

Towards an Artificial Muse for new Ideas in Science



Mario Krenn

Artificial Scientist Lab, Theory Division

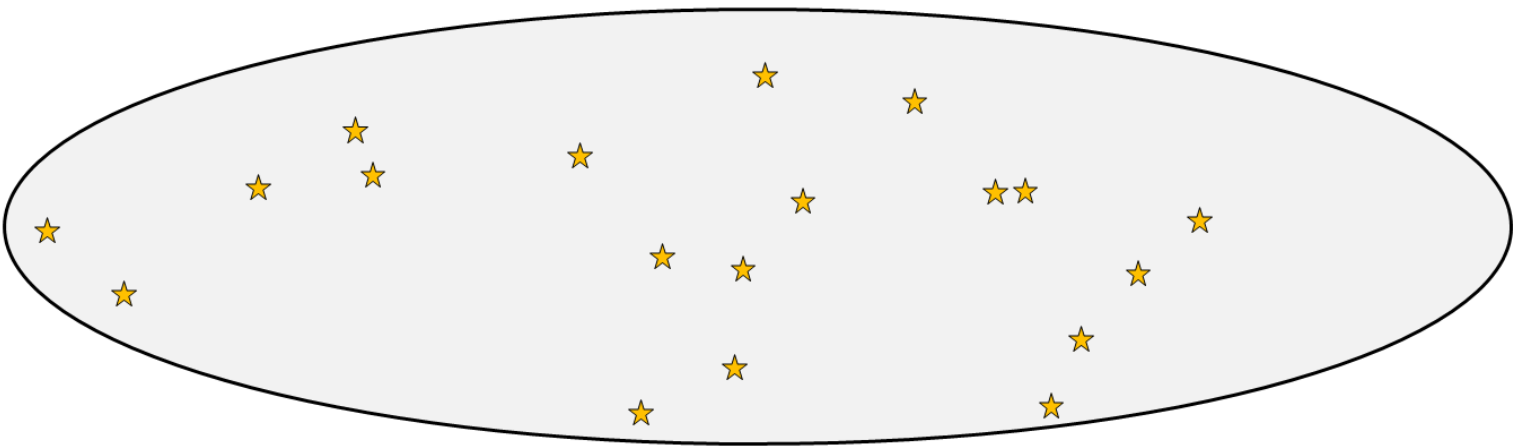
 @mariokrenn6240

<http://mariokrenn.wordpress.com/>



MAX PLANCK INSTITUTE
FOR THE SCIENCE OF LIGHT

Abstract space of all experimental setups



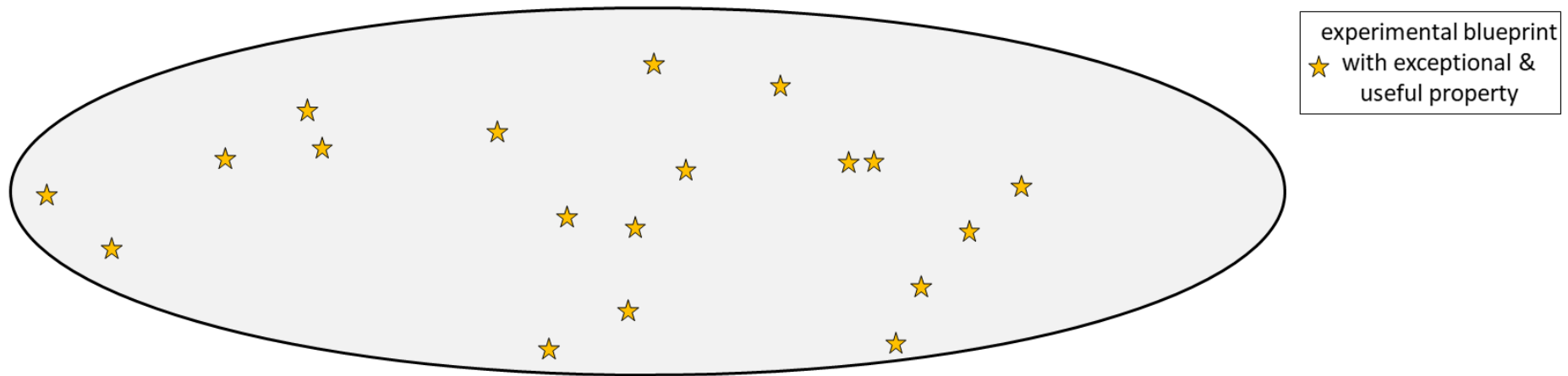
experimental blueprint
★ with exceptional & useful property

Some examples:

3 lasers, 3 BS, 3 detectors: 1000 combinations

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

Abstract space of all experimental setups

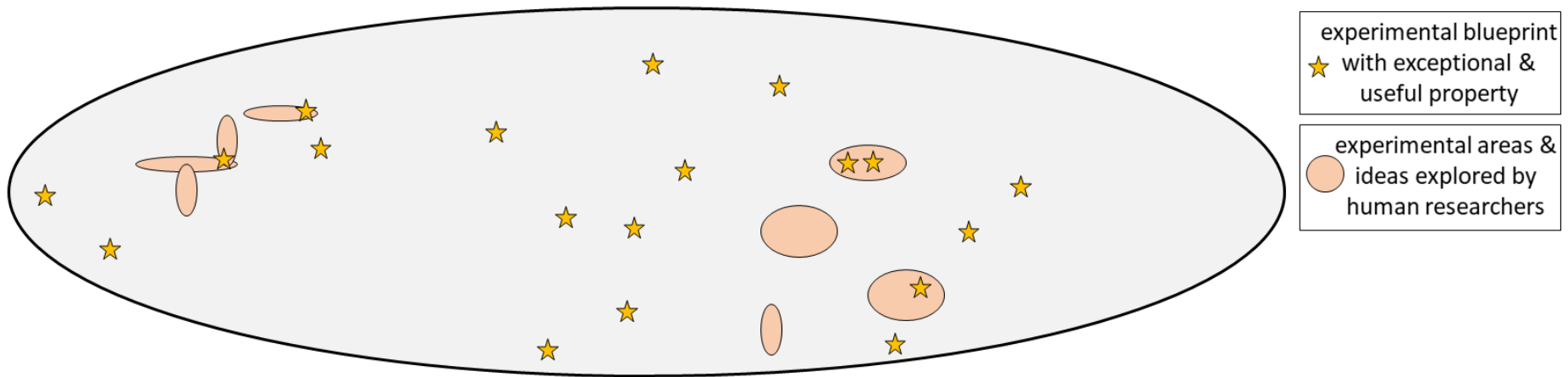


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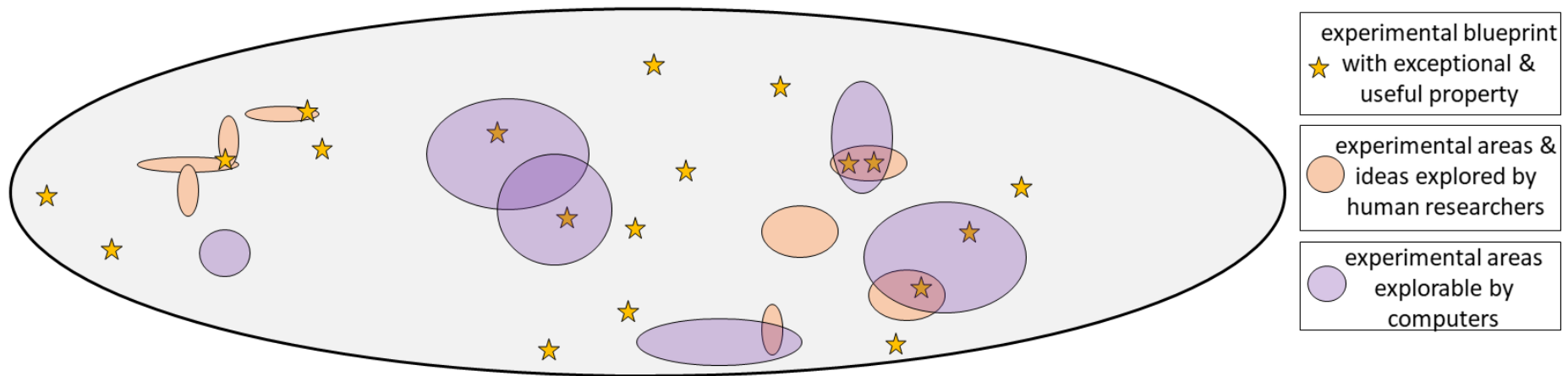


Some examples:

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Abstract space of all experimental setups



How to design quantum experimental setups?

