ISC High Performance

REINVENTING HPC

MAY 12 – 16, 2024 | HAMBURG, GERMANY

HPC-Coder: Modeling Parallel Programs using Large Language Models

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[*] University of Maryland

[†] Lawrence Livermore National Laboratory

Timeline and Motivation

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August 2021

OpenAI Codex Release

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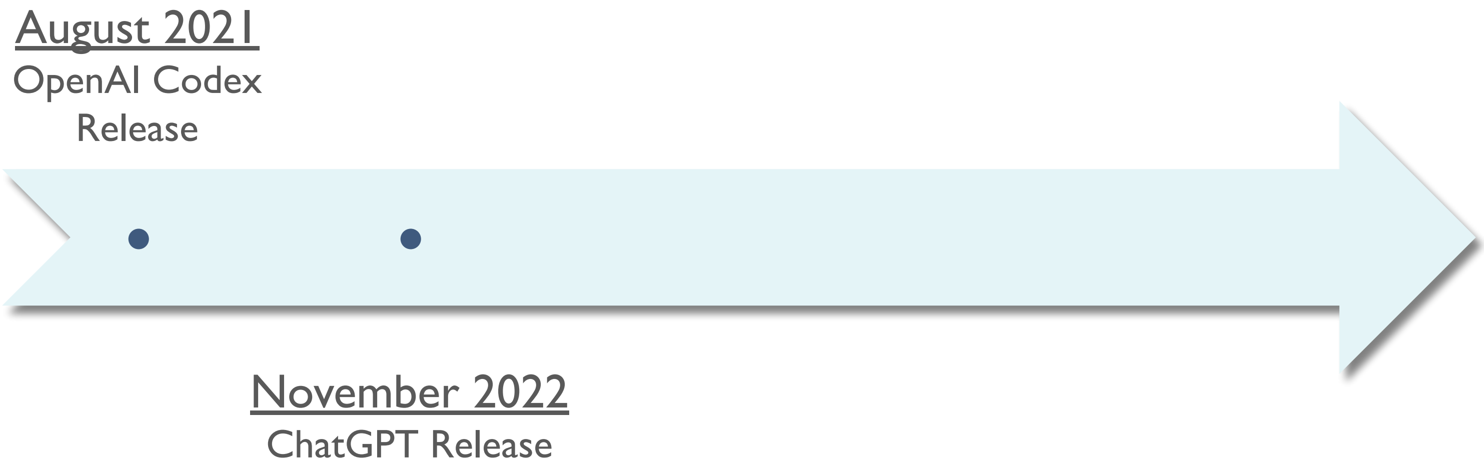

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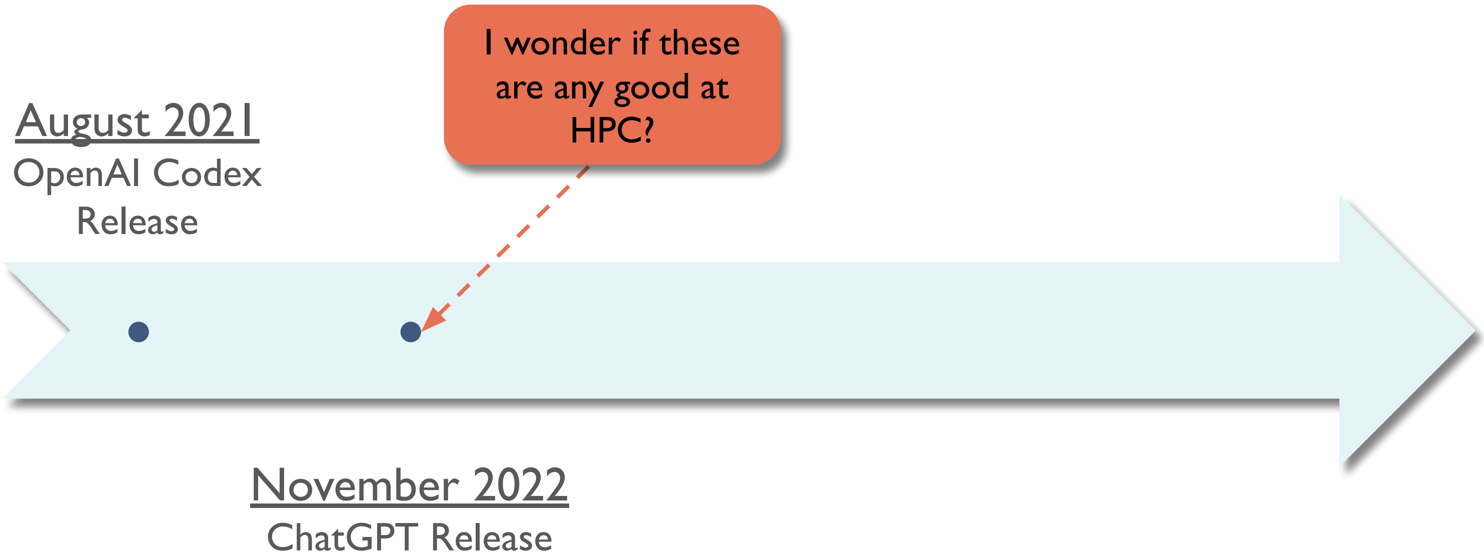

