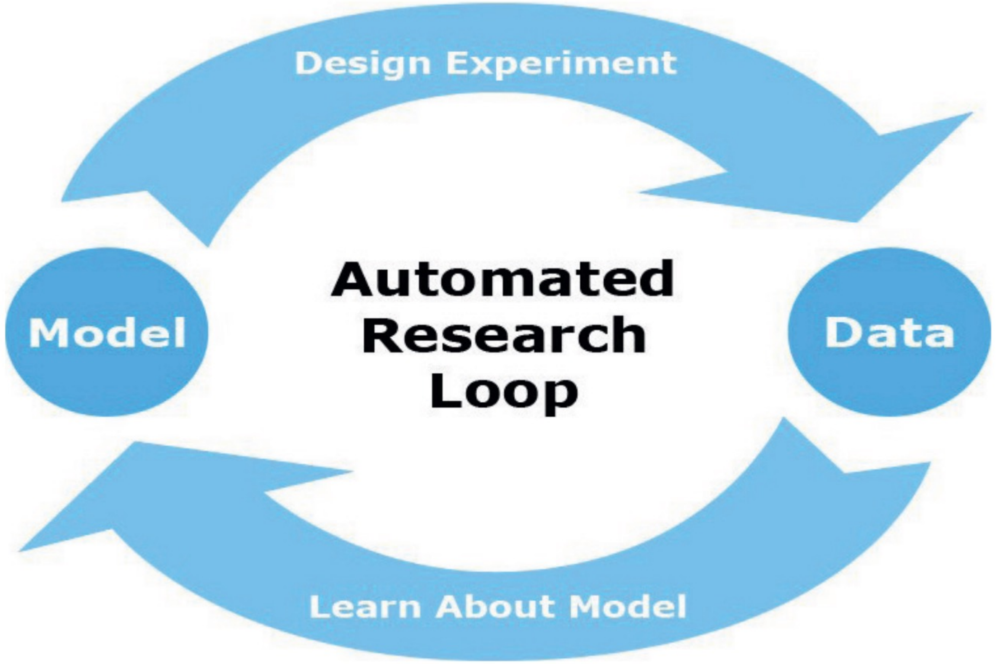
Discrete space: strange new worlds => facing NP-hard problems (Integer programming, Combinatorial optimization…)

Bayesian optimization (modern design of experiments)

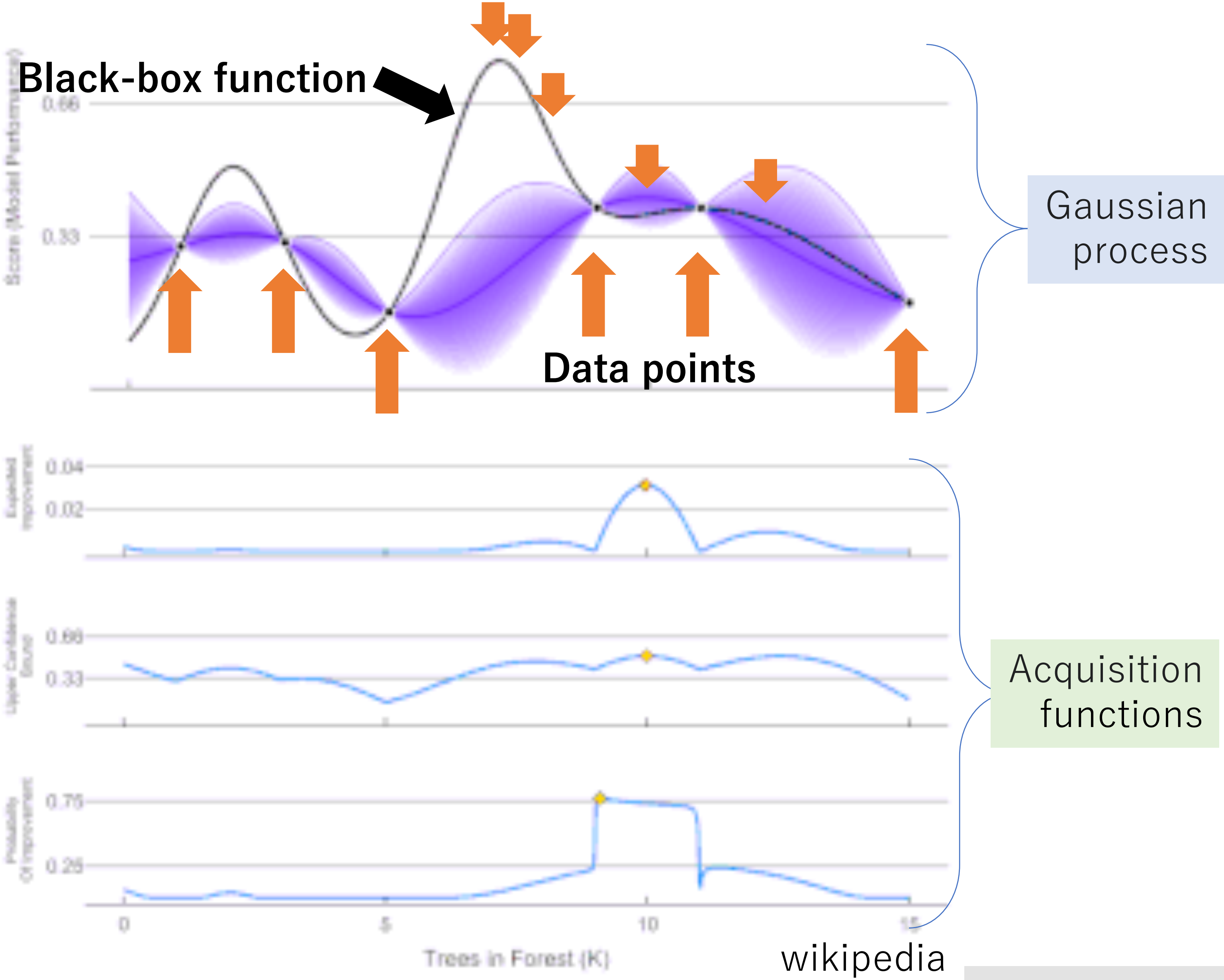
$$x^* = \underset{x \in \mathcal{X}}{\mathrm{argmax/argmin}}\, f(x)$$

Acquisition function

Experiment



Gaussian process (surrogate model)



wikipedia

Bayesian Optimization of Combinatorial Structures (BOCS)

Solving combinatorial optimization of black-box function

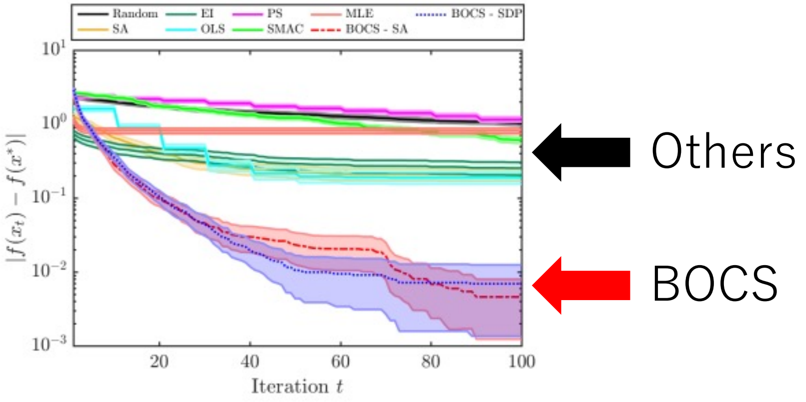


Figure 1. Random BQP instances with $L_c = 10$ and $\lambda = 0$: Both variants of BOCS outperform the competitors substantially.

Making a reduced model

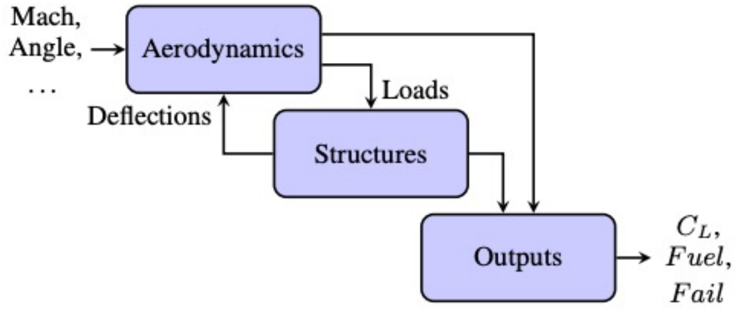


Figure 5. The aero-structural model of Jasa et al. (2018): The arrows indicate the flow of information between components. Note that the loop requires a fixed point solve whose computational cost increases quickly with the number of involved coupling variables.

Algorithm 1 Bayesian Optimization of Combinatorial Structures

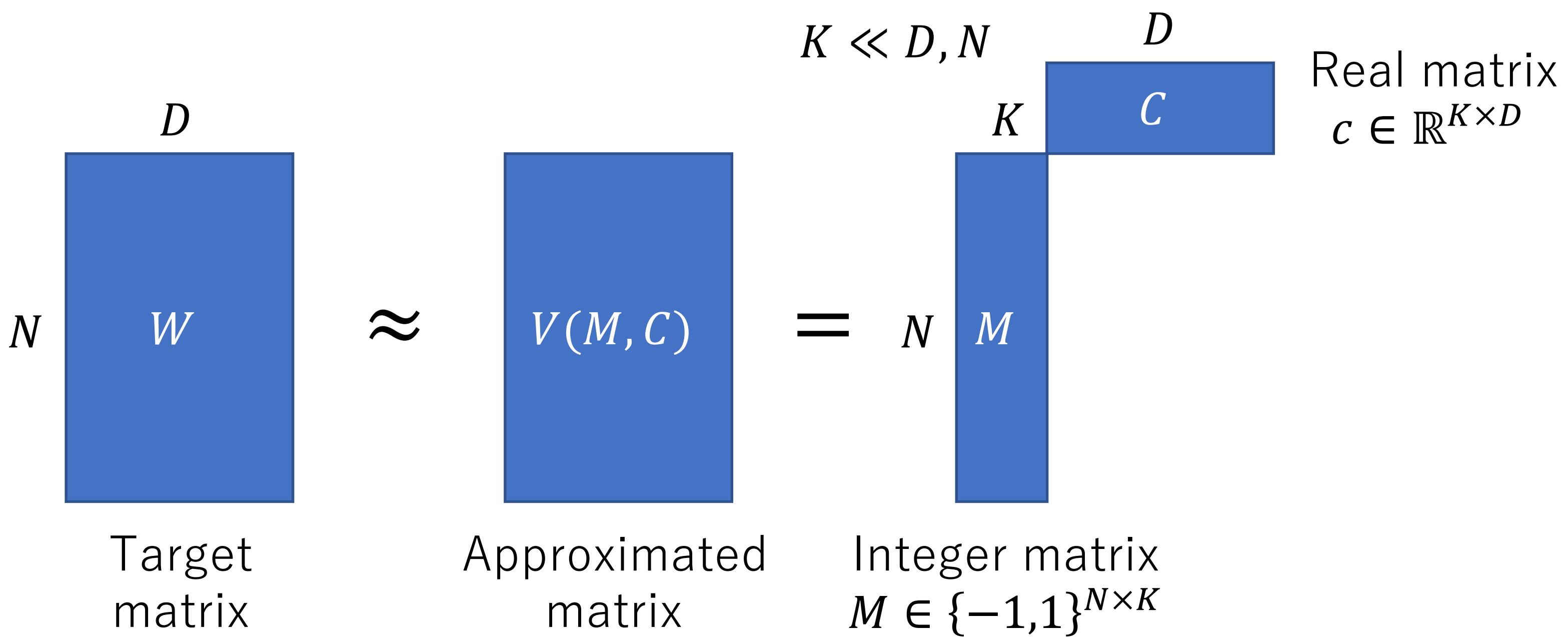
Input: Objective function $f(x) - \lambda\mathcal{P}(x)$; Sample budget N_{max}; Size of initial dataset N_0.
Sample initial dataset D_0.
Compute the posterior on $\boldsymbol{\alpha}$ given the prior and D_0.
for $t = 1$ **to** $N_{max} - N_0$ **do**
  Sample coefficients $\boldsymbol{\alpha}_t \sim P(\boldsymbol{\alpha} \mid \mathbf{X}, \mathbf{y})$.
  Find approximate solution $x^{(t)}$ for $\max_{x \in \mathcal{D}} f_{\boldsymbol{\alpha}_t}(x) - \lambda\mathcal{P}(x)$.
  Evaluate $f(x^{(t)})$ and append the observation $y^{(t)}$ to $\mathbf{y}$.
  Update the posterior $P(\boldsymbol{\alpha} \mid \mathbf{X}, \mathbf{y})$.
end for
return $\text{argmax}_{x \in \mathcal{D}} f_{\boldsymbol{\alpha}_t}(x) - \lambda\mathcal{P}(x)$.

Closed loop

Experiment (data) → Modeling (QUBO)
↑ ↓
QUBO optimization (acquisition)

Baptista and Poloczek, ICML, 462–471, (2018)

Integer decomposition (lossy matrix compression)



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

mixed-integer non-linear programming;

MINLP This compression problem is NP-hard.

Ambai and Sato, ECCV2014

Yoon et. al., Sci. Rep. 2022

Mixed integer formulation to integer formulation
(we want to remove continuous variables)

$$W \approx V = MC$$

For given M, least squares method finds,

$$C = (M^T M)^{-1} M^T W$$

By instituting this,

$$V(M, C) = MC = M(M^T M)^{-1} M^T W = V(M)$$

$$\underset{M \in \{-1,1\}^{N \times K}}{\operatorname{argmin}} |W - V|^2$$
$$= \underset{M \in \{-1,1\}^{N \times K}}{\operatorname{argmin}} |W - M(M^T M)^{-1} M^T W|^2$$

Non-linear integer programming problem (NLIP)

Kadowaki, T., Ambai, M., Sci Rep 12, 15482 (2022)

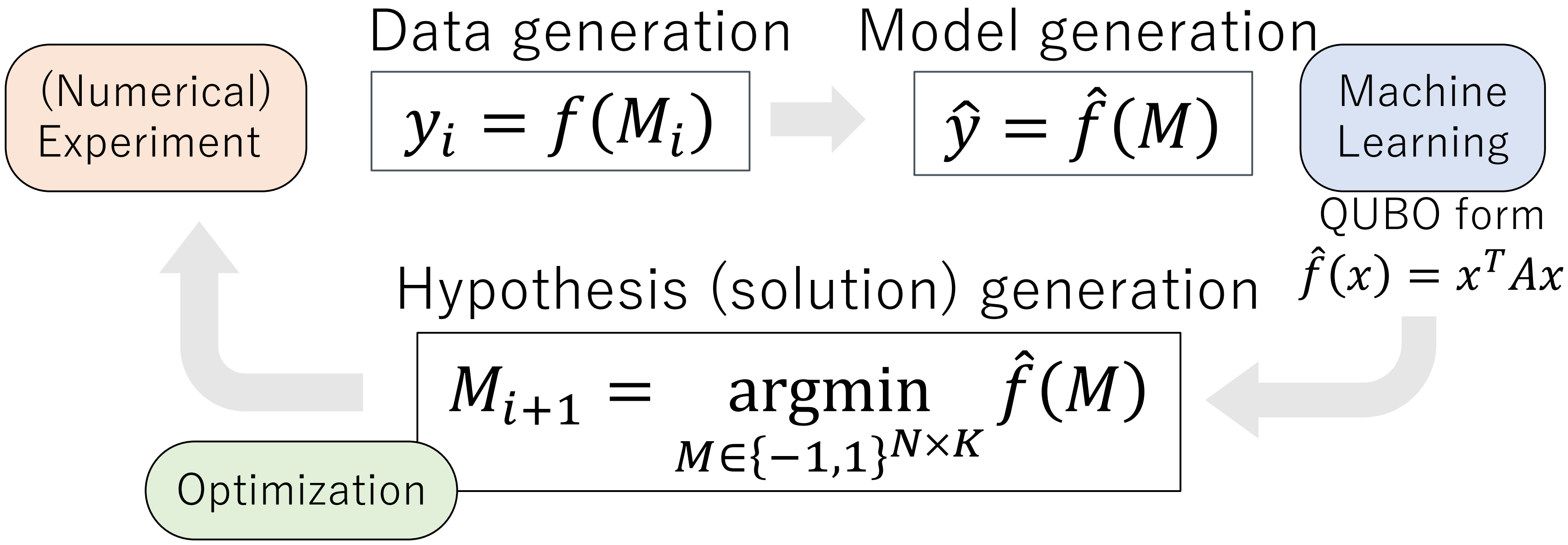
Black-box optimization (BBO)

$$\underset{M}{\operatorname{argmin}} |W - M(M^T M)^{-1} M^T W|^2$$

Data driven approach to solve unknown cost functions

$$f(M) = |W - M(M^T M)^{-1} M^T W|^2$$

(Do not use this function explicitly in the optimization process)

