



The  
Center  
for AI  
@ PNNL

# The AI Summer is Here, will National Security Science and Engineering Bask in the Sunshine, or get Burned?

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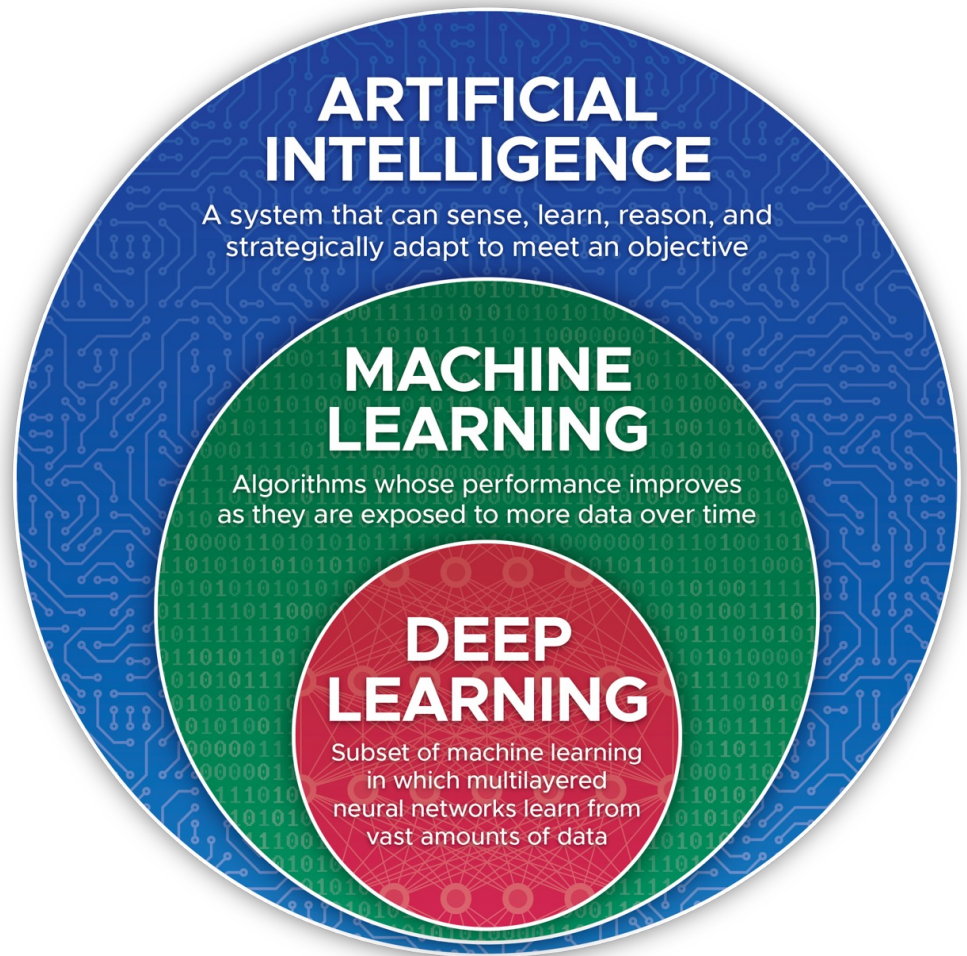
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**Artificial intelligence  
encompasses a  
broad range  
of advanced  
computing topics**



## Machine learning has a formal definition

“A computer program is said to learn from experience  $E$  with respect to some class of tasks  $T$  and performance measure  $P$  if its performance at tasks in  $T$ , as measured by  $P$ , improves with experience  $E$ ” -- Tom Mitchell, “Machine Learning” 1997

Task $T$	Experience $E$	Performance $P$
Image classification	1 million labeled images	Classification accuracy
The game of Go	30 million recoded moves	Winning Rate
Simulating fluid flow	Example solutions to fluid flow equations	Calculation Accuracy
Generate text	Gigabytes of natural language	Prediction of missing words
Detect bugs in code	Thousands of examples of source code with labeled bugs	Classification accuracy
Create artificial faces	50,000 images of faces	The probability the generator creates a face that can't be distinguished from a real one

