AI goes MAD^2, Madrid, Spain, 15.10.2024

# 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

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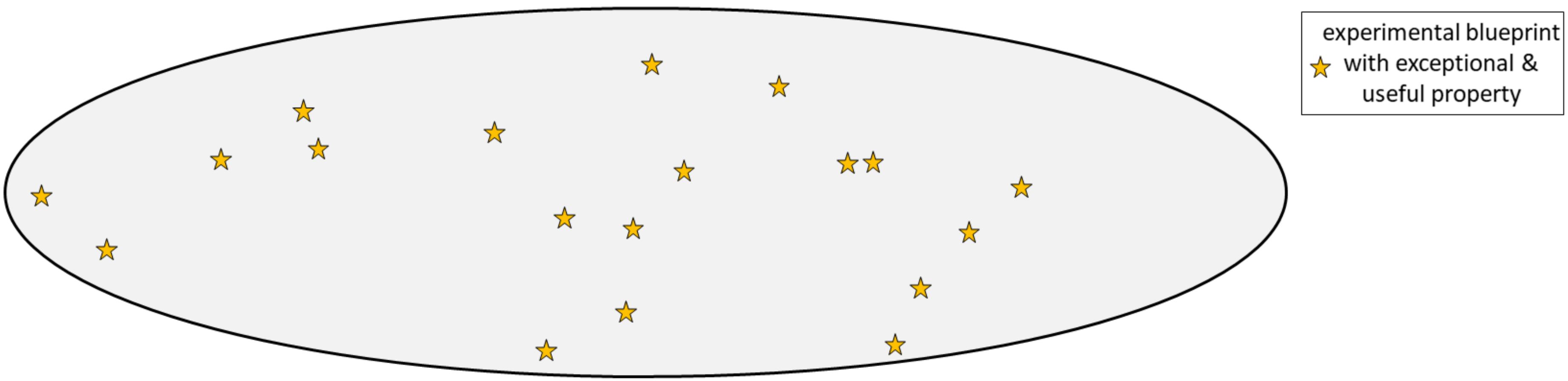
**Abstract space of all experimental setups**



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**Some examples:** (without symmetry)

3 lasers, 3 BS, 3 detectors: 1000 combinations

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

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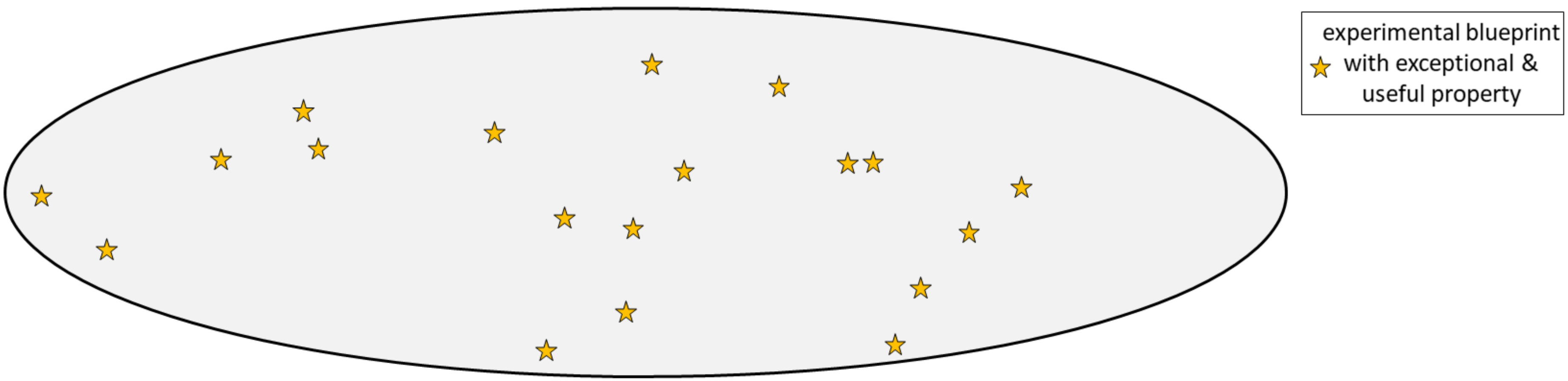

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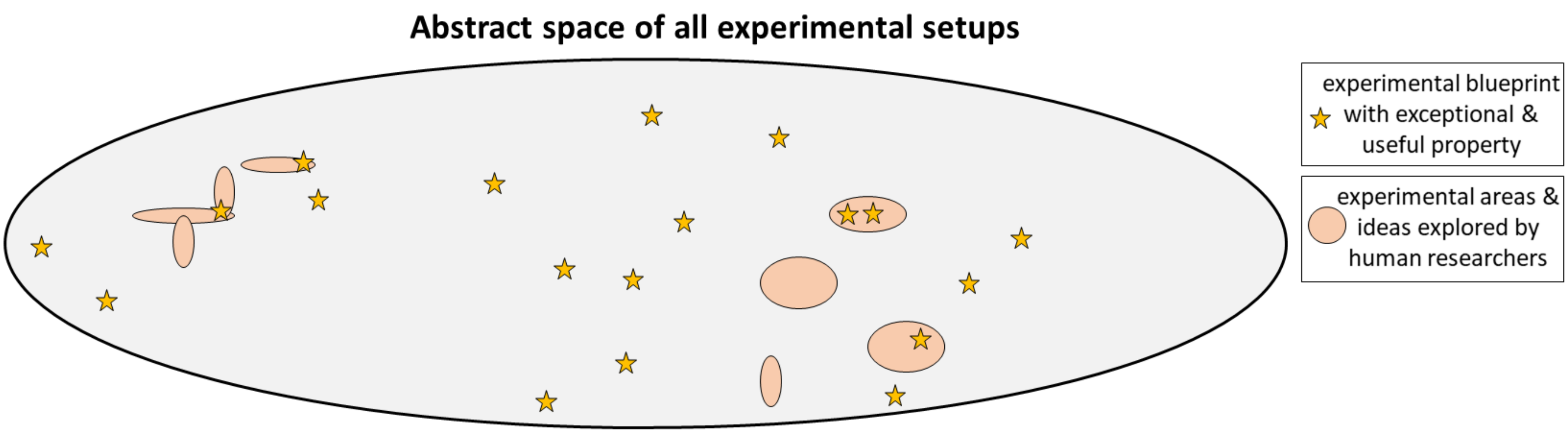

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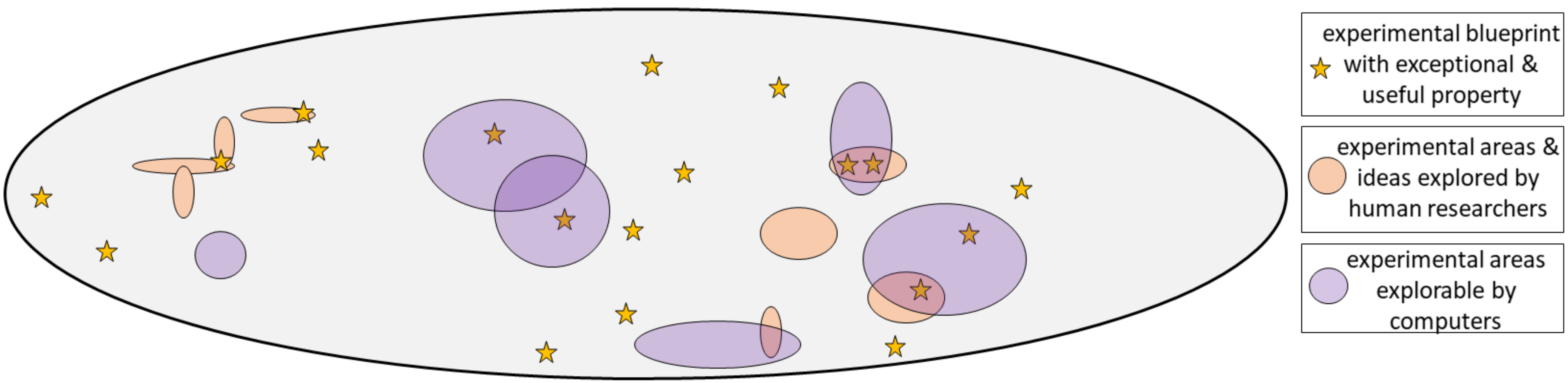

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# How to design quantum experimental setups?

Quantum Entanglement:

n=2, d=2:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

or

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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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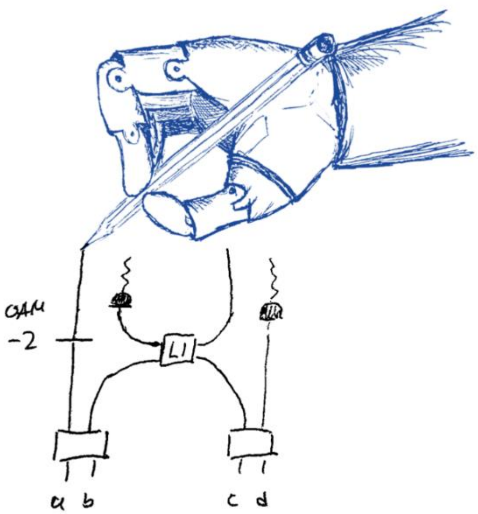

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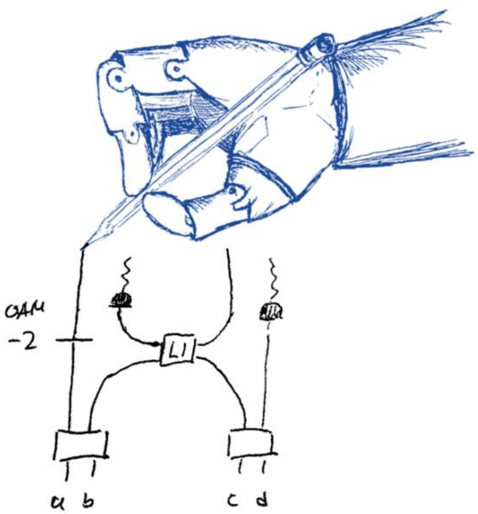
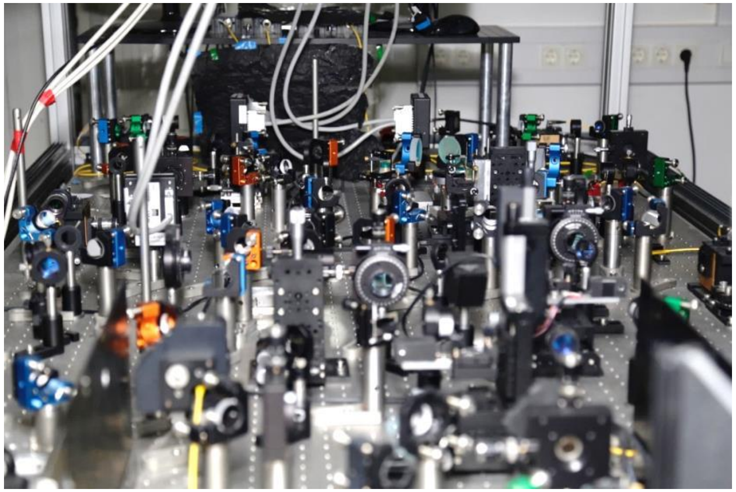



Erhard et al., *Nature Photonics* **12**, 759 (2018)



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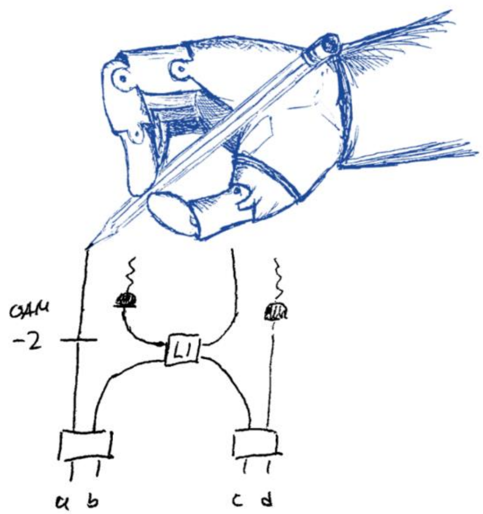