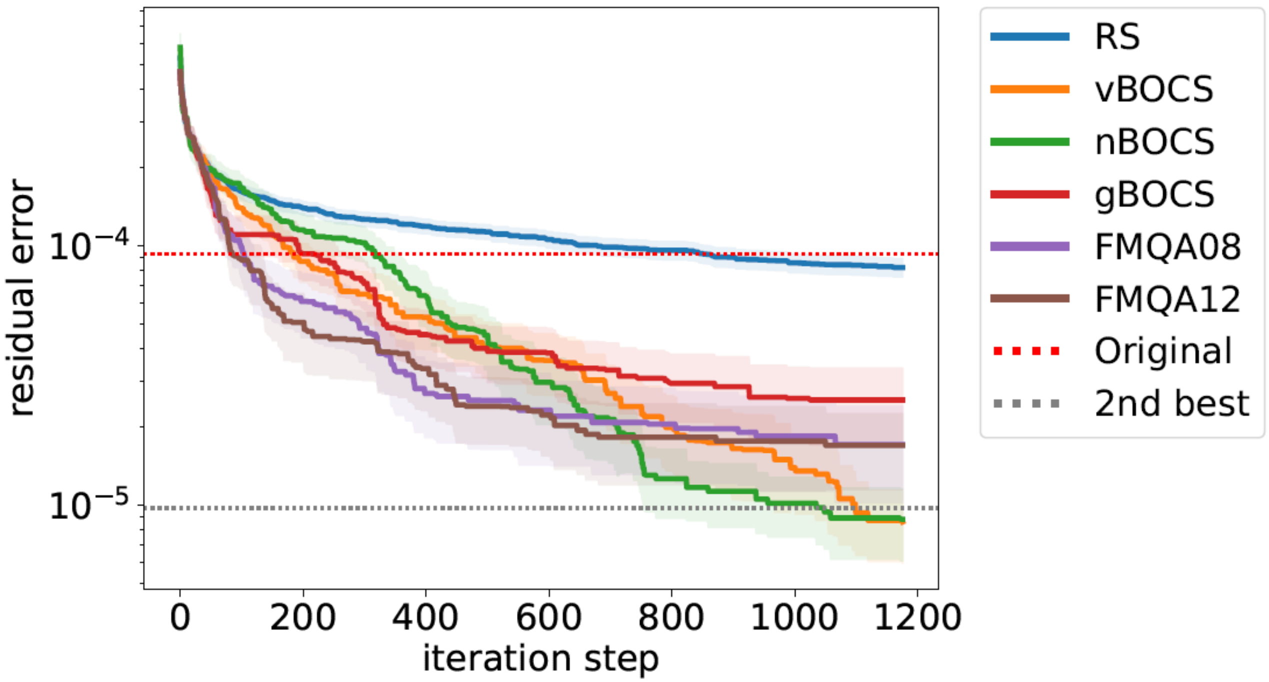


Kadowaki, T., Ambai, M., Sci Rep 12, 15482 (2022)

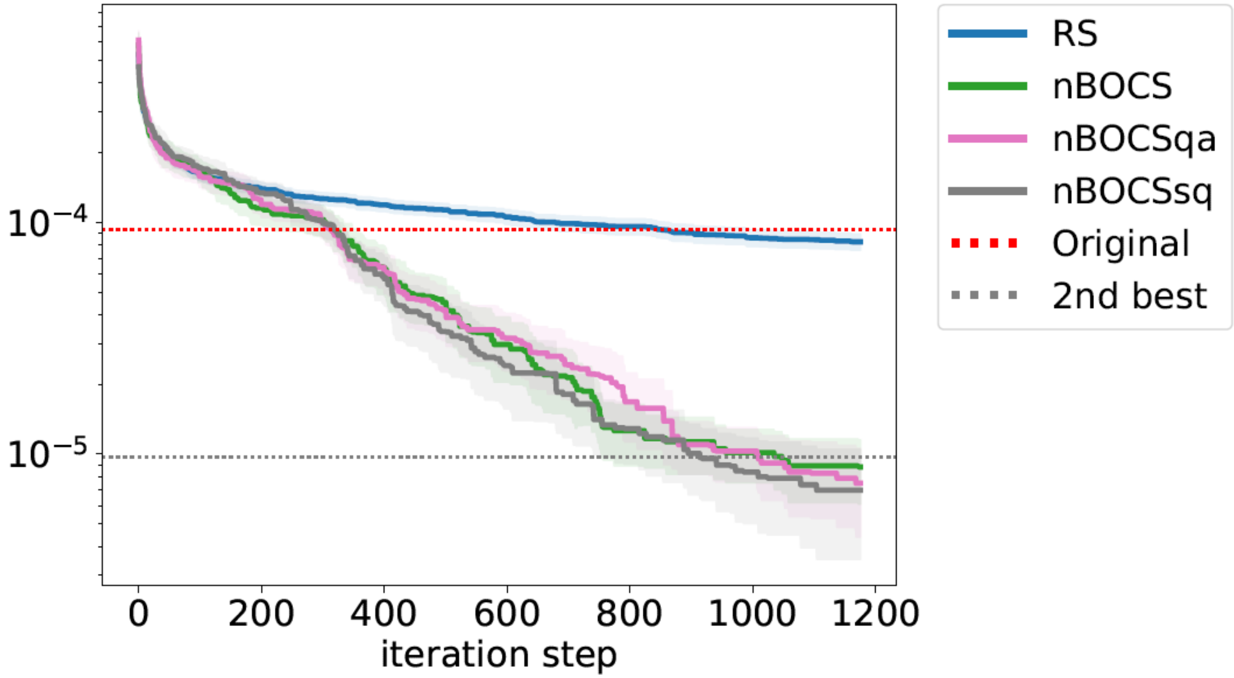
Results 1: residual error among algorithms

$W: 8\times 100, M: 8\times 3, C: 3\times 100$

BBO algorithm variations



SA vs QA vs Simulated Quenching (SQ)*



There is no significant difference among SA, QA and SQ

* Similar to SA, but quenching the temperature to zero immediately, greedy algorithm

Kadowaki, T., Ambai, M., Sci Rep 12, 15482 (2022)

Results 2: solution accuracy and execution time

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10 randomly generated instances, 25 independent runs

Table 1. Counts of finding exact soulution per 25 runs

Instance No.	RS	vBOCS	nBOCS	gBOCS	FMQA08	FMQA12	nBOCSqa	nBOCSsq	nBOCSa
1	0	7	7	2	1	3	9	**11**	0
2	1	6	11	5	6	9	12	**15**	1
3	0	0	**13**	5	6	9	10	2	4
4	1	16	**20**	10	10	13	14	17	0
5	0	0	1	0	3	**4**	2	1	0
6	0	14	12	4	6	4	18	**20**	0
7	0	1	4	6	7	**8**	7	6	0
8	1	**4**	2	2	**4**	1	**4**	1	0
9	1	5	1	3	3	4	**6**	4	0
10	5	21	20	15	20	21	22	**25**	6
Total	9	74	91	52	66	76	**104**	102	11

Table 2. Average execution time (s) per run

	RS	vBOCS	nBOCS	gBOCS	FMQA08	FMQA12	nBOCSqa	nBOCSsq	nBOCSa
CPU	0.72	7165.06	55.39	112.39	3711.31	3625.92	241.46	55.94	319.98
QPU	-	-	-	-	-	-	11.60	-	-

(Numerical) Experiment — Light

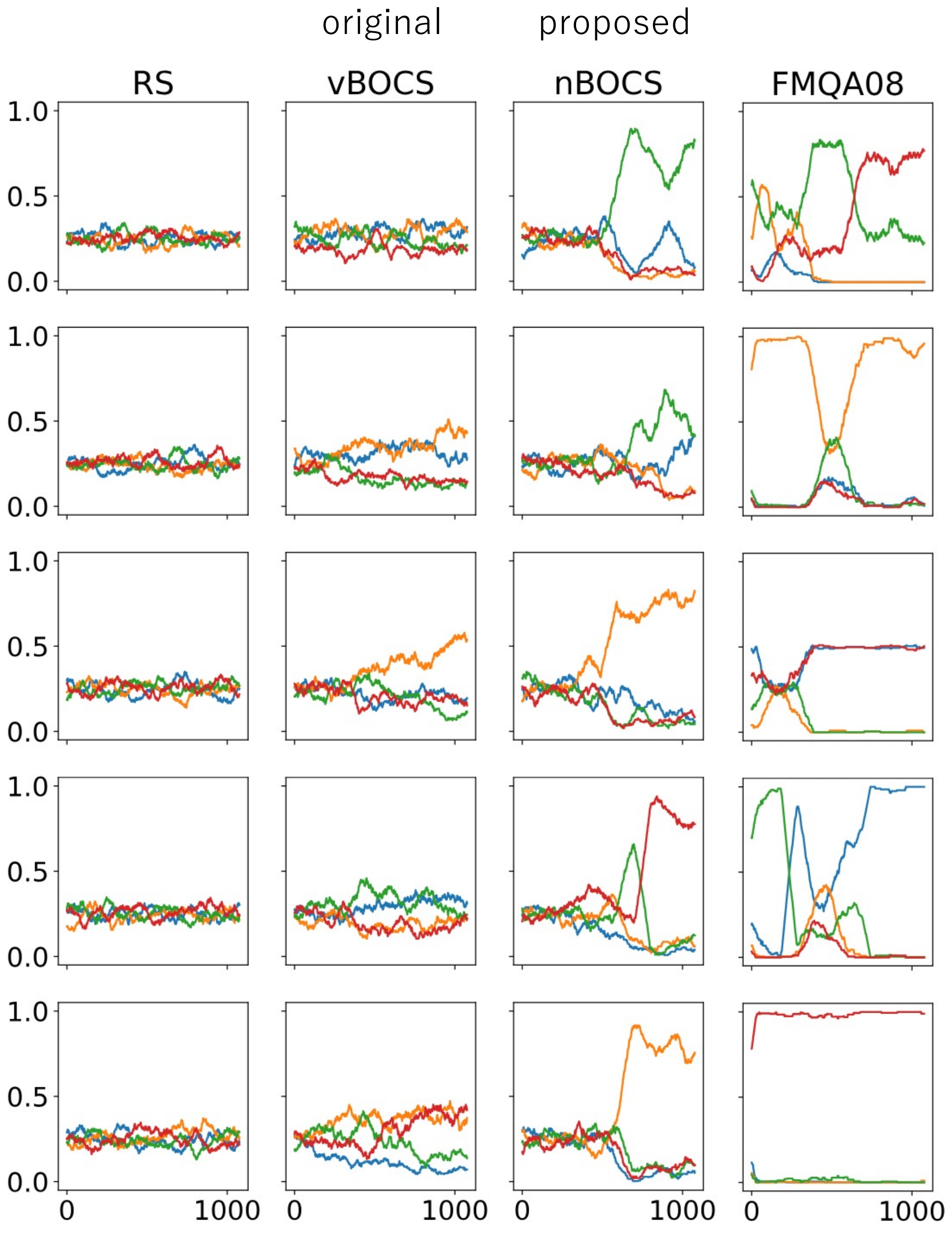
Machine Learning — Heavy!

Optimization — Light

original BOCS :	2 hours
proposed BOCS :	1 min.
FMQA :	1 hour

The proposed BOCS is fast and accurate!

Kadowaki, T., Ambai, M., Sci Rep 12, 15482 (2022)



Balance between exploration and exploitation

		original		proposed		
Exploration: RS	>	BOCS	>	BOCS	>	FMQA
Exploitation: RS	<	BOCS	<	BOCS	<	FMQA

The proposed BOCS is well balanced!

Kadowaki, T., Ambai, M., Sci Rep 12, 15482 (2022)

Agenda

- Automation in Science

  How science is automated by AI.

- Level 3 automation and Computer Aided Engineering (CAE)

  Current automation level in science and engineering

- 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)

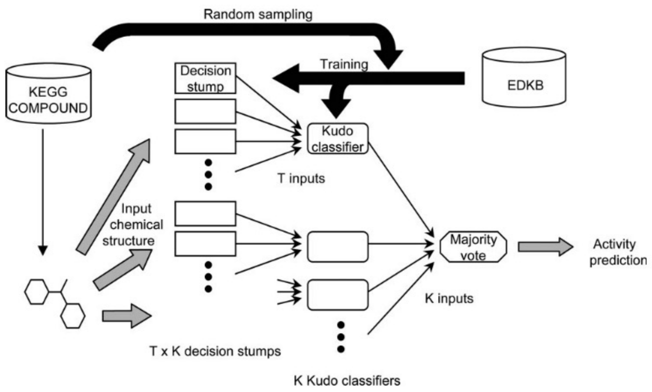


FIGURE 1. Overview of the prediction system. Each decision stump determines if a given chemical contains a specific substructure. A Kudo classifier integrates the weighted *T* inputs and provides an output consisting of a binary prediction, (e.g., active or inactive). These *K* outputs are used to generate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

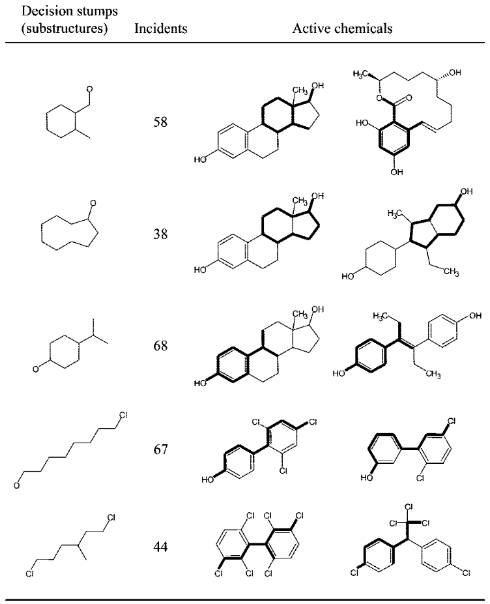
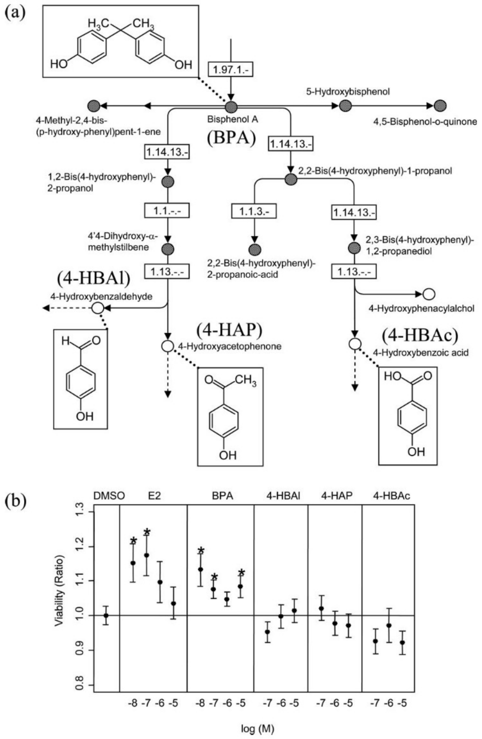


FIGURE 2. Decision stumps for active chemicals commonly used in Kudo classifiers. Matched substructures are drawn with thick lines. The frequencies of decision stumps in 100 Kudo classifiers are also displayed.



(Knowledge) (Hypothesis) (Data)

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

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)

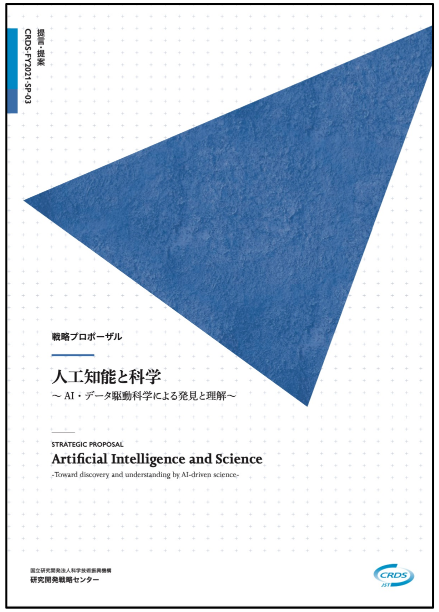
  Automated Research Workflows for Accelerated Discovery

  Closing the Knowledge Discovery Loop

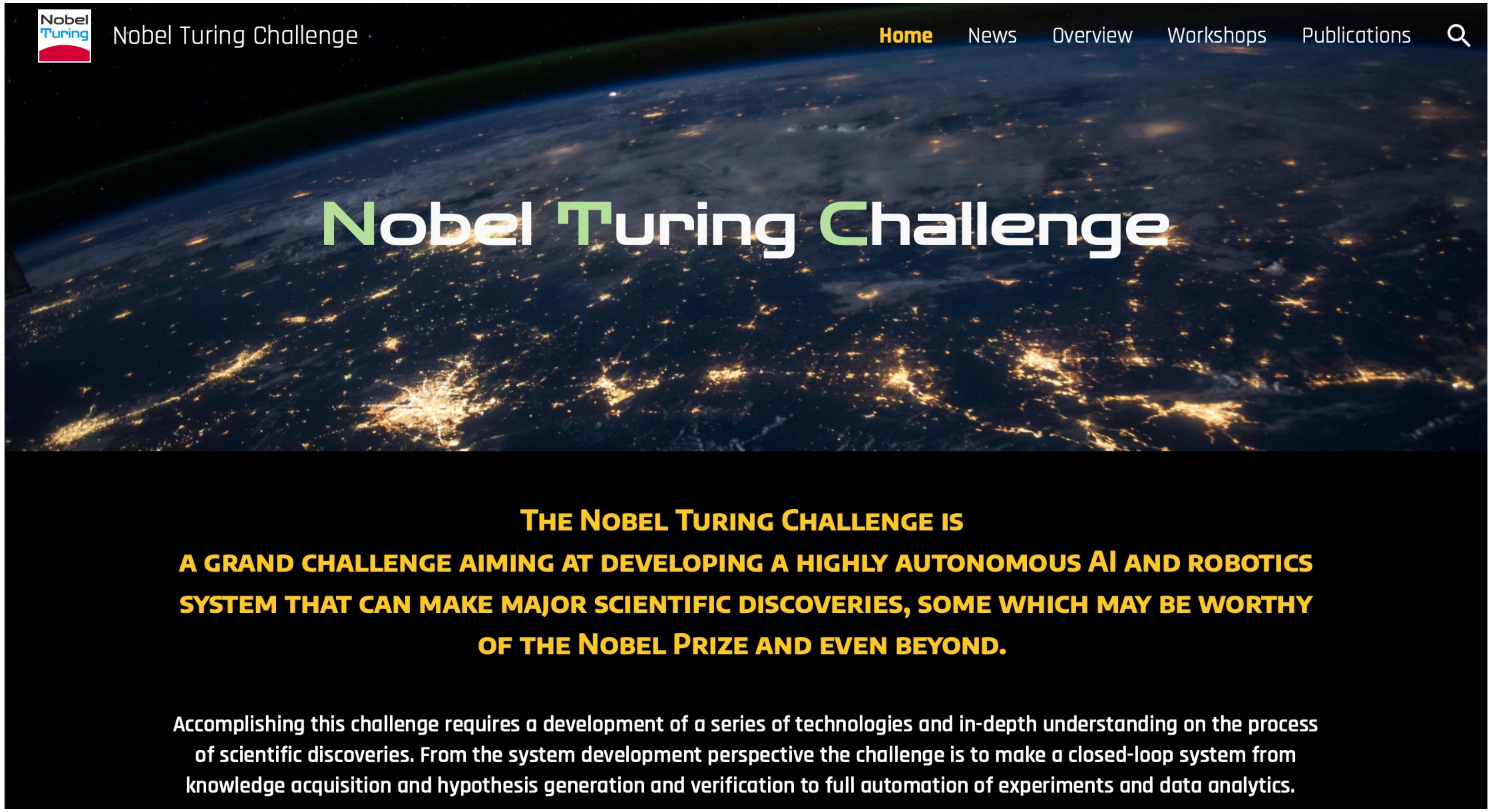
- **OECD** DOI:10.1787/a8d820bd-en (2023)