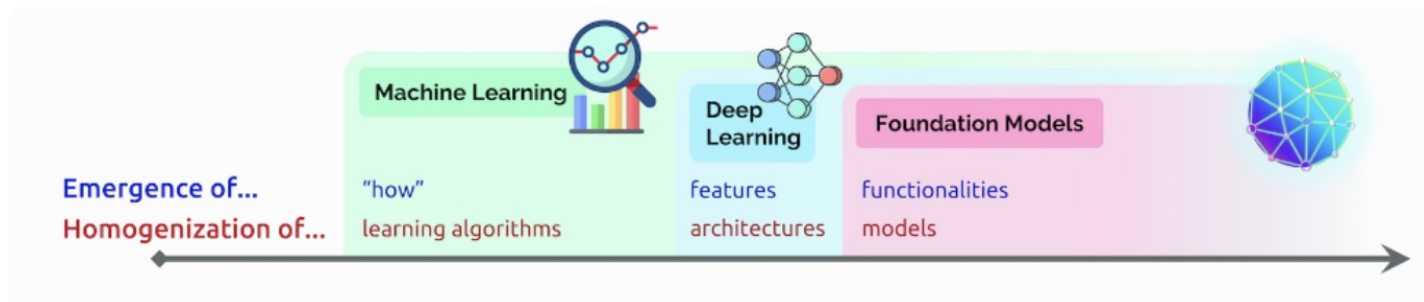
## What's new with foundation models? They wear many hats, not just one

### Narrow (Single-Purpose) AI

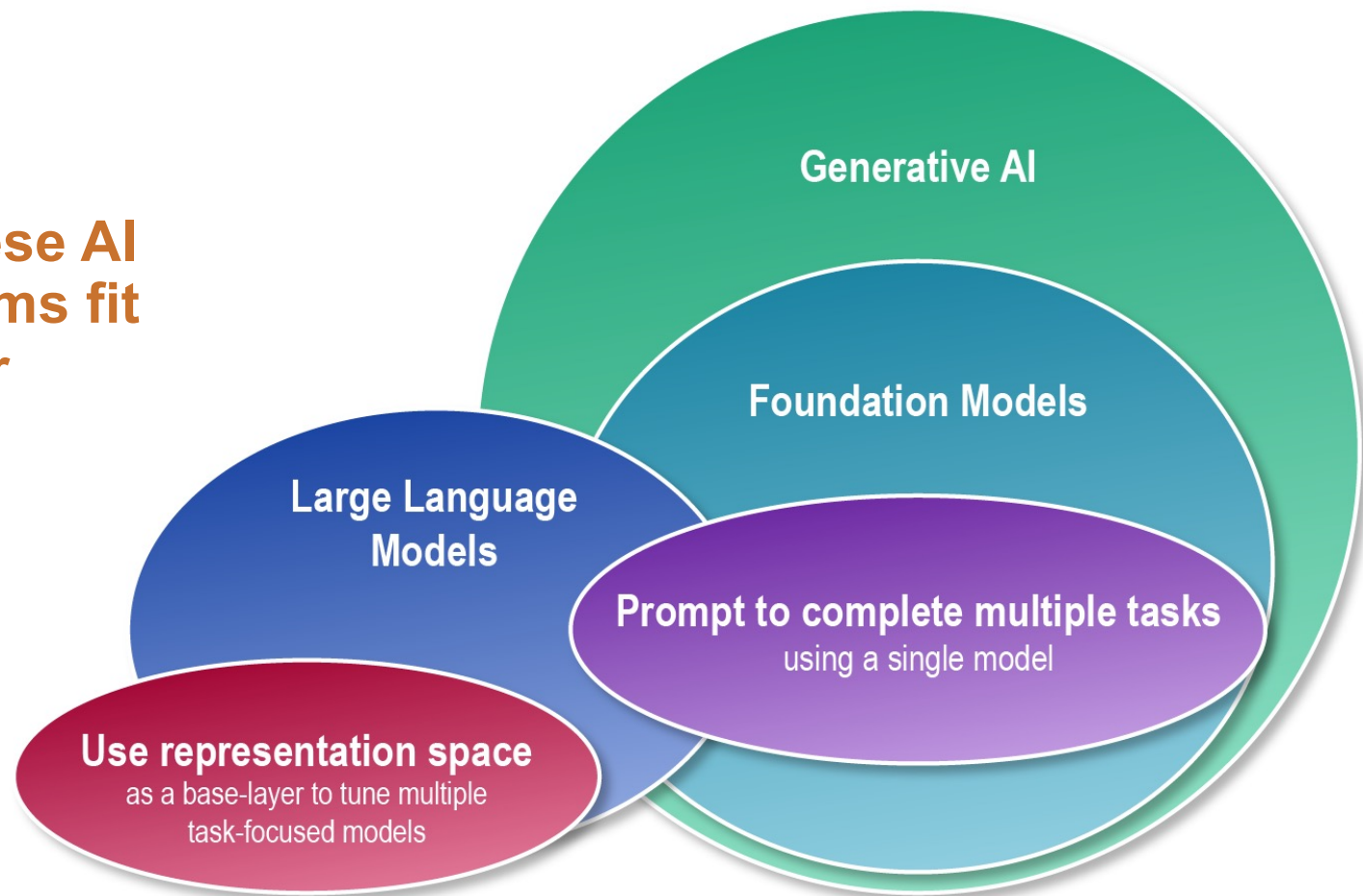
- Application specific
- Single/limited task
- Can't solve unfamiliar problems
- Need to build new models for each new task

