

# Neural Networks in Physics Research

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AI Ambassadors  
HUN-REN Wigner RCP

# About Me

- ◇ 2011: MSc in Physics (BME)  
MSc in Engineering (EC Lille, France, double degree program)
- ◇ 2017: PhD in Physics (BME)
  - ◇ statistical physics, computer simulations of networks in C++ and hybrid phase transitions
  - ◇ taking some machine learning courses in Python
- ◇ Since 2016: Wigner RCP
  - ◇ theoretical neuroscience, complex systems, machine learning
  - ◇ using cloud computing, some GPU programming (in Python :D)
  - ◇ since September 2024 an AI Ambassador



# HUN-REN AI Ambassador program

## Ambassadors

Example: <https://ai.wigner.hu>

- ◇ **spread information** about the services provided by the headquarters
- ◇ **organize** inspiration events and workshops
- ◇ **forward the researchers' needs** to the headquarters



AI Ambassadors  
HUN-REN Wigner RCP



HUN-REN AI Ambassadors



HUN  
REN **A4S**  
FOR SCIENCE



HUN-REN AI 4 Impact

**Experts** are available as a technical support team

- ◇ *Gergő Szabó* (BME mechatronics engineer; freelance Data Scientist):  
**idea validation**
- ◇ *Gergő Kóczán* (Óbuda University, IT engineer; experience in DevOps):  
**infrastructure**



# Contents

## ◆ Large Language Models

- ◆ Use cases: literature review, novelty research, market analysis
- ◆ Infrastructures: Web-based, GenAI4Science, local machine (ollama)

## ◆ Generative AI

- ◆ Use cases: writing aid, pair programmer, illustrator
- ◆ Infrastructures: SciSpace, GitHub Copilot, ChatGPT

## ◆ Physics-Informed Neural Networks

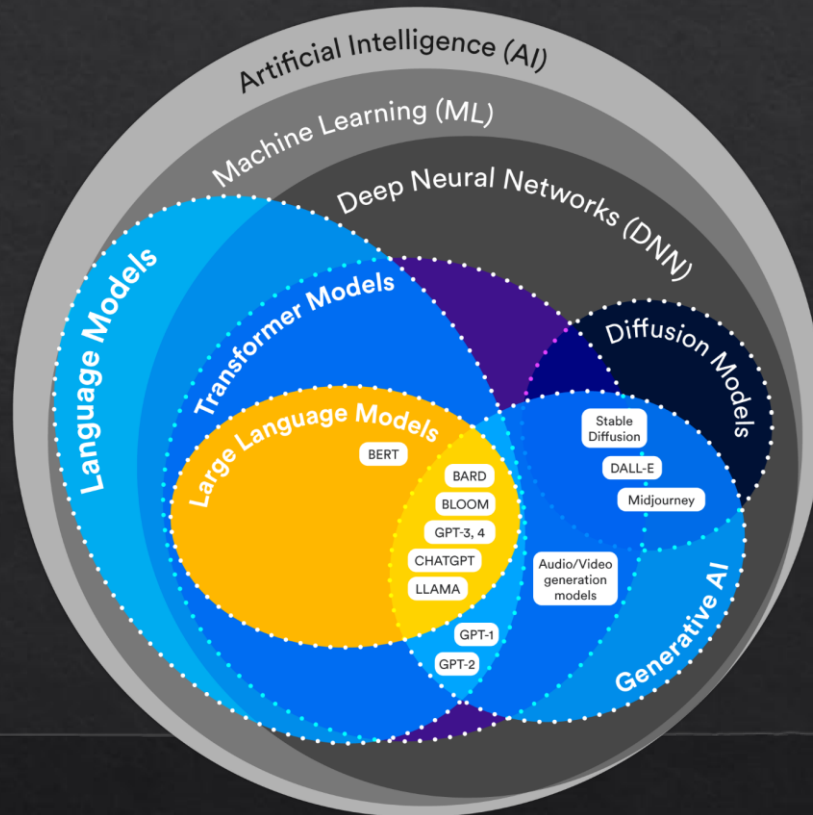
- ◆ Fit on training data
- ◆ Comply physical laws



# Large Language Models

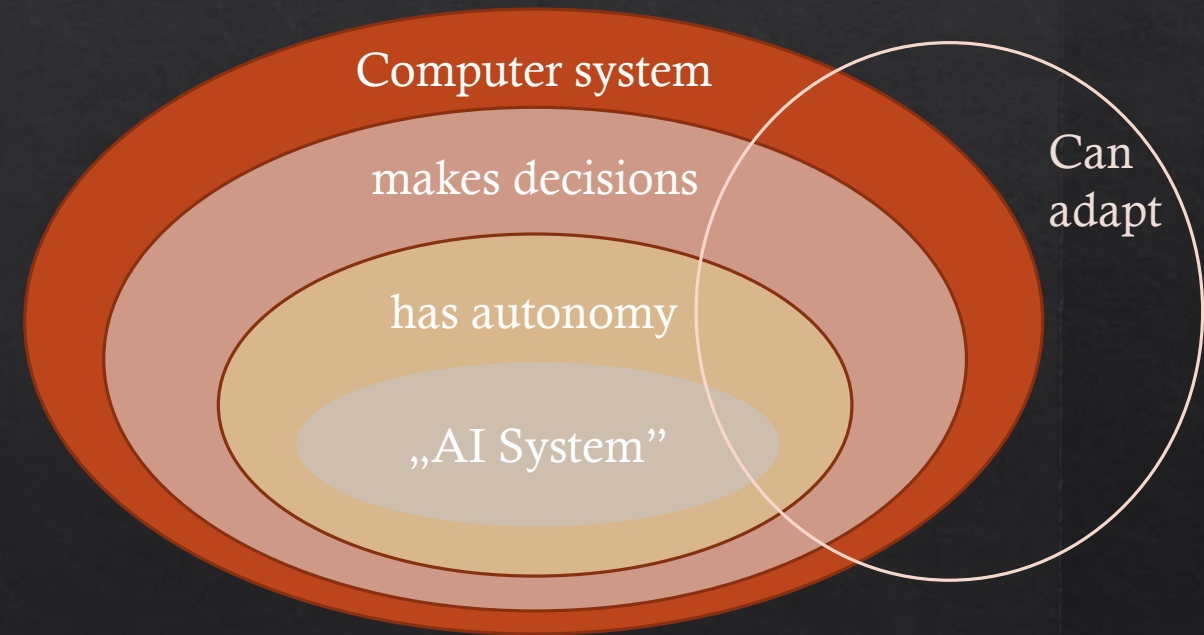
# How do we define artificial intelligence?