  Artificial Intelligence in Science:

  Challenges, Opportunities and the Future of Research



Nobel Turing Challenge



2009

- King, R.D., Rowland, J., Oliver, S.G., Young, M., Aubrey, W., Byrne, E., Liakata, M., Markham, M., Pir, P., Soldatova, L.N., Sparkes, A., Whelan, K.E. and Clare, A. **The Automation of Science.** Science 324, 85-89 (2009). https://doi.org/10.1126/science.1165620

https://www.nobelturingchallenge.org

npj Syst Biol Appl **7**, 29 (2021)

npj Systems Biology and Applications

www.nature.com/npjsba

PERSPECTIVE OPEN

Check for updates

Nobel Turing Challenge: creating the engine for scientific discovery

Hiroaki Kitano[1]

Scientific discovery has long been one of the central driving forces in our civilization. It uncovered the principles of the world we live in, and enabled us to invent new technologies reshaping our society, cure diseases, explore unknown new frontiers, and hopefully lead us to build a sustainable society. Accelerating the speed of scientific discovery is therefore one of the most important endeavors. This requires an in-depth understanding of not only the subject areas but also the nature of scientific discoveries themselves. In other words, the "science of science" needs to be established, and has to be implemented using artificial intelligence (AI) systems to be practically executable. At the same time, what may be implemented by "AI Scientists" may not resemble the scientific process conducted by human scientist. It may be an alternative form of science that will break the limitation of current scientific practice largely hampered by human cognitive limitation and sociological constraints. It could give rise to a human-AI hybrid form of science that shall bring systems biology and other sciences into the next stage. The Nobel Turing Challenge aims to develop a highly autonomous AI system that can perform top-level science, indistinguishable from the quality of that performed by the best human scientists, where some of the discoveries may be worthy of Nobel Prize level recognition and beyond.

npj Systems Biology and Applications (2021)7:29 ; https://doi.org/10.1038/s41540-021-00189-3

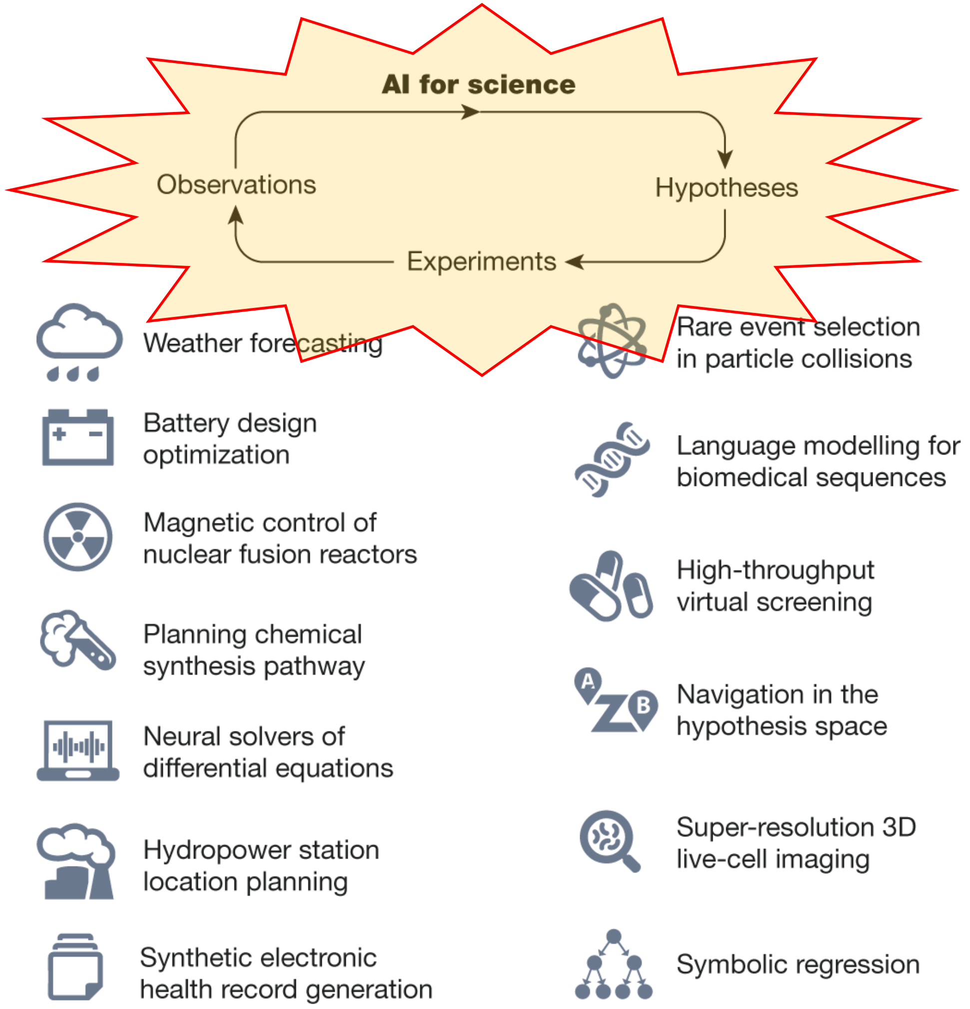
(1) Science of science (2) Beyond the human cognitive limitation

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.



Wang, et al. Nature 620, 47 (2023)

Simplified process of scientific discoveries

AIST
Create the Future, Collaborate Together

iPS

SEARCH and OPTIMIZATION

Goal: Reprogram Cell to gain Stemness

SEARCH — Search 24 genes from FANTOM DB

24 genes enabled reprogramming

OPTIMIZATION — Leave-one-out experiments

Yamanaka Factors identified

Nobel Prize in Physiology and Medicine 2012

Conducting polymer

ACCIDENT, SEARCH and OPTIMIZATION

Accidental discovery of thin film formation in polyacetylene polymerization process

ACCIDENT

Goal: Polyacetylene thin film formation condition

OPTIMIZATION — Search optimal thin film formation condition

Prof. Alan MacDiarmid

Goal: Conducting polymer

SEARCH & OPTIMIZATION — Prof. Alan Heeger

Conducting polymer thin film

Nobel Prize in Chemistry 2000

Kitano, H. Nobel Turing Challenge: creating the engine for scientific discovery. *npj Syst Biol Appl* **7**, 29 (2021)

FANTOM: Hight quality mouse genome database

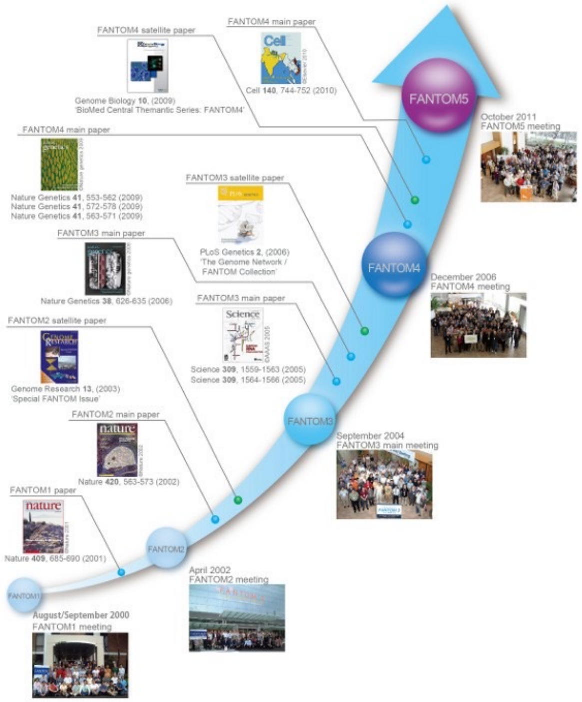
FANTOM
FUNCTIONAL ANNOTATION OF THE MAMMALIAN GENOME

日本語

Home | Data | Views | Protocols | Software | Papers | FAQ

shortcut links to COVID-19/SARS-CoV-2 related genes

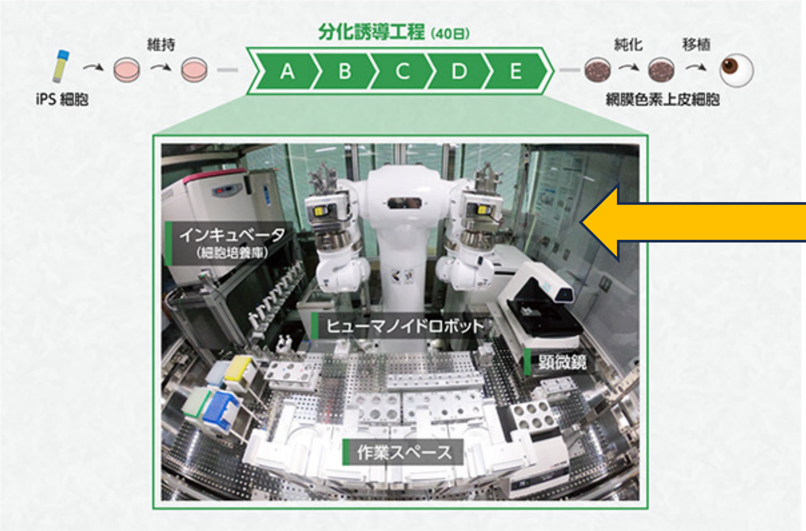
gene	FANTOM5 SSTAR	ZENBU	UCSC Genome Browser
ACE2	ACE2 gene	hg19 / hg38	hg19 / hg38
TMPRSS2	TMPRSS2 gene	hg19 / hg38	hg19 / hg38



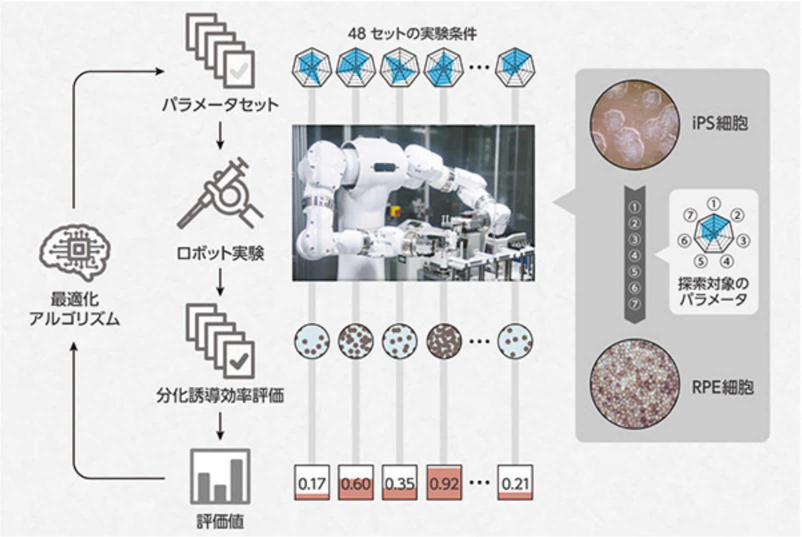
Simultaneously with producing data, FANTOM established the FANTOM database and the FANTOM full-length cDNA clone bank, which are available worldwide. The FANTOM resources have been used in several important research projects. For instance, the full-length cDNA database was used in a computer prediction of the genomic position (transcriptional unit) of genes by the International Human Genome Sequencing Consortium. Also they have been used by a research group led by Dr. Shinya Yamanaka at Kyoto University, Japan, for establishing Induced pluripotent stem (iPS) cells. In the study, 24 transcription factors were selected from FANTOM database as candidate initiation factors. Furthermore, the Allen Institute for Brain Science in the United State has created a digital atlas that encompasses the whole brain, and has made it publicly available. The atlas graphically illustrates the expression of genes within the mouse brain using Informatix software. This project has also made use of the FANTOM database.

https://fantom.gsc.riken.jp

Robot scientist and laboratory of the future



YASUKAWA Electric & AIST
https://www.aist.go.jp/aist_j/highlite/2015/vol3/index.html

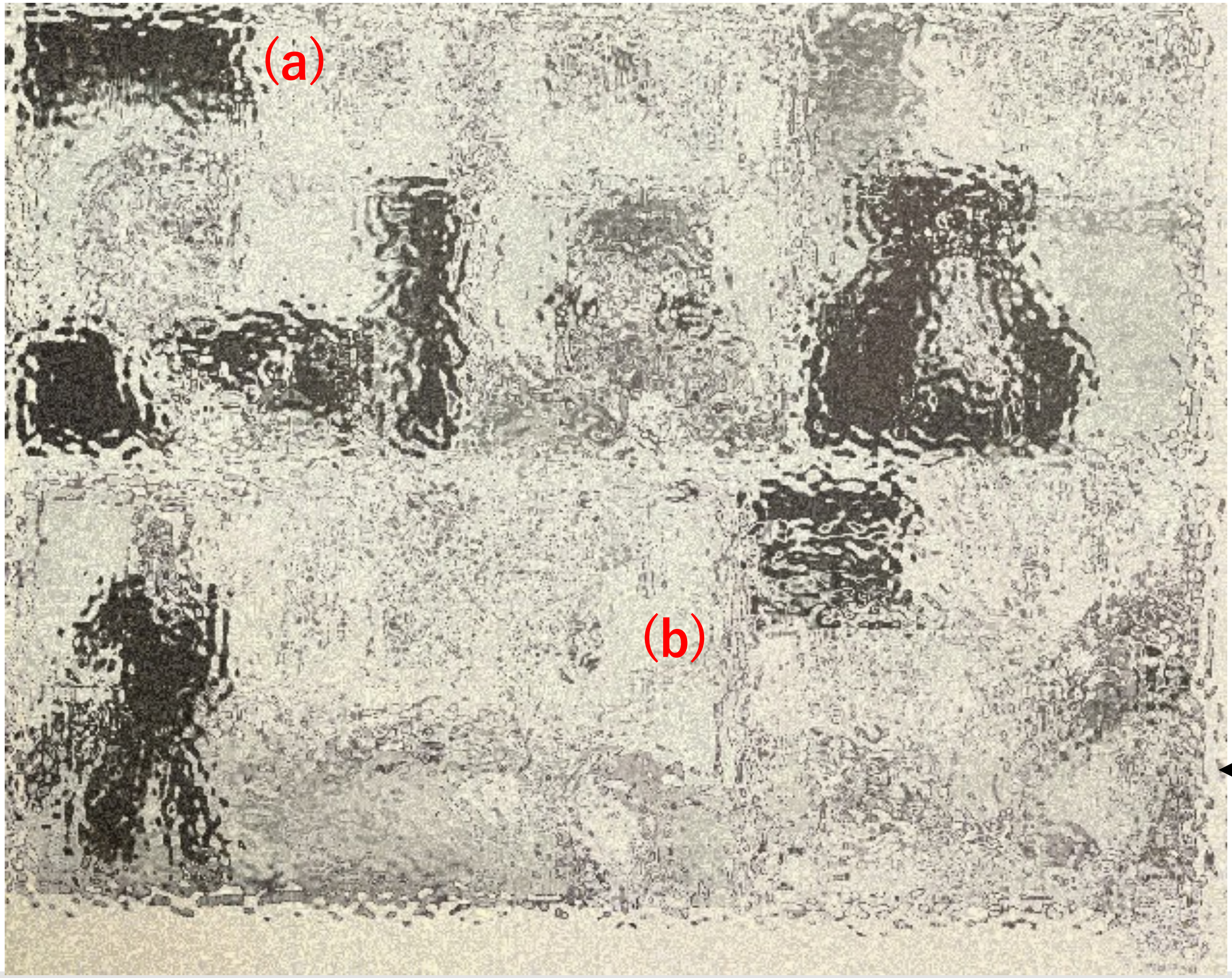


Robot & AI ＋ Human

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

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

Robot scientist was predicted in old Sci-Fi, such as
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)



