HAMLET-PHYSICS, Copenhagen, Denmark, 20.08.2025

Towards an Artificial Muse for new ideas in Physics

Mario Krenn

Artificial Scientist Lab

@mariokrenn6240

http://mariokrenn.wordpress.com/

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

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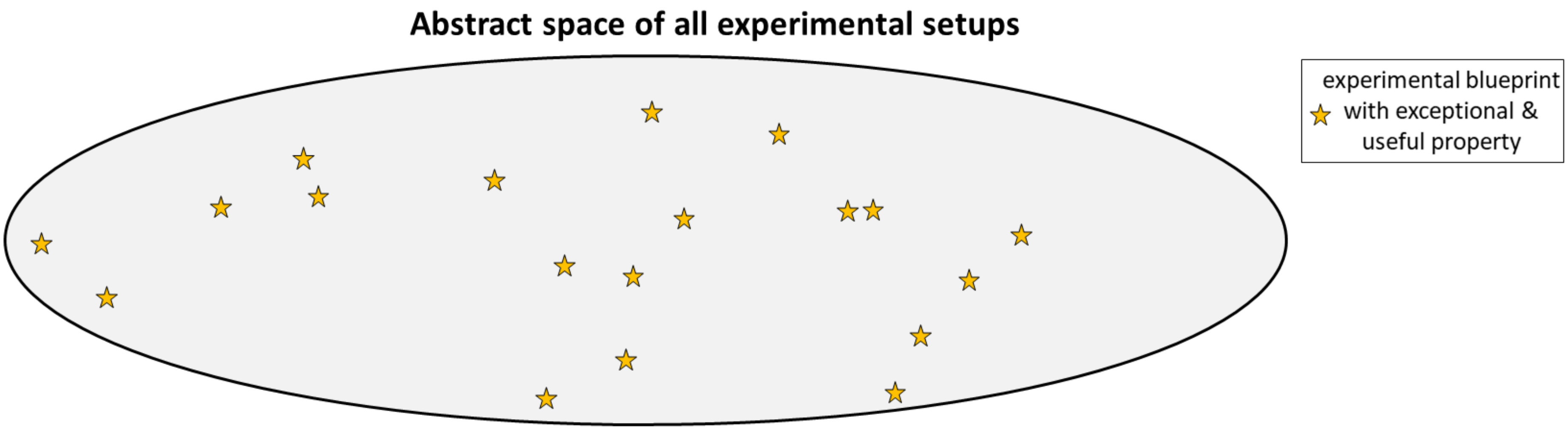
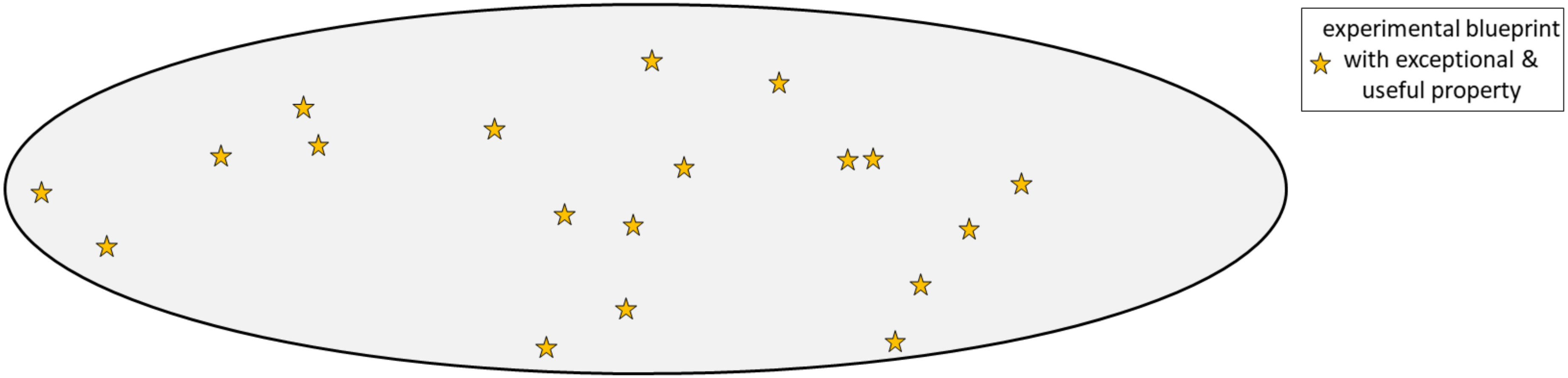

Abstract space of all experimental setups
experimental blueprint
with exceptional &
useful property

Some examples: (without symmetry)

3 lasers, 3 BS, 3 detectors: 1000 combinations

5 lasers, 5 BS, 5 detectors: 81,000 combinations (!)

Abstract space of all experimental setups



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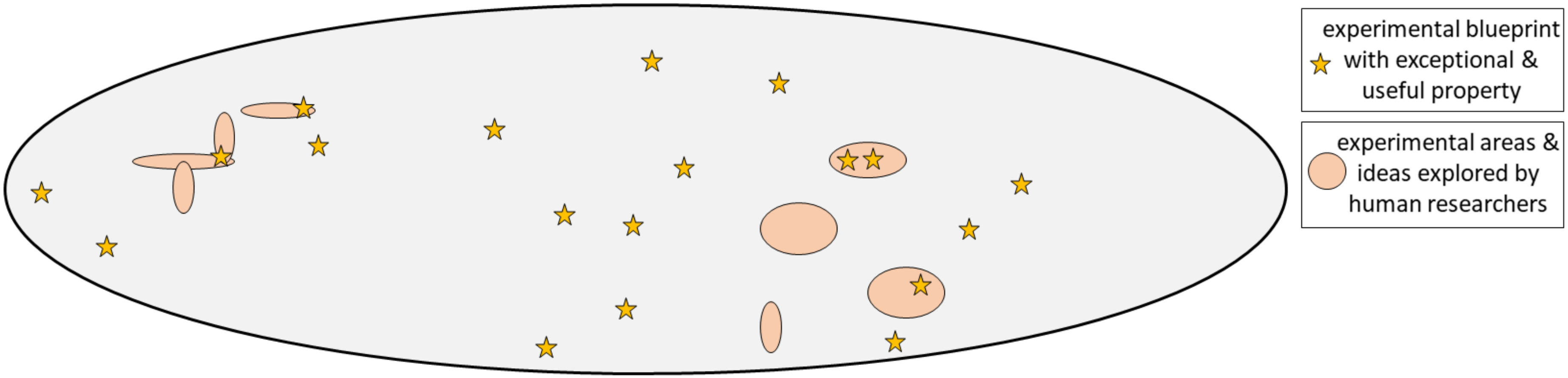

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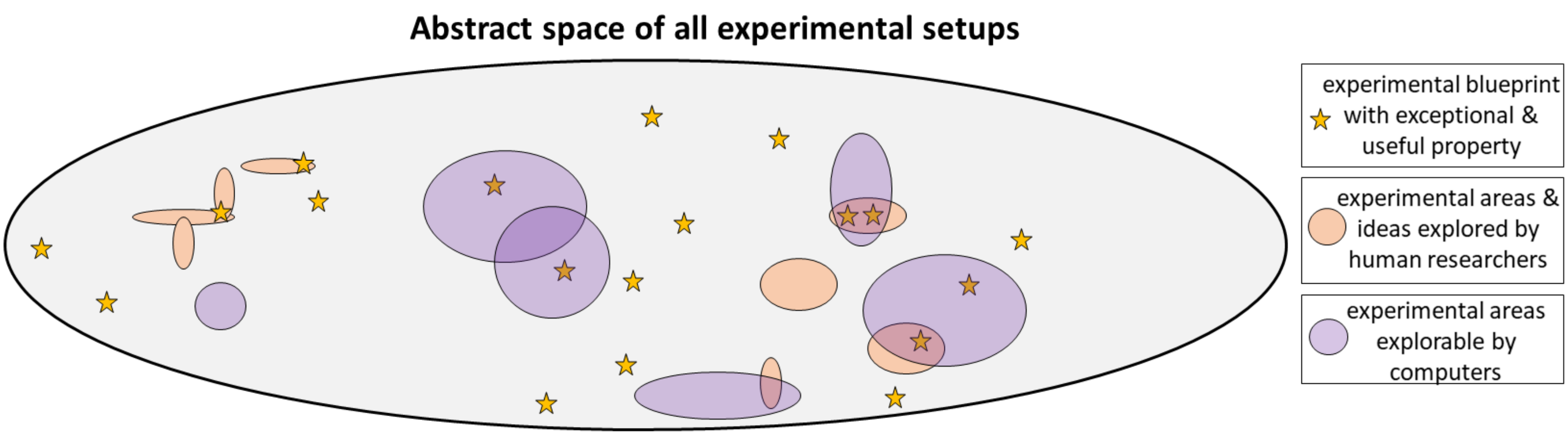

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How to design quantum experimental setups?

High-dimensional multipartite entanglement

$$|\psi\rangle_{GHZ-3D} = \frac{1}{\sqrt{3}}\left(|000\rangle + |111\rangle + |222\rangle\right)$$

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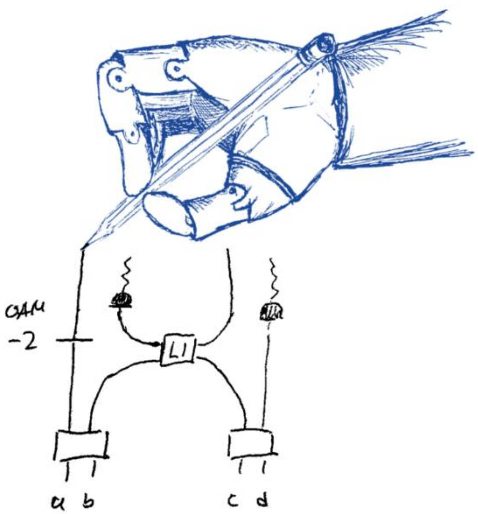

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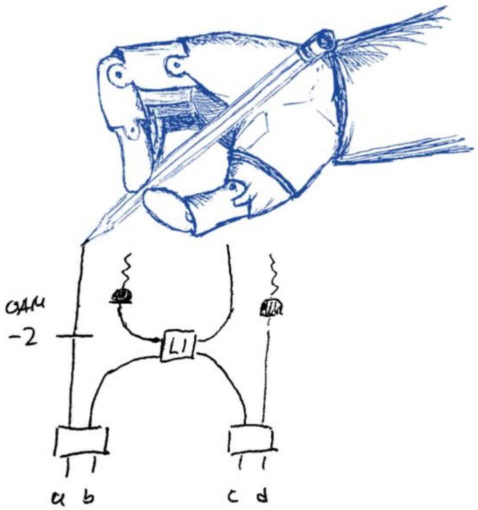
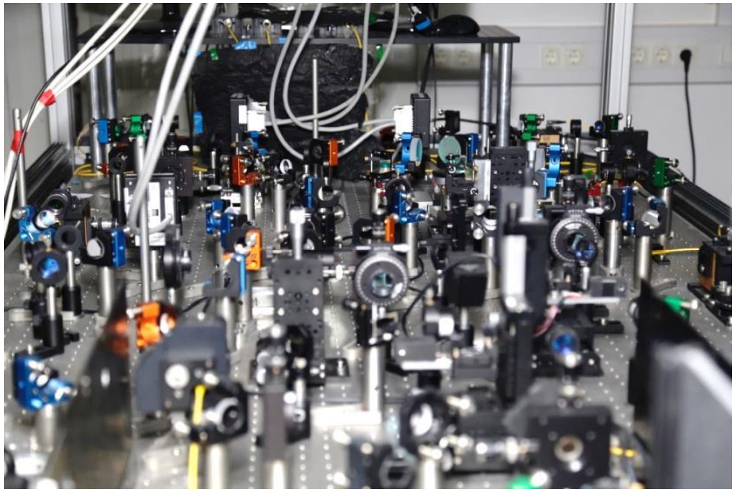


Erhard et al., *Nature Photonics* **12**, 759 (2018)



Krenn, Malik, Fickler, Lapkiewicz, Zeilinger, Automated Search for new Quantum Experiments, *Phys. Rev. Lett.* **116**, 090405 (2016)
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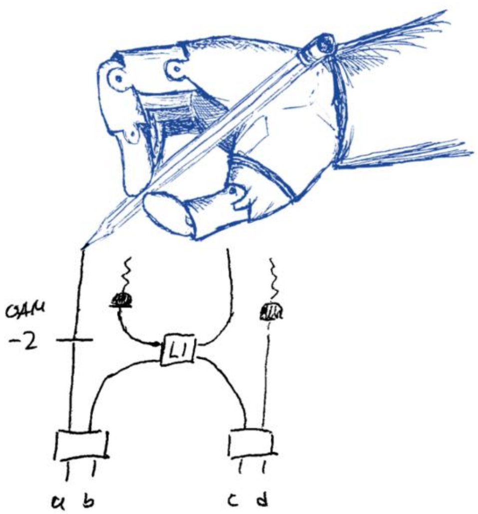