## Scientific picture



## Legal picture (AI Act)

- ◆ If you sell AI or offer it as a service don't forget to ask your lawyer

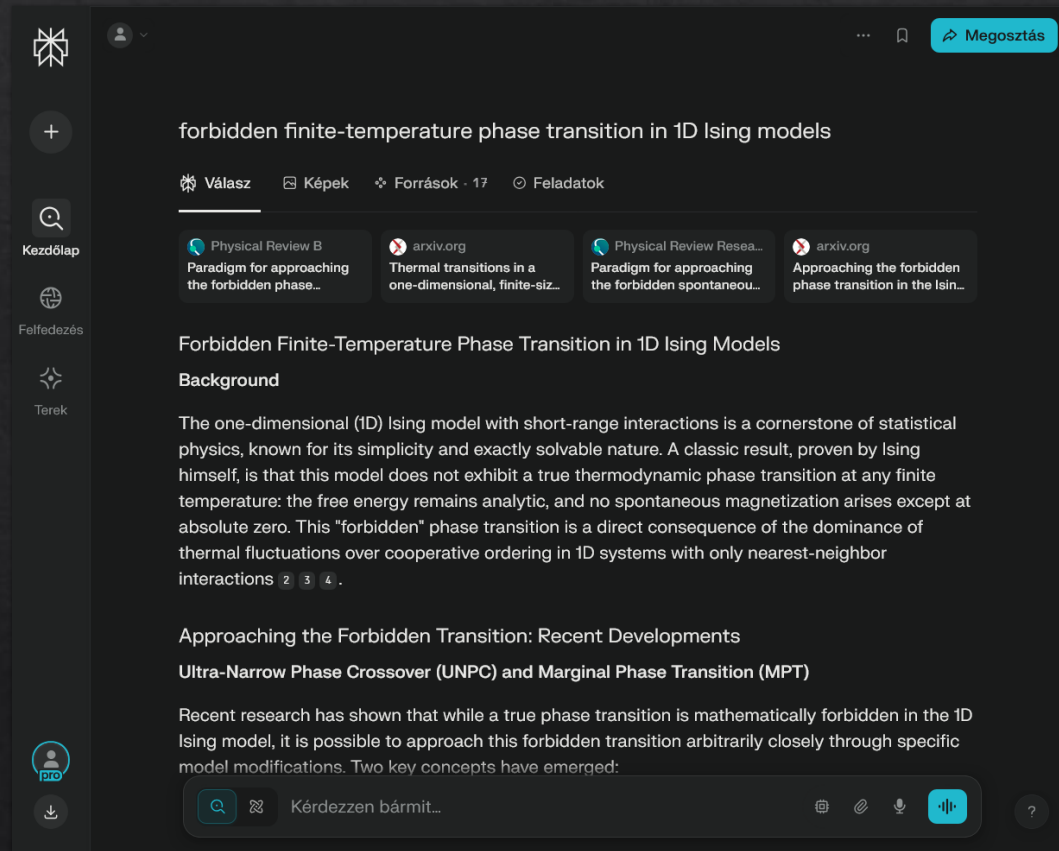


# Large Language Models

- ◇ A text prediction tool (AI → ML/NNs → NLP → LLM → Transformer → GenAI → ChatGPT)
  - ◇ Trained on web corpus, including books, Wikipedia, StackOverflow and similar
  - ◇ It is good at typical tasks and getting better for automated reasoning
- ◇ No logical reasoning per se or understanding of text expected
- ◇ It can be instructed
  - ◇ Prompt engineering: formulating task for a GenAI in natural language (no programming skills)
  - ◇ Instructions shall be clear, specific and describe all important aspects, use examples
  - ◇ Can take roles (“Please, explain as an expert speaking to a 6-year old.” or “Be sarcastic.”)
- ◇ Takes no responsibility for the output
  - ◇ Not a coauthor (see EU’s AI Act)
  - ◇ May be wrong, biased or stereotypic
- ◇ Rapidly developing: what we see tomorrow may be surpassed tomorrow.




# Literature review (Perplexity)




- ◇ Web search (query language matters)
- ◇ References for each statement
- ◇ Deep research available
  - ◇ Breaks down task into queries
  - ◇ Visits and summarizes multiple sources
  - ◇ Evaluates whether necessary info retrieved
- ◇ Pro version for T-users (Magenta moments)

# Literature review (SciSpace)



Papers

Pricing 

[My Searches](#)

**Technical aspects of power delivery network synchronization on a continental scale focusing on grid stability, frequency regulation, and voltage conditions. Include how these aspects are modeled and managed in large-scale power systems.**

Standard High Quality Deep Review

en

Research Steps [See all steps](#)

Deep Review Search has found [311 relevant papers](#) after going through 1050 papers.

Answer from top **20 papers**


Table of Contents

**Technical Aspects of Power Delivery Network Synchronization on a Continental Scale**


- Grid Stability, Frequency Regulation, and Voltage Conditions
- Modeling and Management of Large-Scale Power Systems
- Comparative Analysis of Key Strategies
- Conclusion

**Technical Aspects of Power Delivery Network Synchronization on a Continental Scale**

**Grid Stability, Frequency Regulation, and Voltage Conditions**  
The synchronization of power delivery networks on a continental scale is a complex task that involves maintaining grid



Papers

Pricing 

**Conclusion**  
The synchronization of power delivery networks on a continental scale is a complex task that requires advanced modeling and management strategies to ensure grid stability, frequency regulation, and optimal voltage conditions. Various approaches, such as the use of VSC–HVDC links with MPC, PINN-based RFSM, adaptive inertia VSGs, low-order frequency and voltage models, phasor domain models for GFM, and DOBC for frequency and voltage regulation, have been proposed to address these challenges. These strategies have been validated through simulations and experimental setups, demonstrating their effectiveness in enhancing the stability and reliability of large-scale power systems.

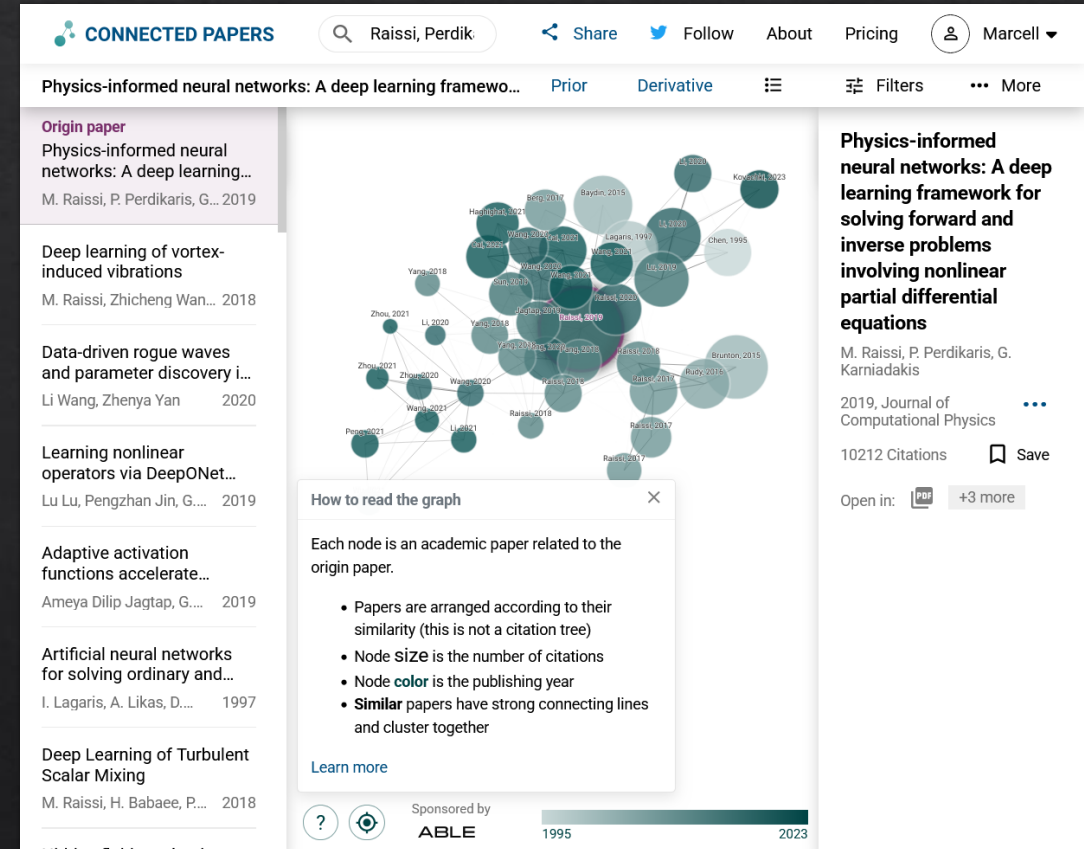
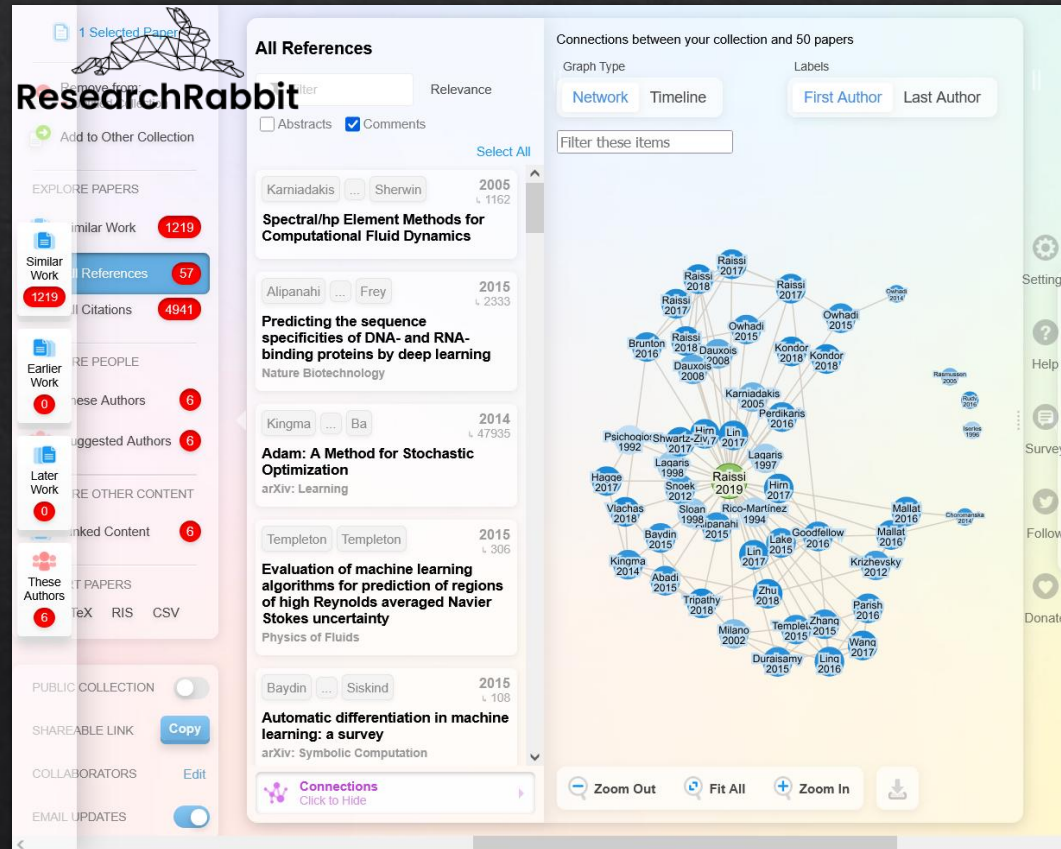
Read Less

