

Frontiers in Computer Science and Technology

计算机科学与技术前沿

Spring 2025

[Tailin Wu](#), Westlake University

Website: ai4s.lab.westlake.edu.cn/course

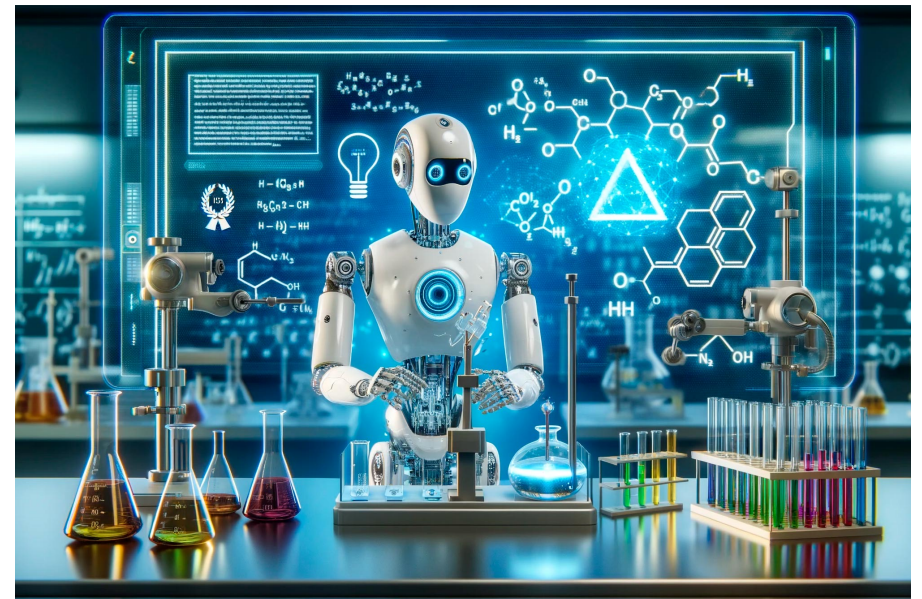


Image from: SciTechDaily

Outline

- **Course logistics**
- Why study this course?
- Course introduction
 - Tasks
 - Neural Architecture
 - Learning paradigm
 - Application in AI and Science

Course logistics

We are going to learn important branches of **AI techniques** and their **application in science**, both the **fundamentals** and **the frontiers**:

AI techniques:

- Deep Learning
- Generative models
- Foundation models
- Reinforcement learning
- Robotics
- Computer vision and autonomous driving
- Graph Neural Network
- Evolutionary Machine Learning and Multi-objective Optimization

AI for Science:

- AI + PDEs/scientific computing
- AI + life science
- AI + materials science

Course timeline

All teachers are PIs in the AI direction in Westlake University

#	Topic	Date	Teacher
1	Course introduction	Thur, 2/20	Tailin Wu
2	Frontiers in Deep Learning	Thur, 2/27	Tailin Wu
3	Frontiers in Generative Modeling	Thur, 3/6	Tailin Wu
4	Frontiers in Graph Neural Networks	Thur, 3/13	Tailin Wu
5	Introduction to Reinforcement Learning	Thur, 3/20	Tailin Wu
6	Reinforcement Learning: Advanced techniques and applications	Thur, 3/27	Tailin Wu
7	Computer Vision and Autonomous Driving	Thur, 4/03	Kaicheng Yu
10	Foundation models	Thur, 4/24	Zhengzhong Lan
12	AI + Life Sciences	Thur, 5/08	Ziqing Li
13	Evolutionary Machine Learning and Multi-objective optimization	Thur, 5/15	Yaochu Jin
14	AI + PDE/Scientific computing	Thur, 5/22	Tailin Wu

*For project timeline see the slides later.

Course arrangement

Time: Every Thursday 15:10pm – 16:55pm

Typical time split:

15:10 – 15:55pm (45min): First part

15:55 – 16:00pm (5min): Discussion

16:00 – 16:45pm (45min): Second part

16:45 – 16:55pm (10min): Discussion

No prerequisite for the course

But would be good to have a basic understanding of neural network, its training, and write basic neural network with PyTorch

If you don't have any of the above background, that is fine. You only need **half a day** to master them, using the materials provided in this lecture.

Project guidance

Choose a **problem related to your research**, and **use AI to solve it**.

Team size: 1-3 people, encouraging **interdisciplinary** collaboration

Course project design @ midterm:

- Give a presentation (10min) that formulates the problem for the 5 questions, each with one slide:
 1. What is the problem?
 2. Why is it important
 3. Why is it hard?
 4. What is the limitation of the prior method?
 5. What is the main component of the proposed method?

Then detail the proposed method (3-4 slides) that uses an AI technique to solve the problem

#	Topic	Date	Teacher
8	Course project design (1)	Thur, 4/10	Tailin Wu
9	Course project design (2)	Thur, 4/17	Tailin Wu

Project guidance

Course project report and discussion @ final:

Give a presentation (15min) that

- Formulates the problem in terms of the 5 questions before, each with one slide.
- Then detail the proposed method (3-4 slides) that uses an AI technique to solve the problem.
- Then report the main experiment results (3-4 slides)

Submit a project report that summarize the project.

#	Topic	Date	Teacher
15	Course Project Reporting and Discussion (1)	Thur, 5/29	Tailin Wu
16	Course Project Reporting and Discussion (2)	Thur, 6/05	Tailin Wu

Course grading

Assessment Criteria	Percentage
Attendance	5%
Project proposal and discussion	30%
Project conclusion presentation	30%
Project conclusion report	35%

Grade	Assessment Standard
A	90-100 points
B	80-89 points
C	70-79 points
D	60-69 points
F	Below 60 points

The grading will be **generous**. The important thing is that you learn **useful AI techniques** that you can use for your own **research**.

Other logistics

Office hour: Wed 2:30-4:30pm, E2-203, Tailin Wu

Email: wutailin@westlake.edu.cn

Website: <https://ai4s.lab.westlake.edu.cn/course>

Join the Feishu group: For announcements, group collaboration, course materials

Outline

- Course logistics
- **Why study this course?**
- Course introduction
 - Tasks
 - Neural Architecture
 - Learning paradigm
 - Application in AI and Science

Your research interest

Self-introduction:



Department & lab

Research interest

Familiarity (1-10)
with deep learning

Why study this course?

If you are from **science/engineering background, not so familiar with AI, you will:**

- Know major AI techniques, their application areas, and limitations
- Able to use state-of-the-art AI techniques for your own research

If you are from **AI background, you will:**

- Learn state-of-the-art AI techniques in different subfields
- Know the open research problems for each subfield
- Collaborate and explore interdisciplinary research

Outline

- Course logistics
- Why study this course?
- **Course introduction**
 - Tasks
 - Neural Architecture
 - Learning paradigm
 - Application in AI and Science

Course introduction

Tasks

- Classification/regression
- Simulation
- Inverse design/inverse problem
- Control/planning

×

Neural architecture

- Multilayer perceptron
- Graph Neural Networks
- Convolutional Neural Networks
- Transformers

×

Learning paradigm

- Supervised learning
- Generative modeling
- Foundation models
- Reinforcement learning
- Evolutionary and multi-objective optimization

Application (AI & Science)

- Robotics
- Games (e.g., Go, atari)
- Autonomous Driving
- PDEs
- Life science
- Materials science

Course introduction: tasks

Tasks

- Classification/regression
- Simulation
- Inverse design/inverse problem
- Control/planning

×

Neural architecture

- Multilayer perceptron
- Graph Neural Networks
- Convolutional Neural Networks
- Transformers

×

Learning paradigm

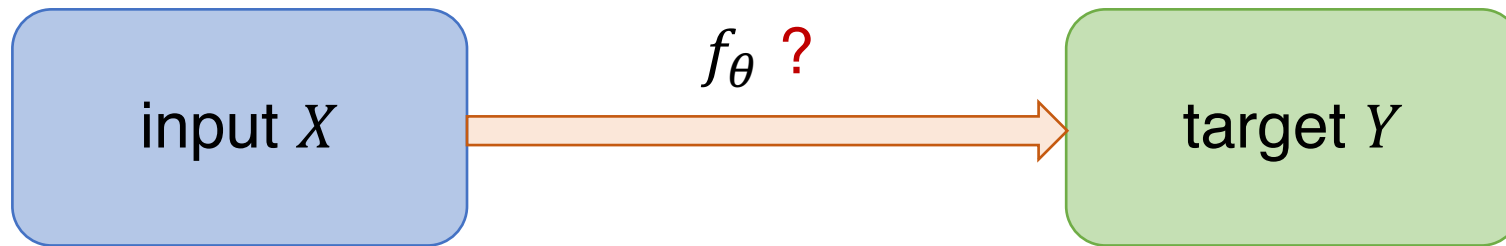
- Supervised learning
- Generative modeling
- Foundation models
- Reinforcement learning
- Evolutionary and multi-objective optimization

Application (AI & Science)

- Robotics
- Games (e.g., Go, atari)
- Autonomous Driving
- PDEs
- Life science
- Materials science

Task 1: Classification & regression

- image
- video
- graph
- time series
- natural language
- ...



- **classification**
↑
• label (discrete)
- scalar/tensor (continuous)
↓
• **regression**

Given many examples of (X, Y) pairs, learn a neural network (NN) f_θ that minimizes the prediction loss:

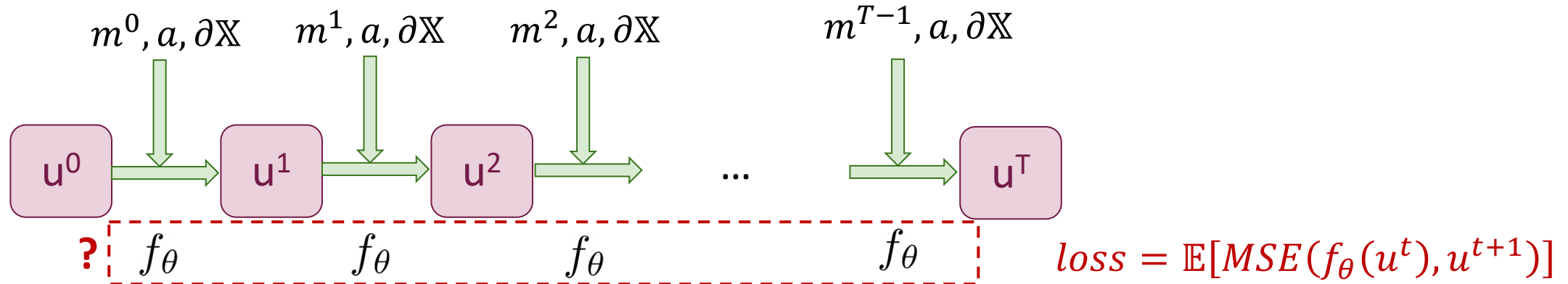
$$\theta^* = \operatorname{argmin}_\theta \mathbb{E}_{(X,Y) \sim P(X,Y)} [\ell(f_\theta(X), Y)]$$

f_θ : neural network to be learned

ℓ : loss function

Task 2: (Learning) simulation

Goal: learn the mapping f_θ from u^t to u^{t+1} :



u^t : original **state** (状态) of the system. Can be a graph (e.g., mesh, particle-based systems, molecules), a tensor, or an infinite-dimensional function $u(t, x)$ as solution to a PDE

f_θ : **neural surrogate models** (神经网络代理模型)

m^t : **external control** (外界控制)

