Europe, February 2025

Material Foundation Models (MFMs)

Introduction deck

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Executive summary

- Foundation models (FMs) or base models, are task-agnostic, pre-trained, large-scale neural networks that can be adapted to numerous downstream tasks.
- Within FMs, large language models (LLMs) trained on terabytes of internet-based textual datasets like CommonCrawl have become popular in recent years due to product examples like ChatGPT. As LLMs have attracted hundreds of billions of EUR, and FMs like GPT-3/GPT-4 have led to a myriad of derivative models tailored to specific downstream tasks (e.g., specific assistants). These recent investments in LLMs have also shed light on the unit economics in an AI-world: CAPEX required to train SOTA (state of the art) models increases~2,5x/annum[1], compute required to train SOTA models is growing at ~4,6x per year[1], rapid commoditization of models occurs due to open-source competition, different geographic regions tend to build their FMs[2], and rapid declines in token costs for existing models occur at -86%/annum[3].
- New categories of FMs will occur in the coming years, typically with alternative use cases. The main examples include geospatial foundation models (GFMs), time series foundation models (TFMs), and material foundation models (MFMs). An alternative way to segment foundation models is to focus on the data modality being used, the main categories using that logic are language foundation models, vision foundation models and multimodal foundation models – the latter category using multimodal input data and typically allowing multimodal generalizations (e.g. text to image, image to text).
- Materials Foundation Models (MFMs), also known as Foundation Models for Materials (FM4M), use computational techniques to simulate and predict properties and behavior of materials under various conditions. MFMs can speed up new material research and design exponentially for both organic materials (e.g., proteins, enzymes, bio-based materials such organic photovoltaics) and inorganic materials (e.g., metal alloys, crystals, ceramics, catalysts). Well-known models today are Alphafold (DeepMind), MatterGen (Microsoft), LINUS (Orbital Materials) and GNoME (DeepMind). It is likely that MFMs will have an impact in materials R&D, chemicals, pharma, biotech, electronics, defense, aerospace and fashion. The current market size for AI-generated materials in these sectors is small today, but growing at a ~30% CAGR.
- Lastly, we dive into the AI economics making these use cases viable and highlight three main trends relevant to understanding AI economics: i) the increase in training costs for new state-of-the-art (SOTA) models, ii) the increase in the total amount of available models, and iii) the decrease in token costs over time. First, investment for developing foundation models is significant, with the first ~1bln EUR models in sight – while at the same time cheaper variants keep popping up (e.g., DeepSeek, Llama). Second, in the last four years open-source model repositories have grown very rapidly in with a 70X increase in the number of models available. Language-based models are still the dominant category, but this can change when more high-quality and affordable satellite data becomes available at scale. Finally, given the intense competition from open-source models, API token costs tend to fall rapidly, as was shown in recent years for GTP-3 and GPT-4 where token costs fell ~90% per year. These trends support the premise that geospatial models can have a wide set of economically viable use cases in the coming years, as the willingness to invest is present and usage costs are declining rapidly.

[1] Source: Epoch.ai; [2] ChatGPT in the US, Mistral in Europe, DeepSeek in China – with largely similar capabilities, [3] source: deeplearning.ai.