### Foundation (Multi-Purpose) Models

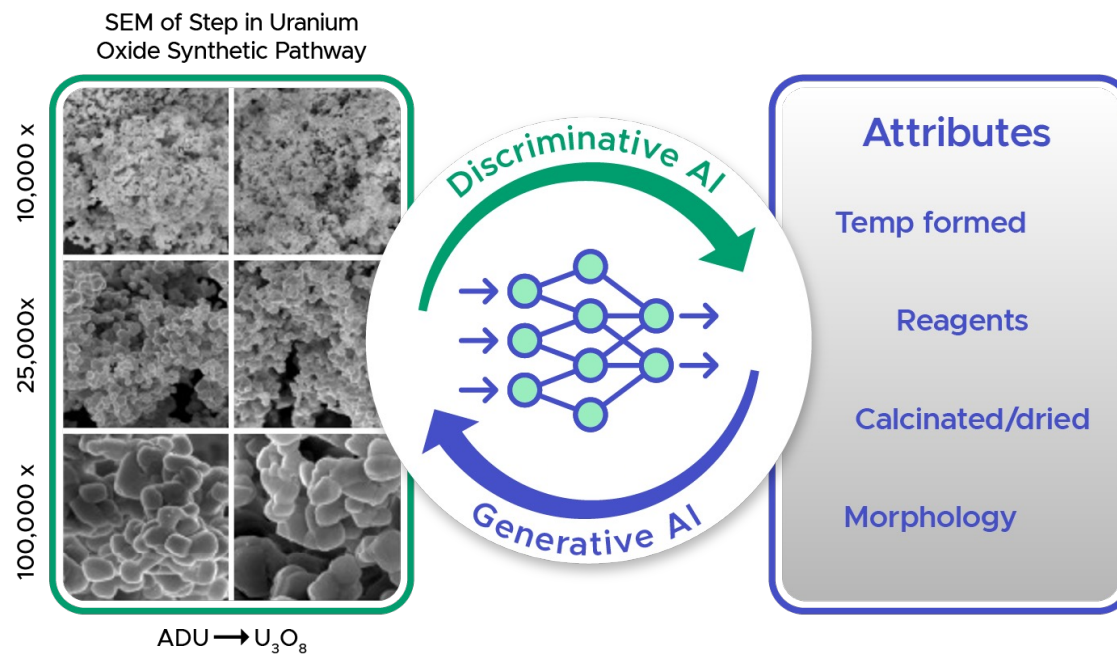
- Self-supervised learning on unlabeled data
- Generative
- Multipurpose (multiple tasks)
- Support new tasks and complex logic



## How these AI paradigms fit together



## Toy example: generating plausible materials from a set of attributes as opposed to characterization



## Diffusion model

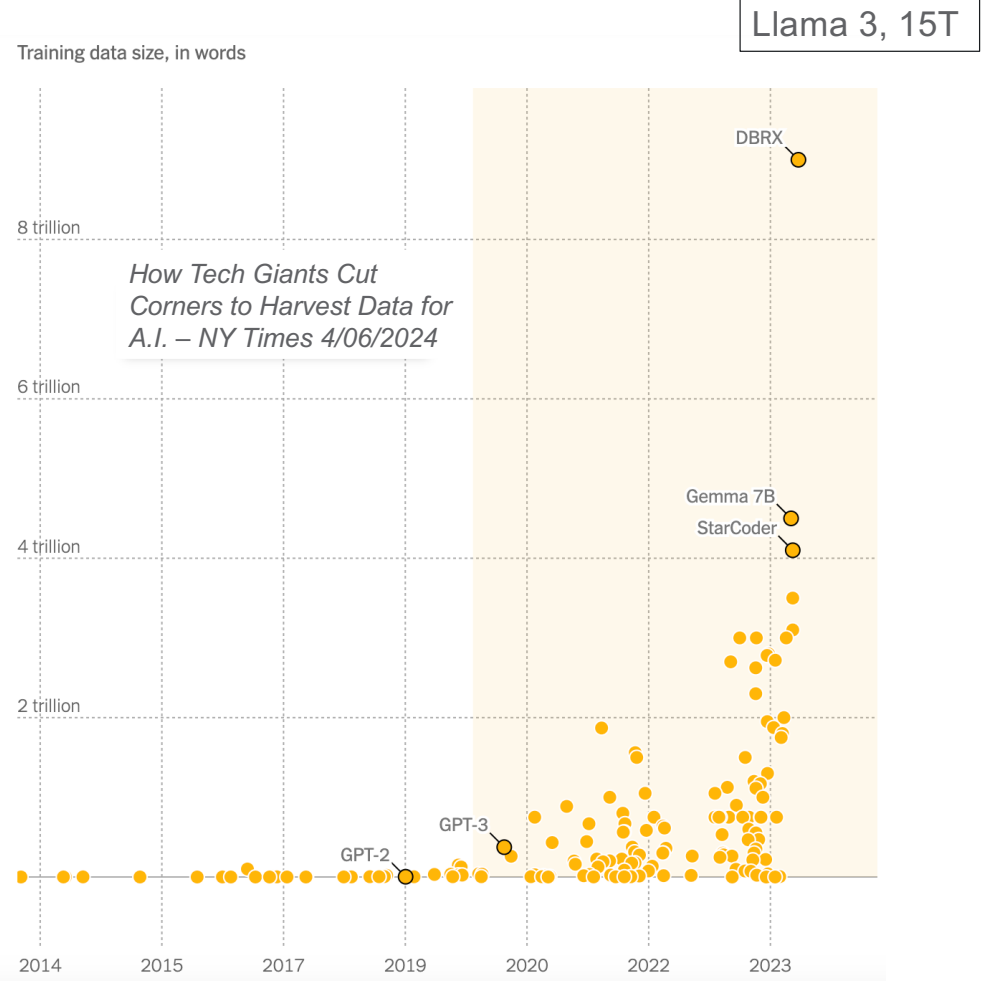
- Diffusion models can generate data similar to what it was trained on
- High quality video and image generation
- Text-to-image generation