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and hopefully many more…

Code LLMs are Bad at Parallel Code

- PolyCoder
  - State-of-the-art, open-source, code LLM released in 2022
  - 2.7B parameters and outperformed OpenAI's Codex

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    Use MPI to compute the average of X across ranks
    and return the result on all ranks.
    Use the default communicator.
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double mpiAverage(double X) {
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    int nprocs;
    double average;
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We observed an ability to generate parallel code constructs, but not use them correctly

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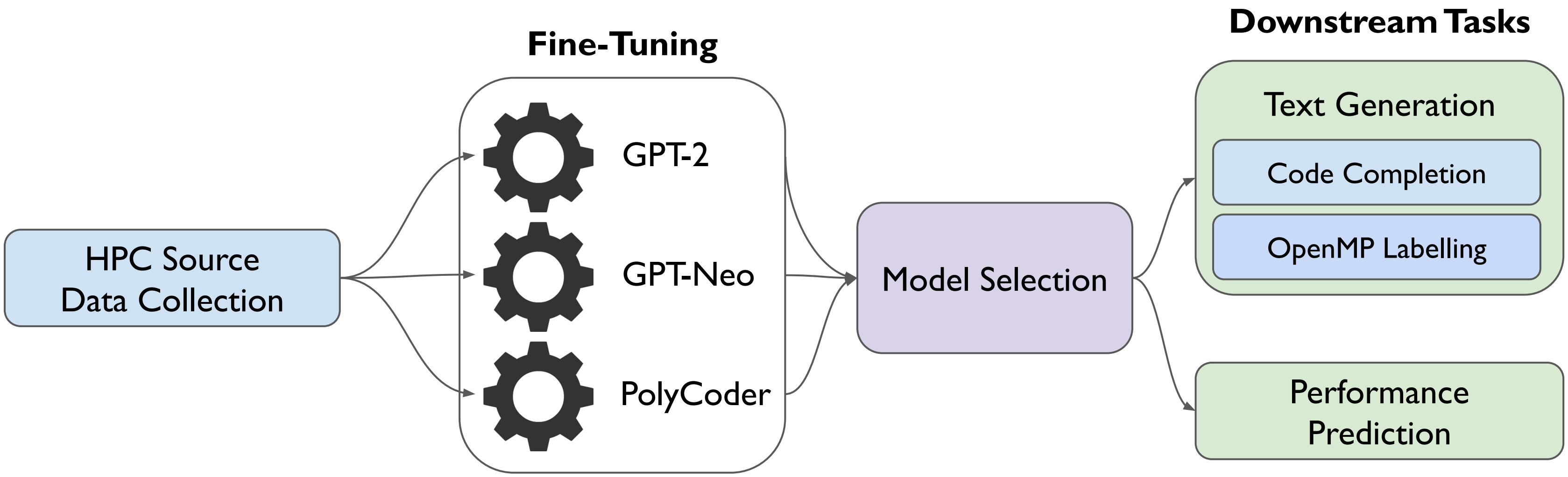
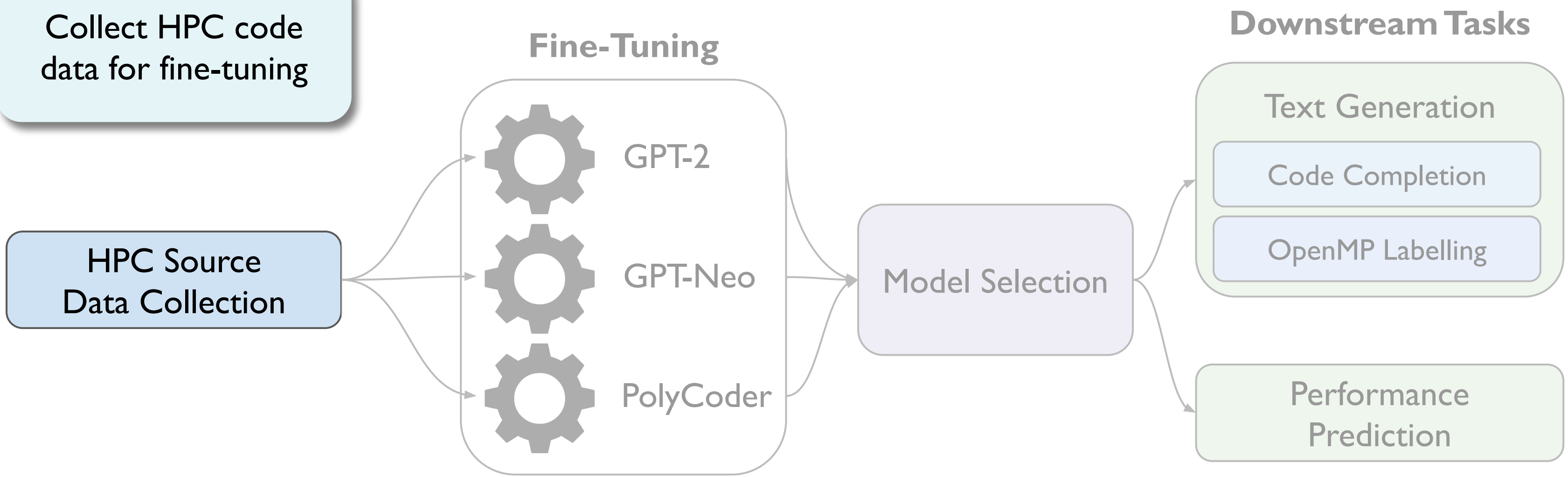
RQ 2 – *How can we effectively measure the capabilities of LLMs at modelling parallel and HPC code?*

