# GRANITE 3.0 LANGUAGE MODELS

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#### **ABSTRACT**

This report presents Granite 3.0, a new set of lightweight, state-of-the-art, open foundation models ranging in scale from 400 million to 8 billion active parameters. Equipped with native support of reasoning, multilingual, coding, function calling, and strong safety performance, these models target enterprise on-premise and on-device use cases. Evaluations on a comprehensive set of tasks demonstrate that Granite 3.0 models consistently reach state-of-the-art performance for their size. This report also disclosed many technical details of pre-training and post-training that could help the research community push the collective efforts of developing open foundation models. We publicly release both pre-trained and post-trained versions of our models with the Apache 2.0 license. Together with the support from the research community, we also integrated our model with existing tools for quantization, fine-tuning, and deployment to facilitate potential application and research endeavors.

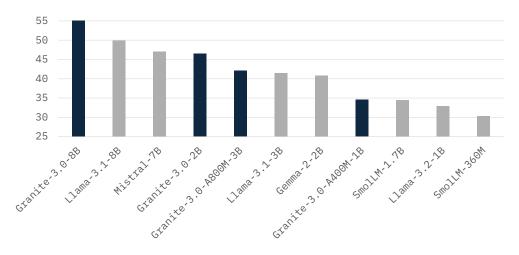


Figure 1: Average accuracy of base models across 19 tasks from 6 domains

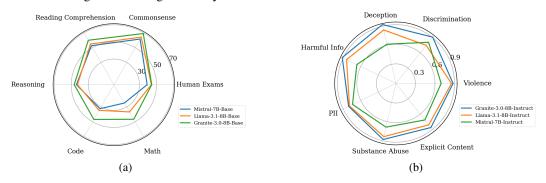


Figure 2: Instruction models performances and safety evaluations.

# 1 Introduction

The adoption of large language models (LLMs) across different applications has spread quickly. While commercial options that are consumer-facing via a web interface or API call are widely available, there is a demand for on-premise models. For accessibility, being able to fine-tune a pretrained LLM for on-premise use requires models with lower hardware requirements.

There are many lightweight models like Gemma (Team et al., 2024) and Llama (Dubey et al., 2024b) that perform well and fit the bill. However, in an enterprise setting, the adoption of LLMs can have further constraints. The provenance and transparency around data usage and processing can have legal and compliance implications. In particular, the license that an LLM is released under can also restrict companies from using a model on their specific use cases.

In this report, we present the **Granite 3.0** family of language models natively supporting multilinguality, coding, reasoning, and tool usage, including the potential to be run on constrained compute resources. All the models are publicly released under an Apache 2.0 license for both research and commercial use. The models' data curation and training procedure were designed for enterprise usage and customization in mind, with a process that evaluates datasets for governance, risk and compliance (GRC) criteria, in addition to IBM's standard data clearance process and document quality checks. Specifically, Granite 3.0 includes 4 different models of varying sizes:

- Dense Models: A 2B and 8B parameter model, trained on 12 trillion tokens in total.
- **Mixture-of-Expert (MoE) Models:** A sparse 1B and 3B MoE model, with 400M and 800M activated parameters respectively, trained on 10 trillion tokens in total.

Accordingly, these options provide a range of models with different compute requirements to choose from, with appropriate trade-offs with their performance on downstream tasks. At each scale, we release a base model — checkpoints of models after pretraining, as well as instruct checkpoints — models finetuned for dialogue, instruction-following, helpfulness, and safety. The base models are trained from scratch with a two-stage training procedure. In stage 1, our dense and MoE models are trained on 10 trillion and 8 trillion tokens, respectively. Stage 1 training data consists of unstructured multilingual language data from diverse sources across academia, the internet, enterprise (e.g., financial, legal), and code, including publicly available datasets with permissive licenses. In stage 2, we train on a mixture of 2 trillion tokens of data. Some of the data sources for stage 2 are the same as the stage 1 data sources, mixed with a small amount of high-quality open-source and synthetic corpora with permissive licenses. The data mixtures are derived through a data mixture search focusing on robustness across different domains and tasks. The instruct models are derived by supervised fine-tuning (SFT) of the pre-trained checkpoints, followed by model alignment using reinforcement learning (PPO, BRAIn (Pandey et al., 2024)). We find that both SFT and PPO/BRAIn are important for improved performance on downstream automatic evaluations, including better chat capabilities.

Additionally, the models were trained with techniques that leverage different methods found in the existing literature:  $\mu P$  (Yang & Hu, 2020; Yang et al., 2022; 2023) allowed for hyperparameter transfer after a hyperparameter search on smaller models, and Power scheduler (Shen et al., 2024c) allowed for learning rate transfer across batch size and total number of training tokens. For our MoE models, we used a dropless MoE (Gale et al., 2023) approach for better model performance using the ScatterMoE (Tan et al., 2024) implementation.

Experiment results show that our Granite 3.0 models outperform models of similar parameter sizes on many benchmarks, demonstrating strong performance in knowledge, reasoning, function calling, multilingual, code support, as well as enterprise tasks like cybersecurity and retrieval augmented generation (RAG). The key advantages of Granite 3.0 models are:

- **Lightweight:** Our largest dense model has 8 billion parameters, and our smallest MoE model has an activated parameter count of 400 million, enabling hosting, or even fine-tuning, on more limited compute resources.
- Robust Models with Permissive License: All our models, including instruct variants, use an Apache 2 license, allowing for more flexibility in consumer and enterprise usage over the more restrictive licenses of other available models in the same class. Combined with excellent performance across various benchmarks, our models provide a great foundation for enterprise customization.

• Trustworthy Enterprise-Grade LLM: All our models are trained on license-permissible data collected following IBM's AI Ethics principles<sup>1</sup> and guided by IBM's Corporate Legal team for trustworthy enterprise usage. We describe in great detail the sources of our data, our data processing pipeline, and our data mixture search to strengthen trust in our models in mission-critical and regulated contexts.

We describe the model architecture and background on MoE models in Section 2. Then, we describe our data collection, filtering, and preprocessing pipeline in Section 3. We then go into detail about our data mixture and hyperparameter search for pretraining in Section 4, followed by our post-training methodology in Section 5, and our compute infrastructure in Section 6. Section 7 describes the results of our comprehensive evaluation of the trained models, including a comparison with other open-source LLMs. Finally, Section 8 discusses the social harms and risks of this project.

## 2 Model Architecture

The Granite 3.0 language models are based on two architectures: a decoder-only dense transformer and a decoder-only sparse Mixture-of-Expert (MoE) transformer.

Model	2B Dense	8B Dense	1B MoE	3B MoE
Embedding size	2048	4096	1024	1536
Number of layers	40	40	24	32
Attention head size	64	128	64	64
Number of attention heads	32	32	16	24
Number of KV heads	8	8	8	8
MLP hidden size	8192	12800	512	512
MLP activation	SwiGLU	SwiGLU	SwiGLU	SwiGLU
Number of Experts	_	_	32	40
MoE TopK	_	_	8	8
Initialization std	0.1	0.1	0.1	0.1
Sequence Length	4096	4096	4096	4096
Position Embedding	RoPE	RoPE	RoPE	RoPE
#Parameters	2.5B	8.1B	1.3B	3.3B
#Active Parameters	2.5B	8.1B	400M	800M
#Training tokens	12T	12T	10T	10T

Table 1: Hyperparameter for Granite models.

## 2.1 Dense Models

Granite 3.0 2B and 8B dense models share a similar architecture as popular language models like Llama and our previous Granite Code models Mishra et al. (2024), ensuring strong compatibility with open-source inference and fine-tuning pipelines. We use Grouped Query Attention (GQA; Ainslie et al. 2023) with 8 key-value heads to get a good balance between memory cost and model performance, and Rotary Position Embedding (RoPE; Su et al. 2024) to model the relative position between tokens. For the MLP layers, Granite 3.0 Dense models use SwiGLU as the activation function. Before each MLP and attention layer, we use RMSNorm to normalize the layer's input. We also share parameters between the input embedding and the output linear transform. This reduces the size of the model, and we have observed that the tying of these embeddings have zero, or even a positive impact on model performance.

## 2.2 MIXTURE-OF-EXPERT MODELS

Granite 3.0 1B and 3B MoE models use similar architecture as Granite Dense models, with the MLP layers substituted with MoE layers. A Mixture of Experts (MoE) layer comprises N modules  $f_1, \ldots, f_N$  and a router  $g(e \mid \mathbf{x})$ . Given an input  $\mathbf{x}$  to the MoE layer, the router predicts a probability distribution over the N modules. Of these, we select the top k experts. When k < N, we are using a

<sup>1</sup>https://www.ibm.com/impact/ai-ethics

Sparse Mixture of Experts (SMoE; Shazeer et al. 2017). For this series of Granite MoE models, we use a linear layer to model the router:

$$\mathbf{s} = \mathbf{W}_{\text{router}} \mathbf{x},\tag{1}$$

$$g(e \mid \mathbf{x}) = \begin{cases} \operatorname{softmax} (\operatorname{Top} k(\mathbf{s}))_i, & \mathbf{s}_i \in \operatorname{Top} k(\mathbf{s}) \\ 0, & \mathbf{s}_i \notin \operatorname{Top} k(\mathbf{s}) \end{cases}$$
(2)

where  $\mathbf{W}_{\mathrm{router}}$  is the expert embedding matrix of shape  $(N, D_{\mathrm{emb}})$ , and  $\mathrm{Top}k$  is the operator that select the top k logits from  $\mathbf{s}$ . The final output of the SMoE is then given by

$$y = \sum_{e=1}^{N} g(e \mid \mathbf{x}) \cdot f_e(\mathbf{x})$$
(3)

When  $g(e \mid \mathbf{x}) = 0$ ,  $f_e(\mathbf{x})$  will not need to be evaluated, thus reducing computation cost during training and inference. The key designs of the Granite MoE models are summarized below:

**Dropless Token Routing.** Since each token selects experts independently, some experts could receive more tokens than others. In previous MoE models, like Switch Transformer (Fedus et al., 2022) and Deepseek-V2 (Liu et al., 2024), a capacity cap is set for each expert or device, and the extra tokens that exceed the cap are dropped. As observed in Gale et al. (2023), this cap negatively affects the model training stability and loss. In our training, we use ScatterMoE (Tan et al., 2024), a dropless MoE implementation, to avoid token dropping and improve training efficiency.

**Fine-grained Experts.** Recent studies (Krajewski et al., 2024; Dai et al., 2024) suggest that setting the size of experts in MoE to mirror the feed-forward layer is not optimal. Instead, increasing the expert granularity, number of experts, and number of activated experts could increase the possible combinations of experts and result in better model performance. Following these observations, we use fine-grained experts and a larger number of activated experts in Granite 3.0 MoE models. Specifically, we use a top-k of 8, and 32 and 40 experts respectively for the 1B and 3B MoE models.

**Load Balancing Loss.** To avoid routing tokens repeatedly to same expert and wasting the extra capacity in other experts, we use the frequency-based auxiliary loss introduced in Fedus et al. (2022)

$$\mathcal{L}_b = N \sum_{i=1}^{N} f_i P_i \tag{4}$$

where N is the number of experts,  $f_i$  is the fraction of tokens dispatched to expert i, and  $P_i$  is the fraction of the router probability allocated for expert i. Intuitively, this loss penalises over-usage of experts, thus 'balancing' the load. To improve the training stability, we also use the router z-loss introduced in Zoph et al. (2022):

$$\mathcal{L}_{z} = \frac{1}{B} \sum_{i=1}^{B} \left( \log \sum_{j=1}^{N} \exp(x_{j}^{i}) \right)^{2}$$
 (5)

where B is the number of tokens, x is the logits given by router. This loss penalises logits of the router when it has extreme values, allowing the router to adapt better during training in order to better assign experts. The final loss is the weighted sum of language model loss and two auxiliary losses.

## 3 Training Data

Granite 3.0 language models are trained using data from various sources such as unstructured natural language text and code data from web curated by IBM, a collection of synthetic datasets generated by IBM, and publicly available high-quality datasets with permissible licenses. For governance, all our data undergoes a data clearance process subject to technical, business, and governance review. This comprehensive process captures critical information about the data, including but not limited to their content description, ownership, intended use, data classification, licensing information, usage restrictions, how the data will be acquired, as well as an assessment of sensitive information (i.e,

personal information). For code, we annotate each code file with license information associated with the respective repository, found via Github APIs and only keep files with permissive licenses for model training. In addition, we also filter out all data obtained from sources that match URLs in IBM's URLs blocking-list. Below, we provide a brief overview about our data processing steps and refer to the Appendix A.1 for details on individual datasets used in different stages of model training.

#### 3.1 CURATED WEB DATA

We curate a massive collection of unstructured data crawled from the web, obtained from academic, enterprise (e.g., financial, legal, biomedical), code, and other publicly available sources, e.g., open-source datasets like FineWeb (Penedo et al., 2023), DCLM (Li et al., 2024) for language and Github Code Clean<sup>2</sup>, StarCoderdata<sup>3</sup> for code domain. To ensure the quality of our curated web data, we have developed a comprehensive data preprocessing procedure, as follows.

**Text Extraction.** Text extraction is the first step in the processing of unstructured data crawled from web, and is used to extract language from various documents into a standardized format for further processing. After text extraction, we apply language identification at a document level to detect the dominant language using the Watson Natural Language Processing library. With language identification, we specifically select documents annotated with 12 languages namely English, German, Spanish, French, Japanese, Portuguese, Arabic, Czech, Italian, Korean, Dutch, or Chinese as the dominant language. While our training data consists of primarily-English data, we utilize high-quality documents from these other eleven languages to improve multilinguality of Granite 3.0 models.

**Deduplication.** Deduplication aims to identify and remove duplicate documents to improve overall quality of a dataset. We adopt an aggressive deduplication strategy including both exact and fuzzy deduplication to remove documents having (near) identical content. For exact deduplication, we first compute SHA256 hash on the document content and remove records having identical hashes. Then, we follow a two-step fuzzy deduplication strategy: (1) computing MinHashes of all the documents and then utilize Locally Sensitive Hashing (LSH) to group them based on their MinHash fingerprints, and (2) measuring Jaccard similarity between each pair of documents in the same bucket to annotate documents except one as duplicates based on a similarity threshold. We apply this near-deduplication process to both language and code data to enhance the richness and diversity of the training dataset.