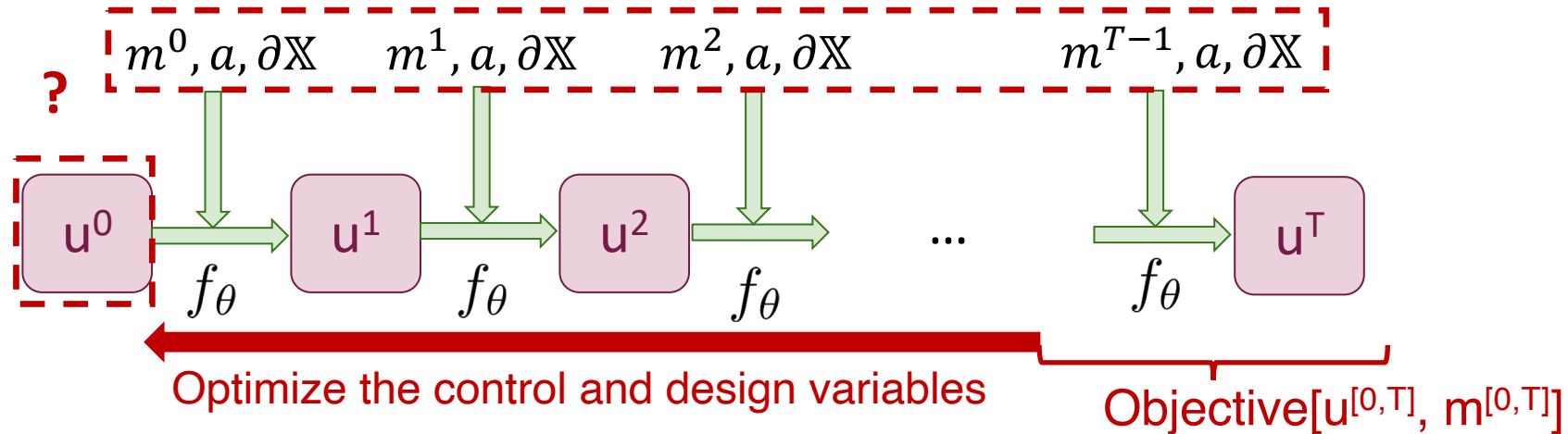
a : **static parameters** (静态参数) of the system that does not change with time (e.g. parameters of PDE, spatially varying diffusion coefficient)

$\partial\mathbb{X}$: **boundary condition** (边界条件) of the system

PDE: partial differential equation

ODE: ordinary differential equation

Tasks 3 & 4: Inverse design, inverse problem, and control



u^t : original **state** of the system. Can be an infinite-dimensional function $u(t, x)$ as solution to a PDE, or a graph (e.g., mesh, particle-based systems, molecules)

f_θ : neural surrogate models

m^t : external **control** (外界控制)

a : **static parameters** (静态参数) of the system that does not change with time (e.g. parameters of PDE, spatially varying diffusion coefficient)

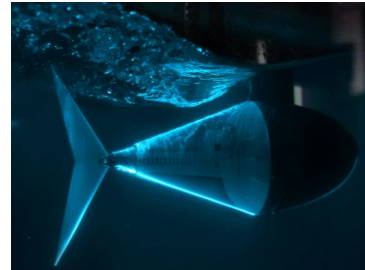
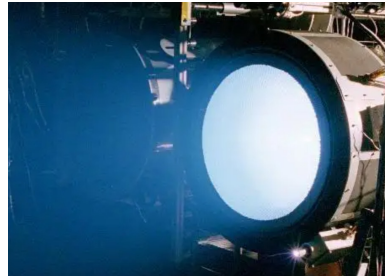
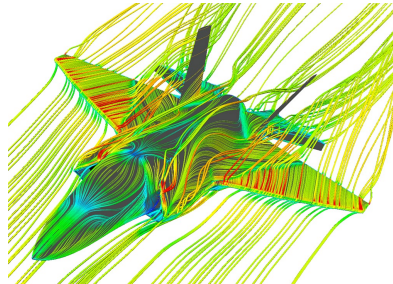
$\partial\mathbb{X}$: **boundary condition** (边界条件) of the system

} control (控制)

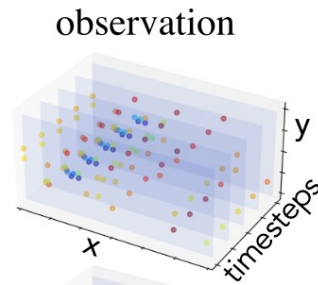
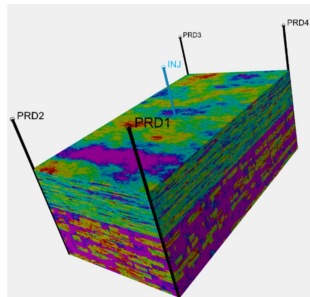
} inverse design (反向设计)

Tasks 3 & 4: Inverse design, inverse problem, and control

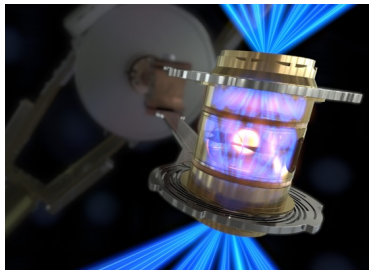
- **Inverse design:** boundary $\partial\mathbb{X}$, initial condition u^0 , parameter a to **optimize design objective:** plane design, rocket shape, underwater robot shape



- **Inverse problem :** infer initial condition u^0 or parameter a to **match prediction with observation**

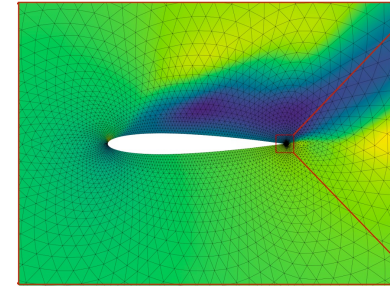
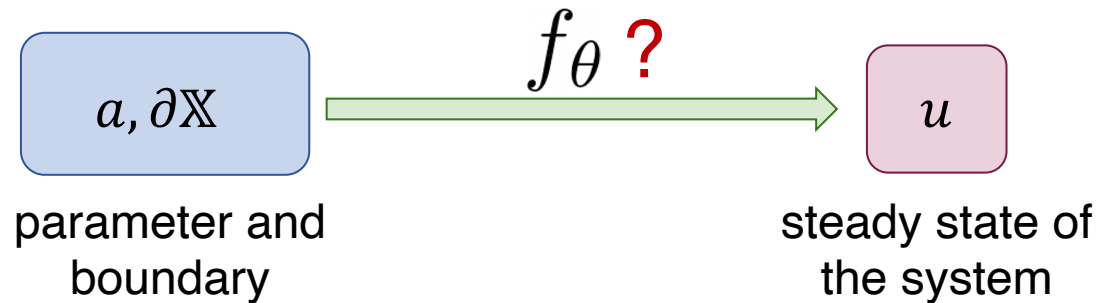


- **Control:** optimize control m^t to **optimize control objectives:** controlled nuclear fusion, robotics

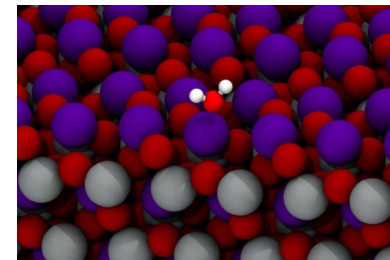


Tasks 2 & 3: **Steady-state** simulation and inverse design

Simulation:

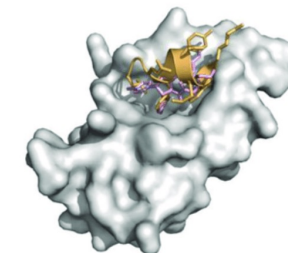
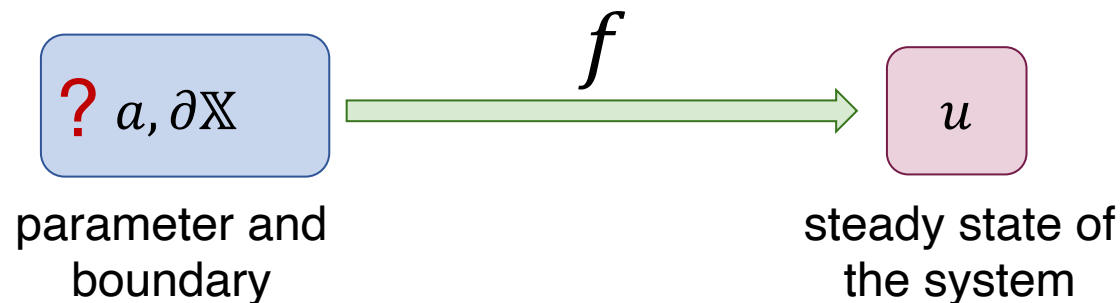


Aerodynamics simulation



Materials design

Inverse design/inverse problem:



Protein design

Course introduction: Neural architecture

Tasks

- Classification/regression
- Simulation
- Inverse design/inverse problem
- Control/planning

Neural architecture

- Multilayer perceptron
- Graph Neural Networks
- Convolutional Neural Networks
- Transformers

Learning paradigm

- Supervised learning
- Generative modeling
- Foundation models
- Reinforcement learning
- Evolutionary and multi-objective optimization

×

×

Application (AI & Science)

- Robotics
- Games (e.g., Go, atari)
- Autonomous Driving
- PDEs
- Life science
- Materials science

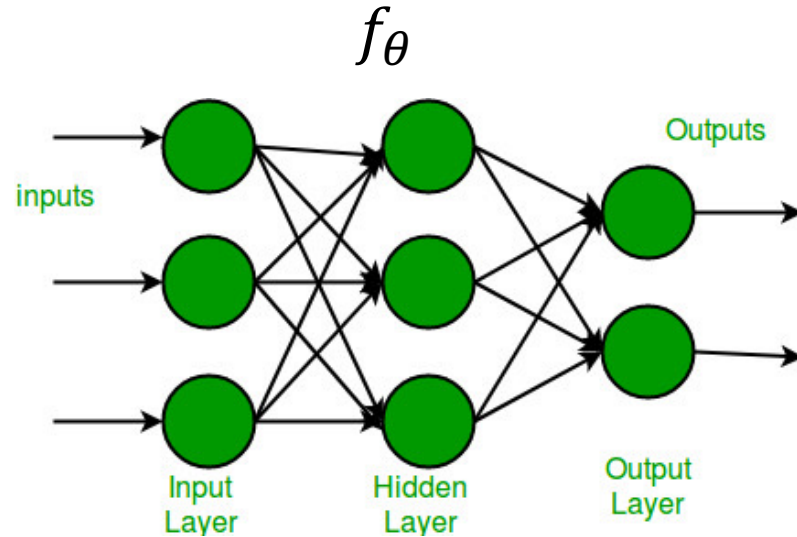
Neural architecture: overview

The choice of neural architecture depend on the data structure:

Data structure	Examples	Suitable neural architecture
Vector	simple vectors	Multilayer Perceptron (MLP)
Graph	molecules, irregular mesh	Graph Neural Network (GNN)
Grid	image, videos	Convolutional Neural Network (CNN)
Sequence	time series, natural language	Transformer

Neural architecture 1: Multilayer Perceptron (MLP)

input $x \in R^d$
(vector)



prediction \hat{y}

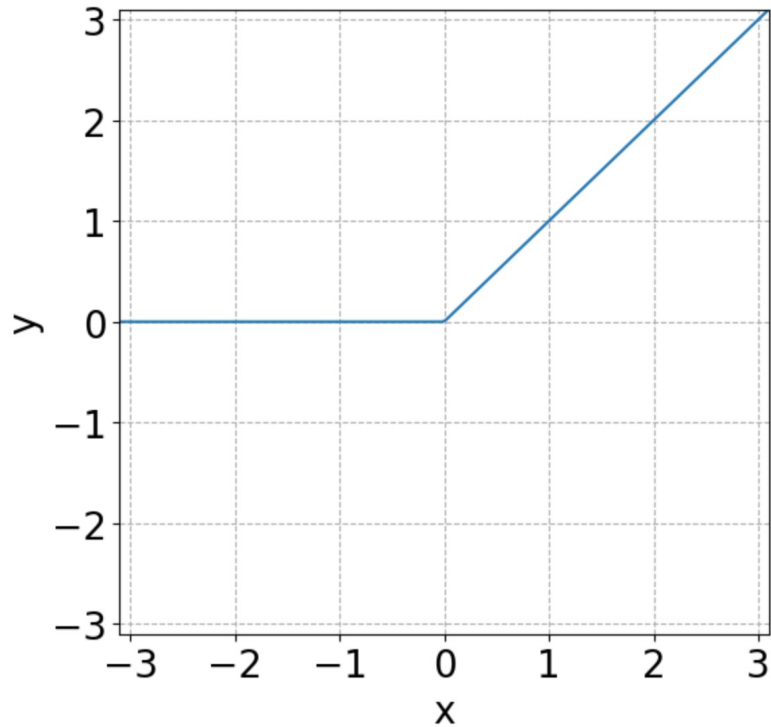
An MLP f_θ with n layers: $\hat{y} = W_n \sigma(\dots \sigma(W_2 \sigma(W_1 x + b_1) + b_2) + b_n$

W_i : weight matrix to be learned

b_i : bias vector to be learned

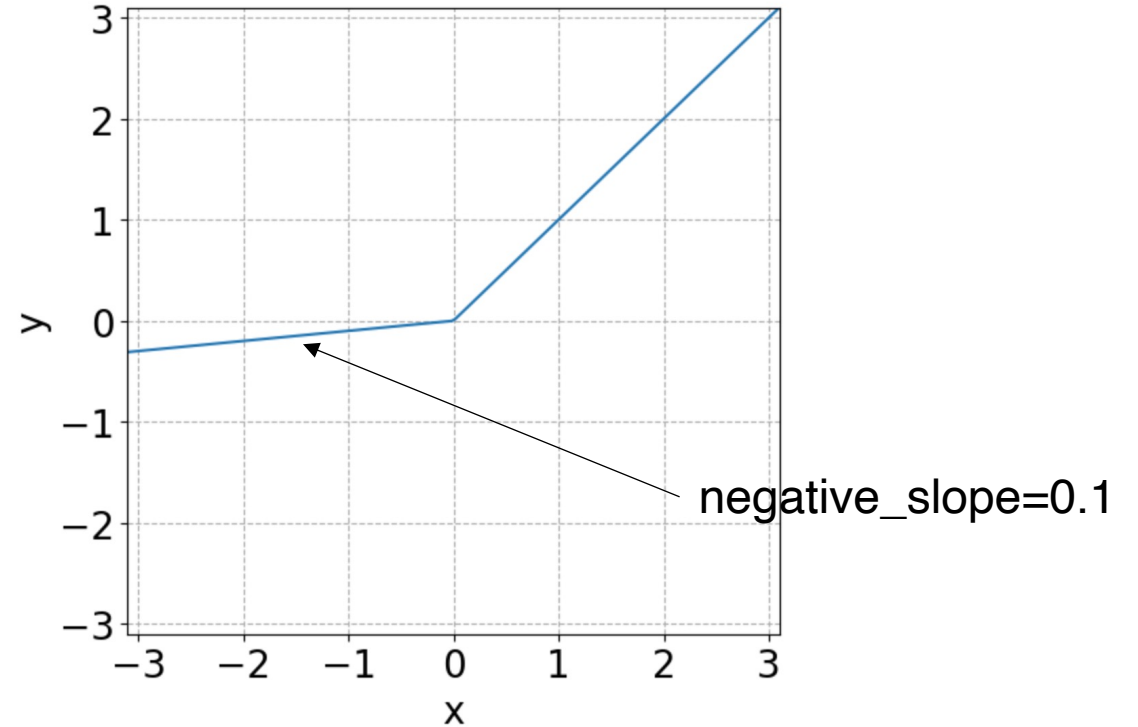
σ : (nonlinear) activation function, e.g., ReLU, softplus, ELU

Activation function



ReLU (Rectified Linear Unit)

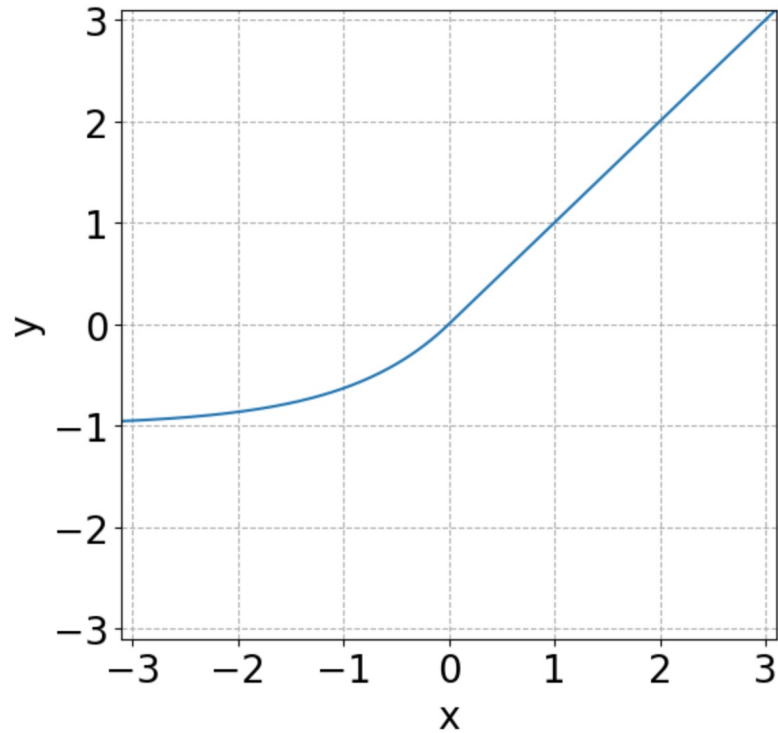
$$\text{ReLU}(x) = \max(0, x)$$



LeakyReLU

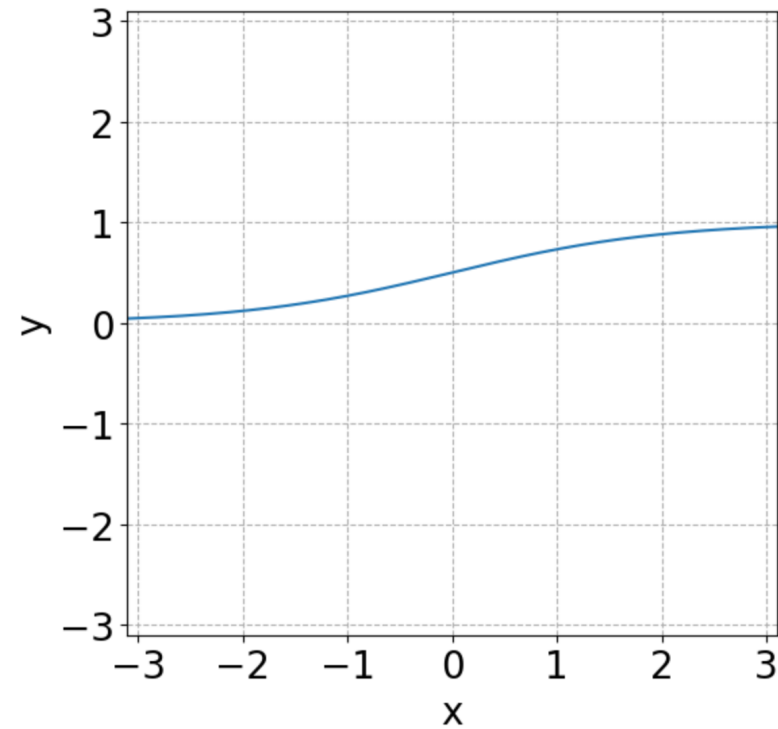
$$\text{LeakyReLU}(x) = \begin{cases} x, & \text{if } x \geq 0 \\ \text{negative_slope} \times x, & \text{otherwise} \end{cases}$$

Activation function



ELU (Exponential Linear Unit)

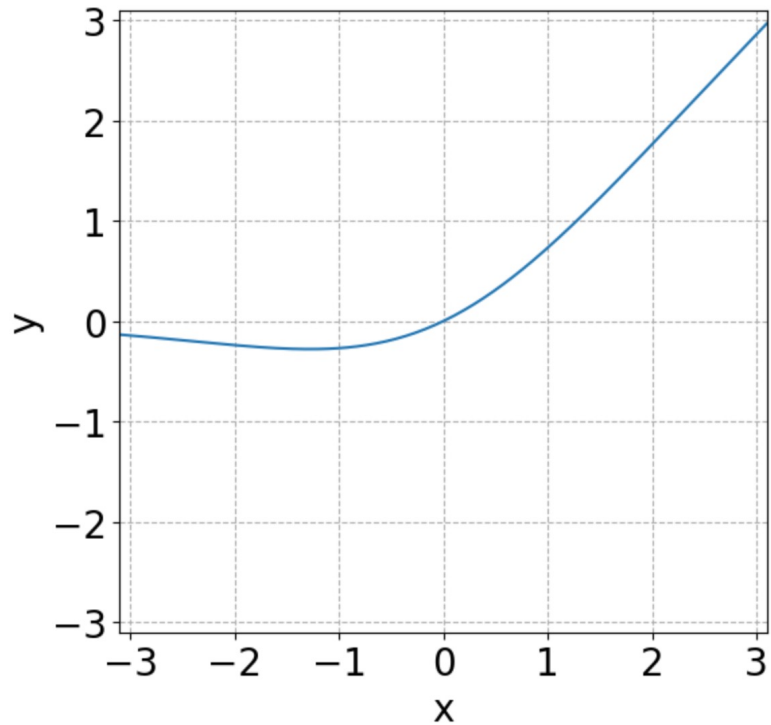
$$\text{ELU}(x) = \begin{cases} x, & x > 0 \\ e^x - 1, & x \leq 0 \end{cases}$$