Overview of Our Approach



Overview of Our Approach

Collect HPC code data for fine-tuning



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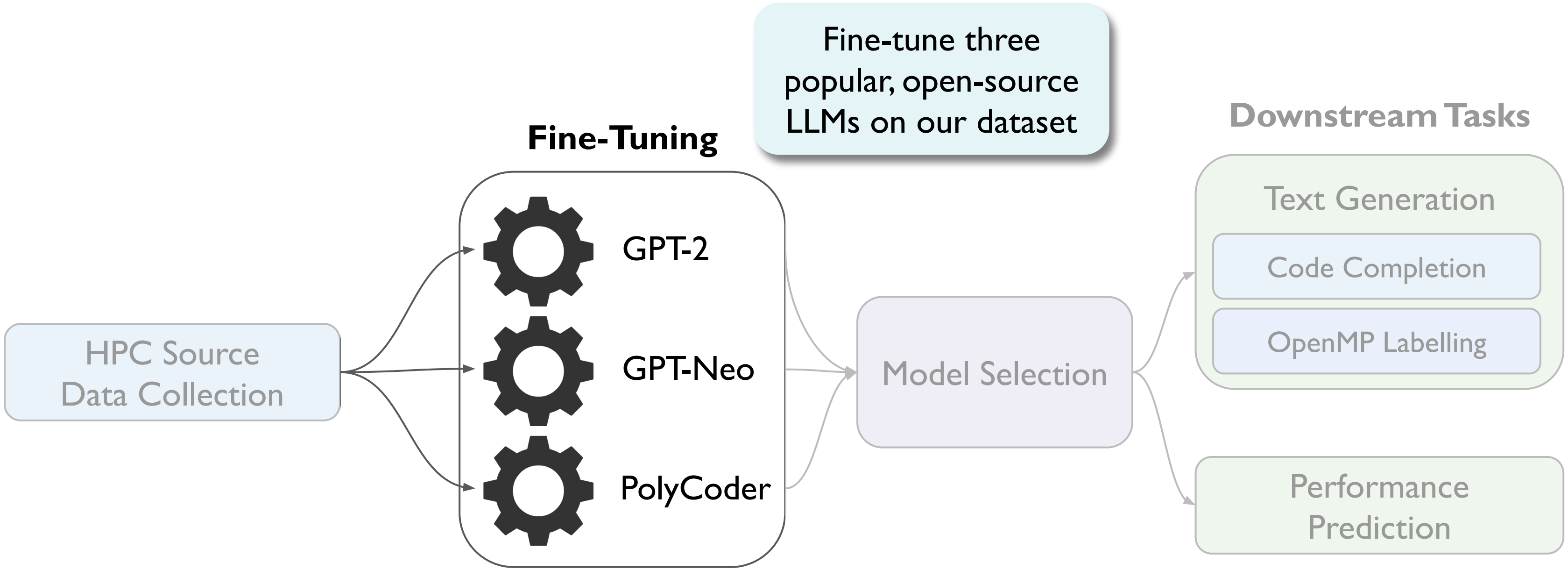

