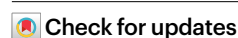


SciSciGPT: advancing human–AI collaboration in the science of science

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We introduce SciSciGPT, an open-source, prototype artificial intelligence (AI) collaborator that uses the domain of science of science as a testbed to explore the potential of large language model-powered research tools. SciSciGPT automates complex workflows, supports diverse analytical approaches, accelerates research prototyping and iteration and facilitates reproducibility. Through case studies, we demonstrate its ability to streamline a wide range of empirical and analytical research tasks while highlighting its broader potential to advance research. We further propose a large language model agent capability maturity model for human–AI collaboration, envisioning a roadmap to further improve and expand upon frameworks such as SciSciGPT. As AI capabilities continue to evolve, frameworks such as SciSciGPT may play increasingly pivotal roles in scientific research and discovery. At the same time, these new advances also raise critical challenges, from ensuring transparency and ethical use to balancing human and AI contributions. Addressing these issues may shape the future of scientific inquiry and inform how we train the next generation of scientists to thrive in an increasingly AI-integrated research ecosystem.

Scientific advances are foundational to improving quality of life, driving global health outcomes and fostering growth and prosperity^{1–6}. Understanding the mechanisms underlying these advances is critical for shaping effective science policies and empowering scientists to address high-risk and high-impact questions. The field of the science of science (SciSci) has emerged to tackle this challenge^{1,7,8}, leveraging interdisciplinary approaches to explore how science is conducted, funded and applied. SciSci has seen rapid growth, partly fueled by the increasing availability of large-scale datasets that capture a wide array of activities in science and innovation^{9–17}, from the inner workings of science to its upstream investments and downstream societal impacts. These advances mirror broader progress in computational social science¹⁸, where increasingly sophisticated datasets and computational methods are enabling researchers to analyze complex systems of human behavior, dynamics and interactions.

However, the very advances in data and tools that make this research possible also introduce substantial technical challenges.

The growing scale and complexity of datasets, coupled with the rapid evolution of computational methods, create barriers to entry for researchers and demand extensive technical expertise. At the same time that science is becoming more complex, individual expertise is becoming more narrowly focused, leading to an increase in specialization^{19–21}. Together, these challenges highlight the need for new approaches to help researchers efficiently navigate, analyze and derive insights from these rich data sources²².

Recent advances in large language models (LLMs) and artificial intelligence (AI) agents have opened new possibilities for advancing human–AI collaboration^{23–25}, offering potential tools to navigate the complex and rapidly evolving research landscape. Recent studies show that LLMs are increasingly adept at performing high-level cognitive tasks, including in-context learning²⁶, complex reasoning^{27,28}, planning, tool usage^{29,30} and coding^{31–34}. Researchers have begun harnessing these capabilities, using LLMs as central controllers in autonomous task-executing LLM agents across various domains,

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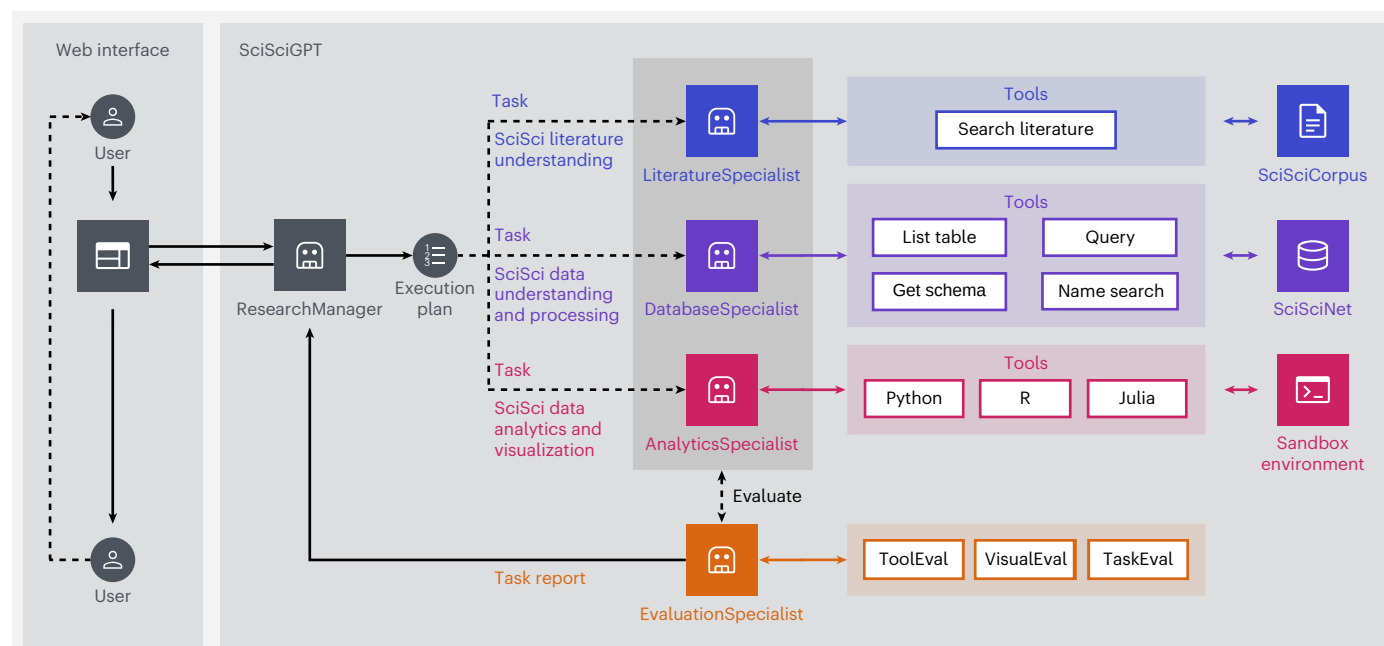


Fig. 1 | SciSciGPT system architecture. A diagram illustrating the modular design of SciSciGPT, an AI collaborator for SciSci. Users submit requests through a web chat interface to the ResearchManager agent, which breaks user requirements down into tasks and delegates them to the appropriate specialist agents: LiteratureSpecialist, DatabaseSpecialist, AnalyticsSpecialist

and EvaluationSpecialist. These specialists provide assistance with literature understanding, data processing, data analytics, visualization, and quality assessment through their interactions with tools, data sources and sandbox environments. Each then returns its results to the ResearchManager to manage the workflow.

including retrieval-augmented generation (RAG)^{35,36} and automated data science^{37–40}.

These developments suggest the potential to leverage LLM agents for SciSci research. An effective LLM agent in this context would be able to understand the SciSci literature, the data available to use for research and the tools and methods for analysis and visualization. It would organize and execute progressive workflows for SciSci research questions, taking on the technical workload and supporting a low-code or no-code research process. If designed appropriately, such a system could substantially increase research efficiency, lower barriers to entering the field, facilitate reproducibility and support early-stage exploration and idea generation. Moreover, its capabilities and reach could expand further as LLMs continue to evolve.

In this Resource, we present our initial effort to explore LLM agents' potential in this realm, including developing SciSciGPT as a proof-of-concept AI collaborator for SciSci, under the guidance of a comprehensive LLM agent capability maturity model. SciSciGPT offers a chat interface for public use that functions similarly to ChatGPT alongside a fully open-source implementation, ensuring transparency and enabling other researchers to reproduce and build on the work. Our framework incorporates a range of functionalities: retrieving pertinent SciSci publications on the basis of user inquiries, writing code to extract data from complex databases, conducting data analytics using advanced methods, creating visualizations of results and insights and evaluating its own analytical and visual outputs. By combining these capabilities into a seamless, AI-powered research workflow, SciSciGPT has the potential to lower technical barriers and enhance efficiency, enabling a new mode of human–AI collaboration in SciSci. Here, we offer an overview of SciSciGPT's architecture and assess its efficacy, including case studies that showcase SciSciGPT's ability to support and enhance research efforts.

It is important to emphasize that our intent is to develop SciSciGPT as a prototype. While its early results appear promising, SciSciGPT's performance and value are expected to grow with the advancement

of LLMs—particularly their complex reasoning abilities—and with ongoing refinements to the SciSciGPT framework. Furthermore, while this Resource focuses on SciSci as a testbed, SciSciGPT offers a generalizable framework for advancing human–AI collaboration across diverse fields. The open-source nature of SciSciGPT allows researchers to flexibly adapt and extend the tool to meet their specific needs. With appropriate adjustments and the integration of domain-specific knowledge, SciSciGPT could be applied to other scientific domains, in particular in data-intensive domains and disciplines traditionally less reliant on computational methods, which may enable more interdisciplinary research and collaborations.

To this end, we further propose an LLM agent capability maturity model to envision a roadmap for developing AI research collaborators, which encompasses four key maturity levels: functional capabilities, workflow orchestration, memory architecture and human–AI collaborative paradigms. As a proof of concept of the capability maturity model, SciSciGPT embodies several key features from the model, and the proposed maturity model provides a framework to guide further developments and extensions, offering a strong foundation for agentic AI system development across broad research environments.

Results

System overview

SciSciGPT is a multi-agent AI system designed to serve as a research collaborator for SciSci researchers and practitioners. Drawing inspiration from the core research tasks of domain researchers, SciSciGPT comprises five specialized modules, each focusing on a distinct component of the research workflow (see Fig. 1 for an overview of the system architecture):

- The ResearchManager agent functions as a project leader and central coordinator. It orchestrates the research workflow, breaking complex research questions down into tasks and assigning them to the four specialist agents listed below.