Sigmoid

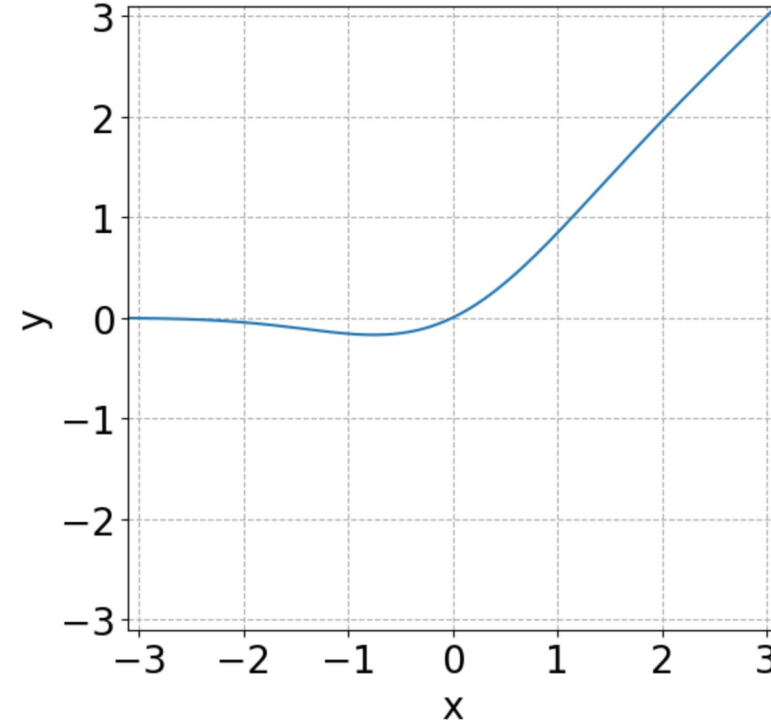
$$\text{Sigmoid}(x) = \frac{1}{1 + \exp(-x)}$$

Activation function



SiLU (Sigmoid Linear Unit)

$$\text{SiLU}(x) = x \cdot \text{Sigmoid}(x)$$



GELU (Gaussian Error Linear Unit)

$$\text{SiLU}(x) = x \cdot \Phi(x)$$

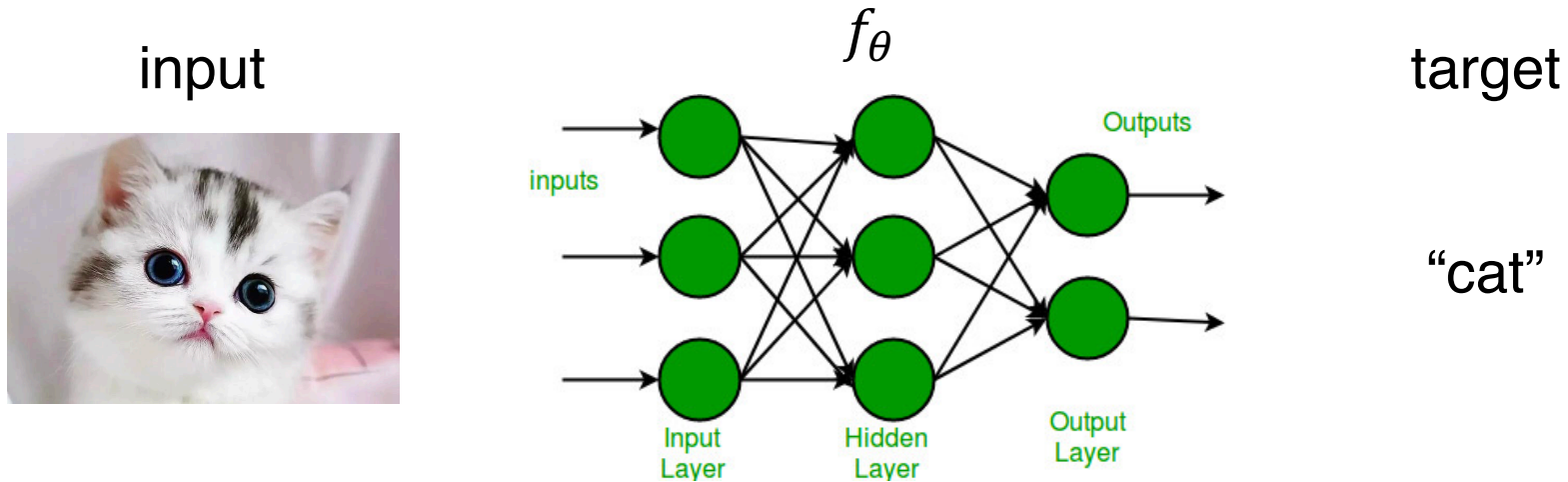
$\Phi(x)$ is the cumulative distribution function for Gaussian distribution

Activation function

Activation function	Advantages	Drawbacks
ReLU	Simple, suitable for classification	Can have some “dead neurons” The network is piecewise linear
LeakyReLU	Does not have dead neurons	The network is piecewise linear
ELU	Typically useful for regression	
Sigmoid	Output constrained to [0,1]	If input is far from 0, then have saturation (vanishing gradient)
SiLU	Typically useful for regression	
GELU	Typically useful for regression	

Typically try ReLU, LeakyReLU, ELU, and SiLU in hyperparameter search

MLP: universal approximation theorem



An MLP f_θ that has 1 hidden layer (with arbitrary width) and a nonlinear activation function can approximate any function to arbitrary precision [1][2].

Here $f_\theta(x) = W_2\sigma(W_1x + b_1)$

- With one hidden layer, may need **exponential** number of neurons w.r.t. input size
- With more layers, the neurons needed may be **polynomial** [3]

[1] Funahashi, Ken-Ichi. "On the approximate realization of continuous mappings by neural networks." Neural networks 2.3 (1989): 183-192.

[2] Hornik, Kurt, Maxwell Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators." Neural networks 2.5 (1989): 359-366.

[3] Rolnick, David, and Max Tegmark. "The power of deeper networks for expressing natural functions." ICLR 2018

Learning with gradient descent

$$f_{\theta}(x) = \sigma(W_n \sigma(\dots \sigma(W_2 \sigma(W_1 x + b_1) + b_2) \dots + b_n)$$

To fit dataset $\{(x_i, y_i)\}, i = 1, 2, \dots, N$, we can use Mean Squared Error (MSE):

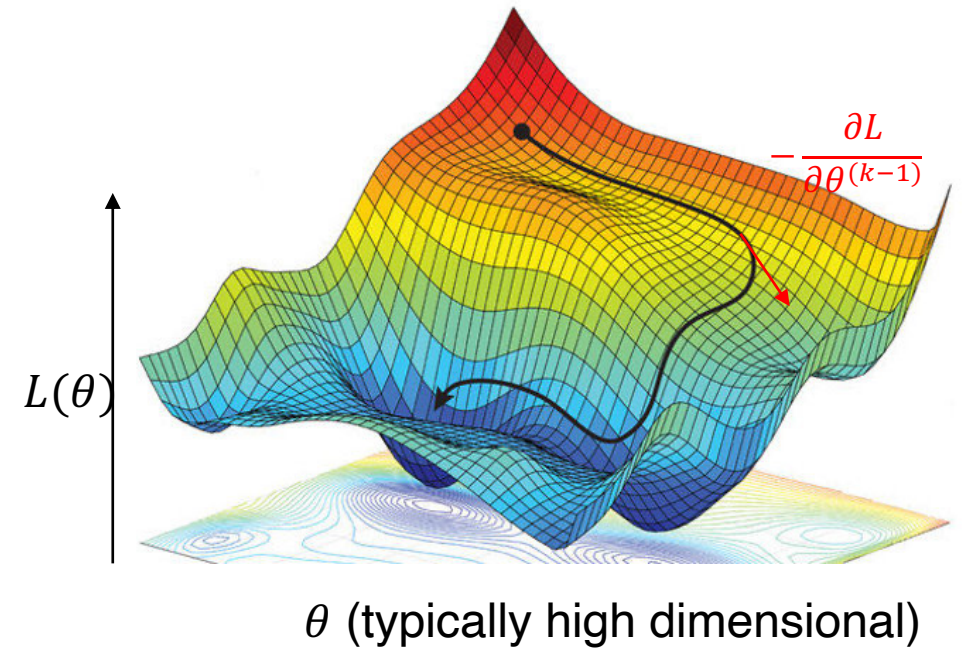
$$L(\theta) = \frac{1}{N} \sum_{i=1}^N (y_i - f_{\theta}(x_i))^2$$

How can we optimize the parameter $\theta = (W_1, \dots, W_n, b_1, \dots, b_n)$?

Answer: compute $\frac{\partial L}{\partial \theta}$, then we can perform gradient descent :

$$\theta^{(k)} \leftarrow \theta^{(k-1)} - \eta \frac{\partial L}{\partial \theta^{(k-1)}}$$

η : learning rate



Backpropagation

Consider:

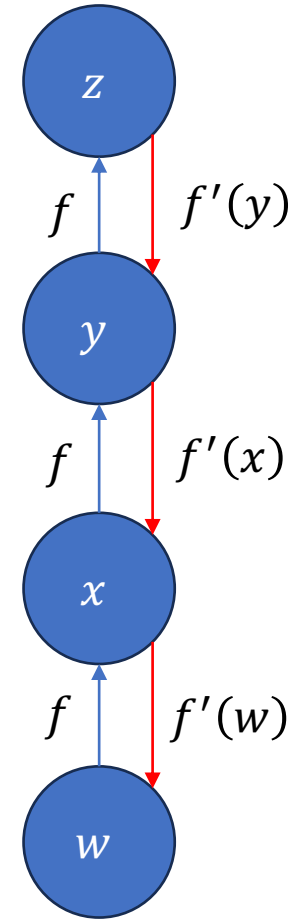
$$z = f(y), y = f(x), x = f(w)$$
$$z = f(f(f(w)))$$

Chain rule:

$$\frac{\partial z}{\partial w} = \frac{\partial z}{\partial y} \frac{\partial y}{\partial x} \frac{\partial x}{\partial w} = f'(y)f'(x)f'(w)$$

Observation:

1. We need to **store intermediate result** x, y to avoid recomputing them.
2. Goes layer-by-layer **from output to input**.