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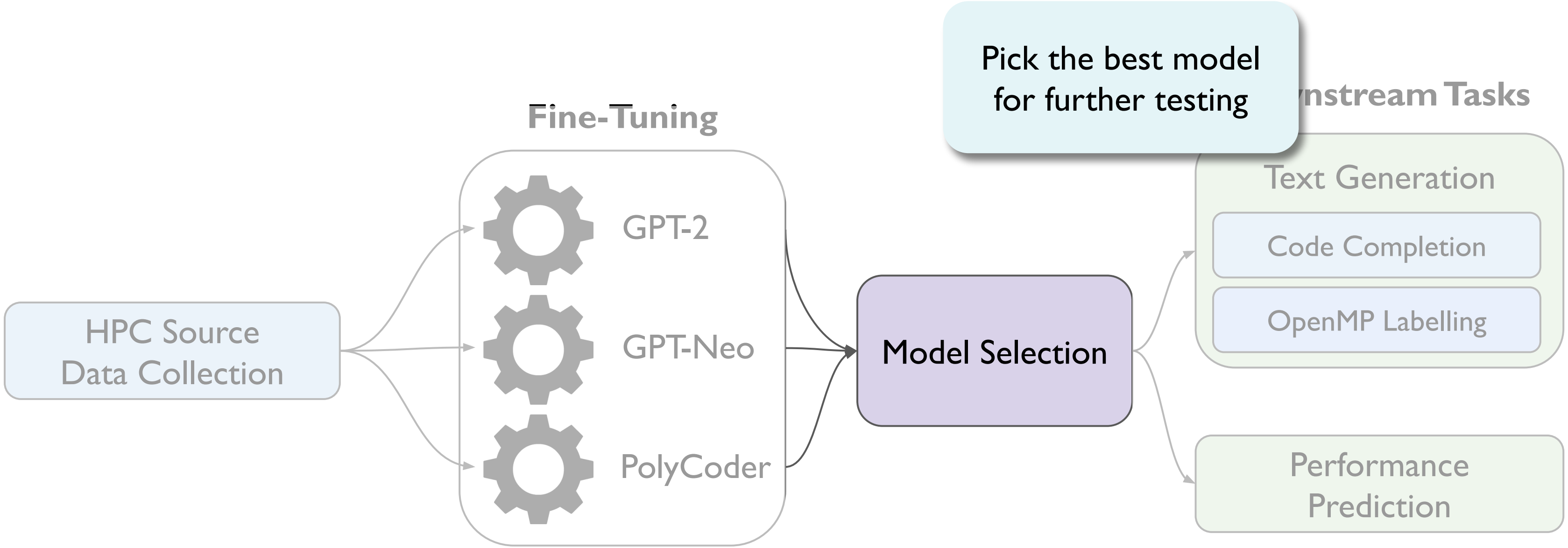

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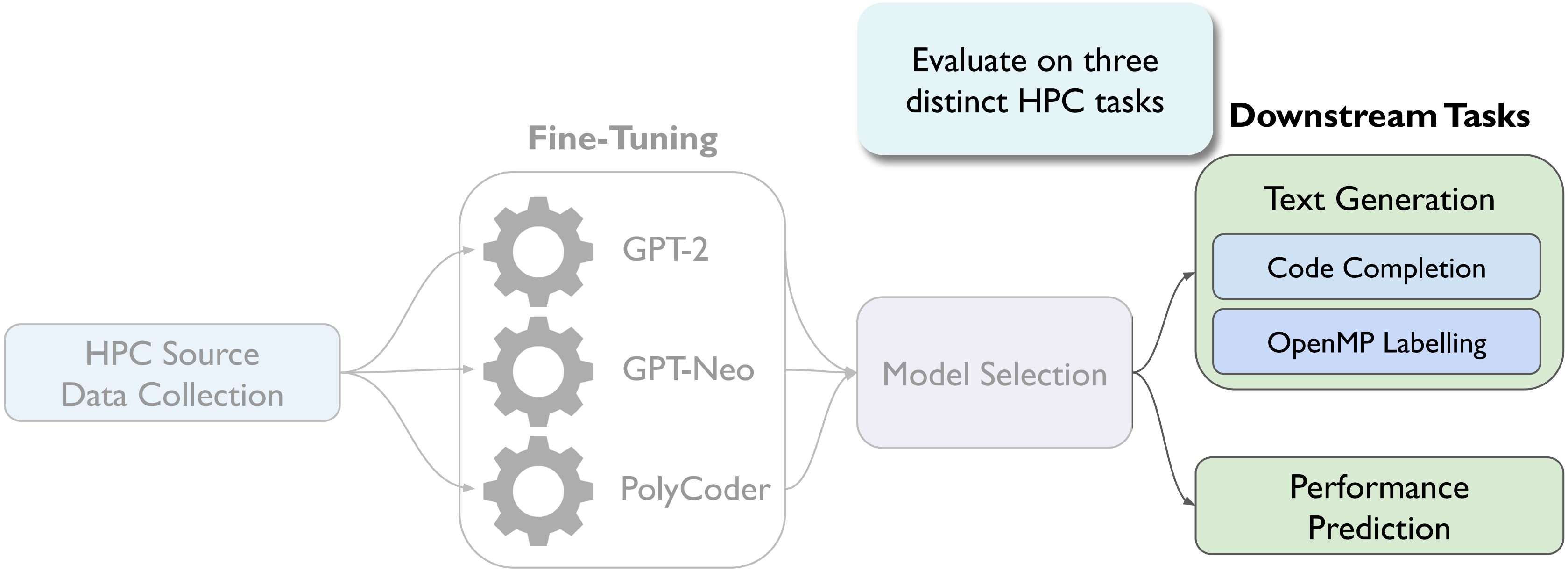