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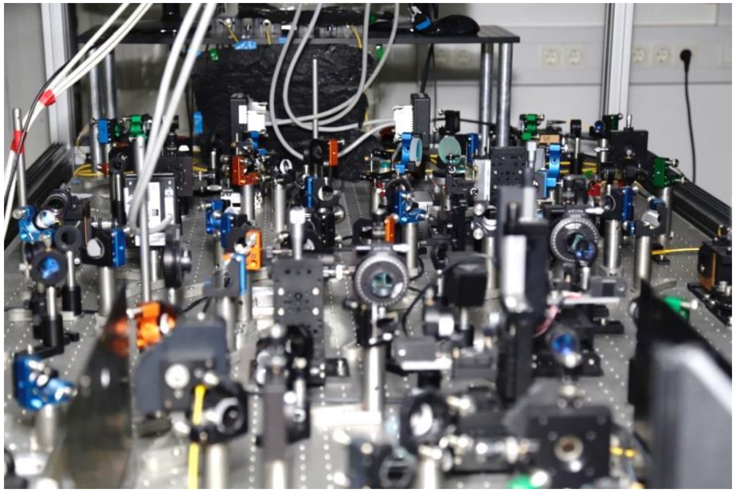

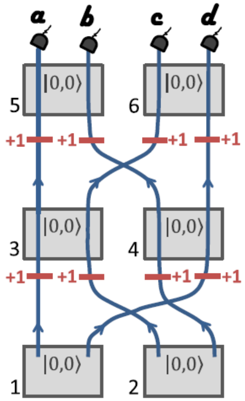


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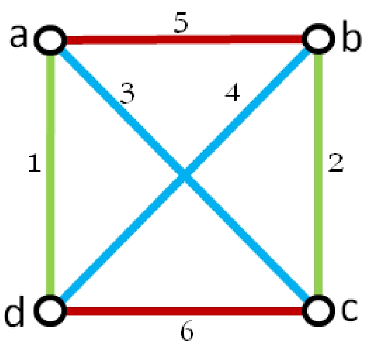


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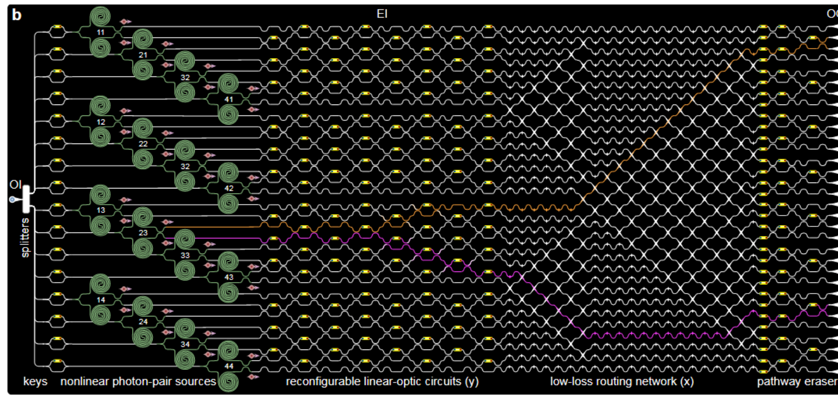


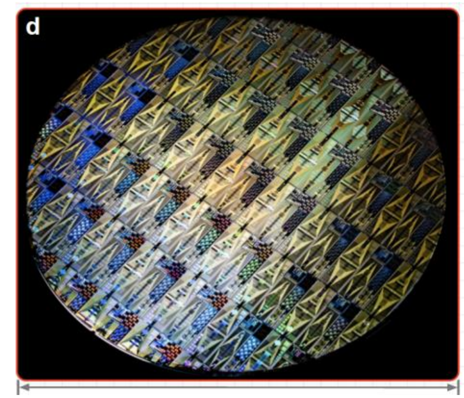


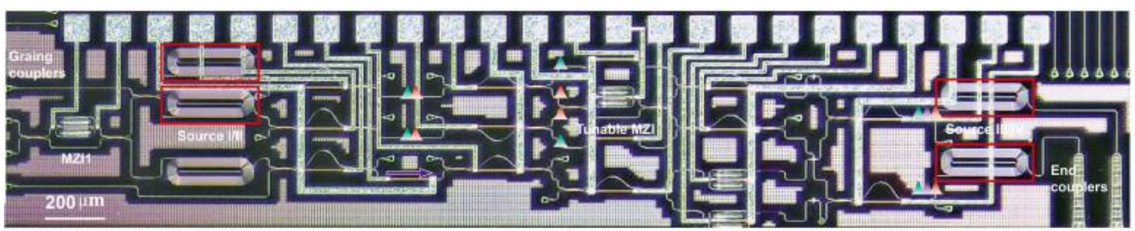


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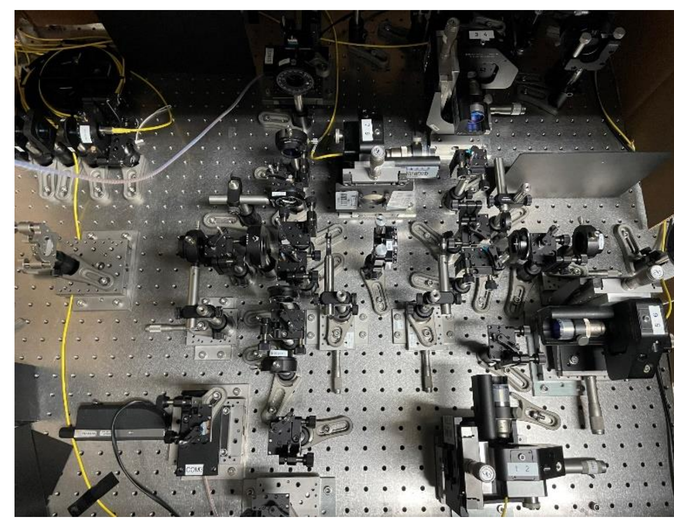

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https://doi.org/10.1088/1402-4896/ab7a35

Perspective

## 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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Perspective

CrossMark

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

**Chemistry Nobel 2019**

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# Highly efficient computer-designed quantum experiments

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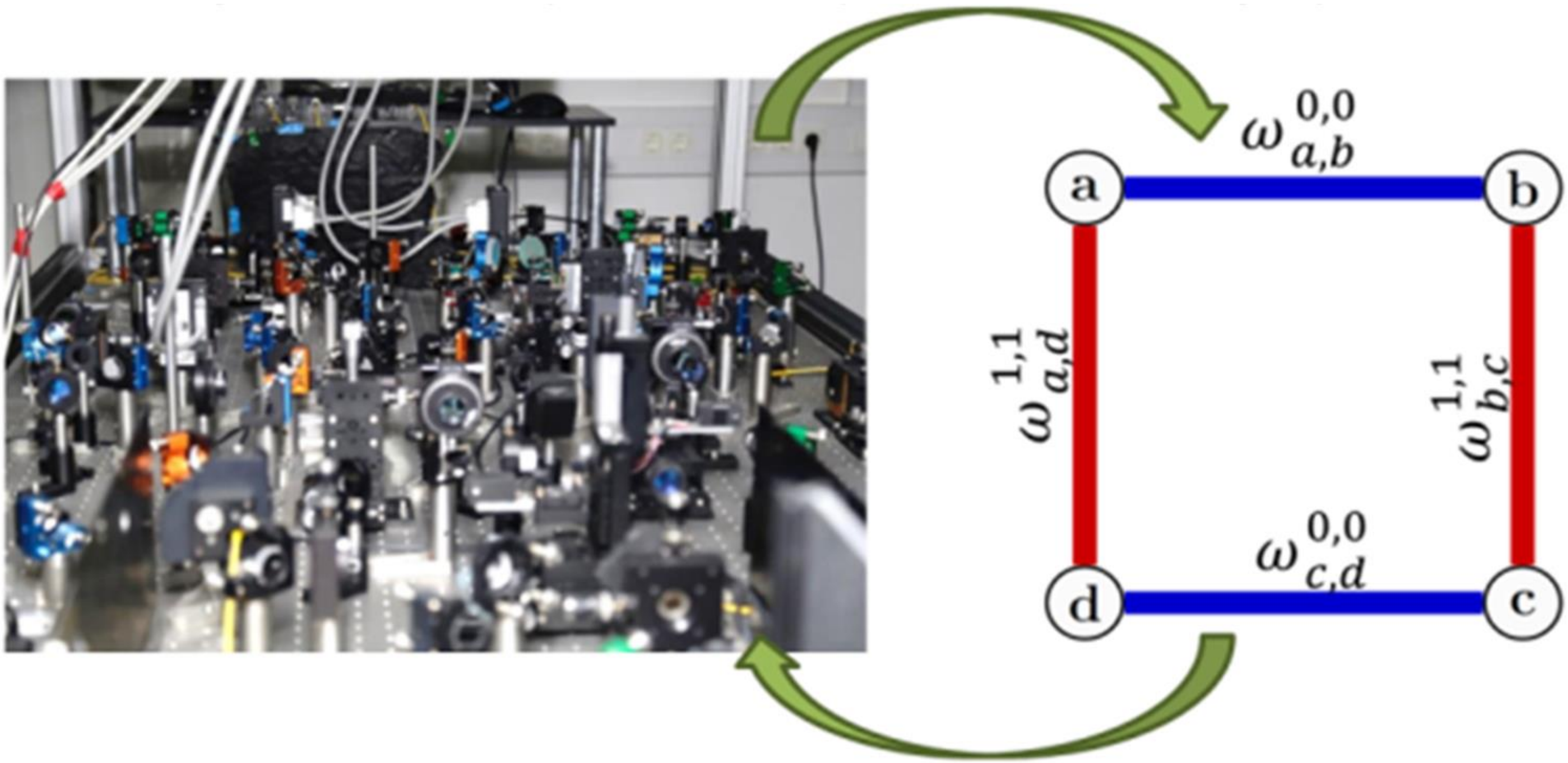
## Change Perspective:

New representation -> orders of magnitude speed-up.



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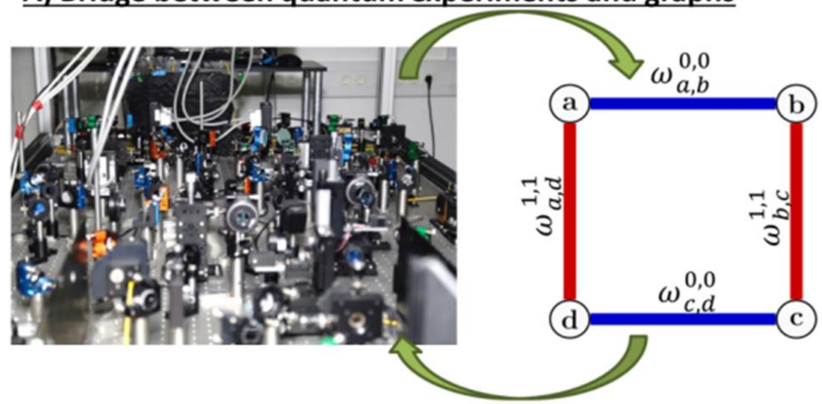
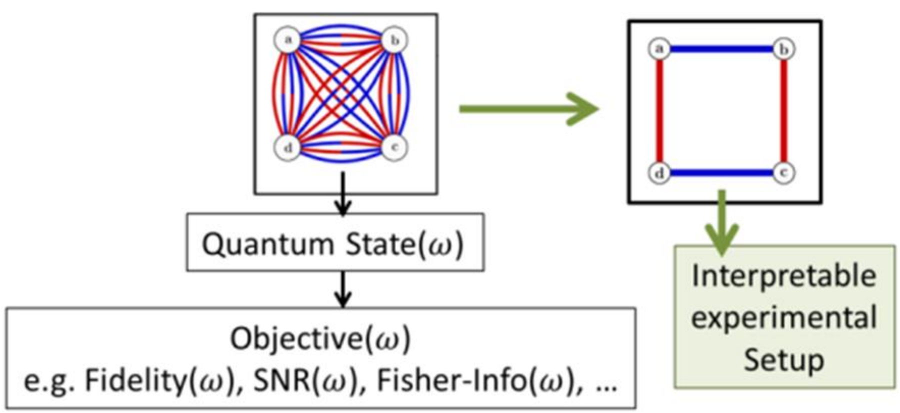
**A) Bridge between quantum experiments and graphs**

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




**B) Gradient-based optimization + discrete topological optimization**



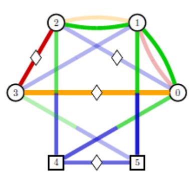
# Highly efficient computer-designed quantum experiments

Quantum
the open journal for quantum science

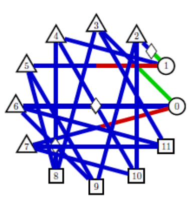
## Digital Discovery of 100 diverse Quantum Experiments with PyTheus

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

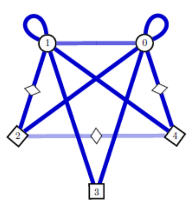
Quantum 7, 1204 (2023).