Backpropagation

Let's take a two layer MLP $f_{\theta}(x) = W_2\sigma(W_1x + b_1)$ as an example:

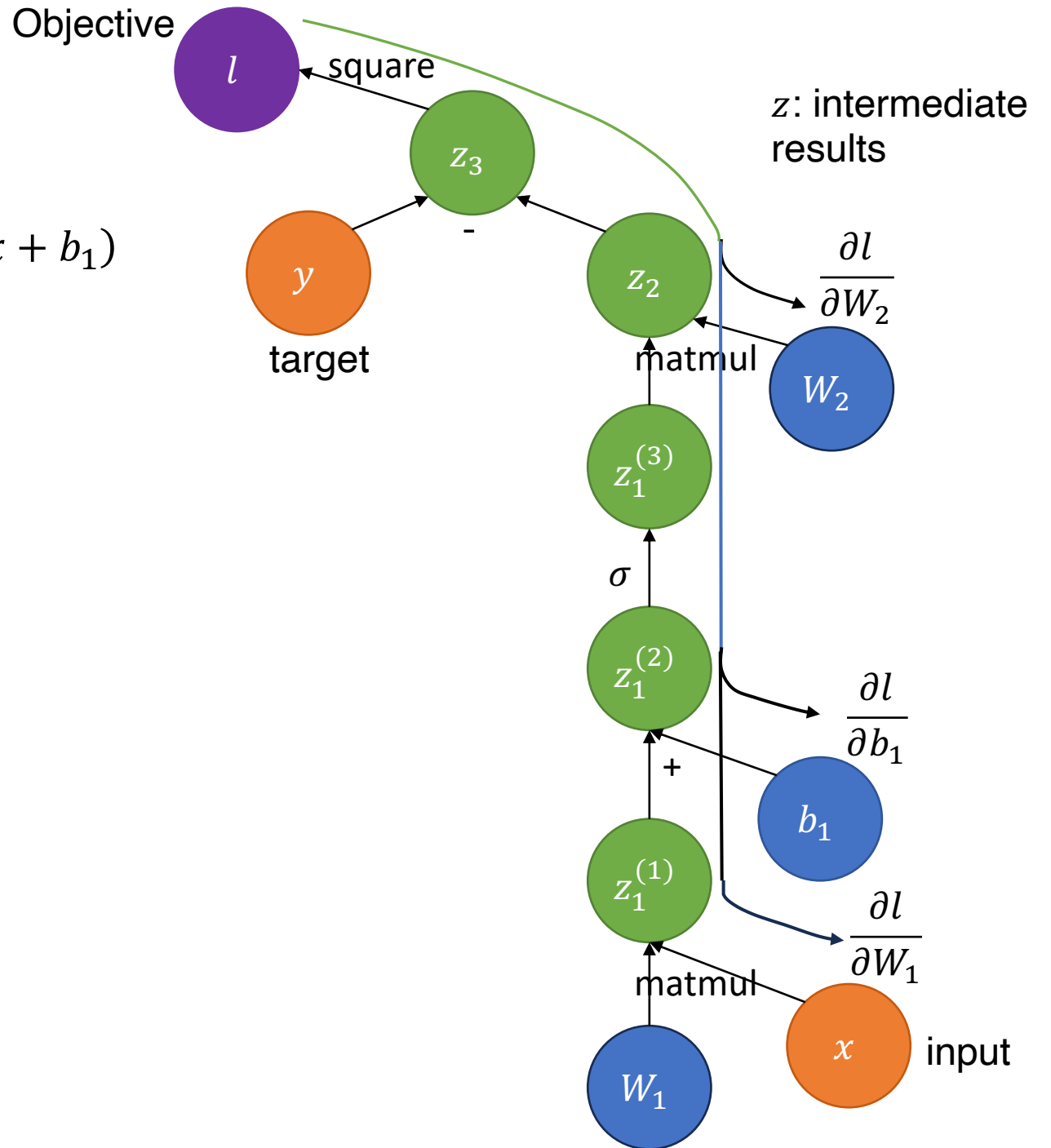
Objective: $l = (y - f_{\theta}(x))^2$

$$\frac{\partial l}{\partial W_2} = \frac{\partial l}{\partial z_3} \cdot \frac{\partial z_3}{\partial z_2} \cdot \frac{\partial z_2}{\partial W_2}$$

$$\frac{\partial l}{\partial b_1} = \frac{\partial l}{\partial z_3} \cdot \frac{\partial z_3}{\partial z_2} \cdot \frac{\partial z_2}{\partial z_1^{(3)}} \cdot \frac{\partial z_1^{(3)}}{\partial z_1^{(2)}} \cdot \frac{\partial z_1^{(2)}}{\partial b_1}$$

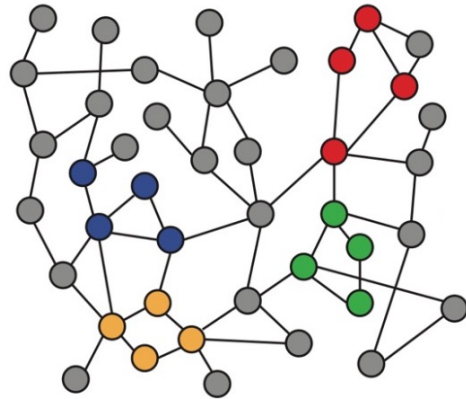
$$\frac{\partial l}{\partial W_1} = \frac{\partial l}{\partial z_3} \cdot \frac{\partial z_3}{\partial z_2} \cdot \frac{\partial z_2}{\partial z_1^{(3)}} \cdot \frac{\partial z_1^{(3)}}{\partial z_1^{(2)}} \cdot \frac{\partial z_1^{(2)}}{\partial z_1^{(1)}} \cdot \frac{\partial z_1^{(1)}}{\partial W_1}$$

shared, no need to recompute

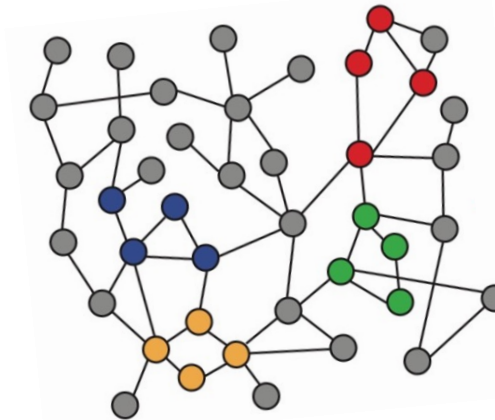


Neural architecture 2: Graph Neural Networks (GNN)

Predictions on the node/edge with updated features

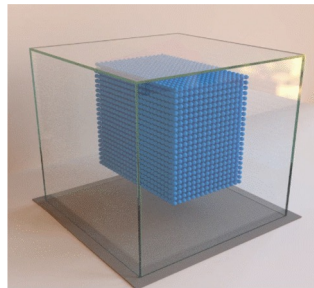


GNN f_{θ}

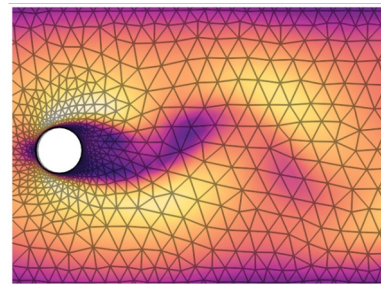


input graph $G = (V, E)$

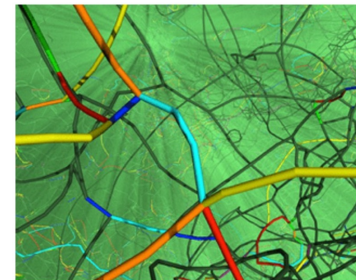
V : set of nodes with node features
 E : set of edges with edge features



Fluid dynamics,
computer graphics



Mesh-based
simulation for PDEs

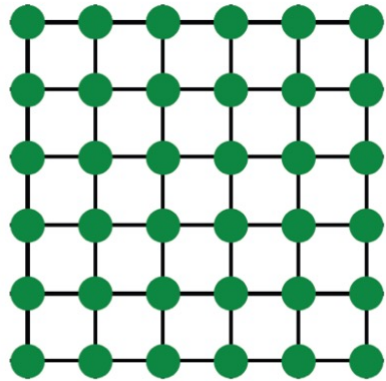


Dislocation in
materials

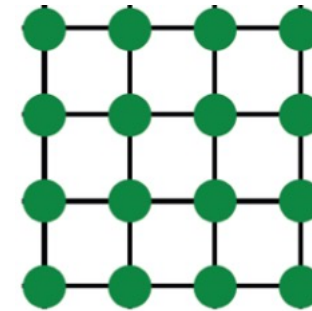


Proteins and small
molecules

Neural architecture 3: Convolutional Neural Networks (CNN)



CNN f_θ



input tensor $X \in R^{d_1 \times d_2 \times \dots \times d_n}$

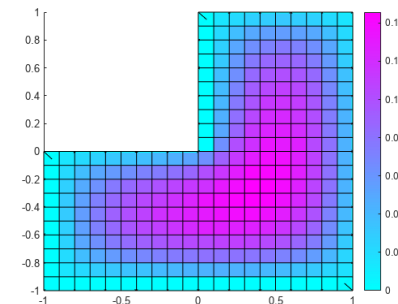
output tensor $\hat{Y} \in R^{d'_1 \times d'_2 \times \dots \times d'_n}$



image



video



PDE discretized on a regular grid

Neural architecture 4: Transformer



input sequence X

Transformer f_θ



output sequence \hat{Y}

The animal didn't cross the street because it was too tired .

Natural language

... GTGCATCTGACTCCTGAGGAGAAG ...
... CACGTAGACTGAGGACTCCTCTTC ...

DNA sequence

... V H L T P E E K ...

Protein sequence

Neural architecture: Summary

Data structure	Suitable neural architecture	Course #
Vector	Multilayer Perceptron (MLP)	2 (Tailin Wu & Tao Lin)
Graph	Graph Neural Network (GNN)	10 (Tailin Wu)
Grid	Convolutional Neural Network (CNN)	7 (Kaicheng Yu)
Sequence	Transformer	4 (Zhenzhong Lan)

For each neural architecture (same goes for topics in the course), we will introduce its:

- Motivation
- Architecture
- Typical tasks
- Research frontiers

Course introduction: Learning paradigm

Tasks

- Classification/regression
- Simulation
- Inverse design/inverse problem
- Control/planning

×

Neural architecture

- Multilayer perceptron
- Graph Neural Networks
- Convolutional Neural Networks
- Transformers

×

Learning paradigm

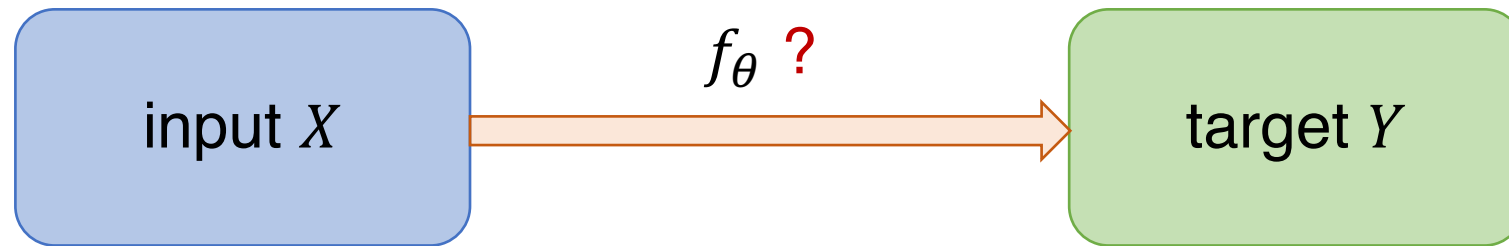
- Supervised learning
- Generative modeling
- Foundation models
- Reinforcement learning
- Evolutionary and multi-objective optimization

Application (AI & Science)

- Robotics
- Games (e.g., Go, atari)
- Autonomous Driving
- PDEs
- Life science
- Materials science

Learning paradigm 1: Supervised learning

- image
- video
- graph
- time series
- natural language
- ...