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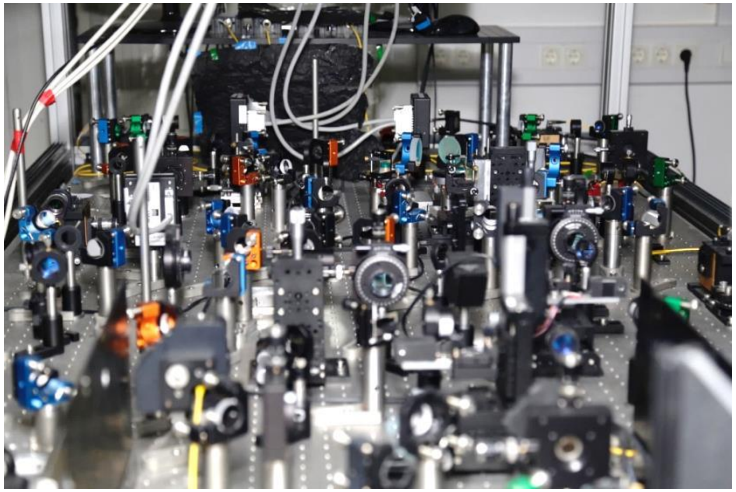

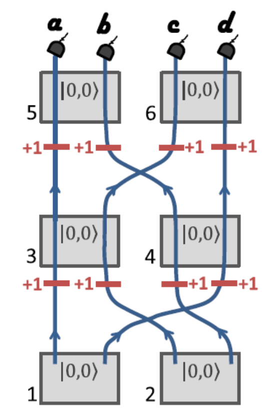

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Computer-inspired ideas and concepts

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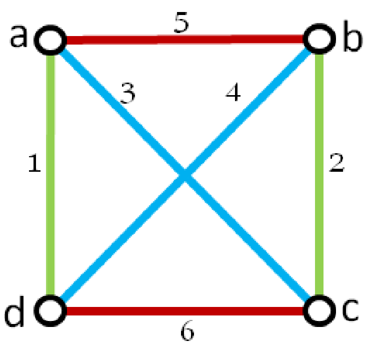
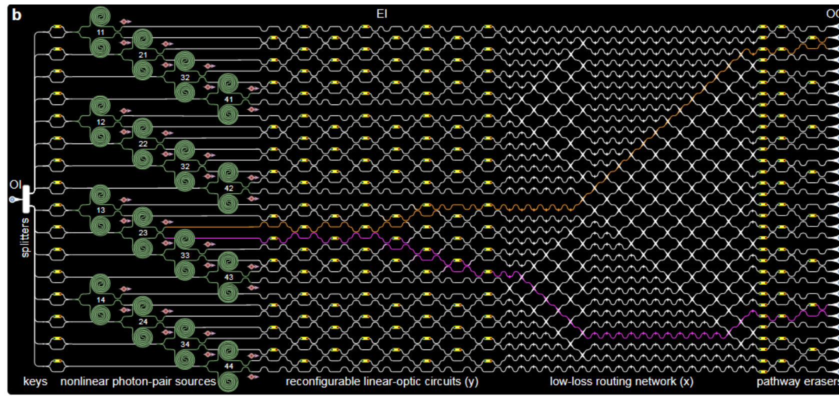
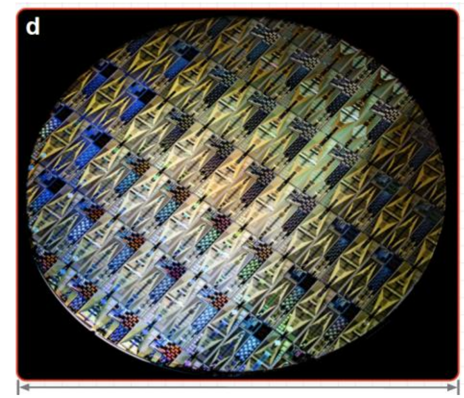
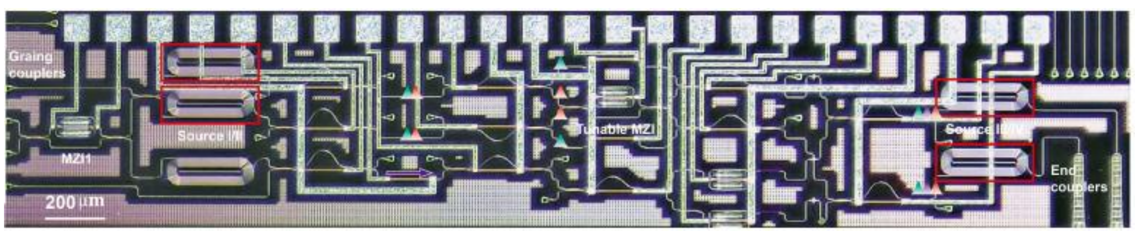


Gu, Erhard, Zeilinger, MK, *PNAS* **116** (2019).

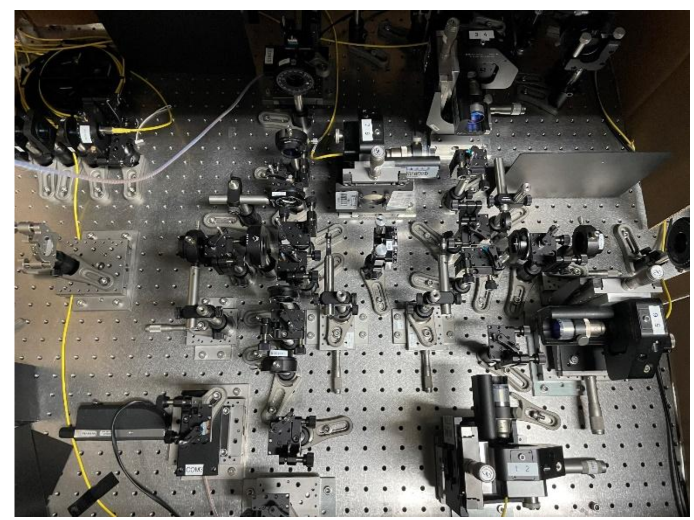
Bao et al., Very-large-scale integrated quantum graph photonics, *Nature Photonics*, **17**, 573 (2023) .







Feng, et al., *On-Chip nonlocal quantum interference between the origins of a four-photon state, Optica* (2023).



Qian et al., *Multiphoton non-local quantum interference controlled by an undetected photon, Nature Communications* **14** (1), 1480 (2023)

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Phys. Scr. 95 (2020) 062501 (50pp) https://doi.org/10.1088/1402-4896/ab7a35

Perspective

CrossMark

The sounds of science—a symphony for many instruments and voices

Gerianne Alexander[1], Roland E Allen[2], Anthony Atala[3], Warwick P Bowen[4,5], Alan A Coley[6], John B Goodenough[7], Mikhail I Katsnelson[8], Eugene V Koonin[9], Mario Krenn[10,11], Lars S Madsen[5], Martin Månsson[12], Nicolas P Mauranyapin[4], Art I Melvin[10,13], Ernst Rasel[14,15], Linda E Reichl[16], Roman Yampolskiy[17], Philip B Yasskin[18], Anton Zeilinger[10,13] and Suzy Lidström[19,20]

14. How can a computer find autonomously new, surprising or creative solutions or insights? by Mario Krenn, Art I. Melvin and Anton Zeilinger

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Chemistry Nobel 2019

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Physics Nobel 2022

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Highly efficient computer-designed quantum experiments

MK, Kottmann, Tischler, Aspuru-Guzik, Conceptual understanding through efficient inverse-design of quantum experiments, *Phys. Rev. X* **11**, 031044 (2021).

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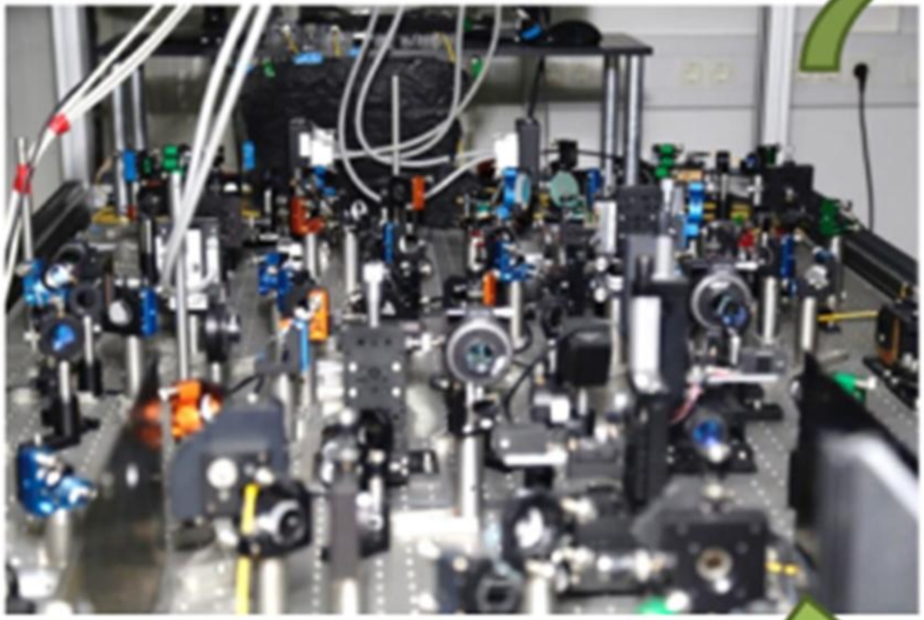
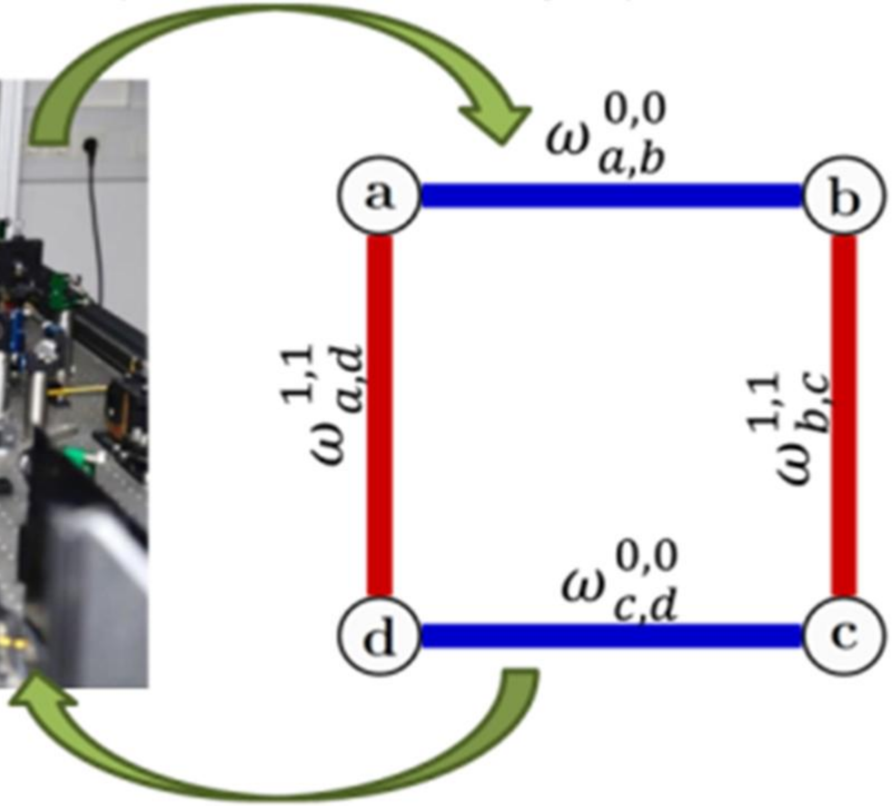
Change Perspective:

New representation -> orders of magnitude speed-up.





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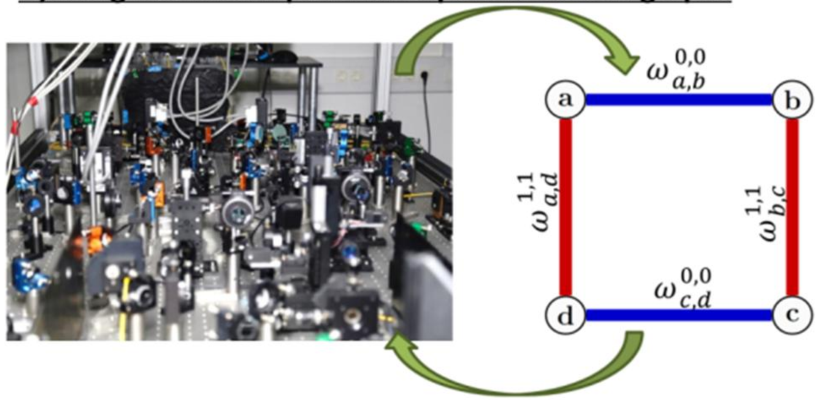
Change Perspective:

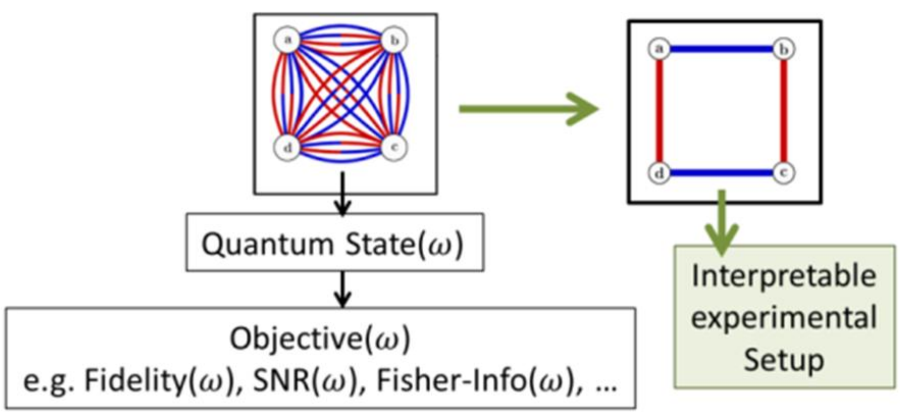
New representation -> orders of magnitude speed-up.