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Collecting a Parallel and HPC Code Dataset

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  - De-duplication by SHA-256 hash
  - Remove large (> 1MB) and small (< 15 tokens) files

Collecting a Parallel and HPC Code Dataset

Filter	# Files	# LOC	Size (GB)
None	239,469	61,585,704	2.02
Deduplicate	198,958	53,043,265	1.74
Deduplicate + remove small/large files	196,140	50,017,351	1.62

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Approximately 18% of files are removed during preprocessing.

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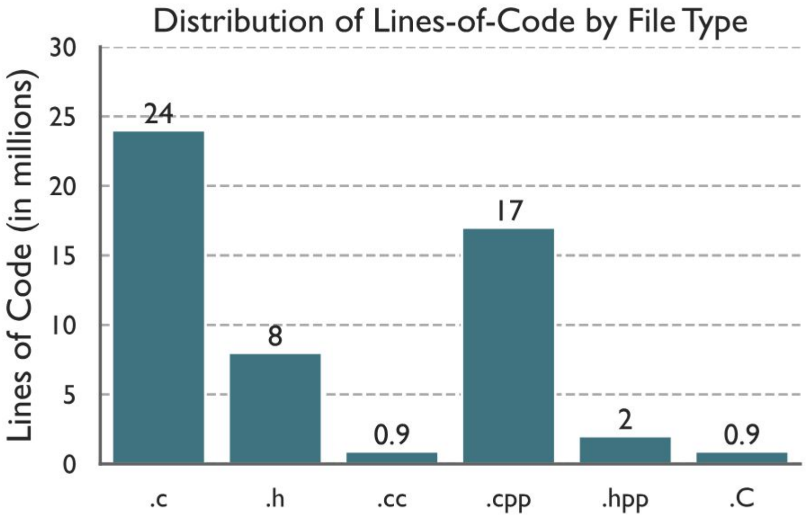

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Selecting LLMs to Fine-Tune

- Focus on LLMs that fit on consumer GPUs

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Model Name	No. of Parameters	Pre-Training Data
GPT-2	1.5B	natural language
GPT-Neo	2.7B	natural language + code
PolyCoder	2.7B	code

Fine-Tuning Methodology

- Fine-tune the existing LLMs on our dataset
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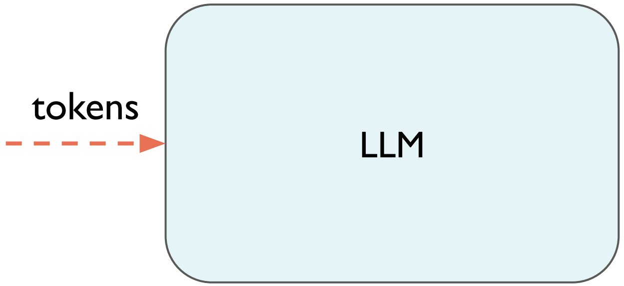

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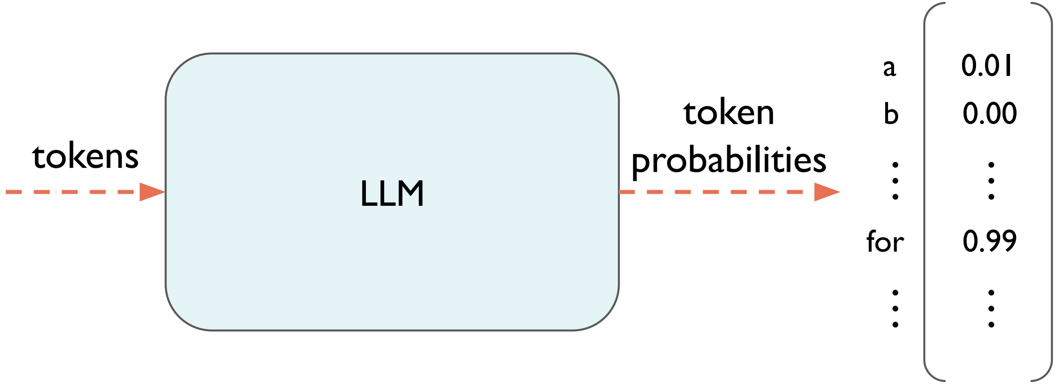