- The LiteratureSpecialist agent focuses on comprehension and synthesis, searching for and organizing relevant information from the SciSci literature.
- The DatabaseSpecialist agent handles data processing tasks, managing complex data extraction, transformation and basic statistics across scholarly databases. This agent is equipped to interact with a comprehensive scholarly data repository.
- The AnalyticsSpecialist agent focuses on statistical analysis and modeling, implementing empirical methods and analytical techniques and generating visualizations to support empirical investigations.
- The EvaluationSpecialist agent assesses the quality, relevance and rigor of SciSciGPT's analyses, visualizations and methodological choices, allowing the system to identify potential improvements and adjust its approach iteratively.

When the ResearchManager receives a research question, it formulates an execution plan, assigning tasks to appropriate specialists. Each specialist agent formulates subplans, invokes tool use and engages in iterative reasoning until the task is completed. As each plan is executed, the EvaluationSpecialist is invoked to assess progress across multiple levels, guiding the specialist's next step. After the specialist finishes each task, control returns to the ResearchManager for subsequent task allocation and execution. This hierarchical structure supports flexible task decomposition and delegation for any user question, enabling SciSci researchers to interact seamlessly with the system through conversation, refine their research questions and explore different approaches as needed. This conversational, multi-agent architecture enables domain-specific functionalities while maintaining the original LLM's general capabilities, such as instruction following, question-answering and common-sense reasoning. Figure 2 illustrates the workflows of the four specialist agents, with details described in 'Multi-agent AI system' section in the Methods.

It is important to note that the specific datasets, literature sources and empirical toolkits currently implemented for each specialist are not fixed. Rather, they represent one instantiation of a flexible framework that can be adapted or extended as data sources evolve, new methods emerge or user needs change. In this sense, SciSciGPT should be understood not as a static offering but as a configurable foundation for developing domain-specific AI collaborators that can continually integrate new data and techniques.

Case studies

To illustrate the functionality and value of this multi-agent system, we present two case studies that showcase how researchers can leverage this tool in real-world scenarios. These examples highlight the interaction between the user and the system, the workflow, the methodological approach and the tangible outcomes that SciSciGPT produces.

Case study 1. The first case study considers a collaboration network among Ivy League universities (refer to Supplementary Data 1 for the full chat history for this case study).

Imagine the following research question: What does scientific collaboration look like among Ivy League universities? This question might be asked by a SciSci researcher who studies scientific collaboration and teamwork, an increasingly important area in the field. Research shows that great breakthroughs today rarely stem from lone geniuses; rather, they disproportionately emerge from collaborative efforts that often transcend institutional or geographic boundaries^{1,7,8,41}. This question could also be asked by a practitioner, such as an institutional leader who is interested in quantitative answers to the question that could inform efforts to foster more strategic partnerships.

To answer the question using conventional approaches, the researcher would need to consider all papers published by each of the Ivy League universities, filter out papers that feature collaborations

between at least two of these universities and calculate the frequency of co-authorship for each pair of universities. As co-authorship analyses are often represented as networks, the researcher might also consider creating a visualization of the collaboration network among the eight universities. Each node would represent a university, and the links between them would denote the collaborative strength (that is, the number of papers that were co-authored by two universities). As part of this process, the researcher would need to identify the necessary datasets, write scripts to query the data and extract information, compute the measures of collaboration and apply network analysis tools for visualization, which requires specialized expertise in network science⁴². In total, this task could take a researcher hours to complete, depending on their experience and skill set.

To see SciSciGPT tackle this task, we gave it the following prompt, as shown in Fig. 3a: 'Generate a network for collaborations among Ivy League Universities between 2000 and 2020. Optimize colors and annotations'.

The workflow began with the ResearchManager, which identified key requirements for the request, including data acquisition, network construction and visualizations based on reasoning through meta-prompting⁴³. The ResearchManager agent then broke down the input question into high-level tasks to delegate to other agents. First, it asked the DatabaseSpecialist to prepare a collaboration dataset with a specified data schema and provided a list of executable steps, including identifying pairs of Ivy League universities, filtering by publication time and cleaning and aggregating the data (see Fig. 3b and the chat history in Supplementary Data 1 for more details). In response, the DatabaseSpecialist executed this task in three steps: (1) it explored the database to identify relevant schemas and tables, (2) it used specialized tools that standardized the university names to ensure consistent institutional identification and (3) it wrote the structured query language (SQL) queries and queried the data through complex SQL operations with common table expressions. After conducting this data extraction procedure and structuring the data, the DatabaseSpecialist saved the extracted data to a temporary file.

As the DatabaseSpecialist moved through this process, the EvaluationSpecialist assessed the agent's performance after each step, giving it a score as well as suggestions for improvements. For example, the EvaluationSpecialist gave the first tool call a score of 0.8, which is high enough for the agent to continue to the next step. Once the DatabaseSpecialist completed the entire task, the EvaluationSpecialist performed a more systematic assessment of the specialist's workflow, providing an overall score and generating a detailed report that reviewed the delegated task, documented key methodological choices and challenges, and assessed the quality of its output. The EvaluationSpecialist then forwarded the complete workflow and assessment report to the ResearchManager.

After receiving the assessment report, the ResearchManager delegated the visualization task to the AnalyticsSpecialist, instructing it to use the extracted data and providing a list of actionable steps for loading the data, constructing and visualizing the network and optimizing the annotation and visual elements (Fig. 3c). The AnalyticsSpecialist then initiated a dynamic visualization workflow, using Pandas for data loading, NetworkX for graph construction and Matplotlib for creating the initial visualization. As with the DatabaseSpecialist's work, the EvaluationSpecialist provided a multimodal assessment of each step, with a caption, feedback, score and suggestions for improvements that the AnalyticsSpecialist could use to redo the visualization. After the first visualization attempt, for instance, the EvaluationSpecialist gave it a score of 0.75, indicating that a revision was needed, and suggested improvements to edge weights, labeling and annotations. The AnalyticsSpecialist used this iterative refinement and debugging process across multiple cycles to continuously enhance the figure, improving the size of elements, colorization, annotations, legends and other esthetic parameters. Figure 3d,e presents the AnalyticsSpecialist's

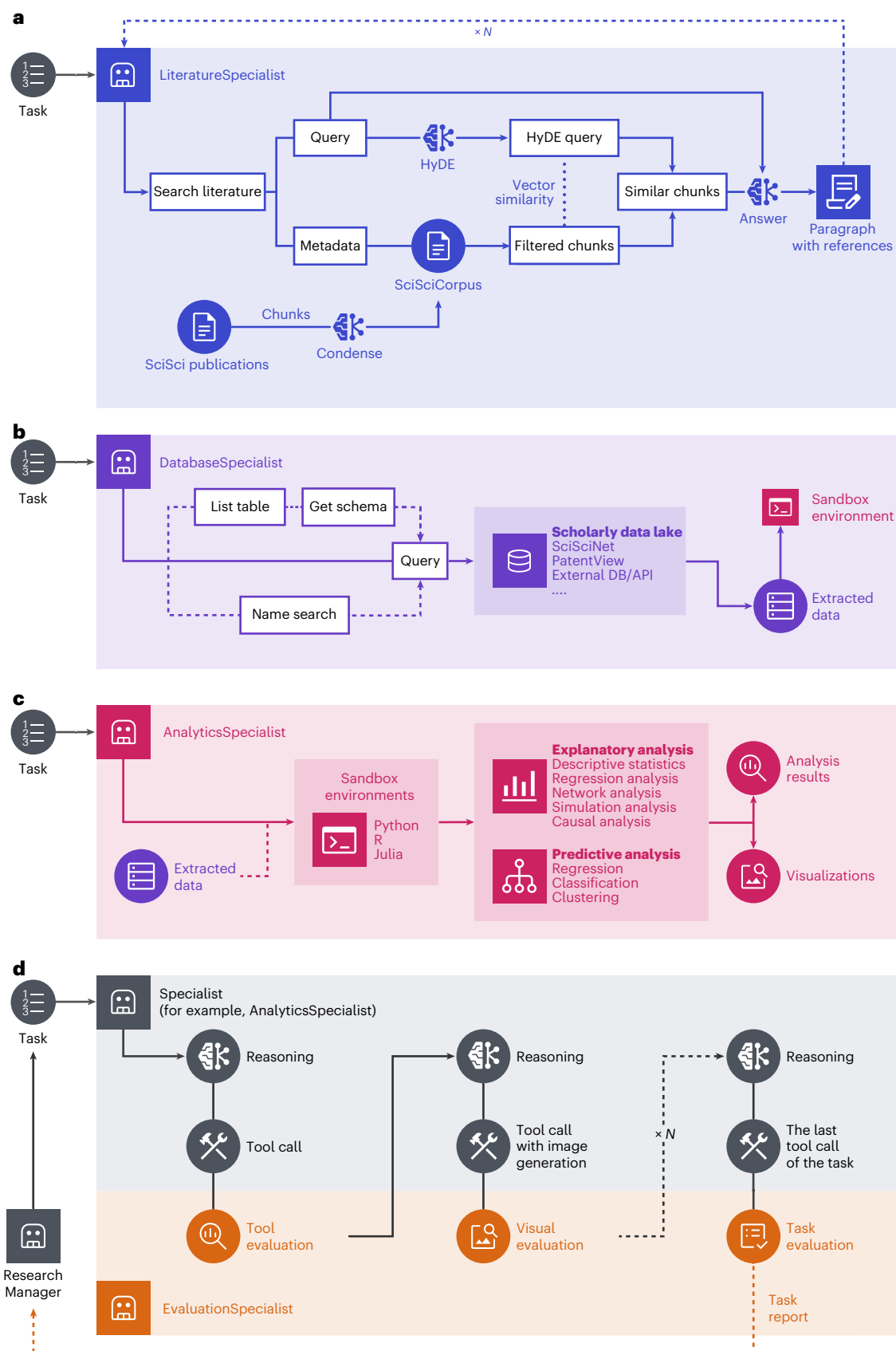


Fig. 2 | Detailed workflows of the four SciSciGPT specialist agents. a, The architecture of the LiteratureSpecialist agent for RAG in SciSci research. **b,** An example of the DatabaseSpecialist's workflow for data extraction. **c,** An example of the AnalyticsSpecialist's workflow for analysis and visualization. **d,** An example

of the EvaluationSpecialist's workflow for multilevel self-evaluation. The $\times N$ indicates that a given process or module could be repeated iteratively depending on the usage scenarios. 'Multi-agent AI system' section in the Methods describes the details and implementations of these workflows.