HAP, PII, and Malware Filtering. To reduce the likelihood of generating hateful, abusive, or profane (HAP) language from the models, we make diligent efforts to filter HAP content from our training set. We compute HAP scores based on a HAP detector trained by IBM <sup>4</sup> at the sentence level and filter out documents which exceeds a certain threshold. For code documents, we first create a dictionary of HAP keywords and then annotate each document with the number of occurrences of such keywords in the content including comments. We filter out documents which exceeds the HAP threshold, computed based on a distributional analysis as well as manual inspection of code files. Moreover, to protect privacy, we make diligent efforts to redact Personally Identifiable Information (PII) from the code training set. Specifically, we leverage the StarPII<sup>5</sup> model to detect IP addresses, keys, email addresses, names, user names, and passwords found in the content. We also scan our datasets using ClamAV<sup>6</sup> to identify and remove instances of malware, especially in the source codes.

**Document Quality Filtering.** Quality annotation aims to identify documents with low linguistic value using both heuristics and a classifier. Specifically, we follow Gopher quality filtering criteria (Rae et al., 2021) to remove low quality documents that contain for example bullet points ratio of greater than 90%, ellipsis line ratio of greater than 30% and symbol to word ratio of greater than 10%, etc. Besides heuristics, we also adopt a classifier-based filtering that assigns a perplexity score using the KenLM linear classifier, pre-trained on a small collection of known high quality documents (e.g., Wikipedia articles). For any document, the KenLM linear classifier provides a score of the document's similarity to a training corpus, indicating overall quality for model training.

<sup>&</sup>lt;sup>2</sup>https://huggingface.co/datasets/codeparrot/github-code-clean

<sup>&</sup>lt;sup>3</sup>https://huggingface.co/datasets/bigcode/starcoderdata

<sup>4</sup>https://huggingface.co/collections/ibm-granite/granite-guardian-66db06b1202a56cf7b079562

<sup>&</sup>lt;sup>5</sup>https://huggingface.co/bigcode/starpii

<sup>6</sup>https://www.clamav.net/

We also apply several heuristics to filter out lower-quality code (Mishra et al., 2024): (1) remove files with fewer than 25% alphabetic characters, (2) filter out files where the string "<?xml version=" appears within the first 100 characters, (3) for HTML files, only keep files where the visible text makes up at least 20% of the HTML code and has a minimum length of 100 characters, (4) for JSON and YAML files, only keep files that have a character count ranging from 50 to 5000 characters.

#### 3.2 SYNTHETIC DATA

Existing permissive datasets are becoming increasingly inadequate for training models with specific capabilities, e.g., coding, reasoning, and safety etc during post-training. While collecting high-quality data from humans is a potential solution for this, it is a time-consuming and costly endeavor. To address this challenge, we conduct an in-depth exploration of synthetic data generation (SDG) as an alternative for Granite models. Recently, the introduction of synthetic data pipelines such as, Self-Instruct (Wang et al., 2023), Evol-Instruct (Xu et al., 2023), and MagPie (Xu et al., 2024) leveraged ways to synthetically produce datasets nearly as comprehensive, competitive, and diverse as those created by humans. Inspired by these recent methods, our synthetic datasets are composed of input-output pairs, cover single and multi-turn scenarios, and target a generic or specific nature. In this section, we provide an overview about the synthetic datasets, what data domains they contribute to, and how we built them using a unified SDG pipeline.

Generic Instruction Data. We build generic instruction data in form of instruction-response pairs primarily using Evol-Instruct (Xu et al., 2023) and MagPie (Xu et al., 2024) methods. Specifically Evol-Instruct takes an initial seed of instruction data to generate improved complex versions of them by randomly selecting in-depth or in-breadth evolving prompt templates. We verify the quality of evolved instructions through a set of heuristics (e.g., character length, word count, seed instruction leakage) and exclude instructions that do not pass this quality verification from the final dataset. We repeat this evolution 5 times, and at each iteration, a mix of either original seed instructions or evolved instructions (that passed the quality check) are used as input for the following iteration. A list of synthetic datasets generated using Evol-Instruct can be found in Appendix A.2.

Unlike Evol-Instruct, MagPie generates high-quality instruction data without relying on prompt engineering or seed questions. Instead, it directly constructs instruction data by prompting a LLM with a pre-query template for sampling instructions. Following (Xu et al., 2024), we use 12 combinations of temperature and top-p parameters by prompting a couple of teacher models with their respective pre-queries followed by greedy sampling to generate the corresponding responses. Our final unfiltered samples target varied between 5M and 10M depending on the LLM used for generation. In addition, we also extend filtered versions of our single-turn datasets to create multi-turn datasets to enhance chat capabilities. Note that we only use open-source teacher models with a non-restrictive license to generate instructions and their respective responses <sup>7 8 9</sup>. A list of synthetic datasets generated using Evol-Instruct and MagPie can be found in Appendix A.2.

Code. As demand for software development surges, it is more critical than ever to increase software development productivity, and LLMs provide promising path for augmenting human programmers. To improve coding capabilities of Granite 3.0 models, we focus on generating high quality synthetic code data and creating quality filters to remove bad samples from our training data. Specifically, inspired by Starcoder2-Instruct<sup>10</sup>, we extend the OSS self-instruct pipeline to 6 coding languages: JavaScript, TypeScript, C, C++, Go, and Python, and use filtered pretraining data as the seed data with granite-34b-code-instruct, as the teacher model for generating instruction-response pairs. We generate 235,000 samples with this method, which serves as one of the major code generation dataset in our supervised finetuning. Beyond code generation, we also generate samples to cover tasks like code explanation, docstring, and pseudocode generation by using a generate, backtranslate, and filter process, as in (Dubey et al., 2024b). Specifically, we prompt a teacher model to generate code explanation, docstring, and pseudocode from the seed functions. These tasks are intentionally grouped together so the model's reasoning can improve with the combination of tasks. For filtering,

<sup>&</sup>lt;sup>7</sup>https://huggingface.co/mistralai/Mistral-7B-Instruct-v0.3

<sup>8</sup>https://huggingface.co/mistralai/Mixtral-8x22B-Instruct-v0.1

<sup>&</sup>lt;sup>9</sup>https://huggingface.co/mistralai/Mistral-Nemo-Instruct-2407

<sup>10</sup> https://huggingface.co/blog/sc2-instruct

we prompt the model to grade the original seed function against the synthetic code for both fidelity and complexity, and we keep samples that only pass a predefined threshold. We also adopt a similar pipeline for generation synthetic data for tasks like unit test generation and code debugging, helping our models to perform better on code fixing and explanation.

We also leverage SDG to collect multi-turn data, by incorporating execution output as feedback along with human feedback. Following (Zheng et al., 2024), we generate 50k multi-turn dialogues with code execution and synthetic code reviews. We identify python samples via model classification and heuristics in two open source datasets, namely Glaive Code Assistant <sup>11</sup> and Code Instructions Alpaca <sup>12</sup>. We filter the instructions by complexity using LLMaJ with a complexity scale of 1-5. We then use the instruction from the filtered dataset as the initial prompt in an mulit-turn agentic pipeline that consists of agents for writing, executing and reviewing code built with the AutoGen framework. Dialogues that produce trajectories with executable code with passing unit tests after a round of synthetic code review and update are included in the final dataset.

**Reasoning.** Reasoning with LLMs has been in the forefront (Plaat et al., 2024; Zhang et al., 2024a), given both the evolution of benchmarks and the inconclusive discussions around the reasoning abilities of LLMs (Kojima et al., 2023; Mirzadeh et al., 2024). However, the progress with chain-of-thought and evolution of Agentic behaviors has shifted focus towards innovative mechanisms to generate reasoning and planning traces with human validation of each step (Dubey et al., 2024a; Lightman et al., 2023). We employ two main techniques for generating synthetic reasoning data:

- Code-Assisted Synthetic Data Generation: We use code-assisted SDG for primarily algorithmic tasks (Li et al., 2023b). Within each reasoning category, we use domain-specific seed prompts and seed data to introduce diversity. Python code execution is used both to generate and validate chain-of-thought and the final answer for various reasoning tasks.
- Knowledge-based Data Generation: We utilize multiple knowledge graphs such as ATOMIC (Hwang et al., 2021) and Wikidata (Vrandečić & Krötzsch, 2014) to generate multi-hop reasoning data with the chain-of-thought that includes commonsense and encyclopedia knowledge. The initial knowledge graph seed structures are a combination of template-based and random-walk-based techniques, enabling the grounding of the reasoning traces being generated. Grounding helps in eliminating incorrect reasoning traces with both right and wrong final answers.

**Retrieval Augmented Generation (RAG)** RAG is widely recognized as a promising approach to address common challenges in large language models, such as factual inaccuracies, outdated knowledge, and limitations in domain-specific expertise (Chen et al., 2024a). To generate synthetic data for improving RAG capabilities, following (Lee et al., 2024b), we first input a document and prompt an LLM 13 to generate a user question. These questions span various types commonly found in information-seeking tasks, and to ensure that the generated questions align with the designated question types, we incorporate question-type-specific CoT prompts, to guide the language model in reasoning through the grounding document (Lee et al., 2024b). We then employ a retriever (ELSER with sentence-transformers/all-MiniLM-L6-v2 sentence embeddings) to dynamically select the top-k relevant passages from a pre-constructed document index, extending the user questions generated in the first step into multi-turn, multi-document grounded conversations. The retrieved passages, along with the query, are provided to the LLM, which is then prompted to generate a response. For subsequent turns, we first prompt the LLM to generate a query given dialog history and retrieved passages and then generate the answer as described above. Furthermore, an LLM-as-a-Judge module is used to filter out dialogues with incorrect responses by evaluating all context-response pairs within each dialogue. A larger language model <sup>14</sup> assesses the accuracy of responses based on dialogue history and the current query, and any dialogues containing incorrect question-answer pairs are discarded. The multi-turn RAG data generation use two pblicly available datasets, QuAC (Choi et al., 2018) and MultiDoc2Dial (Feng et al., 2021) as seed datasets.

<sup>&</sup>lt;sup>11</sup>https://huggingface.co/datasets/glaiveai/glaive-code-assistant-v3

<sup>12</sup>https://huggingface.co/datasets/TokenBender/code\_instructions\_122k\_alpaca\_style

<sup>&</sup>lt;sup>13</sup>https://huggingface.co/mistralai/Mixtral-8x7B-Instruct-v0.1

<sup>&</sup>lt;sup>14</sup>https://huggingface.co/mistralai/Mixtral-8x22B-Instruct-v0.1

**Tool Use.** Tool (or function) calling is now considered one of the fundamental capabilities that LLMs need to possess (Abdelaziz et al., 2024). In real-world applications, tool invocation can vary in complexity, ranging from a single turn with a single tool (the simplest case) to more challenging multi-turn interactions involving multiple sequential/nested tool calls. To train LLMs to utilize tools requires a broad spectrum of training data covering different tool calling scopes.

In the recent past, there has been extensive research on transforming existing curated and manually annotated datasets into a function calling format. While we leverage curated datasets such as API-BLEND (Basu et al., 2024) and APIGen (Chen et al., 2024b), these datasets do not address the evolving landscape of function calling benchmarks such as parallel tool calls, multiple tool calls in sequence, multi-turn tool calls, nested tool calls, and tool relevance, etc. To address this, we extend existing SDG techniques such as ToolLLM (Qin et al., 2023) and API-Bank (Li et al., 2023c) to introduce new features of function calling in LLMs. These pipelines also include generating data that calls APIs via different programming languages (Guo et al., 2024).

Cybersecurity. To create a comprehensive and diverse dataset capable of supporting instruction tuning for various security-related tasks, we adopt the process in Levi et al. (2024), which consists of two main steps, as follows. In the first generation step, we concentrate on producing high-quality instructions derived from predefined schemas. These schemas are formulated through expert-driven analysis of a diverse set of security datasets, examining the relationships between different entities across datasets. This approach ensures that the instructions capture the nuances of various security concepts and tasks. More specifically, each predefined schema has rules that dictate how the data source should be processed into instructions, using parsers developed specifically for these security data sources. This guarantees that the generated instructions focus on the important and unique characteristics of the data source and are representative of real-world security scenarios. In the second generation step, the diversity and complexity of the initial generated dataset is expanded by employing a hybrid synthetic content-grounded data generation process. Specifically, we combine Evol-Instruct (Xu et al., 2023) and Self-Instruct (Wang et al., 2022) alongside content-grounded generation and evaluation pipelines. Additionally, we implement a routing mechanism between the two generation methods to help reduce hallucinations.

This process leverages the initial set of instructions and data from the first generation step to generate additional instructions that follow the established schemas while increasing the model's overall generalizability. By incorporating content-grounded synthetic data, we increase the diversity and volume of the final dataset, ultimately leading to more robust and capable security models.

We leverage various publicly available security data sources, namely MITRE ATT&CK<sup>15</sup>, CWE<sup>16</sup>, CVE<sup>17</sup>, CAPEC<sup>18</sup>, Security Wikipedia, Security interview Q&A, Threat reports, BRON (Hemberg et al., 2020), SIEM alert rules, Sigma rules<sup>19</sup>, and Security Stack Exchange to generate both rules-based and synthetic security instructions. Our final synthetic security dataset consists of various instruction types, such as open/closed book question answering, yes/no questions, multi-choice Q&A, CoT, logic validation, odd/leave one out multi-choice Q&A, question generation, query/rule explanation and generation, TTP mapping, and others.

**Multilingual.** To improve our model's machine translation quality, we include parallel text from datasets such as ParaCrawl <sup>20</sup>, WikiMatrix (Schwenk et al., 2019a), and NLLB/CCMatrix (Schwenk et al., 2019b). We apply extensive filtering based on language specific heuristics and model based scoring to select only the highest quality translation pairs from these datasets. For example, filtering heuristics include steps such as removing samples which do not have a minimum amount of words or where source and target have too many tokens in common, contain too many repeated characters or tokens or contain too many UTF-8 control characters. We also all apply more language specific filtering heuristics, e.g. for CJK languages or Arabic, we set a minimum threshold for percent of

<sup>15</sup> https://attack.mitre.org

<sup>16</sup>https://cwe.mitre.org

<sup>17</sup>https://cve.mitre.org

<sup>18</sup>https://capec.mitre.org

<sup>&</sup>lt;sup>19</sup>https://github.com/SigmaHQ/sigma

<sup>&</sup>lt;sup>20</sup>http://paracrawl.eu

characters in the target language script. Model based filtering comprises language id and calculating alignment scores via a multilingual sentence embedding model (Artetxe & Schwenk, 2019).

Moreover, to enhance multilingual capabilities in multi-turn conversation scenarios, we translate a subset of the the publicly available Daring Anteater <sup>21</sup> SFT dataset into our targeted languages. For translation, we use Mixtral-8x22B-Instruct model and translate each turn separately, but make sure that text formatting and especially code blocks within each turn are preserved during translation.