# AI is data hungry, whether you have labels or not

Foundation models require  
beyond internet scale data



## Medium to small AI models are relevant and vital for national security science and engineering

- Deep learning efficiently leverages large quantities of data to learn representations of classes
  - Deep learning *can* be applied to small data ... but restrictions *will* apply ...
- But what if the class you care about has few examples?
  - Ignore differences and just apply existing model (e.g., information retrieval)
  - Adapt a pre-trained models (e.g., transfer learning)
  - Train model to generalize to new classes (e.g., few-shot learning)

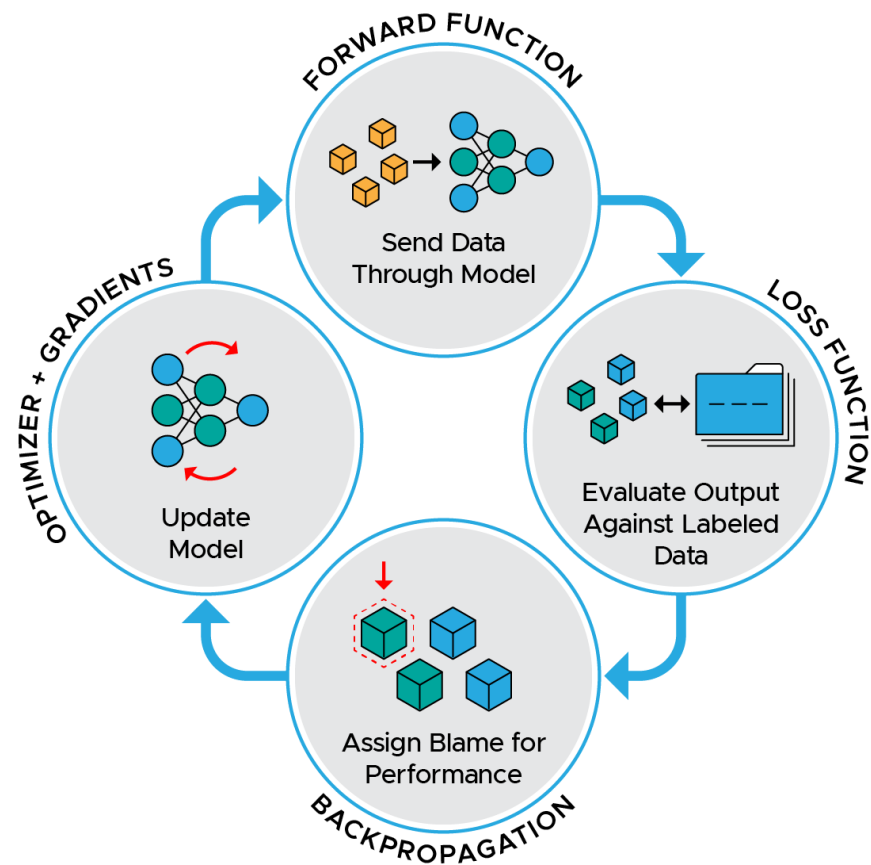
Quantity	# Labels	# Data
Supervised	High	High
Semi-supervised	Low	High
Self-supervised	---	High
Transfer learning	Low/Medium	Low/Medium
Few/low/zero-shot	Very low	Very low



These models continue to train on PNNL's very first DGX-1, *ohmahgerd*, purchased in 2016