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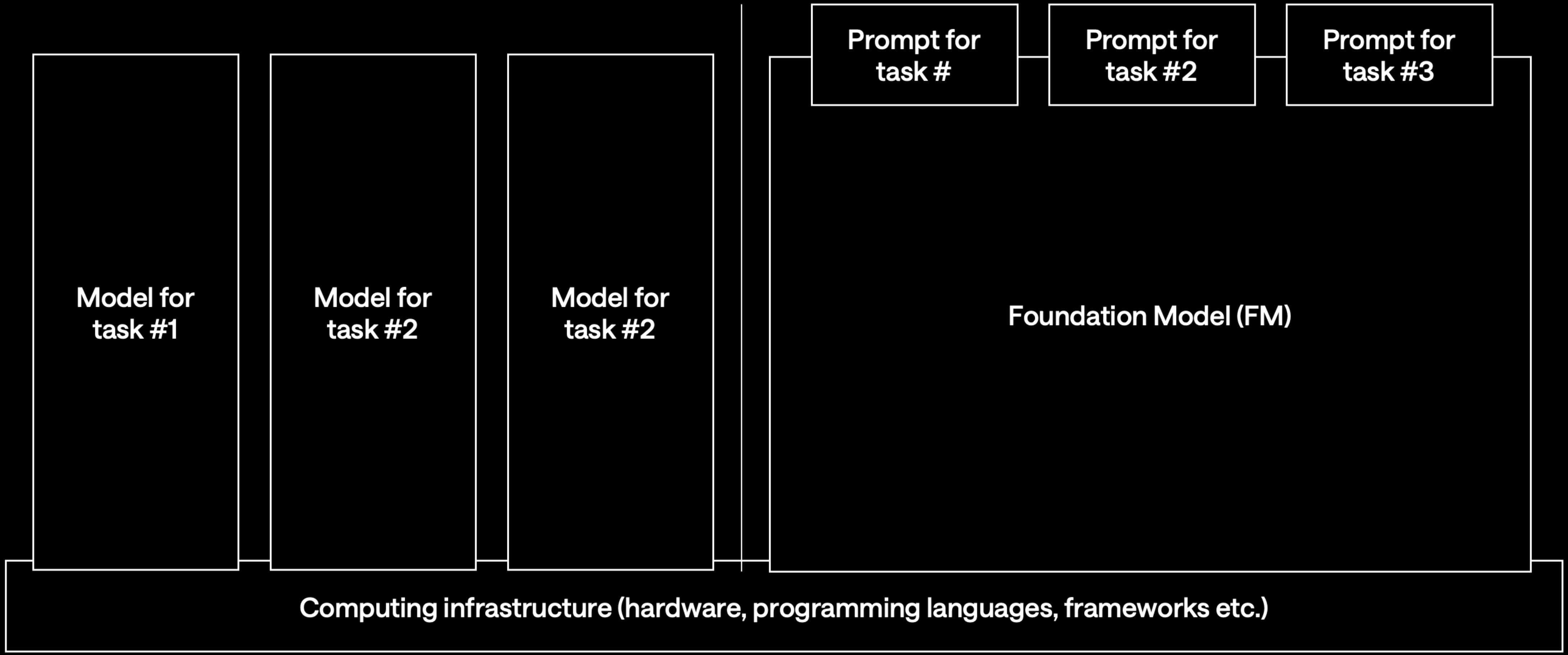
Foundation models are multi-purpose models...