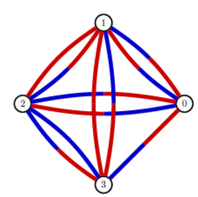
(a) Four-dimensional four-photon GHZ state (overcoming the 3-dimensional barrier for multiphoton entanglement)



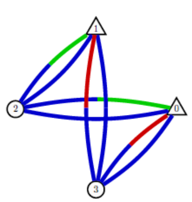
(b) Heralded 3D Bell state with single photons (improves state-of-the-art design by requiring less ancilla photons)



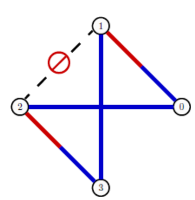
(c) Two-mode five-photon N00N state $|50\rangle + |05\rangle$ (very symmetric shape with an inscribed pentagram)



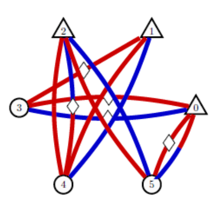
(d) A 4-qubit entangled states with unit coefficients, which requires complex-valued weights for generation



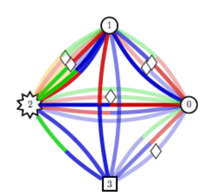
(e) Quantum measurement for a quantum communication task with quantum advantage (Mean King's Problem)



(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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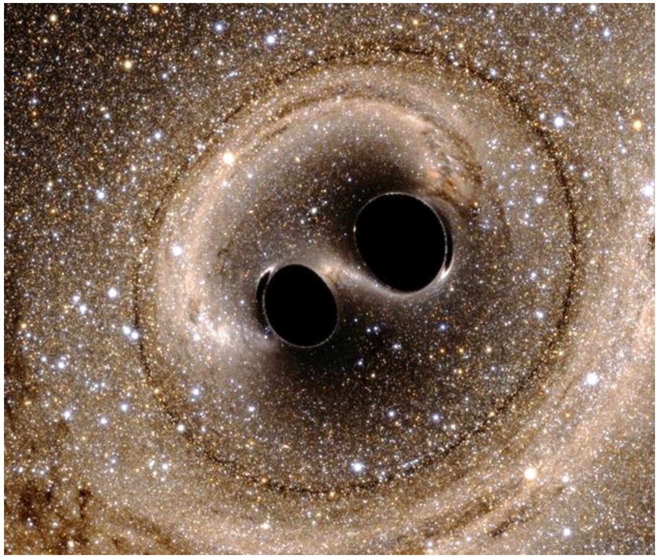
# AI-driven design of new Gravitational Wave Detectors

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



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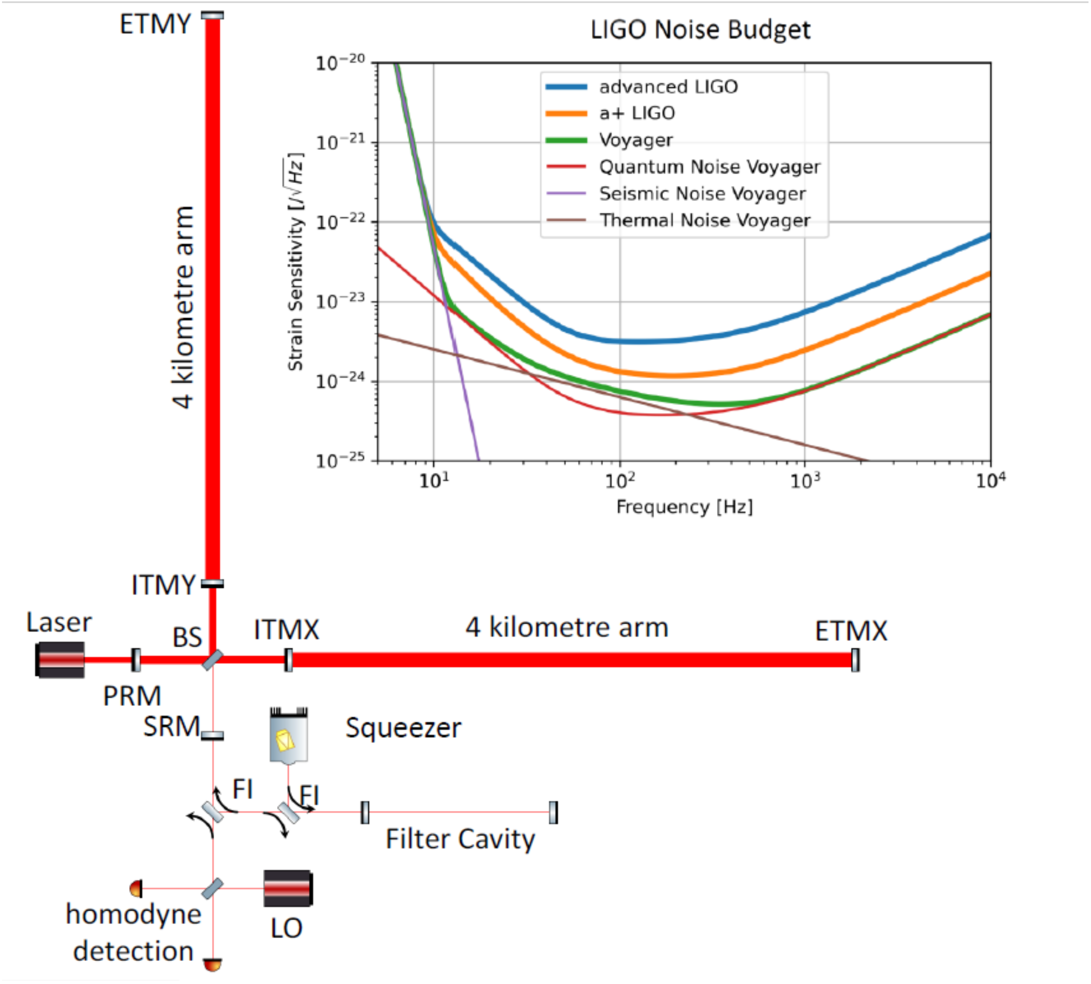
## LIGO's next Generation Detector Update: Voyager



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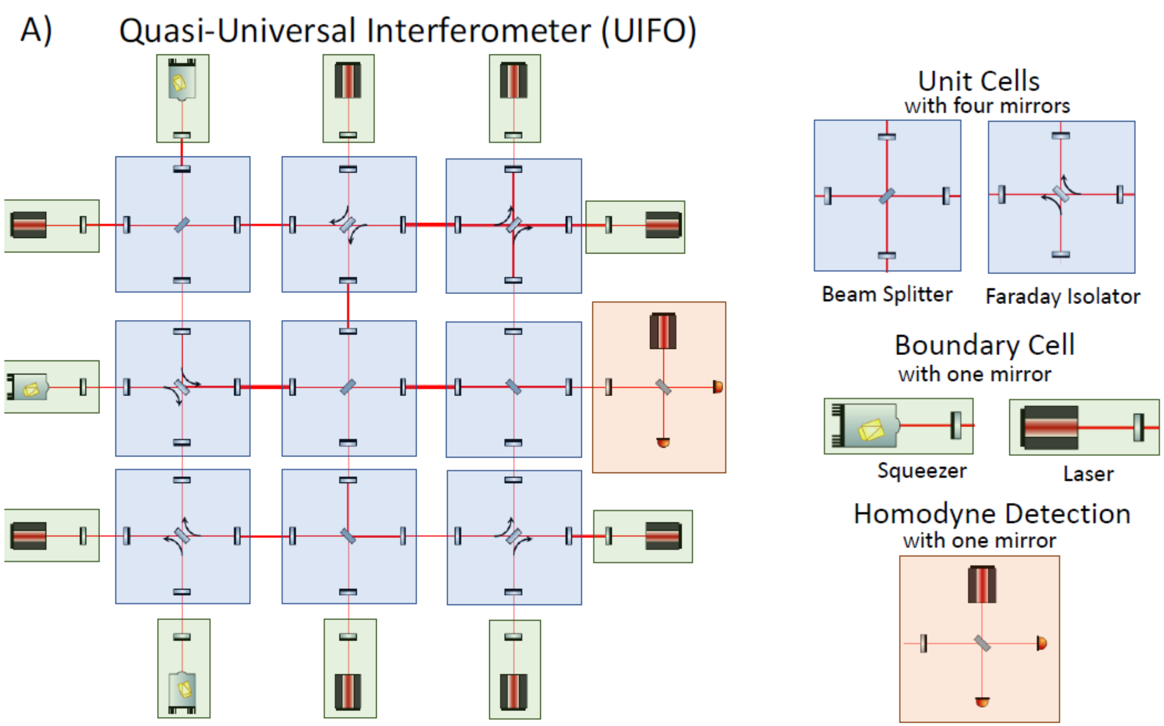

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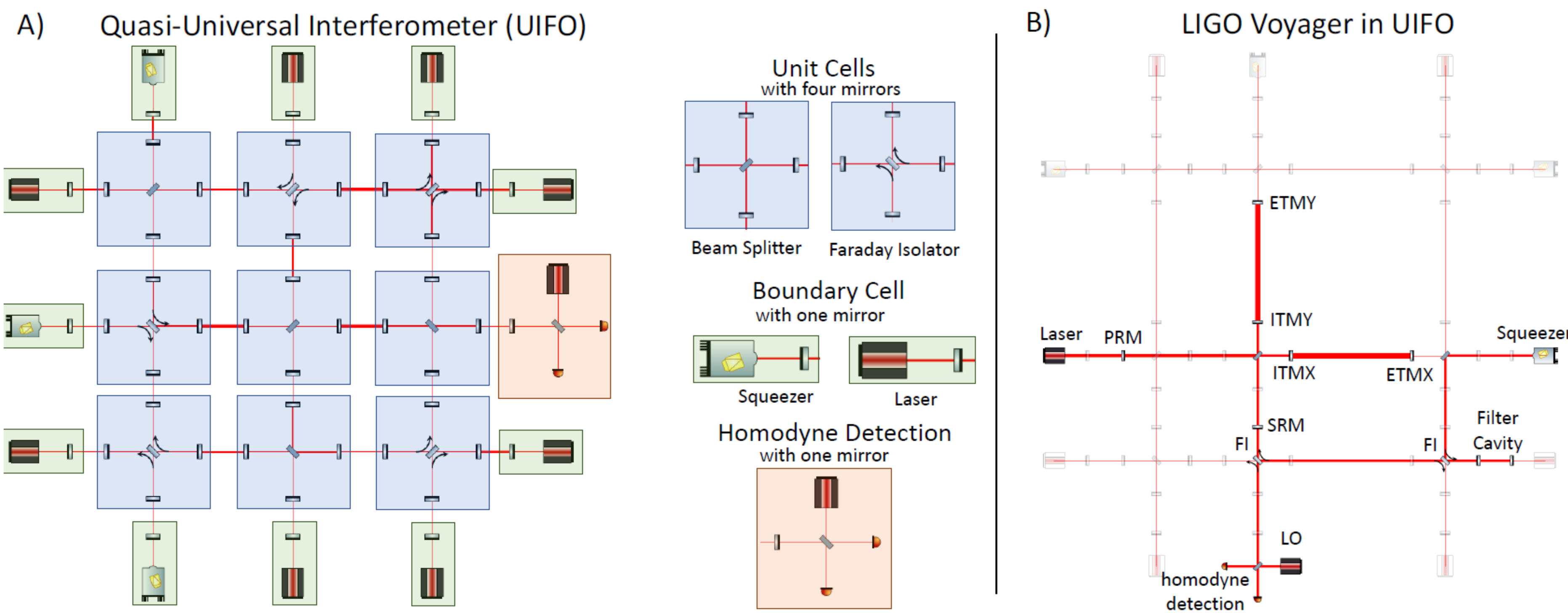