**Safety.** To safeguard our models, we leverage synthetic data as a powerful source for augmenting AI safety training and aligning models in a targeted way. An AI risk taxonomy is a repository that classifies and structures categories of risk. IBM Research uses its AI risk taxonomy as part of a broader set of safety measures that apply to its development of foundation models. The taxonomy helps to categorize known risks, which are used to generate synthetic data, for the purpose of aligning language models. We leverage the following taxonomy for SDG that covers 7 high-level categories:

- Malicious Use: illegal activities, unethical or unsafe actions, and violence and extremism.
- System Risks: security and operational risks.
- Information Hazards: sensitive and personal information.
- Discrimination: a wide range of discrimination, including implicit and explicit bias.
- Societal Risks: disinformation, propaganda, and voter suppression.
- Human-Chatbot Interactions: mental health, child harm, and self-harm.
- Multi-Modal Requests: various forms of undesirable requests related to multi-modal support.

Our safety taxonomy has been informed by internal research as well as opensource AI risk taxonomies research conducted by MIT and MLCommons <sup>22</sup>. A diverse set of people distributed across different IBM locations worldwide with diverse expertise and socio-cultural background contributed quality seeds to address inappropriate prompts. Additionally, research into adversarial attacks also informed the seeds gathered to safeguard our model against jailbreaks and prompt injection attacks. Specifically, our synthetic safety data includes prompt-response pairs across a broad range of scenarios, covering direct requests across a safety taxonomy with direct questions, comparative questions, hypothetical prompts, adversarial attacks, and multi-turn interactions designed to expose unsafe behavior. Once generated, quality and consistency checks of the synthetic data are also applied which includes both extensive automated and manual reviews. An iterative approach was also used to improve the safety alignment data by analyzing the resulting model's behavior and producing more synthetic data to increase the safety coverage as needed.

**Quality Filtering.** When using synthetic data, we run several stages of filtering over it, removing samples that are very short, easy for a reference model, unclear instructions or duplicated samples. We follow (Xu et al., 2024) and leverage (1) LLM-as-judge (Zheng et al., 2023) to determine the category, quality, and difficulty of instructions, and (2) the computation of minimum neighbor distance in the embedding space to identify near duplicates (Douze et al., 2024). Our sample annotation pipeline uses Mistral-7B-Instruct-v0.3 <sup>23</sup> as the reference model (judge) and consists of the following steps:

- Instructions Annotation: We annotate the generated instructions with category (creative writing, advice seeking, planning, and math, etc), difficulty ('very easy', 'easy', 'medium', 'hard', or 'very hard'), and instruction quality ('very poor', 'poor', 'average', 'good', and 'excellent').
- Responses Annotation: We asses the quality of responses conditioned on their respective instruction using an LLM as judge (in a scale of 1-5).
- Sample-level Annotation: Particularly important for multi-turn datasets, we prompt an LLM for assessing overall quality of a conversation between a user and an assistant (including all turns).
- Duplicates Annotation: We measure the similarity using minimum neighbor distance in the embedding space (Xu et al., 2024). For multi-turn data, however, we concatenate the inputs from all turns and compute minimum neighbor distance in the embedding space using the full conversations.

<sup>&</sup>lt;sup>21</sup>https://huggingface.co/datasets/nvidia/Daring-Anteater

<sup>22</sup>https://mlcommons.org/

<sup>&</sup>lt;sup>23</sup>https://huggingface.co/mistralai/Mistral-7B-Instruct-v0.3

## 4 PRE-TRAINING

Granite 3.0 language models are trained on 10T to 12T tokens of language and code data, sourced from different domains. Data is tokenized via byte pair encoding (BPE, (Sennrich et al., 2015)), employing the same tokenizer as StarCoder (Li et al., 2023d). In this section, we provide details on our two stage training, data mixture and power scheduler used in pretraining the models.

#### 4.1 DATA MIXTURE

Beyond training data quality, the data mixture is another important aspect of model performance. We craft the pretraining data mixture with two goals: 1) maximize the model's performance across a diverse set of domains and tasks without bias toward a specific type of data or task; 2) leverage both high-quality and medium-quality data for optimal performance. To achieve these two goals, we adopt the 2-stage data mixture strategy used in MiniCPM (Hu et al., 2024) and JetMoE (Shen et al., 2024b). In stage 1, we pre-train the model on a large quantity of medium-quality data to learn and memorize the knowledge from diverse domains. In stage 2, we continue pre-training the model on a smaller set of high-quality data mixed with medium-quality data to encourage the model to mimic the behavior of high-quality data and improve the model's performance on downstream tasks.

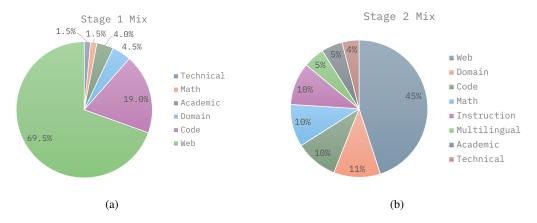


Figure 3: Data mixture for pretraining stages. The percentage for individual datasets has been merged into different categories. Best viewed in color.

#### 4.1.1 STAGE 1 DATA MIXTURE

The stage 1 data mixture search focuses on achieving robust language model performance across different domains  $D_i$ . Inspired by distributionally robust language model (Oren et al., 2019) and DoReMi (Xie et al., 2024), our target was to minimize the weighted sum of relative domain losses, with respect to a baseline:

$$\min_{\theta} L(\theta, \alpha) := \sum_{i=1}^{|D|} \alpha_i \cdot \left[ \frac{1}{\sum_{x \in D_i} |x|} \sum_{x \in D_i} \left( \ell_{\theta}(x) - \ell_{\text{ref}, i}(x) \right) \right]$$
 (6)

where  $\theta$  is the mixture percentage of pre-training data,  $\ell_{\theta}(x)$  is the negative log-likelihoods of the proxy model for data mixture search,  $\ell_{\mathrm{ref},i}(x)$  is the reference model for domain  $D_i$ , |x| is the number of tokens in an example x, and  $\alpha$  is the weights for different domains. Reference models are small language models trained with in-domain data from  $D_i$ . Our assumption here is that the loss reflects the difficulty of the target domain. By subtracting the reference model loss, we normalize the proxy model loss by removing the difficulty factor. This way, we can avoid forcing the model to learn difficult domains even if the model cannot improve further in this domain (Oren et al., 2019).

In the data mixture search, we train thousands of small proxy models with randomly sampled data mixtures to find the optimal data mixture. Each proxy model is a small language model with 10M parameters trained on 15B tokens. The ratio of the number of tokens to parameters is approximately

the same as our 8B dense model. Oren et al. (2019) and Xie et al. (2024) suggest that the maximum relative domain loss should be minimized to achieve a distributional robust language model. However, in practice, we notice that some domains are more difficult to learn in this multi-domain learning setting due to conflicts between domains or format mismatches. In other words, if we focus on reducing the maximum relative domain loss, the performance of other domains will be sacrificed. To account for that, we minimize the average relative domain loss:

$$\min_{\theta} L(\theta) := \sum_{i=1}^{|D|} \frac{1}{|D|} \cdot \left[ \frac{1}{\sum_{x \in D_i} |x|} \sum_{x \in D_i} (\ell_{\theta}(x) - \ell_{\text{ref},i}(x)) \right]$$
(7)

After running many experiments, we select the proxy model with minimum  $L(\theta)$  and use its data mixture as our stage 1 data mixture. Figure 3(a) shows the data mixture of stage 1.

#### 4.1.2 STAGE 2 DATA MIXTURE

The stage 2 data mixture search focuses on improving model performance on a diverse set of downstream tasks from natural language, code, and math domains. Similar to the stage 1, we maximize the weighted sum of performance on the three domains:

$$\max_{\theta} L(\theta, \alpha) := \sum_{i=1}^{|D|} \alpha_i \cdot \left[ \frac{1}{|D_i|} \sum_{t \in D_i} Acc_t(\theta) \right]$$
 (8)

where  $Acc_t$  is proxy model performance on the task t. We use the average across multiple tasks from each domain as the targeted metric to avoid over-fitting on a specific task.



Figure 4: The predicted and ground-truth accuracy for different data mixture samples. The x-axis is the ground truth accuracy, and the y-axis is the predicted accuracy.

However, in stage 2, we cannot use the small proxy models for the mixture search, because most downstream tasks require a model that is large enough to achieve meaningful performance. Thus, we conduct the mixture search with our 2B dense model. Even with the 2B dense model, we still cannot run thousands of experiments to find the optimal search. Instead, we run a few hundred experiments with 30B tokens from a randomly sampled mixture and use linear regression to fit the correlation between the data mixture and task performance. Figure 4 shows the correlation between the predicted and ground-truth accuracy for different domains. We can see a strong correlation between the two sets of values. Based on the linear regression results, we craft the final stage 2 mixture to achieve robust performance across different domains. Figure 3(b) shows the data mixture of stage 2.

## 4.2 TRAINING HYPERPARAMETERS

In Shen et al. (2024c), we proposed a systematic way of doing a hyperparameter search on a small scale and 0-shot transfer the hyperparameter to a large scale. The core part of this method is maximum update parameterization and a power scheduler.

**Maximal Update Parameterization.** ( $\mu$ P) (Yang & Hu, 2020; Yang et al., 2022; 2023) controls initialization, layer-wise learning rates, and activation magnitudes to ensure analytically stable training, independent of a model's width and depth. In addition to improving training stability,  $\mu$ P

improves the transferability of training hyperparameters from small proxy models to large models, a technique called  $\mu$ Transfer. The hyperparameter transferability of  $\mu$ P is theoretically justified and empirically demonstrated for width (Yang et al., 2022) and depth (Yang et al., 2023).

Table 2: List of changes applied when using  $\mu$ P.  $m_{\text{width}}$  is width multiplier, defined as  $d_m/d_{\text{base}}$ , where  $d_{\text{base}}$  is the embedding width,  $d_m$  is the target model size.

Name	Function
Embedding multiplier	Multiply the embedding output with $m_{ m emb}$
Residual Multiplier	Multiply the output of each attention and MLP layer with $m_{\rm res}$ before adding to residual connection
Initialization std	Initialize internal weight matrices (excluding input and output embedding) with standard deviation init <sub>std</sub> $/\sqrt{m_{\rm width}}$
Learning rate scaling	Set learning rate of internal weight matrices to $\eta/m_{ m width}$
Attention logit scaling	Divide attention logits by $d_{\text{head}}$

We follow the  $\mu$ P config used in CerebrasGPT (Dey et al., 2023) to study the transferability of batch size and learning rate across different numbers of training tokens and model sizes. Table 2 lists the  $\mu$ P changes we applied to model initialization, learning rate, and multipliers.

**Power Scheduler.** is a new learning rate schedule that includes a linear warmup, a slow power decay, and a fast exponential decay:

$$\operatorname{Power}(n) = \begin{cases} \frac{n}{N_{\text{warmup}}} \cdot \eta_{\text{max}} & \text{if } n \leq N_{\text{warmup}} \\ \min\left(\eta_{\text{max}}, \beta a n^b\right) & \text{if } N_{\text{warmup}} < n \leq N - N_{\text{decay}} \\ f(n, N, N_{\text{decay}}) \cdot \beta a \left(N - N_{\text{decay}}\right)^b & \text{if } N - N_{\text{decay}} < n \end{cases}$$
(9)

where  $\beta$  is the batch size, n is the number of tokens already trained, a is the amplitude of the learning rate, b is a power-law exponent for decaying the learning with respect to the number of trained tokens, and  $\eta_{\text{max}}$  is the learning rate upper bound that rejects very large learning. Shen et al. (2024c) shows two benefits of a power scheduler: 1) it enables zero-shot transferability of learning rate between different batch sizes and numbers of training tokens, such that we can use small batch size and number of training tokens to search for optimal learning rate, then use it for large scale training runs; 2) it doesn't require a predefined number of training tokens or steps, such that we can start the training and do early exist or add additional tokens to the training and still get optimally converged model.

Combining these two methods, we conducted the hyperparameter search on a very small scale (36M parameters, up to 128B tokens) to get the optimal hyperparameters. We then zero-shot transferred this set of hyperparameters to all of our model training. More details about the hyperparameter search can be found in Shen et al. (2024c).

For all our models, we use AdamW optimizer (Diederik, 2014) with  $\beta_1=0.9, \beta_2=0.95$  and weight decay of 0.1 for training all our models. For the learning rate, we use the power scheduler with a=4, b=-0.51, and  $\eta_{\rm max}=0.02$ , and an initial linear warmup step of 2500 iterations. We use a batch size of 4M tokens during both stages of pretraining.

#### 4.3 MODEL PARALLELISM

We use a combination of 3D parallelism (Tensor Parallelism (Shoeybi et al., 2020), Pipeline Parallelism (Narayanan et al., 2021b) and Data Parallelism (Li et al., 2020)) for training all our models. We use tensor parallelism to split the weight matrices and activations and pipeline parallelism to slice the model along the layers. We put an equal compute load on each pipeline stage except the first and last pipeline stages, which contain the embedding matrix and the LM head, respectively. The 2B dense model is trained with 256 GPUs using tensor parallel sharding on 2 GPUs, and the 8B dense model is trained on 768 GPUs using 4x tensor parallelism and 4x pipeline parallelism. We use the 1F1B (1-Forward 1-Backward) schedule (Narayanan et al., 2021a;b) for efficient pipeline parallelism to reduce the memory consumption for the in-flight microbatches. The 1F1B schedule makes the memory consumption proportional to the pipeline depth instead of the number of in-flight

microbatches, which can be quite large when training such models. We shard the optimizer on the Data Parallel process group similar to ZeRO-1 (Rajbhandari et al., 2020) for reducing the optimizer memory footprint during training. Because tensor parallelism is extremely latency sensitive and blocking in nature, we only do tensor parallelism within a server node while pipeline parallelism and data Parallelism can span across nodes. We only use data parallelism without any model parallelism to train the MoE models. They are trained using 128 and 256 GPUs using ZeRO-1 sharding (Rajbhandari et al., 2020) to shard the optimizer across multiple GPUs. To accelerate training, we use FlashAttention 2 (Dao et al., 2022; Dao, 2023), the persistent layernorm kernel, Fused RMSNorm kernel (depending on the model), and the Fused Adam kernel available in NVIDIA's Apex library.

# 5 Post-training

We develop the post-training (instruct) variants of our Granite 3.0 models by further training the pre-trained checkpoints, focusing on instruction-following capabilities and alignment with human values. We employ a diverse set of techniques with a structured chat format, including curriculum-based supervised finetuning, model alignment using proximal policy optimization (PPO), best-of-N sampling, BRAIn (Pandey et al., 2024), and model merging.