High-dimensional multipartite entanglement

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

 or  or 

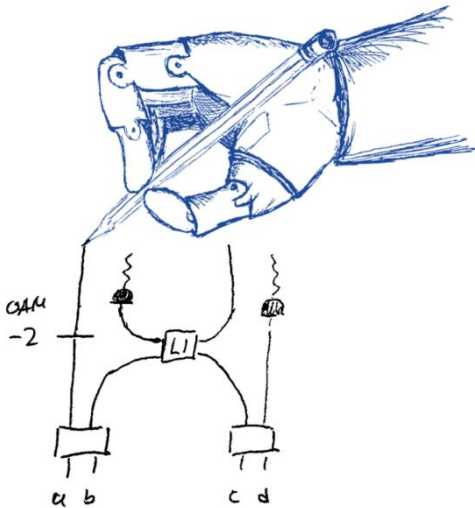
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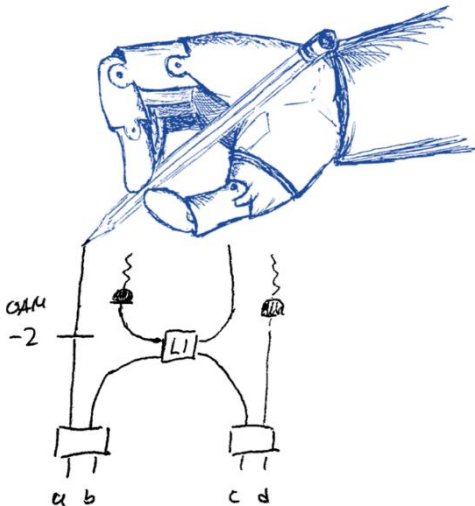
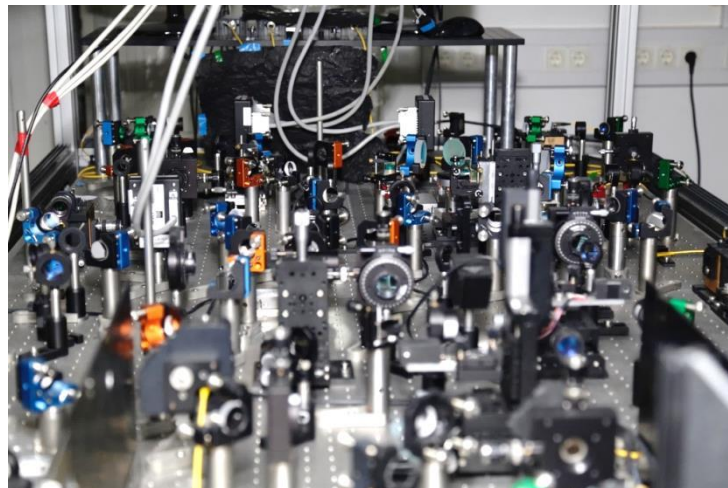
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Erhard et al., *Nature Photonics* **12**, 759 (2018)



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

Krenn, Erhard, Zeilinger, Computer-inspired quantum experiments, *Nat.Rev.Phys* **2**, 649 (2020).

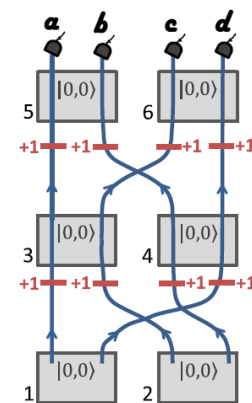
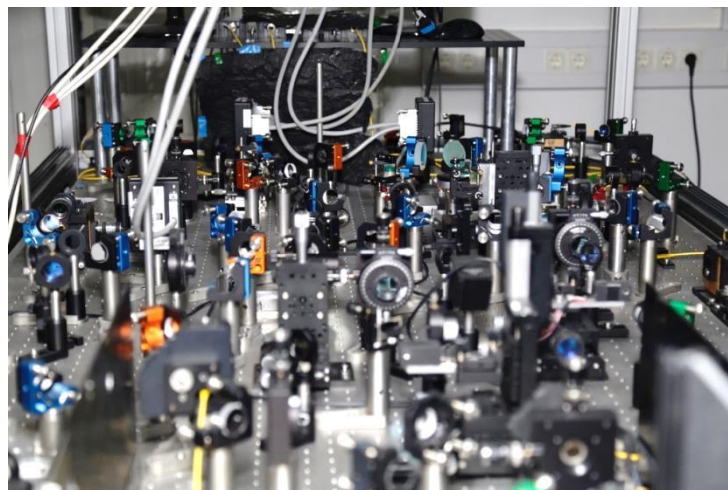
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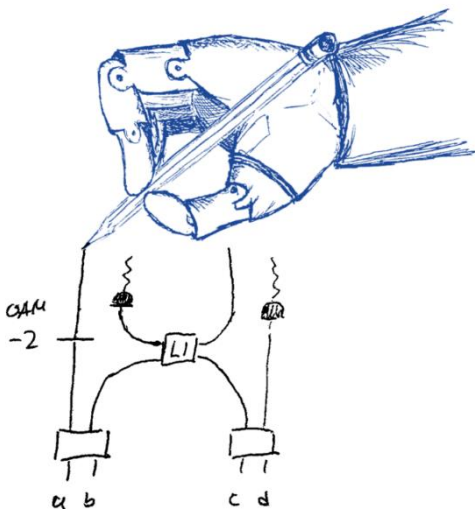
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MK, Hochrainer, Lahiri, Zeilinger, Entanglement by Path Identity, *PRL* **118** (2017)

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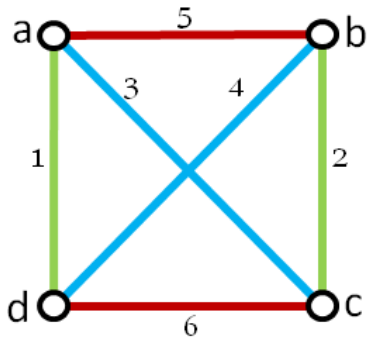
Krenn, Erhard, Zeilinger, Computer-inspired quantum experiments, *Nat.Rev.Phys* **2**, 649 (2020).



Computer-inspired ideas and concepts

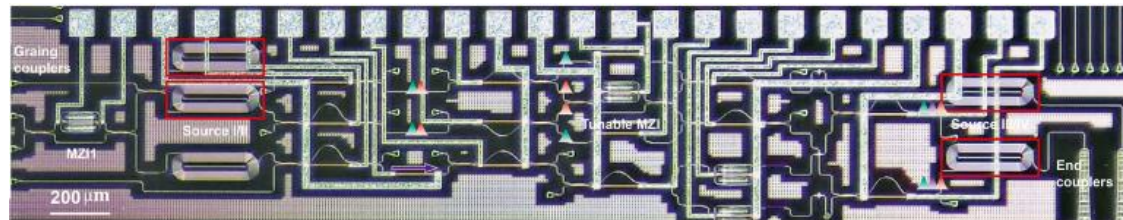
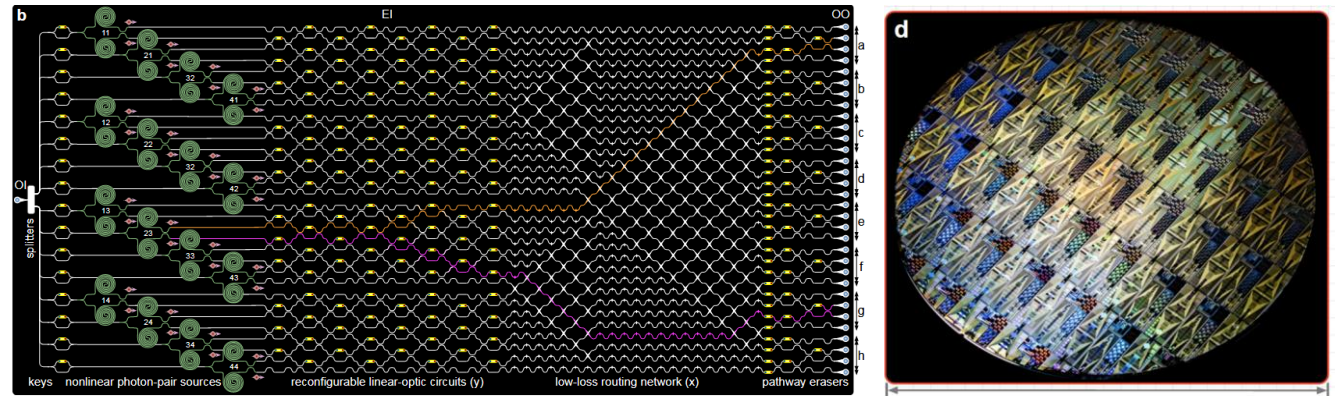
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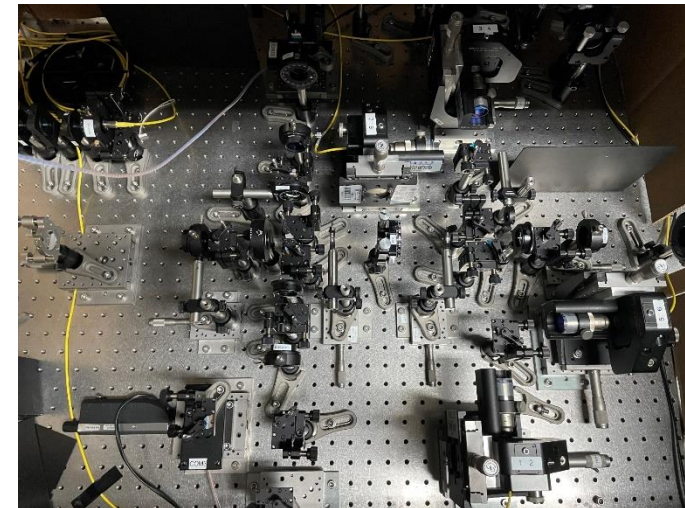


Gu, Erhard, Zeilinger, MK, *PNAS* **116** (2019).