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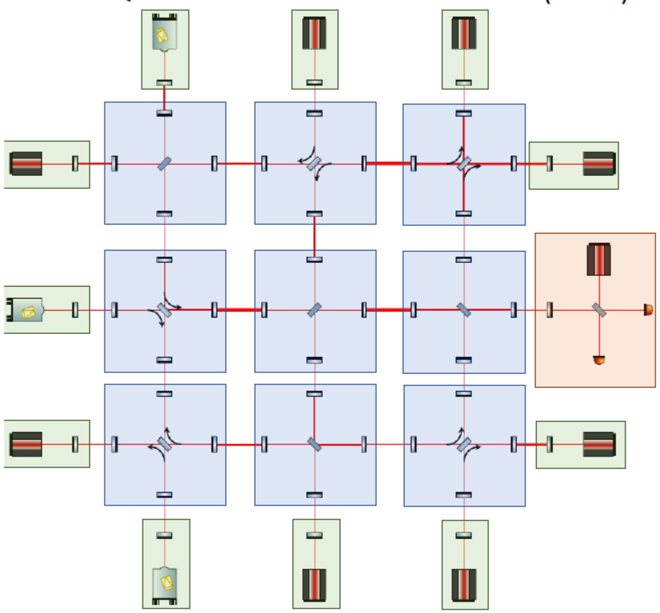
Quasi-Universal Interferometer (UIFO)



## Physical Targets:

Broadband: 20Hz-5kHz

Cosmology: 10Hz-30Hz -- Terra incognita

Supernova: 200Hz-1kHz

Post-Merger Analysis (Neutron Stars): 800Hz-3kHz

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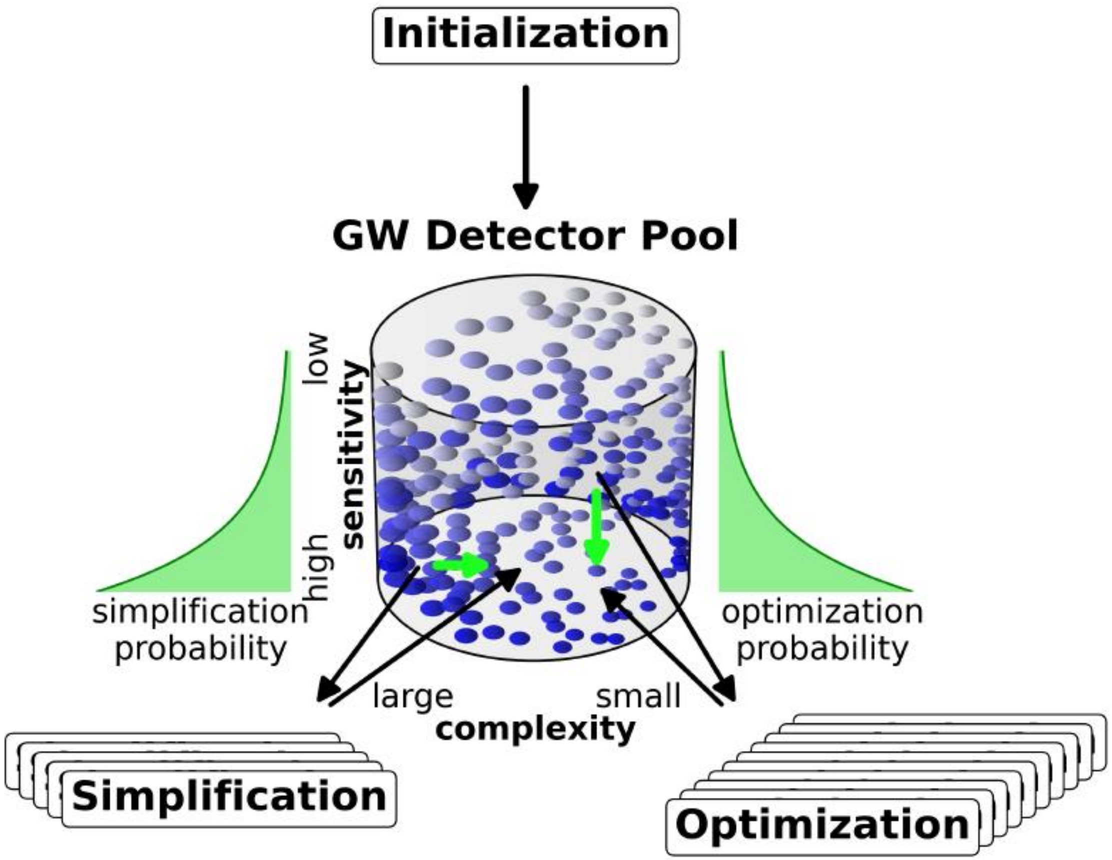
with Yehonathan Drori, Rana X. Adhikari (Caltech, LIGO): arXiv:2312.04258

**Maximization of strain sensitivity in frequency range, under realistic experimental constraints**



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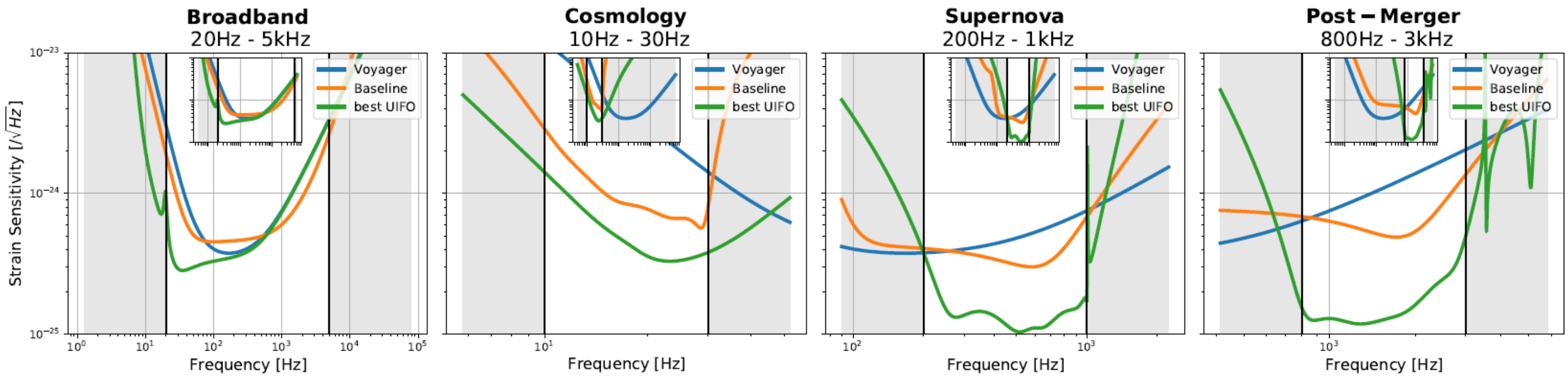

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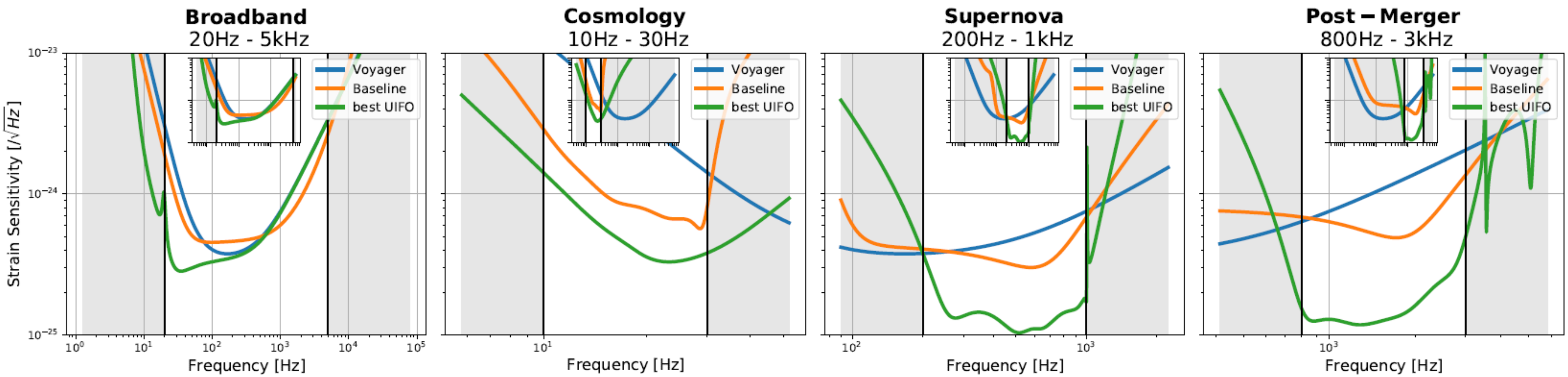
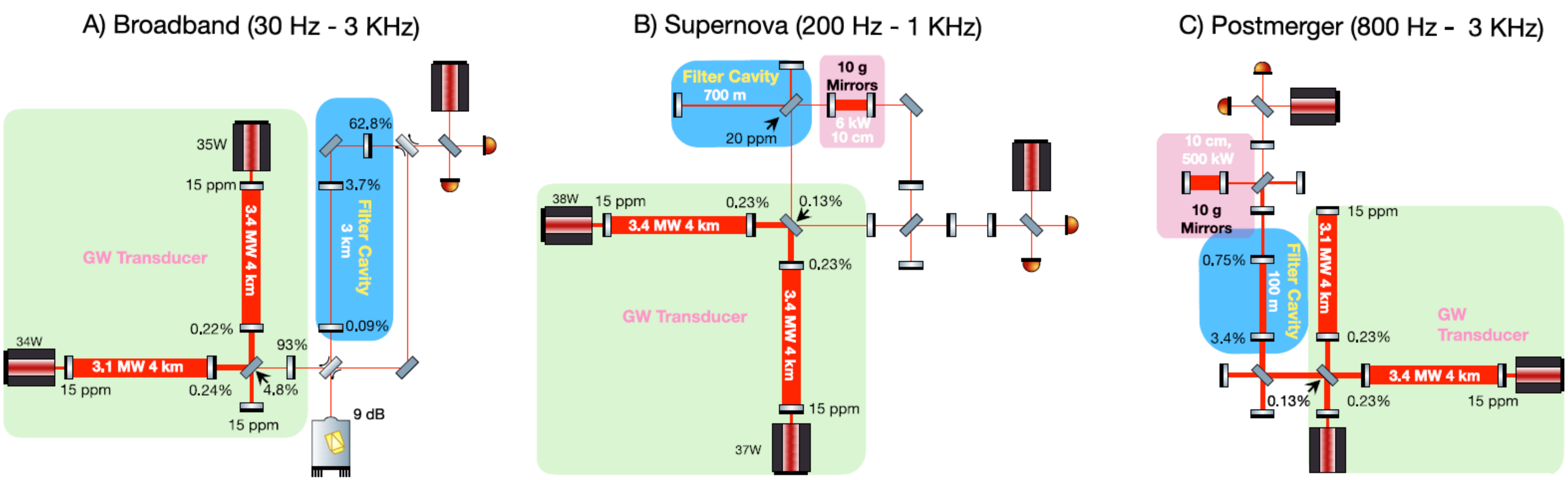
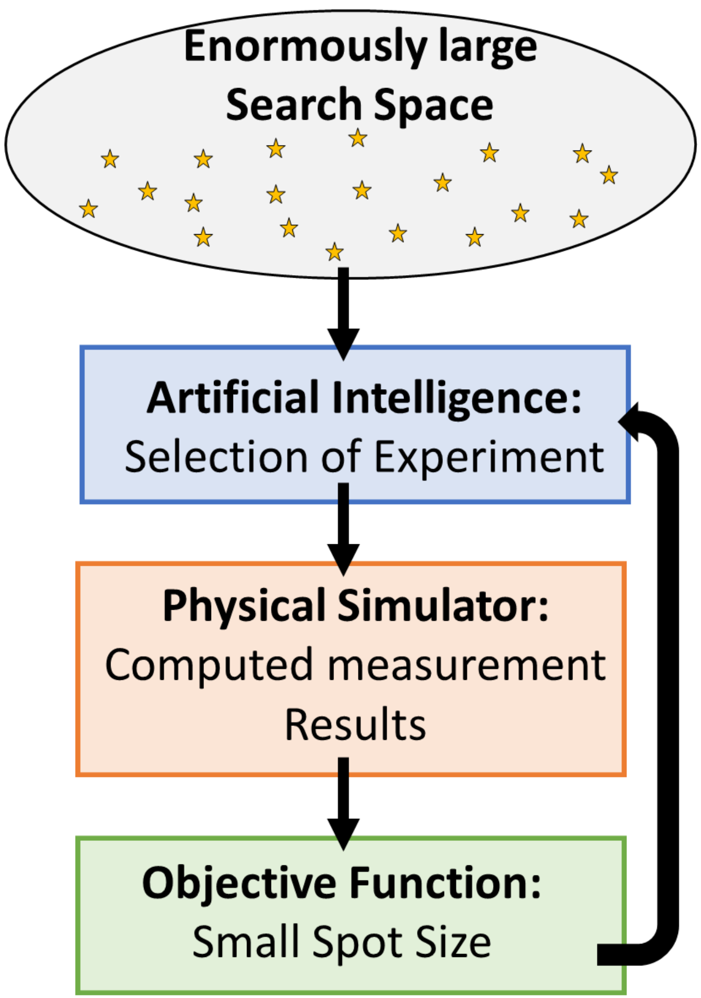