### 5.1 STRUCTURED CHAT TEMPLATE

While a pre-trained model may generate reasonable responses to directives—or, instructions—a standardized chat format is commonly used in post-training. A common format not only reinforces the structure of query and response pairs used in the applications of instruct-styled models but also allows for further control sequences to denote different actors within a single input provided to the model, such as information from external systems. To support both human-AI and machine-AI interactions with the instruction-following variants of Granite, we develop a structured interface that enhances the model's ability to follow directives as including follow ups. The structure is split in multiple sections, or turns, where knowledge is commonly formatted and then aggregated for the model. For basic uses, turns include sections for just the human and the model; however, for enterprise uses, flexibility was added so that turns can include system information, external tools and functions available, further context, and even other agents and their responses (see Table 3).

```
<|start_of_role|>user<|end_of_role|>What is 1+1?<|end_of_text|>
<|start_of_role|>assistant<|end_of_role|>2<|end_of_text|>

<|start_of_role|>system<|end_of_role|>Your name is Granite.<|end_of_text|>
<|start_of_role|>available_tools<|end_of_role|>[{"name": "get_temp", ...}, ...]<|end_of_text|>
<|start_of_role|>user<|end_of_role|>What is temperature in Boston?<|end_of_text|>
<|start_of_role|>assistant<|end_of_role|><|tool_call|>[{"name": "get_temp", ...}]<|end_of_text|>
<|start_of_role|>tool_response<|end_of_role|>{"temp": 20.5, "unit": "C"}<|end_of_text|>
```

Table 3: Chat template for conversational tasks. Top of the table refers basic single turn chat between user and assistant, while the bottom shows an example of our model in tool use.

Additionally, we carefully study the impact of specific/control tokens used in the structure of the prompt template, as shown in Table 4. Through ablations studies of different tokenizers, we find most BPE tokenizers fail to create guaranteed boundary lines when simple separators such as a newline are used. This not only makes masking during supervised finetuning unreliable but also leaks prompt control sequences into the prompt's text resulting in unwanted behavior and subpar performance. As such, we add special tokens into the vocabulary that allow us to create a structured language in the prompt that guarantees a separation between the formatting of the prompt and the prompt text itself.

```
      <|start_of_role|>
      Denotes the start of a new turn, and precedes a role label.

      <|end_of_role|>
      Follows the role label and indicates the end of the turn's header.

      <|end_of_text|>
      Denotes the end of the turn and is trained as the end of sequence token.

      <|tool_call|>
      Produced by the model and is a designation that a function call follows
```

Table 4: Control tokens added to the vocabulary for user and assistant interactions.

Specifically, during post-training, the model has learned multiple roles, including: **user** role for any human input or, the query in the instruction-following system, **assistant** which indicates any output generated by the model, **available\_tools** a turn for a structured list of tools and functions available to model to use, **tool\_response** role of any external system that produces information based on a called tools, and a **system** role for guiding information that does not necessarily pertain to the user's query.

#### 5.2 Supervised Finetuning

To enable instruction-following capabilities in our model, we further trained the pre-trained models using supervised finetuning with a curriculum-based approach where, in the first stage, we use all selected data and in the second phase, we focus on high quality, multiturn reasoning data with some data replay from the first stage. Furthermore, to support the model's ability to stop after a single turn in a multiple conversation, we unlearn the end of sequence token from pretrained model by setting its embedding weight to the arithmetic mean of the full embeddings vector. We then use the end of sequence token as the indicator for the end of a turn in the prompt structure.

We compute the loss at each step only on tokens produced by the model at any point in the prompt structure. That is, for multiturn samples, the loss is calculated for each model turn starting after the turn's header and until the next end of sequence token is reached. Everything else, including prompt control sequences, user and tools inputs, is masked out. To optimize training, we use variable length flash attention as well as the fit-first-decreasing bin packing algorithm to pack samples to create a near static batch size based on tokens instead of samples.

#### 5.2.1 Data Mixture

Data mixture plays a critical role in supervised finetuning for improving model usability and general performance. We first create an internal set of benchmarks that focus on various domains useful for enterprise deployments of AI, including math, reasoning, and instruction following. We then create a static set of training examples as a baseline and mixed in one epoch of a single dataset to see how the model improves over that said baseline for each dataset in our finetuning mixture.

We filtered datasets that did not see improvement and grouped together datasets that showed improvement in the same domains. We then trained models with various sampling proportions to find a mixture of datasets with best average improvement over the baseline across the targeted domains. To find the optimal data mixture, we train for 5 million samples and test sampling rates that correspond to the range from a half epoch to four epochs of a dataset group. Note that we use a combination of only permissively licensed data from publicly available sources and internally collected SFT data, where each sample is formatted in form of instruction and response pairs (with optional context). Table 5 lists the overall statistics of our SFT data across six broad categories from general English to safety, used in Granite 3.0 post-training. See Section A.2 for the full list of individual datasets.

Domains	Avg. # turns	Avg. # tokens	Avg. # input tokens	Avg. # output tokens
General English	1.33			
Multilingual	1.75			
Code	1.15			
Tools	2.13			
Math	1.00			
Safety	1.00			

Table 5: Statistics of supervised finetuning data. Overall, our SFT data is largely comprised of three key sources: (1) publicly available datasets with permissive license, (2) internal synthetic data targeting specific capabilities, and (3) very small amounts of human-curated data.

# 5.2.2 Hyperparameter Search

We perform extensive search over the hyperparameters after the data mixtures are finalized. We search parameters such as learning rates, weight decay, warmup ratio, and batch size using the same metrics as the data mixture search. Ultimately, the first stage of SFT use a batch size of 1 million tokens with a learning rate in the magnitude of 1e-2. We employ a cosine decay schedule for the

learning rate with a warmup ratio of 0.1 for 8b and 0.2 for 3b, and we decay to 0.1 of the peak learning rate for all models. Additionally, we set a constant weight decay of 0.1. For the second stage, we drop the batch size down to 32 thousand tokens, and the learning rate to magnitude of 1e–7. We train for 20 million samples in first stage and 100 thousand samples in stage two, which equates to approximately 30 thousand total training steps. We follow similar hyperparameters and settings for training both dense and MoE models.

#### 5.3 Model Alignment

We further train our SFT models with reinforcement learning for human preference alignment. Specifically, the backbone of our model alignment is an unique combination of PPO (Rafailov et al., 2024; Korbak et al., 2022), BRAIn (Pandey et al., 2024), and Best-of-N Sampling, with an ensemble of reward models. Below we provide a brief description of the alignment data, followed by alignment techniques and different reward models with their ensemble used to align Granite 3.0 models.

#### 5.3.1 ALIGNMENT DATA

The alignment data composition plays a critical role in the usefulness and behavior of language models. Table 6 shows the composition of our data mixture that we used to align the Granite 3.0 models. We primarily use publicly available high quality datasets with permissible license including synthetic prompts tailored for improving specific capabilities like knowledge-based question and answering. We perform several small-scale experiments to find the optimal mixture across four key categories, such as general English, code, math and safety. This optimal mixture is used for all the algorithms described in the subsequent sections.

CategoriesProportionsDatasetsGeneral English40%HelpSteer2 24, ShareGPT Prompts 25, Truthy-DPO 26, Synthetic PromptsCode25%Synthetic Coding Prompts generated using modified OSS Instruct 27Math5%MetaMathQA 28Safety30%Anthropic-HH-RLHF 29

Table 6: Data mix used for aligning the SFT models.

## 5.3.2 ALIGNMENT TECHNIQUES

Following supervised finetuning, we employ model alignment techniques that rely on reward model(s) for supervision. The training objective aims at maximizing the expected reward, often augmented with a penalty term controlling the KL divergence of the learned policy from the initial SFT policy,

$$\mathbb{E}_{(x,y) \sim D_{\pi_{\theta}}} \left[ r(x,y) - \beta \log \frac{\pi_{\theta}(y|x)}{\pi_{SFT}(y|x)} \right]$$

where r denotes the reward score,  $\pi_{\theta}$  represents the policy being learned and  $\pi_{SFT}$  is the initial (instruct) model, serving as a baseline policy.  $\beta$  moderates the Kullback-Leibler divergence to prevent excessive deviation of  $\pi^{\theta}$  from  $\pi^{SFT}$ . The optimal policy under this objective can be written as (Rafailov et al., 2024; Korbak et al., 2022):

$$\pi_{\theta}^* \propto \pi_{\text{SFT}}(y|x) \exp\left(\frac{r(x,y)}{\beta}\right)$$
 (10)

Proximal Policy Optimization (PPO) learns a policy that minimizes the reverse KL-divergence to the above optimal policy. BRAIn, on the other hand, optimizes forward KL between optimal policy and

<sup>&</sup>lt;sup>25</sup>https://huggingface.co/datasets/nvidia/HelpSteer2

 $<sup>^{26}</sup> https://hugging face.co/datasets/anon8231489123/Share GPT\_Vicuna\_un filtered$ 

<sup>&</sup>lt;sup>27</sup>https://huggingface.co/datasets/jondurbin/truthy-dpo-v0.1

<sup>&</sup>lt;sup>28</sup>https://github.com/bigcode-project/starcoder2-self-align

<sup>&</sup>lt;sup>29</sup>https://huggingface.co/datasets/meta-math/MetaMathQA

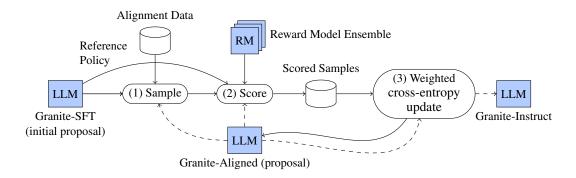


Figure 5: Granite 3.0 model alignment framework includes multiple iterations involving (1) Sampling, (2) Sample scoring optionally involving a proposal distribution, a reference distribution (SFT), an esemble of Reward Models and a Value Function. (3) SFT using a weighted cross-entropy loss. Process is repeated using updated model as new proposal (dashed line). The methods used in succession are BRAIn, PPO and a last iteration of Best-of-N sampling.

current policy (Pandey et al., 2024) and results in very effective LLM alignment (Shen et al., 2024a). For aligning Granite 3.0 models, we combine the optimization of forward KL (BRAIn) and reverse KL (PPO) in a sequential manner – starting with a single iteration of Best-of-N (BoN) training, we first apply PPO followed by a short run of BRAIn training. We find this recipe to be quite effective for model alignment, achieving higher performance compared to any of the individual methods involved. See figure 5 for an illustration of our alignment framework.

**Best-of-N Sampling.** We use a single iteration of Best-of-N (BoN) sampling, as the first step in our model alignment pipeline. Training on BoN samples is by far the simplest yet very effective alignment technique (Stiennon et al., 2020; Sessa et al., 2024). We generate 64 responses for each sample and then rank them using an ensemble of the first two reward models from section 5.3.3. We experiment with both arithmetic mean and geometric mean to ensemble reward scores. Both methods perform similarly, with arithmetic mean giving more consistent gains across experiments.

**Proximal Policy Optimization.** PPO is a policy gradient method that employs a surrogate loss to efficiently minimize the reverse KL divergence to the optimal policy in 10. We use the trlX library (Havrilla et al., 2023) for PPO training; we modified the trlX to allow for LoRA training, with alpha and rank both set to 8. Each PPO run performs 1000 updates with a batch size of 8 and learning rate of 5e-7. The KL penalty coefficient is initialized at 0.05 and goes to a target value of 2 during the course of training. The number of rollouts is set to 64, with the reward as an arithmetic mean of normalized scores from three different reward models, described in section 5.3.3.

**BRAIn.** While PPO optimizes the reverse KL-divergence between the model and the target policy, BRAIn and its variants (Pandey et al., 2024; Wang et al., 2024) optimize a self-normalized version of the forward-KL divergence and has been shown to achieve improved performance on several tasks such as abstractive summarization, helpfulness and chat benchmarks. The proposal distribution in BRAIn is updated after every 100 steps of training and the samples from the proposal distribution are labeled using an arithmetic mean of the reward models. These samples are then used for the next 100 steps of training. The cycle repeats until all the data available is exhausted.

## 5.3.3 REWARD MODELS

Unlike most alignment approaches, in this work, we do not collect any human annotations over the model responses – to make up for the lack of direct human annotations, we instead resort to an ensemble of three vastly different rewarding mechanisms – 1) an aspect-level reward model akin to the SteerLM (Wang et al., 2024), 2) a standard Bradley Terry reward model trained on preference pairs and 3) ratios of log-probabilities from two related models, as a contrastive reward signal. In the following, we discuss each of these in some detail followed by a discussion on ensembling strategies.

**Multi-Aspect Reward Model.** We train a multi-aspect regression-based reward model using Mistral-Nemo-Instruct <sup>30</sup> following the SteerLM recipe from HelpSteer2 (Wang et al., 2024), where each model predicts the scalar value of the response's rating (a float ranging from 0 to 4) for each fine-grained aspect: Helpfulness, Correctness, Coherence, Complexity, and Verbosity. When using this reward model for alignment, the individual scores are collapsed into one score using the weights prescribed in (Wang et al., 2024). These collapsed weight give a RewardBench score of 87.

**Bradley-Terry Reward Model.** We train an autoregressive reward model with the standard Bradley-Terry objective (Bradley & Terry, 1952; Rafailov et al., 2024) on pairs of preference data. The training data comprises one million preference pairs, including open-source gold preference data from various domains as well as synthetically generated preference pairs. For synthetic data generation, we adopt the model-gap strategy from (Naseem et al., 2024), where the accepted response come from a strong model (Mixtral 8x22b Instruct <sup>31</sup>, Mixtral 8x7b Instruct <sup>32</sup>) and the rejected response comes from a weaker model (Mistral 7b Instruct v0.1 <sup>33</sup>). We train a Mistral-7B-Instruct-v0.2 <sup>34</sup> on the whole preference data; The training hyper-parameters and the proportions of each data in the training mix are discussed in Appendix A.3.2. Our trained reward model gives a score of 84.5 on RewardBench.

Contrastive Reward Model. Two independent lines of prior work have shown contrastive log probabilities as an informative signal: First, in decoding research, a number of papers have shown that the difference between probabilities of a strong model and a related weak model can pick the next token more accurately than any of the two models being contrasted (Li et al., 2023e). Second, following the Direct Preference Optimization work (Rafailov et al., 2024), it has been shown that the sample level density ratio of the DPO instruct model with its corresponding base model gives high performance on RewardBench (Lambert et al., 2024). In this work, we contrast the Granite-3.0-8B-Instruct (SFT only) model with the Granite-3.0-2B-Instruct (SFT only) model and aggregate token level reward to get a sample level reward that is then used in the alignment algorithms.