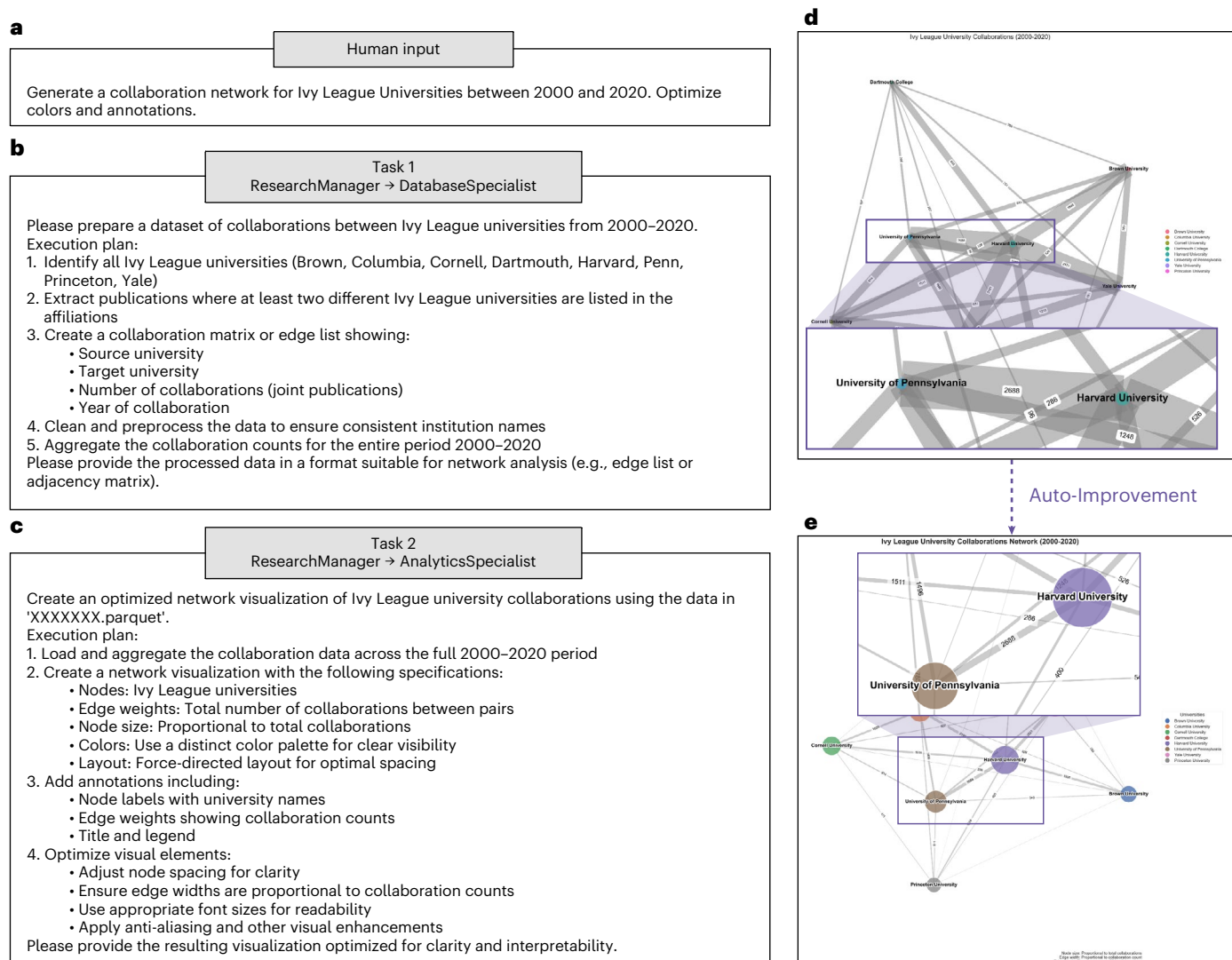


Fig. 3 | SciSciGPT's visualization of Ivy League university collaborations. **a–c**, In response to the human input (**a**), the ResearchManager decomposed the request and then delegated the data extraction task (**b**) and visualization task (**c**) to the DatabaseSpecialist and AnalyticsSpecialist, respectively.

d,e, The AnalyticsSpecialist created an initial visualization (**d**), and the system refined the figure through two rounds of improvements to generate a final visualization (**e**) with an enhanced color scheme, proportional node sizes and clearer text annotations. The zoomed window in **e** was added manually for clarity.

first visualization attempt and its output after two more iterations of this automated refinement process. As this last figure received a high score of 0.85 from the EvaluationSpecialist, the ResearchManager determined that no additional tasks were necessary and finalized the response, summarizing the workflow and synthesizing a final answer for the user.

In this case study, SciSciGPT successfully processed and visualized collaboration patterns among Ivy League universities, producing a network visualization that communicates both institutional productivity through node sizes and collaboration intensity through edge weights. The case study highlights not only SciSciGPT's automation of complex workflows but also its ability to execute quality checks and refine its results through iterative improvements.

Just as researchers using conventional data science methods often develop follow-up questions after considering their initial findings, researchers may have additional questions after examining SciSciGPT's output. In this case, for example, a researcher might be interested in a more in-depth exploration of the research fields involved in Ivy League collaborations, or they may be interested in writing an op-ed on university collaboration using these findings.

Supplementary Data 1 also presents SciSciGPT's responses to these follow-up questions.

Case study 2. This case study deals with multimodal replication of existing findings (refer to Supplementary Data 2 for the full chat history for this case study).

Now imagine another researcher who is reading a SciSci paper and is curious about the interpretation and replication of the findings. This scenario is typical for researchers at various career stages. For example, active researchers who want to build on a particular finding often begin by replicating key results, and junior researchers who are just entering the field frequently find that replicating the primary findings serves as a valuable learning exercise. More broadly, the growing emphasis on open science^{44,45} has made the replication of existing results and findings increasingly important.

In this case, imagine the researcher is reading the paper, 'Large teams develop and small teams disrupt science and technology'⁴⁶, and they are intrigued by its main finding, depicted in Fig. 2a in ref. 46. The figure shows that median citations increase with team size while the average disruption percentile decreases with team size. Recognizing

