

AMERICAN GEOSCIENCES INSTITUTE SHARON TAHIRKHELI, FORMER DIRECTOR SCHOLARLY INFORMATION

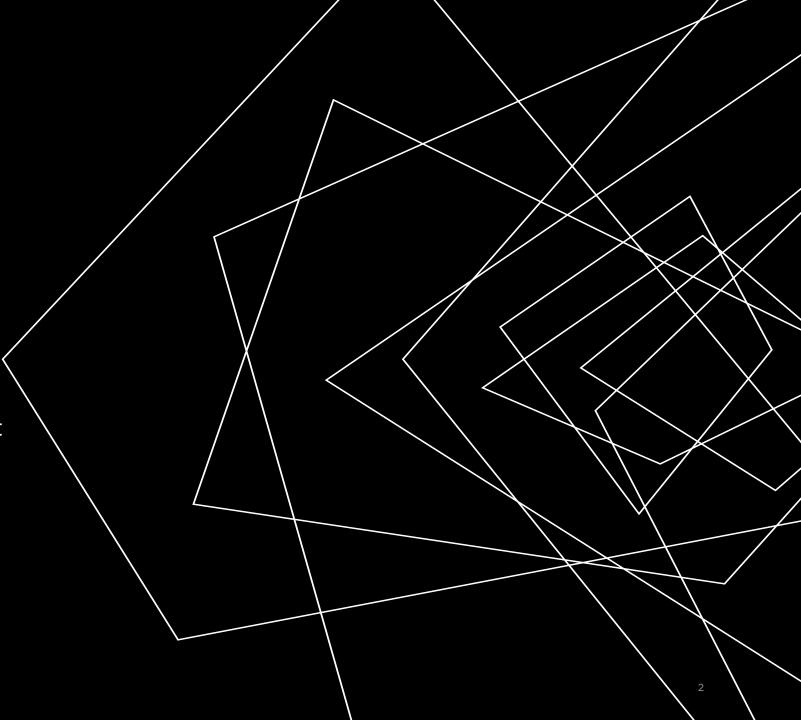


LLM & RAG Functions

Global Applications

Imperatives for Development

Next Steps





LLM (Large Language Models)

- Encoder Models Data condensing (classification)
- Decoder Models Data expansion (chat)
- Generates text in response to queries
- Requires large quantities of text for training
- Provides high impact with accurate instruct-model data prep
- Performs as well as the input language represents the logic and knowledge process of the domain
- Interprets language
- Are stochastic models predicting tokens
- Unable to return sourcing of information
- May be standalone

RAG (Retrieval-Augmented Generation)

- Pulls text passages based on a query to provide context to an LLM for processing the query
- Can provide citations for responses
- Dramatically lowers
 hallucinations when using a low
 temperature
- Requires hosting of original text;
 long-term data and rights
 management

GLOBAL APPLICATIONS OF PARTICULAR SIGNIFICANCE FOR THE SDGS

Foster global collaboration and communication

Accelerate science across language barriers

Improve science accessibility

Provide Education Opportunities

Generating learning materials

Provide explanations of scientific concepts

IMPERATIVES FOR DEVELOPMENT

Created with respect to the intellectual and legal rights of all parties

Transparency on data sources and methodologies employed in development

Based on unbiased, broad and deep data sources

Recognize critical limitations of knowledge domain between current open access/free data and rights-retained data

MOVING FORWARD

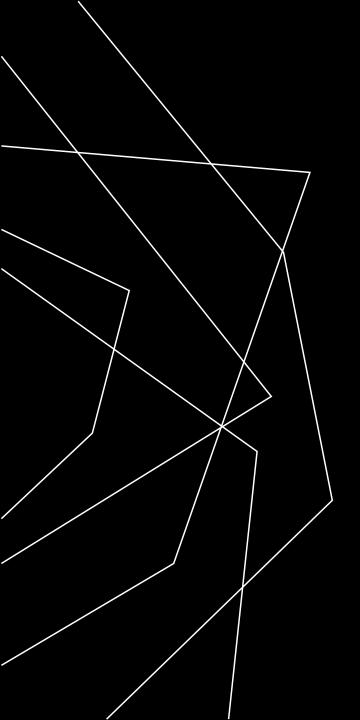
Review/ Governance Board

- Establish a Committee/Board with the ongoing responsibility to evaluate:
 - Data sources
 - Legal and intellectual property issues
 - Ethical considerations
- Mitigate conflicts of interest
- Engage the broad geoscience community

MOVING FORWARD

Tool Development from LLM/RAG

- Develop a domain-based embedding model for the geosciences community
 - Interoperability for myriad of use cases
- Ensure that such a tool can be captured and used without legal/ethical/rights concerns
- Focus on building trusted open source models that can be either centrally-hosted or run locally to democratize the science
 - e. g. Provide release pathways that include GGUF quantized versions



THANK YOU

Sharon Tahirkheli

On behalf of AGI (American

Geosciences Institute)

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GeoGPT: Current Status and Future Plan

GeoGPT Research Group

Outline of Presentation

1. Introduction:

- DDE introduction
- Brief overview of AI's evolution over the past decade.
- Discussion on how these advancements have set the stage for models like GeoGPT.

2. Al Transforming Scientific Research:

- Case studies demonstrating AI's impact on different scientific disciplines.
- Examination of how LLMs like GPT-4 facilitate scientific discovery.

3. GeoGPT: Vision and Architecture:

- In-depth look at the architecture of GeoGPT-0.5 and its foundational models.
- Explanation of the training stages.

4. Challenges and Suggestions:

- Discussion of the challenges of obtaining high-quality geoscience data and literature.
- Future plans for expanding GeoGPT's capabilities and collaboration opportunities.