**Ensemble of Reward Models.** When ensembling the reward models, we experiment with two simple approaches. 1) we compute the arithmetic mean of normalized reward scores, where each reward model's score is individually normalized using its mean and standard deviation over a range of samples. This approach can be used with all three alignment techniques. 2) we rank multiple responses for the same input separately using each reward signal, we then compute the score of each sample as the geometric mean of its ranks across reward models, the lower is better in this case. This approach is suited for best-of-N sampling and BRAIn.

### 5.4 MODEL MERGING

We systematically train multiple models at each stage of the post-training pipeline, each specialized in a specific domain, such as multilingual understanding or reasoning. Before moving to the next stage of training and alignment, we merge the different model weights to create the best overall model across the tasks. The model's performance is validated on the same set of internal training benchmarks used in the data mixture and hyperparameter searches.

## 6 INFRASTRUCTURE, ENERGY CONSUMPTION AND CARBON EMISSIONS

**Infrastructure.** We train the Granite 3.0 models using Blue Vela, one of IBM's supercomputing clusters building with NVIDIA H100 SuperPod and IBM Spectrum LSF. Each node in Blue Vela consists of dual 48-core processors, 8x NVIDIA H100 SXM5 80GB and 10 NVIDIA ConnectX-7 NDR InfiniBand Host Channel Adapters (HCA). Blue Vela employs 3.2Tbps InfiniBand interconnect to facilitate seamless communication between nodes, known for their high throughput and low latency. In addition, Blue Vela employs a separate, dedicated storage subsystem which is designed around the IBM Spectrum Scale ecosystem and the new IBM Storage Scale System 6000 (SSS) (Gershon

 $<sup>^{30}</sup> https://hugging face.co/mistralai/Mistral-Nemo-Instruct-2407$ 

<sup>&</sup>lt;sup>31</sup>https://huggingface.co/mistralai/Mixtral-8x22B-Instruct-v0.1

<sup>32</sup>https://huggingface.co/mistralai/Mixtral-8x7B-Instruct-v0.1

<sup>&</sup>lt;sup>33</sup>https://huggingface.co/mistralai/Mistral-7B-Instruct-v0.1

<sup>&</sup>lt;sup>34</sup>https://huggingface.co/mistralai/Mistral-7B-Instruct-v0.2

et al., 2024). Utilizing InfiniBand and PCIe Gen 5 technology for optimal performance, each SSS appliance is capable of delivering upwards of 310 GB/s throughput for reads and 155 GB/s for writes. The Blue Vela cluster runs on 100% renewable energy to minimize the environmental impact.

**Energy Consumption and Carbon Emissions.** The training has consumed energy result in emission of carbon dioxide. We show the energy consumption and carbon emission in Table 7. To calculate Watt-hour, we follow Touvron et al. (2023) which uses the formula:

Wh = GPU-hours 
$$\times$$
 (GPU power consumption)  $\times$  PUE

where Power Usage Effectiveness (PUE) is set with 1.1. To calculate the emission we use the US national average carbon intensity factor of 0.39 kg CO<sub>2</sub>eq/KWh according to U.S. Energy Information Administration<sup>35</sup> without taking location of data centers in consideration. A number of mitigation strategies can be used to reduce the energy and carbon footprint of training future Granite models. For example, the amount of resources used in training may be adjusted as a function of the availability of renewable energy, or the resources usage may be capped to not exceed certain energy usage or emissions limits. Moreover, we hope that releasing all our Granite 3.0 models in open source will help to reduce future carbon emission since the training is already done, and the models are relatively small and can be run on a single GPU (maximum 8B params).

Table 7: Energy consumption and carbom emissions of training Granite 3.0 models in the same data center. We take PUE of 1.1 and 0.39kg  $CO_2eq/KWh$  as carbon intensity factor.

Model	GPU power consumption	GPU-hours	Total power consumption (MWh)	Carbon (tCO <sub>2</sub> eq)
Granite 3.0 2B	700W	192,030	147.8	57.6
Granite 3.0 8B	700W	832,102	640.6	249.8
Granite 3.0 1B-400M	700W	71,171	54.6	21.3
Granite 3.0 3B-800M	700W	133,308	102.6	40.0

## 7 EVALUATION

## 7.1 PRE-TRAINED LANGUAGE MODEL

We compare our pre-trained Granite models (base) against models with similar active parameters from the following releases: Llama 3.1 and 3.2 (Dubey et al., 2024b), Gemma-2(Team et al., 2024), Mistral (Jiang et al., 2023), SmolLM <sup>36</sup>. All benchmark scores for baseline models were also evaluated ourselves using LM evaluation harness (Gao et al., 2024) using the same pipeline

For the Granite 3 2B model, we compare its performance against Llama 3.2 3B, and Gemma 2 2B. Llama 3.2 performs very well at benchmarks evaluating across a broad variety of different capabilities like MMLU and AGI-eval. However, on many other metrics, our 2B model outperforms both Gemma-2 and Llama-3.2. Our base Granite 3 8B model was compared against Mistral 7B and Llama 3.1 8B. On most benchmarks, we outperform these two models. On benchmarks where the Granite-3 8B model does not outperform, the performance is comparable to the Llama 3.1 8B.

Considering the architectural similarity, the main difference in these available models is in the training data. This suggests that our data mixture is well optimized for improvements on a variety of different tasks.

<sup>35</sup> https://www.eia.gov/tools/faqs/faq.php?id=74&t=11

<sup>36</sup>https://huggingface.co/blog/smollm

Benchmark Param	Metric	Gemma-2 2B	Llama-3.2 3B	Granite-3.0 2B	Mistral 7B	Llama-3.1 8B	Granite-3.0 8B
Human Exams							
MMLU	5-shot	53.01	56.16	55.00	62.33	65.95	65.54
MMLU-Pro	5-shot	21.97	24.98	23.79	29.49	32.60	33.27
AGI-Eval	5-shot	21.47	24.40	22.56	25.34	33.44	34.45
Commonsense							
WinoGrande	5-shot	71.59	71.59	74.90	78.37	79.24	80.90
OBQA	0-shot	41.80	43.00	43.00	44.20	44.40	46.80
SIQA	0-shot	52.66	39.69	59.84	39.38	53.90	67.80
PIQA	0-shot	79.11	77.48	79.27	82.15	81.18	82.32
Hellaswag	10-shot	74.66	76.39	77.65	83.01	81.70	83.61
TruthfulQA	0-shot, mc2	36.27	39.21	39.90	42.58	45.25	52.89
Reading Comp	rehension						
BoolQ	5-shot	78.59	74.28	81.35	84.28	85.63	86.97
SQuAD 2.0	0-shot	18.36	17.84	25.22	20.96	24.09	32.92
Reasoning							
ARC-C	25-shot	53.33	50.34	54.27	60.15	57.68	63.40
GPQA	0-shot	24.66	28.86	30.58	29.61	28.78	32.13
BBH	3-shot	36.45	39.54	40.69	44.99	46.42	49.31
MUSR	0-shot	41.27	35.58	34.34	40.74	37.96	41.08
Code							
HumanEval	pass@1	18.90	17.68	38.41	27.44	31.71	52.44
MBPP	pass@1	27.40	33.40	35.40	37.40	37.60	41.40
Math							
GSM8K	5-shot	23.88	25.17	47.23	36.85	50.64	64.06
MATH	4-shot	14.88	6.86	19.46	12.60	22.90	29.28
Average							
All	avg	41.59	41.18	46.47	46.41	49.53	54.77

Table 8: Base version performance for Granite-3.0 dense and baseline models.

## 7.2 POST-TRAINED LANGUAGE MODEL

## 7.2.1 Instruction Following

We evaluate the model's instruction following capabilities with the help of two benchmarks: IFEval (Zhou et al., 2023) and MT-Bench (Zheng et al., 2023). Tables 10, 11 show the results of all the models for the two benchmarks.

**IFEval** It contains 25 types of verifiable instructions and 500 prompts, where each prompt contains one or more verifiable instructions. **Prompt-level strict-accuracy** (the percentage of prompts that follow all verifiable instructions) and **Inst-level strict-accuracy** (the percentage of verifiable instructions that are followed) are the two metrics we average to evaluate the models.

MT-Bench MT-Bench contains 80 high-quality multi-turn questions to test the multi-turn conversation and instruction-following abilities of the models. The benchmark uses GPT-4 as a judge to evaluate the models. The judge is asked to evaluate the turn-1 and turn-2 responses of the models (given a reference answer wherever applicable) on a scale of 1-10. The judge checks for the correctness and helpfulness of the generated responses. We present the average of turn-1 and turn-2 scores for all the models (this average is further averaged over 5 independent runs).

The dense 2B model underperforms Gemma-2 and Llama-3.2, but our 8B models outperforms Mistral and Llama-3.1. For our MoE models, compared to equivalent activated parameter models, our models perform better on the instruction benchmarks.

Benchmark Metric	SmolLM	Granite-3.0	Llama-3.2	SmolLM	Granite-3.0
Active parameters	360M	400M	1B	1.7B	800M
Total parameters	360M	1B	1B	1.7B	3B
Human Exams					
MMLU	26.01	25.69	30.79	28.80	48.64
MMLU-Pro	11.24	11.38	11.78	11.55	18.84
AGI-Eval	19.21	19.96	19.68	19.06	23.81
Commonsense					
WinoGrande	57.22	62.43	60.69	60.93	65.67
OBQA	37.60	39.00	37.20	42.00	42.20
SIQA	34.88	35.76	34.42	34.63	47.39
PIQA	71.33	75.35	74.59	76.06	78.29
Hellaswag	53.45	64.92	63.66	65.74	72.79
TruthfulQA	38.02	39.49	37.67	38.50	41.34
Reading Comprehension					
BoolQ	62.69	65.44	66.12	68.96	75.75
SQuAD 2.0	3.15	17.78	10.17	11.47	20.96
Reasoning					
ARC-C	35.92	38.14	36.26	46.42	46.84
GPQA	26.26	24.41	23.57	22.82	24.83
BBH	26.20	29.84	30.76	29.30	38.93
MUSR	41.01	33.99	34.39	33.99	35.05
Code					
HumanEval	10.98	21.95	16.46	21.34	26.83
MBPP	13.80	23.20	22.20	29.20	34.60
Math					
GSM8K 5-shot	1.36	19.26	6.90	6.60	35.86
MATH	1.08	8.96	1.82	3.18	17.40
Average					
All	30.25	34.57	32.83	34.40	42.05

Table 9: Base version performance for Granite-3.0 MoE and baseline models

### 7.2.2 **SAFETY**

We evaluate the model's harmlessness behavior using the **AttaQ** benchmark (Kour et al., 2023). Attaq is a semi-automatically curated dataset, consisting of Adversarial Question Attack samples. These samples represent queries that the LLMs must refrain from answering. It consists of 7 labels or categories of harmful input prompts – Harmful Info, PII, Substance Abuse, Explicit Content, Violence, Discrimination, and Deception. To evaluate the model's responses to input prompts belonging to each of the above-mentioned categories, we make use of a reward model judge<sup>37</sup>.

Figures 2(b), 6(a), 6(b) shows the radar plots of the different models for each of the AttaQ categories. Granite-3.0 models perform best for all three plots.

### 7.2.3 Function Calling

The function calling tasks evaluates the LLMs ability to effectively use external APIs/tools to perform user-specified tasks. We evaluate Granite-3.0 function calling capabilities against existing models of similar sizes using the following public benchmarks. All evaluations for all models are done in a zero-shot manner. Tables 12, 13 show the results of the models on Berkeley Function-Calling Leaderboard<sup>38</sup> (BFCL-v2), API-Bank (Li et al., 2023c), API-Bench (Patil et al., 2023), ToolAlpaca (Tang et al., 2023), and Nexus (Srinivasan et al., 2023). The details of each of these datasets are specified below:

<sup>&</sup>lt;sup>37</sup>https://huggingface.co/OpenAssistant/reward-model-deberta-v3-large-v2

<sup>38</sup>https://gorilla.cs.berkeley.edu/blogs/12\_bfcl\_v2\_live.html

Benchmark	Metric	Gemma-2	Llama-3.2	Granite-3.0	Mistral	Llama-3.1	Granite-3.0
Parameter	rs	2B	3B	2B	7B	8B	8B
Open Leaderborads							
Open LLM Leaderb	road 1	58.70	61.47	62.26	65.54	68.58	69.04
Open LLM Leaderb	road 2	33.70	33.73	31.38	34.61	37.28	37.56
LiveBench		20.70	22.90	19.30	22.40	27.60	25.20
MixEval		66.20	65.20	64.80	73.55	73.35	76.55
Instruction Followin	ıg						
IFEval	0-shot	53.83	51.00	46.07	49.93	50.37	52.27
MT-Bench		7.91	8.04	7.66	7.67	7.93	8.22
Human Exams					•		
AGI-Eval	5-shot	30.94	30.82	29.75	37.15	41.07	40.52
MMLU	5-shot	56.83	59.68	56.03	62.01	68.27	65.82
MMLU-Pro	5-shot	27.19	30.06	27.92	30.34	37.97	34.45
Commonsense					•		
OBOA	0-shot	44.20	36.00	43.20	47.40	43.00	46.60
SIQA	0-shot	60.83	57.98	66.36	59.64	65.01	71.21
Hellaswag	10-shot	71.21	73.47	76.79	84.61	80.12	82.61
WinoGrande	5-shot	68.90	70.17	71.90	78.85	78.37	77.51
TruthfulQA	0-shot	53.17	49.71	53.37	59.68	54.07	60.32
Reading Compreher	ısion						
BoolO	5-shot	84.37	80.46	84.89	87.34	87.25	88.65
Squad 2.0	0-shot	16.21	22.39	19.73	18.66	21.49	21.58
Reasoning							
ARC-C	25-shot	57.42	30.47	54.35	63.65	60.67	64.16
GPQA	0-shot	29.36	29.19	28.61	30.45	32.13	33.81
ввн	3-shot	43.48	43.92	43.74	46.73	50.81	51.55
Code					•		
HumanEval	pass@1	40.55	45.12	50.61	34.76	63.41	64.63
MBPP	pass@1	34.00	40.20	41.00	38.60	52.20	49.60
Math							
GSM8k	5-shot,cot	30.86	58.45	59.66	37.68	65.04	68.99
MATH	4-shot	21.76	31.36	23.66	13.10	34.46	30.94
Multilingual							
PAWS-X (7 langs)	0-shot	57.02	53.19	61.42	56.57	64.68	64.94

Table 10: Instruct version performance of Granite-3.0 dense and baseline models. The Open LLM Leaderboard 1 and 2 results are the average accuracy of tasks used in the leaderboard evaluated in the specified way.