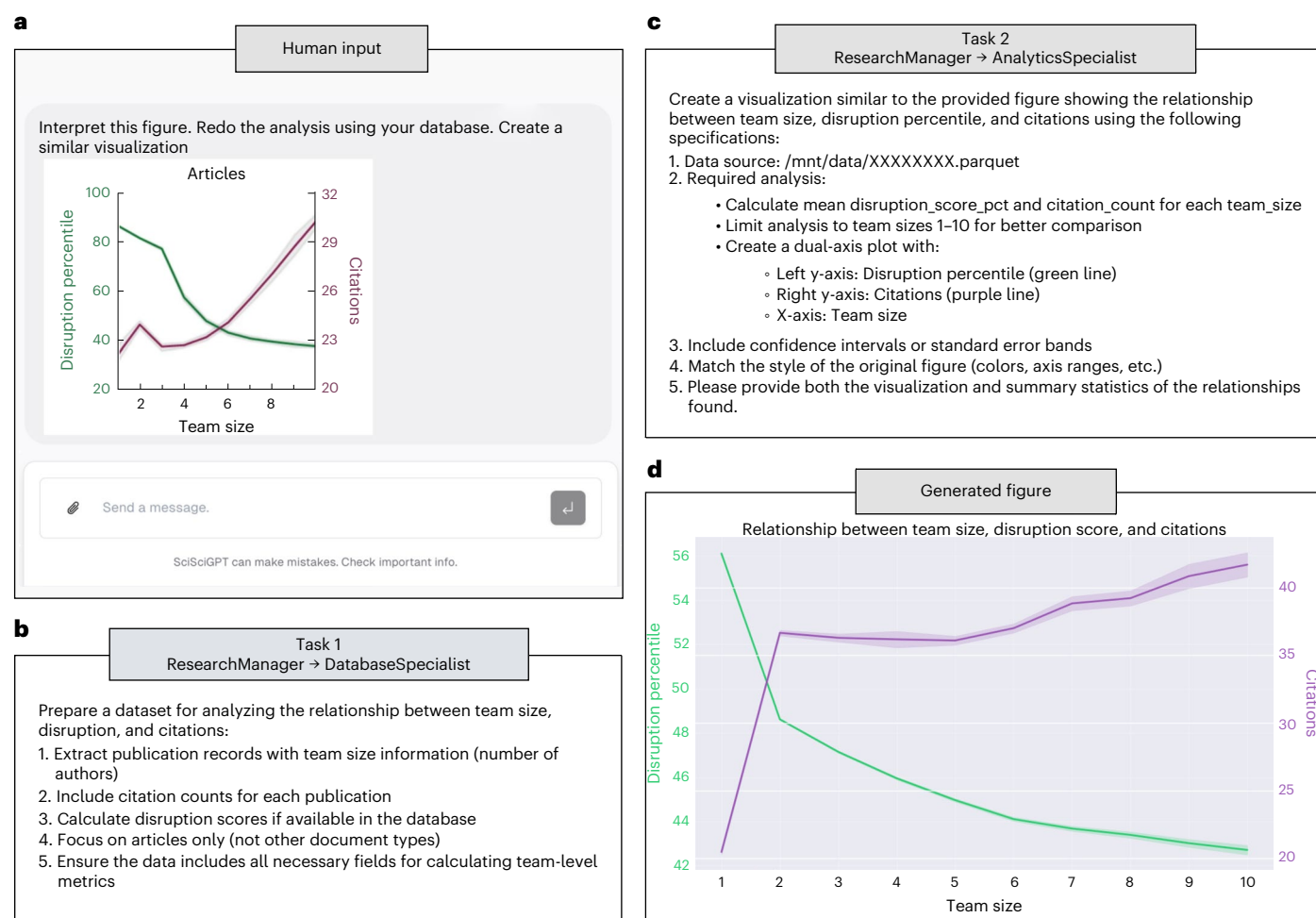


Fig. 4 | SciSciGPT's replication of a figure from a published paper. **a**, The user input includes Fig. 2a from ref. 46 and instructions to interpret the figure, redo the analysis and create a similar visualization. **b,c**, SciSciGPT broke the request down into tasks for the DatabaseSpecialist (**b**) and AnalyticsSpecialist (**c**). **d**, SciSciGPT's final output. Data are presented as mean values, while shaded regions denote 95% confidence intervals ($\text{mean} \pm 1.96 \times \text{s.e.m.}$). For each team size, statistics are derived from all papers in the dataset with that team size:

$n = 1,428,247$ (team size 1), 1,709,831 (2), 1,163,098 (3), 740,447 (4), 464,777 (5), 299,615 (6), 185,061 (7), 116,869 (8), 72,841 (9) and 48,745 (10) for disruption; $n = 2,866,780$ (team size 1), 2,186,114 (2), 1,468,295 (3), 944,649 (4), 601,335 (5), 392,733 (6), 245,204 (7), 156,611 (8), 98,716 (9) and 68,291 (10) for citations. While the exact data points in the two figures differ owing to variations in database timeframes and geographical coverage, SciSciGPT successfully replicated the trade-off between citation impact and disruption.

SciSciGPT's multimodal capabilities, we simply take a screenshot of the figure, upload it to SciSciGPT and give it the following prompt to instruct it to interpret and replicate the findings using data from its repository, as shown in Fig. 4a: 'Interpret this figure. Redo the analysis using your database. Create a similar visualization'.

After receiving the figure and replication request, SciSciGPT coordinated a systematic response. First, the ResearchManager examined the figure, assessing the technical elements (the dual-axis visualization), trend patterns and confidence intervals. It then broke down the user request into specific tasks and delegated the data extraction task to the DatabaseSpecialist (Fig. 4b).

The DatabaseSpecialist surveyed all available data tables and examined their schema. After mapping the database architecture, the DatabaseSpecialist crafted SQL queries to extract data from more than 9 million papers, including their citations, disruption percentile measures, team sizes and other relevant metrics, storing them in a temporary parquet file. After the EvaluationSpecialist assessed these steps, returning a high score of 0.95, the ResearchManager directed the AnalyticsSpecialist to recreate the dual-axis visualization (Fig. 4c).

The AnalyticsSpecialist responded by loading the parquet file from the DatabaseSpecialist and using it to calculate the average impact

by team size, with confidence intervals, and create the visualization (Fig. 4d). The EvaluationSpecialist systematically considered the data representation, visual design, scientific insight and technical execution. As the EvaluationSpecialist's rating met the threshold for continuation, the AnalyticsSpecialist proceeded to calculate additional statistics describing the relationship between team size, citation impact and disruption scores, including correlation coefficients and the percentage change. The ResearchManager then synthesized the final results of this analysis and visualization task for the user.

Here again, after receiving these results, a researcher may have various follow-up questions. A researcher may be interested in further examining the initial result using more advanced statistical methods. For example, they might consider using ordinary least squares (OLS) regression and propensity score matching to investigate whether the result still holds after controlling various confounding factors (Supplementary Data 2), or they may be interested in replicating the same visualization using SciSciGPT's data but calculating the impact metrics, such as disruption scores, from scratch during runtime rather than allowing SciSciGPT to use its predefined impact metrics from the SciSciNet database for computational simplification. In this case, the researcher can simply instruct SciSciGPT to compute the disruption

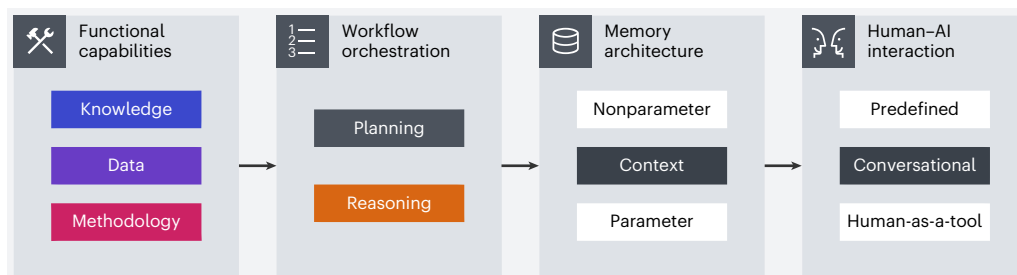


Fig. 5 | LLM agent capability maturity model. A four-level progression framework showing (1) functional capabilities, extending LLMs through specialized tools for knowledge access, data processing and methodology implementation; (2) workflow orchestration, implementing planning and reasoning mechanisms for complicated research tasks; (3) memory architecture,

maintaining information persistence, adaptation and customization throughout multiple interactions; (4) human-AI interaction, defining different modes of system engagement. Colored blocks highlight components implemented in SciSciGPT, balancing technical complexity with research effectiveness.

score, explaining the calculation using natural language (Supplementary Data 3).

Together, these case studies demonstrate how SciSciGPT's multi-agent framework orchestrates diverse functionalities, including understanding user requests, breaking down tasks into concrete steps, retrieving relevant data, analyzing data, creating visualizations, comprehending the literature, evaluating its performance and making iterative improvements.

LLM agent capability maturity model

While SciSciGPT focuses on SciSci as a testbed, its architecture design suggests broader applicability across data-intensive domains, especially those in computational social science. To better understand its generalizability, we propose an LLM agent capability maturity model, building on key concepts from system development^{47–49}, which allows us to formalize essential progression stages for AI research collaborators through a four-tiered developmental roadmap. This roadmap not only guides the current designs of SciSciGPT, which is a proof of concept for this capability maturity model, but also provides further pathways for enhancement.

We envision four progressive maturity levels that define increasingly sophisticated AI capabilities (see Supplementary Section 3 for details). At the first level, functional capabilities extend LLMs beyond text generation through specialized tools for domain knowledge access, data processing and statistical methods implementation. In SciSciGPT, these capabilities are fundamental elements of the specialized agents. At the second level, workflow orchestration introduces planning and reasoning mechanisms. In SciSciGPT, planning is exemplified by our ResearchManager specialists architecture, which decomposes tasks along modular research functions, analogous to different categories of domain research tasks. Reflective reasoning is enabled by meta-prompting and the EvaluationSpecialist. At the third maturity level, memory architecture maintains the overall information environment throughout the research processes, enabling agents to use previous interactions and histories to facilitate adaptation and customization on the basis of their specific needs. SciSciGPT implements selectively controlled prompt and context management to maintain focus and efficiency across progressive explorations. Finally, at the fourth level, human-AI interaction is made possible by the interactive components of the systems, facilitating progressive conversational research workflows.

As a proof of concept of this capability maturity model, SciSciGPT selectively implements core components at each level (highlighted as colored blocks in Fig. 5), while balancing implementation complexity against practical utility and prioritizing research effectiveness over maximum technical sophistication. As AI agents increase their capabilities and reach, the model presented in Fig. 5 may serve as a useful roadmap to facilitate more comprehensive human-AI collaborations.

Expert review

We conducted a preliminary assessment of SciSciGPT's effectiveness, efficiency and usability as an AI research collaborator through (1) an exploratory pilot study that compares its response time and accuracy to those of human researchers answering the same research questions and (2) semistructured interviews with SciSci experts after introducing them to the system.

Exploratory pilot study. We compared the performance of SciSciGPT with that of three domain researchers with different levels of expertise (predoctoral, doctoral and postdoctoral) to develop an initial assessment of the system's effectiveness and efficiency. The participants reported an average of 3.7 years of data science experience and 1.7 years of experience in SciSci research. We provided the participants with identical environments (datasets and Python/R coding platforms) and communicated the task by giving them the same inputs we gave to SciSciGPT. They were permitted to use all their standard research tools, including web resources, existing codebases, LLMs for coding and integrated development environment plugins, but they were not permitted to use SciSciGPT. Because participants completed the same research tasks in their preferred existing data science and coding environments (for instance, Claude 3.5, GPT-4o and ChatGPT-o1), this comparison is best understood as human researchers using general-purpose AI tools versus SciSciGPT, rather than simply human researchers versus SciSciGPT.

After the participants completed the tasks, we invited three postdoctoral researchers to review the participants' results and SciSciGPT's output, assessing each with a five-point scale (with higher scores indicating greater effectiveness) across five dimensions: effectiveness, technical soundness, analytical depth, visualization quality and documentation clarity.