Save to Notebook APA, Bullets Find Topics Write Feedback

Add columns (1) ☐ PDF ☐ Open Access Year More filters Sort by: Citation Count Export

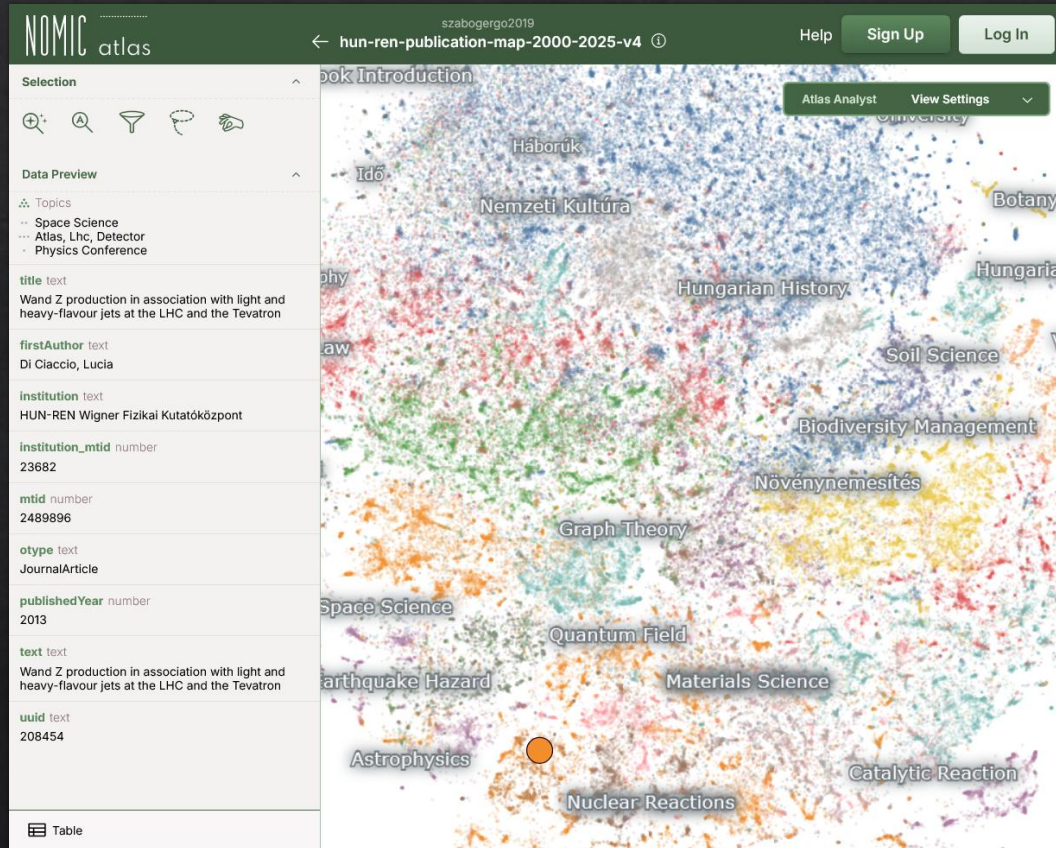
<input type="checkbox"/> Papers (20 / 311)	Insights	Add a Column
<div>Journal Article • 10.1109/TPWRD.2013.2280467</div> <div><input type="checkbox"/> <b>1. Stabilization of Large Power Systems Using VSC–HVDC and Model Predictive Control</b></div> <div>Alexander Fuchs, Markus Imhof, Turhan Demiray +1 more</div> <div>1 Feb 2014 • IEEE Transactions on Power Delivery</div> <div>Request PDF Podcast Chat</div>	<p>The paper focuses on stabilizing large power systems using VSC-HVDC links and model predictive control (MPC) to manage grid stability, frequency regulation, and voltage conditions, utilizing global measurements for effective control and optimization during transients and oscillations.</p>	<div>Create</div> <div>Suggested Columns</div> <ul style="list-style-type: none"><li>+ TL:DR</li><li>+ Conclusion</li><li>+ Summarize</li><li>+ Results</li><li>+ Summarize</li><li>+ Methods U</li></ul>

# Citation network with AI





# HUN-REN publication map



- ◇ Nomic Atlas
- ◇ Embedding with a BERT-like model (no decoder or text prediction)
- ◇ 2d projection for visualization

Work of Gergő Szabó (HUN-REN AI4Science)