Vertex: Photonic path
Edge: Photon pair
Edge weight: amplitude
Color: Photonic Mode

A) Bridge between quantum experiments and graphs



B) Gradient-based optimization + discrete topological optimization



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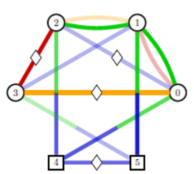
Highly efficient computer-designed quantum experiments

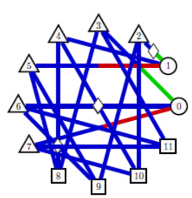
Quantum
the open journal for quantum science

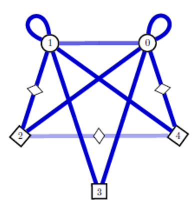
Digital Discovery of 100 diverse Quantum Experiments with PyTheus

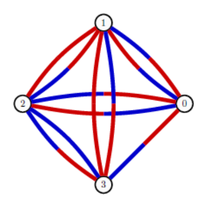
Carlos Ruiz-Gonzalez[§1], Sören Arlt[§1], Jan Petermann[1], Sharareh Sayyad[1], Tareq Jaouni[2], Ebrahim Karimi[1,2], Nora Tischler[3], Xuemei Gu[1], and Mario Krenn[1]

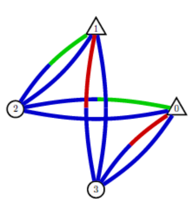
Quantum 7, 1204 (2023).

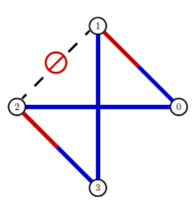

(a) Four-dimensional four-photon GHZ state (overcoming the 3-dimensional barrier for multiphoton entanglement)

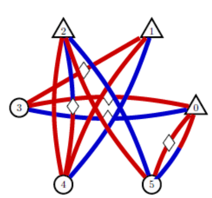

(b) Heralded 3D Bell state with single photons (improves state-of-the-art design by requiring less ancilla photons)

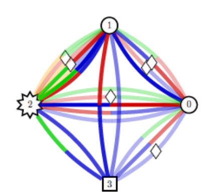

(c) Two-mode five-photon N00N state $|50\rangle + |05\rangle$ (very symmetric shape with an inscribed pentagram)


(d) A 4-qubit entangled states with unit coefficients, which requires complex-valued weights for generation


(e) Quantum measurement for a quantum communication task with quantum advantage (Mean King's Problem)


(f) Entanglement swapping without using two Bell states


(g) Toffoli quantum gate without ancilla photons


(h) Mixed state with bound entanglement that can violate a Bell inequality (counterexample to the Peres conjecture from 1999, solved 2014)

github.com/artificial-scientist-lab/PyTheus

```
pip install pytheusQ
```

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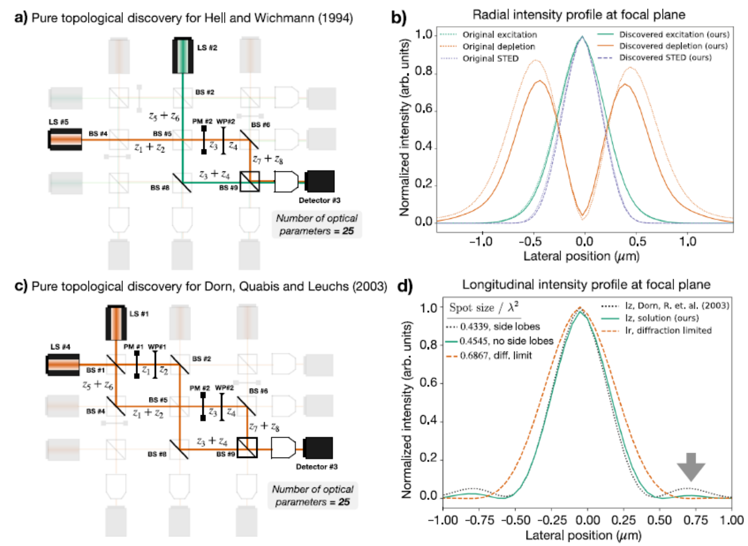
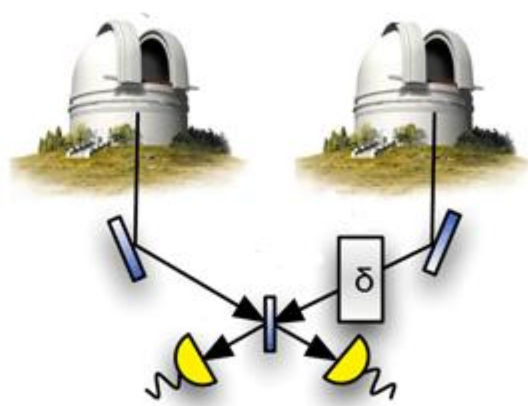
De-novo Design of Physics Experiments with AI

Gravitational wave Detections
Phys. Rev. X **15**, 021012 (2025)



Super-Resolution Microscopy
Nature Comm. **15**, 10658 (2024)



Quantum-Enhanced Telescopes
arXiv 2508:nnnnn (hopefully)

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AI-driven design of new Gravitational Wave Detectors

with Yehonathan Drori, Rana X. Adhikari (Caltech, LIGO)

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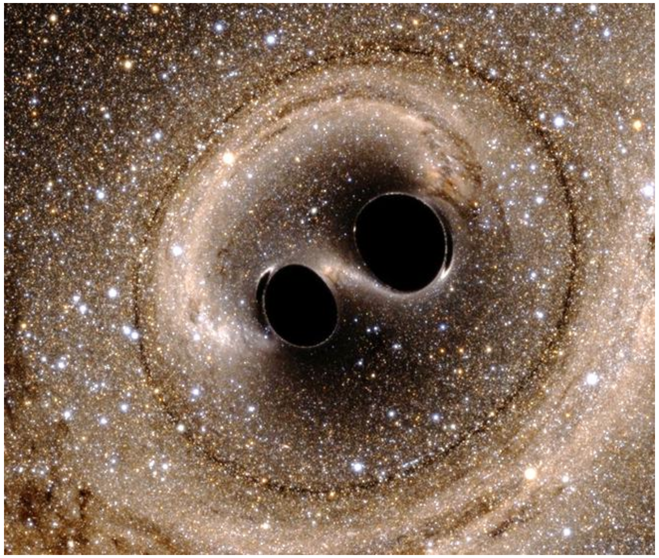

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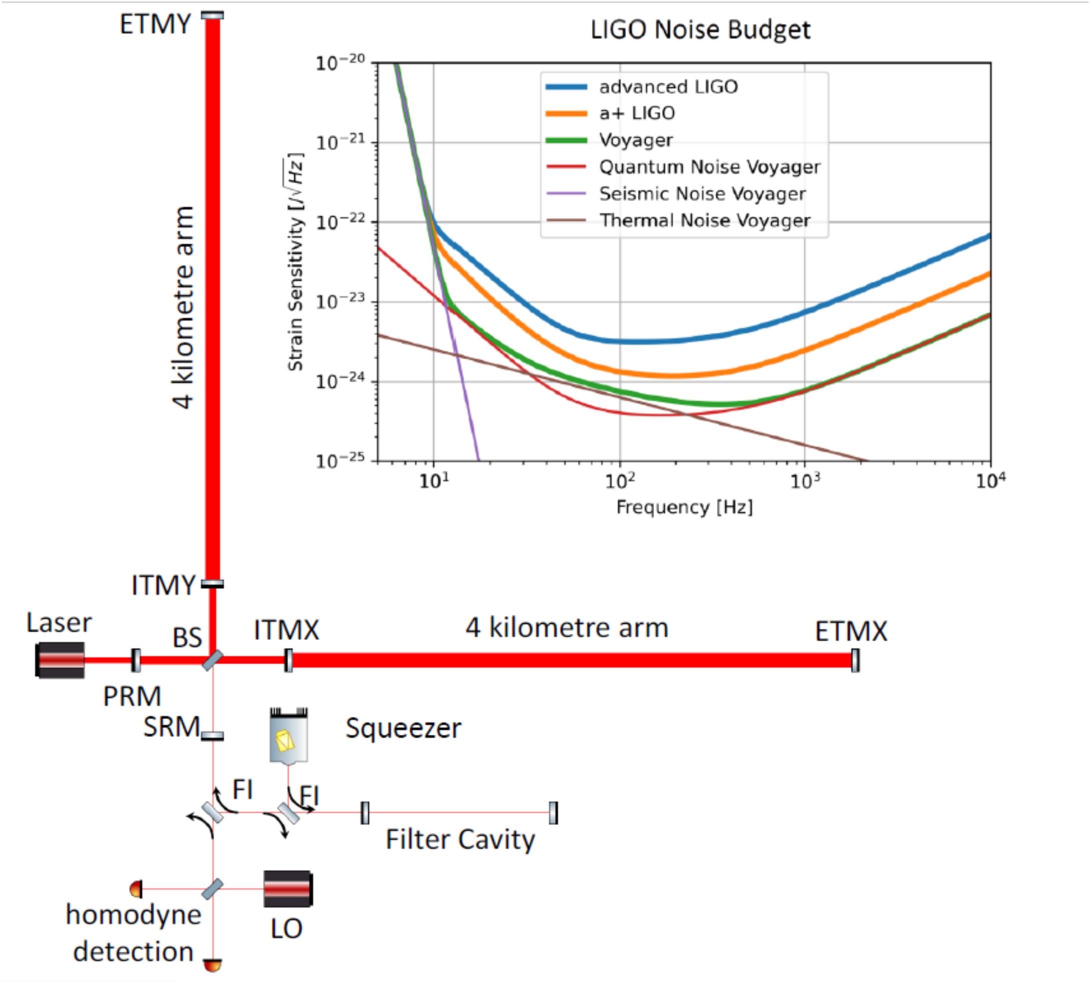
LIGO's next Generation Detector Update: Voyager



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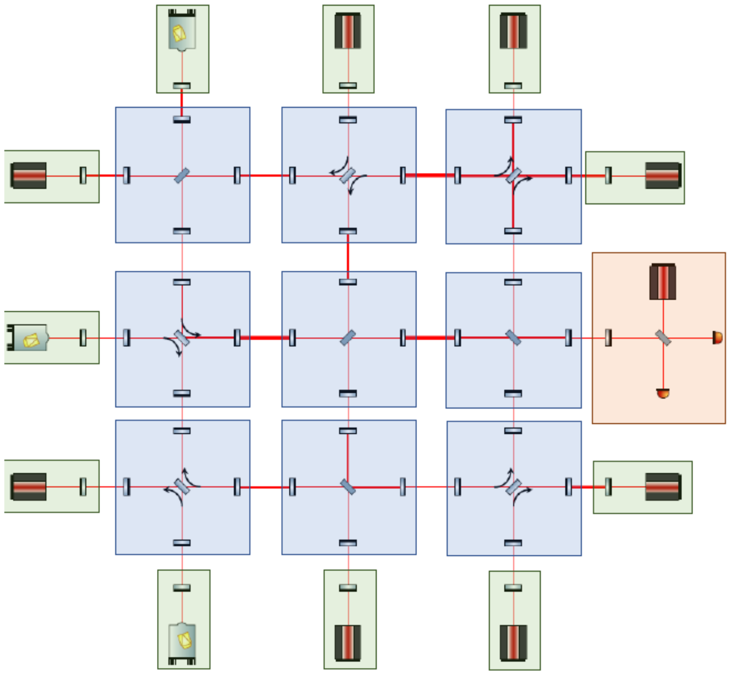
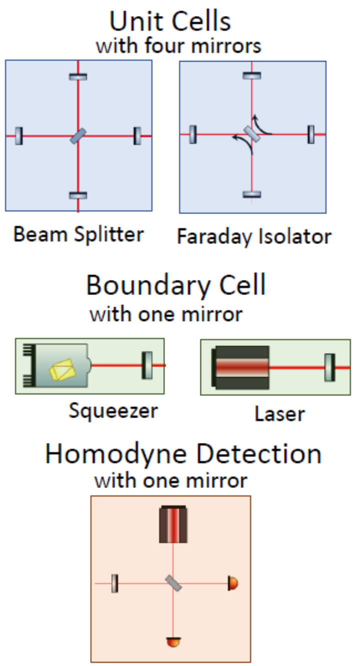
Phys. Rev. X **15**, 021012 (2025)

A) Quasi-Universal Interferometer (UIFO)