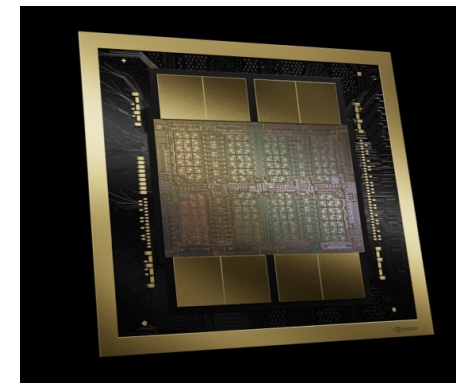
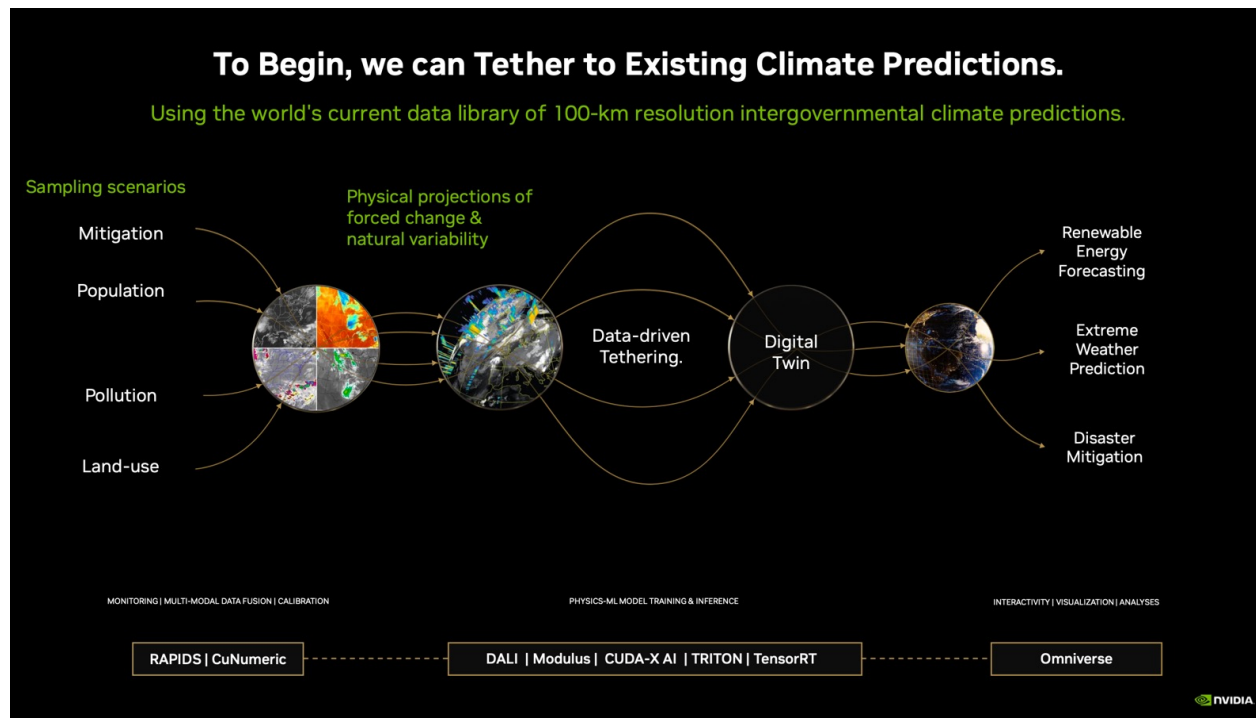
## One step up from everything is linear algebra

- Inside text are the steps that all models use
- Outside text are the terms when training a deep learning model, including transformer-based models



# Differentiable Modeling and Simulation

## *Is this the end of double precision architectures?*



NVIDIA Blackwell advertises 4-bit floating point interfaces w/ 20/40 petaFLOPS (dense/sparse)

## The Cost of AI Compute

- Commodity 8xH100 ~\$250k
- Meta's \$13B and 600,000 GPU purchase is nation state level investment
  - e.g., the unit cost of the U.S. Gerald R Ford aircraft carrier
  - Power? HVAC?

Llama-2 Cloud Deployment Costs (previous generation)