<https://atlas.nomic.ai/data/szabogergo2019>

# Generative AI

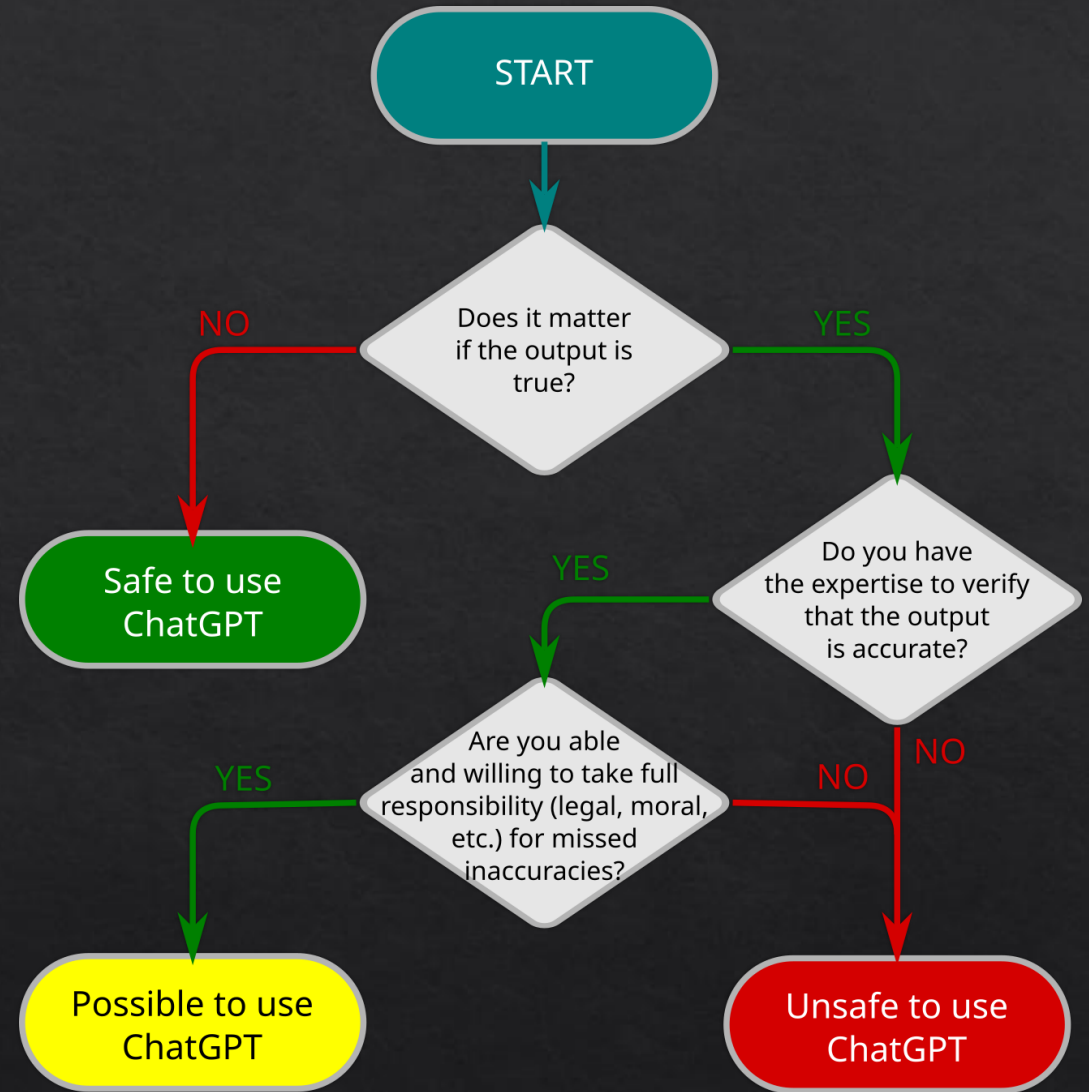
in research

# Shall I use ChatGPT\*?

\* or any other large language model  
for my research tasks

Many clones exist, for the original:

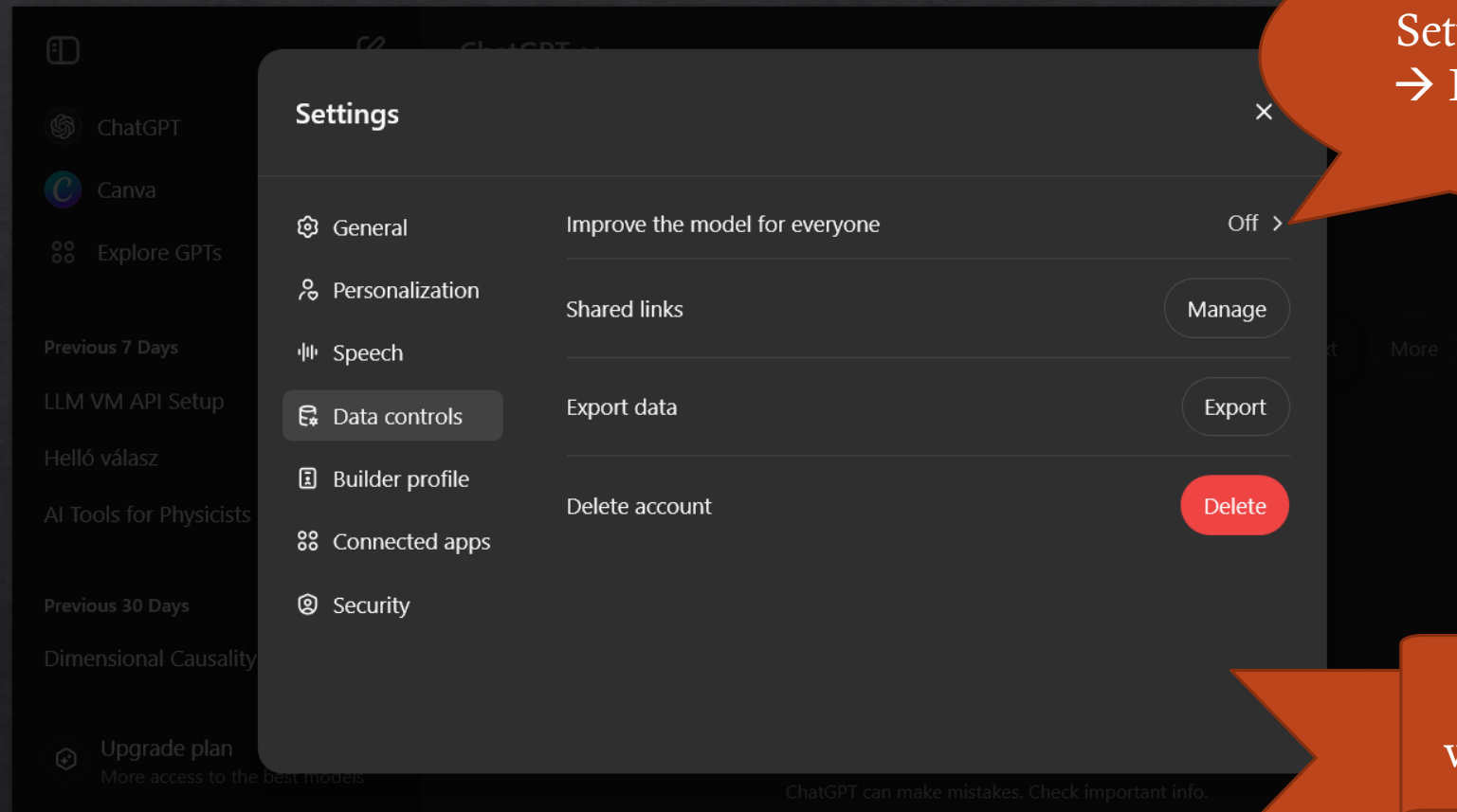
- ◇ <https://chatgpt.com/>
- ◇ <https://chat.openai.com/>





# Ask nicely not to use our data

Here it is:  
Settings → Data controls  
→ Improve the model for  
everyone → Off



I believe it  
when I see it.