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)

Highly efficient computer-designed quantum experiments

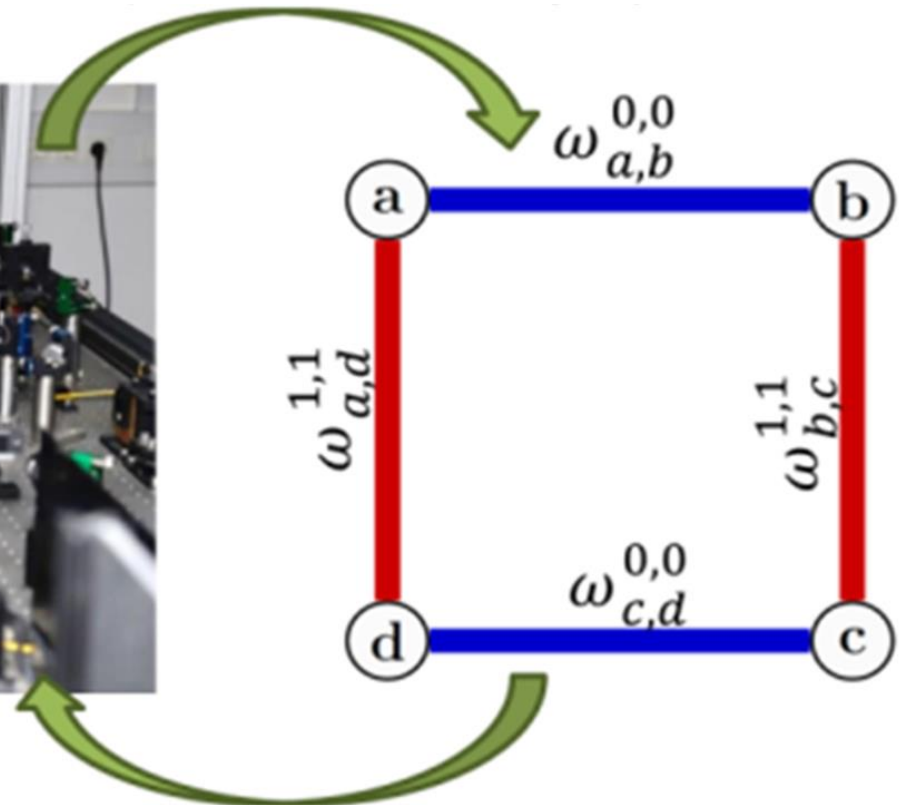
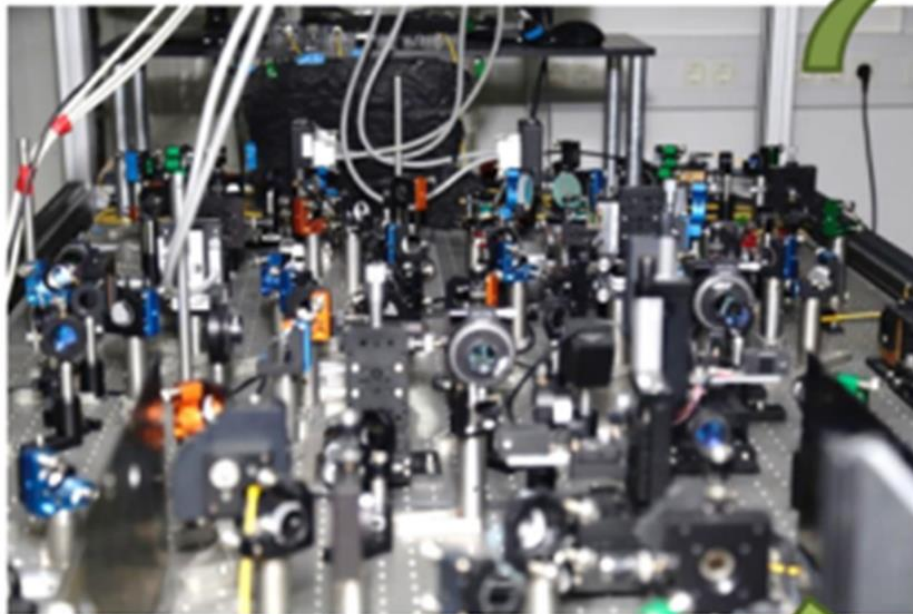
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Change Perspective:

New representation -> orders of magnitude speed-up.



Highly efficient computer-designed quantum experiments

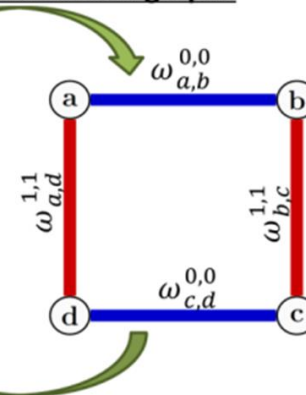
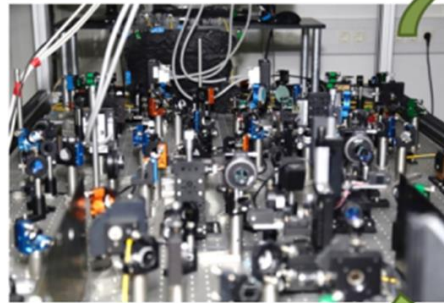
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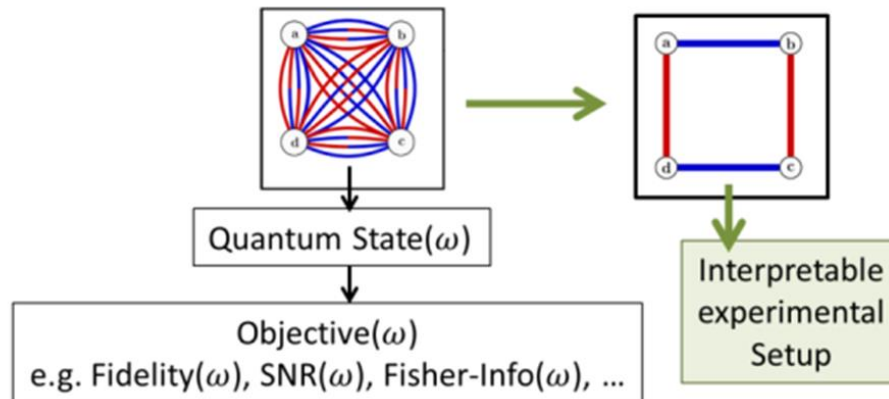
New representation -> orders of magnitude speed-up.

A) Bridge between quantum experiments and graphs

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



B) Gradient-based optimization + discrete topological optimization



Highly efficient computer-designed quantum experiments

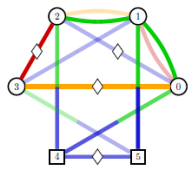
Quantum

the open journal for quantum science

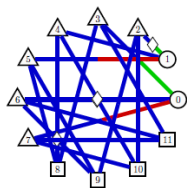
Digital Discovery of 100 diverse Quantum Experiments with PyTheus

Carlos Ruiz-Gonzalez^{§1}, Sören Arlt^{§1}, Jan Petermann¹, Sharareh Sayyad¹, Tareq Jaouni², Ebrahim Karimi^{1,2}, Nora Tischler³, Xuemei Gu¹, and Mario Krenn¹

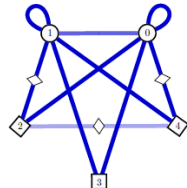
Quantum 7, 1204 (2023).



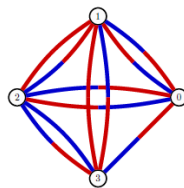
(a) Four-dimensional four-photon GHZ state (overcoming the 3-dimensional barrier for multiphoton entanglement)



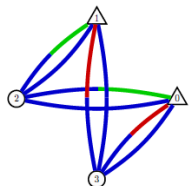
(b) Heralded 3D Bell state with single photons (improves state-of-the-art design by requiring less ancilla photons)



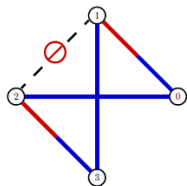
(c) Two-mode five-photon NOON state $|50\rangle + |05\rangle$ (very symmetric shape with an inscribed pentagram)



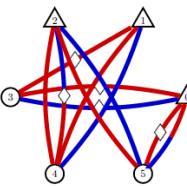
(d) A 4-qubit entangled states with unit coefficients, which requires complex-valued weights for generation



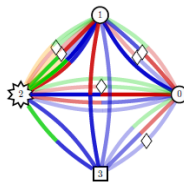
(e) Quantum measurement for a quantum communication task with quantum advantage (Mean King's Problem)



(f) Entanglement swapping without using two Bell states



(g) Toffoli quantum gate without ancilla photons

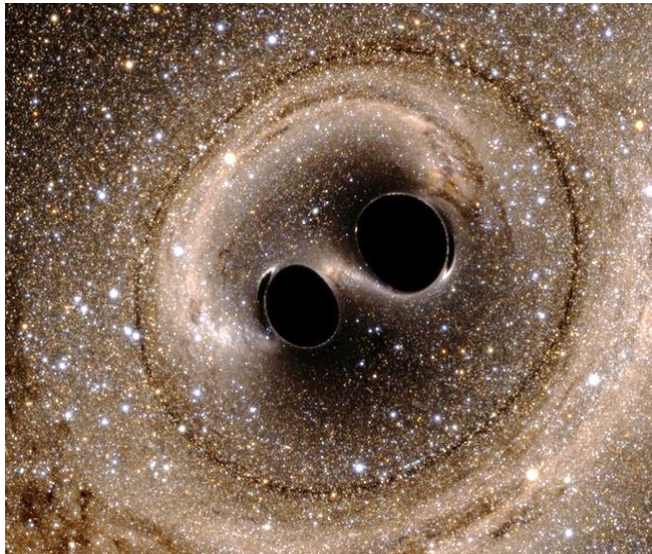


(h) Mixed state with bound entanglement that can violate a Bell inequality (counterexample to the Peres conjecture from 1999, solved 2014)