# XLuminA: An Auto-differentiating Discovery Framework for Super-Resolution Microscopy

**Carla Rodríguez**, Sören Arlt, Leonhard Möckl, Mario Krenn - **arXiv:2310.08408**

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



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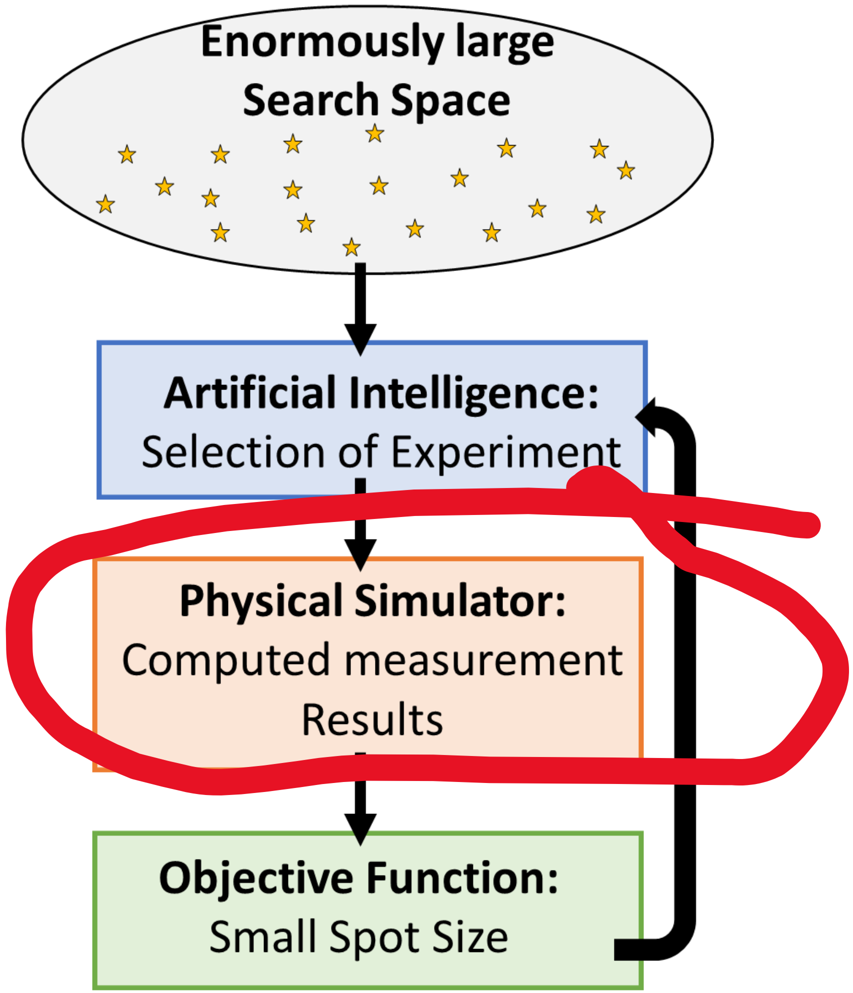


**Simulator:**
- Reliable
- Fast
- General

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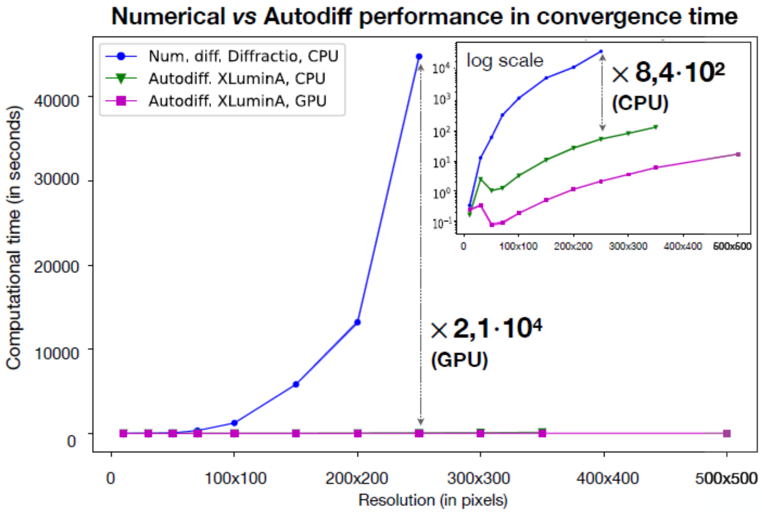
| | RS | CZT | VRS | VCZT |
|---|---|---|---|---|
| **CPU** | | | | |
| *Diffractio* | 4.14 | 1.91 | 12.33 | 6.17 |
| *Our approach* | **2.39** | **1.39** | **5.22** | **4.04** |
| **GPU** | | | | |
| *Diffractio* | / | / | / | / |
| *Our approach* | **0.006** | **0.027** | **0.151** | **0.075** |



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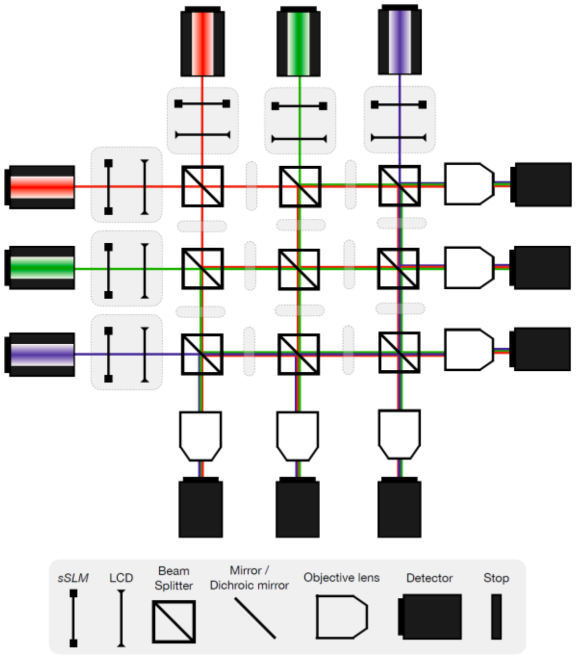
# Towards AI-discovery of new super-resolution microscopy

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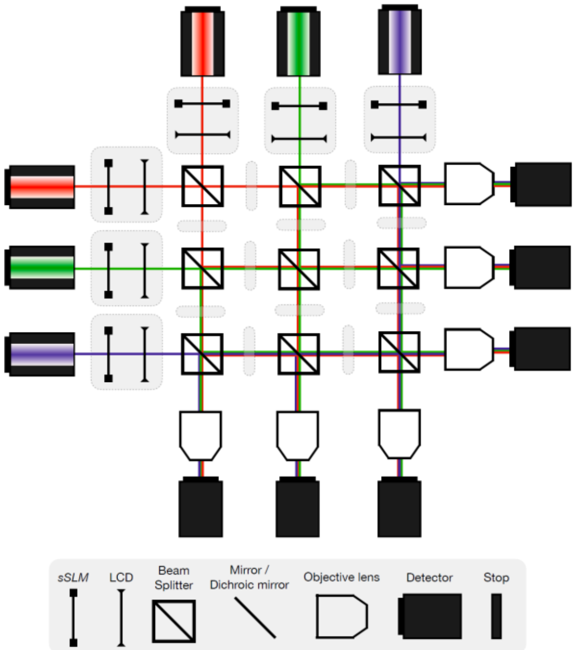
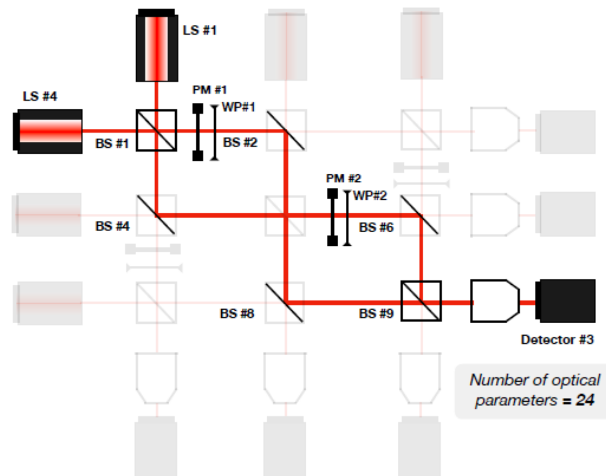
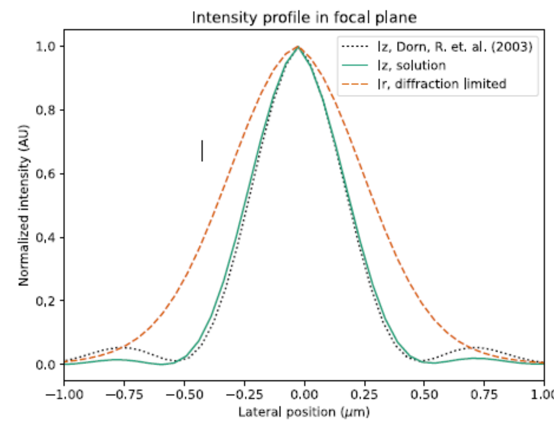