Figure 6 presents the time to completion across all tasks for SciSciGPT and the human participants, as well as the postdoctoral reviewers' average ratings for each dimension of our research quality assessment. In this exploratory study, SciSciGPT accelerated the research process, completing the same tasks in about 10% of the average time required by experienced researchers in the field. Notably, all participants utilized LLMs to assist with coding tasks during the study, making this comparison particularly relevant for understanding SciSciGPT's contributions to modern research workflows. Results suggest that SciSciGPT completed tasks more efficiently, likely owing to its integration of multiple analytical steps, from data processing to analysis to visualization and iterative refinement.

More importantly, when evaluating the quality of work, the three expert evaluators found that SciSciGPT's output was stronger than the human researchers' work across various dimensions we examined. We acknowledge, however, that participants may have been operating under task completion constraints and that their results may not

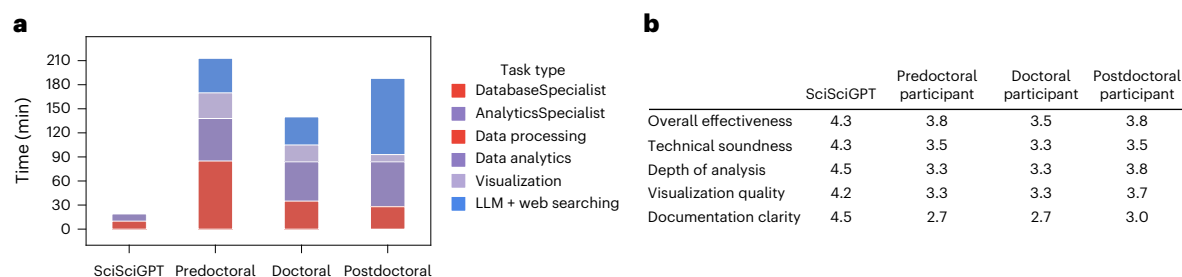


Fig. 6 | Exploratory research efficiency and effectiveness comparison. a, Time allocation across workflow components (data processing, analytics, visualization and LLM + web searching). **b,** Average postdoctoral evaluator workflow effectiveness rating on a five-point scale for each participant and SciSciGPT.

reflect their full capabilities, especially in unconstrained research settings with unlimited time for refinement. Moreover, we note that, given the limited sample size, these results should be interpreted as exploratory rather than offering generalizable insights. Nevertheless, these exploratory results suggest that SciSciGPT may outperform experienced researchers for tasks requiring a 2–3-h completion time, delivering better outcomes across multiple quality dimensions and in much less time.

As part of their review, evaluators noted that SciSciGPT produced excessively detailed documentation. On the one hand, this extended the evaluators' reading time and increased their cognitive load, potentially leading to a suboptimal user experience. On the other hand, the detailed documentation highlights a key advantage of human–AI collaborations enabled by systems such as SciSciGPT, where each step of the analysis is meticulously documented and can be revisited later or by other researchers as needed, substantially facilitating the reproducibility of research. Overall, the lengthy documentation underscores a trade-off between comprehensiveness and brevity and highlights the need for further refinement.

Semistructured interviews. In addition to the exploratory pilot study, we gathered qualitative insights about SciSciGPT from three expert SciSci researchers (E_A , E_B and E_C). We first conducted a 10-min walk-through of the system's architecture and core functionalities, and we then gave the experts 30 min for system exploration, during which they experimented with SciSciGPT and asked clarifying questions. Next, we conducted 60-min semistructured interviews using a standardized questionnaire (Supplementary Section 4.2). The interviews probed the experts' research practices, as well as their thoughts on SciSciGPT's database repository, the AI capabilities and the human–AI collaboration workflow it enables. All sessions were recorded and transcribed for analysis, with key findings summarized below.

We began by exploring the experts' current research processes to identify potential SciSciGPT integration points. All three reported using standard computational tools: Jupyter Notebook/RStudio with Pandas, literature search tools such as Google Scholar and Elicit and web-based coding assistance tools such as ChatGPT and Claude.

When discussing research challenges, experts consistently highlighted data management as a primary pain point, with E_C noting, "Loading large datasets is annoying. Also dealing with messy data." E_A expressed frustration with traditional data processing workflows, describing tasks such as "loading large CSV, TSV into memory" and data cleaning as time-consuming bottlenecks. Our experts estimated that the integrated SciSciNet dataset can be used to address the vast majority of SciSci research questions, highlighting the comprehensiveness of the data coverage. At the same time, they also suggested ways to further improve the data coverage, including expanding SciSciNet with additional public databases and enabling seamless integration of external and user-uploaded data.

All experts found SciSciGPT valuable for early-stage data exploration and prototyping. Experts agreed that the ResearchManager,

as the central controller of the multi-agent framework, effectively decomposed user questions into manageable tasks. E_A noted that the DatabaseSpecialist operates "faster than humans" with generally reliable results. The EvaluationSpecialist received particularly strong positive feedback for its visualization assessment capabilities, with E_B noting that it "spots problems" and "generates helpful suggestions about visualization clarity". The experts also commended the LiteratureSpecialist's ability to generate logical iterative workflows.

After engaging with the system, our experts also identified occasional failure cases. E_B found instances of database downsampling through unnecessary 'limit' clauses in BigQuery. They also observed coordination issues. For example, if the DatabaseSpecialist failed to collect necessary data, the AnalyticsSpecialist could produce unreliable outputs. E_C found that the AnalyticsSpecialist's analytical choices occasionally deviated from their personal preferences and field conventions. They also noted SciSciGPT's inability to implement advanced statistical models, such as exponential random graph models. These specific instances highlighted areas for future improvements.

All experts considered SciSciGPT's interactive features important, reporting that they particularly value the ability to ask follow-up questions, clarify intentions, explore topics in-depth and request more explanations of previous responses. However, the presentation of the system's research workflow documentation received mixed feedback. While all experts agreed on the necessity of complete workflow transparency, they diverged in the appropriate level of information granularity. E_A and E_C expressed concern that the system response could be overwhelming. For example, E_B explained, "Details are good, but maybe it's a little too much. But it's generally good. It would be better if it were collapsible and expandable". Overall, the experts recommended clearer differentiation between the types of information (for instance, content from specific agents or tools) and the levels of information. They suggested, for example, that the system could default to collapsing the detailed reasoning chain and code snippets for a more streamlined presentation.

Guided by this feedback, we designed a new function that allows the system to streamline the information display while preserving the underlying fine-grained logs necessary for reproducibility and transparency. The main idea is that, because SciSciGPT emits its internal state in extensible markup language with semantic tags, we can use this machine-readable structure to demonstrate information to the user selectively, automatically folding or hiding low-level details by default to reduce cognitive load while preserving transparency. This way, the newly designed interface allows collapsible toggles but does not discard any provenance; motivated readers can still access all the workflow information as needed. This design allows us to decouple audit sufficiency (which remains complete) from the information density shown to users (now adjustable).

Our experts also raised important concerns. "I feel uncomfortable trusting something not generated by myself. As a researcher, I'm responsible for all mistakes. Ultimately, it will be my name on the paper". They compared working with the AI collaborator to predoctoral

assistants; both require explicit guidance. While they appreciated SciSciGPT's greater transparency compared to human collaborators, they emphasized the substantial effort required to validate the system's results. Ultimately, trust appears to be an important factor in collaboration—whether it is with a human or AI.

Finally, we conducted a preliminary quantitative assessment by these three domain experts to review every intermediate output generated in the two case studies. After a brief walkthrough of the EvaluationSpecialist's logic, each expert rated the corresponding ToolEval, VisualEval and TaskEval on a five-point scale (from 1 for poor to 5 for excellent) and annotated points of disagreement or confusion. Across all assessments for the EvaluationSpecialist, the mean scores were 4.98 for ToolEval, 4.17 for VisualEval and 5.00 for TaskEval. According to the experts, ToolEval and TaskEval appear to consistently identify reasonable areas for improvement and assign credible scores. By contrast, VisualEval's relatively lower average seems to, at least in part, reflect the multimodality challenges commonly faced by LLMs. Overall, these results suggest that EvaluationSpecialist seems to align with expert judgment on textual capabilities; its VisualEval component shows comparatively less alignment, partly owing to multimodal LLM capabilities, which are currently less mature than textual capabilities, though they have been improving over time. Supplementary Section 4.3 provides more details about the experts' feedback regarding the EvaluationSpecialist.

While a broader evaluation is necessary to strengthen these findings, our preliminary assessments highlight SciSciGPT's ability to leverage multiple LLM functionalities to streamline SciSci research processes. At the same time, our expert reviews and evaluations also suggest several ways that SciSciGPT can be further enhanced, including (1) the adaptation of ongoing LLM advancements, such as large reasoning models and reinforcement learning-based post-training on related tasks, (2) architectural improvements that integrate enhanced RAG techniques and improve the documentation of methodological choices, (3) database module improvements that incorporate broader data sources and support user data imports and (4) interface refinements, including options to adjust the information granularity of implementation details and more flexible visualization options. Overall, our evaluations in this paper are exploratory by nature. While systematic evaluations of alignments are beyond the scope of this work, they represent an important area of future work, potentially as part of a broader exploration into automated research evaluation frameworks.

Discussion

Taken together, by automating technical workflows, SciSciGPT reduces research task completion time from hours to minutes, allowing researchers to focus on the creative and interpretive aspects of their work. This seems particularly beneficial in early-stage research, idea generation and verification processes. Beyond time savings, SciSciGPT lowers technical barriers to entry, broadening participation in the field by enabling those with basic domain knowledge but limited technical skills to explore data more effectively. The acceleration of research and broadening of participation have the potential to shift how researchers work and collaborate.