github.com/artificial-scientist-lab/PyTheus
`pip install pytheusQ`

AI-driven design of new Gravitational Wave Detectors

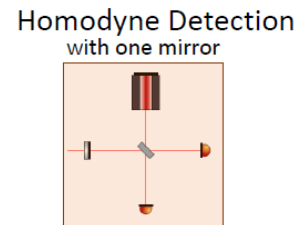
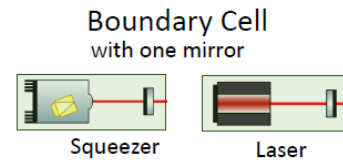
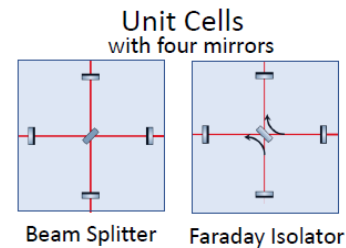
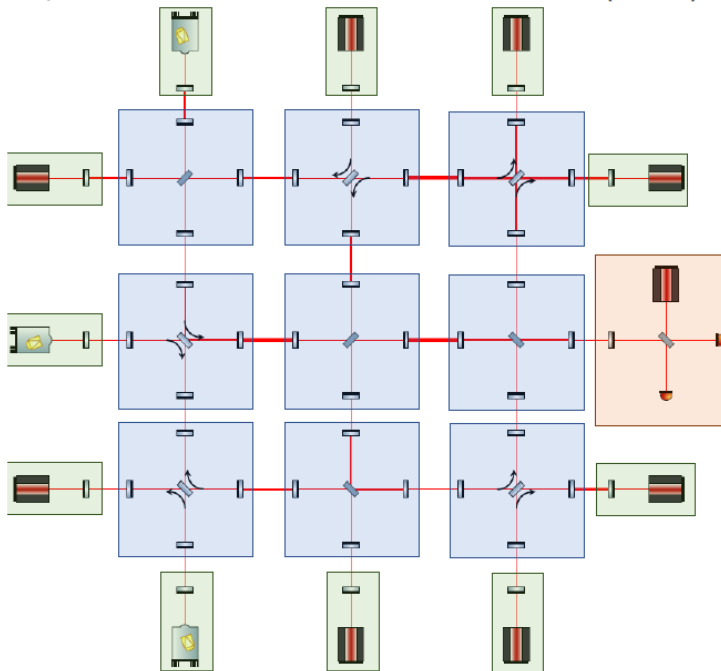
with Yehonathan Drori, Rana X. Adhikari (Caltech, LIGO): arXiv:2312.04258



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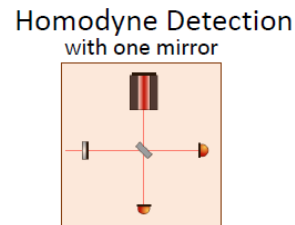
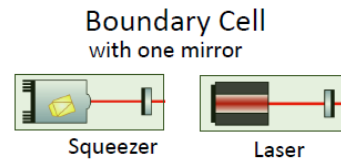
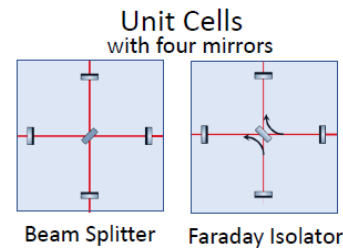
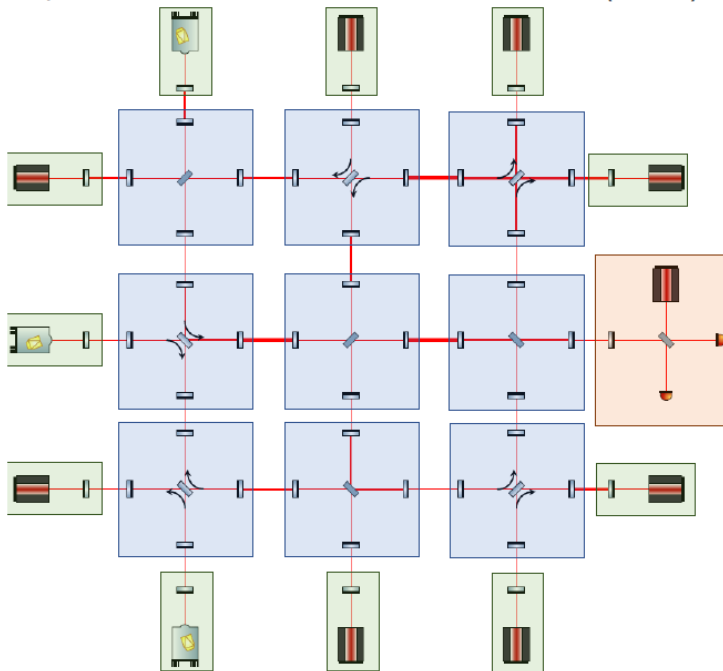
A) Quasi-Universal Interferometer (UIFO)



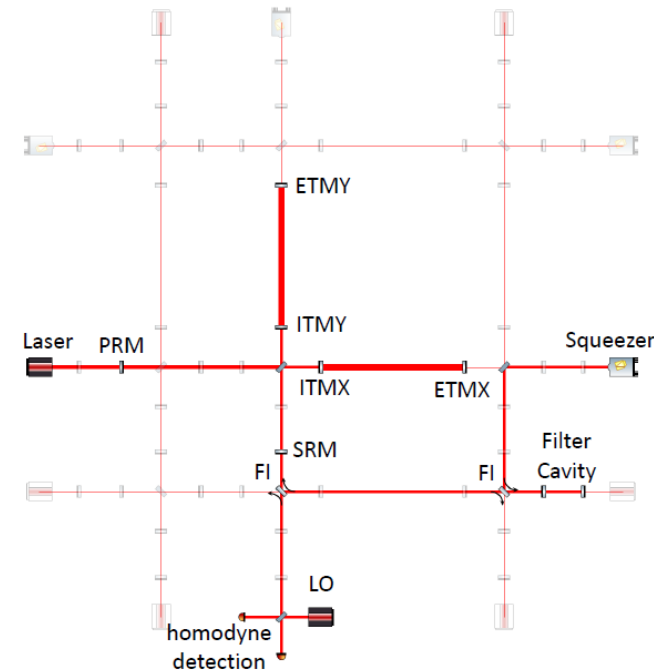
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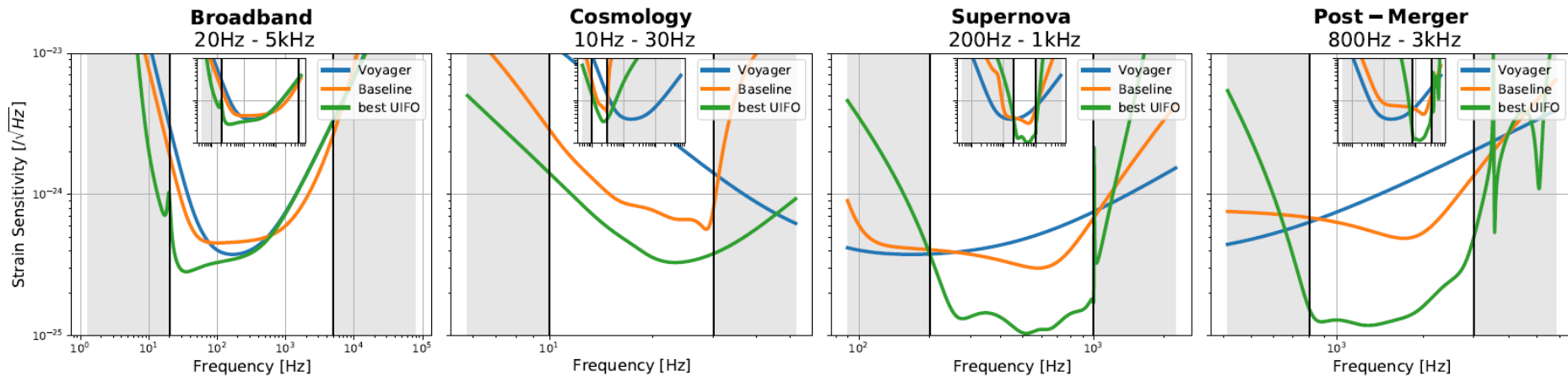


B) LIGO Voyager in UIFO



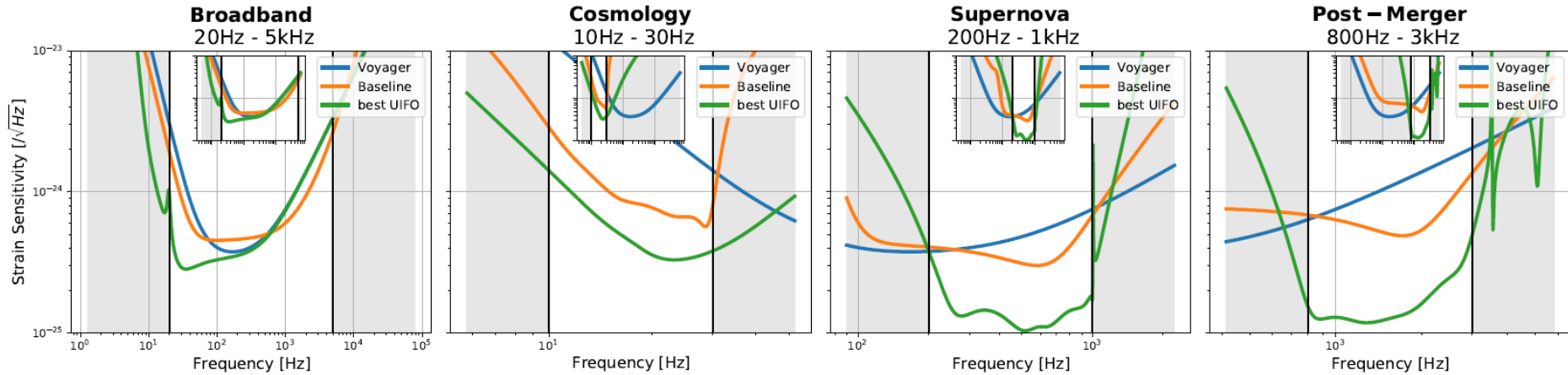
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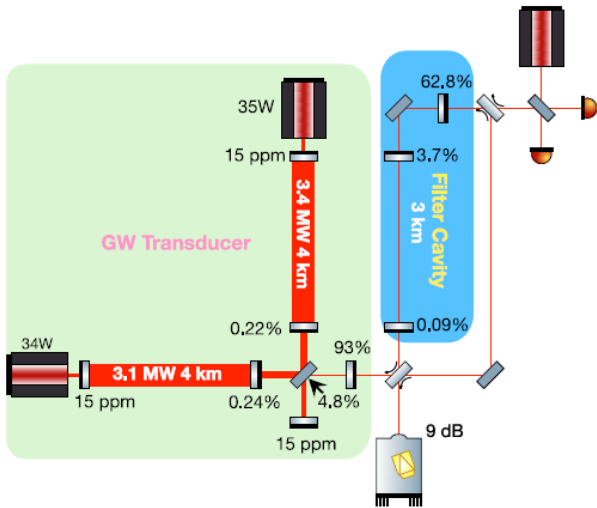