5. Ethics and Data Governance:

- Insights into the ethical challenges and solutions in developing GeoGPT.
- Role and structure of the GeoGPT Data and Integrity Governance Committee.

6. Conclusion and Q&A:

Recap of the main points discussed. Open floor for questions and further discussions.

Deep-Time Digital Earth (DDE)

■ The first big science program recognized by IUGS in 2019



The International Union of Geological Sciences (IUGS) is an international non-governmental academic organization in the field of geological sciences, representing about 400,000 geoscientists worldwide, and is one of the largest and most active scientific societies in the world.

Deep-Time Digital Earth (DDE)



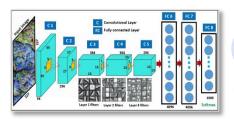
- DDE, through its Open Science Forum in November 2022, committed to the implementation of UNESCO Open Science Recommendation.
- DDE Mission: Harmonize Global Deep-time Earth Data And Share Global Geoscience Knowledge
- DDE Vision: To transform the Earth sciences by fostering a deep-time data-driven research paradigm.





Major Advancements in Al

AlexNet (Hinton, 2012)

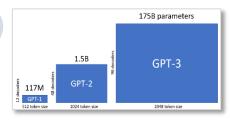


Generative Adversarial Nets (Bengio, 2014)

AlphaGo (DeepMind, 2015)



GPT-1/2/3 (OpenAI, 2018-2020)



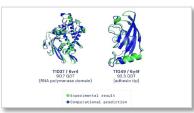
Bert (Google 2018)

Transformer (Google Brain, 2017)



DALL-E (OpenAI, 2021) Imagen (Google, 2022)

AlphaFold2 (DeepMind, 2021)



ChatGPT (OpenAl, 2022)

Claude3 (Anthropic, 2024.3)

Possesses powerful capabilities for inference and generalization, with a 200K-token context window.

Sora (OpenAI, 2024.2)

A landmark in text-to-video GenAl models, powered by Diffusion Transformer (DiT).

Gemini (Google, 2023.12)

A multimodal foundation model with a 32K-token context window; was upgraded to Gemini 1.5 in February 2024, with a context window limit of 1 million tokens.

GPT-4 (OpenAI, 2023.3)

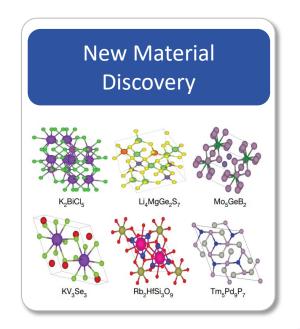
LLaMA (Meta, 2023.2&7)

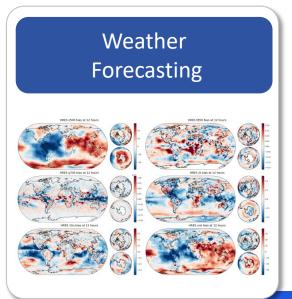
An open-source LLM that promoted the establishment of an open ecosystem for foundation models.

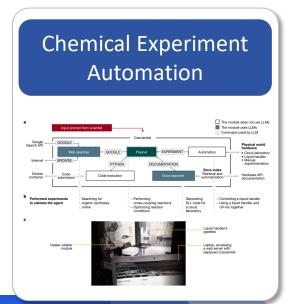


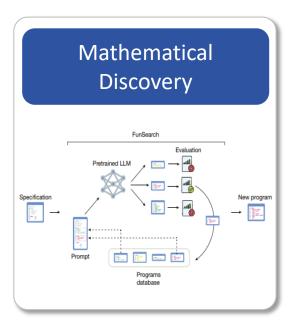


Al Transforms the Paradigm of Scientific Research





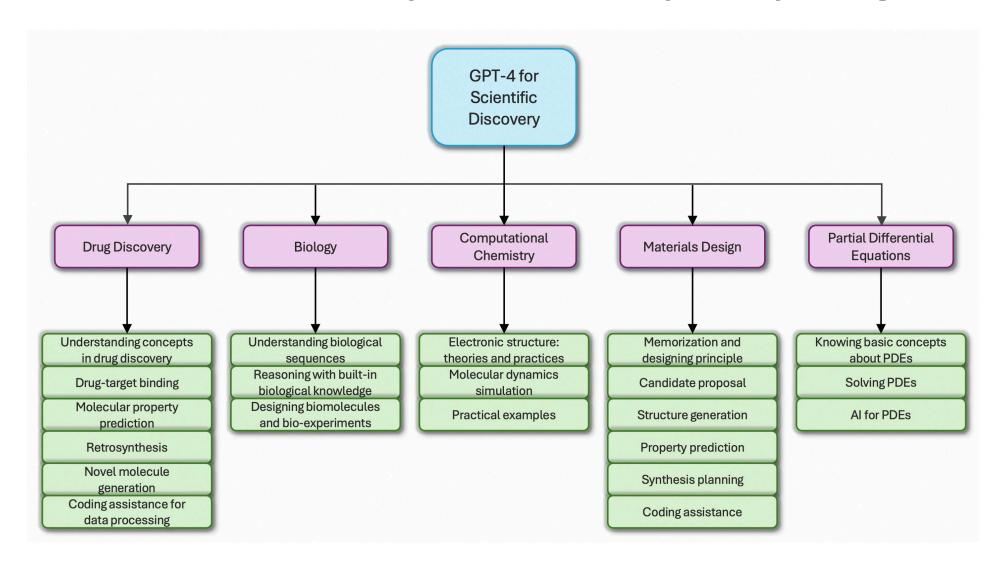




The rapid growth in data, algorithmic models, and computational power is driving a qualitative transformation in research paradigms

- [1] Merchant, A., Batzner, S., Schoenholz, S.S. et al. Scaling deep learning for materials discovery. Nature 624, 80–85 (2023).
- [2] Remi Lam et al., Learning skillful medium-range global weather forecasting. Science 382, 1416-1421 (2023)
- [3] Boiko, D.A., MacKnight, R., Kline, B. et al. Autonomous chemical research with large language models. Nature 624, 570–578 (2023).
- [4] Romera-Paredes, B., Barekatain, M., Novikov, A. et al. Mathematical discoveries from program search with large language models. Nature (2023).