- **classification**
↑
• label (discrete)
- scalar/tensor (continuous)
↓
• **regression**

Given many examples of $(X, Y) = \{(x_i, y_i)\}_{i=1}^N$ pairs, learn a neural network (NN) f_θ that minimizes the prediction loss:

$$\theta^* = \operatorname{argmin}_\theta \mathbb{E}_{(X,Y) \sim P(X,Y)} [\ell(f_\theta(X), Y)]$$

f_θ : neural network to be learned

ℓ : loss function

Learning paradigm 2: Generative modeling

Images and shapes generated by diffusion models:



By DallE 2



By MeshDiffusion [1]

[1] Liu, Zhen, et al. "Meshdiffusion: Score-based generative 3d mesh modeling." *ICLR 2023*

Learning paradigm 2: Generative modeling

Robotic policy by diffusion models [1]



Text to video generation by Sora [2]

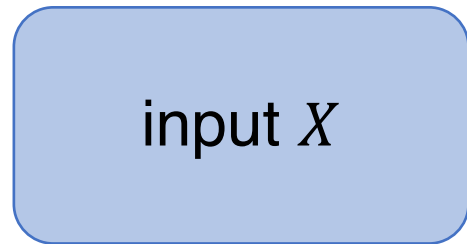


[1] Fu, Zipeng, Tony Z. Zhao, and Chelsea Finn. "Mobile ALOHA: Learning Bimanual Mobile Manipulation with Low-Cost Whole-Body Teleoperation." *arXiv preprint arXiv:2401.02117* (2024).

[2] OpenAI team. "Video generation models as world simulators", 2024

Learning paradigm 2: Generative modeling

- image
- video
- graph
- time series
- natural language
- ...



$p_{\theta}(X)$?

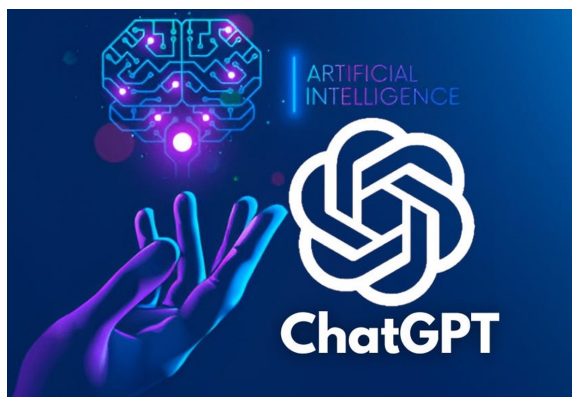
Probability model

Given many examples of the input X , learn a probability model $p_{\theta}(X)$ that can **sample** new instances of X that conform to the data distribution

Major generative models:

- Diffusion models
- Flow
- Generative adversarial network (GAN)
- Variational autoencoder (VAE)

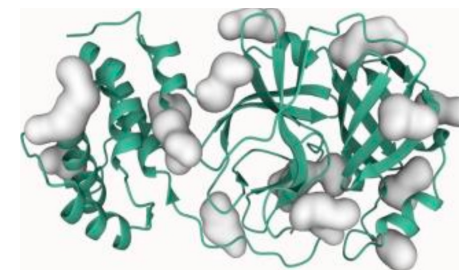
Learning paradigm 3: Foundation models



chatGPT



Sora [1]

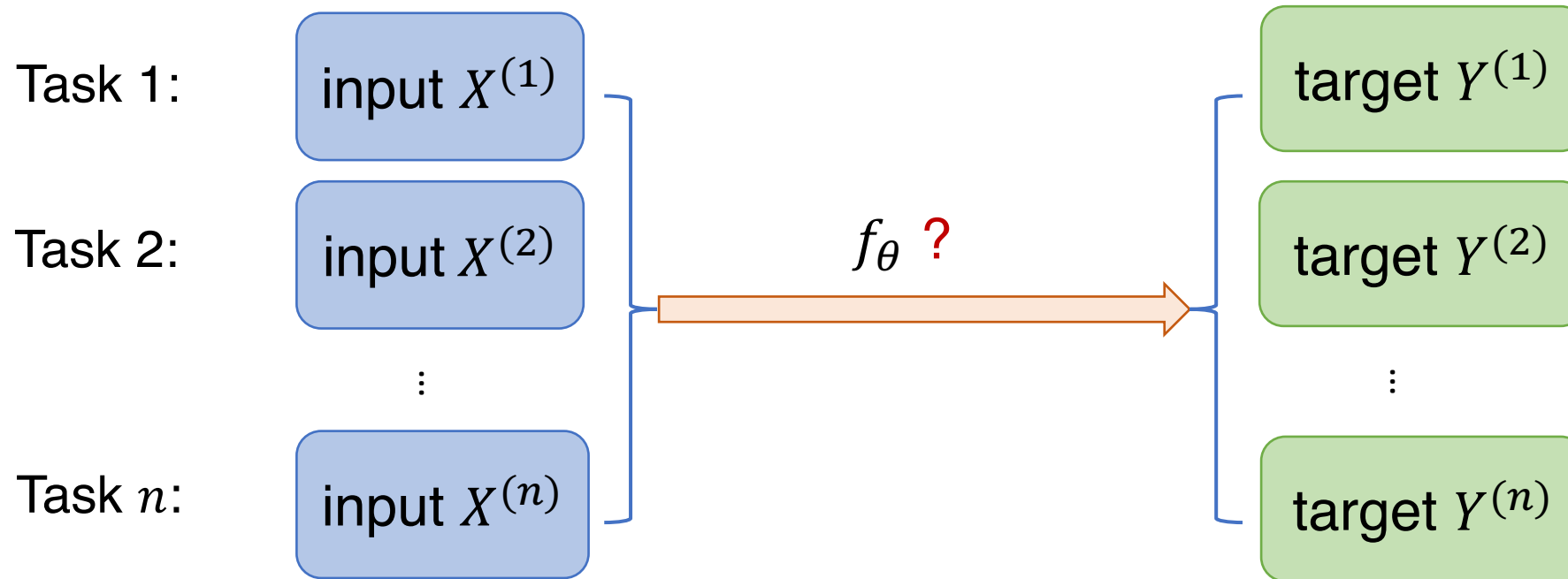


uniMol [2]

[1] OpenAI team. "Video generation models as world simulators", 2024

[2] Zhou, Gengmo, et al. "Uni-Mol: a universal 3D molecular representation learning framework." ICLR 2023

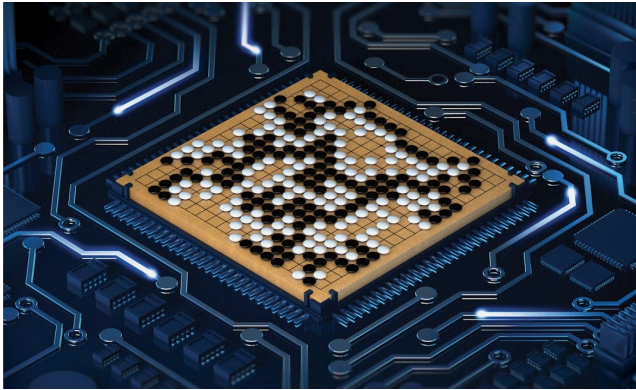
Learning paradigm 3: Foundation models



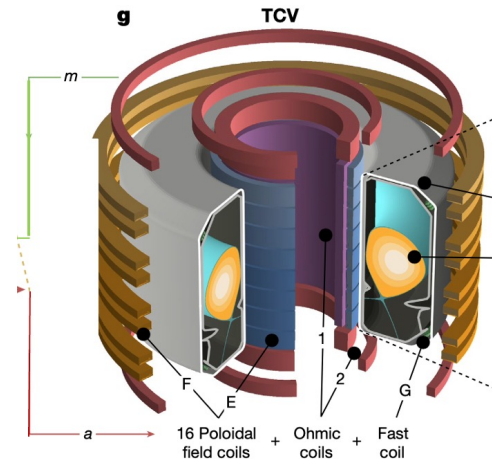
Given many diverse tasks, each consists of its massive number of examples

$(X^{(n)}, Y^{(n)}) = \left\{ \left(x_i^{(n)}, y_i^{(n)} \right) \right\}_{i=1}^{N^{(n)}}$, learn a single foundation model f_{θ} that can faithfully predict the target from the input.

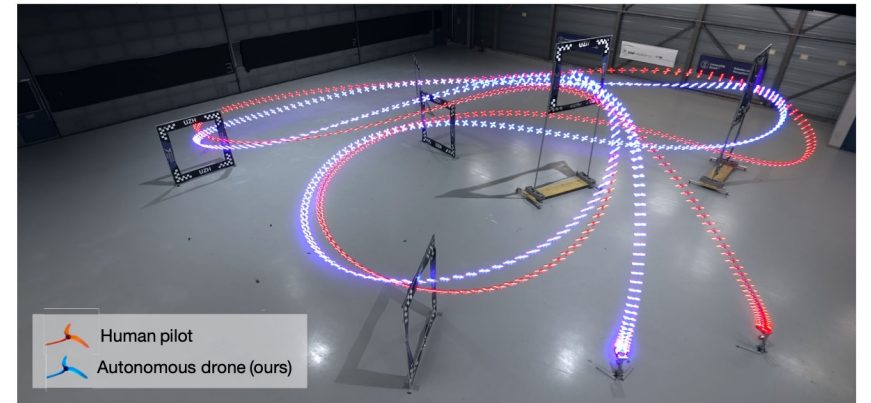
Learning paradigm 4: Reinforcement learning



AlphaGo [1]



Controlled nuclear fusion [2]



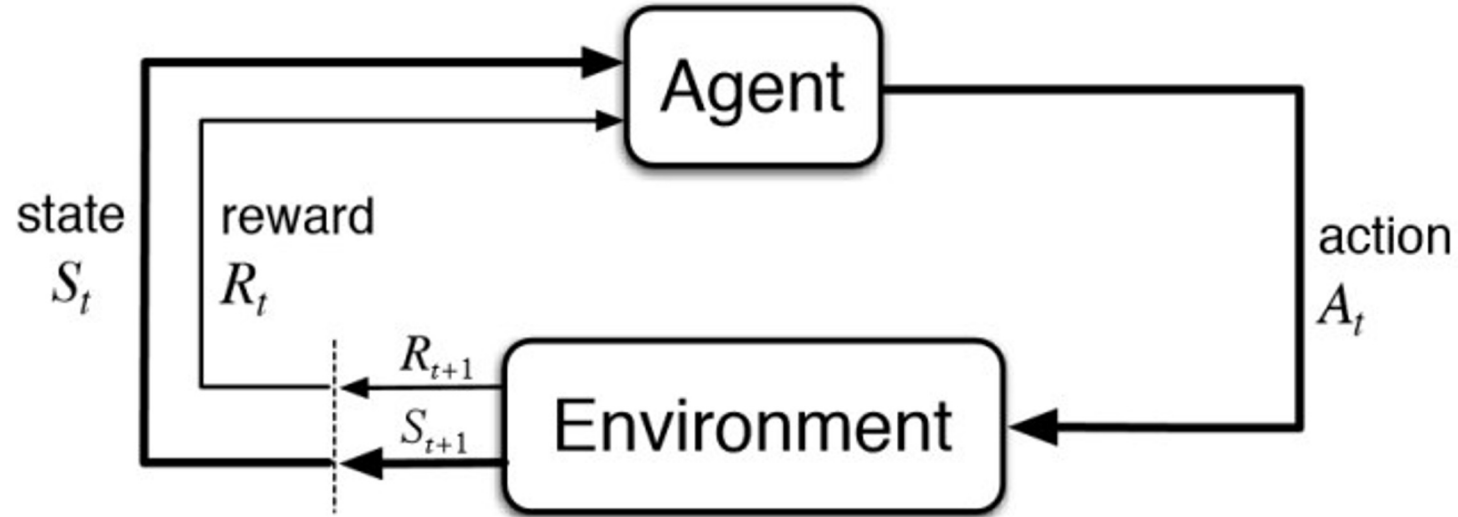
Drone racing [3]

[1] Silver, David, et al. "Mastering the game of Go with deep neural networks and tree search." *Nature* 529.7587 (2016): 484-489.