SciSciGPT is intentionally constructed upon the application programming interface of existing commercial LLMs (for instance, currently Anthropic Claude). As a wrapper, SciSciGPT directly inherits the powerful baseline capabilities and continual improvements of its underlying backbone model. Thus, SciSciGPT naturally performs what general-purpose chatbots such as ChatGPT can perform, including general question-answering, summarization, coding and reasoning. Additionally, our modular architecture, as well as the open-source nature, affords users the flexibility to incorporate new, improved models in the future, ensuring that SciSciGPT benefits directly from advances in the broader LLM ecosystem.

One key advantage of SciSciGPT is that it empowers human researchers at early, exploratory stages of the research process, rather than replacing their expertise or independently producing publication-ready outputs. Consequently, our case studies were deliberately chosen to represent typical early-stage explorations that researchers in the SciSci community frequently undertake. While these initial analyses may appear relatively simple, they illustrate how SciSciGPT supports rapid prototyping, iterative idea refinement and exploratory analyses—tasks that traditionally involve substantial manual effort and time. These iterative interactions also underscore a broader design challenge: effectively managing conversational context in extended, multiturn research workflows. Maintaining the right balance between retaining relevant history and adapting to evolving user goals is an active research frontier for LLM agents, and one we see as an important future direction, especially as models improve. Given the interdisciplinary nature of the SciSci community, researchers and practitioners vary widely in their technical backgrounds. By lowering technical barriers, SciSciGPT can further facilitate the participation of new entrants, broadening the range of ideas and expertise in the field.

While this paper focuses on the field of SciSci, the framework offered by SciSciGPT may extend to other computational disciplines. Indeed, the integration of data, research methods and literature is not unique to SciSci, but rather, with appropriate adjustments, such AI-powered research assistants may find wide applicability in other domains, especially those that are data-intensive or span multiple disciplines. Such systems could democratize access, enable more sophisticated analyses and empower researchers to address complex questions with greater efficiency and effectiveness. Indeed, adapting the designs and thinking behind SciSciGPT to other fields represents an important area for future work, which may require domain-specific adjustments to its specialist agents and underlying datasets, and the modular nature of the key components may further facilitate adaptation. Given its open-source nature, SciSciGPT also invites broader community-driven efforts to extend and customize the framework to suit various research domains and questions. By offering a framework for human–AI collaboration, SciSciGPT thus represents an initial step toward a broader vision of AI-assisted discovery, which may impact a range of computationally supported fields.

The continued relevance of SciSciGPT depends in part on the breadth and timeliness of its underlying data, suggesting that continuously incorporating new data as they become available represents a fruitful area of future research. For example, the newly released SciSciNet-v2⁵⁰ incorporates the latest 2025 OpenAlex snapshot with expanded data tables, additional fields and other refinements. While integrating the full-scale version would require further optimization to meet runtime constraints, the system's modular architecture is designed to facilitate such expansions. It is important to note, however, that even without continuous updates, SciSciGPT remains valuable, as much SciSci research relies on historical data and static datasets can retain substantial utility over extended periods. Moreover, SciSciGPT's open-source nature enables the research community to contribute updates, incorporate new data types and extend coverage, ensuring the framework can evolve through collective effort.

An important consideration for systems such as SciSciGPT is the stability of their outputs when faced with identical prompts. Current mainstream commercial LLMs do not guarantee identical outputs, even at zero temperature, and SciSciGPT naturally inherits this non-determinism from its backbone models. Additional variability can arise from the external tools it invokes, such as data processing pipelines, analytical routines and visualization algorithms. Thus, one might expect the multistep workflows to exhibit some inherent degree of run-to-run variation.

To this end, we performed some initial experiments assessing the run-to-run variability of SciSciGPT (Supplementary Section 2.6). Our experiments highlight the role of prompt specificity in shaping

workflow consistency and provide practical guidance for both users and future system design. These findings suggest that careful prompt engineering, explicit methodological specifications and deliberate workflow management can help minimize variability where precision is essential. At the same time, variability itself can have value: the differences we observe across repeated runs mirror the variability seen among human researchers given the same data and instructions⁵¹. Such variation can expose alternative analytical pathways and surface degrees of freedom in methodological choices that might otherwise remain hidden. This raises an intriguing possibility: whether research agents might be intentionally designed to first explore a broader solution space before iteratively converging toward a preferred approach. This perspective suggests that variability is not simply a limitation to be eliminated but also can be a feature to be strategically harnessed in the early, exploratory phases of research.

It is important to reckon with ethical considerations as AI plays a greater role in research and discovery. Automation of traditional research tasks such as data analysis increasingly blurs the distinction between human contributions and machine-generated work, which may challenge established norms around authorship and intellectual ownership. Widespread adoption of systems such as SciSciGPT could also have implications for early-career researchers and newcomers to the field and may hinder their ability to develop essential analytical skills, potentially leading to a research workforce less equipped to verify, challenge or refine AI-generated insights. Moreover, research^{52,53} reveals disparities in AI tool adoption across groups and fields, suggesting unequal access and adoption in the research community. Lastly, as AI systems continue to grow in relevance for researchers, the question is raised of whether such human–AI collaborations could shape the trajectory of the field, by influencing the questions that researchers prioritize and the methodologies considered valid. For example, if researchers tend to prioritize problems that align with the strengths of SciSciGPT, other crucial areas of inquiry that are less compatible with the use of such tools may be marginalized, potentially narrowing the scope and diversity of the field over time.

Given these considerations, the development and adoption of promising AI systems such as SciSciGPT demand careful and thoughtful approaches that preserve the human element in scientific discovery while leveraging AI to augment researchers' productivity. The human–machine partnership envisioned in SciSciGPT emphasizes the importance of complementing AI-driven analyses with human oversight and expertise. With time, the research community may develop guidelines and best practices to ensure accountability and maintain research integrity. By fostering a culture of transparency and collaboration, the research community can harness the potential of human–AI collaboration while mitigating its risks.

Methods

SciSciGPT architecture

SciSciGPT supports efficient data-driven insight extraction by integrating three modules:

- (1) A database repository, which includes (a) a scholarly data lake organized into a relational database and (b) a corpus of SciSci publications that we have chunked, embedded and organized into a vector database
- (2) A multi-agent AI system that serves as the core of the hierarchical multi-agent SciSci collaborator framework on which SciSciGPT is built (Fig. 1)
- (3) A web interface (<https://sciscigpt.com>) offering a user-friendly chat interface that enables users to collaborate with the AI system through multiturn conversations to generate insights, refine analyses and reach empirically validated conclusions

We describe the architecture in greater detail below.

Database repository

SciSciGPT's data infrastructure enables seamless interaction with scholarly data lakes to support data analysis. It is designed to build on comprehensive databases such as SciSciNet^{9,54} or OpenAlex¹⁰, open-source scholarly data lakes that encompass most of the data and linkages needed for SciSci research, and to integrate with SciSciCorpus, a curated database of literature in the field. SciSciGPT also maintains the ability to integrate with other data sources^{10,11,13,55}.

SciSciNet encompasses over 134 million scientific publications and millions of external linkages to funding sources and public uses. As such, it contains data capturing the essential elements of scientific research, including publications, authors, affiliations, upstream funding and downstream impacts. We use Google BigQuery, a cloud-based, high-performance relational database, to manage SciSciNet's inter-connected data tables. We implemented several refinements to the SciSciNet database to enhance its integration with SciSciGPT. First, since SciSciGPT is currently a prototype, we limited the data scope to papers published in the USA to optimize computational efficiency. Further, we structured the database into 19 tables to ensure that it accurately reflects the relationships between entities, and we wrote and incorporated descriptions that map tables and columns to established SciSci concepts to enable SciSciGPT to interpret the data. The resulting repository encompasses more than 11 million research papers, 78 million citation relationships and numerous other quantifiable metrics of scientific activity. Extended Data Fig. 1 presents the database architecture.

SciSciCorpus contains a corpus of publications as a vector database that the system uses to access prior knowledge in the field. To create SciSciCorpus, we assemble a collection of SciSci papers, download portable document format (PDF) files and employ GeneRation Of Bibliographic Data⁵⁶ to extract and parse the full text into natural paragraphs. We then used the OpenAI application programming interface (API) to generate two- to three-sentence summaries of each paragraph and classified each paragraph into one of a predefined set of categories, such as abstract, methodology, results and discussion. This taxonomic structure, while not necessarily aligned with the organization of the original document, provides a standardized framework for SciSciGPT's content navigation. Each paragraph is then projected into an embedding space and indexed into a vector database for effective RAG during runtime. Supplementary Section 1 contains more details regarding the processing procedures and schemas for these databases. Note that the inclusion of SciSciNet and SciSciCorpus serves as an initial framework, and given the open-source nature of SciSciGPT, users may adjust, replace or extend this corpus to align with their specific preferences and research use cases.

Multi-agent AI system

SciSciGPT includes a ResearchManager and four specialist agents (Fig. 2).

LiteratureSpecialist. Understanding and contextualizing research questions within the SciSci domain is critical for determining the novelty of the research question and ensuring efficient use of existing knowledge, including previous approaches to similar scientific questions, conclusions from prior studies and other researchers' assessments of the implications of their findings.