LLMs on Scientific Discovery: a Preliminary Study using GPT-4



Microsoft Research Al4Science, Microsoft Azure Quantum. The Impact of Large Language Models on Scientific Discovery: a Preliminary Study using GPT-4, Nov 2023.

Key Capabilities of LLMs for Scientific Discovery

- Accessing and analyzing scientific literature. Can LLM suggest relevant research papers, extract key information, and summarize insights for researchers?
- Concept clarification. Is LLM capable of explaining and providing definitions for scientific terms, concepts, and principles, helping researchers better understand the subject matter?
- Data analysis. Can LLM process, analyze, and visualize large datasets from experiments, simulations, and field observations, and uncover non-obvious trends and relationships in complex data?
- Methodology guidance. Could LLM help researchers choose the right experimental/computational methods and statistical tests for their research by analyzing prior literature or running simulations on synthetic data?
- **Prediction**. Is LLM able to analyze prior experimental data to make predictions on new hypothetical scenarios and experiments (e.g., in-context few-shot learning), allowing for a focus on the most promising avenues?
- Code development. Could LLM assist in developing code for data analysis, simulations, and machine learning across a wide range of scientific applications by generating code from natural language descriptions or suggesting code snippets from a library of prior code?
- **Hypothesis generation**. By connecting disparate pieces of information across subfields, can LLM come up with novel hypotheses (e.g., compounds, proteins, materials, etc.) for researchers to test in their lab, expanding the scope of their research?

Microsoft Research Al4Science, Microsoft Azure Quantum. The Impact of Large Language Models on Scientific Discovery: a Preliminary Study using GPT-4, Nov 2023.



https://www.youtube.com/watch?v=sPiOP_CB54A

USA PCAST Backs Use of AI to Accelerate Scientific Research



- Artificial Intelligence (AI) has the potential to <u>revolutionize</u> our ability to address humanity's most urgent challenges by providing researchers with tools that will accelerate scientific discoveries and technological advances. Generative AI, which can create content based on vast data sets and extensive computation, is poised to be particularly transformative. With well-designed, equitably shared, and responsibly used infrastructure, AI will enable scientists to address urgent challenges.
- If basic AI resources, validated data, and scientific tools and training are made broadly accessible, AI technologies have the potential to <u>democratize scientific knowledge</u>, <u>bringing interconnected technical concepts to many more people</u> and <u>enabling diverse researchers</u> to bring their expertise and perspectives to societal and global challenges.
- Just as with any other new tool or technology, realizing the potentials of AI will require addressing its limitations. These issues include <u>misleading or incorrect results</u>, <u>perpetuation of bias or inequity and sampling errors</u> from patterns embedded in the model-training data, <u>limited access</u> to high quality training data, the challenges of <u>protecting intellectual property and privacy</u>, the <u>significant energy</u> required to train or deploy a model or run the AI algorithms, and the risk that bad or nefarious actors will use readily available AI tools for <u>malicious purposes</u>.

Challenges of Academic Research



Challenges

- Data Availability and Bias
- Computational Resources
- Model Complexity and Interpretability
- Interdisciplinary Collaboration
- Regulatory Compliance
- Politics and discrimination

Closed-source models

GPT-4o, Claude-3.5, Gemini......

Open-source models

LlaMa, Mixtral, Qwen.....

Critical to promote the open science concept of

collaboration, sharing, and co-construction

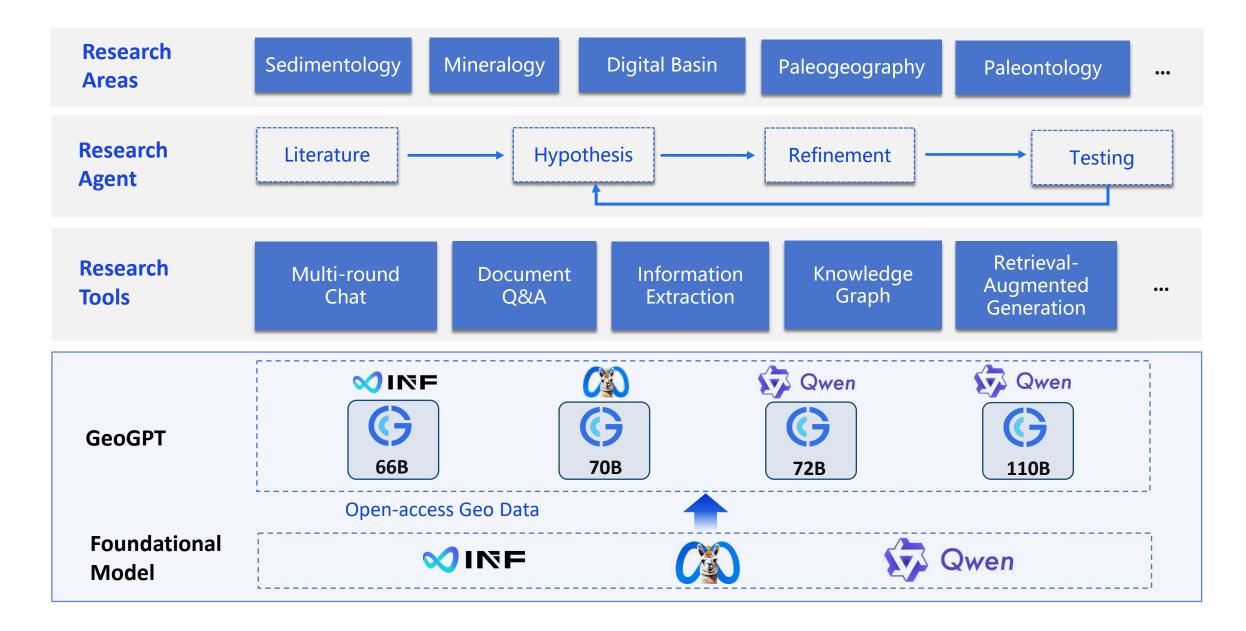
Our Original Intention of Developing GeoGPT