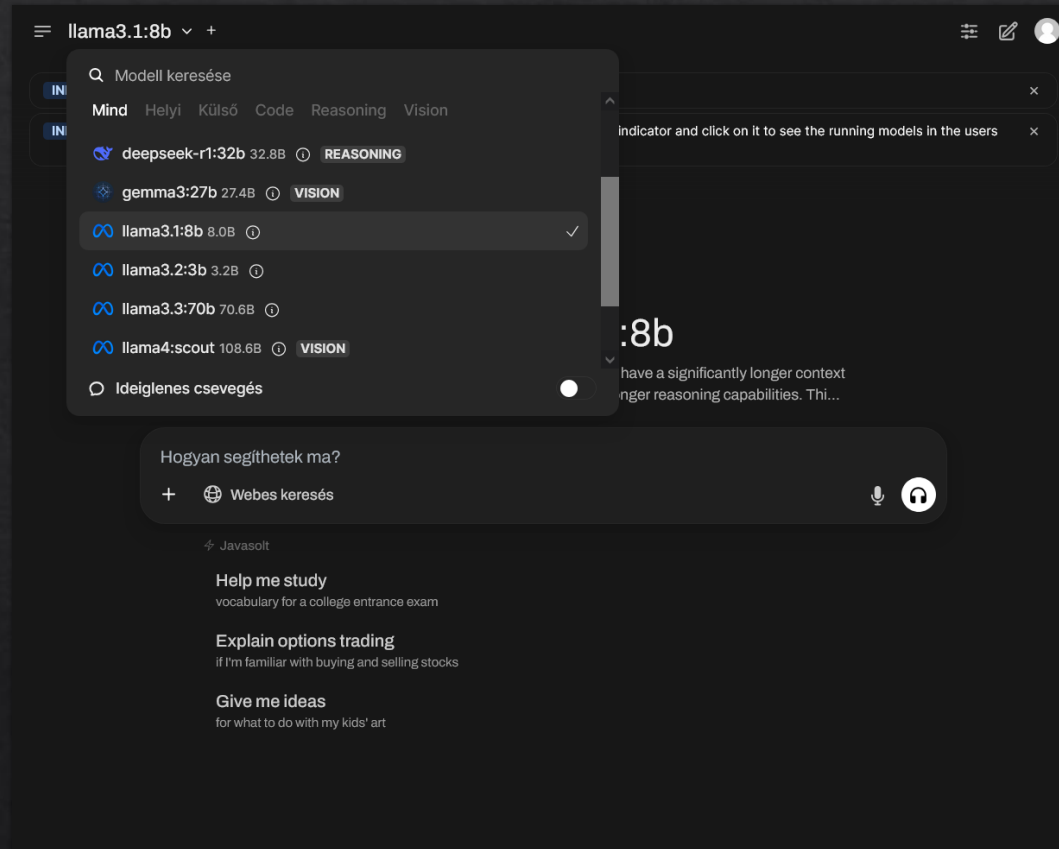
# Ingredients of a prompt

- ◆ priming (personality): “You are an expert at writing clear, concise, Python code.”
- ◆ question (task): “Create a doubly linked list.”
- ◆ decorator (presentation): “Insert comments for each line of code.”

## Notes

- ◆ Model is instructed to tolerate typos, to be helpful and polite.
- ◆ The more data, the better performance (English and Python > Hungarian and Fortran)
- ◆ Providing context restricts the creativity and increases the probability of success.
- ◆ Guide the model with example solutions or provide cases to be avoided.
- ◆ Ask the model to break down the task into steps. (Not a human-way reasoning model.)
- ◆ Same input may produce different output. Lot of improvements, but hallucinations may occur.

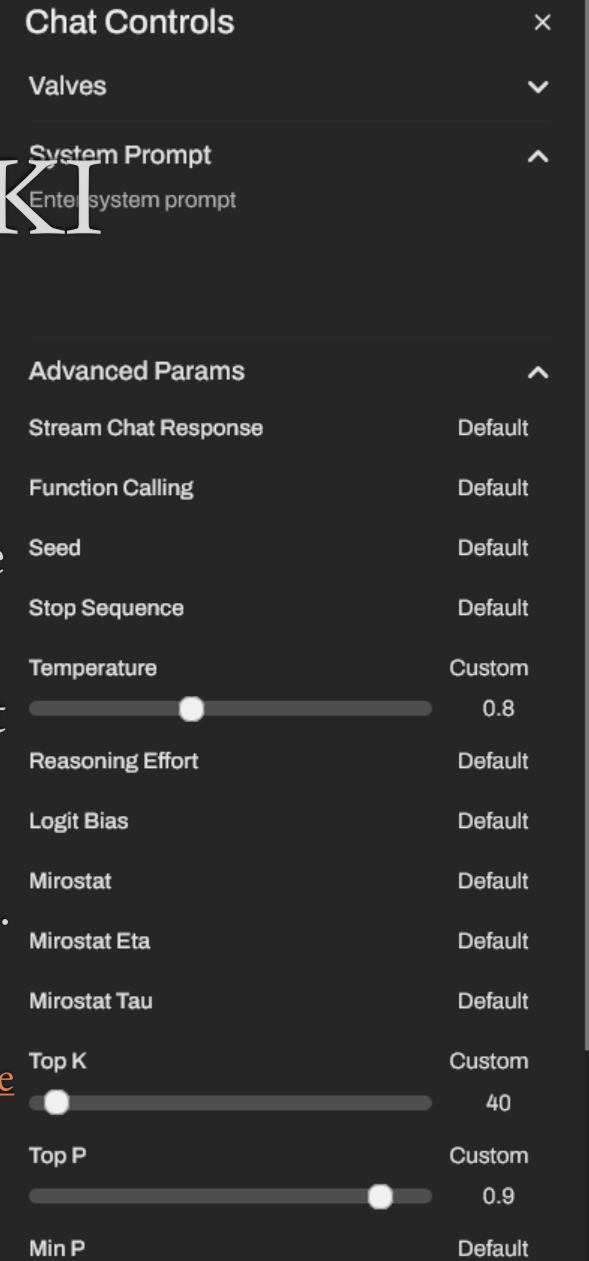
# HUN-REN GenAI platform @ SZTAKI



- ◆ WebUI
- ◆ API access
- ◆ Your data does not leave the HUN-REN Cloud
- ◆ We have \$10.000.- credit for OpenAI models, please, apply for them with your research ideas.

<https://science-cloud.hu/genai4science>

<https://genai.science-cloud.hu>





# HUN-REN GenAI platform @ SZTAKI

## Open WebUI

- ❖ Can work with both data and pdf files
- ❖ Can search the web



pair0077.txt

Fájl

125.9 KB



pair0077\_des.txt

Fájl

722.0 B

Understand the structure of the data based on the attachments. Write and execute a Python code that analyses the periodicity of the uploaded data, performing the following steps. Create plots the original data and also its periodogram. Make sure to include units on both horizontal and vertical axis. Print the peaks of the periodogram.



codellama:13b 2:17 PM

I'm assuming that the data is in a CSV file with two columns: X (temperature in Celsius) and Y (solar radiation in W/m<sup>2</sup>).

Here's a Python code snippet using NumPy, Matplotlib, and Scipy to analyze the periodicity of the data:

```
python
1 import numpy as np
2 from scipy.signal import periodogram
3 import matplotlib.pyplot as plt
4
5 # Load data from file
6 data = np.loadtxt('pair0077_des.txt')
7
8 # Plot original data
9 plt.figure(figsize=(10, 6))
10 plt.subplot(2, 1, 1)
11 plt.plot(data[:, 0], label='Temperature (C)')
12 plt.ylabel('Temperature (C)')
13 plt.title('Original Data')
14 plt.legend()
```

Futtatás Mentés Másolás

Run!

# LLMs on your own machine



Get up and running with large language models.

Run [DeepSeek-R1](#), [Qwen 3](#), [Llama 3.3](#), [Qwen 2.5-VL](#), [Gemma 3](#), and other models, locally.

Download ↓

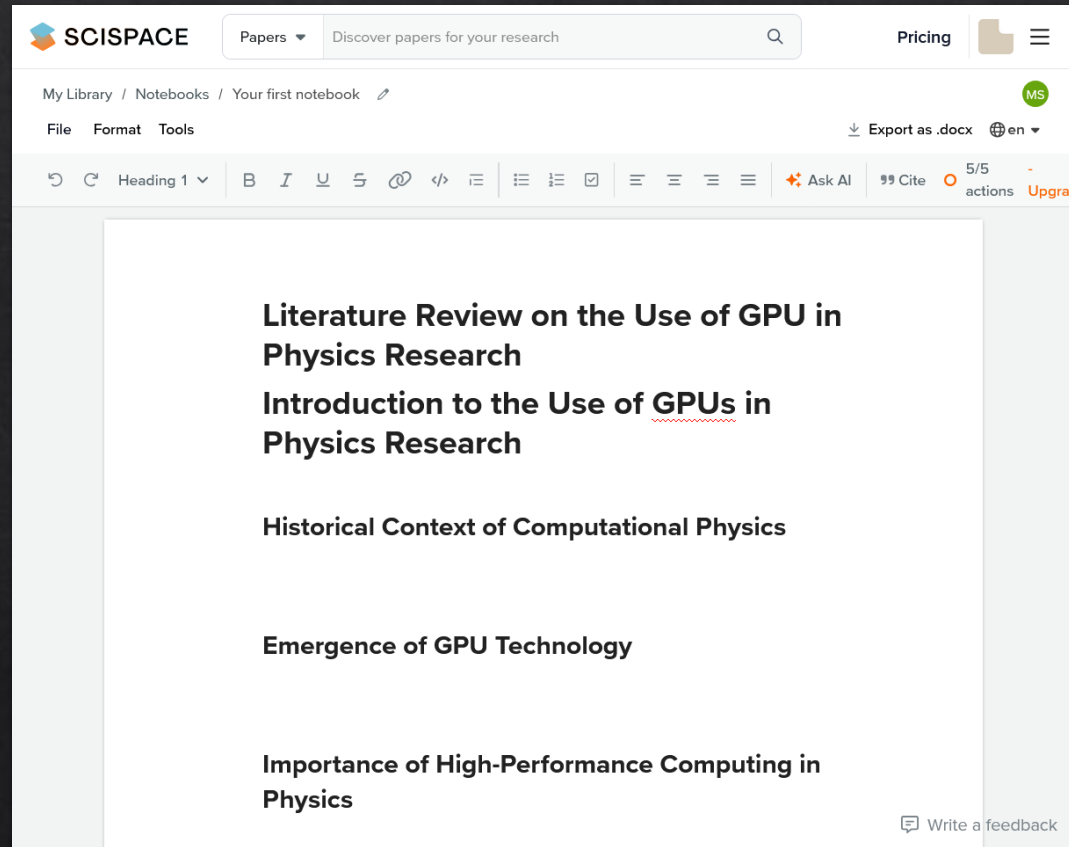
Available for macOS, Linux,  
and Windows