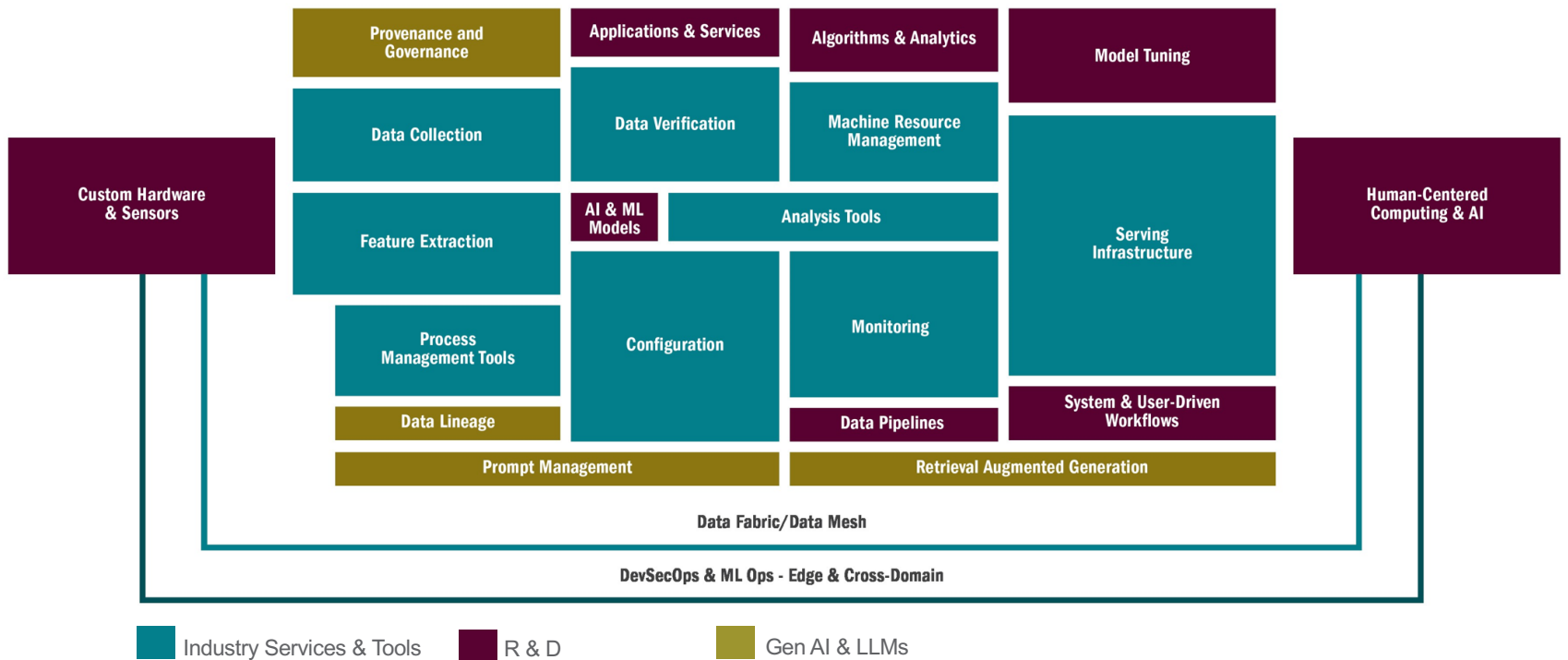
Model	Instance Type	# of GPUs per replica	On-demand (per hour)	On-demand (per year)
<u>Llama 7B</u>	ml.g5.2xlarge	1	\$ 1.52	\$13,315.20
<u>Llama 13B</u>	ml.g5.12xlarge	4	\$ 7.09	\$62,108.40
<u>Llama 70B quantized</u>	ml.g5.48xlarge	8	\$16.29	\$178,353.60
<u>Llama 70B</u>	ml.p4d.24xlarge A100	8	\$32.77	\$287,065.20

Llama-2 Cloud Pre-Training Costs (previous generation)

Model	Instance Type (A100)	GPU Hours	AWS On-demand
<u>Llama 7B</u>	ml.p4d.24xlarge	184,320	\$755,020.80
<u>Llama 13B</u>	ml.p4d.24xlarge	368,640	\$1,510,041.60
<u>Llama 70B</u>	ml.p4d.24xlarge	1,720,320	\$7,046,860.80
DALL-E 2	ml.p4d.24xlarge	150,000	\$614,437.50