- GeoGPT is a large language model specifically designed and trained for the domain of geosciences.
 - Enable users to access, interpret, analyze, and generate geoscience-related information in a highly efficient and interactive manner
 - Contribute to the advancement and democratization of Earth sciences knowledge
- The GeoGPT Research Group (Yunqi Academy of Engineering, Zhejiang Lab), in response to the DDE's mission of sharing global geoscience knowledge and transform geoscience research, has independently developed GeoGPT, in regular consultation with key members from DDE.
- GeoGPT is an open-source, non-profit exploratory research project for global geoscience research. It encourages broad collaboration among experts in broad branches of the geoscience and AI.
- GeoGPT promotes the open science concept of collaboration, sharing, and co-construction.
 - Enhance public availability and reusability of geoscience data.
 - Increase opportunities for collaboration and promote transparency in scientific innovation.
 - Develop AI and internet-based tools to facilitate scientific collaboration.

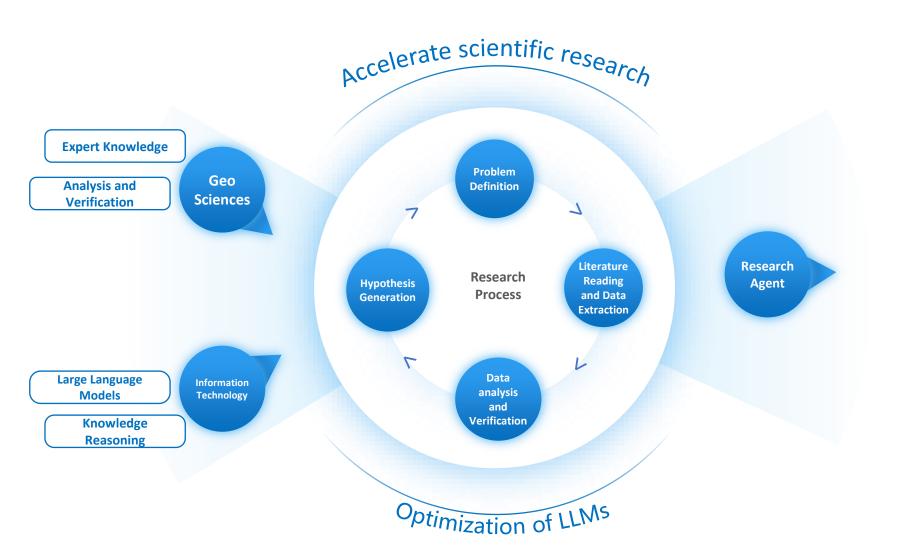
History of GeoGPT Development

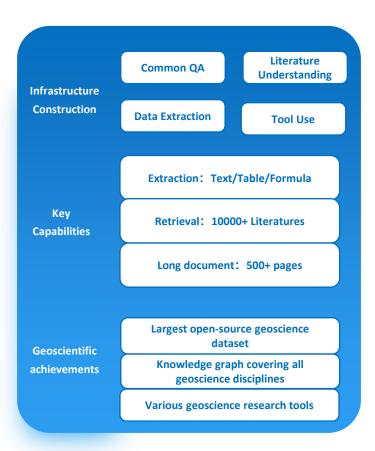
- 2/2023: Several distinguished geoscience and AI scientists from DDE proposed to develop GeoGPT.
- 3/2023: Yunqi Academy of Engineering, in response to the DDE's mission of sharing global geoscience knowledge and transform geoscience research, took the lead in developing GeoGPT. Transition of the GeoGPT project to Zhejiang Lab in 9/2023.
- 7/2023: DDE invited 129 students/scholars to participation in data collection and annotation.
- 9/2023: DDE invited over 400 hundreds Geoscientists to participate in GeoGPT annotation, eventually forming about 89,000 QA pairs.
- 4/2023: Started exploring LlaMA-1-13B for GeoGPT.
- 12/2023: First version of GeoGPT ready for testing (LlaMA-2, Qwen-1, INF-66B from Fudan).
- 4/2024: Three agents (Image-to-Table conversion, PDF parsing for Question Answering and Extraction, Echart Visualization) ready for testing. Demo at EGU-24.
- 5/2024: Completed the first version of RAG (retrieval augmented generation).
- 6/2024: Upgraded foundational models: LlaMA-3, Qwen-2.
- 7/2024: Included Mistral as one of the foundational models.