- ◇ Download & install ollama
- ◇ Run a model from terminal, e.g.,  
`ollama run gemma3:1b`
- ◇ Access via API, even multimodal

```
import ollama

def demo(image_url):
    fn = get_image(image_url)
    res = ollama.chat(
        model="llava:7b",
        messages=[
            {
                'role': 'user',
                'content': 'I made this picture today.'
                'What would i tell about this to my friend?',
                'images': [fn]
            }
        ]
    )
    return ['message']['content']
```

# Scientific Writing



- ◇ Chat with PDF
- ◇ Literature Review
- ◇ AI Writer
- ◇ Find Topics
- ◇ Paraphraser
- ◇ Citation Generator
- ◇ Extract Data
- ◇ AI Detector
- ◇ PDF to Video



# What is GitHub Copilot

## GitHub Copilot

- ◆ LLM trained specifically on programming
- ◆ ChatGPT is Copilot has your repository as context (may replicate errors already made)
- ◆ Suggestions on the fly, while typing
- ◆ A plugin in your favorite IDE
- ◆ Now there is a free version with quota, available for everyone.

## ChatGPT

- ◆ General-purpose AI, even multimodal
- ◆ Context is conversation (plus persona, general settings)
- ◆ Linear (except that now we have canvas)
- ◆ You have to send prompts
- ◆ There are LLM-s hosted in the HUN-REN Cloud: Llama, Gemma, Mistral, DeepSeek  
<https://genai.science-cloud.hu>

# GenAI as a pair programming partner

- ◇ pair programming: two programmers work on the same code together to produce something that is higher-quality than either of them would produce by themselves
  - ◇ the “**driver**,” who actually writes code
  - ◇ the “**navigator**,” who checks the driver’s work as it’s done and keeps an eye on the big picture
- ◇ instead of being twice as slow and expensive, coding this way actually adds just 15% more time to the development process, and in exchange returns 15% fewer bugs and defects
- ◇ GenAI of today is like a newly-hired mediocre junior programmer who’s read tons of documentation, taken every bootcamp, and checked out every Stack Overflow Q&A page
- ◇ you take the navigator role, while the AI is the coder; as the knowledgeable one, you should be planning, thinking about design, and reviewing any code produced, while the tool does what it does best: cranks out code fast
- ◇ *it’s the AI’s job to be fast, it’s your job to be good*
- ◇ hint: embrace multiple LLM tools and interfaces, results can completely change from one week to the next

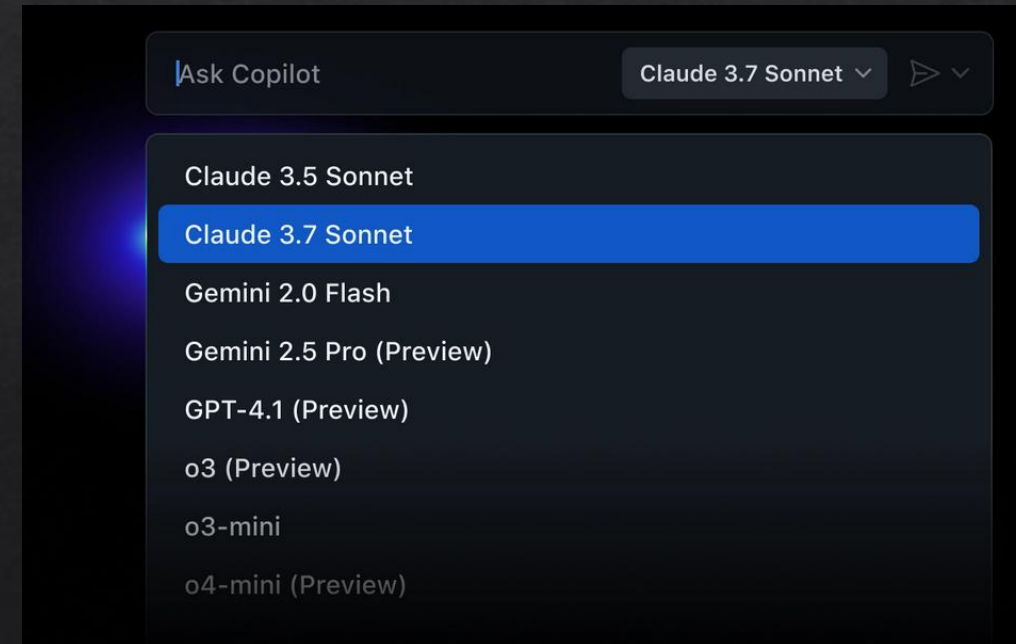
# New in Github Copilot

**Coding agent** tracks issues, plans, writes, tests, and iterates in the background.

Swap between **models** like Claude 3.7 Sonnet, OpenAI o1, and Google Gemini 2.0 Flash.

**Free plan** includes

- ◇ 50 agent mode or chat requests per month
- ◇ 2,000 completions per month
- ◇ Access to Claude 3.5 Sonnet, GPT-4.1, and more





# Ask nicely not to use our data

Here it is:  
(avatar) → Your copilot  
→ Allow GitHub to use  
my code snippets →  
unticked

**Copilot Chat in GitHub Mobile**  
You can use [Copilot Chat in GitHub Mobile](#) personalized to a codebase.

**Suggestions matching public code (duplication detection filter)** Allowed ▾  
Copilot can allow or block suggestions matching public code. Learn more about [code suggestions](#).

☐ **Allow GitHub to use my code snippets from the code editor for product improvements \***  
Allow GitHub, its affiliates and third parties to use my code snippets to research and improve GitHub Copilot suggestions, related models and product features. More information in [About GitHub Copilot privacy](#).

**Copilot access to Bing** Disabled ▾  
Copilot can answer questions about new trends and give improved answers. [See Microsoft Privacy Statement](#).  
ⓘ Your organization(s) have not enabled use of this feature.

I believe it  
when I see it.

