github.com/google/curie

arxiv.org/abs/2503.13517

# CURIE: Evaluating LLMs On Multitask Scientific Long Context Understanding and Reasoning


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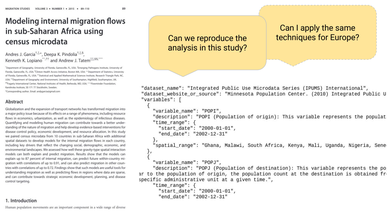
## Can LLMs assist Scientists with some workflows?

### Can we measure problem solving ability?

- Extract details of the data.
- Identify and extract the processes and methodology.
- Write code to solve problem or reproduce study.


Modeling internal migration flows in sub-Saharan Africa using census microdata

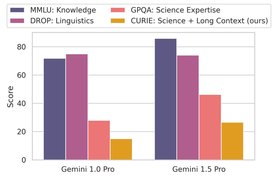



### This requires

- Knowledge of the domain.
- Processing long-context info.
- Reasoning ability to apply knowledge in the context of a problem.

### CURIE: Tests scientific problem solving

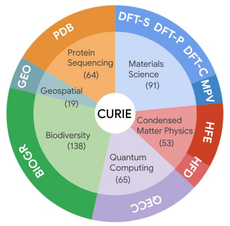
- Existing benchmarks test for knowledge, linguistics.
- CURIE: scientific long-**C**ontext **U**nderstanding **R**easoning and **I**nformation **E**xtraction benchmark

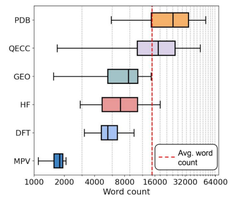


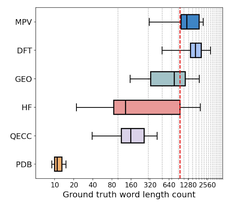

## The CURIE benchmark and dataset

### 580 examples, 429 documents, 10 tasks, 6 domains

- Tasks require expertise + reasoning + long-context understanding
- Avg. input query length ~15k words, gold response length is ~1k



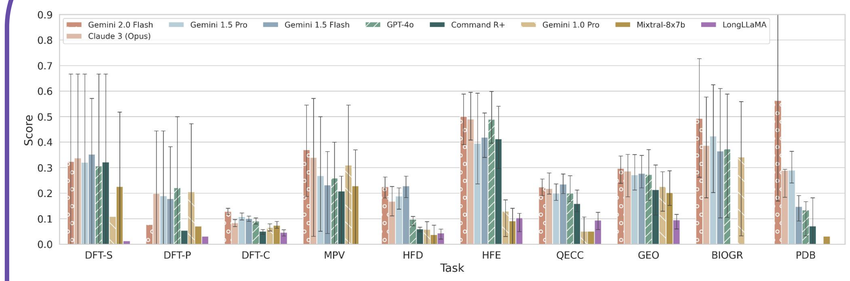




We collaborated closely with domain experts throughout benchmark development. This included:

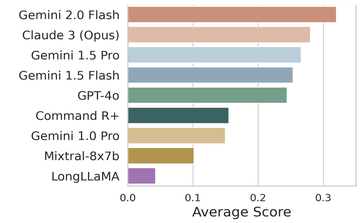
- Defining and identifying tasks reflecting realistic scientific workflows.
- Sourcing relevant papers from the domain.
- Creating accurate, nuanced, and comprehensive ground truth answers.
- Rating task difficulty based on salient features.
- Identifying and verifying evaluation metrics against expert judgments of model responses.

## Results



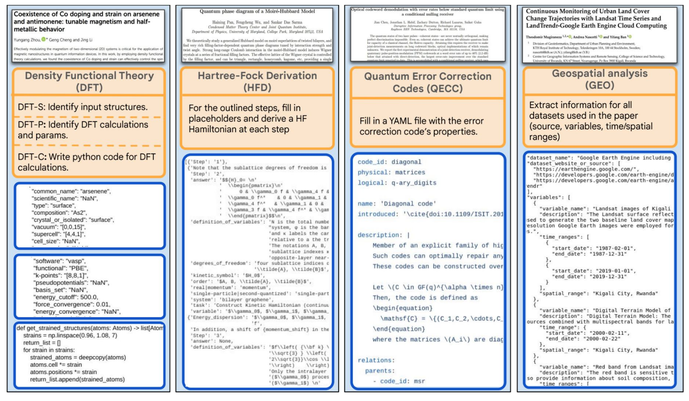

Per task normalized scores of various LLMs on the CURIE benchmark to measure performance on 10 long-context tasks requiring expertise across six scientific disciplines. Higher is better.