Overall Architecture of GeoGPT - 0.5



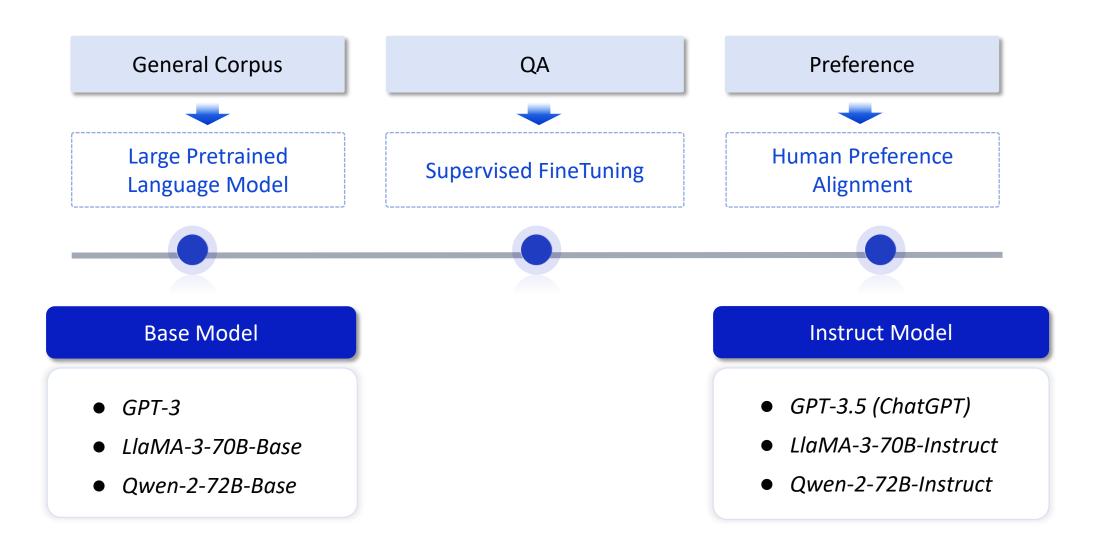
GeoGPT Research Agents to Accelerate Scientific Research







Training Stages of a General LLM



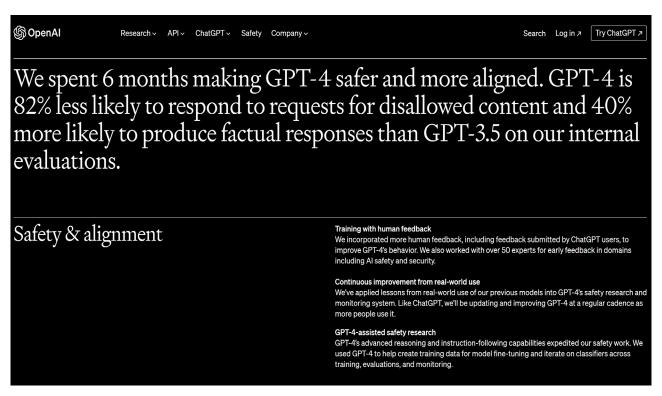


Safety Content Fine-Tuning

Safety Content Fine-Tuning

We compile corpora that adhere to ethical standards and fine-tune the large model's instructions to ensure that the generated content aligns more closely with these ethical principles.

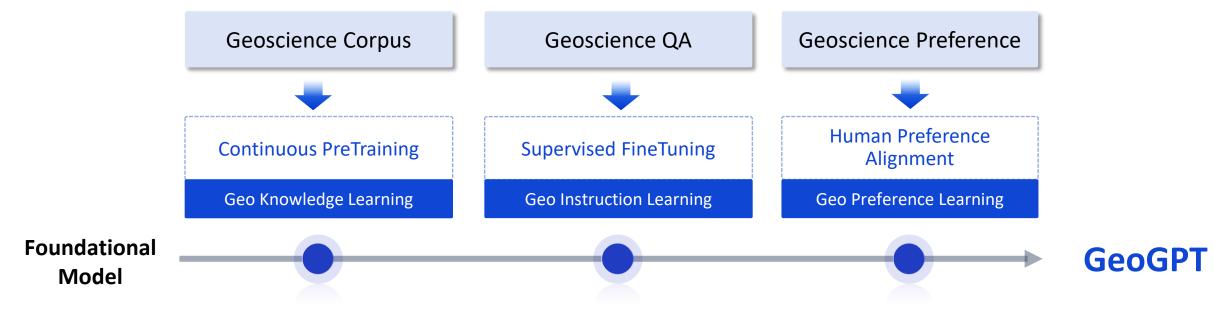
- Bias and Discrimination
- Illegal Activities
- × Physical Harm
- ★ Mental Health
- **×** Ethical Moral



https://openai.com/gpt-4



Training Stages of GeoGPT - 0.5



LlaMA-3-70B-Base

Qwen-2-72B-Base

How to Choose Foundational Models?

Explore Diverse Foundation Models

- Flexibility in Model Choice: Continue to explore and use different foundation models such as LLaMa to avoid over-reliance on a single LLM. This can mitigate potential legal and ethical issues and provide more flexibility in model development.
- **Benchmarking and Performance:** Regularly benchmark different models to ensure the chosen foundation model meets the required performance standards and aligns with the project's goals.

Promote International Collaboration

- <u>Cross-Border Cooperation</u>: Encourage collaboration with international researchers and institutions to share knowledge and best practices in developing and using LLMs. This can help in addressing common challenges and fostering innovation.
- Open Source and Access Initiatives: Support open access initiatives that promote the sharing of scientific knowledge, data, and models, reducing barriers to accessing high-quality data and models.