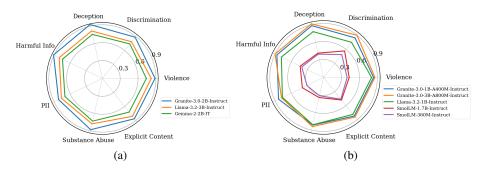


Figure 6: Radar plots showing the performance comparison of (a) 2B instruct and (b) MoE models on the AttaQ benchmark with models of similar (active) parameter counts. Best viewed in colour.

**BFCL V2** Berkeley Function Calling Leaderboard (BFCL) V2 contains 3,951 tool-calling test examples divided into the following two categories (a) Python: Simple Function, Multiple Func-

Benchmark Metric	SmolLM	Granite-3.0	Llama-3.2	SmolLM	Granite-3.0
Active parameters	360M	400M	1B	1.7B	800M
Total parameters	360M	1B	1B	1.7B	3B
Open Leaderboards	ı				
Open LLM Leaderbroad 1	35.58	46.76	47.36	39.87	55.83
Open LLM Leaderbroad 2	19.85	23.46	26.50	18.30	27.79
LiveBench	3.40	10.40	11.60	3.40	16.80
Instruction Following	•				
IFEval	14.98	32.39	41.68	9.20	42.49
MT-Bench	3.49	6.17	5.78	4.82	7.02
Human Exams	•		·		
AGI-Eval	18.25	20.35	19.63	19.50	25.70
MMLU	26.05	32.00	45.40	28.47	50.16
MMLU-Pro	11.05	12.21	19.52	11.13	20.51
Commonsense					
OBQA	37.20	38.40	34.60	39.40	40.80
SIQA	33.23	47.55	35.50	34.26	59.95
Hellaswag	51.94	65.59	59.74	62.61	71.86
WinoGrande	55.96	61.17	61.01	58.17	67.01
Reading Comprehension					
BoolQ	63.18	70.12	66.73	69.97	78.65
Squad 2.0	7.63	1.27	16.50	19.80	6.71
Reasoning					
ARC-C	38.48	41.21	41.38	45.56	50.94
GPQA	25.34	23.07	25.67	25.42	26.85
BBH	30.48	31.77	33.54	30.69	37.70
Code					
HumanEval	11.59	30.18	35.98	18.90	39.63
MBPP	14.40	15.40	37.00	25.20	27.40
Math					
MATH	0.18	10.88	17.62	0.14	19.86
GSM8k 5-shot,cot	0.30	28.66	26.16	0.61	50.94

Table 11: MoE Instruction Models

tion, Parallel Function, and Parallel Multiple Function, and (b) Non-python: Chatting Capability, Relevance/Irrelevance Detection, REST API, SQL, Java, and Javascript

**API-Bank** It has 314 dialogues with 753 API calls to evaluate LLMs' capabilities in planning, retrieving, and calling APIs. We report numbers for API-Bank level-1 which has a total of 399 test samples that test models's abilities to find the right set of APIs and its parameters from a specified list of possible APIs.

**ToolAlpaca** ToolAlpaca is a synthetic data generation approach containing 271 tool-use instances spanning 50 distinct categories. We use the simulated part of ToolAlpaca which has a total of 100 test examples.

**Nexus** NexusRaven<sup>39</sup> is another function calling test set with a total of 318 test examples covering 65 different APIs.

**API-Bench** This dataset tests the model's capability to generate a single line of code for Torchhub, Huggingface, and Tensorhub APIs. We evaluate the models by leveraging the API references obtained using BM25 retriever.

 $<sup>^{39}</sup> https://hugging face.co/datasets/Nexus flow/Nexus Raven\_API\_evaluation$ 

**SealTool** It is a synthetically generated dataset with a separate out-of-domain test set containing 654 diverse examples that use tools from a pool of size more than 4,000 tools. This test set also includes a small pool of 27 examples that require nested API calling (output of one API is used as input to the next). Since not all the models were trained with this capability and we are testing models in a zero-shot mode, we filtered those 27 nested samples and reported metrics on the remaining 627 instances that have single and multiple sequential tool calls.

**Metrics** BFCL reports *Overall Accuracy* which is a weighted average of all individual test splits which in turn uses its own metrics: Abstract Syntax Tree (AST) summary, execution summary, relevance, and irrelevance detection. In API-Bench, we used *AST tree accuracy score* as the metric. For the rest of the datasets, we report an "Exact Match" score which checks if the predicted APIs and their parameters are exact matches of the gold and in the right sequence.

Tables 12 and 13 show the results of the different models on all the above benchmarks. On average, both the 2B and 8B models outperform the other models we compare against. However, Nexus and API Bank tasks, our 8B models underperform Llama-3.1. Interestingly, our dense 2B model outperforms our 8B model on API Bank. This could suggest a high variance in model predictions across models on this task.

Shawn:	MoE	function c	alling resu	lt stuff to go	here
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Benchmark	Gemma-2 2B	<b>Llama-3.2</b> 3B	Granite-3.0 2B	Mistral 7B	Llama-3.1 8B	Granite-3.0 8B
BFCL V2	29.85	65.82	64.00	46.70	67.02	69.19
ToolAlpaca	17.00	38.00	42.00	34.00	37.00	39.00
Nexus	20.40	50.60	48.70	59.70	64.20	60.70
API Bank	21.80	45.90	66.90	60.90	68.20	63.40
SealTools	7.70	41.80	36.40	48.00	37.30	51.40
API Bench	12.75	6.11	13.91	12.40	16.32	25.46
Average	18.25	41.37	45.32	43.61	48.34	51.52

Table 12: Performance comparison of Dense models with models of comparable sizes on the Function calling benchmark

Benchmark	SmolLM	GraniteMoE	Llama-3.2	SmolLM	GraniteMoE
Active parameters	360M	400M	1B	1.7B	800M
Total parameters	360M	1B	1B	1.7B	3B
BFCL V2	10.00	43.83	21.44	10.00	41.11
ToolAlpaca	_	22.00	1.00	_	37.00
Nexus	_	29.20	5.30	_	28.90
API Bank	_	41.10	9.30	_	63.70
SealTools	_	15.00	1.90	_	24.20
API Bench	1.41	12.37	4.13	3.06	6.86

Table 13: Performance Comparison of MoE models with models of comparable sizes on the function calling benchmark

### 7.3 CYBER SECURITY

We evaluate the models performance on cyber-security tasks using the evaluation benchmark constructed by Levi et al. (2024). The benchmark includes of an extensive set of cyber-security tasks (internal) alongside other publicly available security benchmarks, the details of which are given below:

**Internal** It comprises of the following 8 cyber-security tasks comprising of custom please check if custom is a right word. evaluation data which are described as follows:

- Adversarial MITRE ATT&CK: This dataset compiled from various MITRE ATT&CK <sup>40</sup> sources, assess the model's knowledge of malware, attack tactics, and mitigations. Given an MITRE instance (e.g. description) as input the task is to classify the attack source. To further test the model's robustness Goodfellow et al. (2014); Carlini & Wagner (2017); Levi & Kontorovich (2024), the dataset has been extended to include instances of adversarial attacks for multiple-choice questions, where the attack chooses the false options that will confuse the model.
- SIEM Rule TTP Mapping: SIEM solutions detect activities like excessive firewall denials, failed login attempts, and potential botnet activity using rules. The task is to classify each of these rules by its relevant tactic or technique, with multiple-choice options and up to four applicable tags.
- *CTI Detection and Mitigation Mapping* This task assesses the model's abilities to understand the interrelationships among various Cyber Threat Intelligence (CTI) frameworks Hemberg et al. (2020) like MITRE ATT&CK, CWE <sup>41</sup>, CVE <sup>42</sup>, and CAPEC <sup>43</sup>. Specifically, it evaluates a model's proficiency in mapping tactics, techniques, attack patterns, weaknesses, and vulnerabilities to potential detection and mitigation.
- CWE Technical Impact Mapping: Exploitation of CWE weakness can lead to one or more of eight technical impacts modify data, read data, DoS through unreliable execution, DoS via resource consumption, execute unauthorized code or commands, gain privileges or assume identity, bypass protection mechanisms, or hide activities. This evaluation set consists of classification of each CWE to its related technical impact by presenting models with CWEs and their descriptions.
- *CTI Relationship Prediction*: This task tests a model's ability to determine if entities like CVE and CWE are related. The dataset presents two entities and two explanations—one supporting their relationship and one opposing it. The model must identify the correct explanation to assess the relationship.
- CTI Entity Classification: This dataset consists of descriptions of various CTI entities (e.g., weaknesses, vulnerabilities). The task is to classify whether a given description corresponds to the specified entity.
- *MITRE ATTT&CK Entity Classification*: This dataset consists of different MITRE entities. The task is to classify whether a given description is related to the specified entity.
- CWE Description Summarization: This task involves summarizing the extended CWE descriptions into brief, clear summaries that capture their core meaning.

**Public** We evaluated on the following 7 public cyber-security benchmarks:

- SecEval: SecEval Li et al. (2023a) is a benchmark for evaluating cyber-security knowledge in Foundation Models (FMs). It offers over 2,000 multiple-choice, multi-option questions across nine domains, generated by OpenAI GPT-4 using authoritative sources like textbooks, official documentation, and industry standards.
- CISSP Assessment Questions: The Certified Information Systems Security Professional (CISSP) is a recognized cyber-security certification validating deep technical and managerial competence in securing organizations. This classification task involves an evaluation set developed using multiple-choice questions from CISSP assessment tests.
- Cybersecurity Skill Assessment: This is a multiple-choice subset from LinkedIn's professional skill assessments focusing on cybersecurity. These questions evaluate candidates' general knowledge in the cybersecurity domain 44.
- *CyberMetric*: This is a benchmark dataset Tihanyi et al. (2024) for evaluating LLMs' knowledge in cyber-security. Created through a collaborative process merging expert

<sup>40</sup>https://attack.mitre.org

<sup>41</sup> https://cwe.mitre.org

<sup>42</sup>https://cve.mitre.org

<sup>43</sup>https://capec.mitre.org

<sup>44</sup>https://github.com/Ebazhanov/linkedin-skill-assessments-quizzes

knowledge with LLMs, we used the 80- and 500-question datasets, verified by human evaluators, covering a wide range of topics chosen by 30 security experts.

- Cyber Threat Intelligence Multiple Choice Questions (CTI-MCQ): This benchmark Alam et al. (2024) assesses LLMs' knowledge and capabilities in areas like attack patterns, threat actors, APT campaigns, detection methods, mitigation strategies, common software vulnerabilities, attack pattern enumeration, and public CTI quizzes.
- Cyber Threat Intelligence Root Cause Mapping (CTI-RCM) CTI-RCM (Alam et al., 2024)
  maps the root causes of vulnerabilities by correlating CVE records and bug tickets with associated weaknesses (CWEs). Accurate root cause mapping is crucial for guiding investments,
  policies, and practices to address and eliminate these vulnerabilities.
- MMLU Computer Security (SecMMLU): SecMMLU is a subset of MMLU (Hendrycks et al., 2020), specifically focused on the computer security domain. While the original MMLU includes multiple-choice questions from various fields, only those related to computer security are used in this evaluation.

We evaluate the CWE Description Summarization task using ROUGE (Lin, 2004) scores (ROUGE-1, ROUGE-2, and ROUGE-L). We compute ROUGE scores (1, 2 and L) for CWE Description Summarization. For all other tasks, we measure performance using accuracy. The reported results, averaged over internal and public benchmarks, are presented in Tables 14, 15 for both dense and MoE models in the cyber-security domain. All of our models outperform their counterpart models in this benchmark. This may be due to the focus placed on cybersecurity data in stage 2 of training and post-training. shawn: is this correct?

Benchmark	Gemma-2	Llama-3.2	Granite-3.0	<b>Mistral</b>	Llama-3.1	Granite-3.0
	2B	3B	2B	7B	8B	8B
Public (7 Tasks)	55.08	58.73	64.31	64.86	71.31	71.89
Internal (8 Tasks)	53.31	54.30	66.78	56.08	57.04	68.88
Overall (15 Tasks)	54.13	56.37	65.63	60.17	63.70	70.28

Table 14: Performance comparison of dense models with models of comparable sizes on the Cybersecurity benchmark

Benchmark Active parameters Total parameters	360M 360M	GraniteMoE 400M 1B	1B 1B 1B	SmolLM 1.7B 1.7B	GraniteMoE 800M 3B
Public (7 Tasks)	20.95	34.53	46.25	24.55	60.65
Public (8 Tasks)	30.22	41.26	43.45	34.07	58.61
Overall (15 Tasks)	25.90	38.12	44.76	29.63	59.56

Table 15: Performance Comparison of MoE models with models of comparable sizes on the Cybersecurity benchmark.

## 7.3.1 RETRIEVAL AUGMENTED GENERATION

Given the question and the relevant document in the context, we evaluate our models to generate factually correct and relevant answers. To evaluate our model's RAG capabilities, we make use of the test sets of the RagBench (Friel et al., 2024) dataset and the RAG assessment (RAGAs) evaluation framework (Es et al., 2023) to evaluate our models. For the test sets in RagBench, we use the outputs generated by the GPT-3.5 model. Table 16 shows the metrics for the different models on the different datasets of RagBench. We use GPT-4 as the LLM judge to evaluate the models. The metrics we used to evaluate the models are:

- Faithfulness: It measures the factual consistency of the generated answer wrt the given context and is computed from the answer and the retrieved context.
- Correctness: It measures answer correctness compared to the ground truth response as a combination of factuality and semantic similarity.

On average, our dense models outperform their counterparts with similar parameter size. Both our 8B and 2B models outperform other models on the MS MARCO task, a reading comprehension task, by a large margin. However, on the TechQA task, we underperform other models. This might suggest further collection of data from the technical support domain may be required.

