



WELCOME to our Hackathon

1. Hackathon Context

Why this hackathon exists

In recent years, artificial intelligence has begun to change science in a fundamental way.

When AlphaFold demonstrated that protein structures could be predicted not one by one, but at the scale of *all known proteins*, it became clear that AI was doing more than accelerating existing research workflows. It was shifting scientific discovery from solving individual problems to addressing entire problem classes at once.

More recently, we crossed another important threshold. Agentic AI systems have emerged that can plan scientific workflows, integrate literature and data, carry out multi-step investigations, and even generate research papers that pass peer review. This does not mean that science is becoming automated. It means that the **structure of scientific work itself is evolving**.

This hackathon is designed in response to that shift.

What we mean by AI-First Science (AI1Science)

AI-First Science treats AI not as a supporting tool, but as a **core layer of discovery**.

An approach is AI-First when it:

- enables **order-of-magnitude improvements** in speed (weeks becoming hours),
- makes previously **unmanageable or impossible questions** tractable,
- and reshapes the **role of the scientist**, reducing low-level coordination and increasing focus on interpretation, judgment, and strategic decisions.

AI1Science is not about replacing researchers. It is about changing how scientific work is structured.

What is Agentic Discovery?

Agentic Discovery is a practical manifestation of AI-First Science.

Instead of isolated AI tools, it relies on **agentic systems** that can operate across entire research processes. These systems can plan, iterate, connect data and methods, and collaborate with humans over time. Rather than executing single instructions, they help explore complex problem spaces and support non-linear discovery.

In this sense, agentic systems become part of the **infrastructure of scientific discovery**, not just productivity tools.



What the Agentic Discovery Hackathon is (and is not)

The Agentic Discovery Hackathon is an **experimental space**.

It is not a product competition, and it is not focused on polished solutions. Its purpose is to explore ideas that rethink scientific workflows from an AI-First perspective. We encourage participants to move beyond incremental automation and to investigate how AI could fundamentally change how research is conducted in their domain.

Early-stage and exploratory ideas are welcome—especially when they point toward new scientific methods or workflows.

Tools provided during the hackathon

To support exploration, we provide access to tools such as the **Agentic Discovery Platform (see below)**, which integrates multiple agentic capabilities and external tools into a shared research environment.

Use of these tools is **not mandatory**. They are offered as inspiration and as examples of how agentic thinking can be implemented in practice. Teams are free to:

- use the platform to explore a specific scientific domain,
- assemble their own agentic workflows with tools such as n8n,
- or build fully custom solutions through code.

What matters is not the specific tooling, but the **AI-First way of thinking** behind the idea.

Mentors, teams and shared learning

Throughout the hackathon, participants will be supported by a group of mentors who share this mindset and have experience working with agentic systems and related tools.

Mentors are not assigned to individual teams. Instead, they support the collective goal of maximizing learning, exploration, and constructive disruption across the two days. They can help teams validate directions, improve workflows, and ground ambitious ideas in practical considerations - even if they do not know every tool in depth.

If you don't have a pre-formed team, we will assign you to one, with team suggestions powered by AI. For optimal results, ensure your team includes a combination of both domain science expertise and agentic expertise, as the overlap of these skills is crucial.

How ideas and results will be evaluated

Projects will be evaluated along two dimensions:

1. Radical Innovation

This dimension asks how much the idea **redefines scientific practice**.

For example:

- Does it go beyond making existing steps faster?



- Does it introduce a fundamentally new workflow or method?
- Does it meaningfully change the role of the scientist?

2. Feasibility

This dimension considers whether the idea:

- could realistically work in principle,
- can be developed further beyond the hackathon,
- and could fit into real research environments over time.

Our goal is to see project on the high-end of both dimensions, but we prefer radical innovation over feasibility.

2. Schedule

[Online Q&A session](#) – Wednesday, January 14, 2026 16:00-17:30

Venue: 1054 Budapest, Alkotmány utca 29.