Advocate for Policy and Regulation

- <u>Policy Engagement</u>: Engage with policymakers to advocate for regulations that support the ethical development and use of LLMs. This includes policies that balance intellectual property rights with the need for scientific and technological advancement.
- <u>Public Awareness</u>: Increase public awareness about the benefits and challenges of LLMs, fostering informed discussions on their development and deployment.

Top Open LLMs

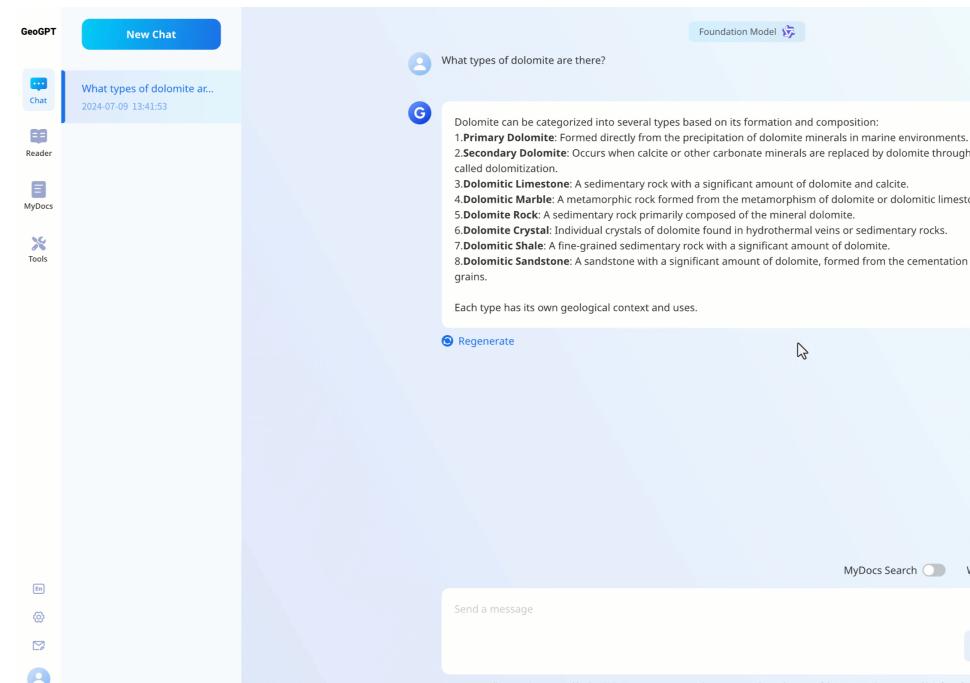
Open LLM Leaderboard

T 🔺	Model	Average 🚹 🔺	IFEval A	BBH 🔺	MATH Lvl 5	GPQA A	MUSR A	MMLU-PRO
9	Owen/Owen2-72B-Instruct	42.49	79.89	57.48	35.12	16.33	17.17	48.92
9	meta-llama/Meta-Llama-3-70B-Instruct	36.18	80.99	50.19	23.34	4.92	10.92	46.74
*	Owen/Owen2-72B	35.13	38.24	51.86	29.15	19.24	19.73	52.56
9	mistralai/Mixtral-8x22B-Instruct-v0.1	33.89	71.84	44.11	18.73	16.44	13.49	38.7
<u></u>	HuggingFaceH4/zephyr-orpo-141b-A35b-v0.1	33.77	65.11	47.5	18.35	17.11	14.72	39.85
<u></u>	microsoft/Phi-3-medium-4k-instruct	32.67	64.23	49.38	16.99	11.52	13.05	40.84
9	01-ai/Yi-1.5-34B-Chat	32.63	60.67	44.26	23.34	15.32	13.06	39.12
<u></u>	CohereForAI/c4ai-command-r-plus	30.86	76.64	39.92	7.55	7.38	20.42	33.24
9	internlm/internlm2_5-7b-chat	30.46	61.4	57.67	8.31	10.63	14.35	30.42
•	Owen/Owen1.5-110B	29.56	34.22	44.28	23.04	13.65	13.71	48.45
•	abacusai/Smaug-72B-v0.1	29.56	51.7	42.42	17.75	9.62	15.39	40.46
(m)	Owen/Owen1.5-110B-Chat	29.22	59.39	44.98	0	12.19	16.29	42.5

	Qwen2-72B	Llama3-70B	Mixtral-8x22E
MMLU	84.2	79.5	77.8
MMLU-Pro	55.6	52.8	49.5
GPQA	37.9	36.3	34.3
TheoremQA	43.1	32.3	35.9
ввн	82.4	81.0	78.9
HumanEval	64.6	48.2	46.3
МВРР	76.9	70.4	71.7
MultiPL-E	59.6	46.3	46.7
GSM8K	89.5	83.0	83.7
MATH	51.1	42.5	41.7
C-Eval	91.0	65.2	54.6
CMMLU	90.1	67.2	53.4
Multi-Exam	76.6	70.0	63.5
Multi-Understanding	80.7	79.9	77.7
Multi-Mathematics	76.0	67.1	62.9

https://huggingface.co/spaces/open-Ilm-leaderboard/open Ilm leaderboard (6/26/2024)

Qwen, LLaMA, and Mistral are the top rated open LLMs!





MyDocs Search

Web Search

Open-source Data for Training GeoGPT - 0.5

CommonCrawl

Common Crawl maintains a free, open repository of web crawl data that can be used by anyone. Over 250 billion pages spanning 17 years.

Free and open corpus since 2007.

Cited in over 10,000 research papers.

3-5 billion new pages added each month.