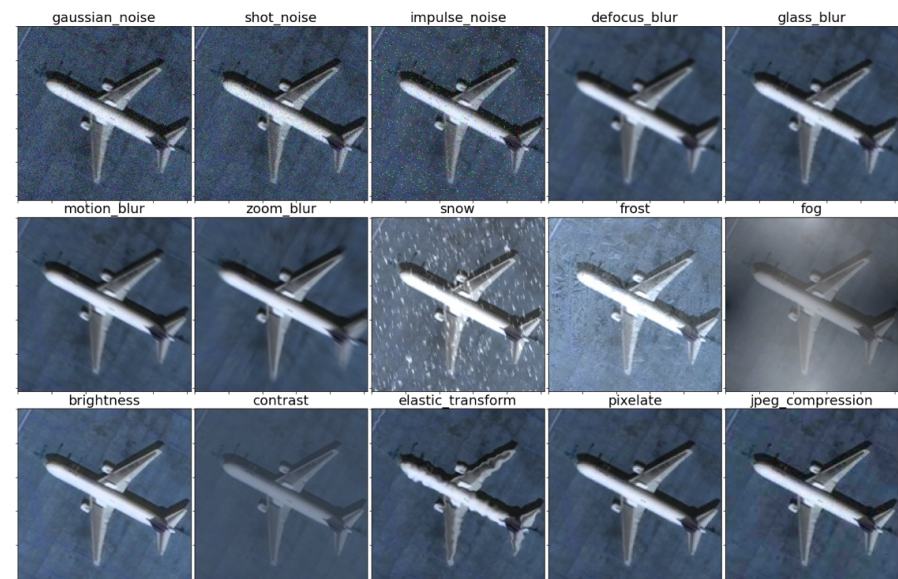
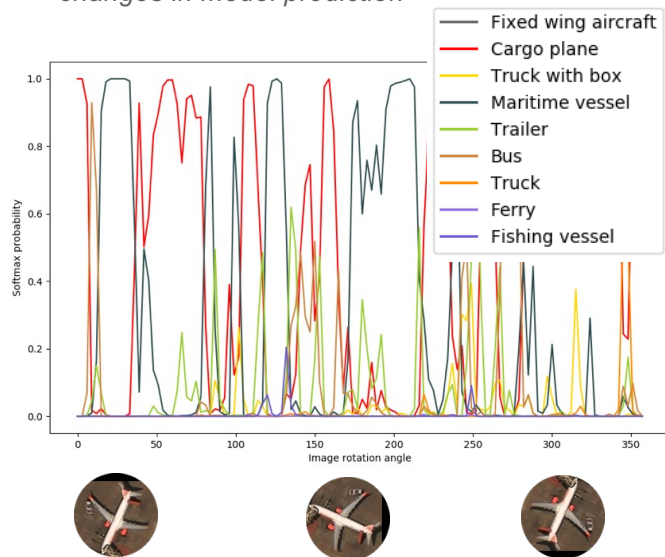
ml.p4d.24xlarge 8GPUs \$32.77/hr  
<https://aws.amazon.com/ec2/instance-types/p4/>

# AI requires services readily available via industry developed tools and platforms



# Even without manipulation, machine learning models lack robustness

Natural changes in the data (such as the rotation of a plane) can result in dramatic and non-intuitive changes in model prediction



Environmental changes such as weather can cause a model to fail if it hasn't seen these conditions before

## Hallucination (caveat emptor)

**erroneous** references, content, and statements, may be intertwined with correct information, and presented in a persuasive and confident manner, making their identification difficult **without close inspection and effortful fact-checking**

```
Human:> Can I get McDonalds at the SeaTac airport?
```

```
ChatGPT:> Yes, there is a McDonalds at the SeaTac airport,  
located in the central terminal near gate C2. It is open from 5  
a.m. to 10 p.m. daily.
```



# Reinforcement Learning with Human Feedback: Alignment and Guardrails

How do you create/  
code a loss function for:

- What is *funny*?
- What is *ethical*?
- What is *safe*?

Don't Code it, Model It

## 1 Collect human feedback

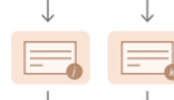
A Reddit post is sampled from the Reddit TL;DR dataset.



Various policies are used to sample a set of summaries.



Two summaries are selected for evaluation.



A human judges which is a better summary of the post.



## 2 Train reward model

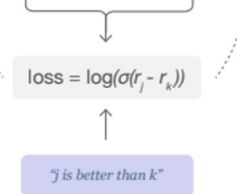
One post with two summaries judged by a human are fed to the reward model.



The reward model calculates a reward  $r$  for each summary.



The loss is calculated based on the rewards and human label, and is used to update the reward model.



## 3 Train policy with PPO

A new post is sampled from the dataset.



The policy  $\pi$  generates a summary for the post.



The reward model calculates a reward for the summary.