← Sultan

(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

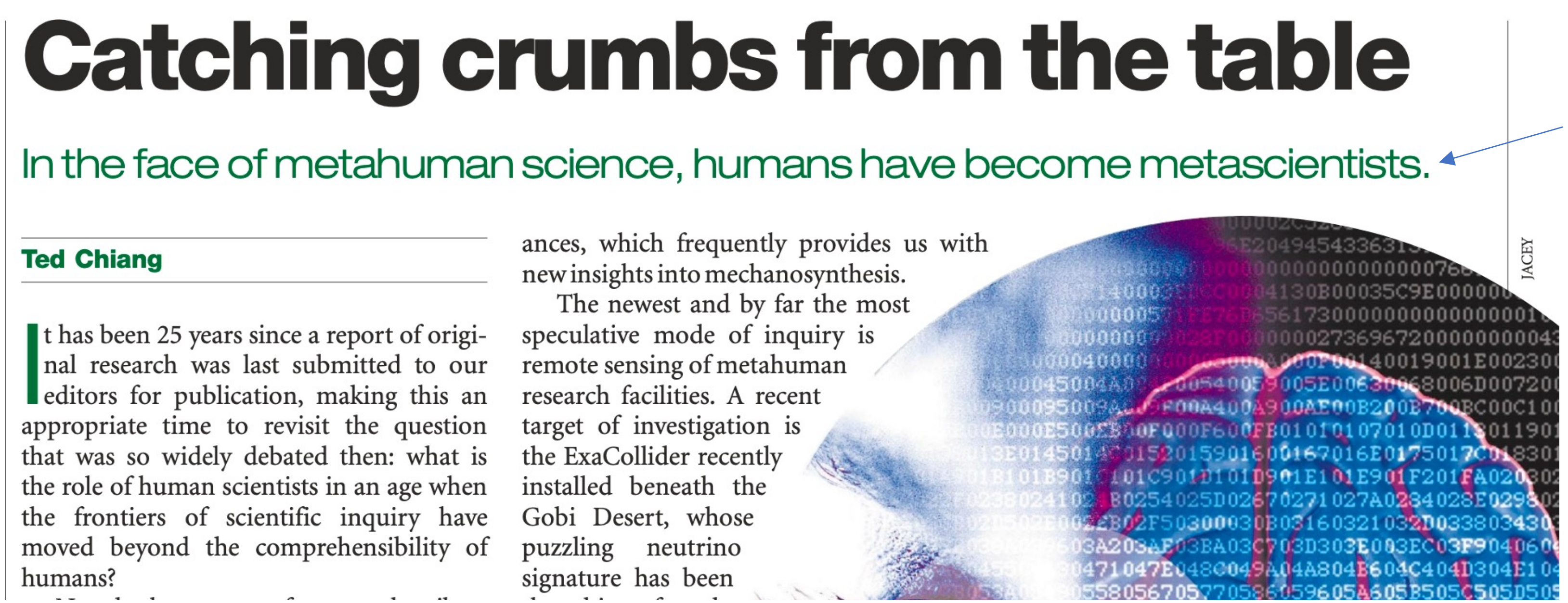
Robot scientist in Sci-Fi, a quarter of a century ago by Ted Chiang

AIST
Create the Future, Collaborate Together

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

JACEY

Palaeography
(古文書の解読)

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

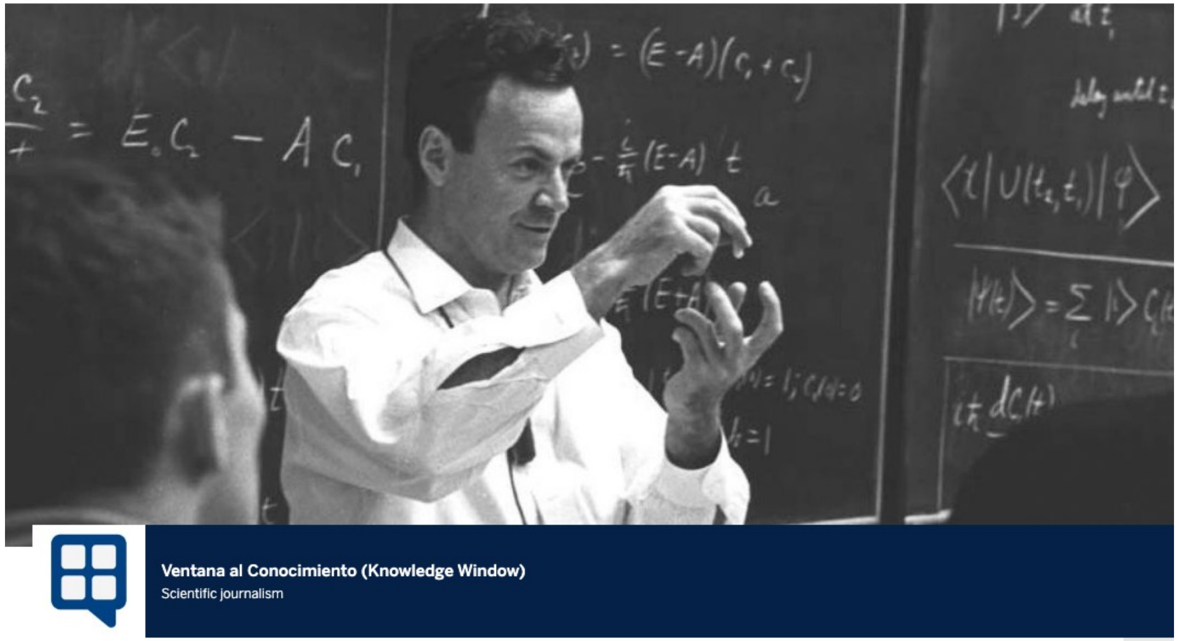
"But as metahumans began to dominate experimental research, they increasingly made their findings available only via DNT (digital neural transfer), leaving journals to publish second-hand accounts translated into human language." => Beyond the human cognitive limitation

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



"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

YouTube JP 検索

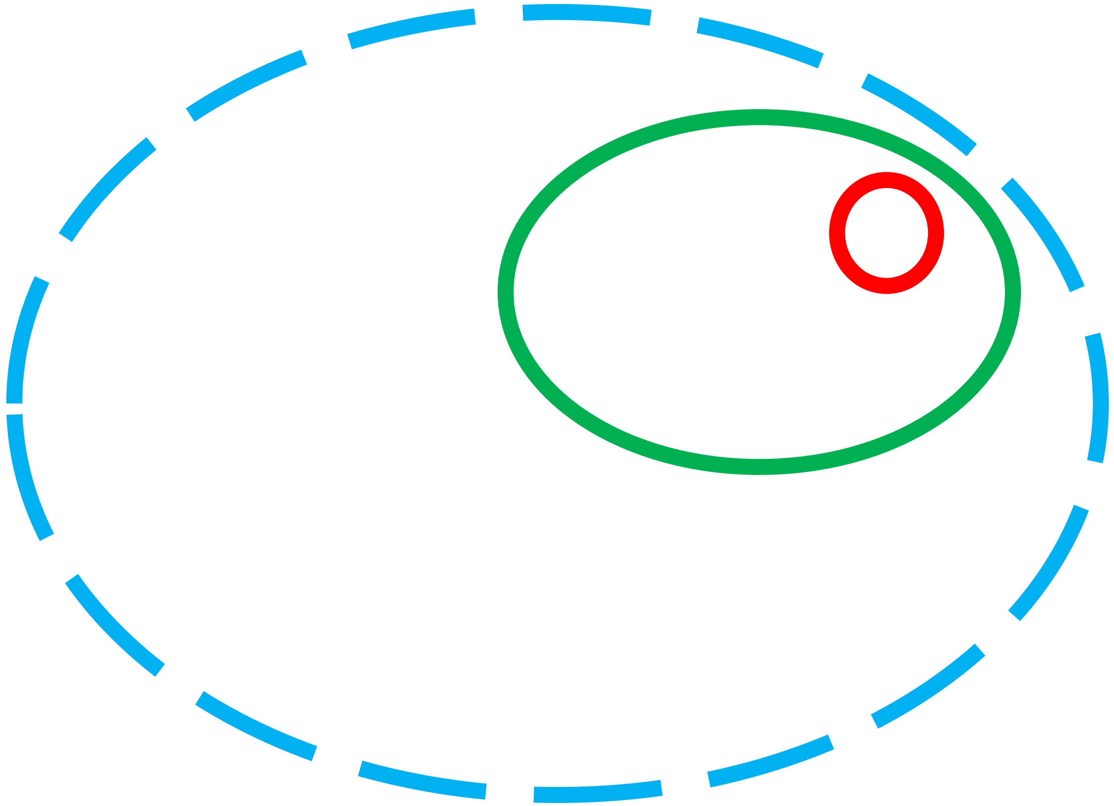
Feynman - Nobody understands Quantum Mechanics

https://www.youtube.com/watch?v=w3ZRLlIWgHI&t=23s

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

Hypothesis space of science

“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



Discovered knowledge
=**State of the art (SOTA) boundary**

Human discoverable knowledge
(Human cognitive limitation)
=**Feynman boundary**

An entire hypothesis space of science
(explored by robot scientists with their own language)

Kitano, H. Nobel Turing Challenge: creating the engine for scientific discovery. *npj Syst Biol Appl* **7**, 29 (2021)

Agenda

- Automation in Science

  How science is automated by AI.

- Level 3 automation and Computer Aided Engineering (CAE)

  Current automation level in science and engineering

- Quantum CAE

  How quantum computing accelerates engineering and science.

- Summary

Automation of Science & self-driving

AIST
Create the Future, Collaborate Together

Perfect information game

Imperfect information game

JST CRDS Artificial Intelligence and Science

SAE Levels of Driving Automation™

Level 3 automation (here now)

特定の閉じた系で完全情報ゲームとしてAI システムが探索・最適化を行う。関係する全ての要素のデータが揃っており、モデルに不明な変数はないと仮定する。ゴールや評価関数は人間が明示的に機械可読な形で与える。

In a specific closed system, an AI system conducts exploration and optimization as a perfect information game. It is assumed that all data on the relevant elements are available, and there are no unknown variables to the model. Goals and measures are explicitly provided by humans in a machine-readable format.

(defined in JST CRDS Artificial Intelligence and Science [translated])

Well-known applications:

- Reinforcement learning in Go (AlphaGo)
- Bayesian optimization
    - Hyperparameter tuning in deep neural networks
    - Optimization in bioinformatics, cheminformatics, material informatics, process informatics, and so on.

What we do in science

Description from National Academies' white paper,
Automated Research Workflows for Accelerated Discovery

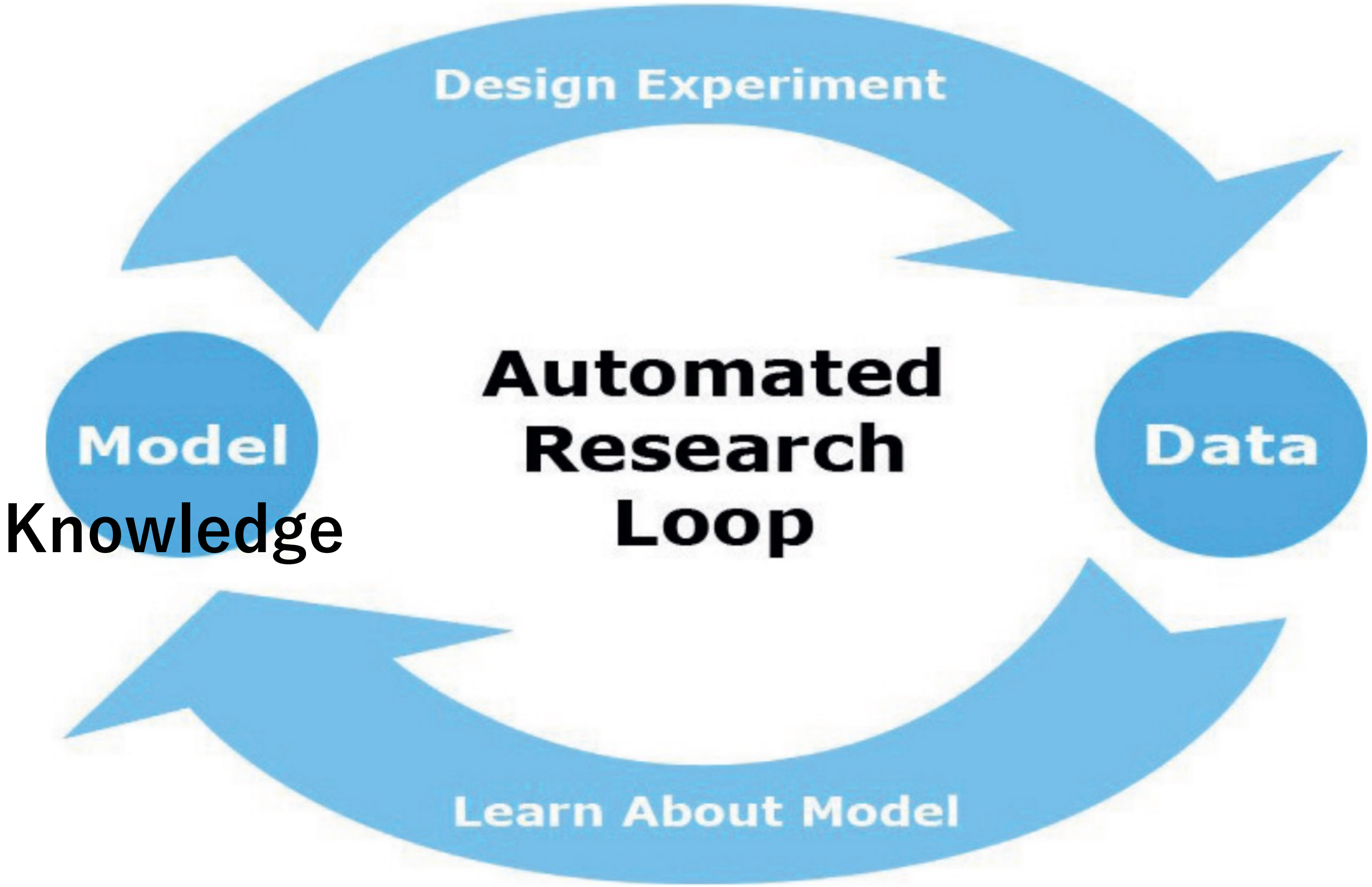


FIGURE 2-1 Knowledge discovery loop.

This loop is equivalent to level 3 automation.

Measure: experiment

Goal: maximize the measure

Beyond a typical scientific study (after automation)

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

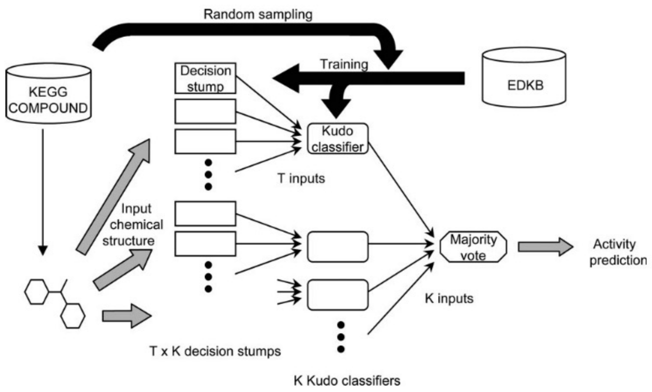


FIGURE 1. Overview of the prediction system. Each decision stump determines if a given chemical contains a specific substructure. A Kudo classifier integrates the weighted *T* inputs and provides an output consisting of a binary prediction, (e.g., active or inactive). These *K* outputs are used to generate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

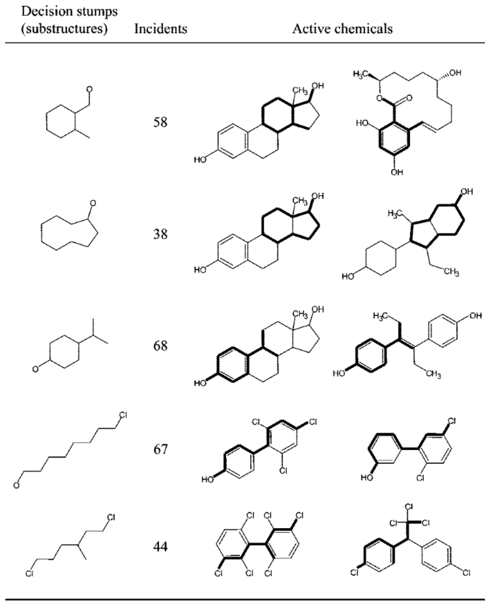
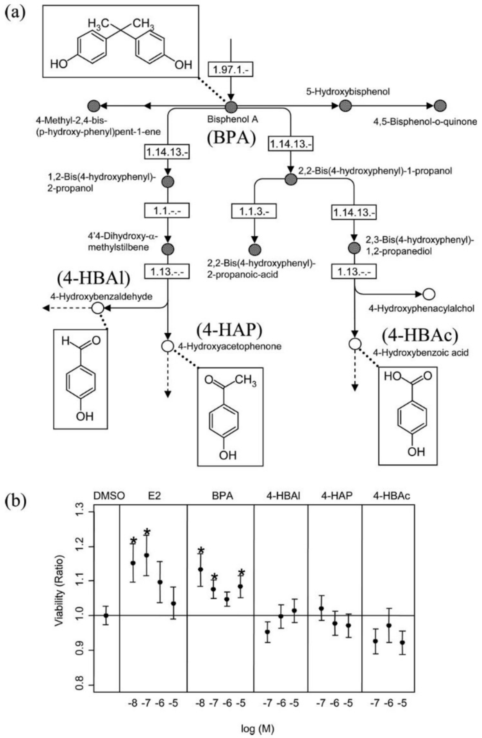


FIGURE 2. Decision stumps for active chemicals commonly used in Kudo classifiers. Matched substructures are drawn with thick lines. The frequencies of decision stumps in 100 Kudo classifiers are also displayed.