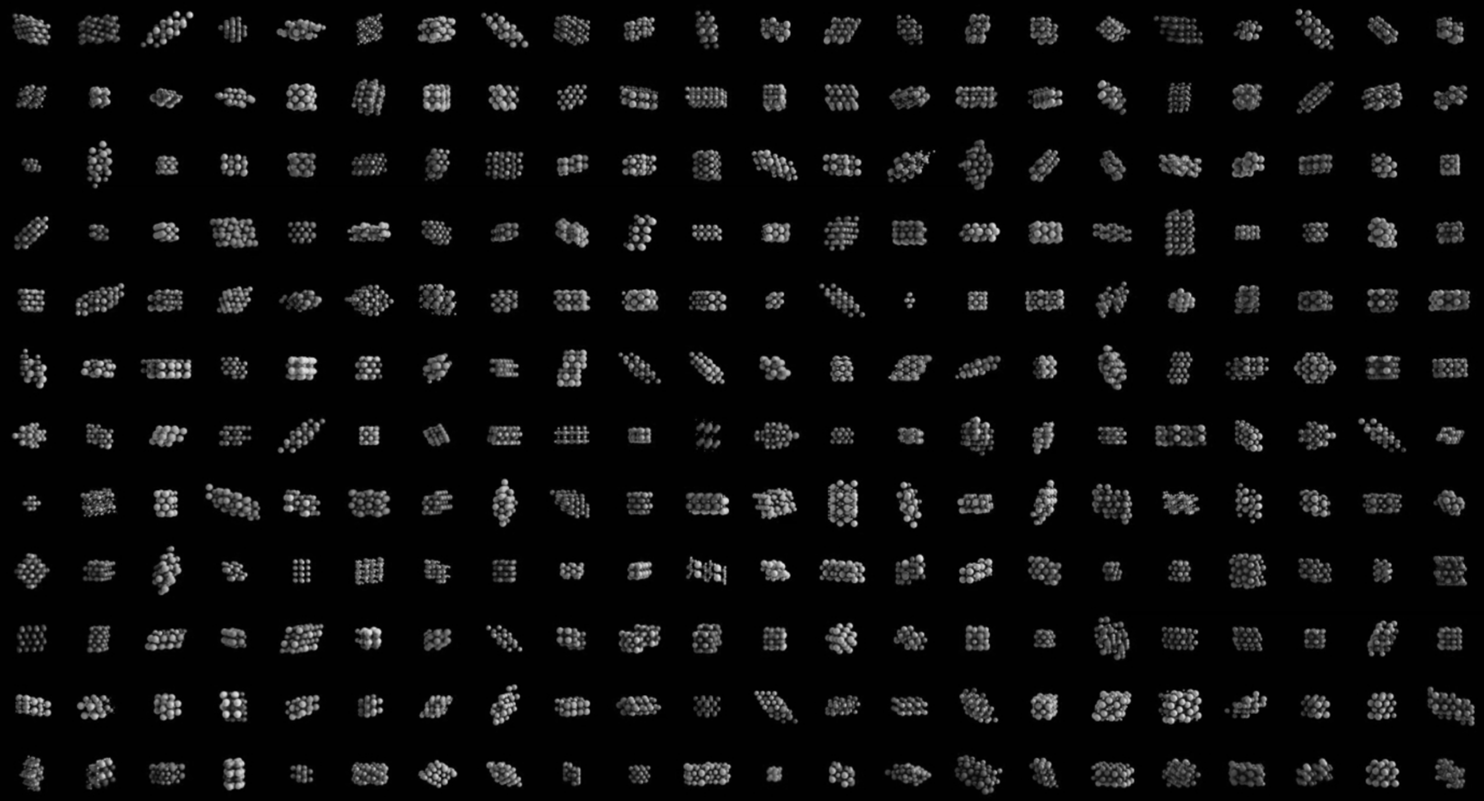
Source: University of Amsterdam (2024): Foundation models are platform models.

...where MFMs focus on the material discovery process

MFMs are trained using the following steps...

1. **Data collection**: diverse datasets, including material property databases (e.g., ICSD, NIST), molecular simulation data (e.g. Materials Project), and textual data (e.g., PubChem).
2. **Model training**[2]: select model type (GNN, transformer-based model[3]), training process (e.g., SSL[4]) and evaluation of how close predictions are to reality.
3. **Prediction**[5]: the model can predict material properties (e.g., strengths, conductivity, heat capacity) and/or suggest new materials.
4. **Experimental validation**: rank the top-50 material candidates lab testing to validate the model's predictions. Feedback loop with model is maintained to learn from errors.
5. **Deployment**: once the material qualities are confirmed, real-world applications can be designed at scale.

...and if successful, can do hundred of years of research in a month[1].