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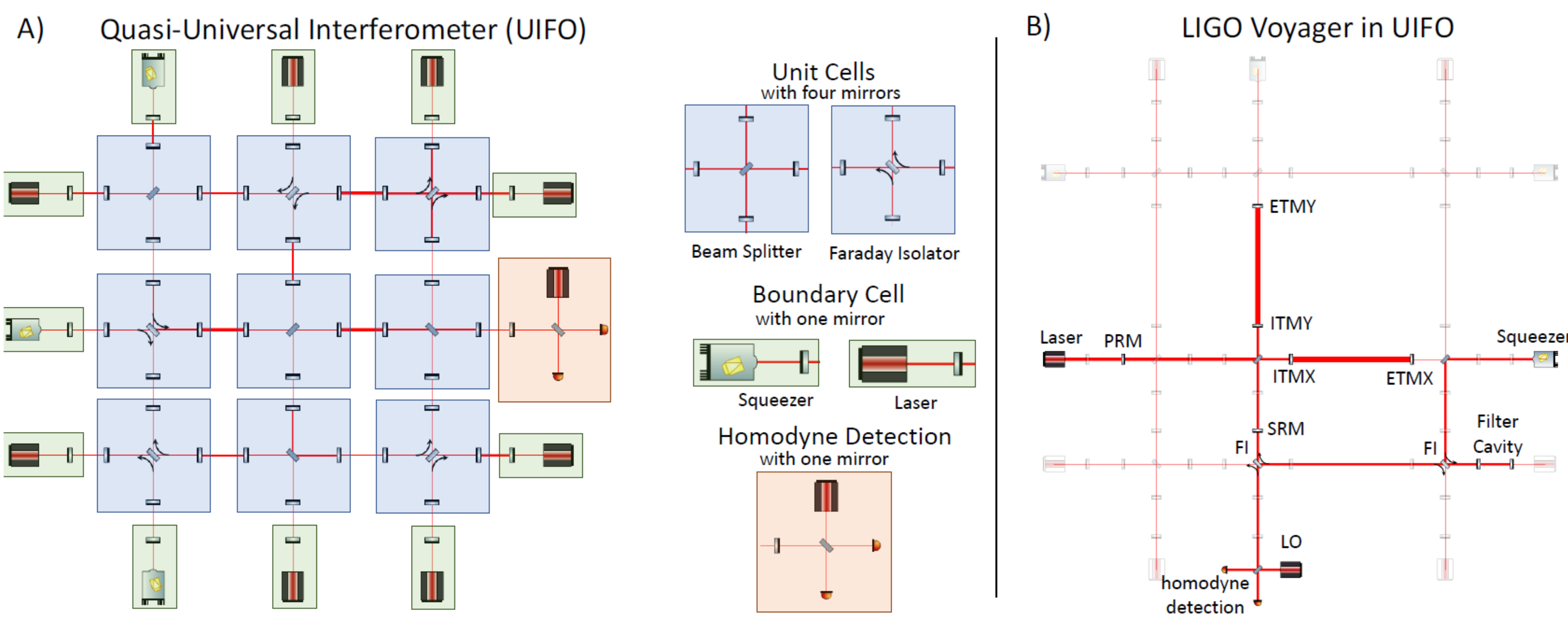

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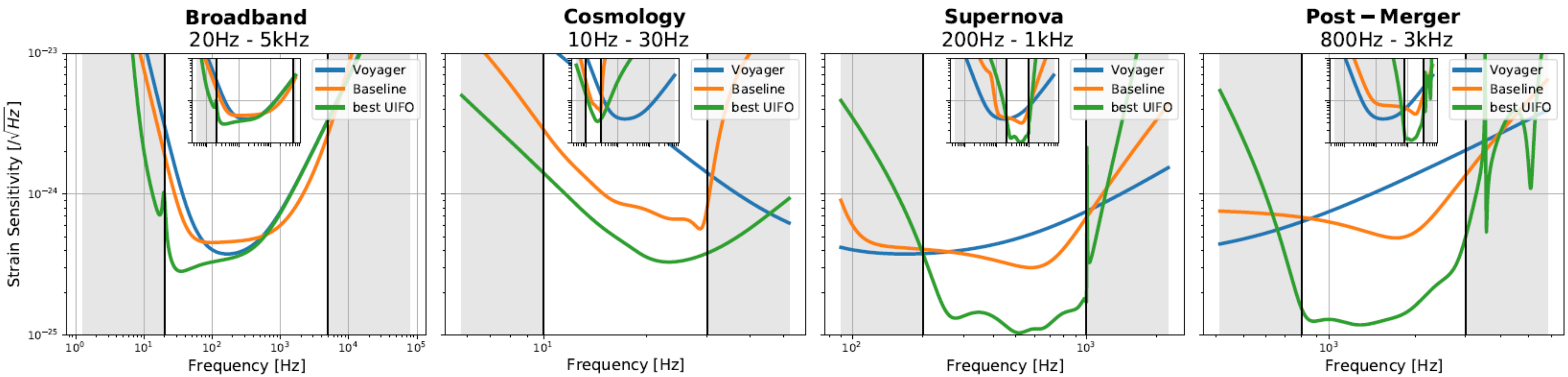

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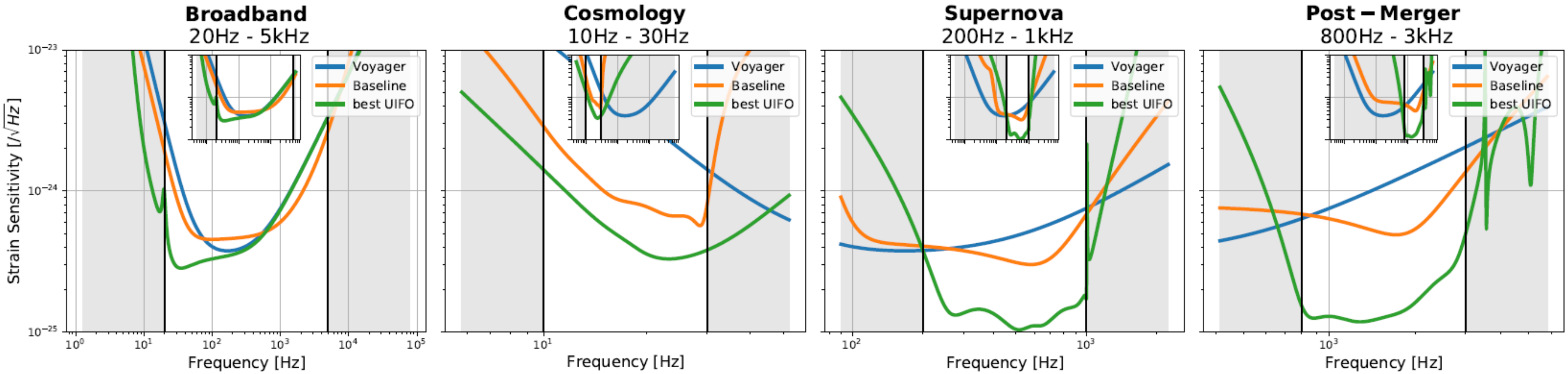
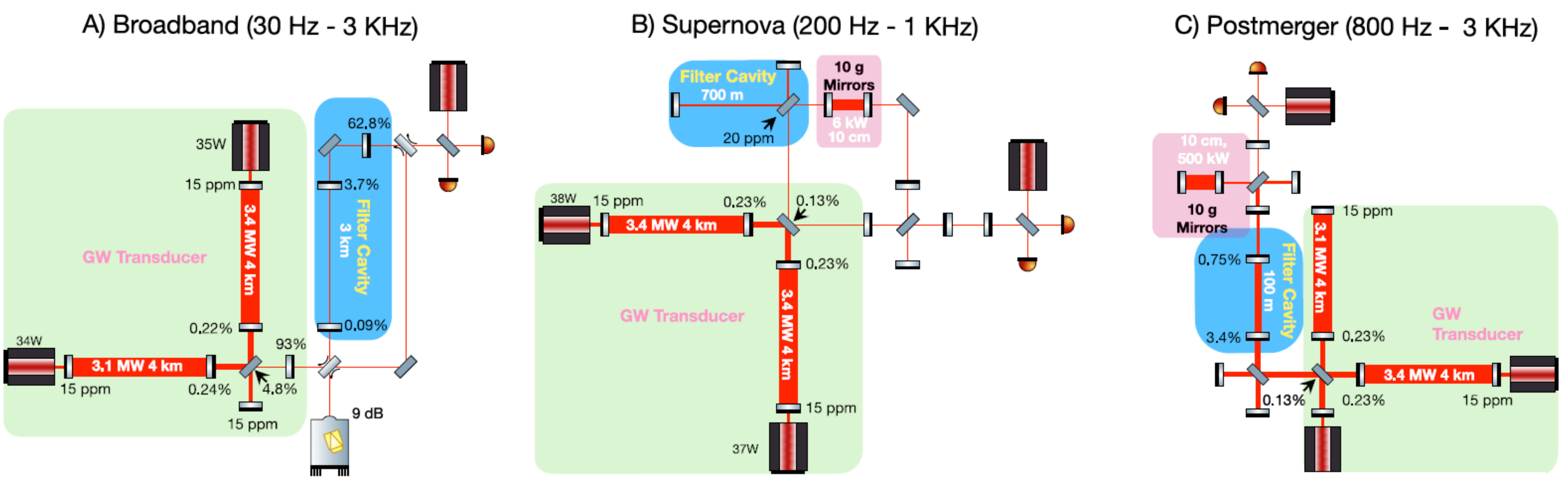


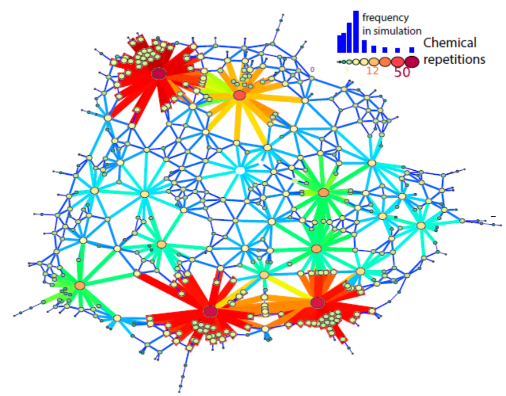


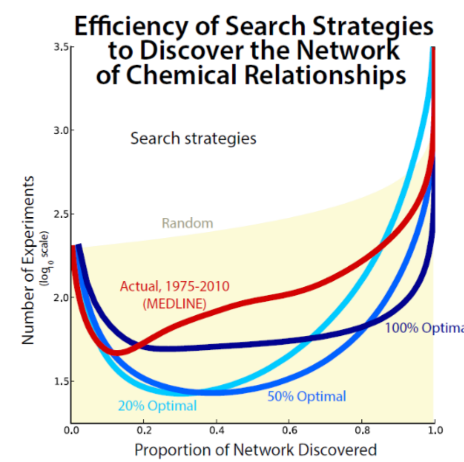
Choosing experiments to accelerate collective discovery

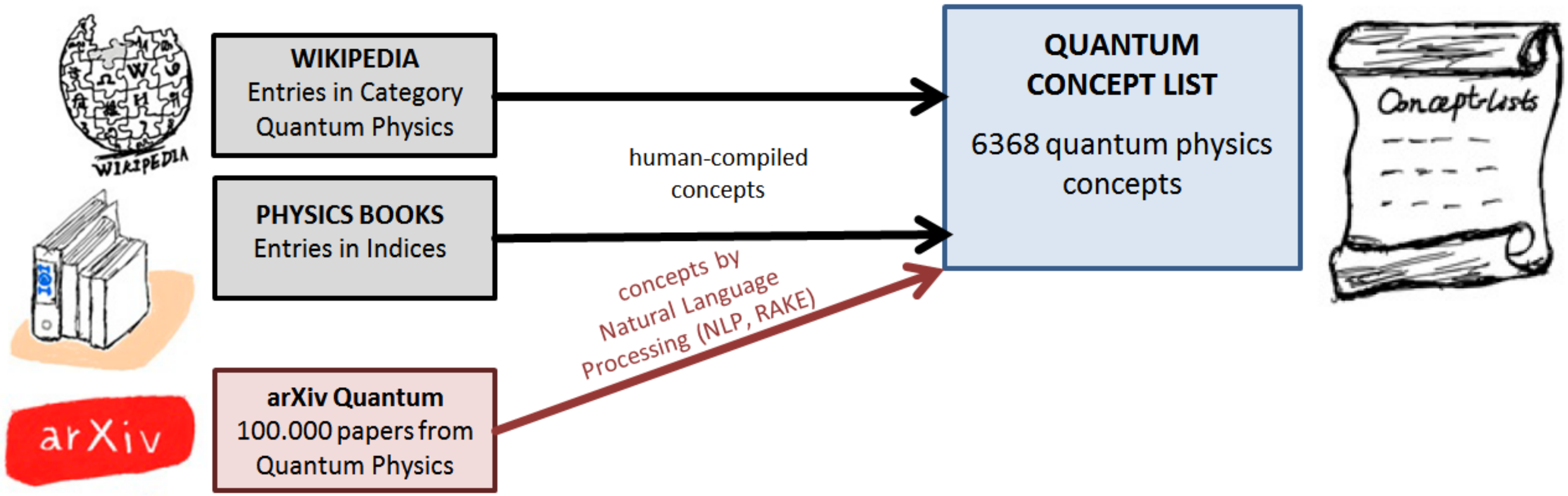
Andrey Rzhetsky[a,b,c,1], Jacob G. Foster[d], Ian T. Foster[b,e], and James A. Evans[b,f,1]

Edited by Yu Xie, University of Michigan, Ann Arbor, MI, and approved September 8, 2015 (received for review May 18, 2015)