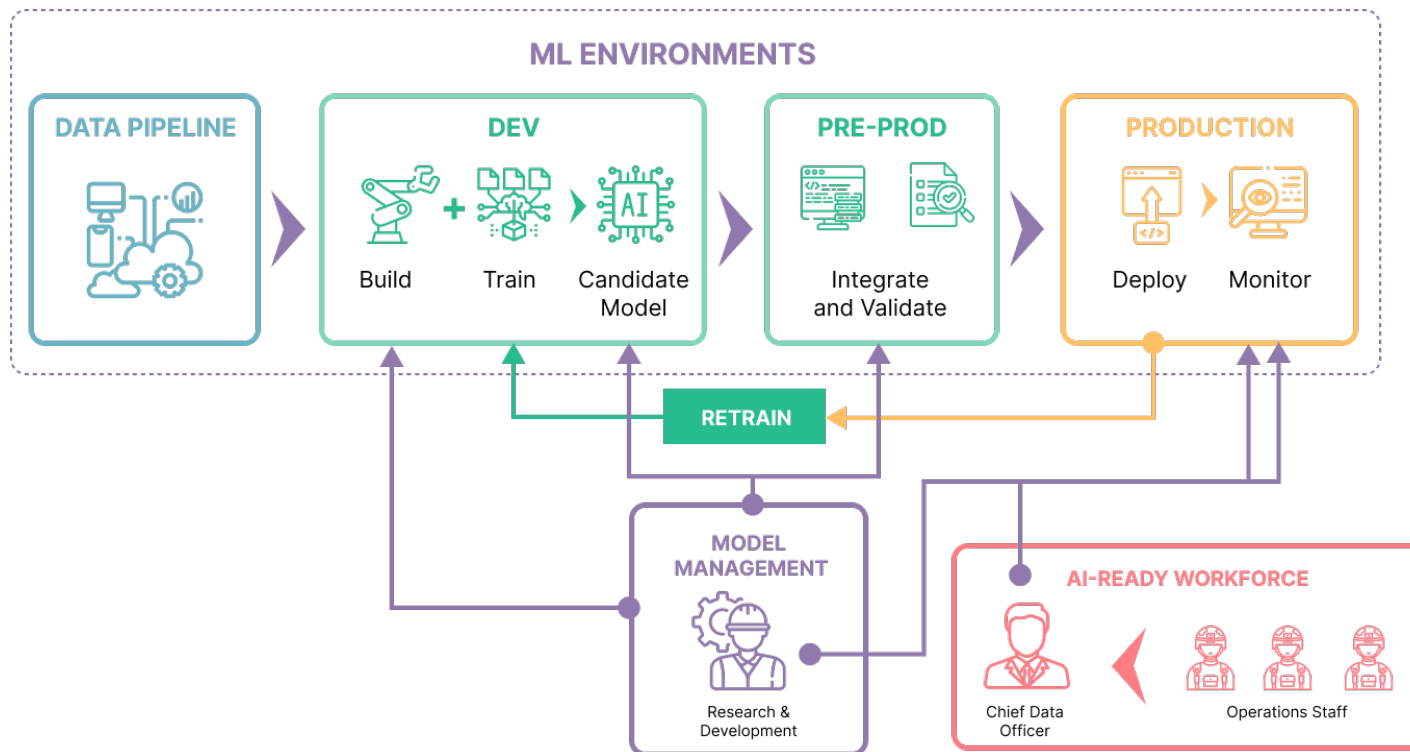


The reward is used to update the policy via PPO.



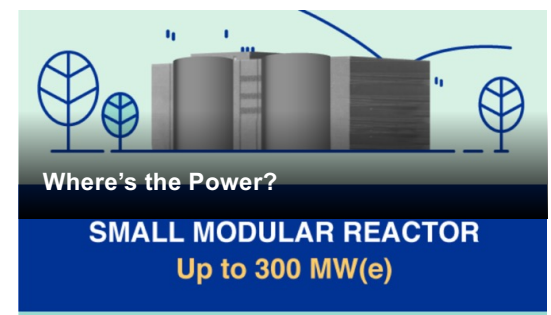
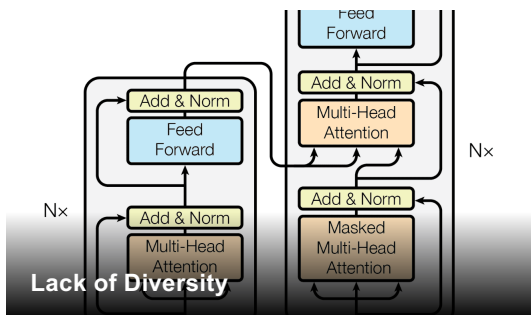
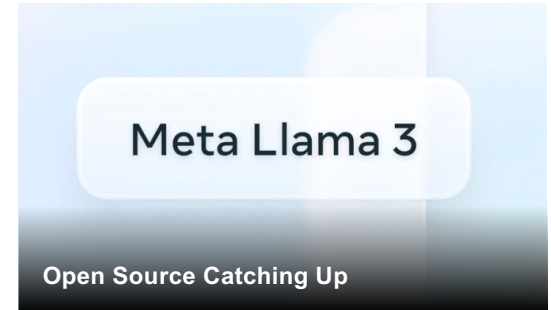
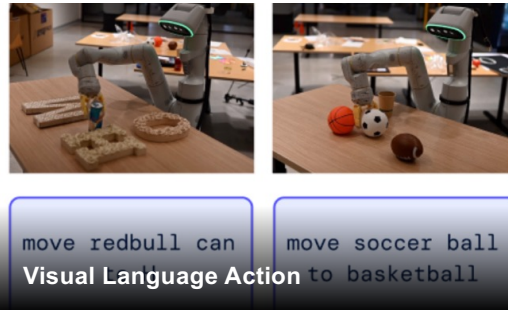
Figure 2: Diagram of our human feedback, reward model training, and policy training procedure.

## AI requires fundamental changes to the workforce *Human-machine workflows and operating constructs*



# Bask in the sunshine, or get burned?

The first and second derivatives are growing, if and when will they normalize?





**Thank you**



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