[2] Degraeve, Jonas, et al. "Magnetic control of tokamak plasmas through deep reinforcement learning." *Nature* 602.7897 (2022): 414-419.

[3] Kaufmann, Elia, et al. "Champion-level drone racing using deep reinforcement learning." *Nature* 620.7976 (2023): 982-987.

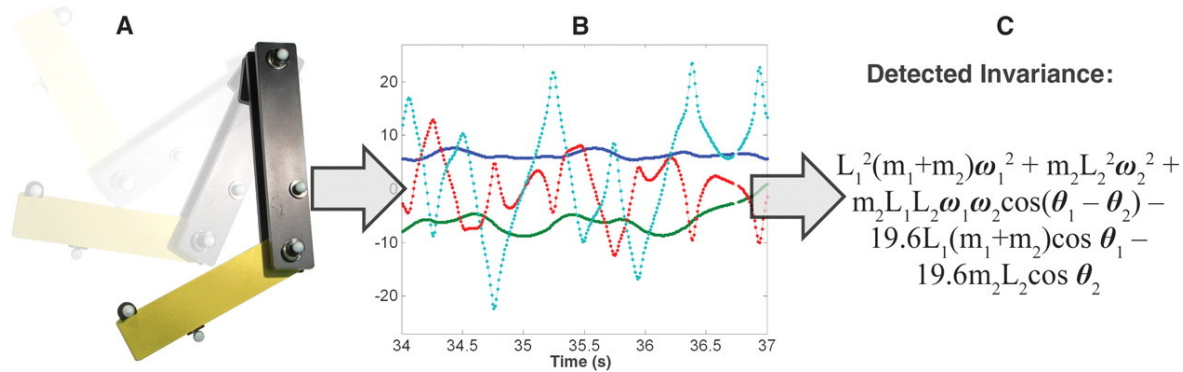
Learning paradigm 4: Reinforcement learning



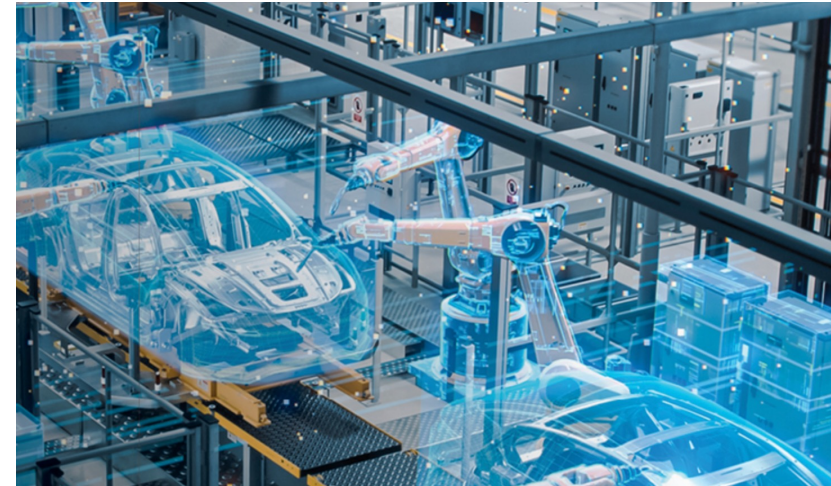
Goal: maximize the long-term expected reward w.r.t. to the policy $\pi(A_t|S_t)$

$$\max_{\pi(A_t|S_t)} \mathbb{E}_t[R_t]$$

Learning paradigm 5: Evolutionary and multi-objective learning



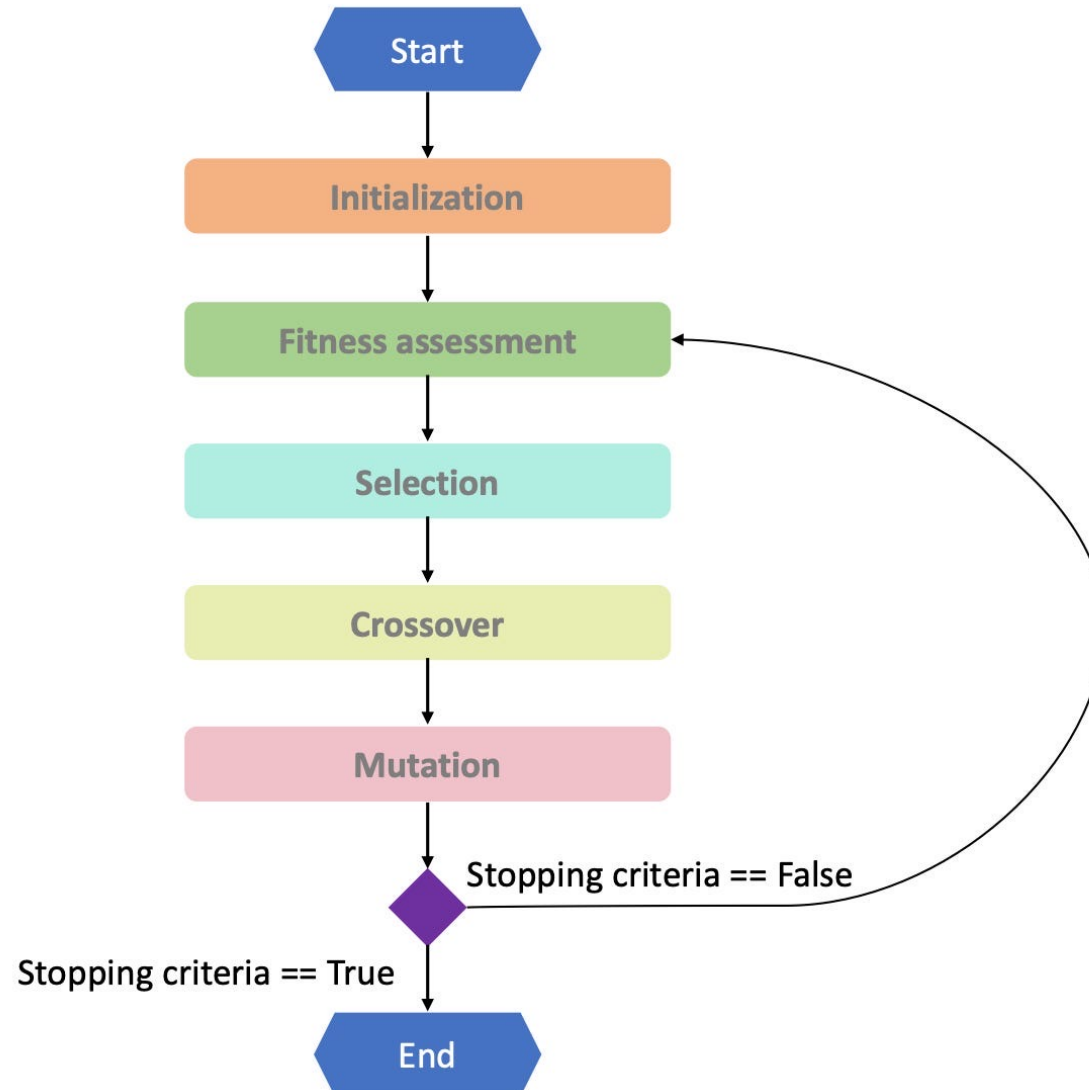
Discovering equations from data [1]



Optimization in engineering

[1] Schmidt, Michael, and Hod Lipson. "Distilling free-form natural laws from experimental data." *science* 324.5923 (2009): 81-85.

Learning paradigm 5: Evolutionary and multi-objective learning



Learning paradigm: Summary

Learning paradigm	Suitable scenarios	Course #
Supervised learning	Most standard	2 (Tailin Wu)
Generative modeling	High-dimensional data, can also be used in any tasks in regression	3 (Tailin Wu)
Foundation models	Large diverse tasks	10 (Zhenzhong Lan)
Reinforcement learning	Agent interacting with environment, cannot pass gradient through	5 (Tailin Wu)
Evolutionary and multi-objective learning	Gradient-free, discrete optimization	13 (Yaochu Jin)

Course introduction: Application in AI and Science

Tasks

- Classification/regression
- Simulation
- Inverse design/inverse problem
- Control/planning

×

Neural architecture

- Multilayer perceptron
- Graph Neural Networks
- Convolutional Neural Networks
- Transformers

×

Learning paradigm

- Supervised learning
- Generative modeling
- Foundation models
- Reinforcement learning
- Evolutionary and multi-objective optimization

Application (AI & Science)

- Robotics
- Games (e.g., Go, atari)
- Autonomous Driving
- PDEs
- Life science
- Materials science