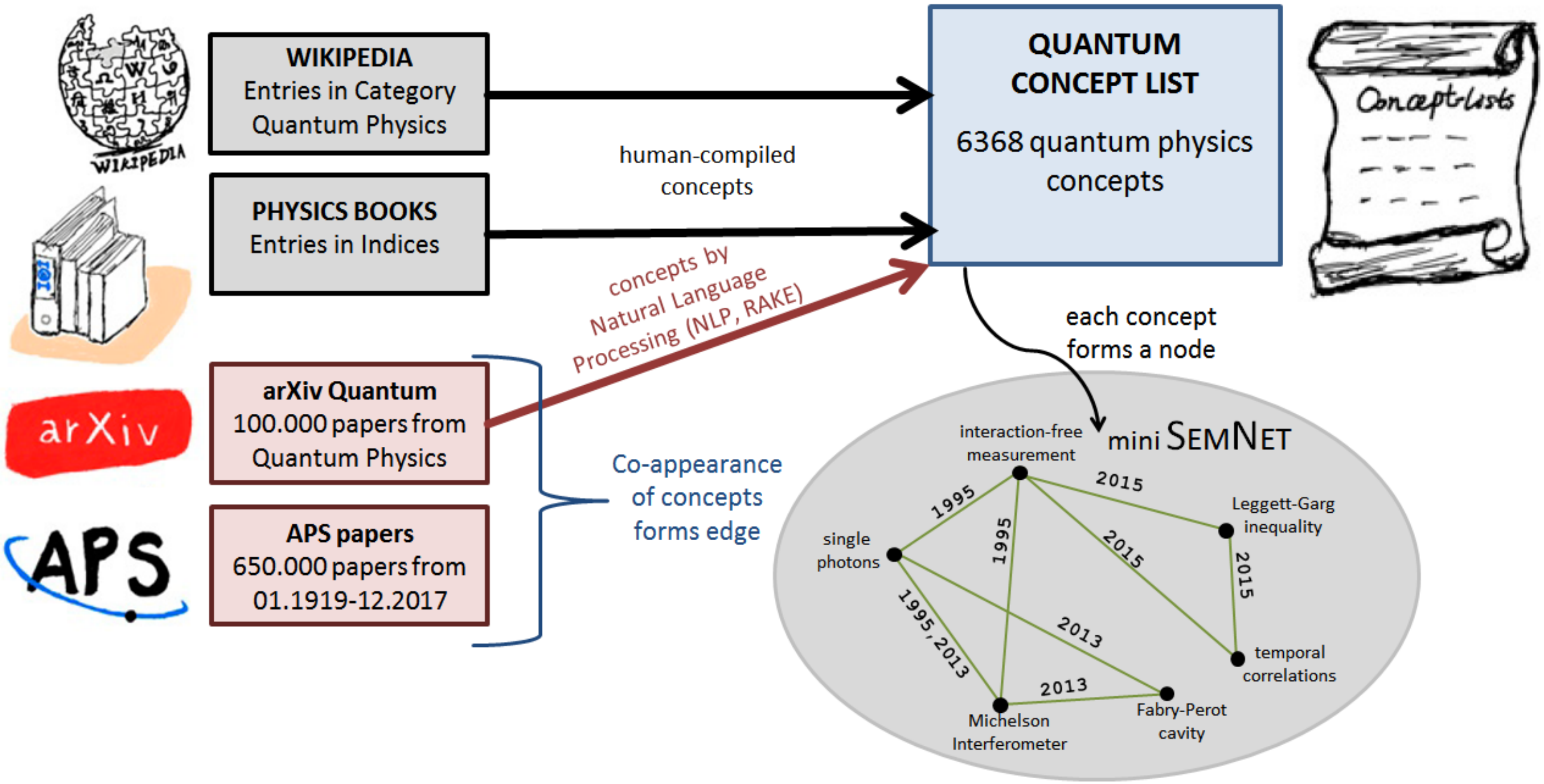
A scientist's choice of research problem affects his or her personal career trajectory. Scientists' combined choices affect the direction and efficiency of scientific discovery as a whole. In this paper, we infer preferences that shape problem selection from patterns of published findings and then quantify their efficiency. We represent research problems as links between scientific entities in a knowledge network. We then build a generative model of discovery informed by qualitative research on scientific problem selection. We map salient features from this literature to key network properties: an entity's importance corresponds to its degree centrality, and a problem's difficulty corresponds to the network distance it spans. Drawing on millions of papers and patents published over 30 years, we use this model to infer the typical research strategy used to explore chemical relationships in biomedicine. This strategy generates conservative research choices focused on building up knowledge around important molecules. These choices become more conservative over time. The observed strategy is efficient for initial exploration of the network and supports scientific careers that require steady output, but is inefficient for science as a whole. Through supercomputer experiments on a sample of the network, we study thousands of alternatives and identify strategies much more efficient at exploring mature knowledge networks. We find that increased risk-taking and the publication of experimental failures would substantially improve the speed of discovery. We consider institutional shifts in grant making, evaluation, and publication that would help realize these efficiencies.







MK, Zeilinger "Predicting Research Trends with Semantic and Neural Networks with an application in Quantum Physics", *PNAS* **117**(4), 1910 (2020).



Phys. Rev. Lett. 74, 4763 (1995):
[...] The fraction of **"interaction-free" measurements** can be arbitrarily close to 1. Using **single photons** in a **Michelson interferometer**, we have performed a preliminary demonstration of some of these ideas. [...]

Phys. Rev. A 88, 023812 (2013):
We study the quantum dynamics of a **Michelson interferometer** with **Fabry-Perot cavity** arms and one movable end mirror, and driven by a **single photon**—an optomechanical device previously studied by Marshall et al. as a device that searches for gravity decoherence. [...]

Phys. Rev. X 5, 011003 (2015):
[...] Measuring **temporal correlations** of the position of single atoms performing a quantum walk, we observe a 6σ violation of the **Leggett-Garg inequality**. [...] The **interaction-free measurement** is based on a novel atom transport system, which allows us to directly probe the absence rather than the presence of atoms at a chosen lattice site. [...]

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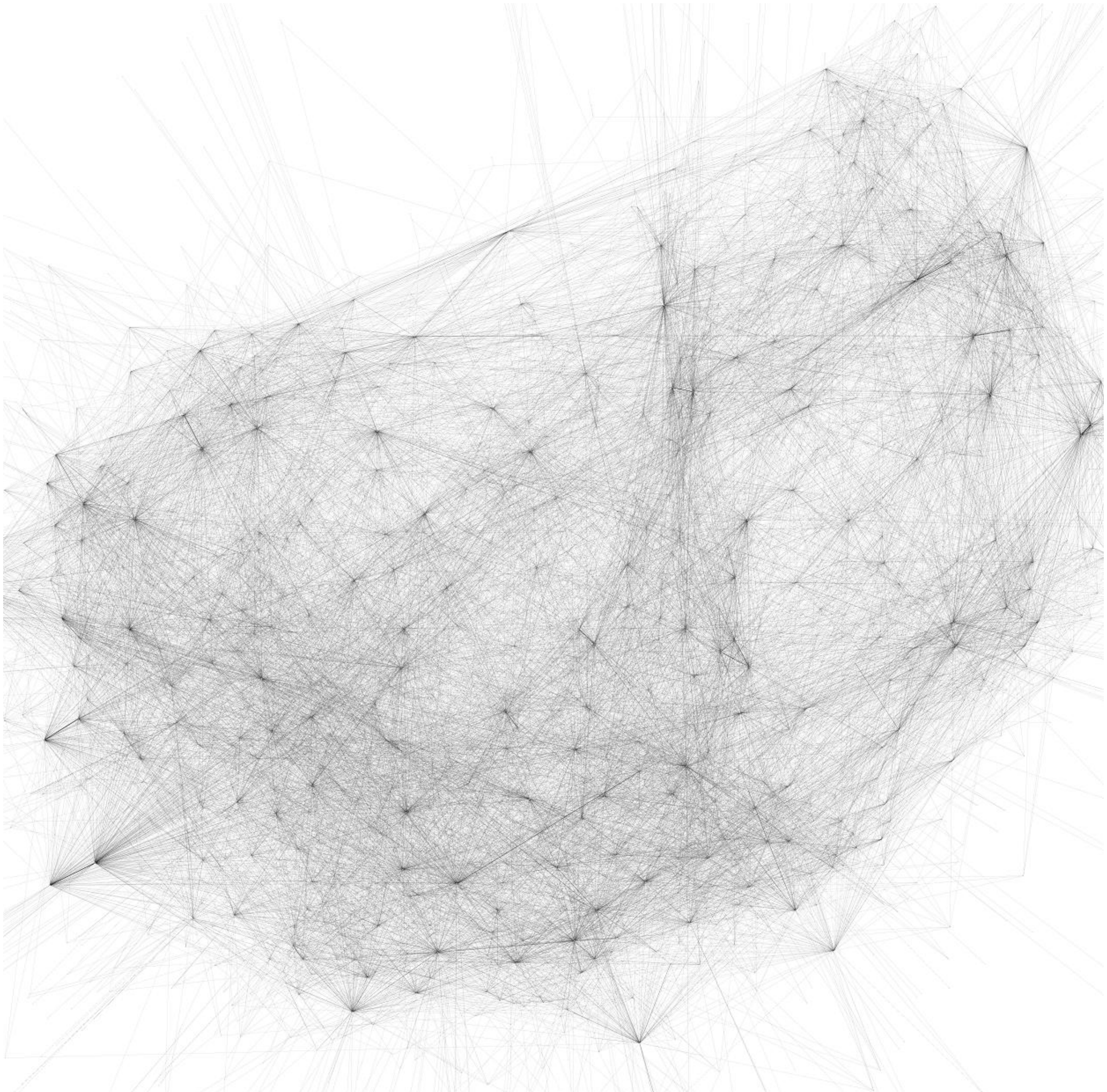

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What will human researchers work on in the future?

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Which unconnected pairs of concepts will be investigated together in 5 years?

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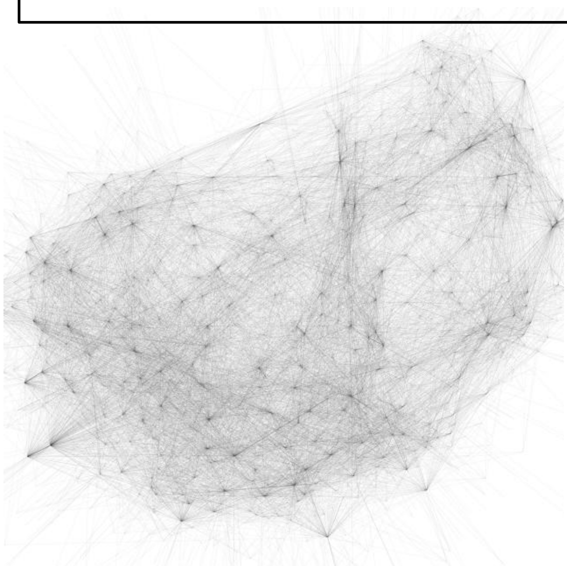
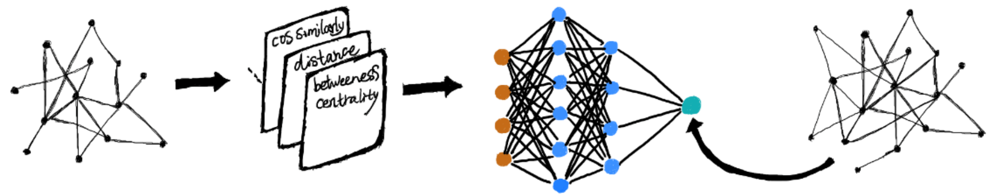


Link Prediction
via Neural Networks

2015

2020



<u>MK</u>, Zeilinger "Predicting Research Trends with Semantic and Neural Networks with an application in Quantum Physics", *PNAS* **117**(4), 1910 (2020).

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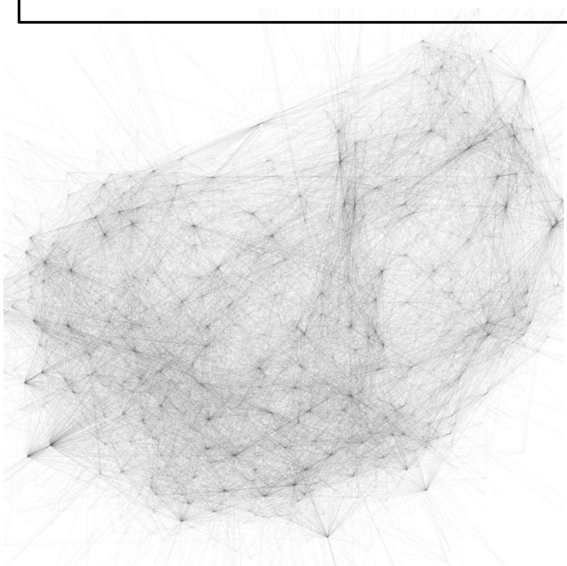
What will human researchers work on in the future?

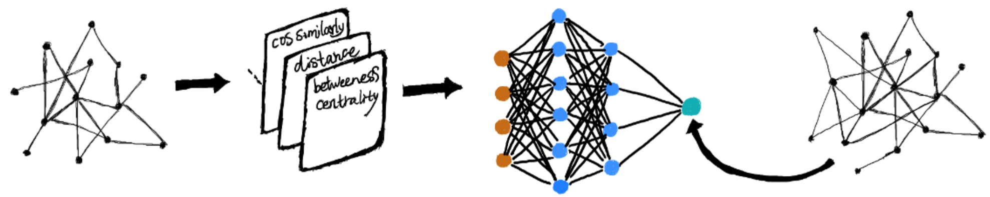
Which unconnected pairs of concepts will be investigated together in 5 years?