# More ideas for GitHub Copilot

1. Run terminal commands from GitHub Copilot Chat
2. Write pull request summaries with a single click
3. Generate commit messages in your IDE
4. Get help in the terminal with GitHub Copilot in the CLI
5. Talk to your repositories on GitHub.com
6. Fix code inline with GitHub Copilot suggestions
7. Bulk close 1000+ GitHub Issues
8. Generate documentation for your code
9. Write code in natural language
10. Create amazing content with GitHub Copilot

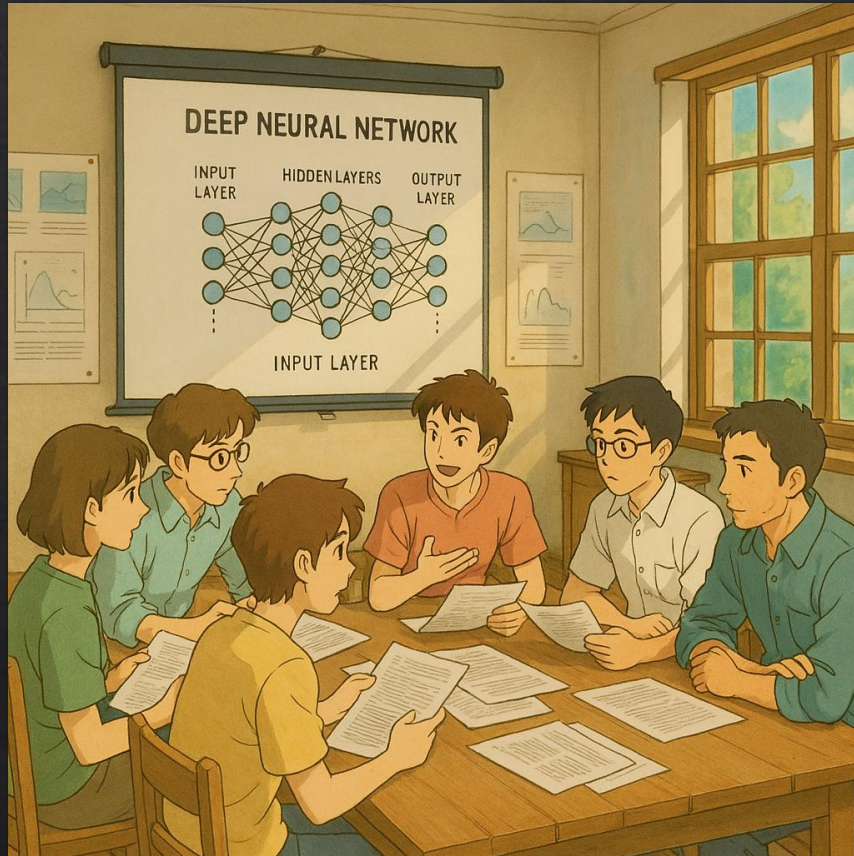
Source:

<https://github.blog/developer-skills/programming-languages-and-frameworks/10-unexpected-ways-to-use-github-copilot/>

# Physics-Informed Neural Networks



# Physics-Informed Neural Networks

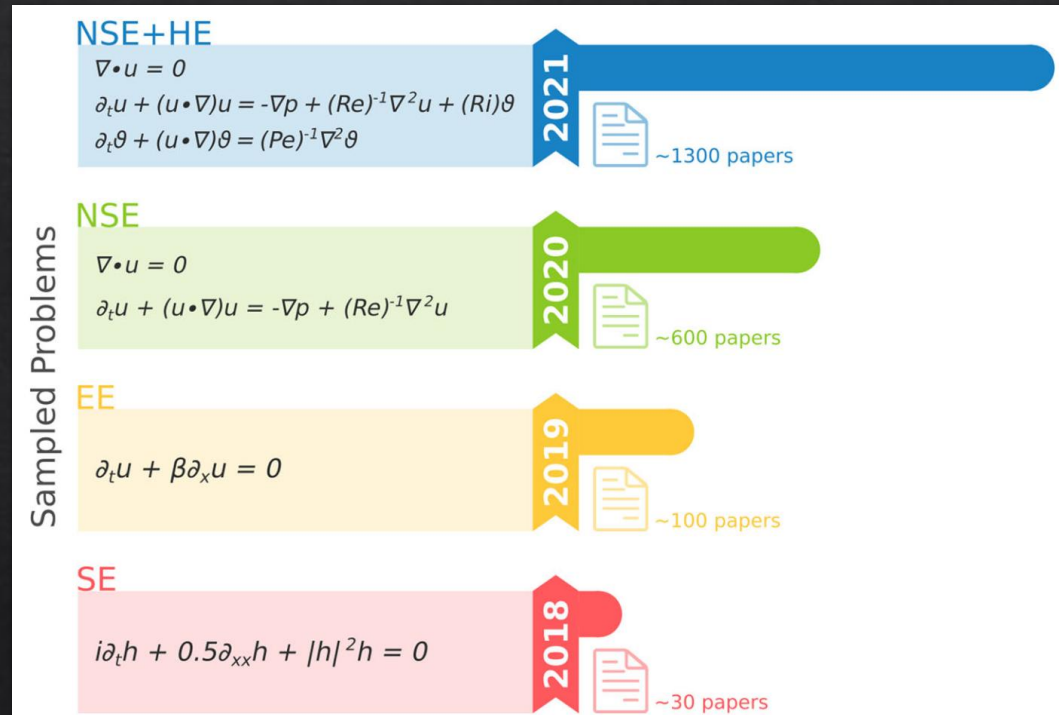


- ◇ Started a Journal Club
- ◇ Feel free to join

(cartoon by ChatGPT)

<https://ai.wigner.hu/journal-club-2025/>

# Physics-Informed Neural Networks



## Task setting

- ◇ (noisy) measurement data
- ◇ (some) physical understanding: laws as partial differential equations or discrete-time mapping function

## Want

- ◇ solution as a function of time

Coumo et al., Journal of Scientific Computing (2022) 92:88

<https://doi.org/10.1007/s10915-022-01939-z>

# PINN formulation

- ◆ Differential equation, boundary and initial conditions

$$\begin{aligned}\mathcal{F}(u(z); \gamma) &= f(z) & z \text{ in } \Omega, \\ \mathcal{B}(u(z)) &= g(z) & z \text{ in } \partial\Omega \\ r_{\mathcal{F}}[\hat{u}_{\theta}](z) &= r_{\theta}(x, t) = \frac{\partial}{\partial t} \hat{u}_{\theta}(x, t) + \mathcal{F}_x \hat{u}_{\theta}(x, t).\end{aligned}$$

- ◆ No need to manually enter derivatives
- ◆ Implementation relies on automatic differentiation available in all recent ANN frameworks (PyTorch, JAX, Tensorflow)

- ◆ Artificial neural network loss function:

$$\theta = \arg \min_{\theta} \mathcal{L}(\theta)$$

$$\mathcal{L}(\theta) = \omega_{\mathcal{F}} \mathcal{L}_{\mathcal{F}}(\theta) + \omega_{\mathcal{B}} \mathcal{L}_{\mathcal{B}}(\theta) + \omega_d \mathcal{L}_{data}(\theta).$$

$$\mathcal{L}_{\mathcal{F}}(\theta) = MSE_{\mathcal{F}} = \frac{1}{N_c} \sum_{i=1}^{N_c} \|\mathcal{F}(\hat{u}_{\theta}(z_i)) - f(z_i)\|^2$$

$$\mathcal{L}_{\mathcal{B}}(\theta) = MSE_{\mathcal{B}} = \frac{1}{N_B} \sum_{i=1}^{N_B} \|\mathcal{B}(\hat{u}_{\theta}(z_i)) - g(z_i)\|^2$$