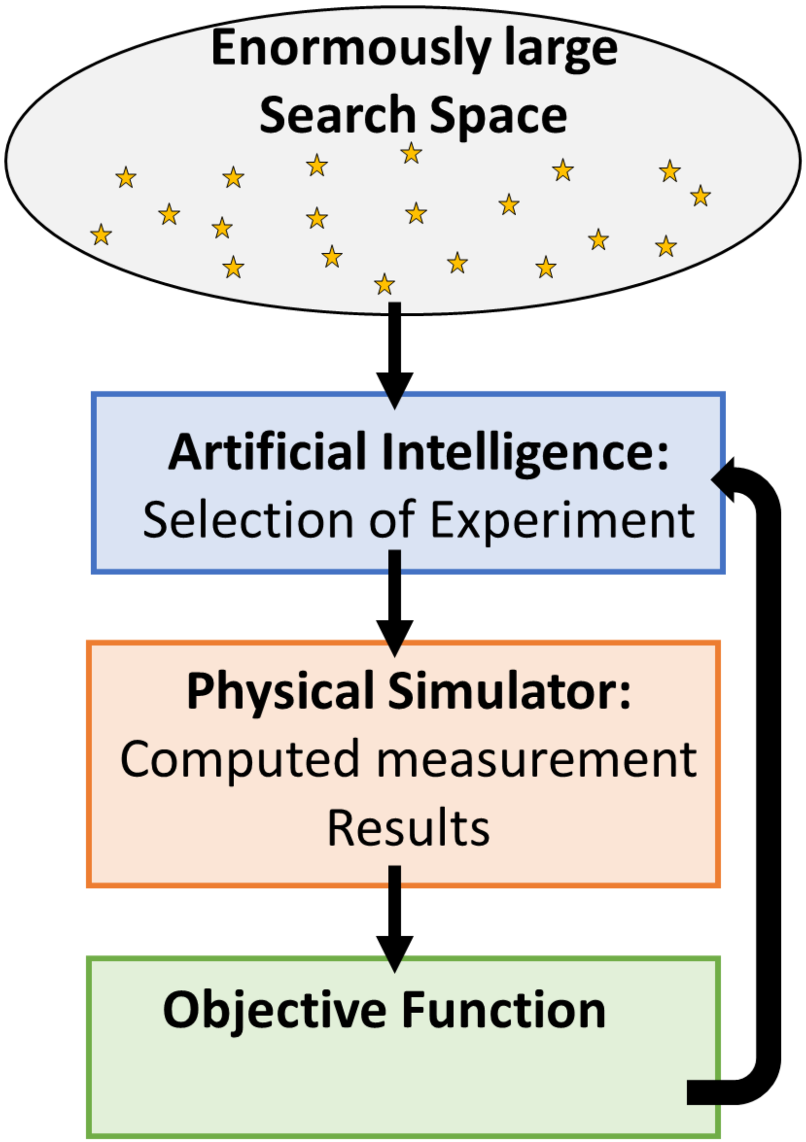




| | Spot size / $\lambda^2$ |
|---|---|
| Dorn, R. et. al. (2003) | 0.4360 |
| Discovered solution | 0.4485 |
| Diffraction-limited | 0.6853 |

Carla Rodríguez, Sören Arlt, Leonhard Möckl, Mario Krenn,
*XLuminA: An Auto-differentiating Discovery Framework for Super-Resolution Microscopy,* **arXiv:2310.08408**

Mario Krenn

# AI-driven Design of Experiments



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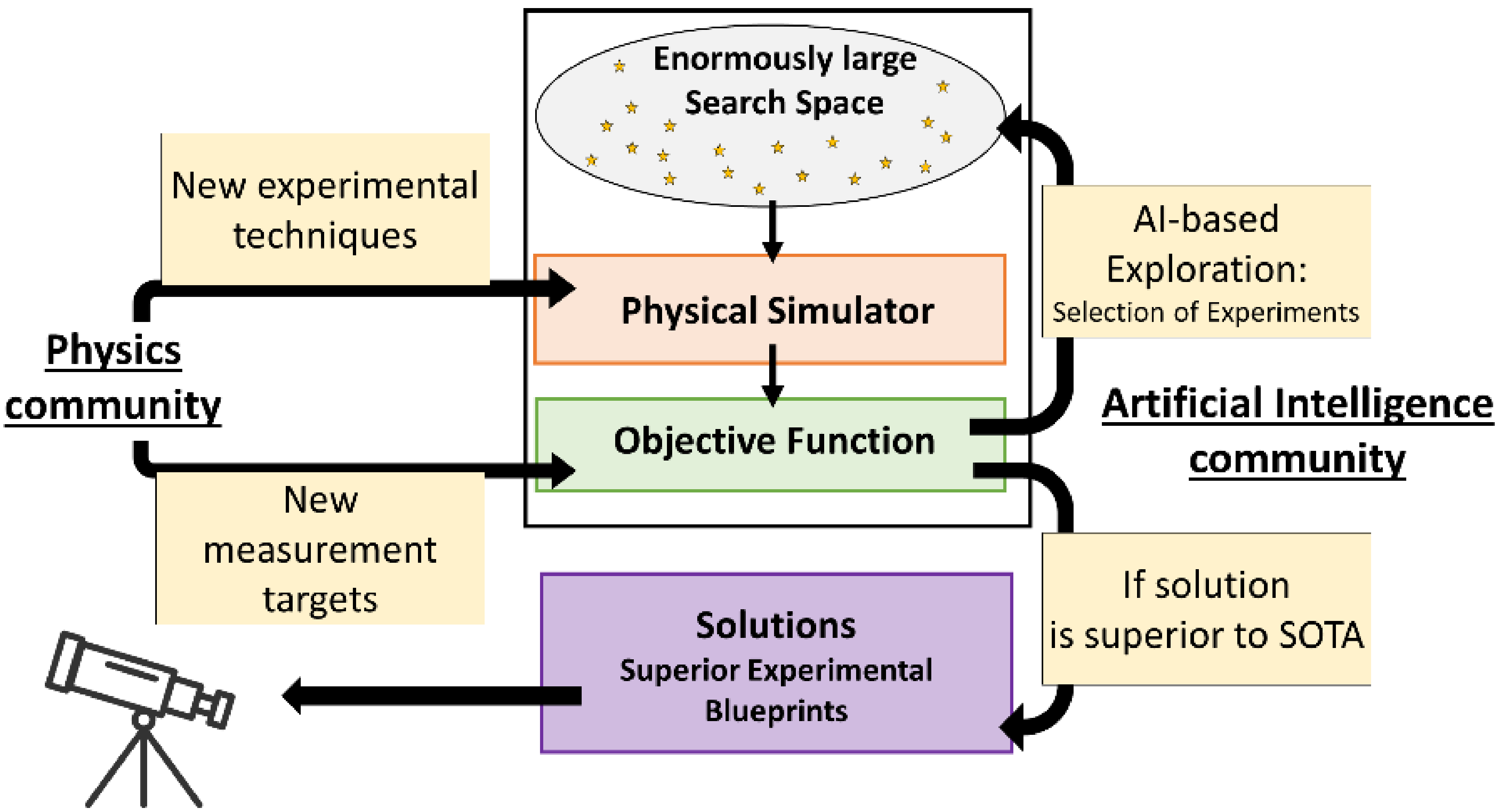

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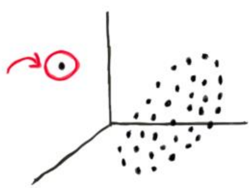

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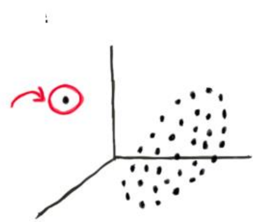
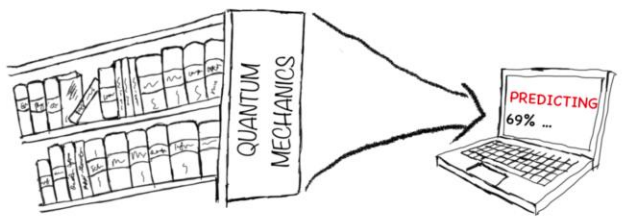


**From Large Collection Of Literature**



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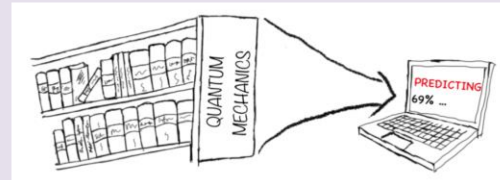
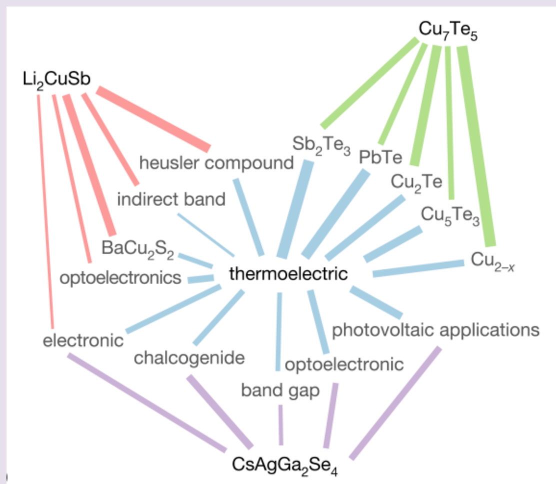
# Class II: Re-Source of Inspiration

**From Large Collection Of Literature**




## Word2Vec of 3,3mio papers




Cosine similarity to 'thermoelectric'

1. $Bi_2Te_3$ ✓
2. MgAgSb ✓
3. PbTe ✓

... ✓

326. $Li_2CuSb$ ?

... ✓

328. $In_4Te_3$ ✓

... ✓

345. $Cu_3Nb_2O_8$ ?

... ✓

✓ Known thermoelectrics

? Predictions

Tshitoyan, et al., *Nature* **571**, 95 (2019)

**Krenn, Pollice, Guo, ..., Aspuru-Guzik, On scientific understanding with artificial intelligence, Nat. Rev. Phys. (2022).**

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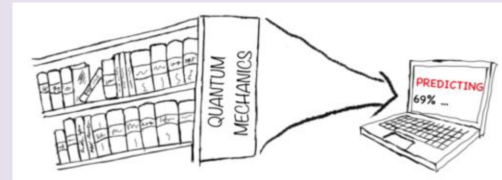


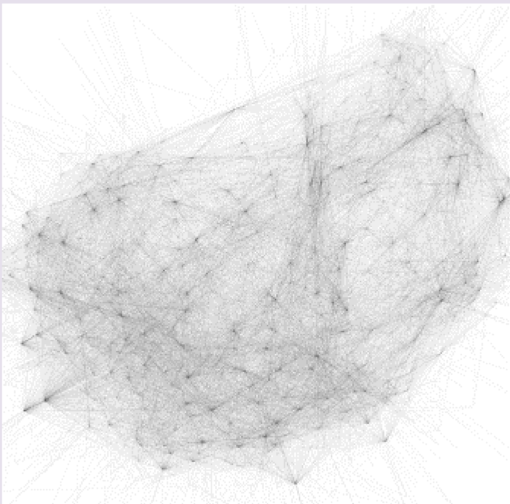

Semantic Network of QM from 750k papers

**Vertices:** Concepts

**Edges:** Co-Occurance

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

Krenn et al., *Nat. Mach. Intell.* (2023)