We designed the LiteratureSpecialist to facilitate literature understanding and contextualize SciSciGPT's workflow within the SciSci research domain using the 'literature_search' tool for RAG. Given a search query, the tool first filters papers using potential meta-data parameters identified by the LLM from the query (for instance, section=Abstract). It then employs hypothetical document embedding to generate multiple hypothetical paragraphs. It retrieves the top *K* similar chunks from SciSciCorpus using the text embedding similarity between the generated paragraphs and the corpus, identifies the most

relevant papers and summarizes the retrieved chunks into paragraphs with references in response to the search query. As a tool designed to support a multistep RAG workflow, the LLM typically dynamically and iteratively invokes it to focus on different levels of paper information. For example, it may first analyze abstracts and then progressively delve into other key sections (for instance, methodology, results and discussion) to deepen its understanding of the literature. Through this step-by-step process, the tool gradually generates a summary paragraph that synthesizes the current SciSci research relevant to the query, which is output to the user and stored in context memory to guide subsequent activities. Through RAG, LiteratureSpecialist not only provides SciSciGPT with domain knowledge but also ensures accurate and verifiable scholarly references (see Supplementary Data 4 for illustrative case studies).

DatabaseSpecialist. Understanding the complex data structure in the SciSci domain is essential for bridging abstract concepts and relationships in the research question to specific data. We designed the DatabaseSpecialist to comprehend the intricate SciSci data lake, extract relevant data and preprocess them through data cleaning and transformation. This agent incorporates a suite of specialized tools: (1) `sql_list_table` retrieves all available table-level descriptions, helping with database navigation, (2) `sql_get_schema` provides detailed structural information for specified tables, including column specifications, data formats and formatted sample rows, (3) `sql_query` executes the SQL queries generated by the agent, returning a preview of the fetched data frame (top k rows and column names) and a temporary file path for further use, and (4) `name_search` performs embedding-based similarity matching within a vector database to identify the most semantically relevant entities on the basis of the user's query. This tool is necessary because key entities in the SciSci field—such as scientific fields and research institutions—are often referred to by multiple names, making standardization crucial for accurate analysis. With these tools, the DatabaseSpecialist can comprehend both the delegated tasks and the SciSci data structure to extract relevant data segments for further analysis. Overall, this design enables SciSciGPT to navigate the scholarly data lake commonly used in SciSci research.

AnalyticsSpecialist. Once SciSciGPT has established an understanding of the relevant SciSci literature and the data lake, it needs to conduct the analysis and derive insights. As SciSci is an inherently multidisciplinary field, research in this area requires familiarity with a diverse range of computational methods, from basic statistical techniques (for instance, descriptive and regression analysis) to advanced modeling approaches (such as machine learning). Thus, we designed the AnalyticsSpecialist to implement appropriate methodologies, write and execute code to conduct the analysis and generate insights through text and visualizations that are tailored to the user's query. The agent integrates three open-source tools within isolated, stateful sandboxes to enable efficient code execution, debugging and refinement: (1) `python` offers extensive machine learning frameworks and general-purpose programming capabilities, (2) `R` provides robust statistical computing and visualization libraries and (3) `Julia` provides high-performance scientific computing capabilities with concise syntax. Together, these tools equip the agent with comprehensive analytics toolkits, allowing it to write and execute code and create new analyses.

EvaluationSpecialist. To ensure the quality and reliability of these AI-generated analyses, processes and findings, we designed the EvaluationSpecialist to conduct multilevel self-evaluations, which include tool evaluations, visual evaluations and task evaluations. The tool evaluation assesses each specialist's tool usage by analyzing the task context, including the task assigned by the ResearchManager, the workflow history, the tool parameters and the tool response. The visual evaluation assesses any visualization that is generated, typically by

the AnalyticsSpecialist. The EvaluationSpecialist examines the figure comprehensively, considering its alignment with the task, the data it uses and its adherence to visual design principles. The visual evaluation results in a list of suggestions for potential improvements that the specialist agent can use to refine the visualization. And the task evaluation analyzes the entire workflow after a specialist agent completes its task, and no more tool calls are created. The EvaluationSpecialist then provides a comprehensive execution report to the ResearchManager.

For each of these assessments, the EvaluationSpecialist assigns a reward score to guide the other agents' next steps. Depending on the score, SciSciGPT either continues with its current approach, makes minor adjustments or backtracks for major revisions. This multilevel self-evaluation mechanism ensures that SciSciGPT maintains quality control throughout complex research tasks.

Implementation

Meta-prompting for reasoning. SciSciGPT uses meta-prompting to facilitate the reasoning chain in slow-thinking LLMs^{57–59}, enhancing their ability to engage in deeper, more structured analytical processes. This approach incorporates two key functionalities: (1) structured reasoning, which guides logical step-by-step analysis, and (2) verbal reinforcement learning, which refines responses through iterative feedback and adaptation. Structured reasoning requires SciSciGPT to use a comprehensive tag taxonomy with predefined extensible markup language (XML)-style tags, such as `<thinking>`, `<step>`, `<reflection>`, `<answer>`, `<count>` and `<reward>`, which represent distinct cognitive stages in the LLM's reasoning process. These labels ensure that responses are organized into clear, logical and maintainable steps. By contrast, verbal reinforcement learning enables SciSciGPT to adjust its progress on the basis of the reward score it receives from the EvaluationSpecialist. We provide detailed meta-prompts for all agents in Supplementary Section 2.

Contextual memory management. Given SciSciGPT's extensive workflows, the multimodal input and output and the iterative feature for progressive research workflow, it must maintain focus and efficiency during iterative and resource-intensive multiturn literature retrieval or data-driven insight exploration. As long-context conversations pose substantial challenges to LLMs, SciSciGPT employs several mechanisms to compress the context, optimize prompt quality, minimize redundancy and improve computational efficiency^{60,61} by pruning content less relevant to ongoing reasoning: (1) The ResearchManager acts as the system's coordinator and maintains a complete record of all interactions with users and specialists. This comprehensive view allows it to track methodological choices, determine relevant prior context and provide specialists with precisely the right excerpts to facilitate coherent long-range reasoning. When delegating tasks, the ResearchManager controls the visibility of history to the specialist, selecting the relevant portions of the specialist's earlier dialog so it can build seamlessly on past computations. (2) Each specialist in SciSciGPT operates independently. A specialist's workflow begins with receiving tasks from the ResearchManager, proceeds through iterative reasoning and tool calling and concludes by returning results to the ResearchManager. Specialists cannot access another specialist's workflow or the interaction between the user and ResearchManager. (3) The `<thinking>` tag functions as a scratchpad for inner monologue, allowing agents to engage in detailed reasoning. This monologue remains invisible to other agents. Since the ResearchManager is designed to maintain a comprehensive awareness of all exchanges between users and specialists, this inner monologue is pruned for the ResearchManager. Using a compact context helps manage token limitations and shields the ResearchManager from unnecessary reasoning details. (4) Rather than presenting raw images of all generated figures in the context, SciSciGPT transforms the modality of all generated figures into a textual representation using

the capability of EvaluationSpecialist to output structured textual summaries of generated figures (that is, retaining the <evaluation> and <caption> outputs).

Web interface for collaborative research. As an AI collaborator, SciSciGPT behaves like a chatbot, building context from the sequential accumulation of messages generated by the user, agents and tools. SciSciGPT's conversational web interface is a standard chat interface, like ChatGPT, with account management, persistent history and multimodal support for text, code and visualizations. This design enables users to iteratively refine or expand their queries and explore insights through the back-and-forth interaction for scientific workflows. To further illustrate these human–AI interactions, we include a few examples and analyses in Supplementary Data 5, showcasing iterative clarifications and corrections and demonstrating SciSciGPT's human–AI collaborative process.

Related work

SciSciGPT builds on recent advances in LLMs that have shown noteworthy capacities for code generation^{31–34}, tool use and planning. Frameworks such as Toolformer²⁹ and ReAct³⁰, for example, have pioneered new ways to harness LLMs for tool usage, and various cutting-edge planning methodologies^{27,28,62} have showcased LLMs' ability to break tasks down into specific procedures.

SciSciGPT also benefits from advances in RAG, which enables LLMs to retrieve relevant external information in real time^{63,64}. This enhances the response accuracy by mitigating LLMs' tendency to hallucinate or generate incorrect information in specialized domains^{65–69} and by helping overcome limitations imposed by knowledge cutoffs that create gaps in their understanding⁷⁰. First introduced by Lewis et al.⁷¹, RAG has evolved from early frameworks such as ReAct³⁰ and MRKL⁷² to more sophisticated approaches, including Self-Ask⁷³, SELF-RAG⁷⁴ and PaperQA^{35,36}, enabling systems to handle complex queries with multistep reasoning and fact verification. Further innovations, such as hypothetical document embedding⁷⁵ and Chain-of-Note⁷⁶, enhance retrieval accuracy and information integration.

Researchers have leveraged these developments to create autonomous LLM data agents—integrated systems that combine code generation, tool use, planning and RAG to orchestrate tasks in a wide range of fields. In the data science domain, two primary types of LLM-based agents are particularly relevant:

- (1) Code-writing agents are designed specifically for code writing tasks⁷⁷, autonomizing the generation of code for data science projects. These frameworks include TaskWeaver⁷⁸, Data-Copilot⁷⁹ and DA-Agent³⁷, which enhance data analysis capabilities through python sandbox integration or enable database interaction and external knowledge extraction. DS-Agent³⁸ integrates LLM agents with case-based reasoning, leveraging Kaggle's expert knowledge for automated machine learning. LAMBDA⁴⁰ develops a multi-agent system with specialized programmer and inspector roles, while Data Interpreter³⁹ uses hierarchical graph modeling and programmable node generation to support a wide range of machine learning tasks.
- (2) Co-scientist pipelines in the data science field are multi-agent frameworks designed to emulate the research process. They follow specific procedures to generate ideas, write code, interpret results and generate reports. For instance, Lu et al.⁸⁰ developed an AI scientist for machine learning research, an AI system designed to automate the entire research process, from idea generation and experimentation to paper writing. Similarly, Schmidgall et al.⁸¹ introduced AgentLaboratory, a framework that simulates collaborative machine learning research by using LLM agents to automate tasks across the research pipeline, from idea generation to reporting.