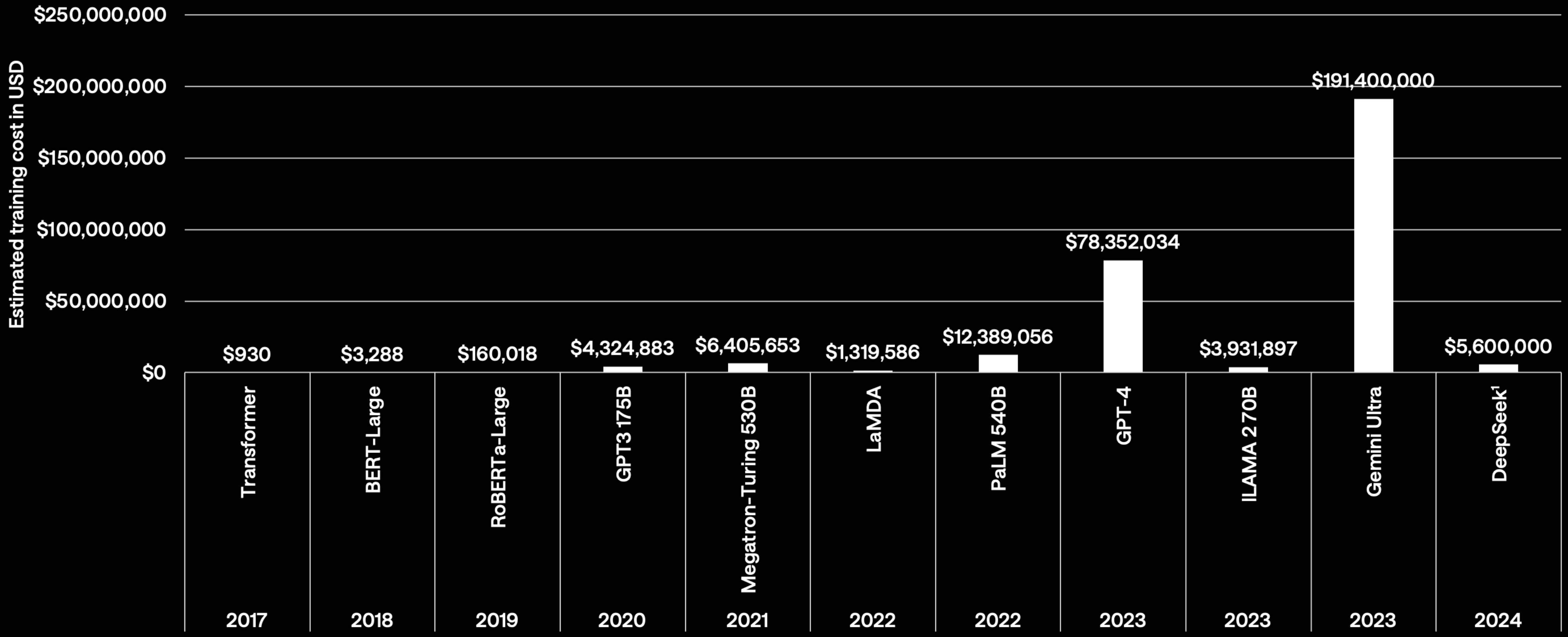
[1] DeepMind's GNoME led to the discovery of 2.2mln new crystal structures, equivalent to 800 years of regular research; [2] Training of models can take multiple weeks, or even months, depending on compute requirements. [3] Where GNNs (Graph Neural Networks) are typically used to understand property estimation, and transformers for predictions of new material designs; [4] SSL (Self Supervised Learning) is a technique where models learn representations without explicit human-labelled data, e.g., by masking parts on the input data; [5] Takes minutes once the model is trained.

MFMs can guide breakthrough research in the coming years

Data modality	Language data		Vision data		Multimodal data
Model type	Geospatial (GFMs)	Time Series (TFMs)	Urban FMs (UFMs)		Material (MFMs)
Sector	Materials	Chemicals	Pharma/Biotech	Electronics	Other
Value estimate	**~10B EUR/year[1].** Accelerated discovery of new materials (TTM), R&D cost reduction, optimisation of materials (sustainability, strength, conductivity) etc.	**10-20B EUR/year[2].** Process optimisation, waste reduction, energy efficiency, product innovation, safety enhancements, compliance, personalised niche markets etc.	**1-10B EUR/year[3].** Drug discovery acceleration, personalised medicine, cost savings, regulatory streamlining, biomarker discovery etc.	**1-10B EUR/year[4].** Discovery of more efficient semiconductors, R&D cost reduction, energy efficiency, miniaturization, enhanced durability of electronics, more sustainable electronics etc.	**1-10B EUR/year.** Aerospace R&D, space R&D, defence R&D, construction materials (e.g., self-healing materials, fire-resistance), fashion materials (e.g., biodegradable, self-cleaning materials) etc.