Link Prediction via Neural Networks

2015

2020



Evaluate with 2025: AUC=85%

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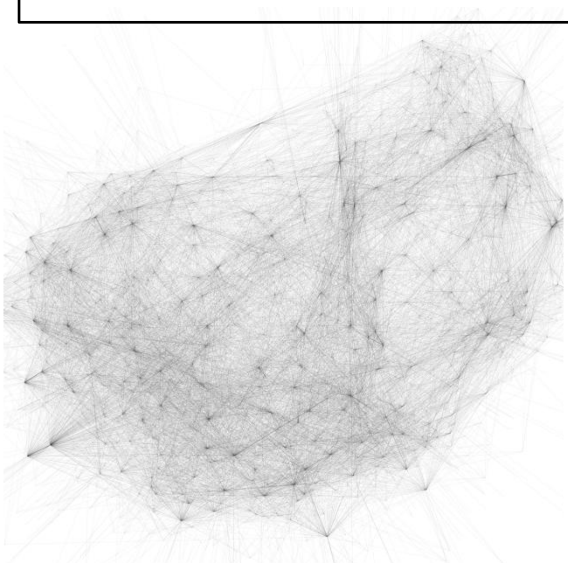
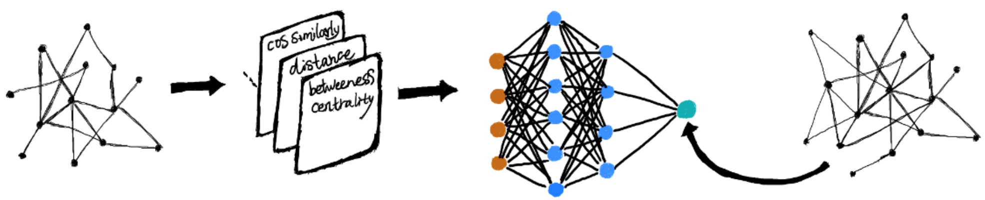


Link Prediction via Neural Networks

2020

2025



<u>Then: From 2025 to 2030!</u>

<u>MK</u>, Zeilinger "Predicting Research Trends with Semantic and Neural Networks with an application in Quantum Physics", *PNAS* **117**(4), 1910 (2020).

What will be impactful?

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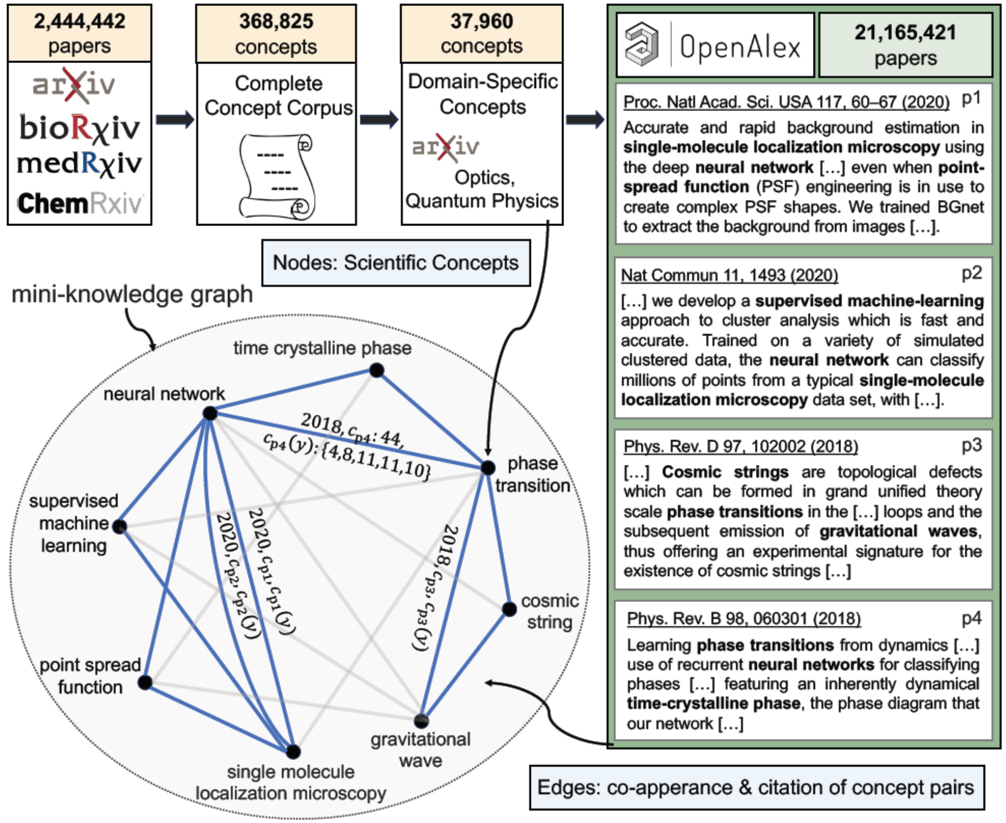

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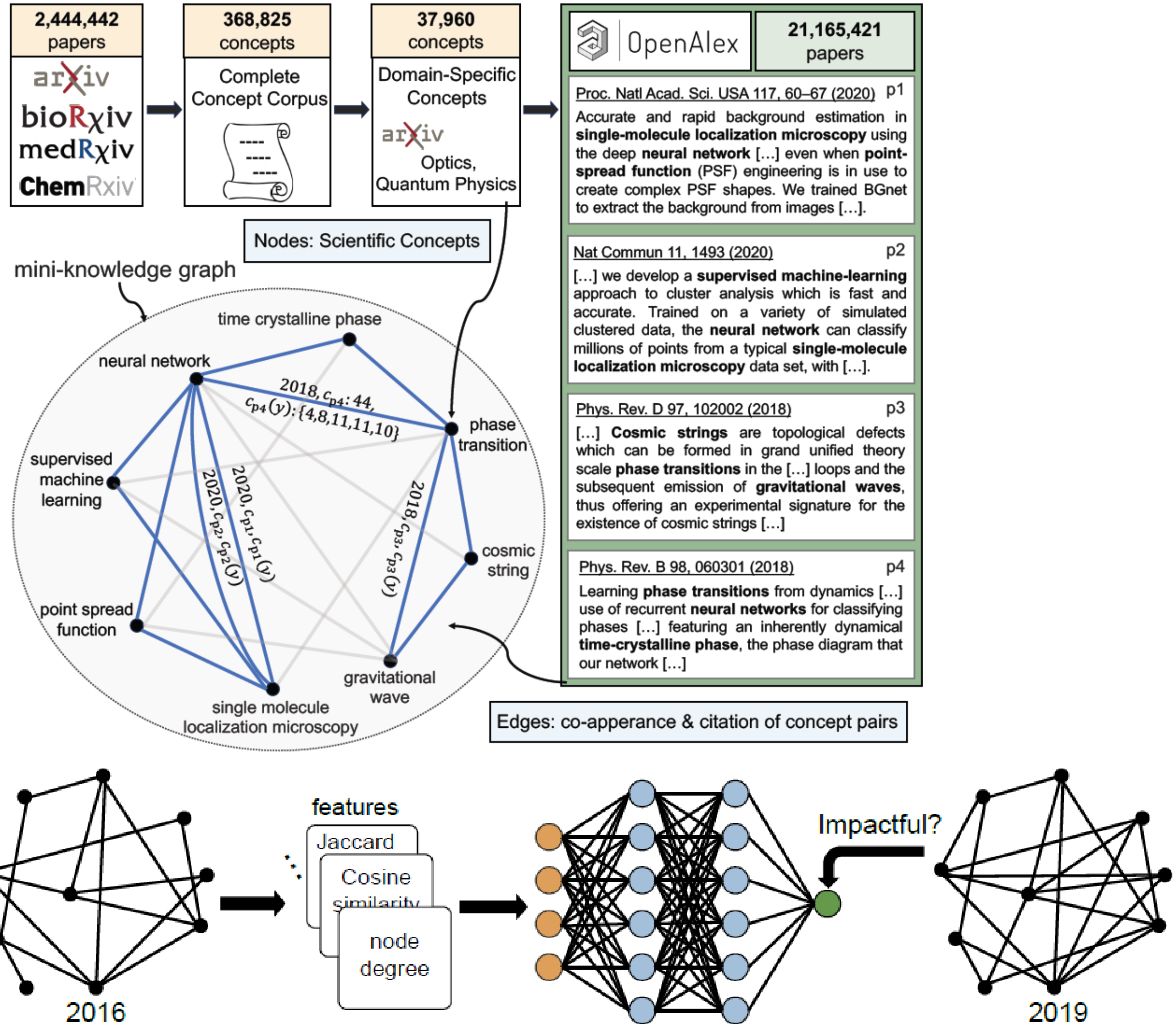

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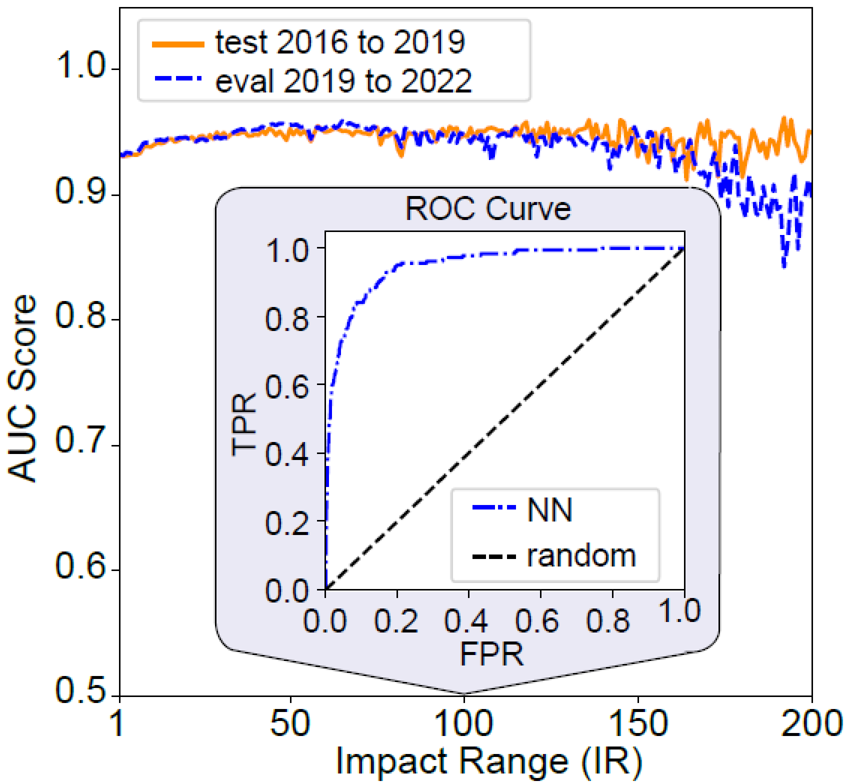

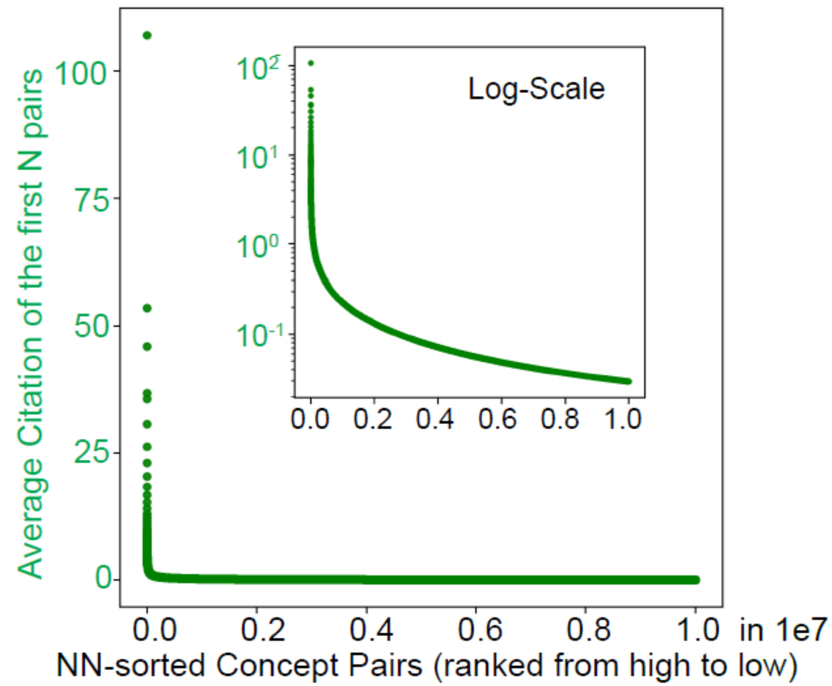

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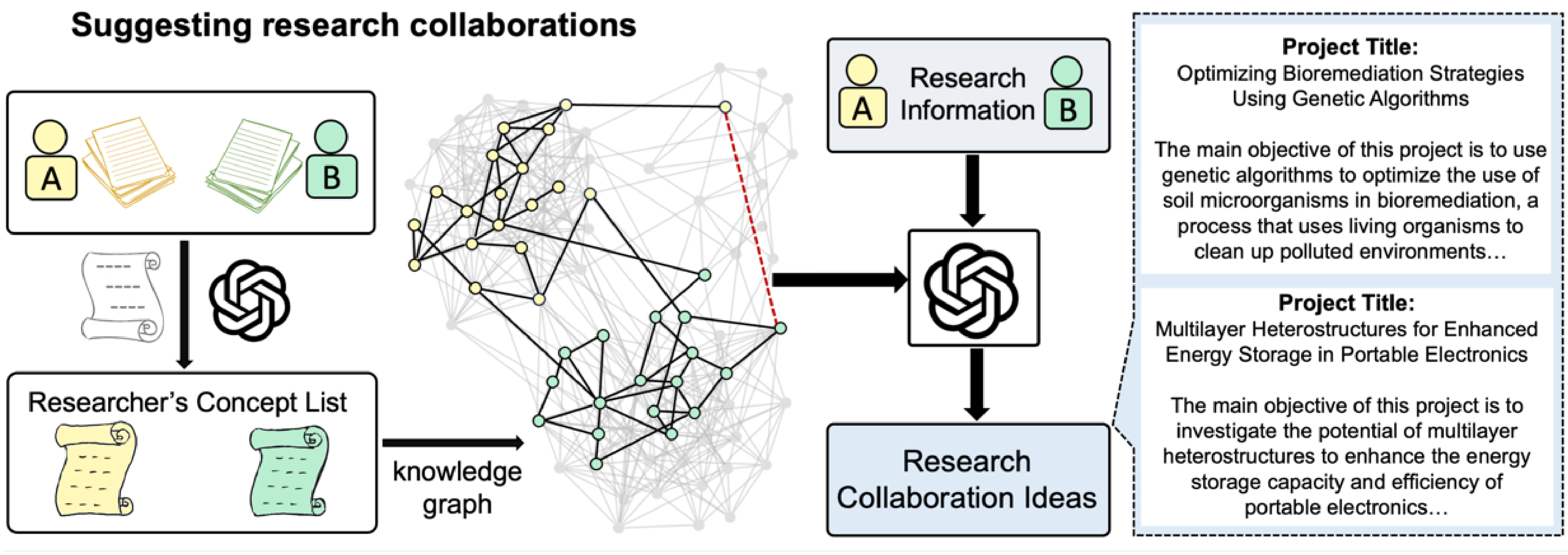
Real project ideas?