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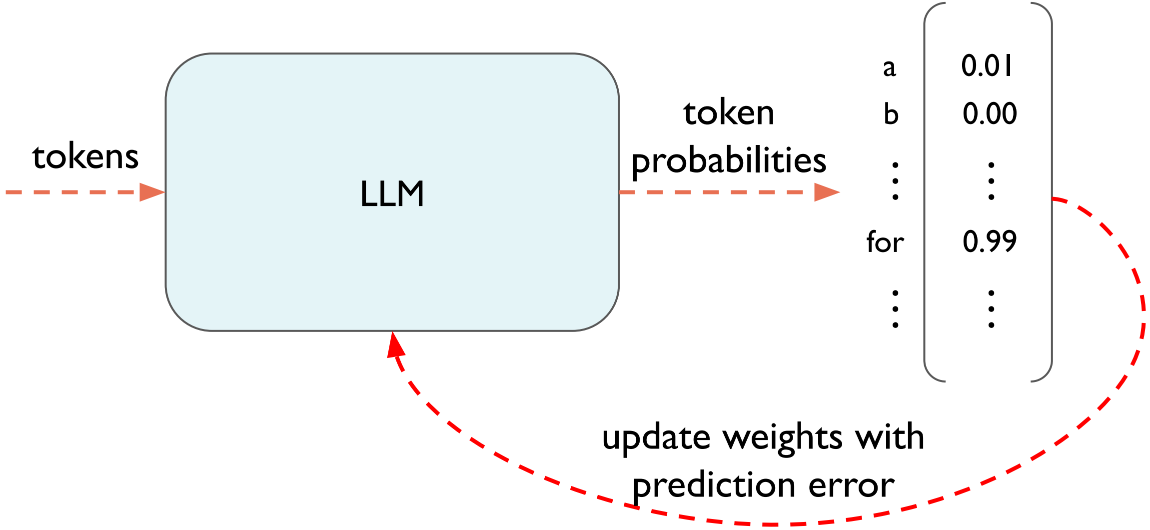

Fine-Tuning Methodology

- Fine-tune the existing LLMs on our dataset
- Auto-regressive fine-tuning
- Fine-tune for 1 epoch
- Record perplexity
  - Inversely proportional to how "perplexed" the LLM is by tokens in the distribution
  - Lower is better
- Run downstream tasks every 1000 steps

Fine-Tuning Results

Model	GPT-2	GPT-Neo	PolyCoder
Final Validation Perplexity	4.47	2.23	2.24

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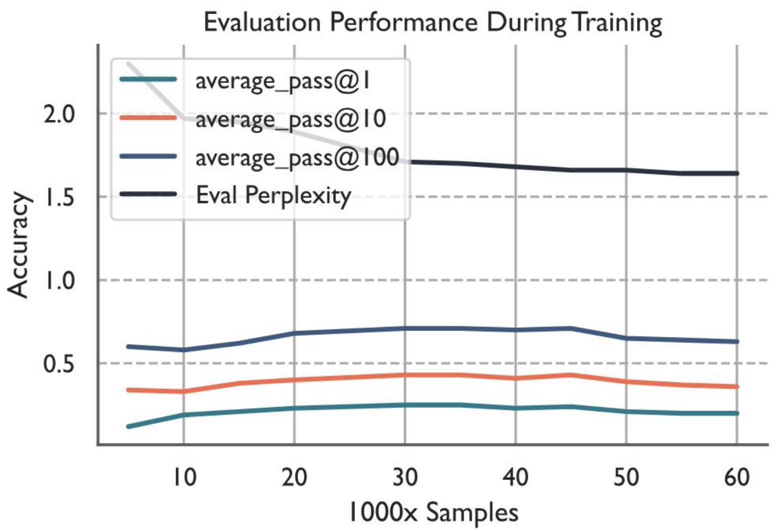

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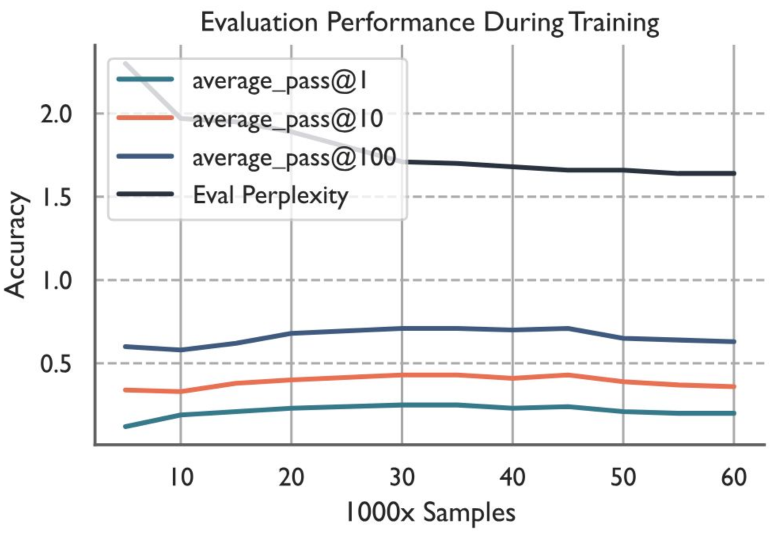
After ~45k steps the downstream performance drops, but perplexity keeps getting better