[1] Still a small market today at ~1B EUR, but expected to grow to ~10B EUR/year in 2030; [2] Small market today at ~2B EUR, expected to grow to ~20B EUR in 2030; [3] AI in drug discovery market today is ~1B EUR, expected to be 7B EUR in 2030; [4] Harder to quantify, as some of the effects (energy efficiency) are second-order effects that would impact the electronics market at scale.

While training costs for foundation models is generally increasing…



Source: epoch.ai; [1] Note the discussion around DeepSeek's true training costs, with estimates from 5,6mln USD to 1,6bln USD.

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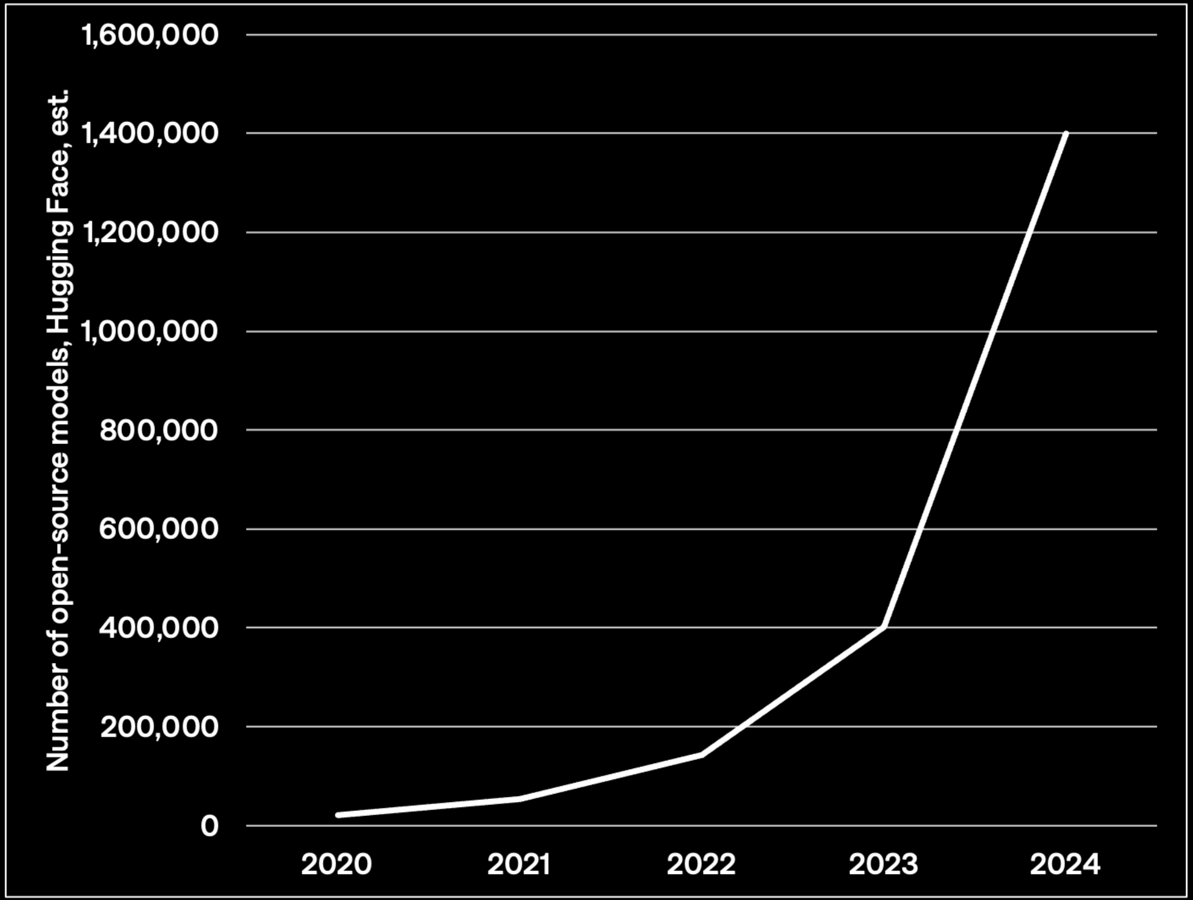
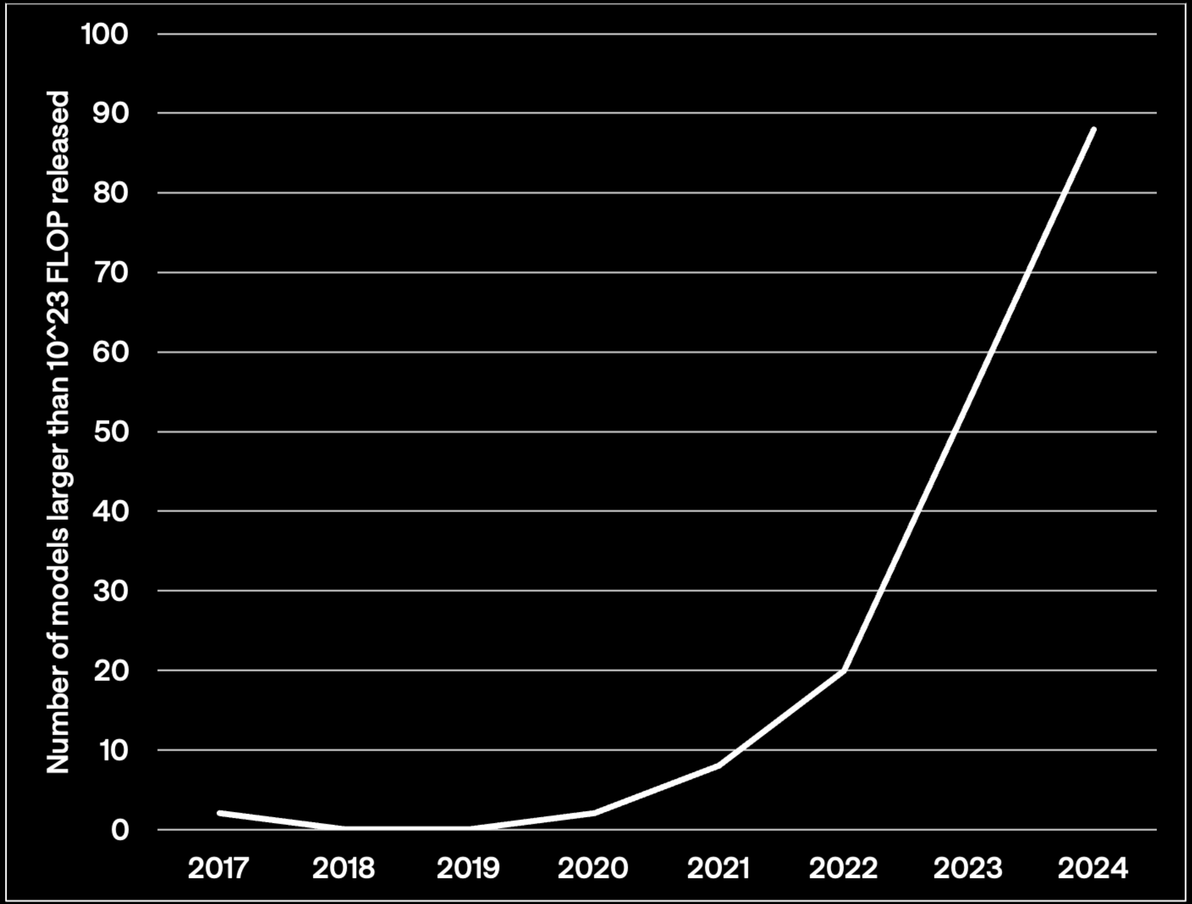
...the competition between models is fierce...