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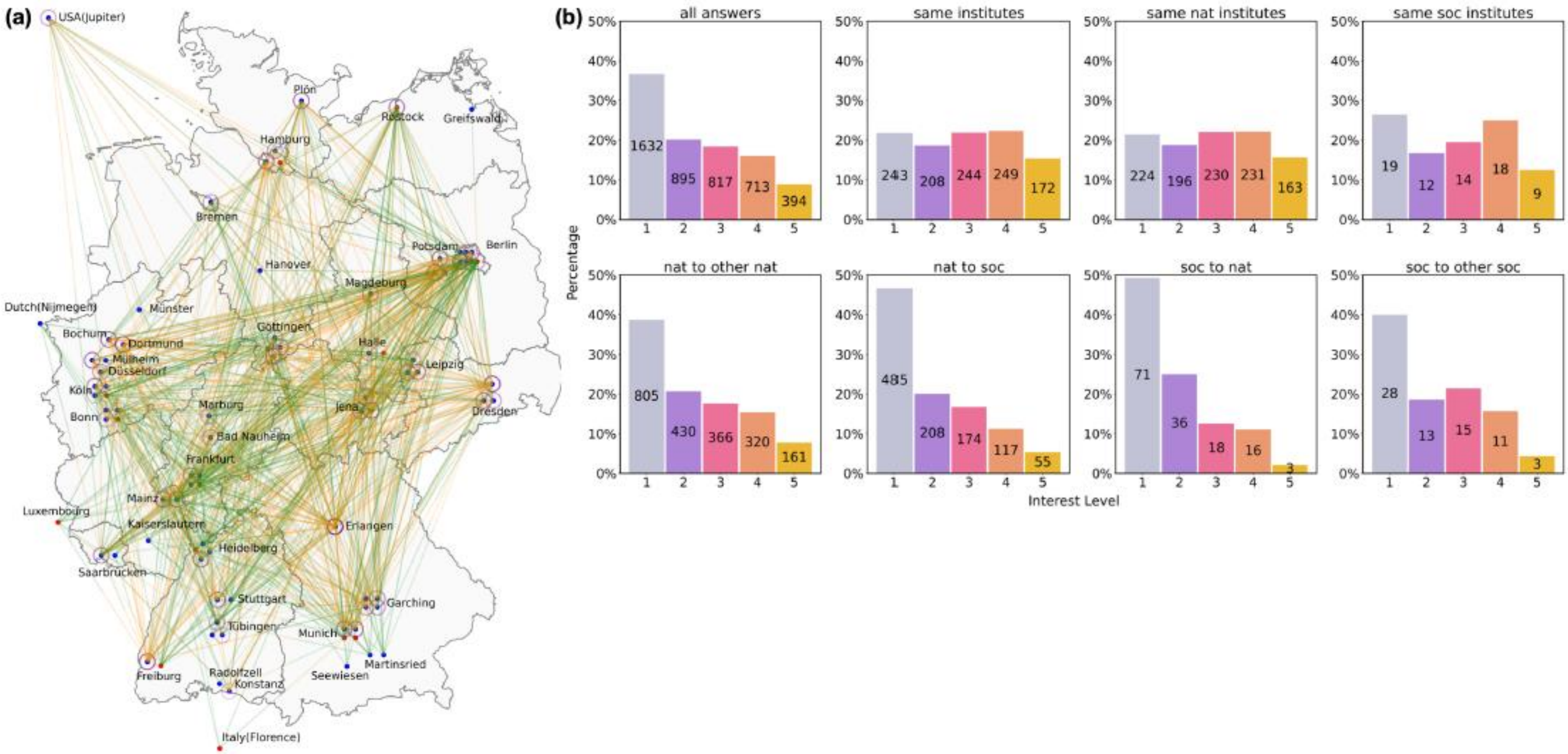

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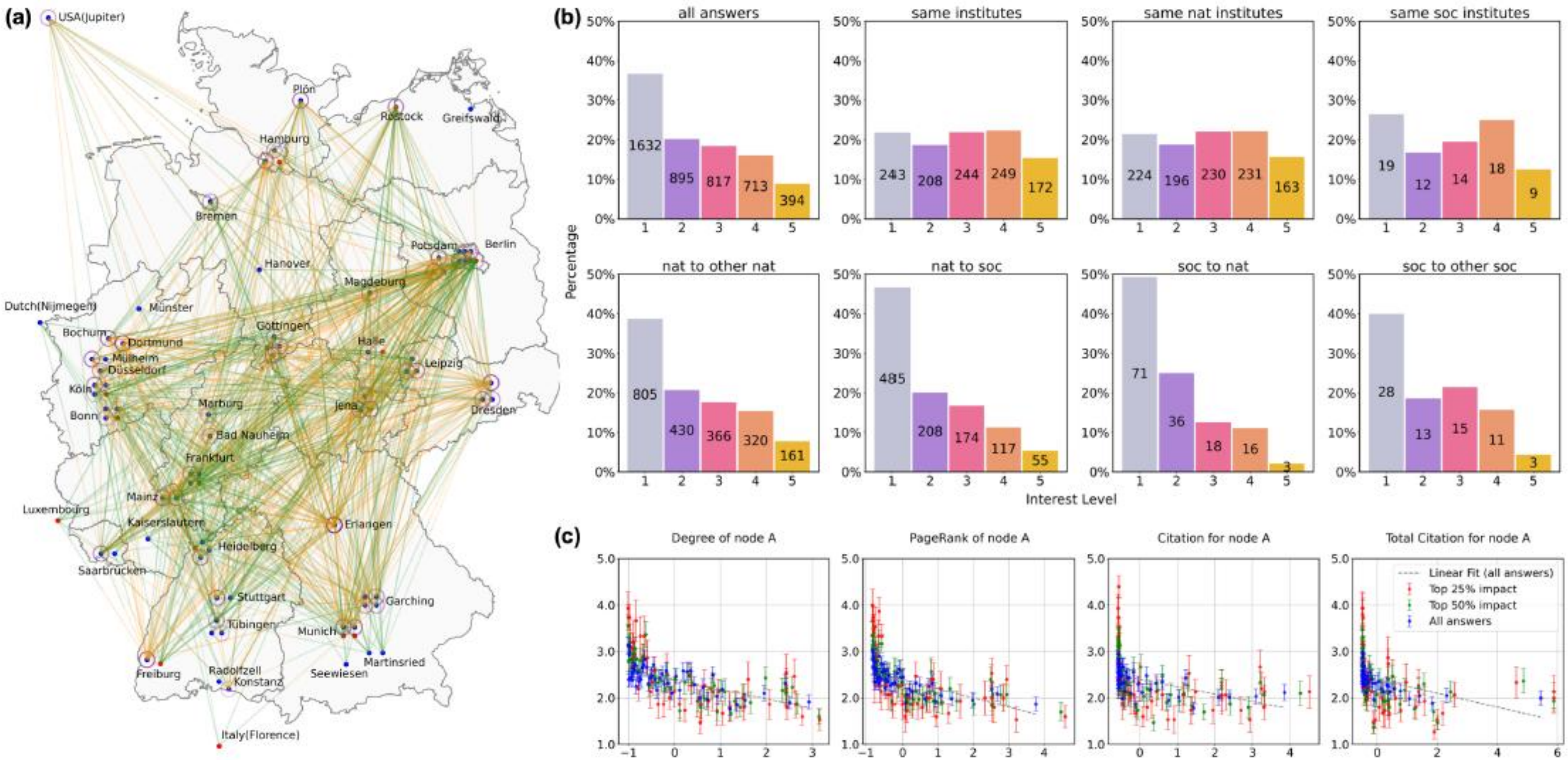

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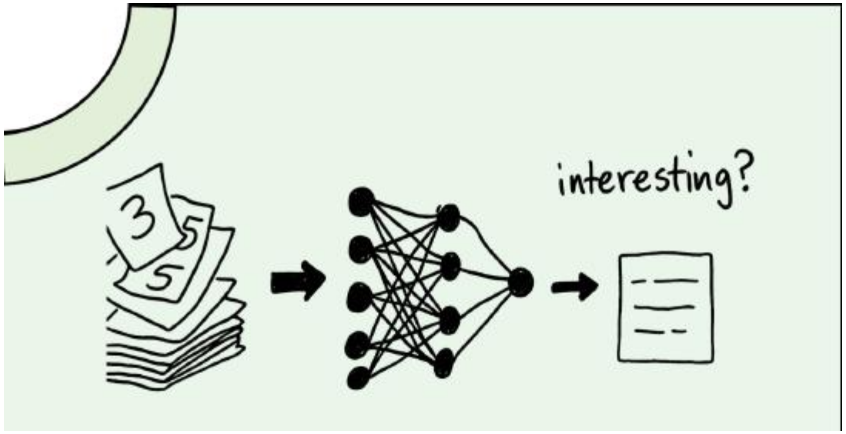

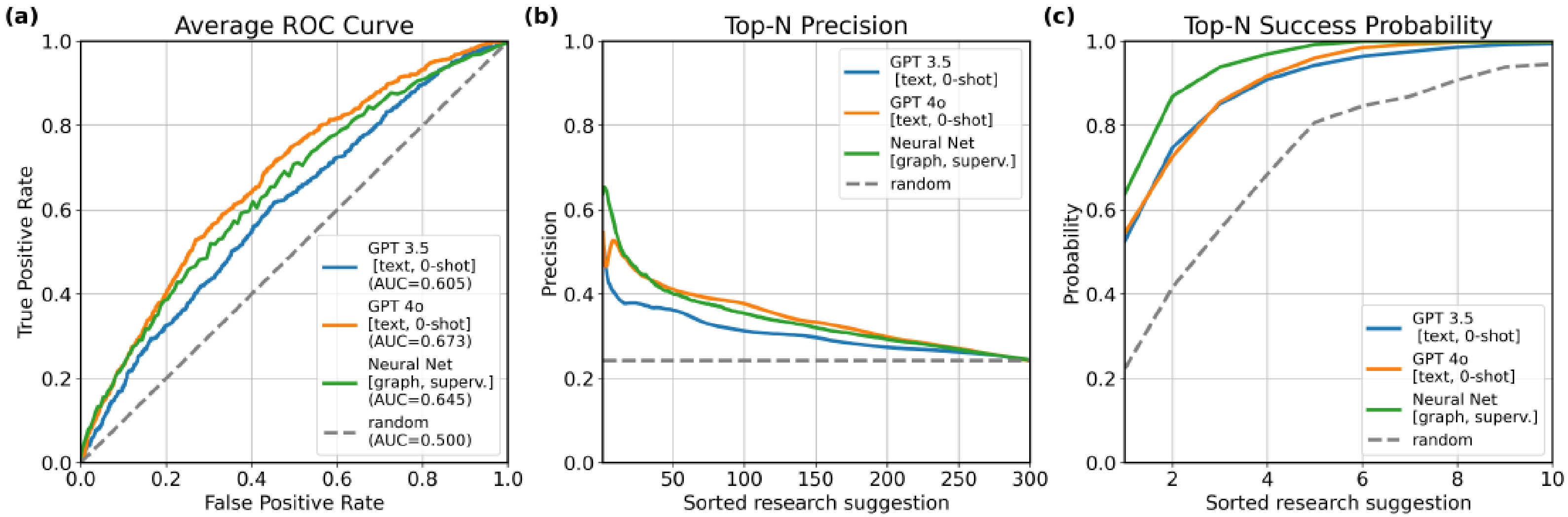

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Ongoing: Agentic Automated Discovery Framework in Quantum Mechanics