Dataset	Gemma-2 2B		<b>Llama-3.2</b> 3B		Granite-3.0 2B		<b>Mistral</b> 7B		Llama-3.1 8B		Granite-3.0 8B	
	F↑	C↑	F↑	C↑	F↑	C↑	F↑	C↑	F↑	C↑	F↑	C↑
CovidQA	75.76	64.18	77.96	62.34	81.62	63.49	83.61	63.49	82.58	62.12	86.80	66.73
DelucionQA	80.62	63.35	83.51	63.24	84.51	61.48	88.32	60.93	87.49	69.44	85.13	67.97
<b>EManual</b>	76.78	66.33	74.61	64.63	85.08	63.93	74.89	63.55	87.40	68.09	85.67	68.24
ExpertQA	53.66	59.57	62.43	58.60	58.08	58.87	65.69	61.28	62.15	59.89	68.90	61.35
HAGRID	83.64	63.42	82.10	63.32	82.84	66.60	84.94	66.92	84.38	62.07	81.95	70.58
HotpotQA	84.98	74.16	80.36	72.19	88.55	76.26	86.90	77.09	80.77	69.29	89.48	77.85
MS Marco	79.00	63.66	82.80	62.38	85.83	65.46	82.99	63.83	86.82	62.89	90.23	68.48
PubMedQA	72.64	63.68	70.32	64.58	83.69	66.03	80.19	66.83	73.34	64.48	89.68	68.29
TAT-QA	67.63	64.40	75.22	65.14	76.12	70.85	75.74	68.14	83.14	66.89	85.82	76.38
TechQA	32.34	41.51	61.38	41.11	34.35	40.26	71.01	43.46	58.07	45.64	33.85	43.45
FinQA	52.08	47.12	57.65	52.57	63.00	56.26	62.37	57.59	72.34	58.84	66.02	58.96
Average	69.01	61.03	73.48	60.92	74.88	62.68	77.88	63.01	78.04	62.69	78.50	66.21

Table 16: RAGAs average for all

## 8 SOCIO-TECHNICAL HARMS AND RISKS

Numerous potential socio-technical harms and risks of LLMs have been identified in recent years, including misinformation, hallucination, lack of faithfulness or factuality, leakage of private information, plagiarism or inclusion of copyrighted content, hate speech, toxicity, human-computer interaction harms such as bullying and gaslighting, malicious uses, and adversarial attacks.

In line with the IBM AI Ethics Board, a central, cross-disciplinary body that defines the AI ethics vision and strategy for the IBM Corporation, we have followed several risk mitigation strategies while creating and releasing Granite 3.0 models. This includes comprehensive data governance which includes clearance, block-listing, filtering of documents with potential hate, abuse and profanity. Through model alignment with a dedicated focus on safety, we have also encouraged prosocial and less harmful model behavior with the aim to mitigate certain aspects of misuse and value alignment risks. We have also endeavoured to safeguard against some of the risks by assessing safety through standardized AI safety benchmarks which can be seen in Section 7, including internal red teaming to better understand the risks associated with external use of Granite 3.0 models in critical enterprise use cases. However, evaluating on benchmarks is only a limited approach for revealing socio-technical harms. Going forward, as the harms from LLMs become well-defined, or as Granite model capabilities advance, we will explore extended training and staged releases to further minimize risks.

In addition, as part of IBM's commitment to responsible AI, we are also introducing a new family of LLM-based Granite Guardian guardrail models <sup>45</sup>, providing the most comprehensive set of risk and harm detection capabilities available in the community today. These models can be used to monitor and manage inputs and outputs to any LLM, whether open or proprietary. We have also released a Generative AI Responsible Toolkit to support developers to build AI responsibly with out Granite 3.0 models. This encompasses a series of assets to help developers design and implement responsible AI best practices and keep their users safe. However, every enterprise often has its own regulations to conform to, whether they come from laws, social norms, industry standards, market demands, or architectural requirements; we believe that users should be empowered to personalize our released Granite models according to their own values (within bounds) (Kirk et al., 2023).

<sup>&</sup>lt;sup>45</sup>https://huggingface.co/collections/ibm-granite/granite-guardian-66db06b1202a56cf7b079562

# 9 CONCLUSION

# AUTHORSHIP, CREDIT ATTRIBUTION, AND ACKNOWLEDGEMENTS

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Infrastructure

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## A APPENDIX

#### A.1 PRE-TRAINING DATA

This section outlines the datasets employed during pre-training. To recognize specific features, we utilize the following annotations:

- P1: dataset used in stage-1 pre-training.
- P2: dataset used in stage-2 pre-training.
- ML12: sources from which we selected data in the following languages: English, German, Spanish, French, Japanese, Portuguese, Arabic, Czech, Italian, Korean, Dutch, Chinese.
- IBM-Curated: IBM's curated compendium of unstructured language data and code files.
- IBM-Synthetic: synthetic data created by IBM.

## A.1.1 WEB

- FineWeb <sup>46</sup> [P1]: The FineWeb dataset consists of more than 15T tokens of cleaned and deduplicated English web data from CommonCrawl (Penedo et al., 2024).
- Webhose [P1,P2][IBM-Curated]: Unstructured web content in English converted into machine-readable data feeds acquired by IBM.
- DCLM-Baseline<sup>47</sup> [P2]: This is a 4T token / 3B document pretraining dataset that achieves strong performance on language model benchmarks (Li et al., 2024).

### A.1.2 CODE

- Code Pile [P1,P2][IBM-Curated]: Our code pile is sourced from a combination of publicly available datasets like Github Code Clean<sup>48</sup>, StarCoderdata<sup>49</sup>, and additional public code repositories and issues from GitHub. We filter raw data to retain a list of 116 programming languages and only keep files with permissive licenses for model training.
- FineWeb-Code [P2][IBM-Curated]: FineWeb-Code contains programming/coding related documents filtered from the FineWeb dataset using a pipeline similar to FineWeb-Edu but using Mixtral-8x22B-Instruct for annotation (Penedo et al., 2024).
- CodeContests<sup>50</sup> [P2]: A competitive programming dataset for machine-learning. Problems include test cases in the form of paired inputs and outputs, as well as both correct and incorrect human solutions in a variety of languages (Li et al., 2022).

## A.1.3 DOMAIN

- USPTO [P1, P2][IBM-Curated]: Collection of US patents granted from 1975 to May 2023, excluding design patents.
- Free Law [P1, P2][IBM-Curated]: Public-domain legal opinions from US federal and state courts.
- Pubmed Central [P1, P2][IBM-Curated]: Biomedical and life sciences papers.
- EDGAR Filings [P1, P2][IBM-Curated]: Annual reports from all the publicly traded companies in the US spanning a period of more than 25 years.
- SEC Filings [P1, P2][IBM-Curated]: 10-K/Q filings from the US Securities and Exchange Commission (SEC) for the years 1934-2022.
- FDIC [P1, P2][IBM-Curated]: The data is from the annual submissions of the FDIC.

 $<sup>^{46}</sup> https://hugging face.co/datasets/Hugging Face FW/fine web$ 

<sup>&</sup>lt;sup>47</sup>https://huggingface.co/datasets/mlfoundations/dclm-baseline-1.0

<sup>48</sup> https://huggingface.co/datasets/codeparrot/github-code-clean

 $<sup>^{49}</sup> https://hugging face.co/datasets/bigcode/starcoder data$ 

<sup>&</sup>lt;sup>50</sup>https://huggingface.co/datasets/deepmind/code\_contests

- Earnings Call Transcripts [P1, P2][IBM-Curated]: Transcripts from the quarterly earnings calls that companies hold with investors. The dataset reports a collection of earnings call transcripts, the related stock prices, and the sector index.
- IBM Documentation [P2][IBM-Curated]: IBM redbooks and product documents, as well as publicly available documentation from Fortune 500 companies.
- Cybersecurity [P2][IBM-Curated]: Compendium of data crawled from web sources about cybersecurity-related topics.

#### A.1.4 MULTILINGUAL

- Multilingual Wikipedia [P2][IBM-Curated, ML12]: Multilingual Wikipedia data of 12 different languages.
- Multilingual Webhose [P2][IBM-Curated, ML12]: Unstructured multilingual web content converted into machine-readable data feeds acquired by IBM.
- Aya Dataset<sup>51</sup> [P2][ML12]: A multilingual instruction fine-tuning dataset curated by an open-science community via Aya Annotation Platform from Cohere For AI. The dataset contains a total of 204k human-annotated prompt-completion pairs along with the demographics data of the annotators Singh et al. (2024).
- MADLAD-12<sup>52</sup> [P2][ML12]: A document-level multilingual dataset based on Common Crawl, covering 12 languages filtered out of 419 languages in total.

#### A.1.5 Instructions

- Code Instructions Alpaca<sup>53</sup> [P2]: A dataset of instruction-response pairs about code generation problems.
- Glaive Function Calling V2<sup>54</sup> [P2]: A function calling dataset in real-world scenarios.
- Glaive Code Assistant V3<sup>55</sup> [P2]: A dataset of approximately 1M code problems and solutions generated using Glaive's synthetic data generation platform. This source includes the first and second versions of the dataset.
- SQL Create Context Instruction<sup>56</sup> [P2]: This dataset contains 78,577 examples of natural language queries, SQL CREATE TABLE statements that serve as context, and SQL Queries answering the question. This dataset is built upon the SQL Create Context dataset, which was constructed using data from WikiSQL and Spider.
- CommitPackFT<sup>57</sup> [P2]: A filtered version of CommitPack containing only high-quality commit messages that resemble natural language instructions (Muennighoff et al., 2023).
- OASST-OctoPack<sup>58</sup> [P2]: A filtered version of code data extracted from OASST (Muennighoff et al., 2023), which only covers high-quality conversation trees.
- FLAN <sup>59</sup> [P2]: A filtered version of the original FLAN dataset, by only keeping permissible license datasets. Wei et al. (2022).
- WebInstructSub<sup>60</sup> [P2]: A high-quality subset of the MAmmoTH2 datasetYue et al. (2024).
- Open-Platypus <sup>61</sup> [P2]: A dataset to improve LLM logical reasoning skills. The dataset was filtered using keyword search and sentence transformers to remove duplicates Lee et al. (2024a).

<sup>&</sup>lt;sup>51</sup>https://huggingface.co/datasets/CohereForAI/aya\_dataset

<sup>52</sup>https://huggingface.co/datasets/allenai/MADLAD-400

<sup>&</sup>lt;sup>53</sup>https://huggingface.co/datasets/TokenBender/code\_instructions\_122k\_alpaca\_style

<sup>&</sup>lt;sup>54</sup>https://huggingface.co/datasets/glaiveai/glaive-function-calling-v2

<sup>55</sup> https://huggingface.co/datasets/glaiveai/glaive-code-assistant-v3

 $<sup>^{56}</sup> https://hugging face.co/datasets/bugdaryan/sql-create-context-instruction$ 

<sup>&</sup>lt;sup>57</sup>https://huggingface.co/datasets/bigcode/commitpackft

<sup>&</sup>lt;sup>58</sup>https://huggingface.co/datasets/bigcode/oasst-octopack

<sup>&</sup>lt;sup>59</sup>https://huggingface.co/datasets/Muennighoff/flan

 $<sup>^{60}</sup>$ https://huggingface.co/datasets/TIGER-Lab/WebInstructSub

<sup>&</sup>lt;sup>61</sup>https://huggingface.co/datasets/garage-bAInd/Open-Platypus

- xP3x-octopack<sup>62</sup> [P2]: A subset of code-related instances extracted from xP3x, a permissive-license instruction dataset. The extraction process was performed as part of the OctoPack project Muennighoff et al. (2023).
- Function Calling/API Data [P2][IBM-Synthetic]: pavan's team will provide
- Reasoning Instructions [P2][IBM-Synthetic]: pavan's team will provide
- Multilingual Instructions [P2][IBM-Synthetic]: A multilingual synthetic dataset of instruction-response pairs that covers generic multilingual tasks.
- Language Instructions [P2][IBM-Synthetic]: A synthetic dataset of instruction-response pairs that covers generic language topics.
- Cybersecurity Instructions [P2]: A dataset of instruction-response pairs about cybersecurity topics.

## A.1.6 ACADEMIC

- peS2o<sup>63</sup>[P1, P2]: The peS2o dataset is a collection of 40M creative open-access academic papers, cleaned, filtered, and formatted for pre-training of language models. It is derived from the Semantic Scholar Open Research Corpus (S2ORC).
- arXiv [P1, P2][IBM-Curated]: Over 1.8 million scientific paper pre-prints posted to arXiv.
- IEEE [P1, P2][IBM-Curated]: Compendium of technical content from IEEE acquired by IBM.
- DeepMind Mathematics [P1, P2][IBM-Curated]: Mathematical question and answer pairs data.
- Financial Research Papers [P1, P2][IBM-Curated]: Publicly available financial research paper corpus.
- Papers With Code<sup>64</sup> [P1, P2][IBM-Curated]: Selection of publicly available academic papers sourced from the papers with code website.

## A.1.7 TECHNICAL

- Wikipedia [P1, P2][IBM-Curated]: Technical articles sourced from Wikipedia.
- Library of Congress Public Domain Books<sup>65</sup> [P1, P2]: This dataset contains more than 140,000 English books digitised by the Library of Congress (LoC) that are in the public domain in the United States.
- Directory of Open Access Books [P1, P2][IBM-Curated]: Selection of publicly available technical books sourced from the Directory of Open Access Books, a community-driven discovery service that indexes and provides access to scholarly, peer-reviewed open access books.
- Cosmopedia<sup>66</sup>: A dataset of synthetic textbooks, blogposts, stories, posts and WikiHow articles Ben Allal et al. (2024).

# А.1.8 МАТН

• OpenWebMath<sup>67</sup> [P1, P2]: This dataset contains the majority of the high-quality, mathematical text from the internet. It is filtered and extracted from over 200B HTML files on Common Crawl down to a set of 6.3 million documents containing a total of 14.7B tokens. We used a filtered version of this dataset.

 $<sup>^{62}</sup> https://hugging face.co/datasets/bigcode/xp3x-octopack$ 

<sup>63</sup>https://huggingface.co/datasets/allenai/peS2o

<sup>&</sup>lt;sup>64</sup>https://paperswithcode.com/

<sup>65</sup>https://huggingface.co/datasets/storytracer/LoC-PD-Books

 $<sup>^{66}</sup> https://hugging face.co/datasets/Hugging Face TB/cosmopedia$ 

<sup>&</sup>lt;sup>67</sup>https://huggingface.co/datasets/open-web-math/open-web-math

- Algebraic-Stack<sup>68</sup>[P1, P2]: A new dataset of mathematical code composed of 11B tokens that includes numerical computing, computer algebra, and formal mathematics. This dataset is part of the Proof-Pile-2 collection Paster et al. (2023).
- Stack Exchange [P1, P2][IBM-Curated]: Anonymized set of all user-contributed content on the Stack Exchange network, a popular collection of websites centered around usercontributed questions and answers.
- MetaMathQA<sup>69</sup>[P2]: a dataset built by rewriting mathematical questions from multiple perspectives Yu et al. (2023).
- StackMathQA<sup>70</sup> [P2]: a meticulously curated collection of 2 million mathematical questions and answers, sourced from various Stack Exchange sites Zhang (2024).
- MathInstruct<sup>71</sup> [P2]: a meticulously curated instruction tuning dataset that is lightweight yet generalizable. MathInstruct is compiled from 13 math rationale datasets, six of which are newly curated by this work. It uniquely focuses on the hybrid use of chain-of-thought (CoT) and program-of-thought (PoT) rationales, and ensures extensive coverage of diverse mathematical fields Yue et al. (2023).
- TemplateGSM<sup>72</sup> [P2]: a novel and extensive collection containing over 7 million grade school math problems with code solutions and natural language solutions designed for advancing the study and application of mathematical reasoning within the realm of language modeling and AI Zhang et al. (2024b).