	Time	Activity
Thursday, January 15	08:30 – 09:00	Arrival & Registration
	09:00 – 09:30	Opening Session
	09:30 – 12:30	Team Work
	12:30 – 14:00	Lunch
	14:00 – 18:00	Team Work
Friday, January 16	08:30 – 09:00	Arrival
	09:00 – 12:30	Team Work
	12:30 – 13:30	Lunch
	13:30 – 15:30	Team Work
	15:30 – 17:30	Final Pitches
	17:30 – 18:00	Jury Deliberation
	18:00 – 18:30	Awards & Closing



3. Messaging Platform

Registration Steps:

1. Register on Discord: <https://discord.com/register>
2. Verify your email address to activate your account.
3. Join our Community: <https://discord.gg/BVvM6uEN>.
4. Set your nickname on the server (please use your full name if it's not already set, optional otherwise):
 - a. You can change your own nickname by clicking your profile in the server → Edit Server Profile → Nickname.
 - b. For a step-by-step guide, see [Discord Nickname Tutorial](#).

Once you join the community:

- You will soon have access to your team's channel:
 - Under the Teams category, look for the channel with your team's name.
 - This is where you can discuss topics only with your team members.
 - A pinned message in your team's channel will contain an API key for accessing OpenAI's models.
- In the General channel, you can discuss topics visible to all community members.
- In the Announcements channel, you can see our latest announcements and updates.
- In the tech-help-desk channel, you can ask technical questions, e.g., your API key does not work.

4. Resources

4.1 DATAGEN

Code: GitHub: <https://github.com/starpig1129/DATAGEN>

Publication: No official academic publication.

4.2 Denario

Code: GitHub: <https://github.com/AstroPilot-AI/Denario>

Article: arXiv: <https://arxiv.org/abs/2510.26887>

4.3 AstroAgents

Code: GitHub: <https://github.com/amirgroup-codes/AstroAgents>

Article: arXiv: <https://arxiv.org/abs/2503.23170>

4.4 AI Scientist v2 (Sakana AI)



Code: GitHub: <https://github.com/SakanaAI/AI-Scientist-v2>

Article: arXiv: <https://arxiv.org/abs/2408.06292>

4.5 Syxplain

Application: Web app: <https://syxplain.ai1science.net/>

Please see the attached descriptions for further details.

5. OpenAI API Key Registration

A pinned message in your team's channel will contain an API key for accessing OpenAI's models. See Section 3, Messaging Platform.

If you have any issues with your API Key, please contact us in the Discord tech-help-desk channel.

6. ADP Registration

Follow these steps to create your account and access the platform:

- Visit the Portal:** Go to ai-scientist.ai1science.net.
- Access the Sign-Up Page:** On the login screen, click the link that says "**Don't have an account? Sign up!**"
- Enter Your Details:** Provide a valid email address and create a secure password, then click **Sign Up**.
- Verify Your Email:** Check your inbox for a verification email from **Supabase**. Click the confirmation link within the email to activate your account.
- Log In:** Once verified, return to the login page and sign in with your new credentials.

Welcome to AI Scientist!

Please sign in to continue...

Username/E-mail

Password

Sign In

Don't have an account? [Sign up!](#)



7. Tools & Quick Tutorials

7.1 OpenAI

<https://platform.openai.com/docs/quickstart>

7.2 LangChain

<https://academy.langchain.com/courses/langchain-essentials-python>

7.3 n8n

From basics: https://youtu.be/ZHH3sr234zY?si=Fj8Xa_begAoCI9yJ

AI agents inspiration playlist (business):

<https://youtube.com/playlist?list=PLvQWpZ46MVvgUUUBxnqLAu-JzA-6QA1o2&si=R9QANd8PJI-6n7aK>