Open-source models grew ~70X in the last four years...



...and more players are releasing large (over 10^23 FLOP) models.



Source: Hugging Face, Epoch.ai.

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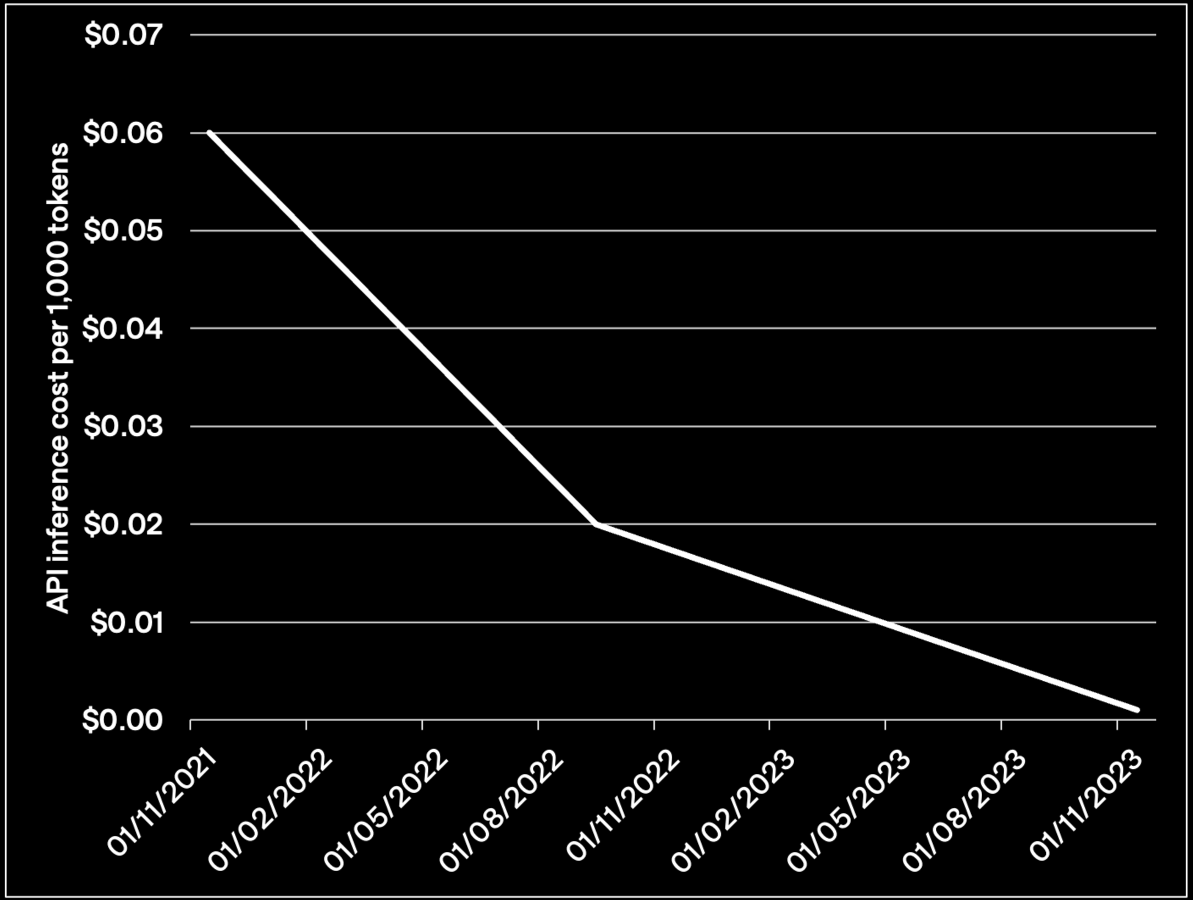