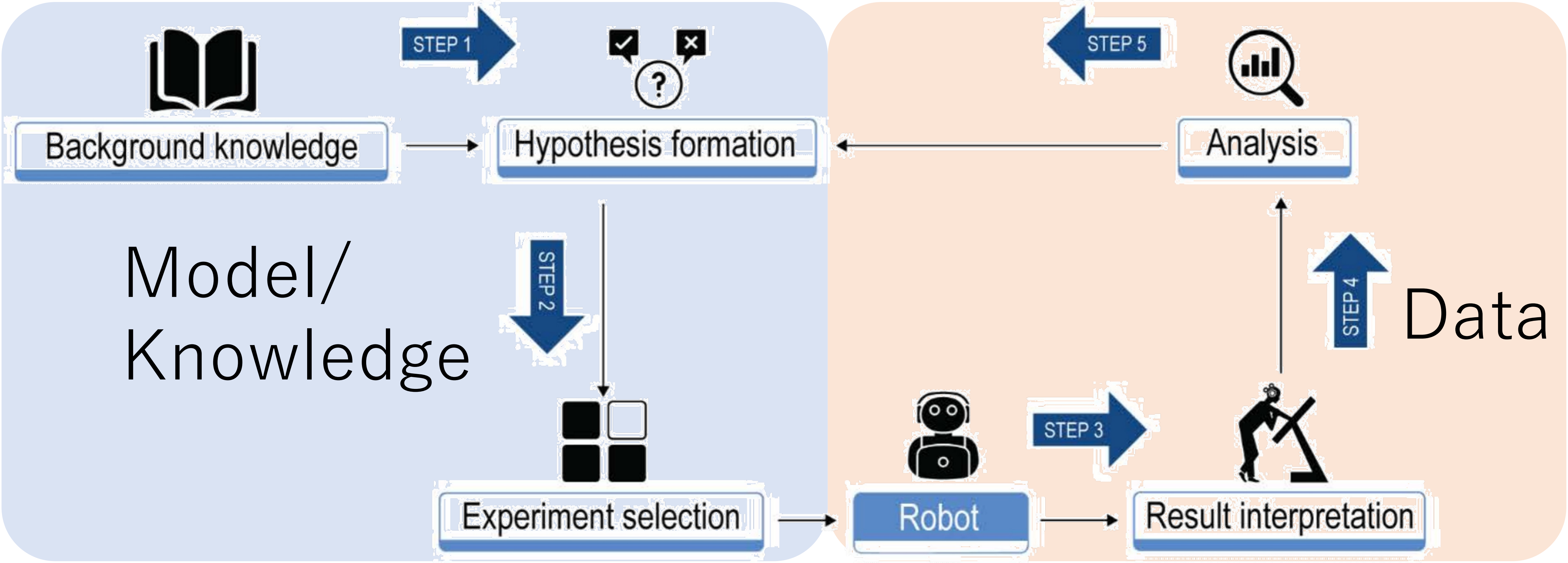


(Knowledge) (Hypothesis) (Data)

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

Ross King's Robot scientist

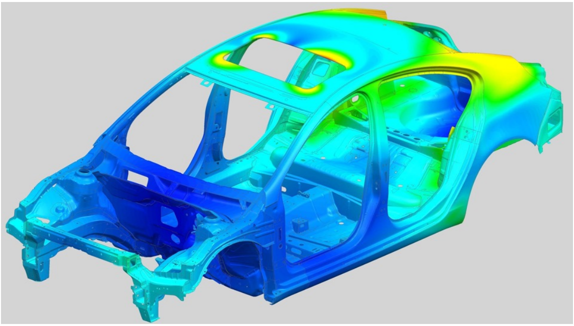
Figure 1. The robot scientist closed-loop cycle of experiments



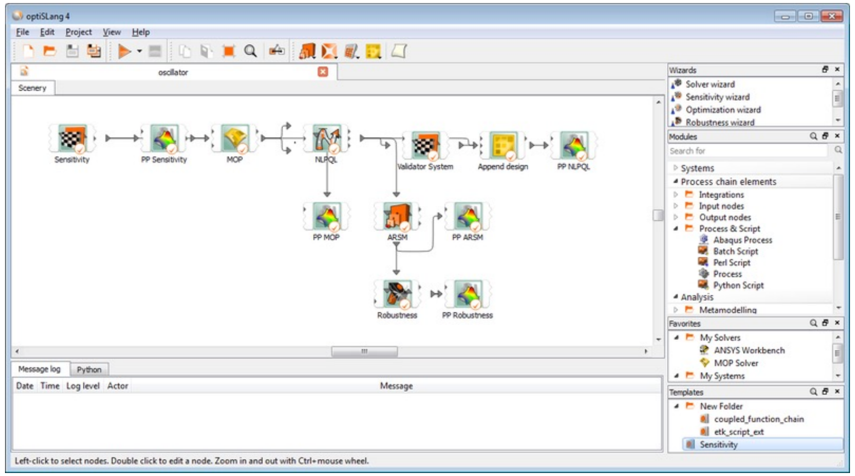
OECD, Artificial Intelligence in Science
King, R., Whelan, K., Jones, F. et al., Nature 427, 247–252 (2004)

Automation in CAE

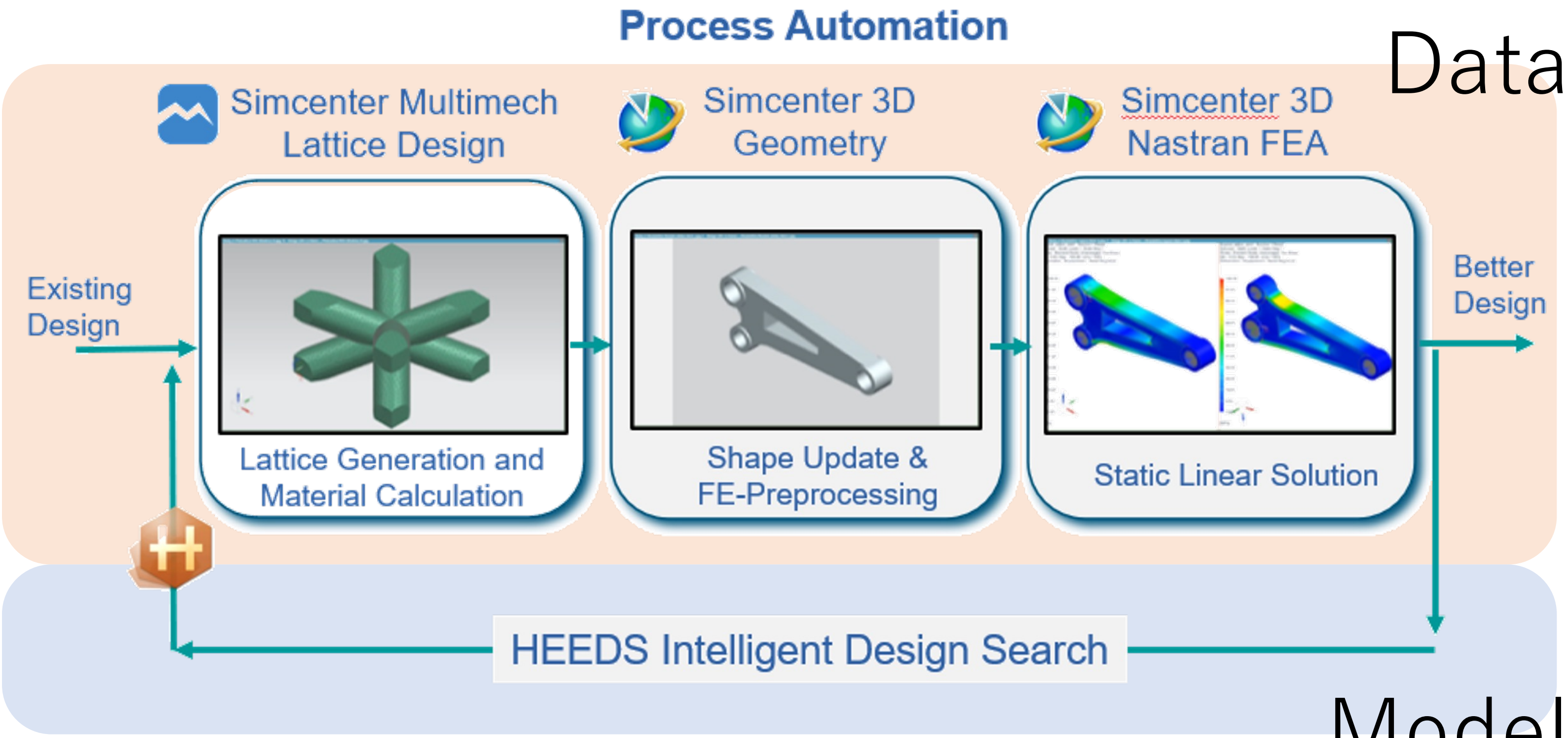
Data (simulation)



Design automation process



Closed loop of Data & Model



Data

Model

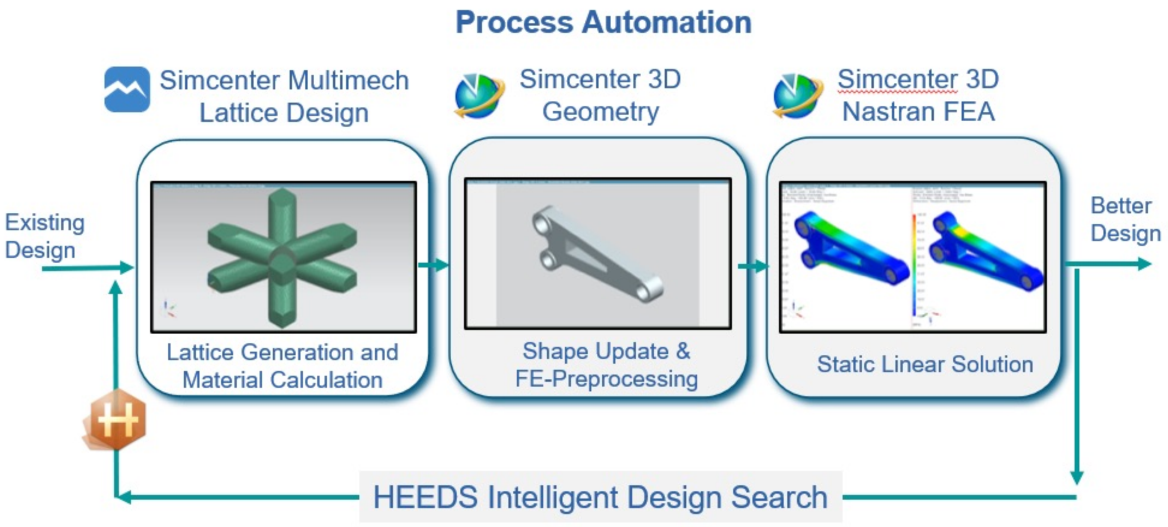
https://webinars.sw.siemens.com/en-US/cae-vehicle-structural-analysis-process/
https://blogs.sw.siemens.com/nx-design/design-for-purpose-heeds-design-exploration-study/
https://www.ansys.com/content/dam/product/platform/optislang/optislang-brochure.pdf

Automation in CAE and science

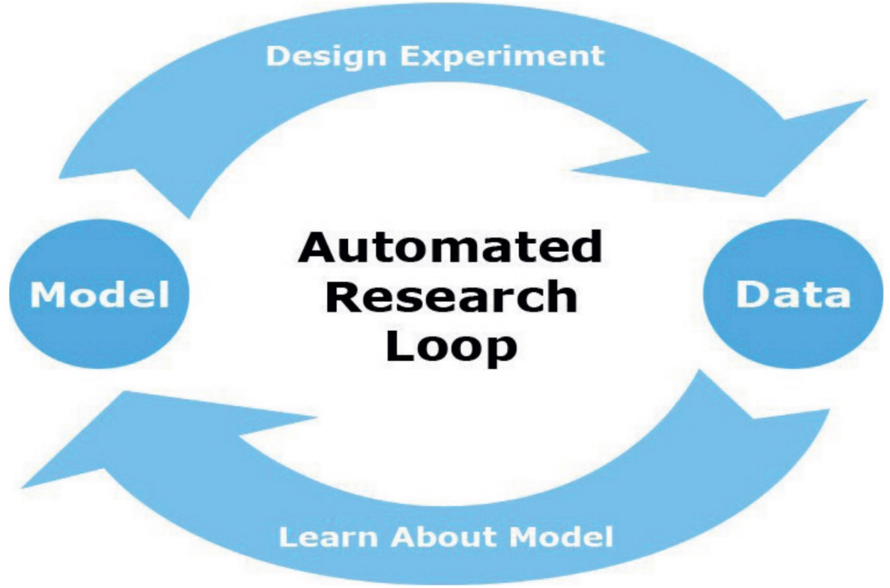
CAE

Science

Closed loop of Data & Model



≈



≈ e.g. Bayesian Optimization

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  How quantum computing accelerates engineering and science.

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Implementation of the loop & CAE

Inverse problem (optimization)

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

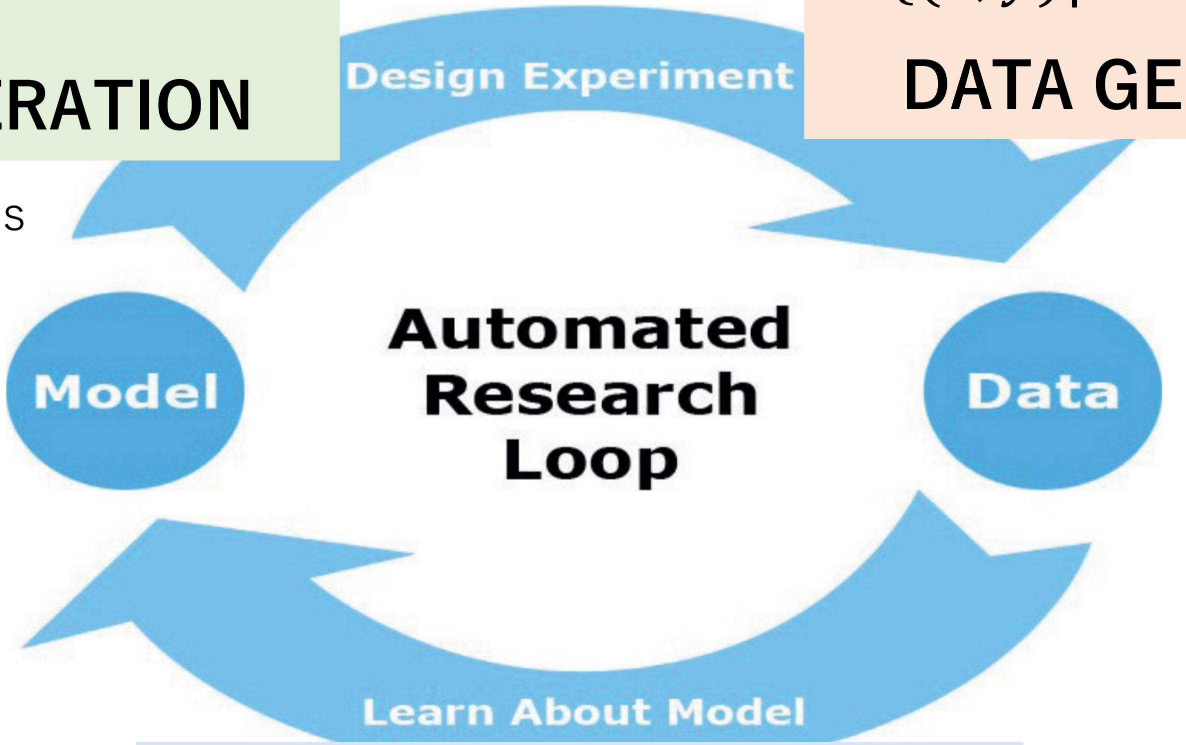
HYPOTHESIS GENERATION

† 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

From classical to quantum

The loop

DATA GENERATRION

MODEL GENERATION

HYPOTHESIS GENERATION

→

Potential speed-up by

Quantum Simulation (QSim)

Quantum Machine Learning (QML)

Quantum Optimization (Qopt)

Factorization Machine Quantum Annealing (FMQA)