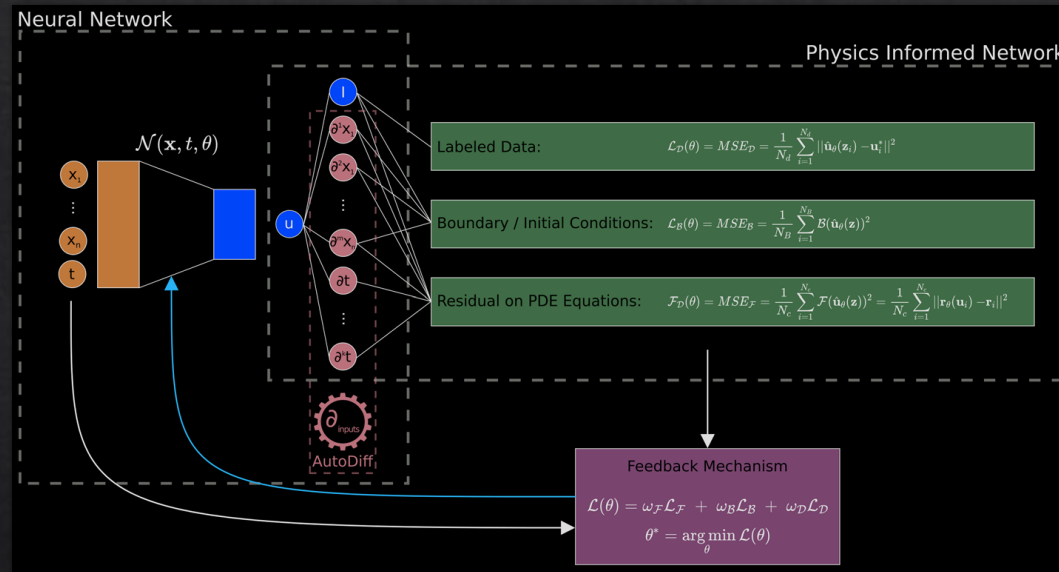
$$\mathcal{L}_{data}(\theta) = MSE_{data} = \frac{1}{N_d} \sum_{i=1}^{N_d} \|\hat{u}_{\theta}(z_i) - u_i^*\|^2.$$



# PINN properties

## Advantages

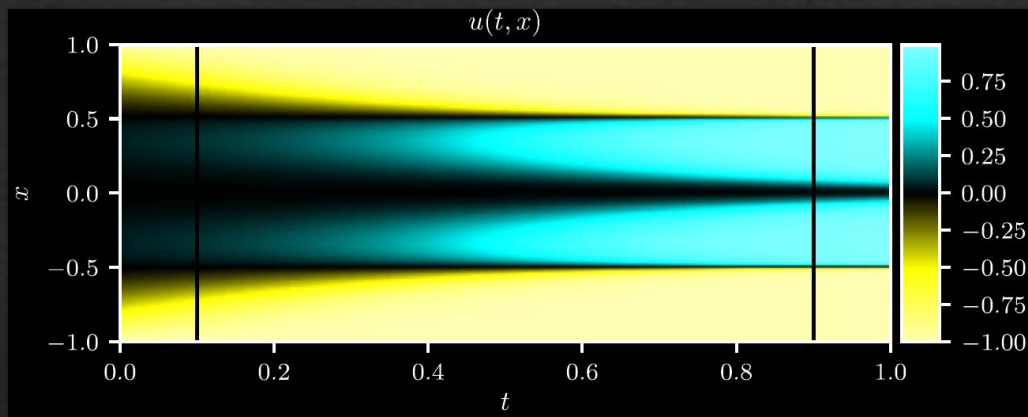
- ◇ Fit noisy measurement data
  - ◇ NNs as universal approximators
  - ◇ NNs perform poorly for extrapolation
- ◇ Regulation via physical laws
  - ◇ Improves extrapolation
  - ◇ Physical description may be incomplete
- ◇ Training on GPU



Coumo et al., Journal of Scientific Computing (2022) 92:88  
<https://doi.org/10.1007/s10915-022-01939-z>

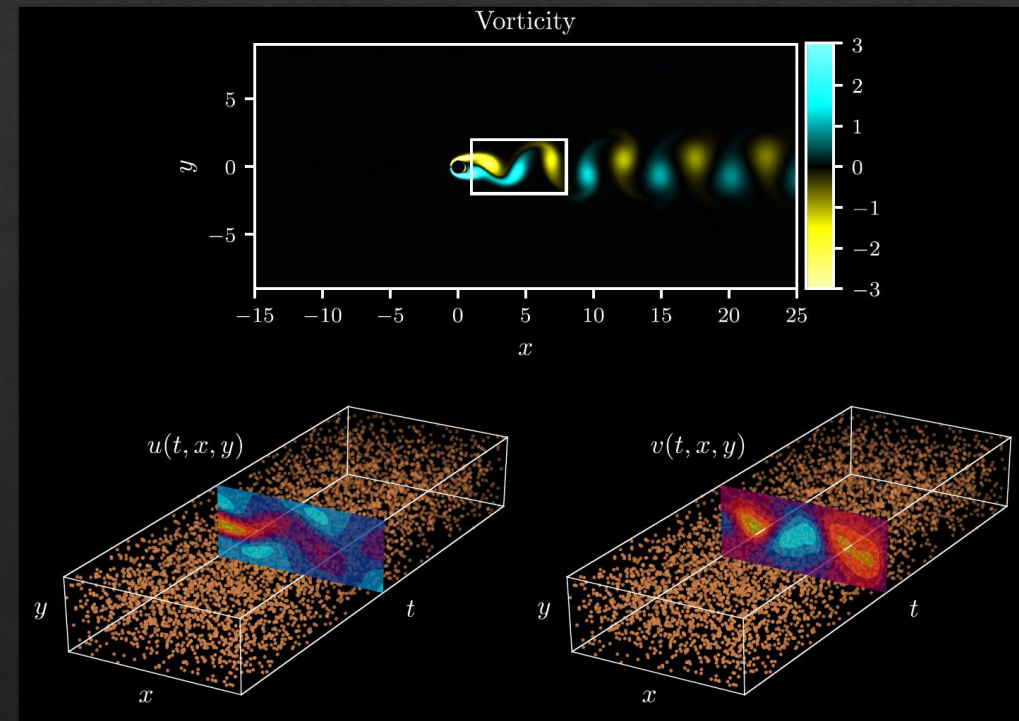
# PINN applications

## Stiff differential equations



Raissi et al., J. of Computational Physics 378 (2019) 686–707  
<https://doi.org/10.1016/j.jcp.2018.10.045>

## Fluid mechanics



and more...

# PINN challenges

## Challenges

- ◆ Network architecture (depth, width, connections, ...)
- ◆ Optimal activation function
- ◆ Optimal training
- ◆ Support multiple initial conditions

## Read more

- ◆ Cuomo et al. Scientific Machine Learning Through Physics-Informed Neural Networks: Where We Are and What's Next. 2022, J. Sci. Computing **92**, (3): 88. [doi: 10.1007/s10915-022-01939-z](https://doi.org/10.1007/s10915-022-01939-z)
- ◆ Raissi et al. PINNs: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations. 2019, J. Comp. Physics **378**: 686–707. [doi: 10.1016/j.jcp.2018.10.045](https://doi.org/10.1016/j.jcp.2018.10.045)
- ◆ Wang et al. An Expert's Guide to Training PINNs. 2023, arXiv <https://doi.org/10.48550/arXiv.2308.08468>
- ◆ Krishnapriyan et al. Characterizing Possible Failure Modes in PINNs 2021, Advances in NIPS **34**: 26548-26560 <https://proceedings.neurips.cc/paper/2021/hash/df438e5206f31600e6ae4af72f2725f1-Abstract.html>
- ◆ Li et al.: Tutorials: Physics-informed machine learning methods ... APL Mach. Learn. **2**, 031101 (2024) [doi: 10.1063/5.0205159](https://doi.org/10.1063/5.0205159)
- ◆ Nakamura et al. PINNs with Variable Initial Conditions Proc. 7th W.Cong. Mech., Chem. & Mat.Eng. (MCM'21) [doi: 10.11159/htff21.113](https://doi.org/10.11159/htff21.113)



# Conclusions

- ◇ ChatGPT and GitHub Copilot support multiple programming languages
- ◇ They can generate text and code, it is your responsibility to provide context and verify
- ◇ Output is well structured, complex tasks can be broken down into steps
- ◇ Specialized apps for scientific purposes: review, deep research, write
- ◇ Artificial neural networks not only for AI but for solving physics problems

# Announcements

- ◆ Visit the homepage of the HUN-REN Wigner AI Ambassadors: <https://ai.wigner.hu>
- ◆ Visit our Wiki for learning materials <https://gitlab.wigner.hu/ai/best-practices>
- ◆ Subscribe to our calendar <https://ai.wigner.hu/events/index.ics>
- ◆ HUN-REN AI <https://hun-ren.hu/ai4impact>

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REN **A4S**  
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FIRST SCIENCE



Csikor Ferenc



Stippinger Marcell

