

General AI assistants

- ChatGPT (OpenAI)
- Gemini (Google)
- Claude (Anthropic)
- Local/open-source models, e.g., Llama/Deepseek, if you are willing to self-host.

All the LLMs above have pros and cons, but what is clear is that today LLMs are *ubiquitous* in science.

Coding agents

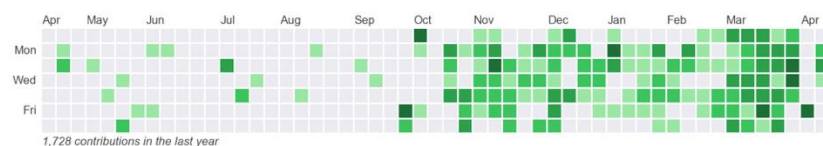
- Codex – OpenAI's agent for editing code
- Claude code – Claude's coding assistant
- Code wiki – Google's LLM for generating documentation

TIP: **When using AI agents, keep track of the context window utilised!**

All tools above should not be a substitute for scientific knowledge and understanding. LLMs are stochastic next-token predictors and often hallucinate.^[1]

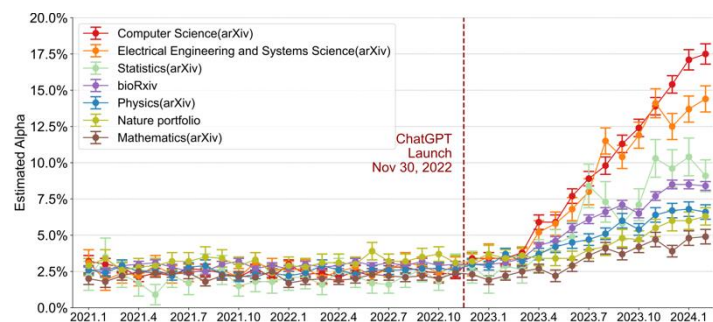
“Used well, agentic coding tools migrate legacy Fortran build systems, write numerically validated simulation code, and maintain CI across multi-language stacks. Used badly, they hallucinate plausible nonsense at scale.”^[2]

GitHub contribution heatmap (jameskermode · Apr 2025 – Apr 2026)



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[1] Huang *et al.*: *ACM Trans. Inf. Syst.* **2025**, 43, 1-55.
[2] <https://github.com/jameskermode/agentic-coding-seminar>.



Estimated fraction of LLM-modified sentences across academic writing venues over time. Reprinted from Liang *et al.*: arXiv 2024, preprint arXiv:2404.01268 under a CC-BY-NC-ND 4.0 license.

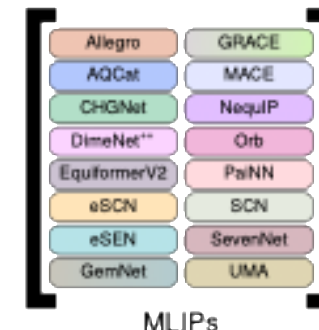
Literature summary and illustrations

- Google Scholar labs – alternative to google scholar for finding papers
- Mathpix – converts equations, tables, and PDFs into LaTeX code
- Paperbanana – Google's AI agent to create scientific illustrations

Machine-learned interatomic potentials

- MACE, UMA, GAP, ORB, etc.
- For a more comprehensive list, see Ref. [3].

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Materials generation

- MatterGen [4] – “*model that generates stable, diverse inorganic materials across the periodic table and can further be fine-tuned to steer the generation towards a broad range of property constraints.*”
- CrystalLLM [5] – “*a methodology for the versatile generation of crystal structures, based on the autoregressive large language modeling (LLM) of the Crystallographic Information File (CIF) format.*”

Chemistry LLMs

- ChemCrow [6] – LLM for Chemistry based on GPT4.
- El Agente [7] – LLM-based tools for generating computational chemistry files and analysing results.

*****Presence of the tool on this page does not mean endorsement!*****

[3] Jacobs *et al.*: *Curr. Opin. Solid State Mater. Sci.* **2025**, 35, 101214.
[4] Zeni *et al.*: *Nature* **2025**, 639, 624-632.
[5] Antunes *et al.*: *Nat. Commun.* **2024**, 15, 10570.
[6] Bran *et al.*: *Nat. Mach. Intel.* **2024**, 6, 525-535.
[7] Zou *et al.*: *Matter* **2025**, 8, 102263.