7.4 Syxplain

<https://peertube.ai.kinin.hu/w/k3K2CD64SXa8AeL2QtvFzB>

7.5 Agentic Discovery Platform

<https://peertube.ai.kinin.hu/w/o2rSh6vMG8ngurai8SGewp>

7.6 Dataverse

<https://peertube.ai.kinin.hu/w/okdscUM1ZANuyb1VGajmk3>

8. Selected Articles

8.1 AI Scientists

- [1] F. Villaescusa-Navarro et al., “The Denario project: Deep knowledge AI agents for scientific discovery,” Oct. 30, 2025, arXiv: arXiv:2510.26887. doi: 10.48550/arXiv.2510.26887.
- [2] C. Lu, C. Lu, R. T. Lange, J. Foerster, J. Clune, and D. Ha, “The AI Scientist: Towards Fully Automated Open-Ended Scientific Discovery,” Sep. 01, 2024, arXiv: arXiv:2408.06292. doi: 10.48550/arXiv.2408.06292.
- [3] Y. Yamada et al., “The AI Scientist-v2: Workshop-Level Automated Scientific Discovery via Agentic Tree Search,” Apr. 10, 2025, arXiv: arXiv:2504.08066. doi: 10.48550/arXiv.2504.08066.
- [4] S. Guo et al., “IdeaBench: Benchmarking Large Language Models for Research Idea Generation,” in Proceedings of the 31st ACM SIGKDD Conference on Knowledge Discovery and Data Mining V.2, in KDD ’25. New York, NY, USA: Association for Computing Machinery, Aug. 2025, pp. 5888–5899. doi: 10.1145/3711896.3737419.
- [5] G. Tie, P. Zhou, and L. Sun, “A Survey of AI Scientists,” Nov. 11, 2025, arXiv: arXiv:2510.23045. doi: 10.48550/arXiv.2510.23045.
- [6] D. Saeedi, D. Buckner, J. C. Aponte, and A. Aghazadeh, “AstroAgents: A Multi-Agent AI for Hypothesis Generation from Mass Spectrometry Data,” arXiv.org. Accessed: Nov. 24, 2025. [Online]. Available: <https://arxiv.org/abs/2503.23170v1>
- [7] S. Schmidgall et al., “Agent Laboratory: Using LLM Agents as Research Assistants,” arXiv.org. Accessed: Nov. 24, 2025. [Online]. Available: <https://arxiv.org/abs/2501.04227v2>



[8] T. Zheng et al., "From Automation to Autonomy: A Survey on Large Language Models in Scientific Discovery," Sep. 17, 2025, arXiv: arXiv:2505.13259. doi: 10.48550/arXiv.2505.13259.

8.2 Agentic Discovery Benchmarks

[1] K. Gandhi et al., "BoxingGym: Benchmarking Progress in Automated Experimental Design and Model Discovery," Oct. 14, 2025, arXiv: arXiv:2501.01540. doi: 10.48550/arXiv.2501.01540.

[2] P. Jansen et al., "DISCOVERYWORLD: A Virtual Environment for Developing and Evaluating Automated Scientific Discovery Agents," Oct. 07, 2024, arXiv: arXiv:2406.06769. doi: 10.48550/arXiv.2406.06769.

[3] J. Shi et al., "KORGym: A Dynamic Game Platform for LLM Reasoning Evaluation," May 21, 2025, arXiv: arXiv:2505.14552. doi: 10.48550/arXiv.2505.14552.

[4] T. Zheng et al., "NewtonBench: Benchmarking Generalizable Scientific Law Discovery in LLM Agents," Dec. 09, 2025, arXiv: arXiv:2510.07172. doi: 10.48550/arXiv.2510.07172.

[5] Y. Chen, P. Piękos, M. Ostaszewski, F. Laakom, and J. Schmidhuber, "PhysGym: Benchmarking LLMs in Interactive Physics Discovery with Controlled Priors," Oct. 26, 2025, arXiv: arXiv:2507.15550. doi: 10.48550/arXiv.2507.15550.

[6] B. P. Majumder et al., "DiscoveryBench: Towards Data-Driven Discovery with Large Language Models," Jul. 01, 2024, arXiv: arXiv:2407.01725. doi: 10.48550/arXiv.2407.01725.