### A.2 POST-TRAINING DATA

This section outlines the datasets employed during post-training. To recognize specific features, we utilize the following annotations:

- IBM-Synthetic: synthetic data created by IBM.
- ML12: sources from which we selected data in the following languages: English, German, Spanish, French, Japanese, Portuguese, Arabic, Czech, Italian, Korean, Dutch, Chinese.

## A.2.1 GENERAL ENGLISH

- Open-Platypus <sup>73</sup> [P2]: A dataset to improve LLM logical reasoning skills. The dataset
  was filtered using keyword search and sentence transformers to remove duplicates Lee et al.
  (2024a).
- WebInstructSub<sup>74</sup> [P2]: A high-quality subset of the MAmmoTH2 datasetYue et al. (2024).
- OASST-OctoPack<sup>75</sup> [P2]: A filtered version of OASST code dataset centered on covering high-quality conversation trees Muennighoff et al. (2023).
- Daring-Anteater<sup>76</sup> [IBM-Synthetic]: A comprehensive dataset for instruction tuning covering a wide range of tasks and scenarios Wang et al. (2024).
- SoftAge-Multiturn<sup>77</sup> [IBM-Synthetic]: A dataset of 400 text-only fine-tuned versions of multi-turn conversations in English based on 10 categories and 19 use cases.
- Glaive-RAG-v1<sup>78</sup>: A dataset with 50k samples built using the Glaive platform, for finetuning models for RAG use cases.

 $<sup>^{68}</sup> https://hugging face.co/datasets/Eleuther AI/proof-pile-2$ 

<sup>&</sup>lt;sup>69</sup>https://huggingface.co/datasets/meta-math/MetaMathQA

<sup>&</sup>lt;sup>70</sup>https://huggingface.co/datasets/math-ai/StackMathQA

<sup>71</sup> https://huggingface.co/datasets/TIGER-Lab/MathInstruct

<sup>&</sup>lt;sup>72</sup>https://huggingface.co/datasets/math-ai/TemplateGSM

<sup>&</sup>lt;sup>73</sup>https://huggingface.co/datasets/garage-bAInd/Open-Platypus

<sup>&</sup>lt;sup>74</sup>https://huggingface.co/datasets/TIGER-Lab/WebInstructSub

<sup>75</sup> https://huggingface.co/datasets/bigcode/oasst-octopack

<sup>&</sup>lt;sup>76</sup>https://huggingface.co/datasets/nvidia/Daring-Anteater

 $<sup>^{77}</sup> https://hugging face.co/datasets/SoftAge-AI/multi-turn\_dataset$ 

<sup>78</sup> https://huggingface.co/datasets/glaiveai/RAG-v1

- EvolKit-20k<sup>79</sup>: A 20k samples dataset build by following the Evol-Instruct method via EvolKit<sup>80</sup> framework.
- Magpie-Phi3-Pro-300K-Filtered<sup>81</sup>: A synthetic single-turn instruction dataset generated by following the MagPie method with microsoft/Phi-3-medium-128k-instruct as the text generation language model. Post-filtering was applied to obtained instances with the highest quality.
- Blue Reasoning [IBM-Synthetic]: Synthetically generated reasoning data to improve the reasoning abilities of LLMs. We used code-assisted synthetic data generation as well as knowledge-based data generation techniques to create this dataset.
- Blue Security [IBM-Synthetic]: A collection of synthetic datasets grounded in security data sources to generate both rules-based and synthetic security instructions by combining Evol-Instruct (Xu et al., 2023) and Self-Instruct Wang et al. (2022) methods alongside content-grounded generation and evaluation pipelines.
- Synthetic LMSys<sup>82</sup> [IBM-Synthetic]: A large-scale dataset containing one million real-world conversations between users and 25 state-of-the-art LLMs. This dataset was collected through the Imarena website, where it is a requirement that users give their consent to release their conversation data.
- Evol Open-Platypus [IBM-Synthetic]: A synthetic single-turn instruction dataset generated by following the Evol-Instruct method sourcing instructions from Open-Platypus<sup>83</sup> dataset and using mistralai/Mixtral-8x22B-Instruct-v0.1 as the text generation language model. Post-filtering was applied to obtained instances with the highest quality.
- MagPie Synthetic [IBM-Synthetic]: We created two synthetic single-turn instruction datasets by following the MagPie method, and respectively using mistralai/Mistral-7B-Instruct-v0.3 and mistralai/Mistral-Nemo-Instruct-2407 as text generation language models. Post-filtering was applied to obtained instances with the highest quality from both datasets. We also extended the turns of the filtered version of MagPie-Mistral-Nemo-Instruct-2407-Filtered-Single-Turn dataset to create a multi-turn version.
- LAB [IBM-Synthetic]:
- Synthetic Everyday Conversations [IBM-Synthetic]: Synthetic dataset about simple multiturn conversations between an user and an AI assistant about a given topic. Conversations cover general and science related topics. We used mistralai/Mixtral-8x22B-Instructv0.1 as the text generation language model to create this dataset.
- IBM Hardcoded [IBM-Synthetic]:
- Incapable Tasks [IBM-Synthetic]: A synthetic dataset to teach LLMs how to respond to taks that they are incapable to perform by themselves. We used mistralai/Mixtral-8x22B-Instruct-v0.1 as the text generation language model to create this dataset.
- IBM Product Feedback [IBM-Synthetic]:

#### A.2.2 MULTILINGUAL

- Aya Dataset<sup>84</sup> [ML12]: A multilingual instruction fine-tuning dataset curated by an openscience community via Aya Annotation Platform from Cohere For AI. The dataset contains a total of 204k human-annotated prompt-completion pairs along with the demographics data of the annotators Singh et al. (2024).
- Blue Multilingual [IBM-Synthetic]:
- Daring Anteater Translated [IBM-Synthetic][ML12]: A multilingual dataset created by translating the Daring-Anteater<sup>85</sup> dataset, a comprehensive instruction dataset covering a wide range of tasks and scenarios, from English to other languages.

<sup>&</sup>lt;sup>79</sup>https://huggingface.co/datasets/arcee-ai/EvolKit-20k

 $<sup>^{80}</sup>$ https://github.com/arcee-ai/EvolKit

<sup>81</sup> https://huggingface.co/datasets/Magpie-Align/Magpie-Phi3-Pro-300K-Filtered

<sup>82</sup>https://lmarena.ai/

<sup>&</sup>lt;sup>83</sup>https://huggingface.co/datasets/garage-bAInd/Open-Platypus

 $<sup>^{84}</sup> https://hugging face.co/datasets/Cohere For AI/aya\_dataset$ 

<sup>&</sup>lt;sup>85</sup>https://huggingface.co/datasets/nvidia/Daring-Anteater

#### A.2.3 CODE

- Glaive Code Assistant V3<sup>86</sup>:
- SQL Create Context Instruction<sup>87</sup>:
- Self-OSS-Instruct-SC2<sup>88</sup>:
- Blue SC Instruct [IBM-Synthetic]:
- Blue OCP Multiturn [IBM-Synthetic]:
- Blue CodeGenPlus [IBM-Synthetic]:
- Evol Blue SC Instruct [IBM-Synthetic]: A synthetic single-turn instruction dataset generated by following the Evol-Instruct method sourcing instructions from Blue SC Instruct dataset and using? as the text generation language model. Post-filtering was applied to obtained instances with the highest quality.
- Evol Blue OCP Multiturn [IBM-Synthetic]: A synthetic single-turn instruction dataset generated by following the Evol-Instruct method sourcing instructions from Blue OCP Multiturn dataset and using? as the text generation language model. Post-filtering was applied to obtained instances with the highest quality.
- Evol Blue Self-OSS-Instruct-SC2 [IBM-Synthetic]: A synthetic single-turn instruction dataset generated by following the Evol-Instruct method sourcing instructions from Blue Self-OSS-Instruct-SC2 dataset and using? as the text generation language model. Post-filtering was applied to obtained instances with the highest quality.
- Evol Blue Glaive Code Assistant v3 [IBM-Synthetic]: A synthetic single-turn instruction dataset generated by following the Evol-Instruct method sourcing instructions from Blue Glaive Code Assistant v3 dataset and using mistralai/Mixtral-8x22B-Instruct-v0.1 as the text generation language model. Post-filtering was applied to obtained instances with the highest quality.

## A.2.4 MATH

- MetaMathQA<sup>89</sup>: a dataset built by rewriting mathematical questions from multiple perspectives Yu et al. (2023).
- StackMathQA<sup>90</sup>: a meticulously curated collection of 2 million mathematical questions and answers, sourced from various Stack Exchange sites Zhang (2024).
- MathInstruct<sup>91</sup>: a meticulously curated instruction tuning dataset that is lightweight yet generalizable. MathInstruct is compiled from 13 math rationale datasets, six of which are newly curated by this work. It uniquely focuses on the hybrid use of chain-of-thought (CoT) and program-of-thought (PoT) rationales, and ensures extensive coverage of diverse mathematical fields Yue et al. (2023).

## A.2.5 Tools

- xlam-function-calling<sup>92</sup>: A 60k samples dataset created with APIGen, an automated data generation pipeline designed to produce verifiable high-quality datasets for function-calling applications. Data verification comprises three hierarchical stages namely format checking, code execution, and semantic verification that ensure the reliability and correctness of the dataset.
- Glaive Function Calling V2<sup>93</sup>: A function calling dataset in real-world scenarios.

<sup>86</sup> https://huggingface.co/datasets/glaiveai/glaive-code-assistant-v3

<sup>&</sup>lt;sup>87</sup>https://huggingface.co/datasets/bugdaryan/sql-create-context-instruction

<sup>88</sup> https://huggingface.co/datasets/bigcode/self-oss-instruct-sc2-exec-filter-50k

<sup>&</sup>lt;sup>89</sup>https://huggingface.co/datasets/meta-math/MetaMathQA

<sup>90</sup> https://huggingface.co/datasets/math-ai/StackMathQA

<sup>&</sup>lt;sup>91</sup>https://huggingface.co/datasets/TIGER-Lab/MathInstruct

<sup>92</sup>https://huggingface.co/datasets/Salesforce/xlam-function-calling-60k

<sup>93</sup> https://huggingface.co/datasets/glaiveai/glaive-function-calling-v2

- Hermes Function Calling V1<sup>94</sup>: A structured output dataset composed by function-calling conversations, json-mode, agentic json-mode, and structured extraction samples, designed to train LLM models in performing function calls that returned as a structured output based on natural language instructions. The dataset features various conversational scenarios where AI agents are required to interpret queries and execute appropriate single or multiple function calls.
- Function Calling/API Data [IBM-Synthetic]:

## A.2.6 SAFETY

- SimpleSafetyTests<sup>95</sup>:
- HarmBench Behaviors<sup>96</sup>: A subset of the standardized evaluation framework for automated red teaming and robust refusal Mazeika et al. (2024).
- Strong Reject<sup>97</sup>: Souly et al. (2024)
- AdvBench<sup>98</sup>: A set of 500 harmful behaviors formulated as instructions Zou et al. (2023).
- DAN:
- MistralGuard<sup>99</sup>:
- Do-Not-Answer<sup>100</sup>:
- Blue Safety [IBM-Synthetic]:

## A.3 REWARD MODEL(S) TRAINING DATA

## A.3.1 MULTI-ASPECT REWARD MODEL

We trained our multi-aspect reward model on HelpSteer2 (https://huggingface.co/datasets/nvidia/HelpSteer2) for two epochs.

## A.3.2 BRADLEY TERRY REWARD MODEL

We trained a Mistral-7B-Instruct-v0.2 reward model, with Bradley Terry preference objective, using a mix of gold and synthetic datasets. During training, the proportion of gold data was 20% and the remaining 80% was sampled from synthetically generated preference data. The model was trained for 120k steps with a batch size of 16 and a learning rate of 1e-7.

The following gold preference datasets were used in training:

- HelpSteer2\_DPO: a binary preference version of helpsteer 2.0 dataset, https://huggingface.co/datasets/gx-ai-architect/HelpSteer2\_DPO containing around 7k samples.
- safetyQA\_DPO: a safety preference dataset, containing roughly 50k samples, https://huggingface.co/datasets/AmberYifan/safetyQA\_DPO
- truthy-dpo-v0.1: A small dataset (1k samples), aim at improving truthfulness, especially in the context of human-like self-awareness. https://huggingface.co/datasets/jondurbin/truthy-dpo-v0.1
- anthropic\_hh: A dataset of over 161k samples, containing preference pairs geared towards helpful and harmless responses. https://huggingface.co/datasets/Anthropic/hh-rlhf

 $<sup>^{94}</sup>$ https://huggingface.co/datasets/NousResearch/hermes-function-calling-v1

 $<sup>^{95}</sup> https://hugging face.co/datasets/Bertievidgen/Simple Safety Tests$ 

<sup>96</sup> https://github.com/centerforaisafety/HarmBench/blob/main/data/behavior\_datasets/harmbench\_behaviors\_text\_all.csv

<sup>97</sup> https://github.com/alexandrasouly/strongreject/blob/main/strongreject\_dataset/ strongreject\_dataset.csv

<sup>98</sup> https://huggingface.co/datasets/walledai/AdvBench

<sup>99</sup> https://huggingface.co/datasets/natolambert/xstest-v2-copy

 $<sup>^{100}</sup> https://hugging face.co/datasets/LibrAI/do-not-answer$ 

• Agentic-DPO-V0.1: A small 5k samples dataset designed to improve AI models for agentic processing. https://huggingface.co/datasets/Capx/Agentic-DPO-V0.1

We also generated preference data synthetically using the model-gap technique Naseem et al. (2024):

- We generated 96k samples, where the chosen response is generated from Mixtral-8x22B-Instruct-v0.1 and the rejected from Mistral-7B-Instruct-v0.1
- Another 770k samples were generated, where the chosen response is generated from Mixtral-8x7B-Instruct-v0.1 and the rejected from Mistral-7B-Instruct-v0.1