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prompt

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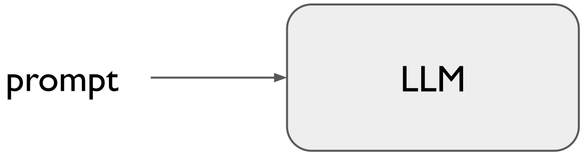


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#pragma omp parallel for
for (int i = 0; i < N; i++) {
    sum += x[i] * y[i];
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return sum;
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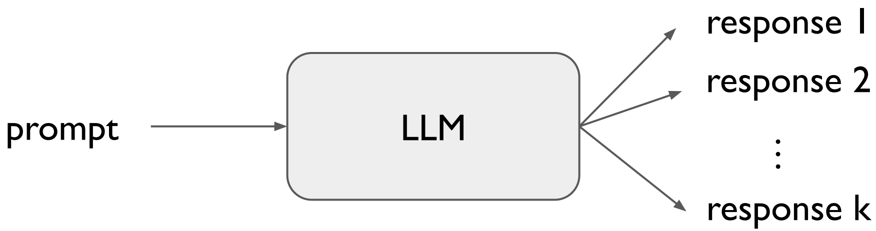


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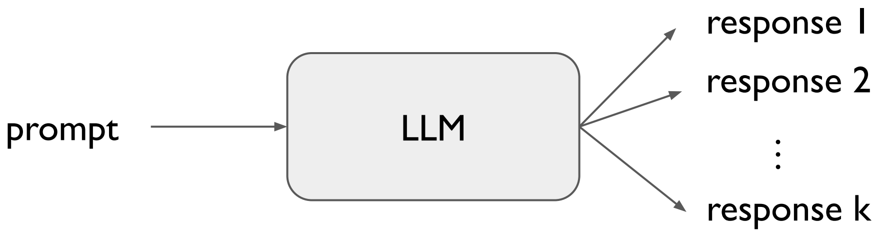

What is the probability at least one of k responses is correct?

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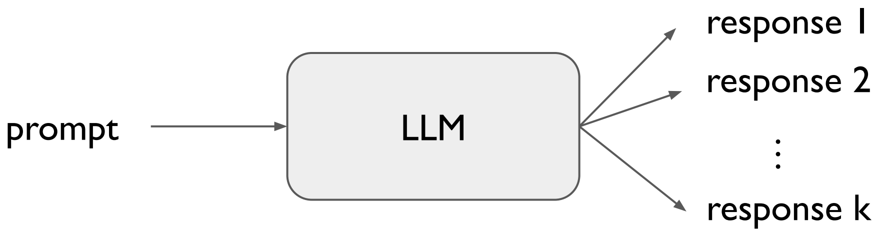
Number of samples generated per prompt

$$\text{pass@}k = \frac{1}{|P|}\sum_{p \in P}\left[1 - \binom{N - c_p}{k} \Big/ \binom{N}{k}\right]$$

Set of prompts

Number of correct samples for prompt p

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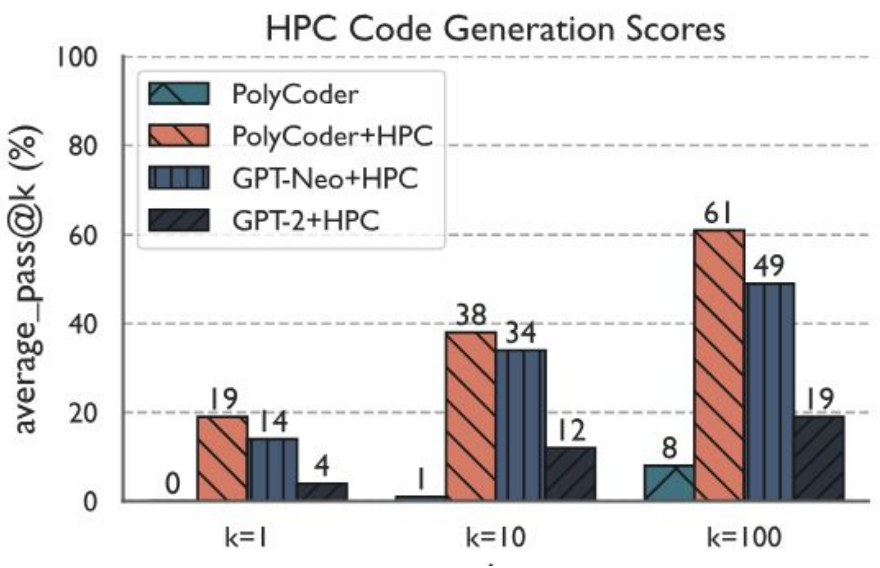