While these models have demonstrated the capacity of LLMs to generate effective code and the usefulness of multi-agent systems for research tasks, these applications are often focused on machine learning tasks. They do not include custom data repositories that allow for the data insight exploration that SciSciGPT facilitates, and few have a self-reflection mechanism for iterative improvement. Moreover, these co-scientist pipelines are fully automated, whereas SciSciGPT is designed to be transparent and interactive. It is intentionally not fully automated, serving instead as a conversational AI collaborator that allows for iterative human–AI collaborations to explore and extract data-driven findings.

SciSciGPT is further distinguished by its focus on advancing research and discovery in a specific research domain, which requires an integrated understanding of the literature and relevant datasets, measurement approaches and empirical methods and toolkits. SciSciGPT uses the field of SciSci as a testbed. This multidisciplinary field offers a rapidly expanding evidence base and insights on science and innovation, leveraging rich sources of data and a range of computational tools. By infusing the agentic features of LLMs, including code generation, tool use, planning and reasoning, with domain-specific knowledge and expertise, including SciSci literature, datasets and empirical methods, SciSciGPT aims to offer a prototype of a new form of human–AI collaboration. From this perspective, SciSciGPT may be viewed as a mesolevel LLM-based research agent—neither too general nor too specific. It is capable of answering a range of research questions with greater depth than general agents while maintaining transparency in its methodology and offering domain-specific knowledge and toolkits that are tailored to the unique analytical needs of the domain researchers.

Reporting summary

Further information on research design is available in the Nature Portfolio Reporting Summary linked to this article.

Data availability

The original SciSciNet is available via Figshare at <https://doi.org/10.6084/m9.figshare.c.6076908.v1> (ref. 54). The variant of SciSciNet used in SciSciGPT is available via Hugging Face at <https://doi.org/10.57967/hf/6649> (ref. 82). SciSciCorpus is available via Hugging Face at <https://doi.org/10.57967/hf/6650> (ref. 83). Source data are available with this paper.

Code availability

The chat interface for public use is available at <https://sciscigpt.com>. A fully open-source implementation is available via GitHub at <https://github.com/Northwestern-CSSI/SciSciGPT> and via Zenodo at <https://doi.org/10.5281/zenodo.17271393> (ref. 84), ensuring full transparency and enabling other researchers to reproduce and build on the work.

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Author contributions

E.S., Y.W. and Y.Q. designed the methodology and conducted the investigation. E.S., Y.W. and Z.P. developed the software. D.W. conceived the study. D.W. administered the project. All authors contributed to writing, reviewed the paper critically for important intellectual content, and approved the final version for publication.

Ethics approval

The study protocol was reviewed and approved by the Institutional Review Board of Northwestern University (no. STU00223588).

Competing interests

The authors declare no competing interests.

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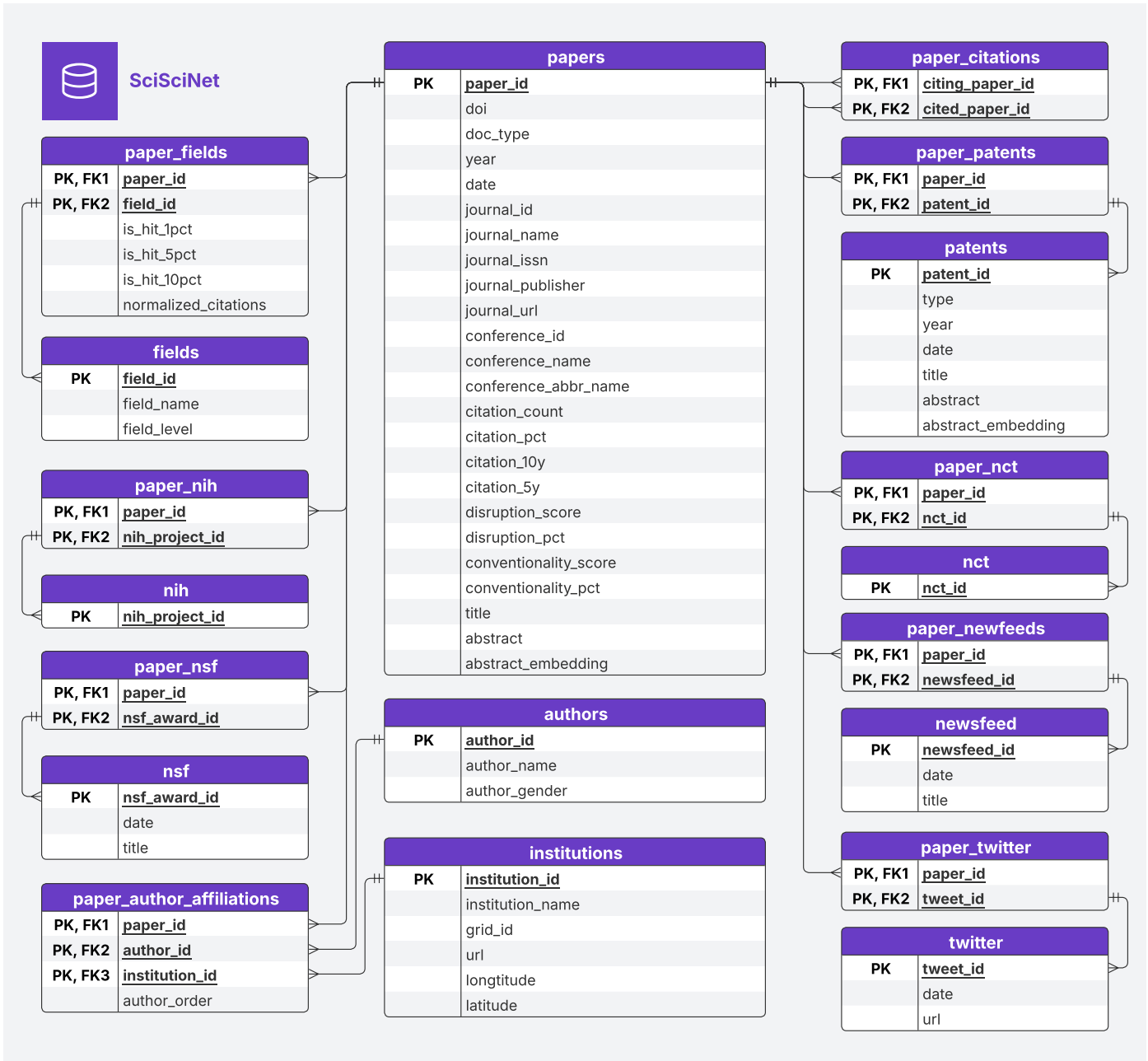
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Extended Data Fig. 1 | Schema diagram of the variant of SciSciNet used in SciSciGPT. SciSciGPT connects to this data lake, which serves as its primary repository of scholarly data. This version of SciSciNet features a refined schema and enhanced paper and patent data. This diagram shows the interconnections

between scientific papers and related entities. Each entity is identified by a primary key (PK), and their relationships are maintained through foreign key (FK) constraints.

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Data analysis	We used open source software for analytics and agentic orchestration. They rely primarily on cloud warehousing and LLM tooling, including langchain == 0.3.27, langgraph == 0.2.22, google-cloud-bigquery == 3.25.0, google-cloud-bigquery-storage == 2.33.1, google-cloud-storage == 2.19.0, SQLAlchemy == 2.0.31, sqlalchemy-bigquery == 1.11.0, langchain_openai == 0.2.0, langchain_google_vertexai == 2.0.28, pinecone-client == 5.0.1. Full dependencies and exact versions are available in the repository: https://github.com/Northwestern-CSSI/SciSciGPT

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Reporting on sex and gender	N/A
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Population characteristics	Six Science of Science researchers (one pre-doctoral, one doctoral, and four post-doctoral researchers).
Recruitment	Participants were recruited on the basis of their career stage and domain expertise for an exploratory pilot study. One pre-doctoral, one doctoral, and one post-doctoral researcher were invited to conduct an initial assessment of the system's effectiveness and efficiency. In addition, three postdoctoral researchers were invited to independently review the participants' results together with SciSciGPT's output.
Ethics oversight	The study protocol was reviewed and approved by the Institutional Review Board of Northwestern University (IRB No. STU00223588).

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Study description	In this paper, we introduce SciSciGPT, an opensource, prototype AI collaborator that uses the science of science as a testbed to explore the potential of LLM-powered research tools. SciSciGPT automates complex workflows, supports diverse analytical approaches, accelerates research prototyping and iteration, and facilitates reproducibility. Through case studies, we demonstrate its ability to streamline a wide range of empirical and analytical research tasks while highlighting its broader potential to advance research.
Research sample	We include only US papers from SciSciNet, which represent approximately 10% of the full dataset.
Sampling strategy	To down-sample the data and increase computational efficiency for demonstration purposes, we include only papers whose authors are all affiliated with US institutions, totaling 11 million out of 134 million papers in the full dataset.
Data collection	SciSciNet data is publicly available at: https://springernature.figshare.com/collections/SciSciNet_A_large-scale_open_data_lake_for_the_science_of_science_research/6076908/1
Timing	Raw datasets were downloaded in 2024.
Data exclusions	The analysis has no data exclusions.
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