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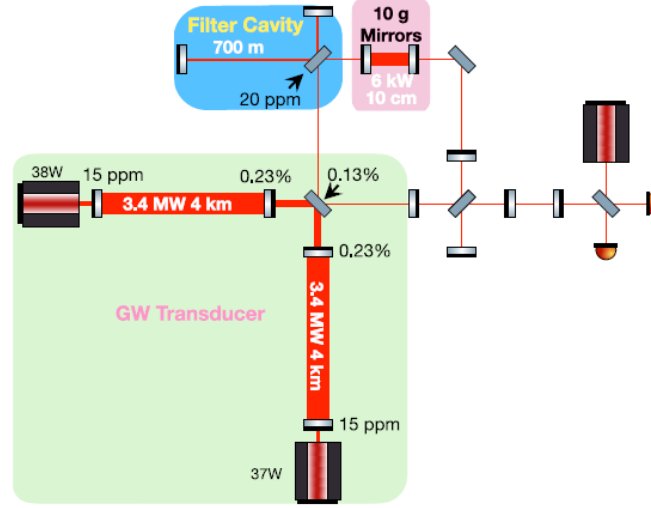
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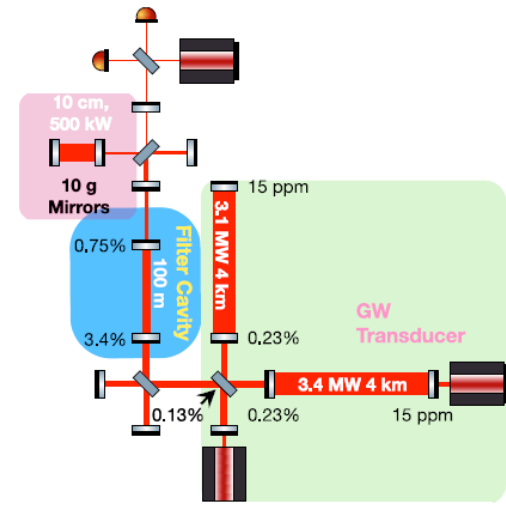
A) Broadband (30 Hz - 3 KHz)



B) Supernova (200 Hz - 1 KHz)

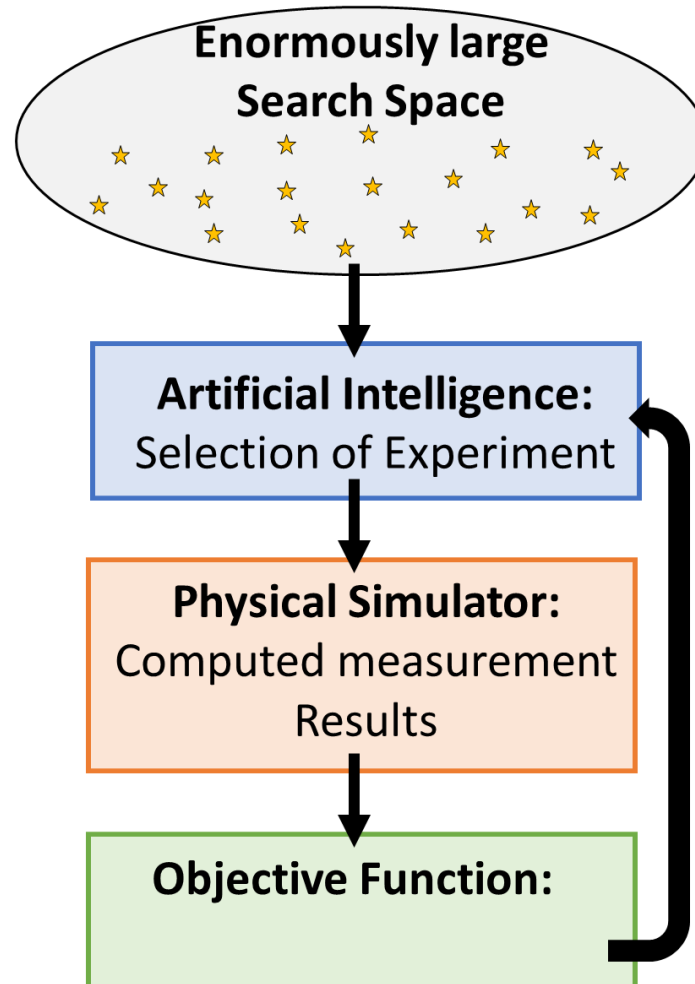


C) Postmerger (800 Hz - 3 KHz)



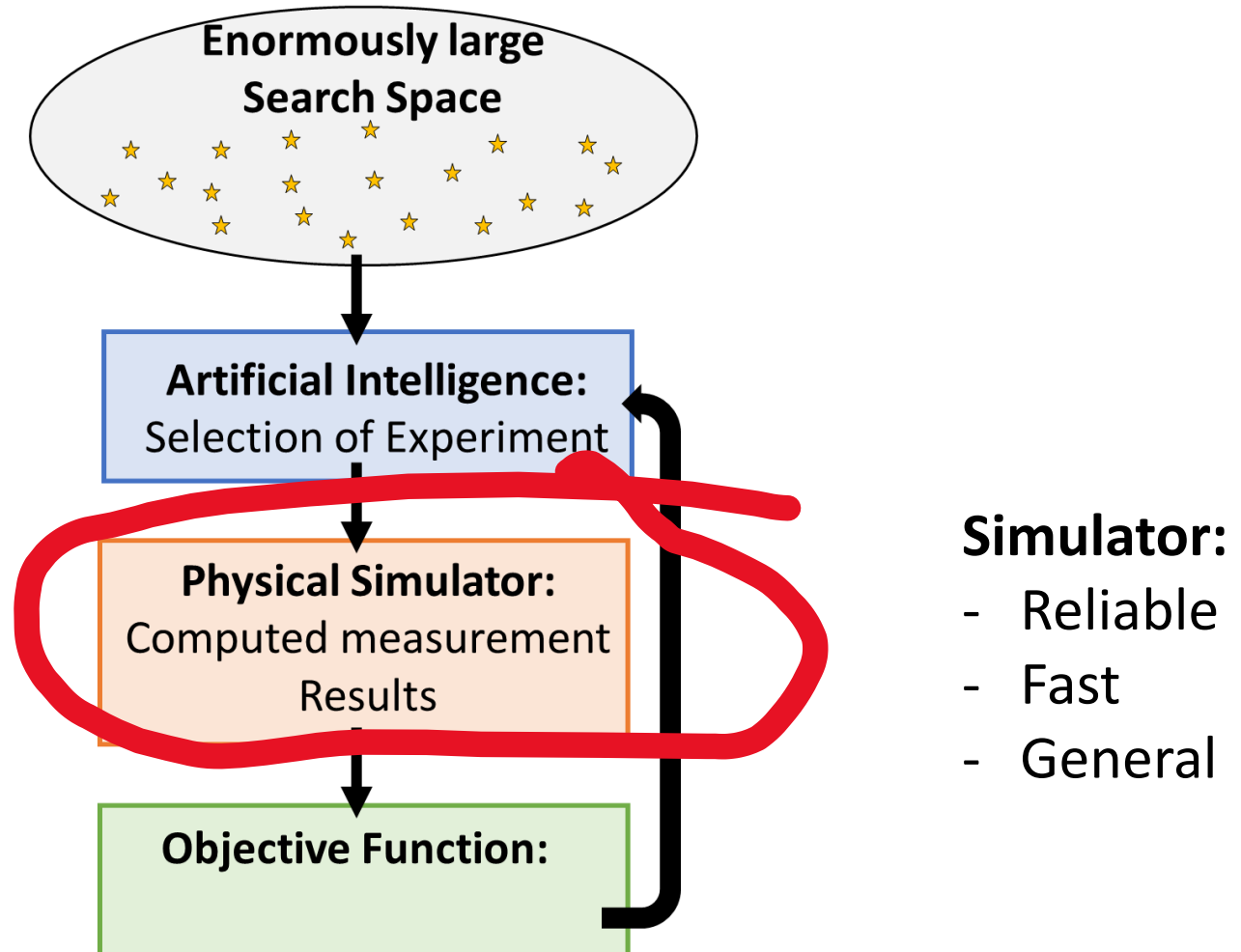
XLuminA: An Auto-differentiating Discovery Framework for Super-Resolution Microscopy

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github.com/artificial-scientist-lab/XLuminA/