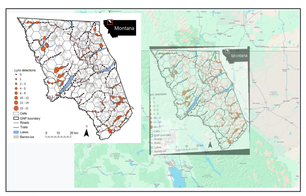
- Highest at 32%
- Gemini Flash 2 and Claude-3 do better. They understand the purpose of the extraction tasks and group responses.
- Exhaustive retrieval e.g. DFT-S, MPV, GEO are challenging for all.
- Flash 2 generated code to solve PDB ~50% of the time and was correct. When enumerating sequence it was similar to other models.
- Experts noted that summaries generated by models were succinct while including a multitude of details hard to comb out e.g. in QECC, and easy to remove afterwards.



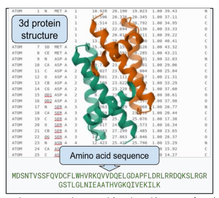

Average normalized performance of long-context LLMs across the 10 tasks from six scientific domains in CURIE.

## Illustrative examples of tasks in CURIE




**BIOGR** task requires identifying latitude and longitude (georeferencing) of a map image.




**PDB** task requires reconstructing a protein's amino acid sequence from the 3D structure.

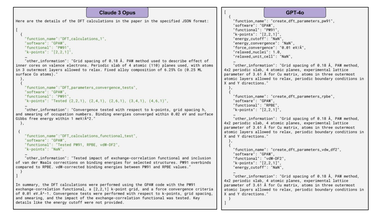
## Brief description of tasks and capabilities measured

| Task | Domain | # Qs | Brief Description | Capability | Output Format | Primary Eval. Metric |
|---|---|---|---|---|---|---|
| DFT-S | Material Science | 74 | Extracts input material structures for DFT calculations. | entity recognition, concept tracking | JSON | LLMSim-F1 |
| DFT-P | Material Science | 74 | Extract parameters for DFT calculations. | concept extraction, tracking, aggregation | JSON | LLMSim-F1 |
| DFT-C | Material Science | 74 | Write functional code for DFT computations. | concept aggregation, coding | TEXT | ROUGE-L |
| MPV | Material Science | 17 | Identify all instances of materials, their properties, and descriptors. | entity recognition, concept extraction, tracking | JSON | LLMSim-F1 |
| HFD | Condensed Matter Physics | 64 | Derive the Hartree-Fock mean-field Hamiltonian for a quantum many-body system. | concept extraction, algebraic manipulation, reasoning | TEXT | ROUGE-L |
| HFE | Condensed Matter Physics | 19 | Extract the most general mean-field Hamiltonian. | concept extraction | TEXT (latex equation) | ROUGE-L |
| QECC | Quantum Computing | 65 | Create a YAML file with the Error Correction Code's properties. | concept aggregation, summarization | YAML | ROUGE-L |
| GEO | Geospecial | 15 | Extract information for all geospatial datasets used along with the spatial and temporal extents. | concept extraction, aggregation | JSON | ROUGE-L |
| BIOGR | Biodiversity | 38 | Determine the latitude, longitude bounding box encompassing the region in the map image. | visual comprehension, reasoning | JSON (lat. lon. co-ordinates) | Intersection-over-Union (IoU) |
| PDB | Protein Sequencing | 138 | Reconstruct a protein's amino acid sequence form the 3D structure. | tracking, aggregation reasoning | Code or TEXT (seq.) | Identity ratio (IDr) |

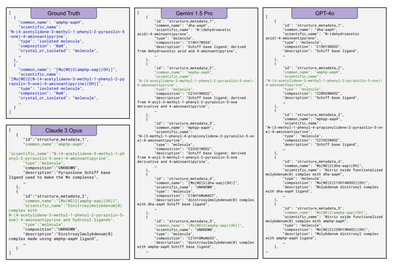
Tasks in CURIE are varied and have ground truth annotations in mixed and heterogeneous form e.g. as JSONs, latex equations, YAML files, or free-form text. We use programmatic metrics for a predominant number of tasks and propose LLM- based evaluation for others.

## Examples

### DFT-P

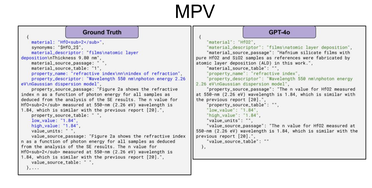



### DFT-S

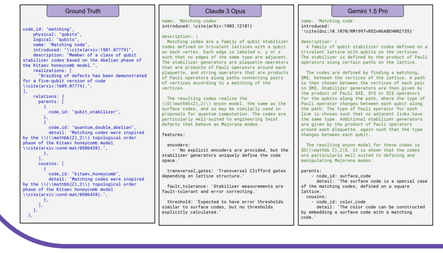



### HFE


### MPV




### QECC




### PDB