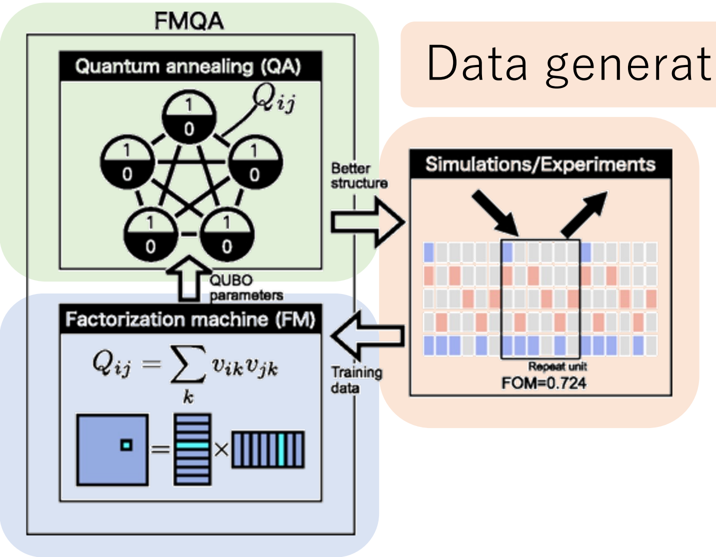
Solving combinatorial optimization

Closed loop

Hypothesis generation

Data generation

Model generation



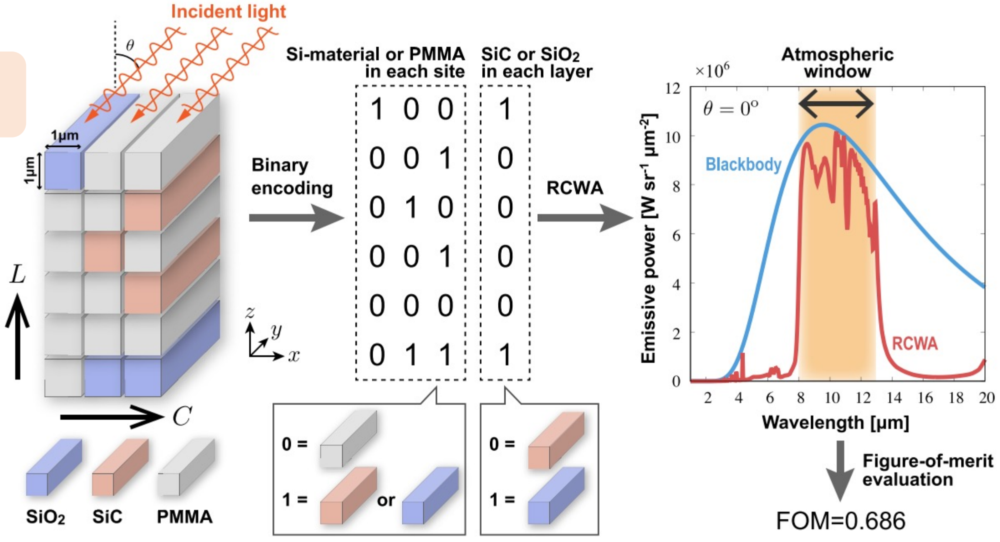
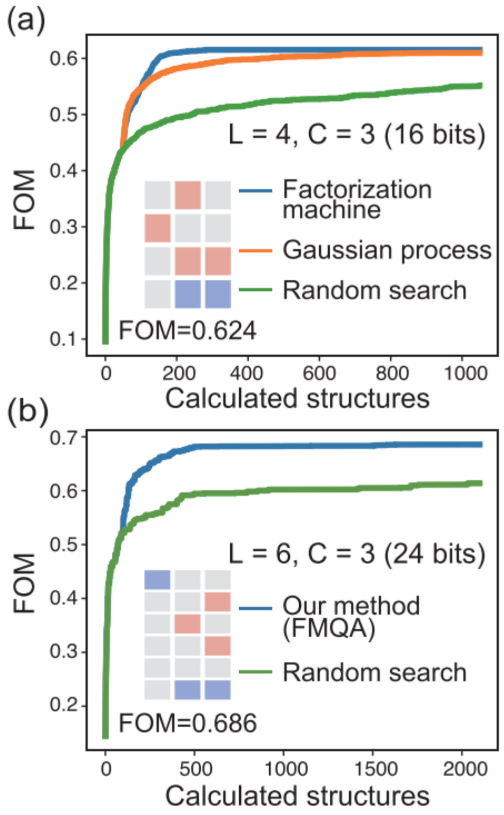


FIG. 2. Example of the target metamaterial structure for $L = 6$ and $C = 3$, the binary variables expressing it, and the emissive powers of target metamaterial (red curve) and blackbody (blue curve) calculated by RCWA.



Kitai et. al., Phys. Rev. Res. 2, 013319 (2020)

BOCS, FMQA and other applications

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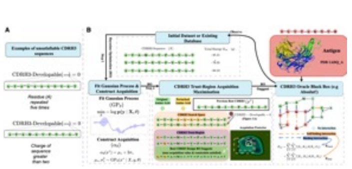
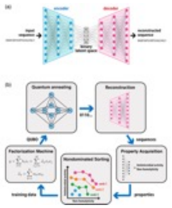
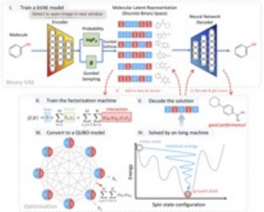


Antibody design
(Khan+ 2023)

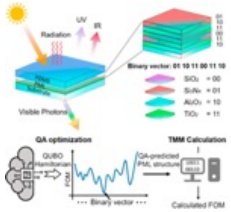


Antimicrobial peptides
(Tučs+ 2023)

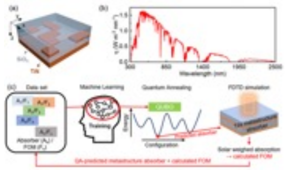


Chemical design
(Mao+ 2023)

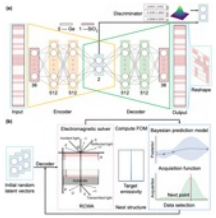
Medicine



Radiative cooler
(Kim+ 2023)

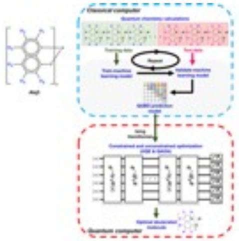


Solar absorber
(Kim+ 2023)



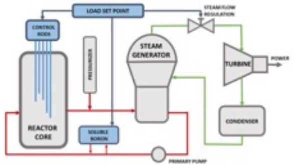
Thermal radiation
(Zhu+ 2022)

Optics



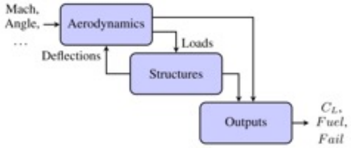
OLED design
(Gao+ 2023)

Chemistry



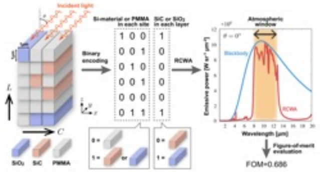
Plant control
(Drouet+ 2020)

Data compression
(Kadowaki+ 2022)

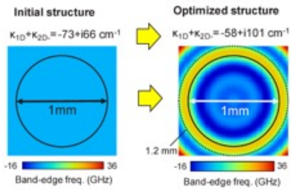


BOCS
Model parameter reduction
(Baptista+ 2018)

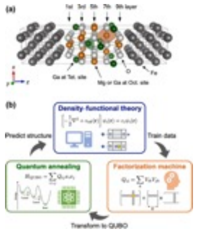
Data science



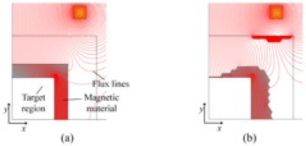
FMQA
wavelength selective radiator
(Kitai+ 2020)



Photonic crystal laser
(Inoue+ 2022)

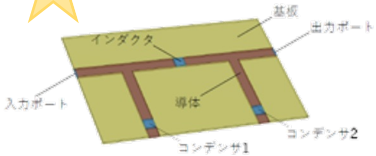


Barrier materials in MTJ
(Nawa+ 2023)



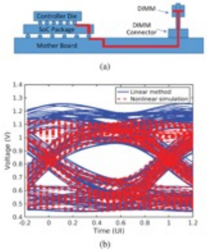
Magnetic shield
(Maruo+ 2022)

Spintronics & Magnetism

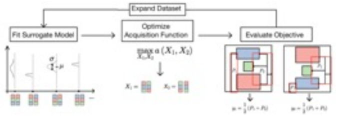


Noise filter
(Okada+ 2023)

Mounting holes
(Matsumori+ 2022)



Circuit analysis
(Dou+ 2022)



Chip design
(Oh+ 2022)

Electronics

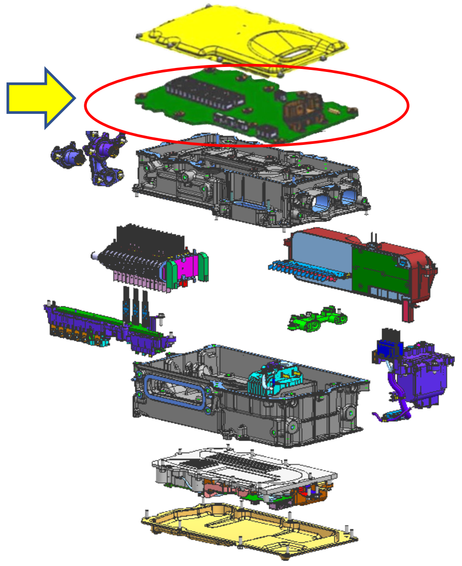
FMQA
https://scholar.google.com/scholar?cites=10314403103808168179
Protonic crystal laser
https://opg.optica.org/oe/fulltext.cfm?uri=oe-30-24-43503&id=520202
Polymer
https://pubs.rsc.org/en/content/articlelanding/2023/RA/D3RA01982A
Vacancies in graphene
https://pubs.aip.org/aip/jap/article/133/22/221102/2896017/Quantum-computing-and-materials-science-A
Multimolecular Adsorption
https://pubs.acs.org/doi/10.1021/jacsau.3c00018
Virtual Screening
https://journals.jps.jp/doi/10.7566/JPSJ.92.023001
OLED
https://spj.science.org/doi/10.34133/icomputing.0037
Noise Filter
https://ieeexplore.ieee.org/document/10113307
Au atomic junctions
https://iopscience.iop.org/article/10.35848/1882-0786/accc6d
Peptides
https://pubs.acs.org/doi/10.1021/acsmedchemlett.2c00487
structure design
https://www.nature.com/articles/s41598-022-16149-8
Polymer
https://onlinelibrary.wiley.com/doi/10.1002/marc.202200385
Radiative cooling
https://www.science.org/doi/10.1126/science.abb0971
Thermal transport
https://pubs.aip.org/aip/jap/article/128/16/161102/568437/Designing-thermal-functional-materials-by-coupling
Radiative cooler
https://pubs.acs.org/doi/10.1021/acsenergylett.2c01969
Solar Absorber
https://pubs.acs.org/doi/full/10.1021/acsami.3c08214
Thermal radiation
https://arxiv.org/abs/2205.01063
Chemical design
https://pubs.rsc.org/en/content/articlehtml/2023/dd/d3dd00047h
Meta surface design
https://ieeexplore.ieee.org/abstract/document/9573086
Barrier Materials
https://journals.aps.org/prapplied/abstract/10.1103/PhysRevApplied.20.024044

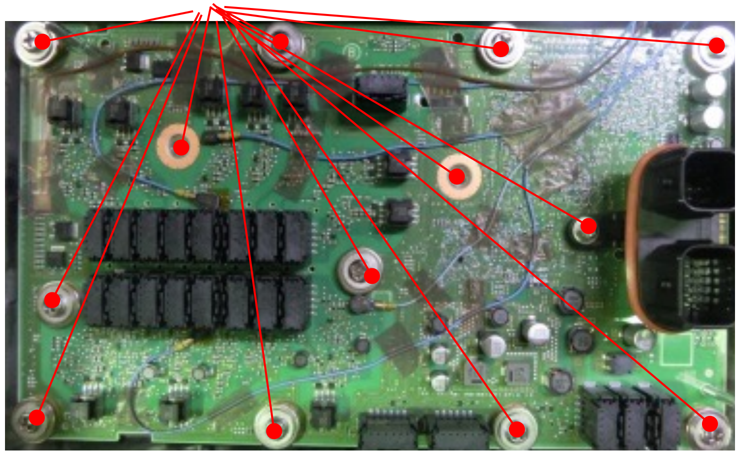
BOCS
https://scholar.google.co.jp/scholar?cites=1602326552169762893
Antibody
https://www.cell.com/cell-reports-methods/pdf/S2667-2375(22)00276-4.pdf
Macro placement (chip design)
https://arxiv.org/abs/2207.08398
Cyber–physical–social systems
https://asmedigitalcollection.asme.org/mechanicaldesign/article/143/7/071702/1094062/Design-of-Trustworthy-Cyber-Physical-Social
Banking
https://www.mdpi.com/2227-7099/9/4/205
Protein folding
https://arxiv.org/abs/2305.18089
Aerospace
https://arc.aiaa.org/doi/epdf/10.2514/6.2022-1614
Plant operation
https://dl.acm.org/doi/pdf/10.1145/3377930.3390206
(Noise filter)
https://ieeexplore.ieee.org/abstract/document/10113307
structure design
https://www.nature.com/articles/s41598-022-16149-8
Bus stop
https://link.springer.com/chapter/10.1007/978-3-030-45715-0_4
Nonlinear circuit
https://ieeexplore.ieee.org/abstract/document/9623363
https://ieeexplore.ieee.org/abstract/document/9574798
Adversarial attack
https://apps.dtic.mil/sti/citations/trecms/AD1194103

Printed circuit board design to protect from resonant vibration

Power control unit

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

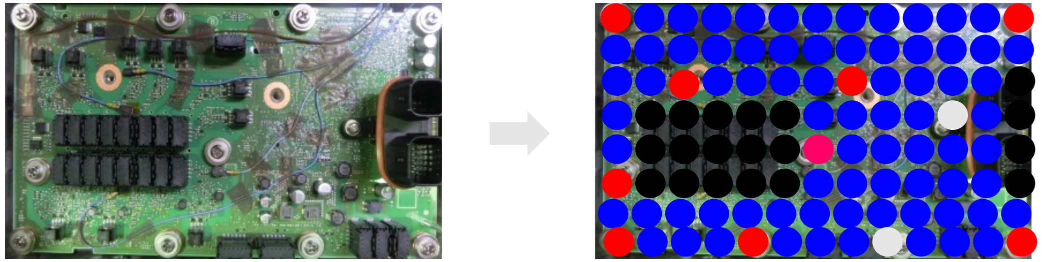




Printed circuit board

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.

Formulation



- candidates ($x_i = 0$)
- holes ($x_i = 1$)
- others

(candidates + holes: 85)

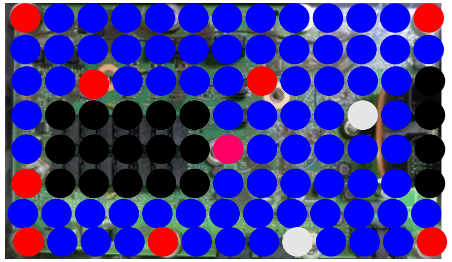
Objective functions

Total holes = cost	$N(\boldsymbol{x}) = \sum_{i=1}^{n} x_i$	
Normal mode freq. = spec.	Calculation of j-th data $(\boldsymbol{x}^{(j)}, f^{(j)})$ $G(\boldsymbol{x}^{(j)}) = [K(\boldsymbol{x}^{(j)}) - \lambda M(\boldsymbol{x}^{(j)})]\boldsymbol{u}$ $= 0$ $\to \lambda_0$ $\to f = \sqrt{\lambda_0}/2\pi$	Surrogate model (regression with cumulated data) $f(\boldsymbol{x}) \approx \hat{f}(\boldsymbol{x}) = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{Q}\boldsymbol{x} + b$

Multi-objective optimization $\underset{\boldsymbol{x} \in \{0,1\}^n}{\text{Minimize}} \{-\hat{f}, N\}$

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

Formulation (2)



- candidates ($x_i = 0$) } 85
- holes ($x_i = 1$) }
- others

1. Weighted sum method (balance two objectives)

$$F(x) = w\alpha N(\boldsymbol{x}) - (1-w)\beta\hat{f}(\boldsymbol{x})$$

$\underset{\boldsymbol{x}\in\{0,1\}^n}{\text{Minimize}}\, F(\boldsymbol{x})$ ⟶ optimize for various w | w is the balancing parameter

2. **ε**-constraint method (fix the total holes $\bar{N}$ and maximize natural frequency)

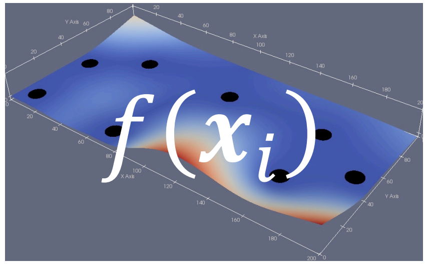
$$F(x) = -p\hat{f}(\boldsymbol{x}) + (N - \bar{N})^2$$

$\underset{\boldsymbol{x}\in\{0,1\}^n}{\text{Minimize}}\, F(\boldsymbol{x})$ ⟶ optimize for various $\bar{N}$ | Search solution around $N = \bar{N}$

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

Black-box optimization（Level 3 automation）

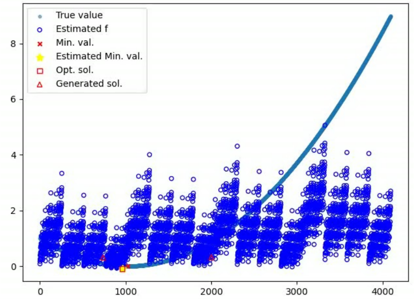
$$\underset{\boldsymbol{x}\in\{0,1\}^n}{\text{Minimize}}\, F\,(\boldsymbol{x})$$



Simulation by FEM

QUBO form

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



(Numerical) Experiment

Data generation

$$y_i = f(\boldsymbol{x}_i)$$

Model generation

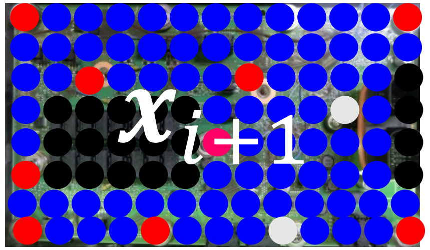
$$\hat{y} = \hat{f}(\boldsymbol{x})$$

Machine Learning

Hypothesis generation

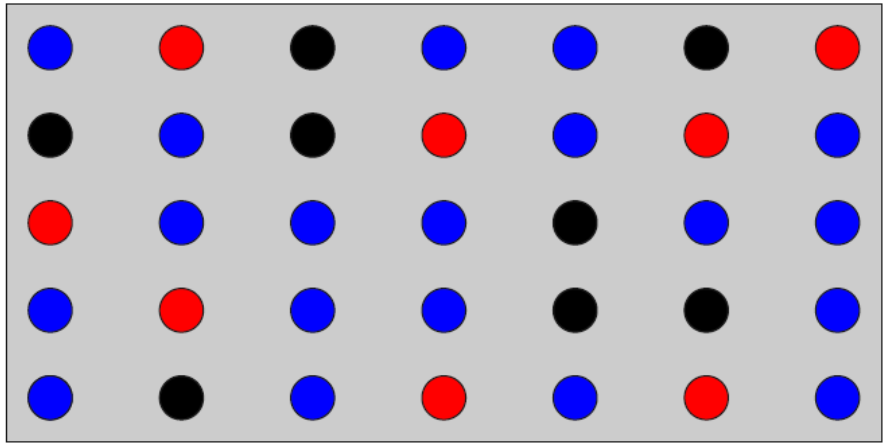
$$\boldsymbol{x}_{i+1} = \underset{\boldsymbol{x}\in\{0,1\}^n}{\operatorname{argmin}}\, \hat{f}(\boldsymbol{x})$$