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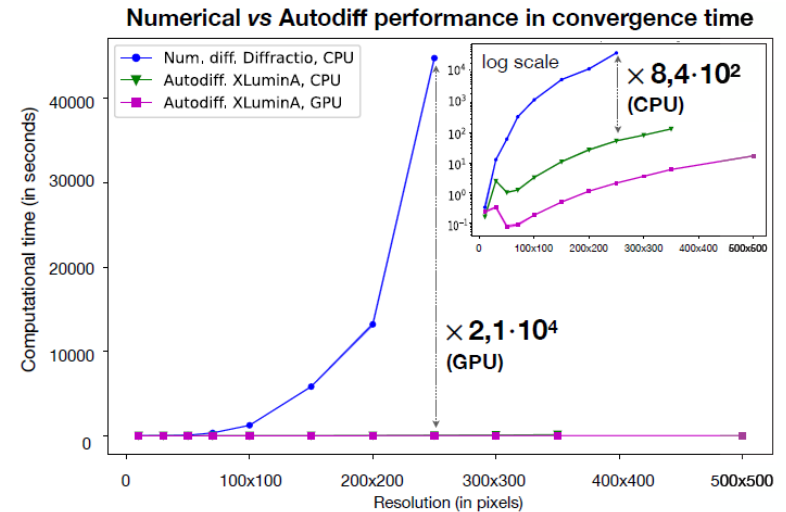
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		CPU			
		RS	CZT	VRS	VCZT
<i>Diffraction</i>		4.14	1.91	12.33	6.17
<i>Our approach</i>		2.39	1.39	5.22	4.04
		GPU			
		RS	CZT	VRS	VCZT
<i>Diffraction</i>		/	/	/	/
<i>Our approach</i>		0.006	0.027	0.151	0.075




Towards an artificial Muse:

An artificial Source of Inspiration for Science

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On scientific understanding with artificial intelligence

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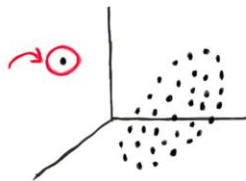
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**Anomaly
Detection**




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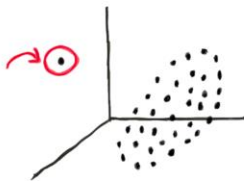
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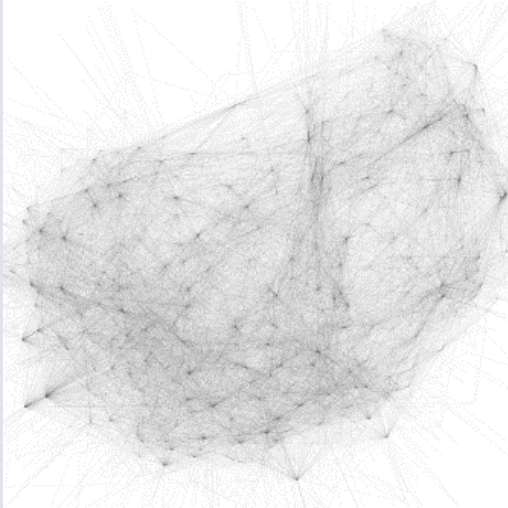


**From Large Collection
Of Literature**



Class II: Re-Source of Inspiration

From Large Collection
Of Literature



Semantic Network of QM

from 750k papers

Vertices: Concepts

Edges: Co-Occurance

Krenn, Zeilinger, *PNAS* **117**, 1910 (2020)

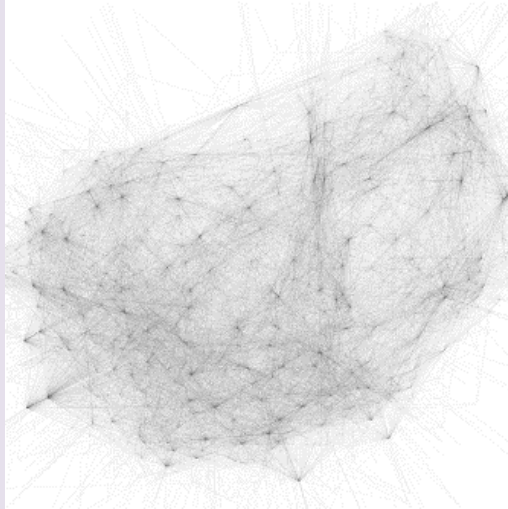
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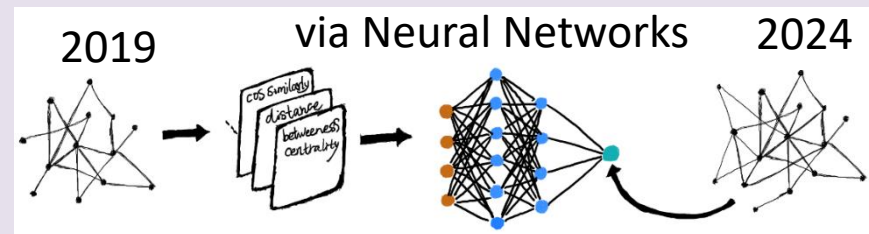
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Link Prediction



Then: From 2024 to 2029!

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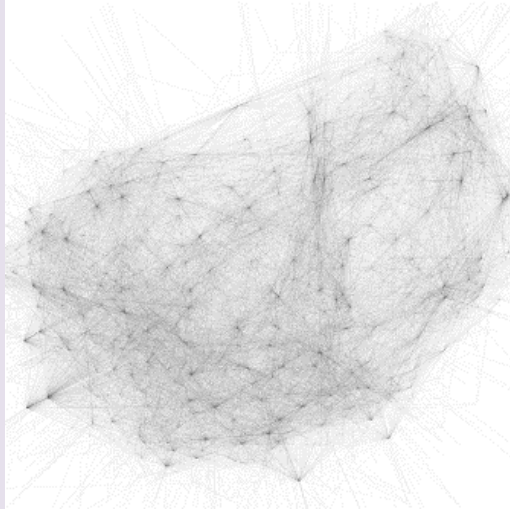
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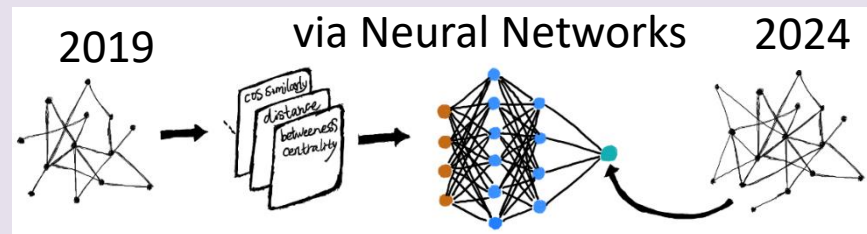
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Gu, Krenn, arXiv:2402.08640: **Impact4Cast**

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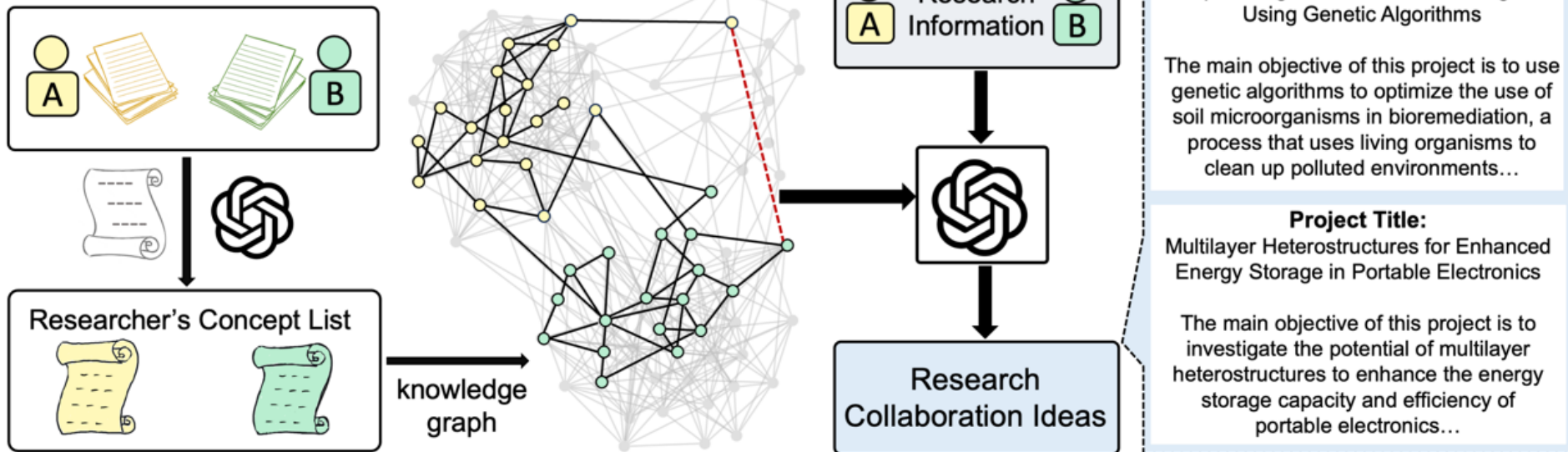
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Suggesting research collaborations