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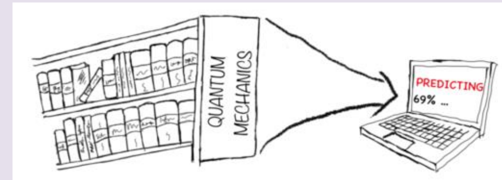
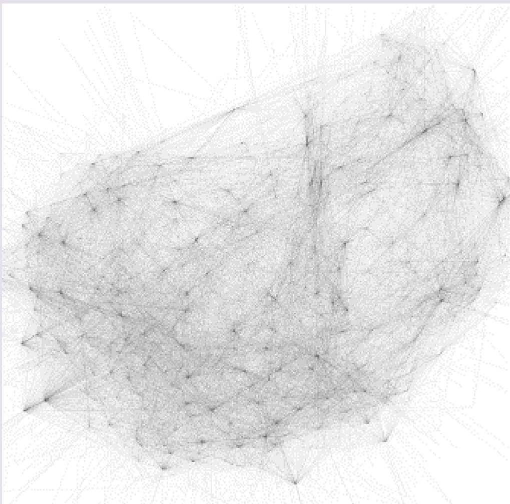
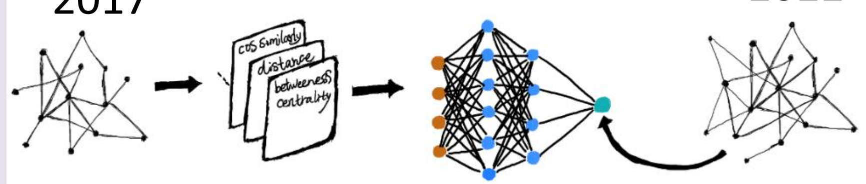


## Semantic Network of QM from 750k papers

**Vertices:** Concepts
**Edges:** Co-Occurance

Link Prediction via Neural Networks




**Then: From 2022 to 2027!**

Krenn, Zeilinger, *PNAS* **117**, 1910 (2020)
Krenn et al., *Nat. Mach. Intell.* (2023)

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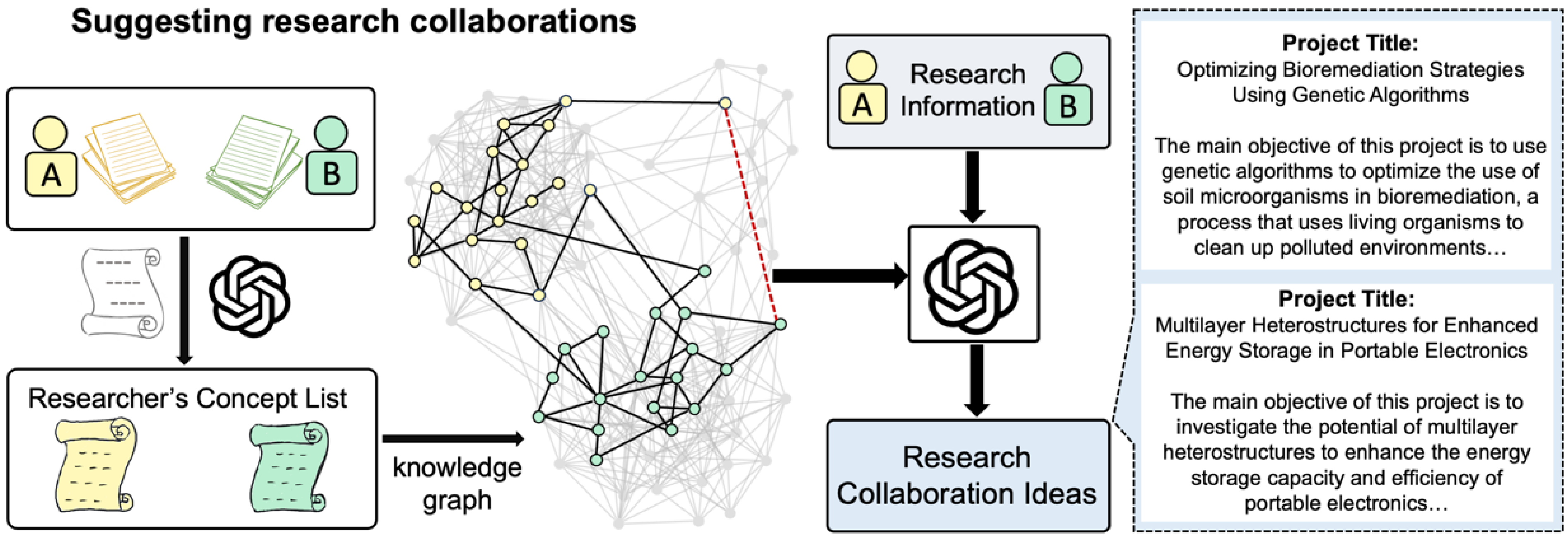


Gu, Krenn, *Interesting Scientific Idea Generation Using Knowledge Graphs and LLMs: Evaluations with 100 Research Group Leaders*, **arXiv:2405.17044.**

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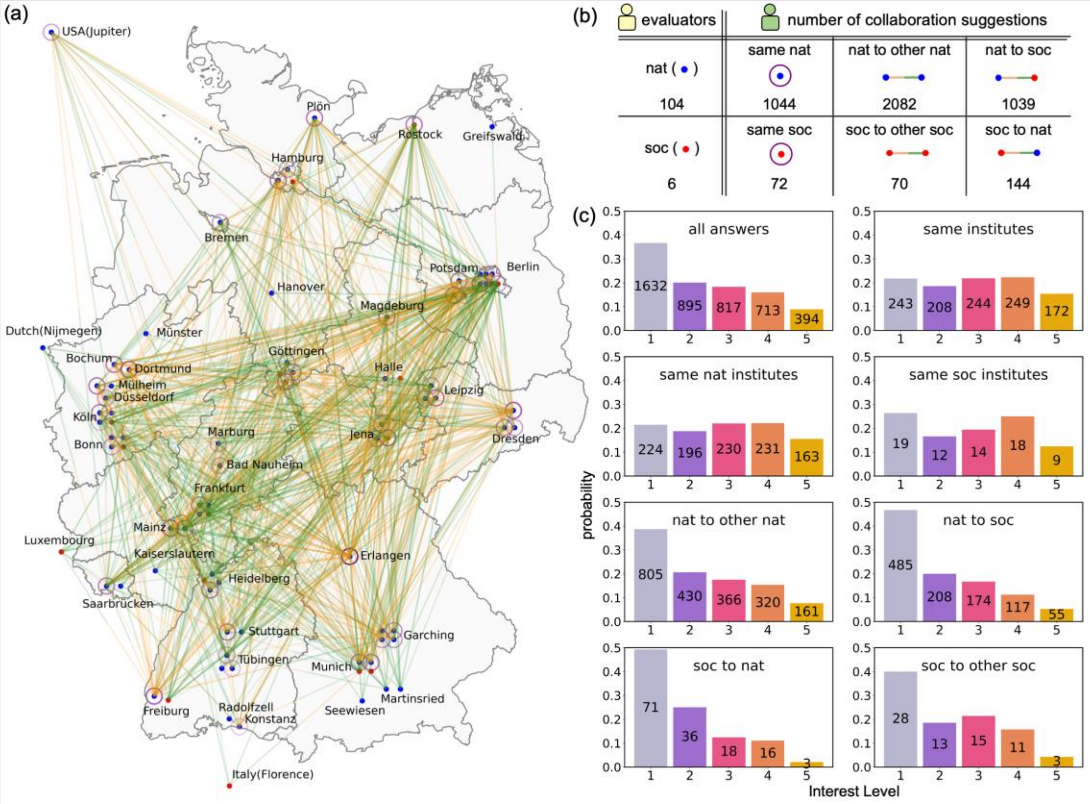


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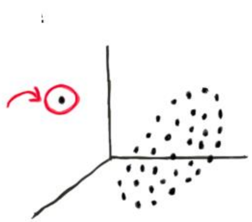

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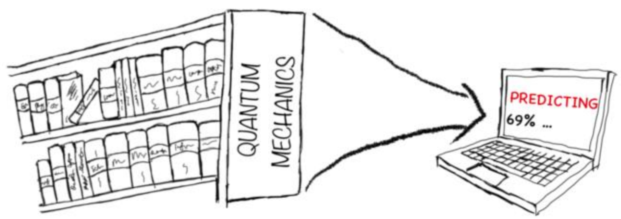

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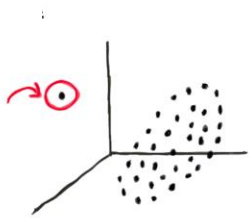

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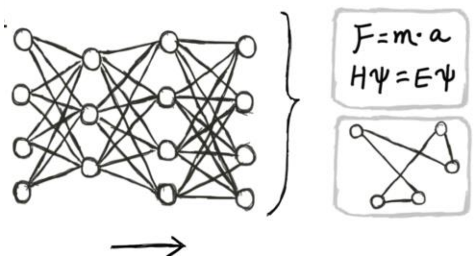
**Interpretable Results**



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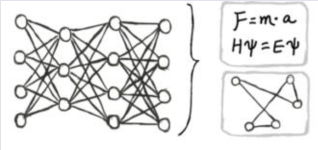


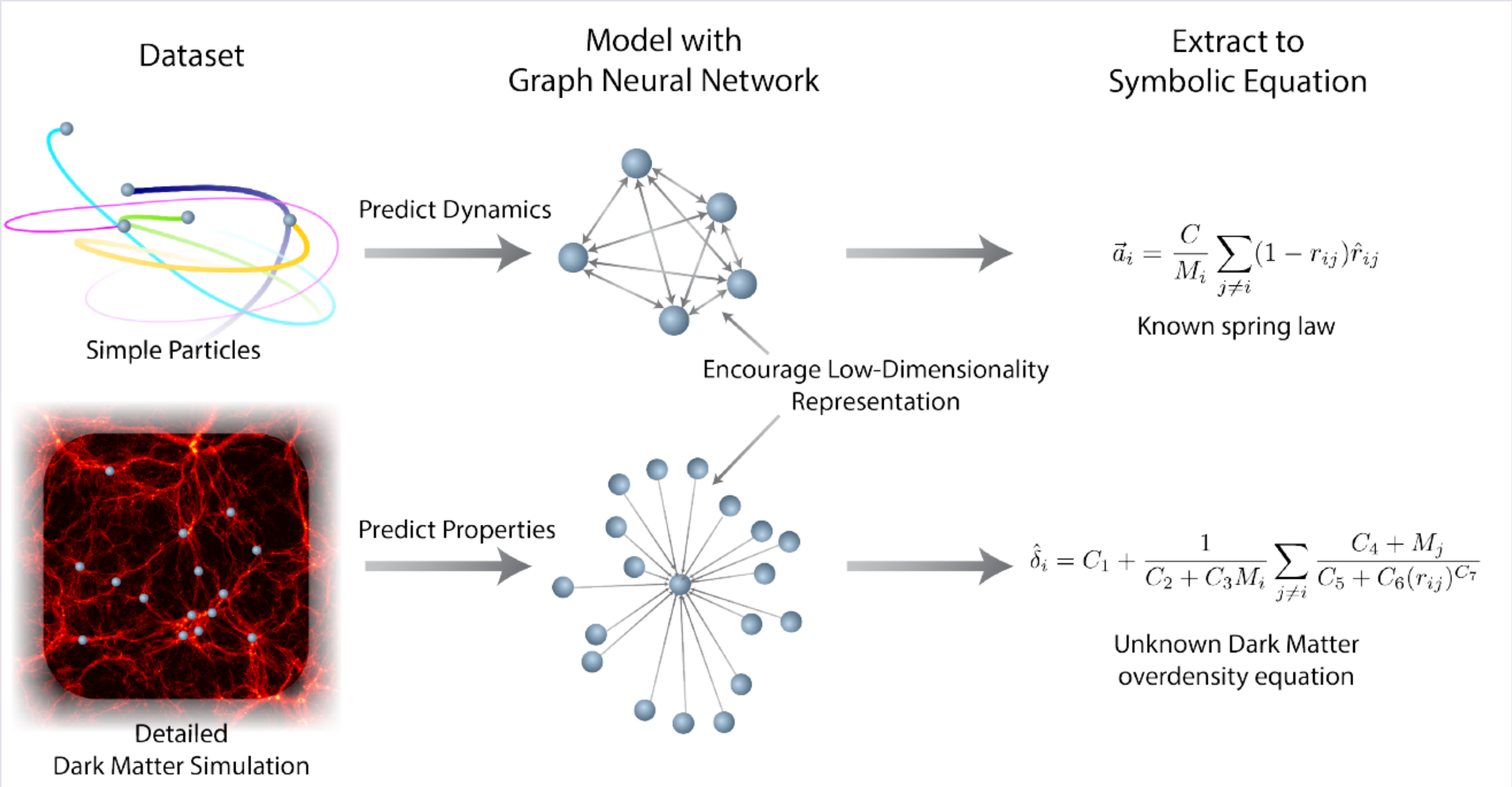


*Cranmer et al., Discovering Symbolic Models from Deep Learning with Inductive Biases, NeurIPS (2020)*