GPT-3						
Dataset	Quantity (tokens)	Weight in training mix				
Common Crawl (filtered)	410 billion	60%				
WebText2	19 billion	22%				
Books1	12 billion	8%				
Books2	55 billion	8%				
Wikipedia	3 billion	3%				

Figure 6. Top 20 languages (excluding English) from processed CommonCrawl based on number of documents and disk size

OLMo

Source	Туре	UTF-8 bytes (GB)	Docs (millions)	Tokens (billions)
Common Crawl	web pages	9,812	3,734	2,180
GitHub	code	1,043	210	342
Reddit	social media	339	377	80
Semantic Scholar	papers	268	38.8	57
Project Gutenberg	books	20.4	0.056	5.2
Wikipedia	encyclopedic	16.2	6.2	3.7

LLaMA							
Dataset	Sampling prop.	Epochs	Disk size				
CommonCraw	1 67.0%	1.10	3.3 TB				
C4	15.0%	1.06	783 GB				
Github	4.5%	0.64	328 GB				
Wikipedia	4.5%	2.45	83 GB				
Books	4.5%	2.23	85 GB				
ArXiv	2.5%	1.06	92 GB				
StackExchange	2.0%	1.03	78 GB				

MPT /// mosaic^{ML} MPT-7B Training Data

Data Source	Number of Tokens in Source	Proportion	Effective Number of Tokens	Epochs
mC4 3.1.0 - English (200+ words)	2417.99 B	33%	330 B	0.14
C4 - English - SemDedup 80%	100.42 B	29.9%	299 B	2.98
RedPajama - CommonCrawl	878.45 B	10%	100 B	0.11

DeepSeek								
Dumps Used	1	2	6	12	16	22	41	91
Deduplication Rate (%)	22.2	46.7	55.7	69.9	75.7	76.3	81.6	89.8

Table 1 | Deduplication ratios for various Common Crawl dumps.

Geoscience Corpus Mining 50B Geoscience Corpus

Document Screening

Corpus Cleaning

Topic-based Filtering



High Quality
Diverse
Training Data

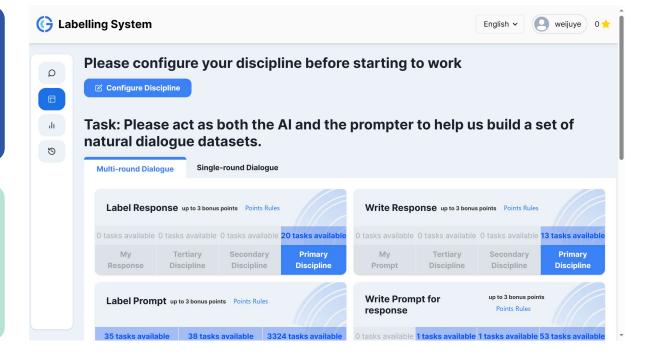
Q&A Data from Geoscientists

A team of geoscience experts were invited to annotate the geoscience field corpus, acquire and calibrate disciplinary data.

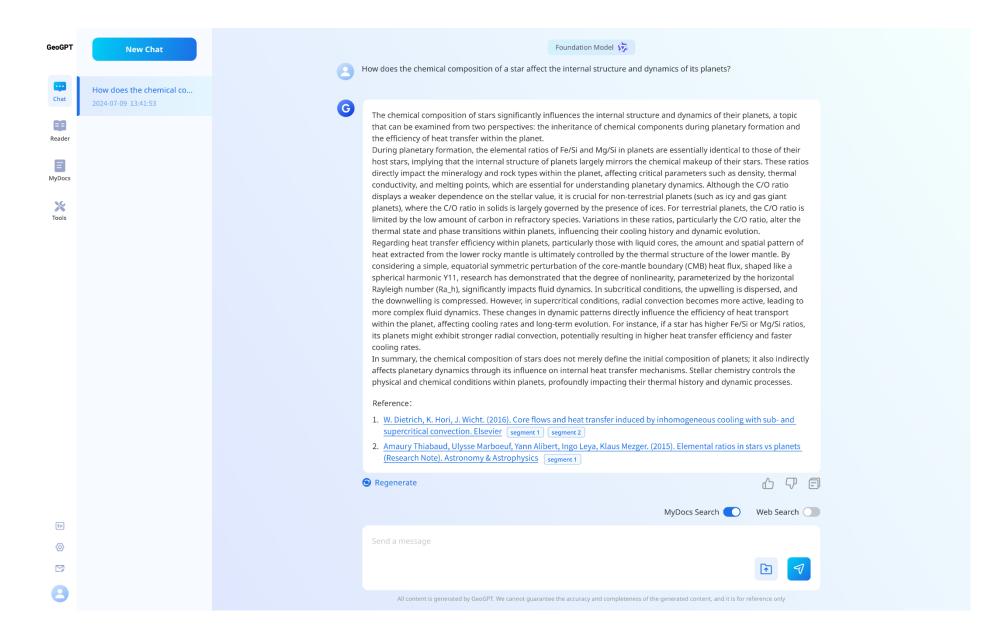
3 Workshops

20+
Organizations

400+ Experts 89k+
Questions&Answers



GeoGPT - 0.5: RAG Implementation



Top Risk Issues Surrounding AI and LLMs

1. Bias and Fairness

- **Issue**: Al models can reflect and amplify cultural differences
- Incident: Amazon's AI recruiting tool showed bias against women.
- Lesson: Use diverse training data and perform regular bias audits.

2. Transparency and Interpretability

- Issue: Al systems often operate as "black boxes."
- Incident: Lack of transparency in DeepMind's NHS kidney prediction system.
- Lesson: Develop explainable AI methods and interpretability tools.

3. Privacy and Data Security

- **Issue**: LLMs require large datasets, raising privacy concerns.
- **Incident**: Facebook-Cambridge Analytica scandal.
- Lesson: Implement strong data governance and comply with privacy laws.