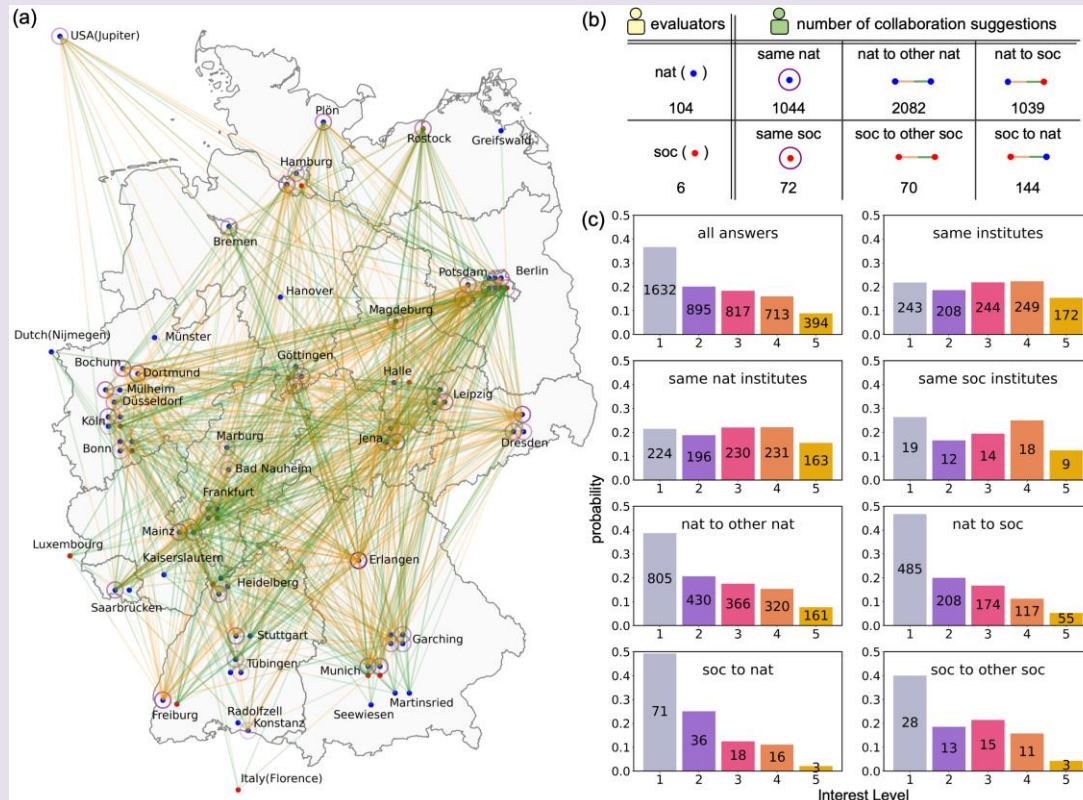
Gu, Krenn, *Interesting Scientific Idea Generation Using Knowledge Graphs and LLMs: Evaluations with 100 Research Group Leaders*, [arXiv:2405.17044](https://arxiv.org/abs/2405.17044).

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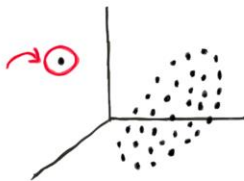
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**Anomaly
Detection**



**From Large Collection
Of Literature**




Towards an artificial Muse:

An artificial Source of Inspiration for Science

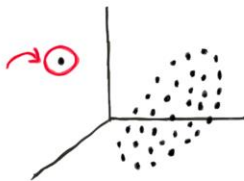
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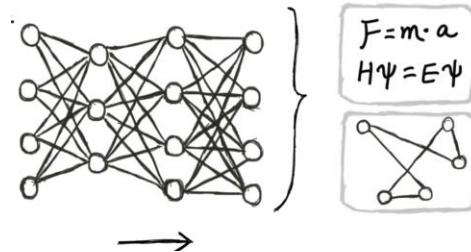
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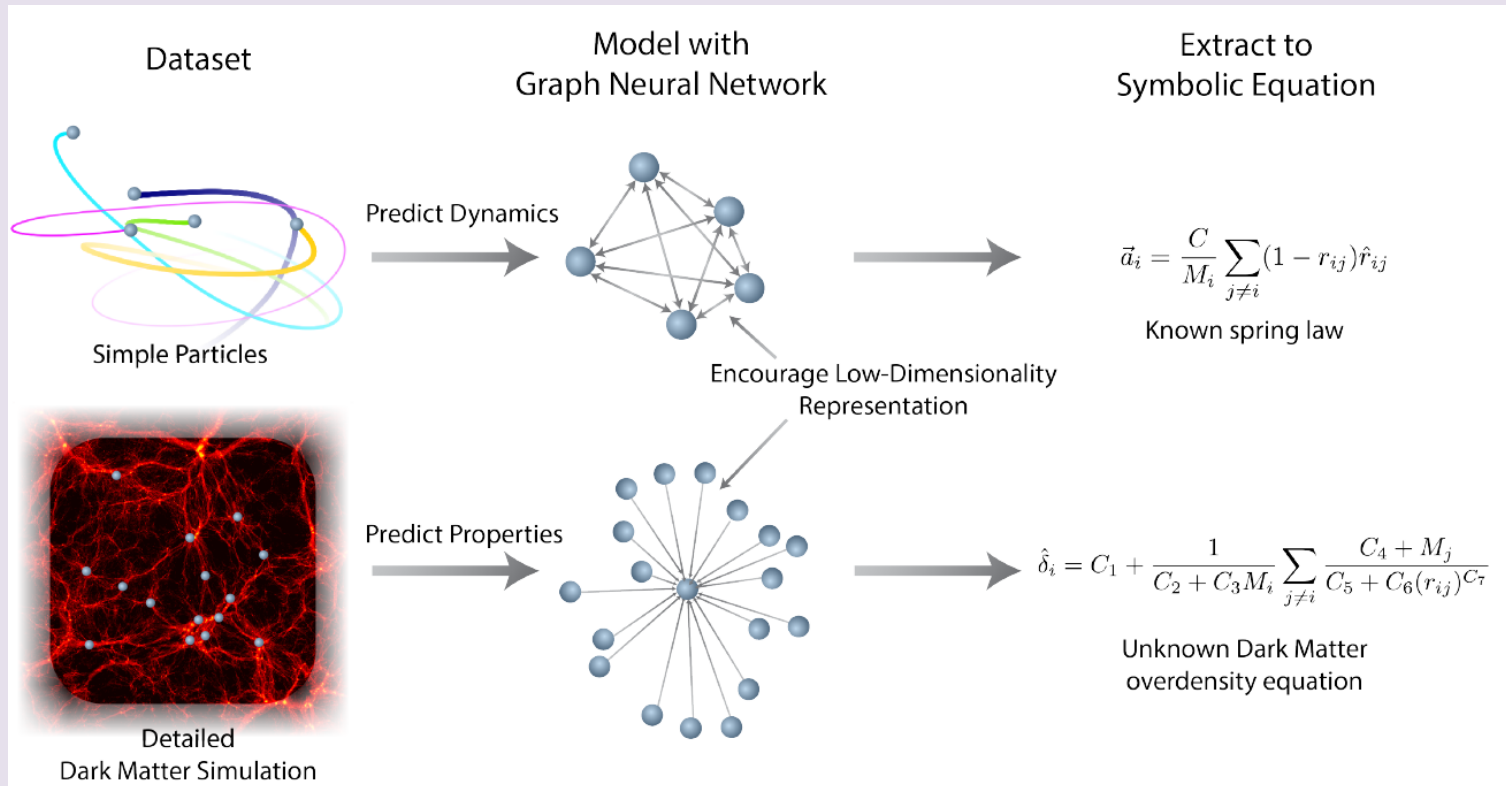
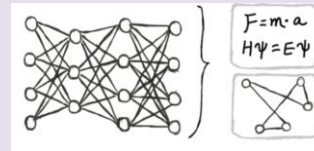


Interpretable Results



Class II: Re-Source of Inspiration

Interpretable
Results



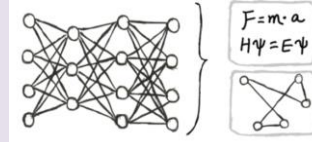
Cranmer et al., Discovering Symbolic Models from Deep Learning with Inductive Biases, NeurIPS (2020)