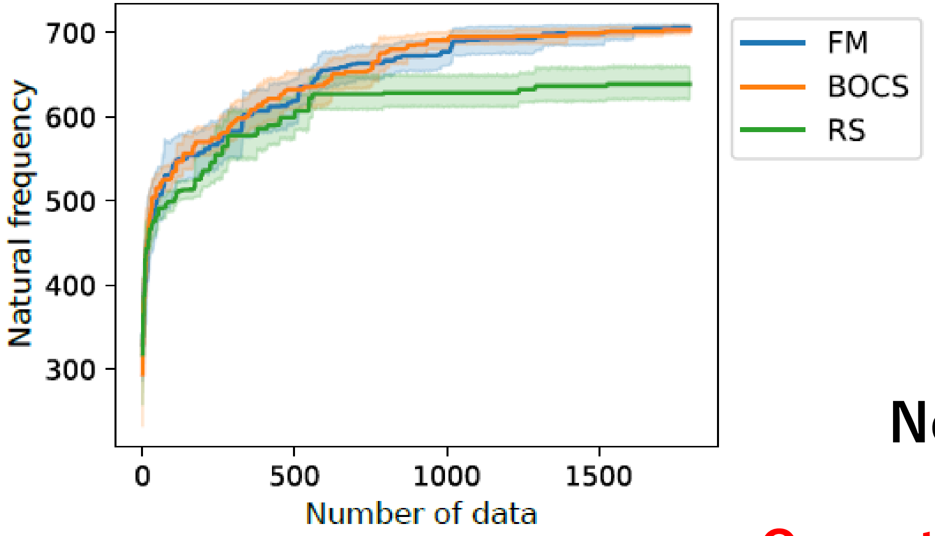
Optimization



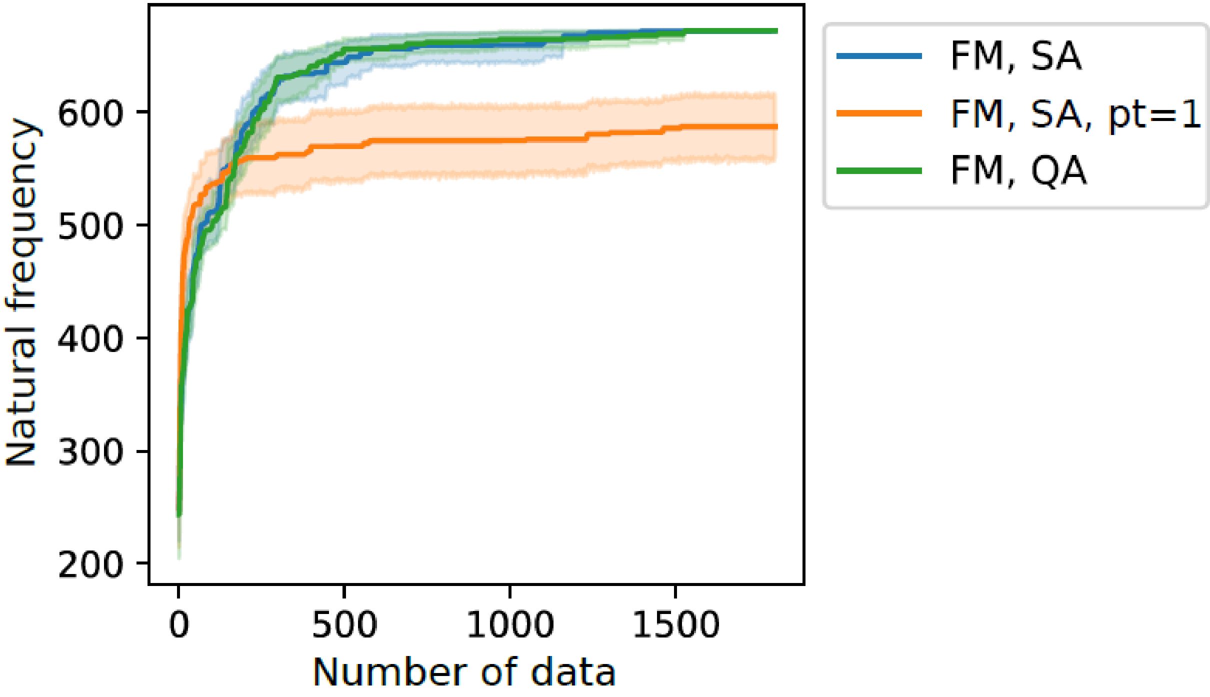
Matsumori, et. al. Sci Rep 12, 12143 (2022)

Results (N=27 problem)





SA vs QA



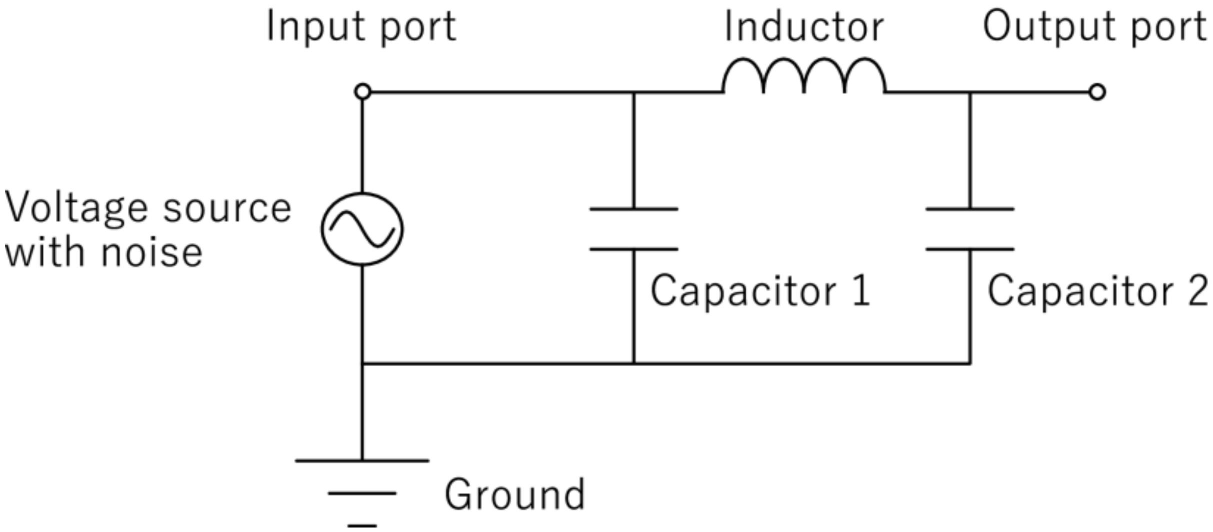
No difference between QA and SA in a small size problem

⇩

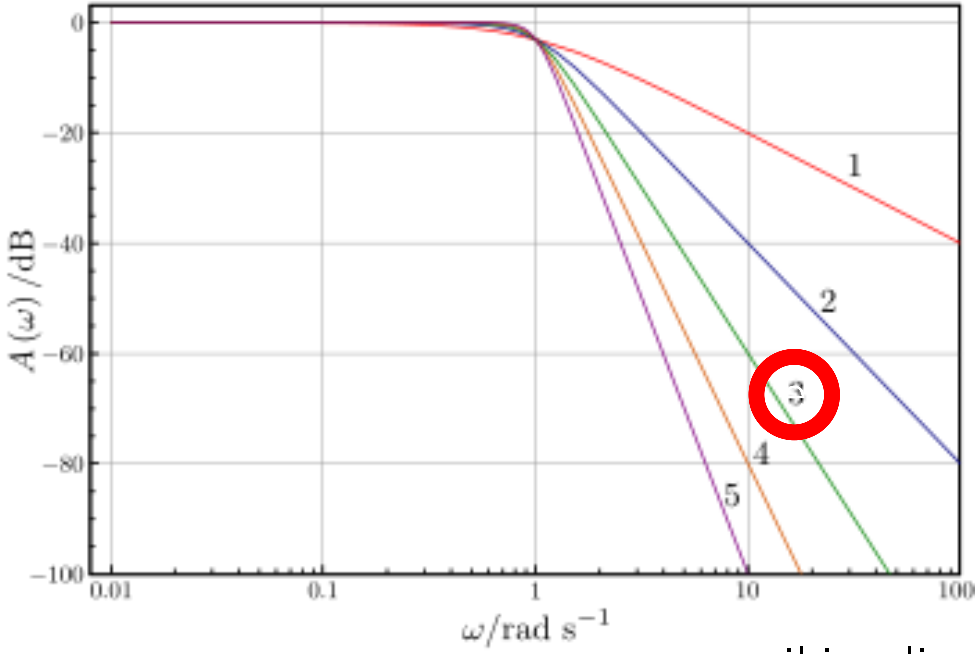
Opportunity to apply this method with the existing technology!

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

Design of noise filter



Third order filter

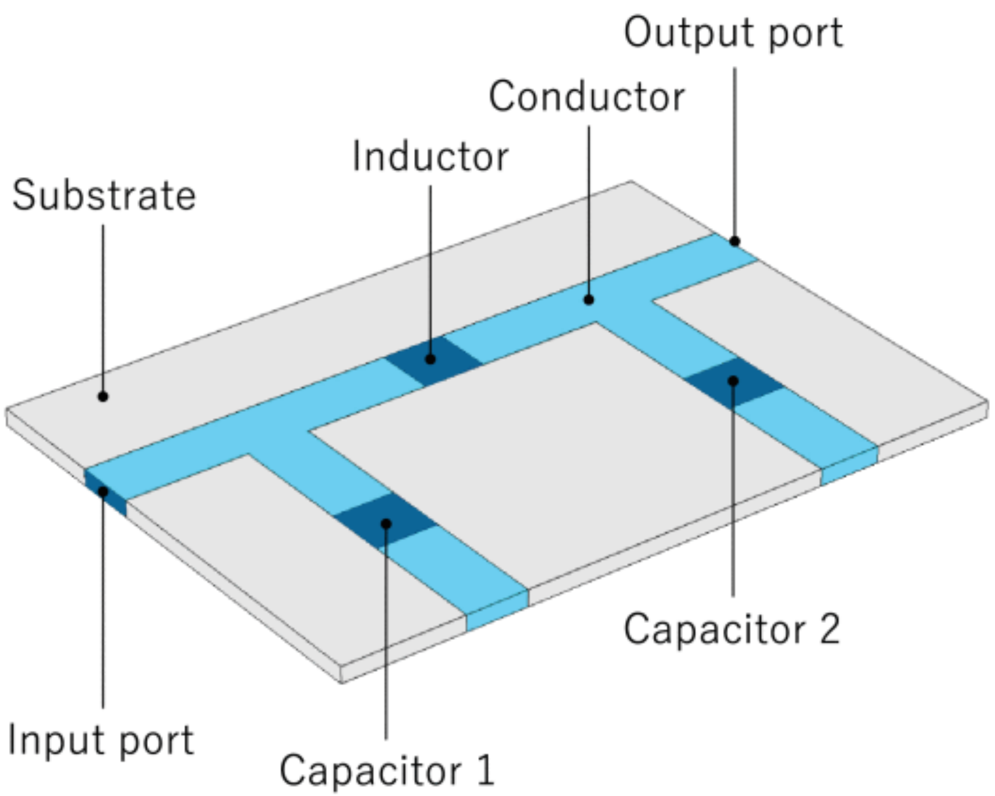


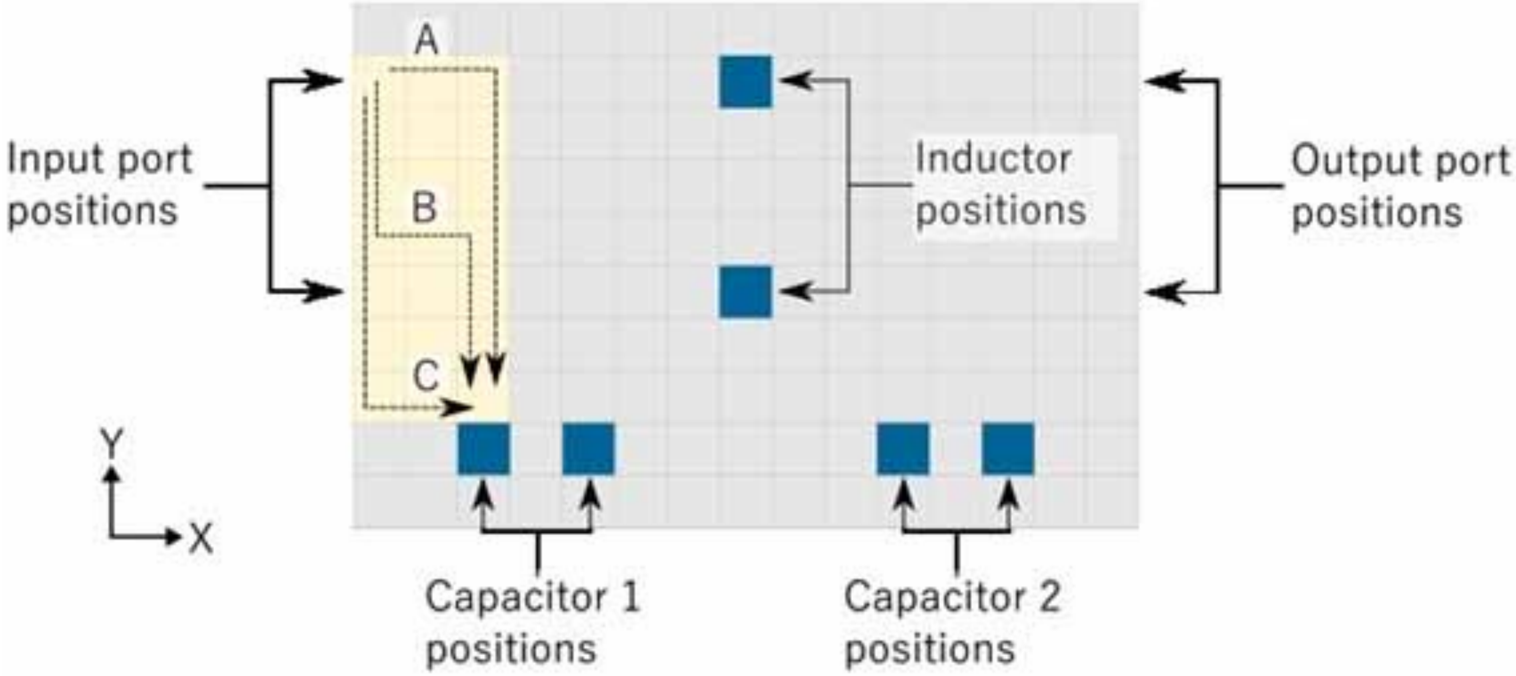
wikipedia

For high-frequency applications,
a lumped-element model may not be suitable.
We need a distributed-element circuit.