4. Safety and Reliability

- Issue: Al can generate harmful or misleading content.
- **Incident**: GPT-3 generating convincing fake news.
- Lesson: Enforce guidelines for safe AI use and implement content moderation.

5. Ethical and Moral Implications

- **Issue**: Al decisions can have significant ethical impacts.
- **Incident**: Google's involvement in Project Maven raised ethical concerns.
- Lesson: Establish ethical guidelines and involve stakeholders in discussions.

6. Regulatory and Legal Challenges

- Issue: Rapid AI development outpaces regulatory frameworks.
- **Incident**: Uber's self-driving car accident highlighted regulatory gaps.
- Lesson: Update regulatory frameworks and promote international cooperation.

Al Governance Committees: Examples from Top Al Companies

OpenAI's AI Ethics and Policy Team

Dedicated team focusing on AI ethics: ethicists, policy experts, and technical researchers

Create guidelines, conducting impact assessments, and engaging with external stakeholders to ensure responsible AI development.

Google's AI Ethics Board

Advanced Technology External Advisory Council (ATEAC): external experts in AI, ethics, and policy. Dissolved, highlighting the complexities in setting up such committees

Google continues to have internal ethics review processes and frameworks.

■ Microsoft's AI, Ethics, and Effects in Engineering and Research (Aether) Committee

Advises on issues related to the responsible development and deployment of AI technologies Ethicists, engineers, and researchers

Works closely with Microsoft's Office of Responsible AI.

Works closely with Microsoft's Office of Responsible P

■ IBM's AI Ethics Board

Ethics, law, and technology

Oversees the company's AI ethics policies, reviews projects for ethical concerns, and ensures compliance with regulatory standards.

GeoGPT Governance Committee Initiative

Establishing a data and integrity governance committee for GeoGPT ensures the program's openness, fairness, transparency, and accuracy. Key elements for forming such a committee could include:

Purpose and Objectives

- ✓ Purpose: Oversee the development and deployment of GeoGPT to ensure it adheres to commonly accepted ethical standards, scientific rigor, and regulatory requirements.
- ✓ Objectives: Maintain data integrity, ensure fairness and bias mitigation, promote transparency in data, methodologies and outcomes, and establish accountability mechanisms.

Committee Composition

- ✓ Internal Members: Include representatives from GeoGPT and its network organizations with expertise in data science, geoscience, ethics, and legal fields.
- ✓ External Experts: Appoint independent experts in AI ethics, data privacy, and geoscience to provide objective perspectives and prevent internal biases.
- ✓ Stakeholder Representation: Include representatives from stakeholder groups, such as IUGS and UNESCO.

Selection Criteria for Members

- ✓ Expertise: Members should have substantial knowledge and experience in their respective fields.
- ✓ Independence: Especially for external experts, ensure they have no conflicts of interest
- ✓ Diversity: Aim for a diverse committee to bring a range of perspectives and avoid groupthink.

Win-win situation: Benefits of Custom LLMs for a Scientific Journal

Improving Manuscript Quality

Provide contributors with writing guidance, topic suggestions, and references, thereby increasing the number of high-quality submissions.

Enhancing Manuscript Review

Offer initial screening and analysis tools for editors and reviewers, assist in drafting review comments, and improve the efficiency.

Optimizing the Publication Process

Automatically organize manuscript content, reducing editorial workload and speeding up publication.

■ Facilitating Content Planning

Analyze data and mine topics to identify research hotspots, providing developing content strategies that better meet market demands.

Enhancing User Experience

Offer readers personalized content recommendations, provide customized services to help readers access research findings of interest.

Expanding the Network of Contributors

Identify potential high-quality researchers, invite them to submit manuscripts, and provide support to attract more scholars.

■ Increasing Engagement and Promotion

Generate relevant scientific news, attract reader participation in journal activities, enhancing the journal's influence and reader engagement.

■ Language Cleanup

Automatically correct grammatical errors, improve readability, and ensure precise scientific terminology and professionalism of the papers.

■ Identify Plagiarism

Detect and flag potential instances of plagiarism by comparing manuscripts against a vast database of published works, ensuring originality.

■ Help in Structuring the Paper

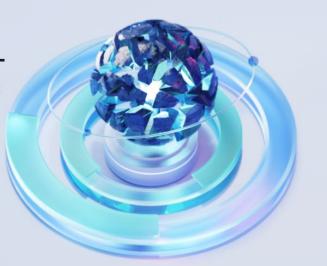
Offer guidance on the appropriate structure of scientific papers, provide templates, and checklists to ensure proper formatting.

■ Identify Additional References

Suggest relevant references and citations, helping authors support their research with comprehensive literature reviews.

Conclusions and Prospects

GeoGPT is an open-source and nonprofit exploratory research project for geoscience, with the goal of offering geoscientists innovative capabilities and tools augmented by large language model technology.



The GeoGPT team is

- committed to empowering geoscience research through AI.
- strives to demonstrate open access, transparency, professionalism, correct values and ethical tendencies, and constantly seeks authoritative advice from ethical experts, legal experts, data compliance experts
- provides a framework possess a versatility that extends beyond their geoscience origins, offering significant contributions to a multitude of other disciplines.

Scientific research has no borders.

large language models are indispensable tools for future scientific research. Geoscience needs to be part of this!





Benefits of better access to geological data, geological tools, modelling capability

- Accessing and analyzing scientific literature.
- Concept clarification.
- Data analysis.
- Methodology guidance.
- **Prediction**
- Code development.
- Hypothesis generation





Thank you!