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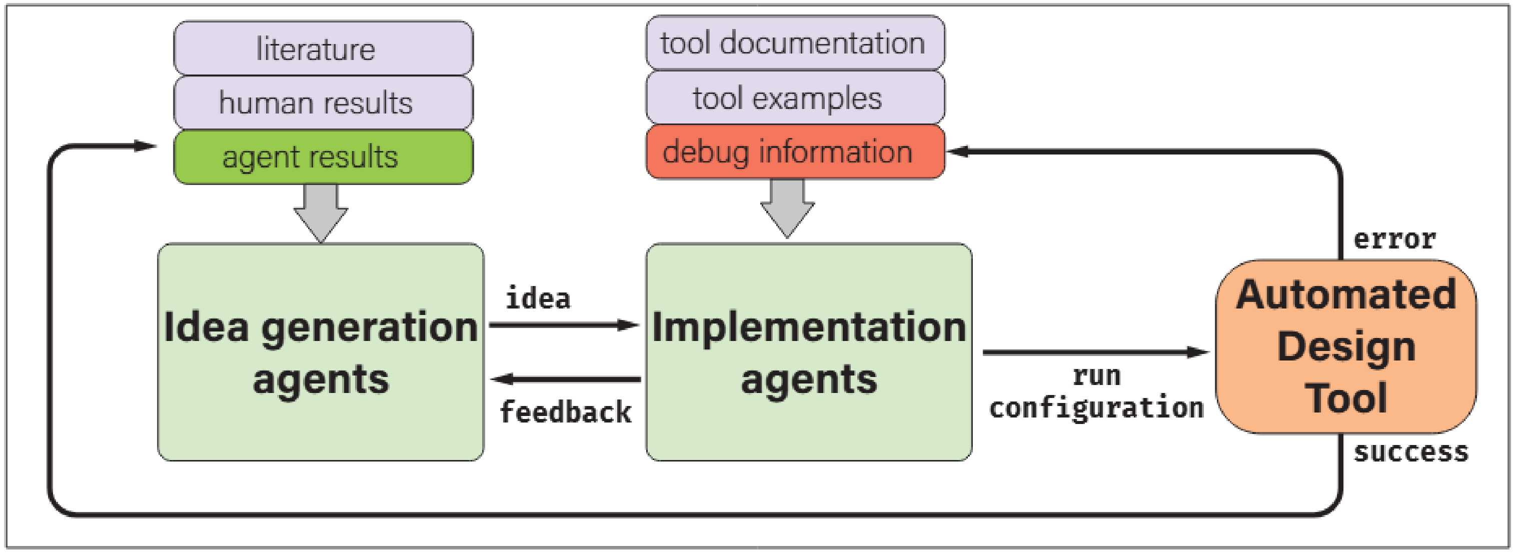

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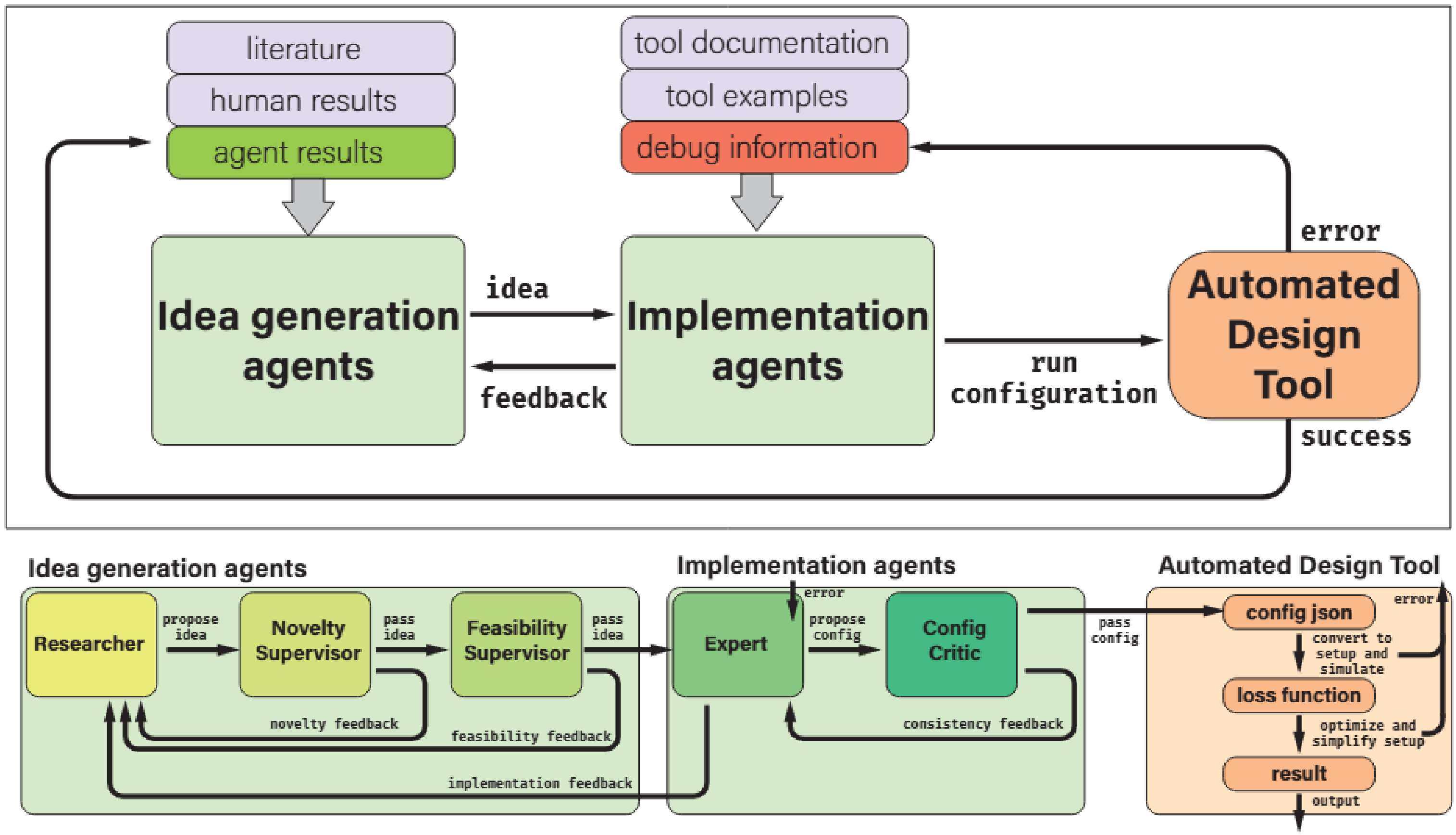

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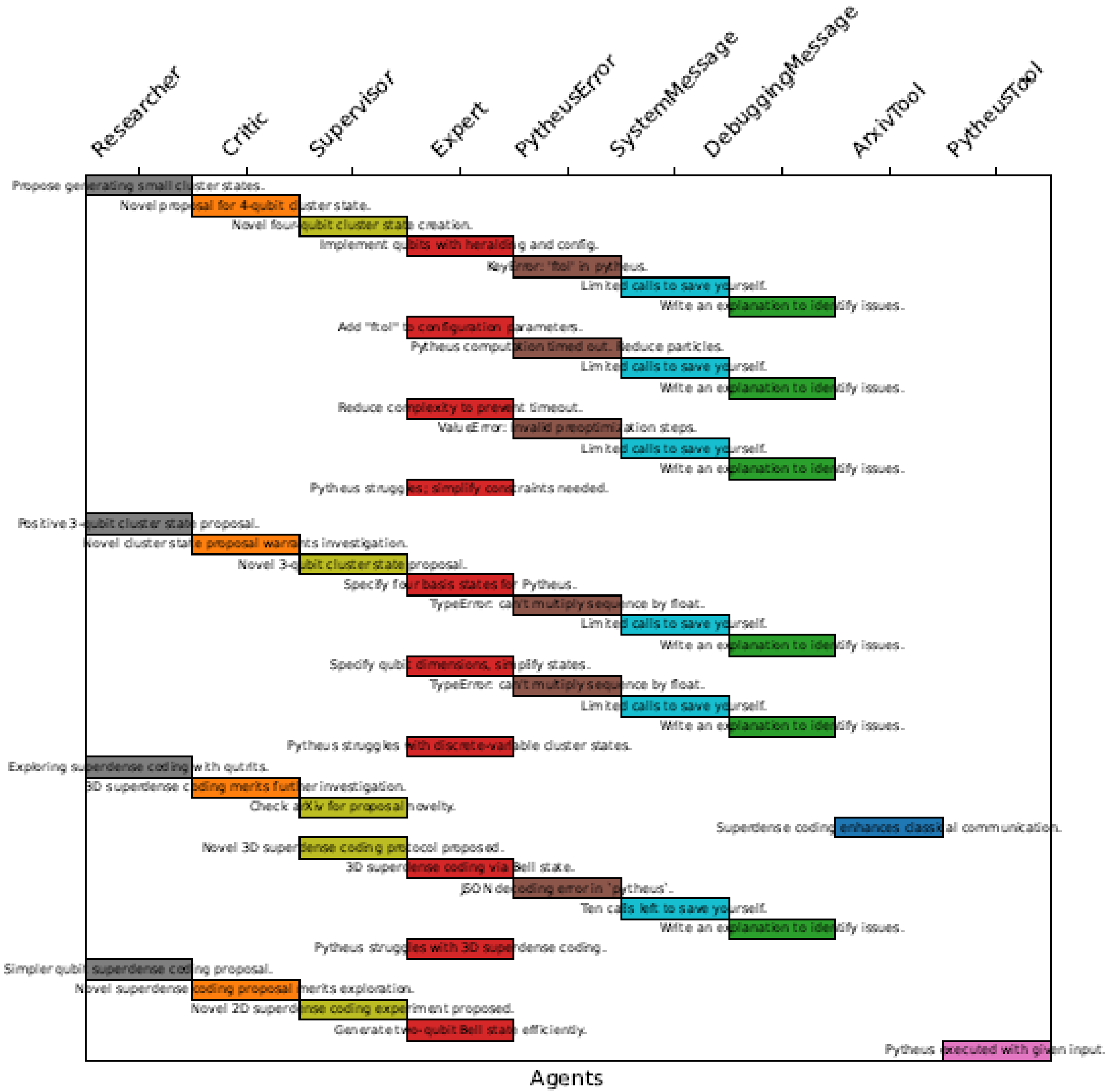

Conclusion

AI-based Experimental Design:

In many domains in physics (*quantum optics, gravitational wave physics, microscopes/telescopes soon*), we have now algorithms for

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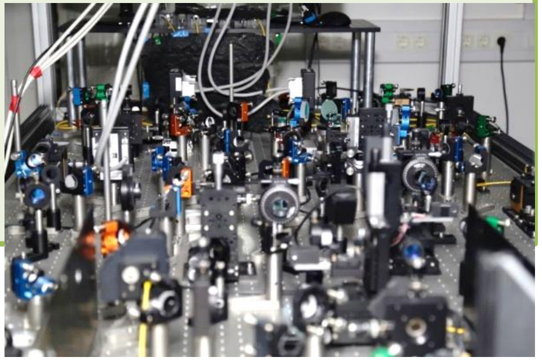

The solutions are presented such that

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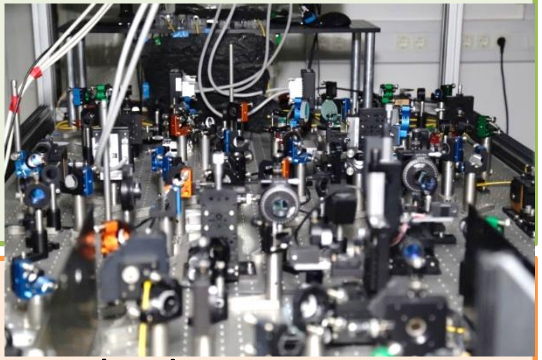

Automated Idea Generation:

Towards personalized, new, high-impact, interesting research idea generation

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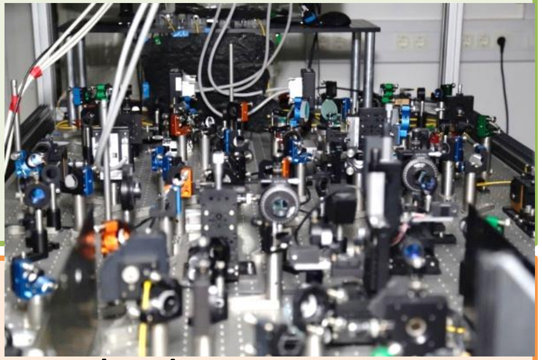


Automated Idea Generation:

Towards personalized, new, high-impact, interesting research idea generation

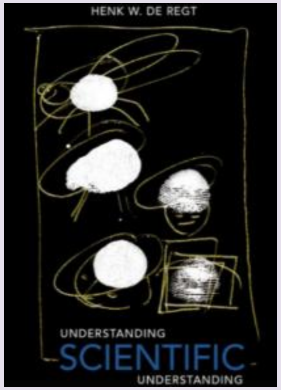
Artificial Scientists

Creativity?

Curiosity?

(a) learn to explore on Level-1 (b) explore faster on Level-2

Understanding?



MK et al., On scientific understanding with artificial intelligence, Nat.Rev.Phys (2022)

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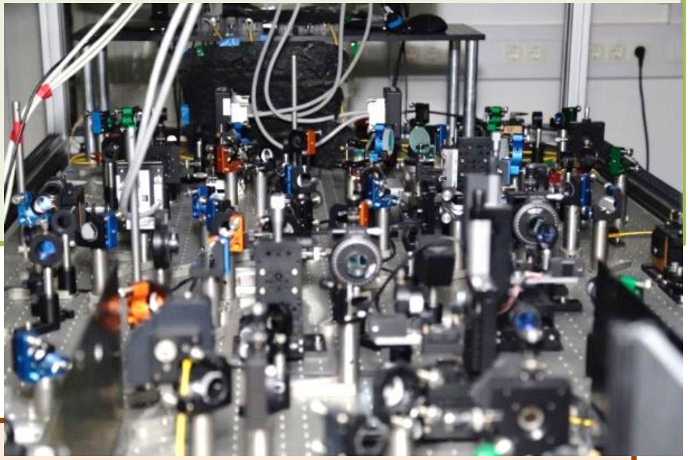

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