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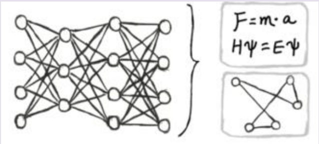



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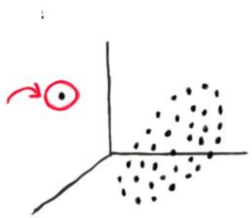

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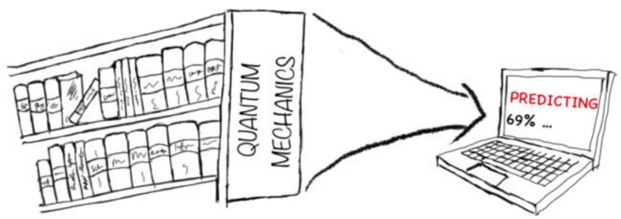


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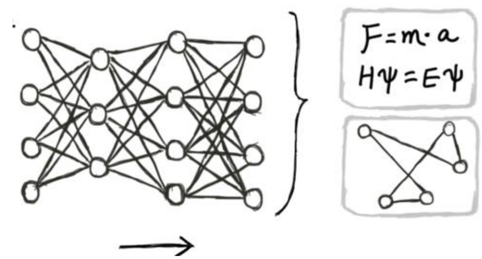
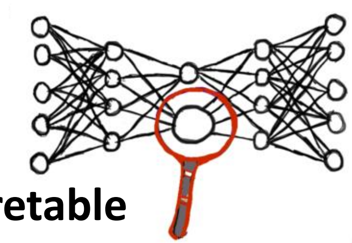
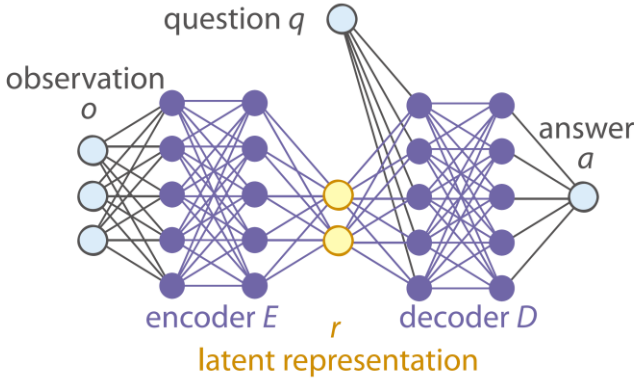


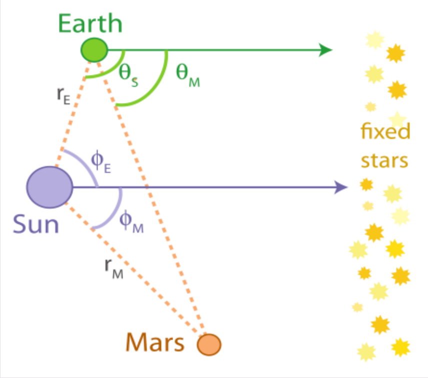



**Interpretable internal states**

## 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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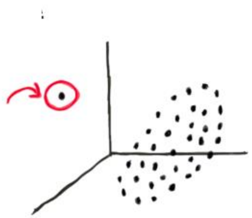

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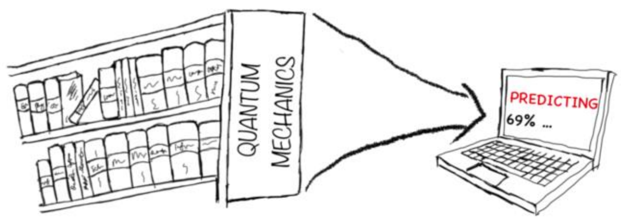


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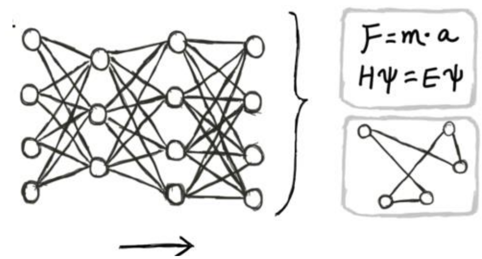


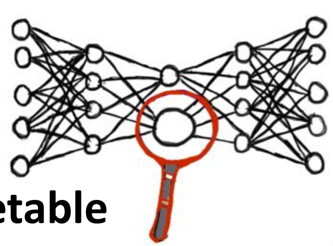

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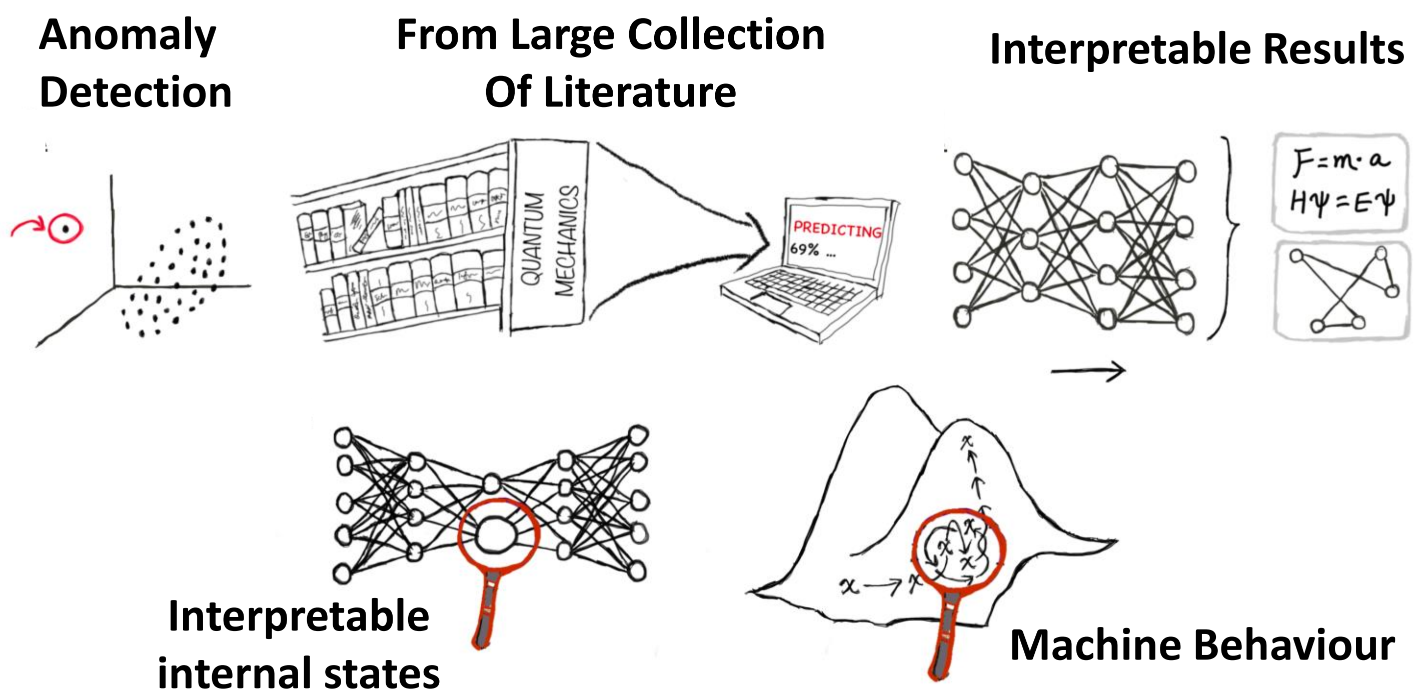


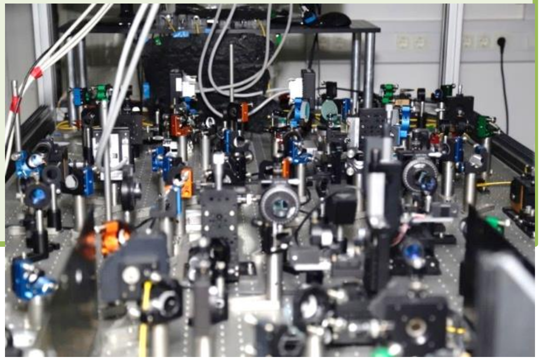
Mario Krenn

# Conclusion

**AI-based Experimental 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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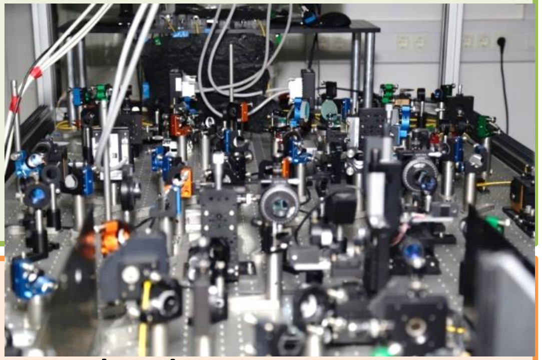

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## Automated Idea Generation:

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

Mario Krenn

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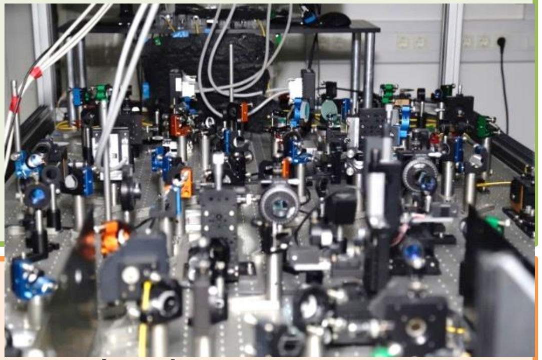


## Automated Idea Generation:

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

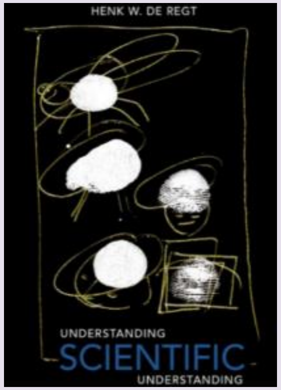
## Artificial Scientists

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)**

Mario Krenn

# Conclusion

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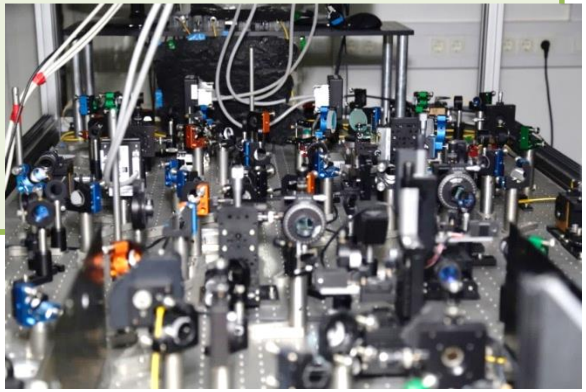

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