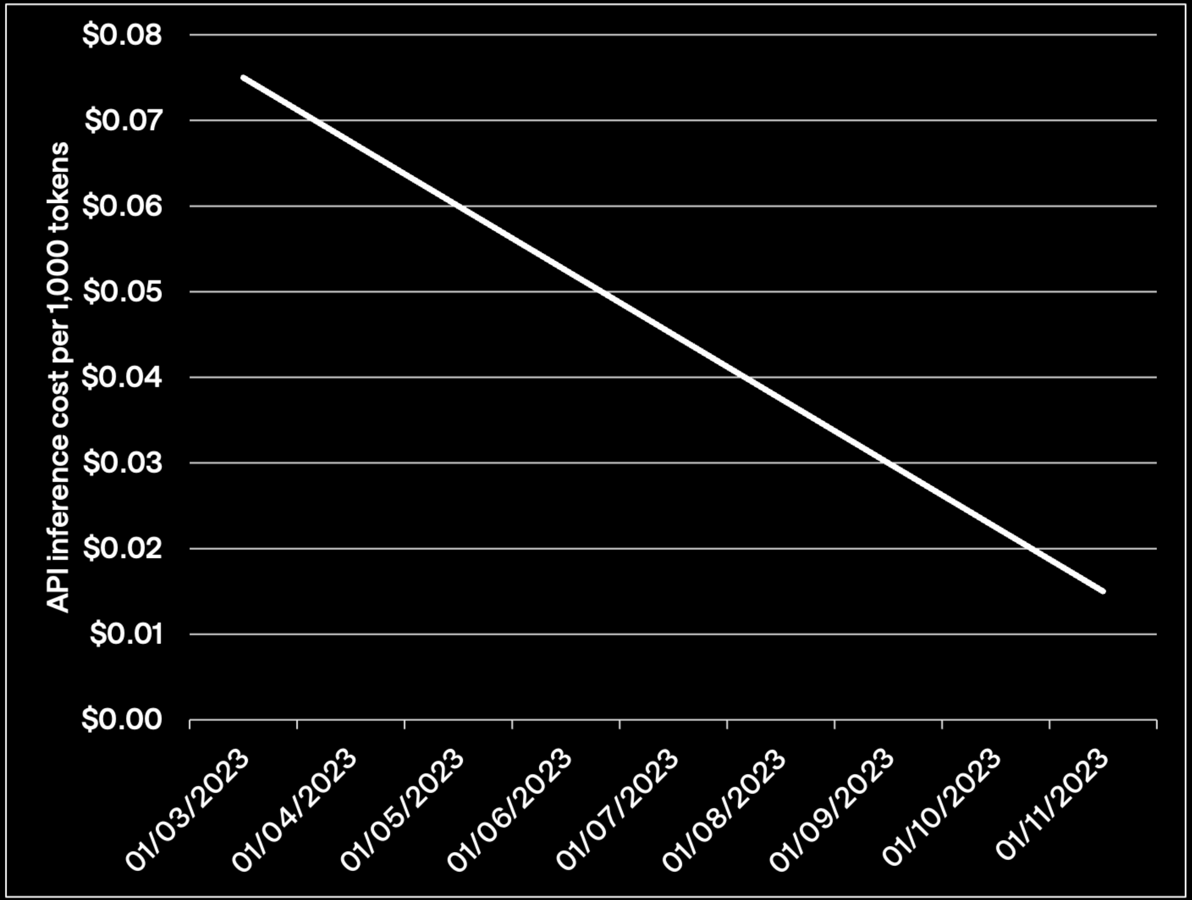
...and falling token costs will make more use cases economical

GPT-3 token cost fell ~86% in cost per year...



...and GPT-4 tokens showed a similar trend of falling 92% per year.



Source: Ark Invest analysis (2024); The Batch (2024).