Krenn, Pollice, Guo, ..., Aspuru-Guzik,

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

Class II: Re-Source of Inspiration

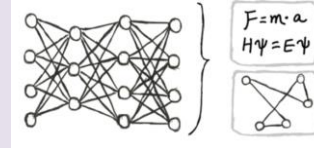
Interpretable
Results



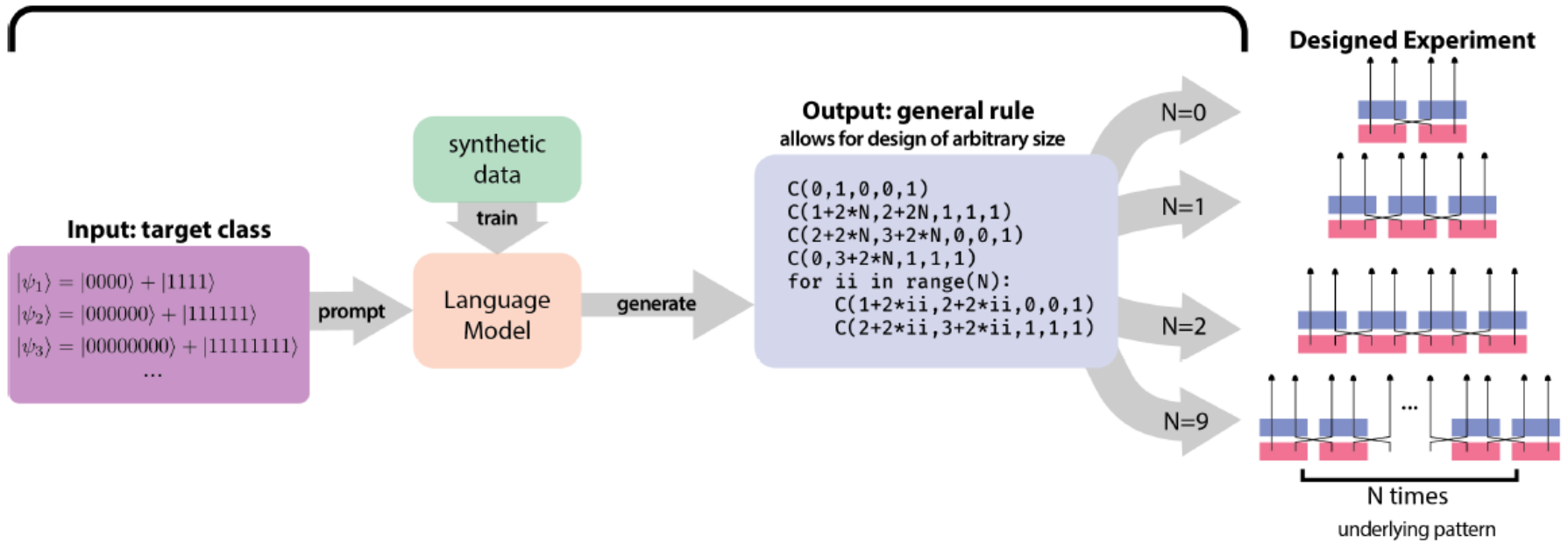
PySR and SymbolicRegression.jl

Class II: Re-Source of Inspiration

Interpretable
Results



Designing a class of experiments




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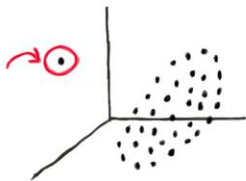
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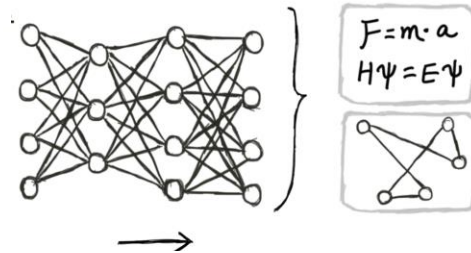
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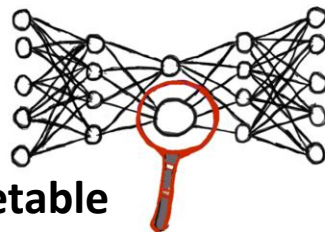
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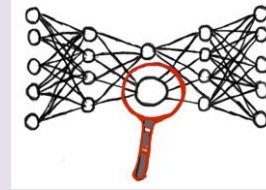
Interpretable Results



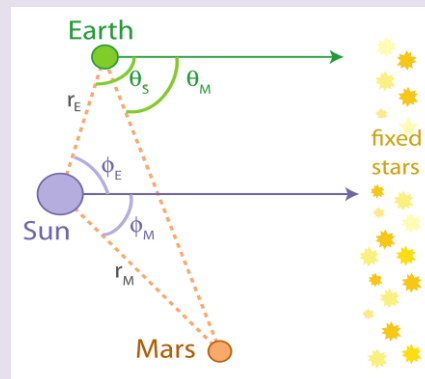
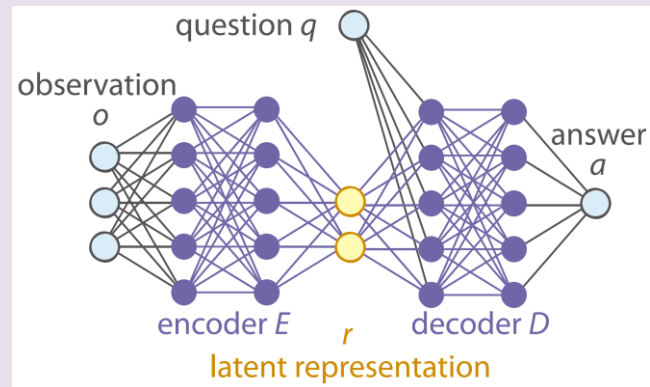
Interpretable
internal states



Interpretable internal states



Interpreting Latent Space



Iten et al., *PRL* **124**, 010508 (2019)

Krenn, Pollice, Guo, ..., Aspuru-Guzik,

On scientific understanding with artificial intelligence, *Nat. Rev. Phys.* (2022).


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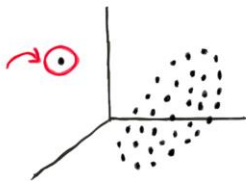
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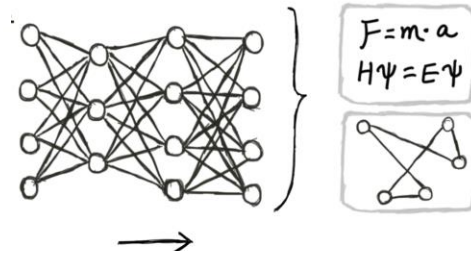
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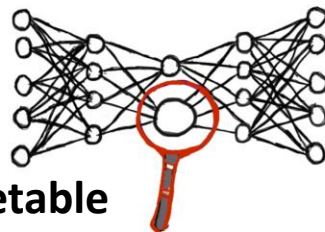
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Interpretable Results



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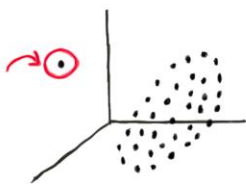
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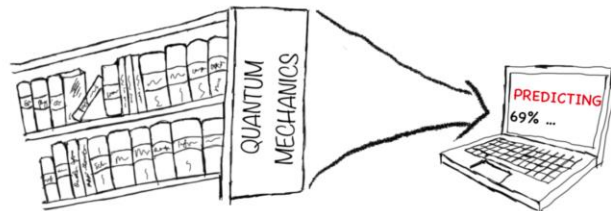
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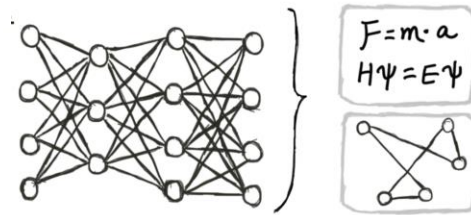
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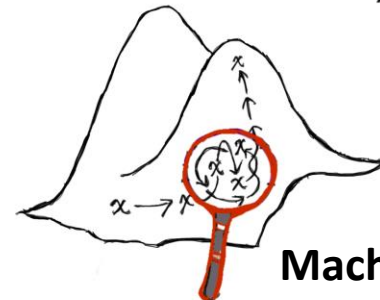
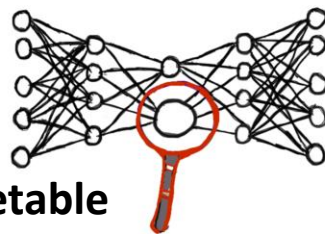
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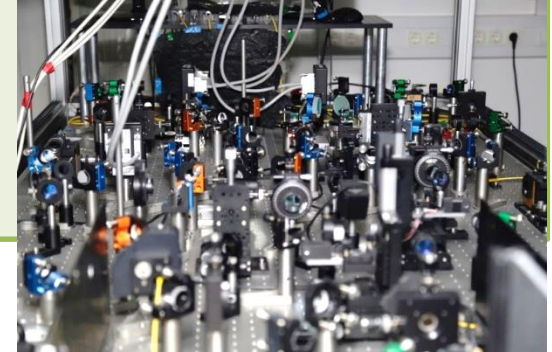
Machine Behaviour

Conclusion

AI-based Quantum Hardware & Experiment Design:

In many domains in physics (*quantum optics, gravitational wave physics, microscopes/telescopes soon*), we have now algorithms for **finding solutions to open questions.**

The solutions are presented such that **we can learn and understand new concepts.**

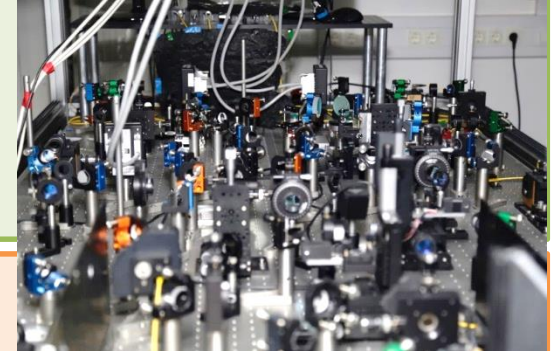


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Automated Idea Generation:

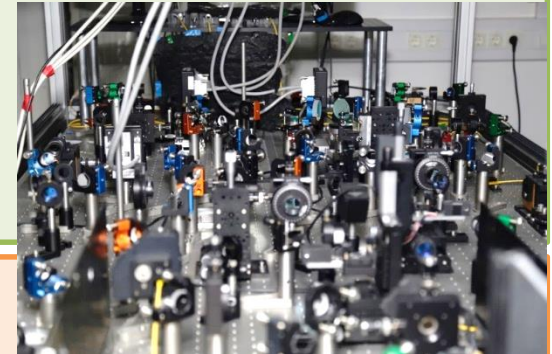
Towards personalized, new, high-impact, interesting research idea generation

Conclusion

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Automated Idea Generation:

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

Artificial Scientists

Creativity?



Curiosity?

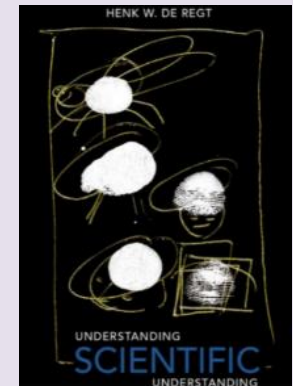


(a) learn to explore on Level-1



(b) explore faster on Level-2

Understanding?

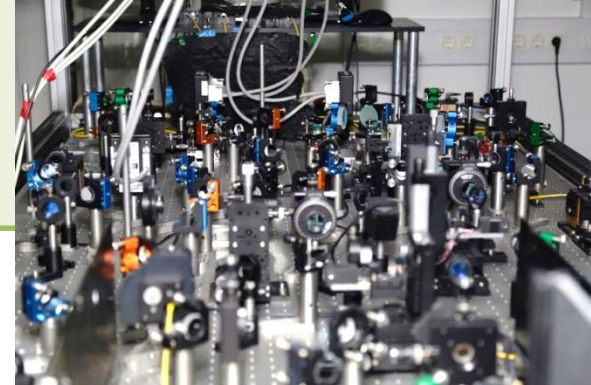


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