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

Printed circuit board

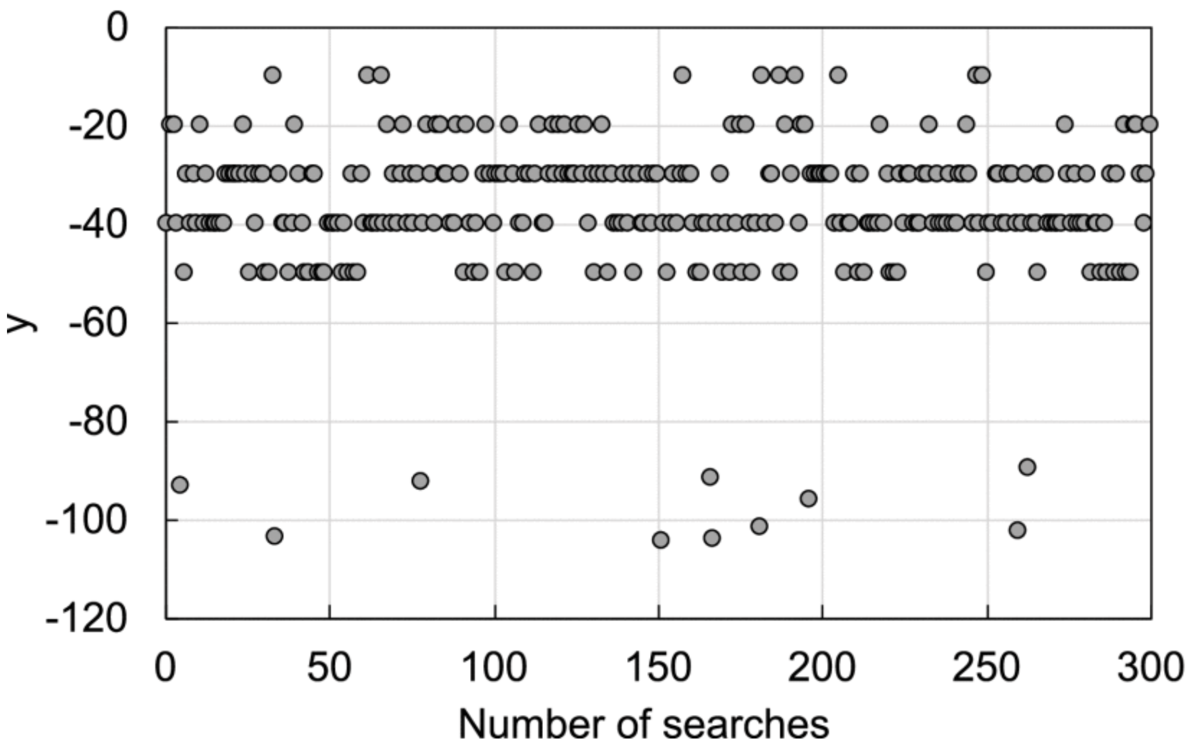




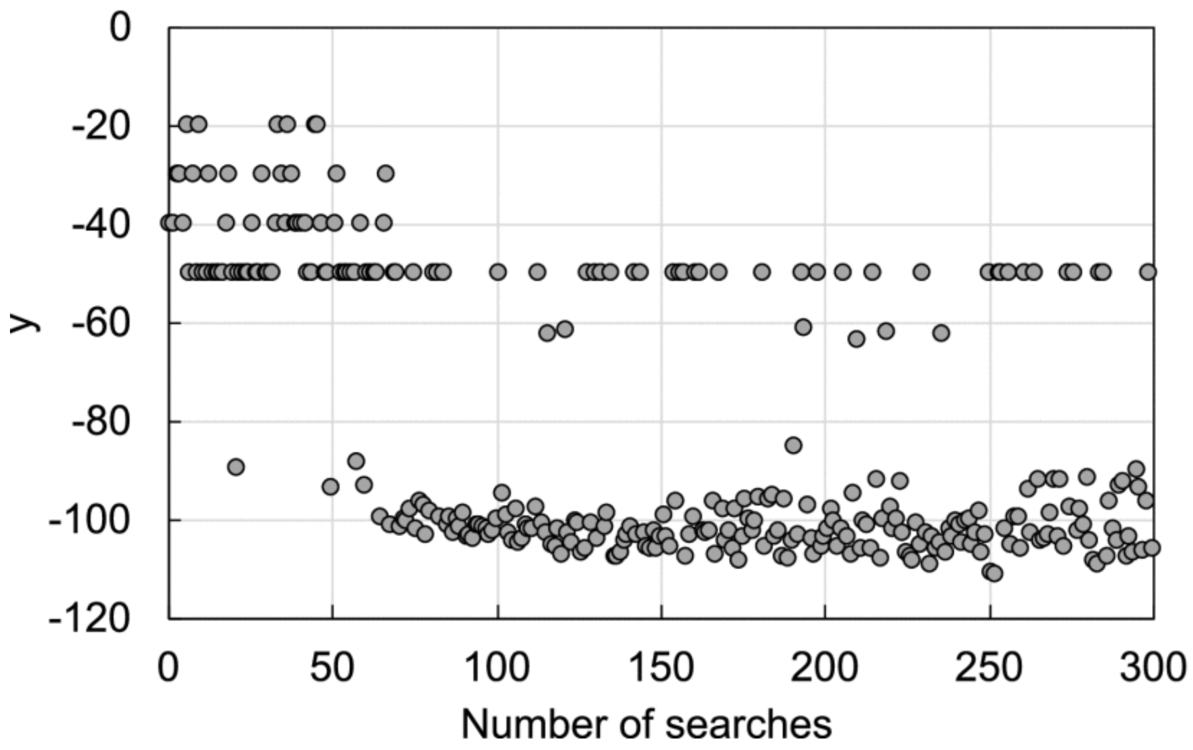
Okada, et. al., IEEE Access, vol. 11, pp. 44343-44349 (2023)

Results (1)

Random search

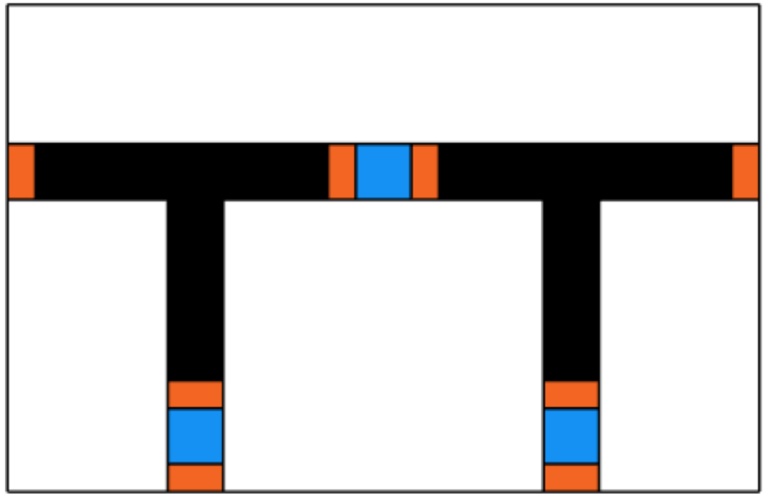
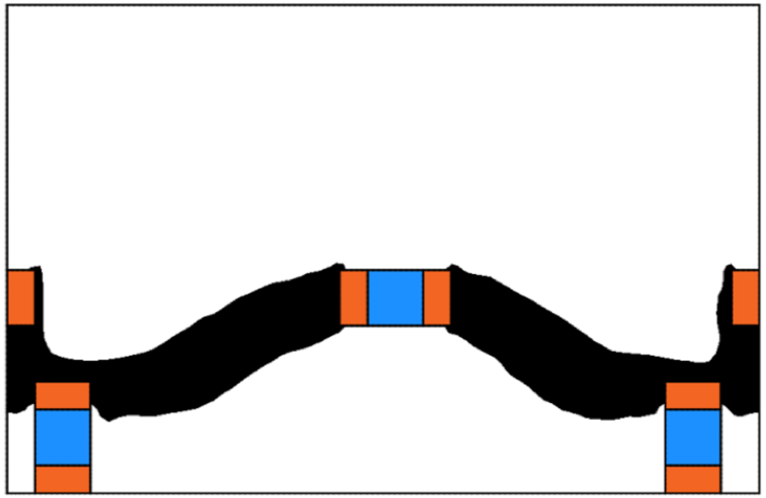
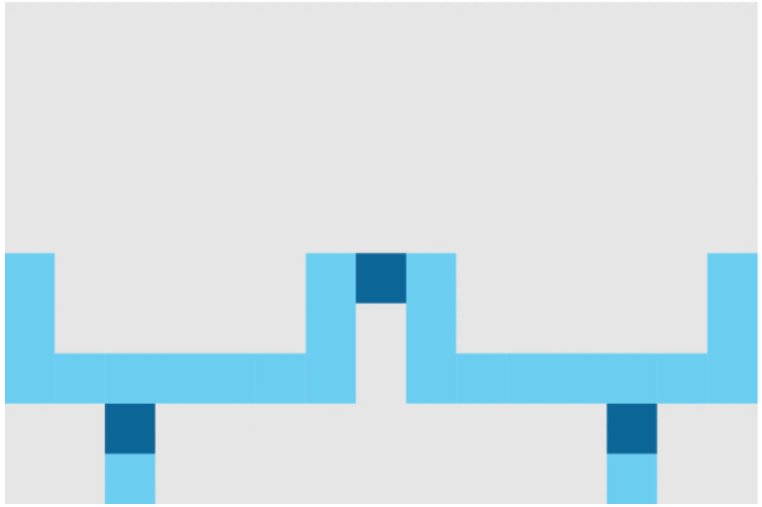


BOCS algorithm



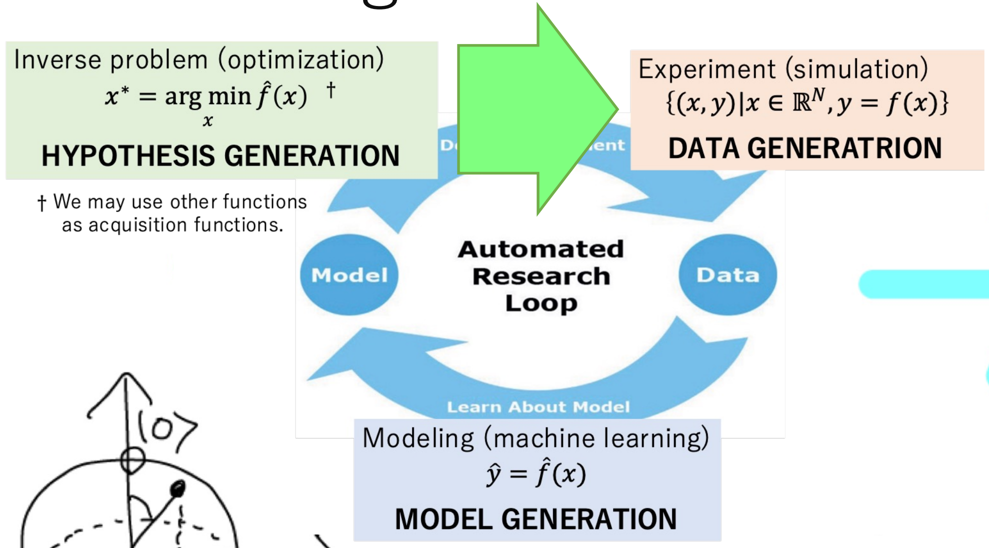
Okada, et. al., IEEE Access, vol. 11, pp. 44343-44349 (2023)

Results

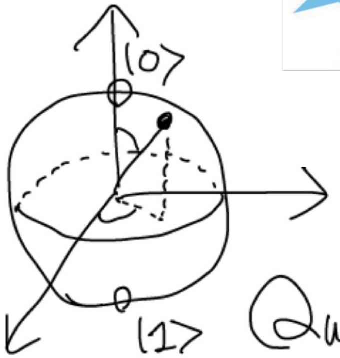
Reference	Topology optimization	Out method
		

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



† We may use other functions as acquisition functions.

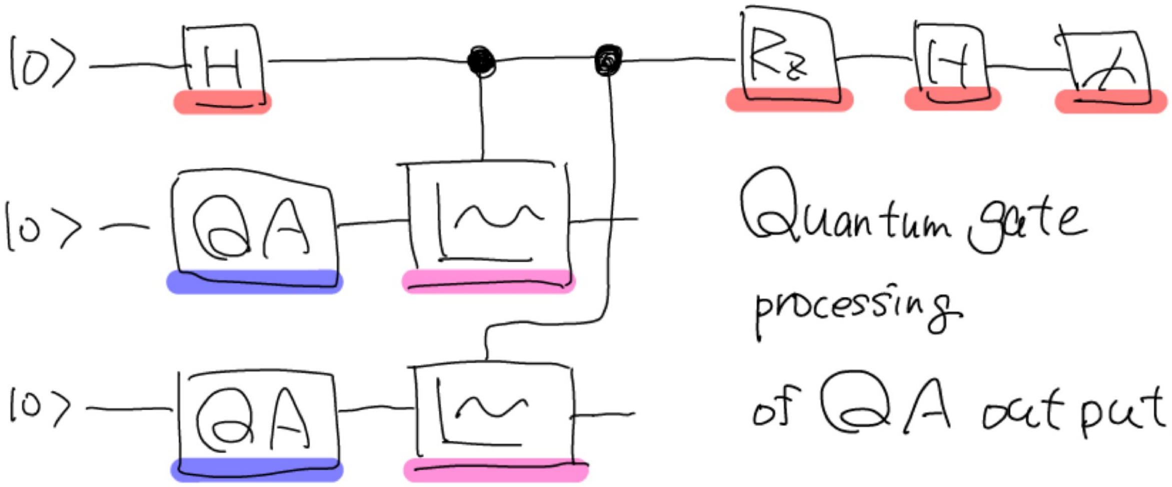


Quantum Data

QQ > QC!

Data Processing

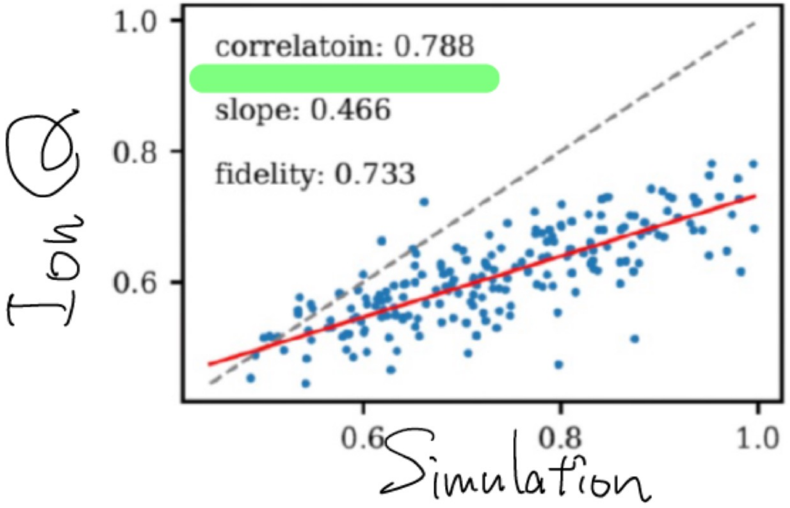
Digital-Analog Quantum Computing



Quantum gate processing of QA outputs

PoC by IonQ on AWS (arXiv:2306.02059)

APL Quantum 1, 026101 (2024)

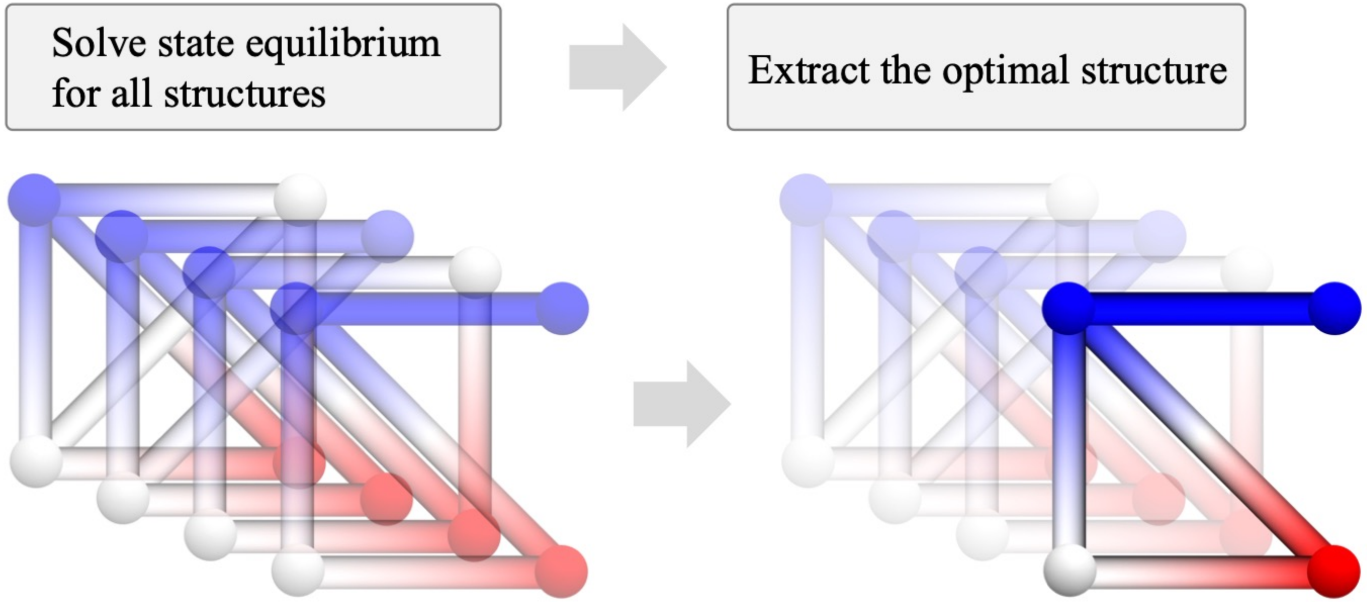


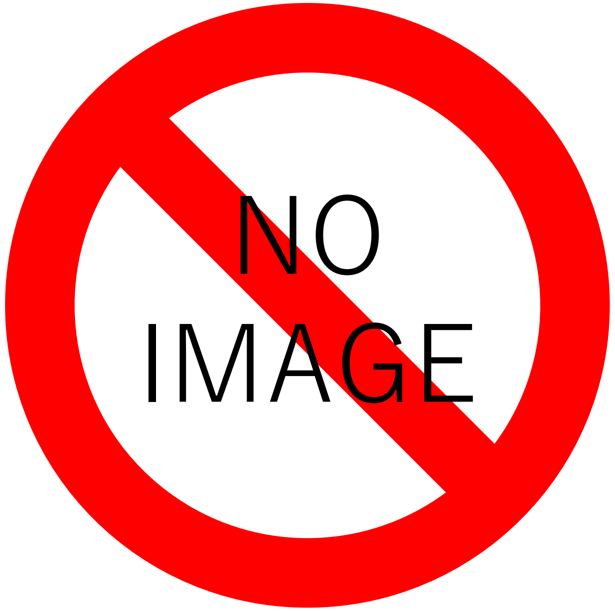
Algorithm validation

Other approach : Quantum topology optimization

Variational Quantum Algorithm

Topology optimization by annealer





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

Agenda

- Automation in Science

  How science is automated by AI.

- Level 3 automation and Computer Aided Engineering (CAE)

  Current automation level in science and engineering

- Quantum CAE

  How quantum computing accelerates engineering and science.

- Summary

Summary

- AI's role in science and engineering is growing, with the future potential of becoming a robot scientist.
- Scientific automation is categorized into five levels; we are currently engaging with level 3.
- Examples of level 3 automation include Game AI and level 3 autonomous driving.
- Quantum computing is expected to enhance the capabilities of level 3 automation in scientific research.
- Quantum CAE aims to accelerate the automation of product design processes, and its techniques have broader applications across various scientific fields.
- The progression to levels 4 and 5 of automation is still an open question.