HPC tuned models perform much better than PolyCoder

Evaluation Task 2: OpenMP Pragma Generation

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<OMP>#pragma omp parallel for<END_OMP>
```

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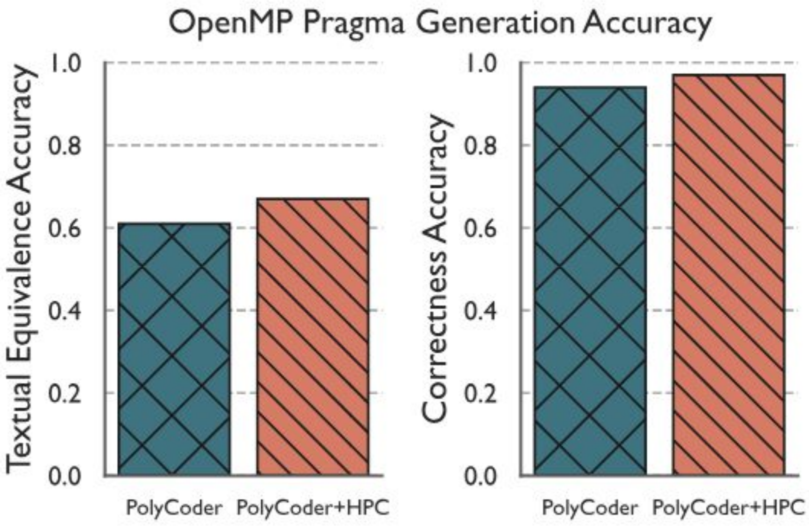
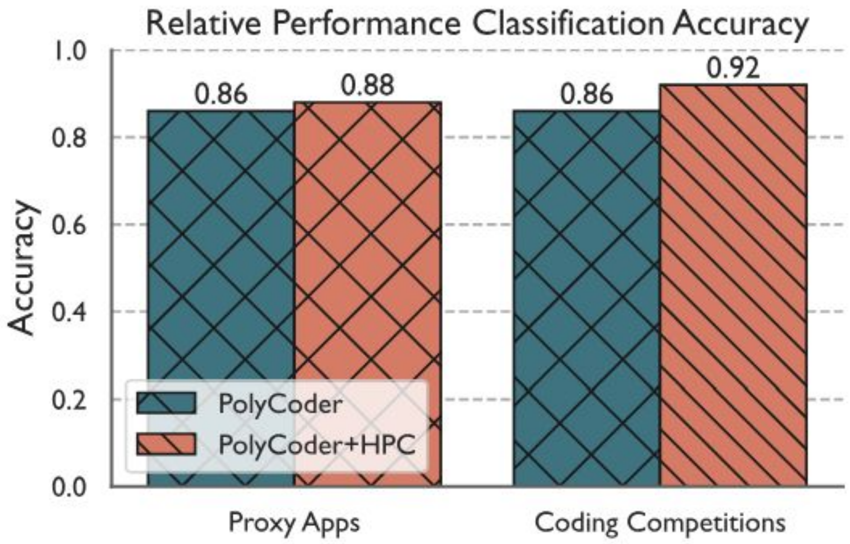


Up to 97% accuracy predicting the OpenMP pragmas.

Evaluation Task 3: Relative Performance Modeling

- Compile and run entire commit history of Kripke and Laghos
- Fine-tune LLM as classifier to predict performance degradation given commit diff
- 1 – performance improved or stayed the same; 0 – performance got worse

Evaluation Task 3: Relative Performance Modeling



Up to 92% accuracy predicting performance regressions.

Conclusion and Takeaways

- Fine-tuning can improve the performance of code LLMs on low data resource problems
- State-of-the-art LLMs are bad at parallel and HPC tasks
- We need custom evaluations on HPC and parallel tasks

Contributions and Next Steps

- A large, HPC source code dataset
- A fine-tuned HPC code LLM: HPC-Coder
- Benchmarks for evaluating LLMs on HPC tasks
- HPC-Coder-v2 in coming weeks…

"Can Large Language Models Write Parallel Code?" HPDC '24

"Performance-Aligned LLMs for Generating Fast Code" arXiv 2404.18864

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