Application in AI



robotics

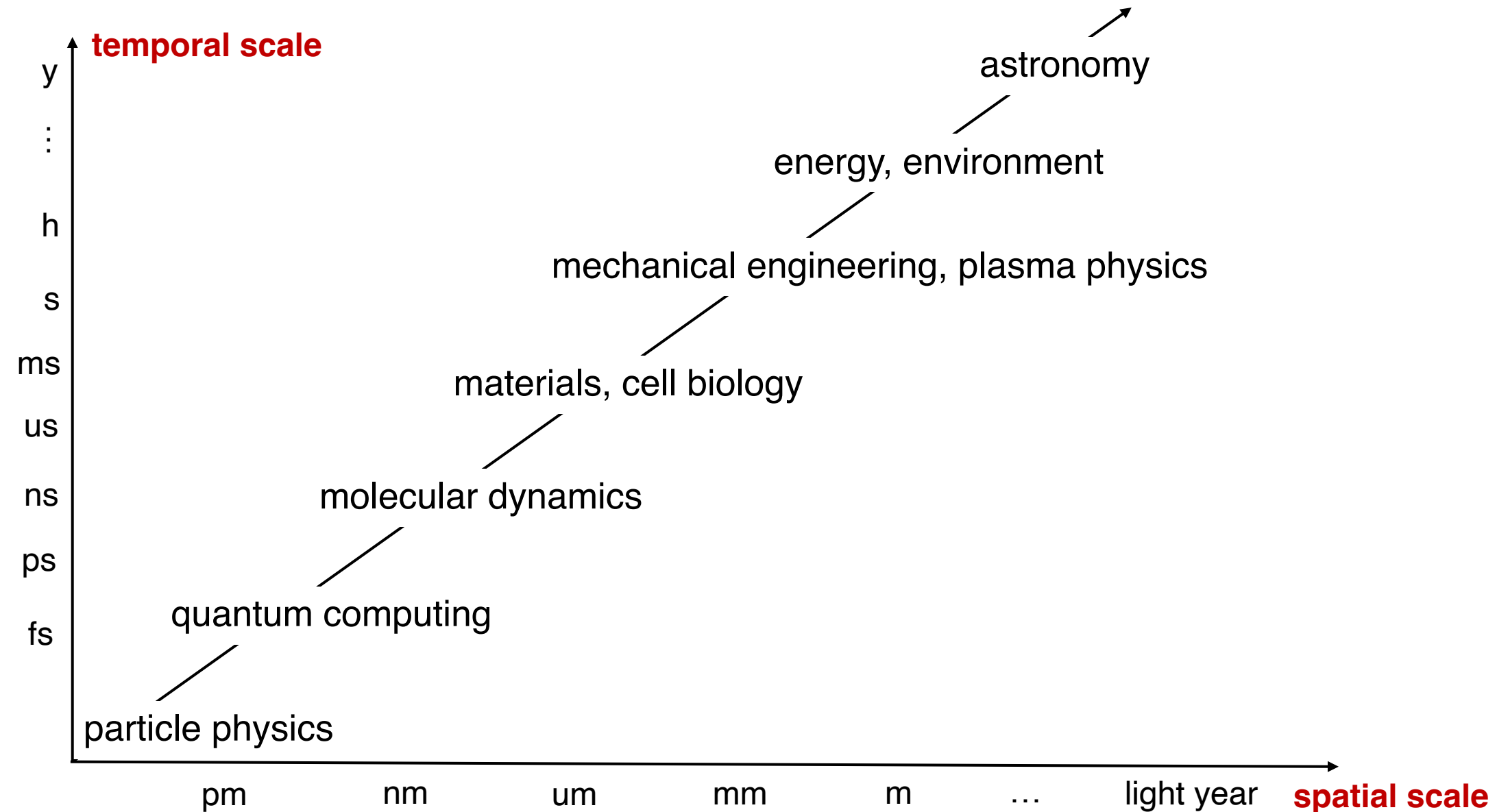


games

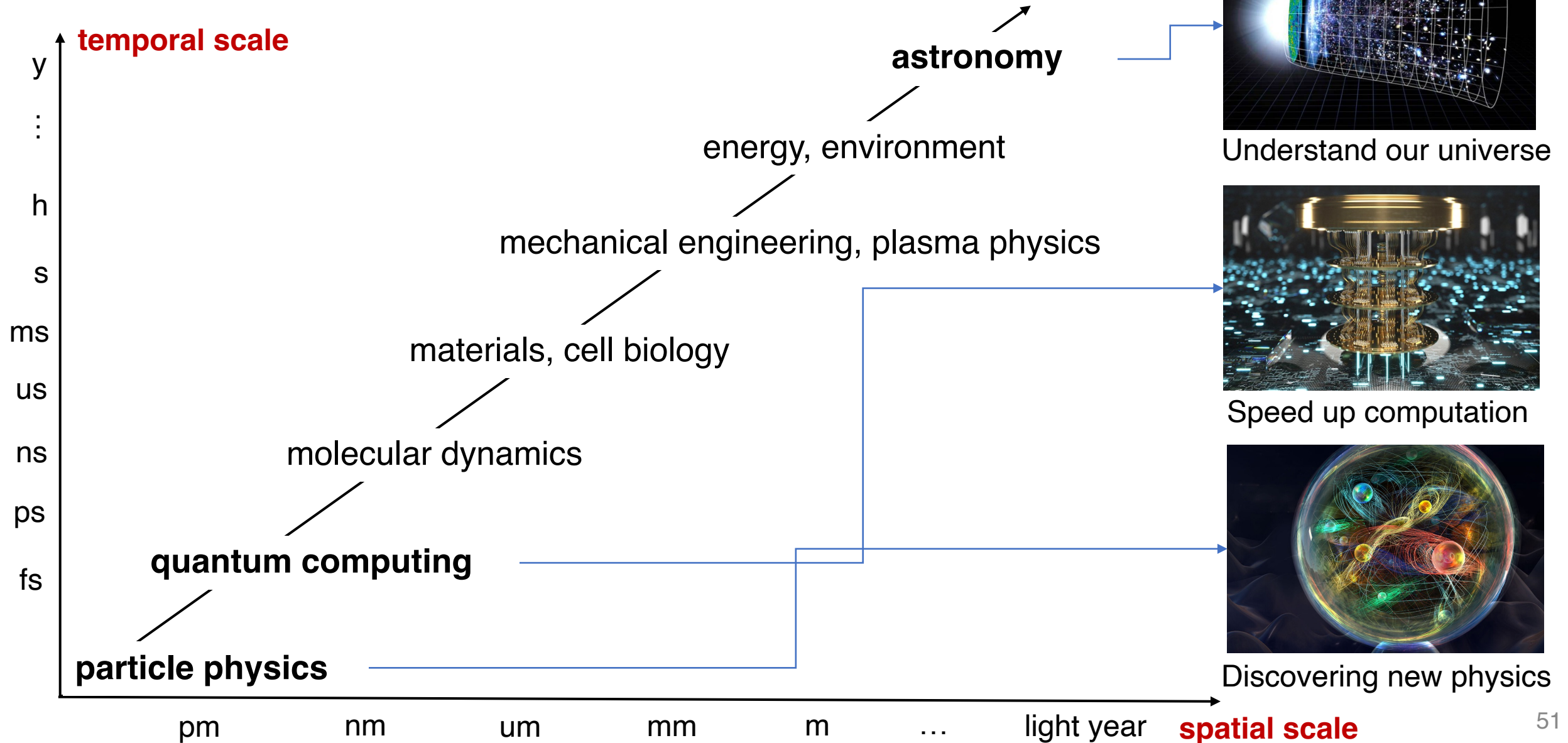


self-driving

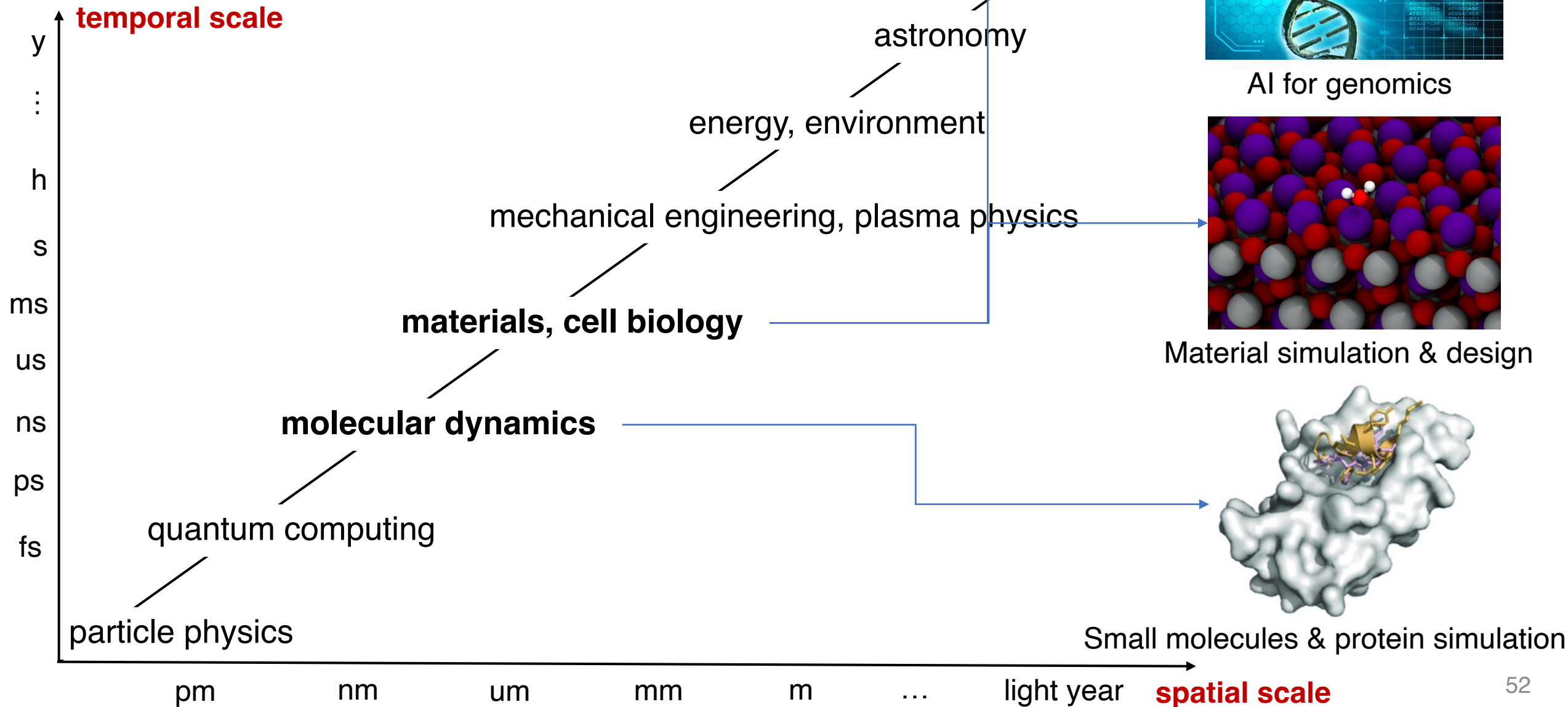
Application in AI for Science: from microscopic to macroscopic



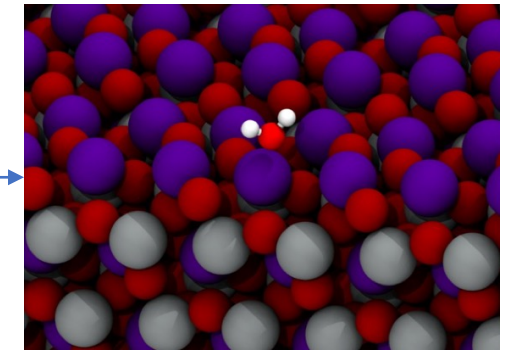
AI for Science: from microscopic to macroscopic



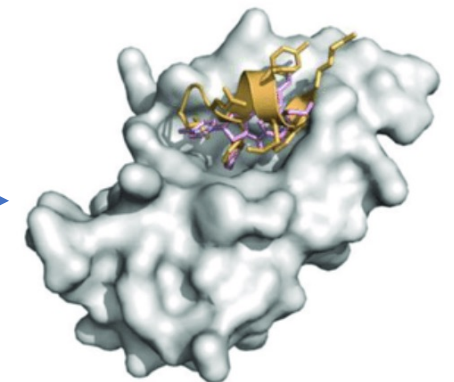
AI for Science: from microscopic to macroscopic



AI for genomics

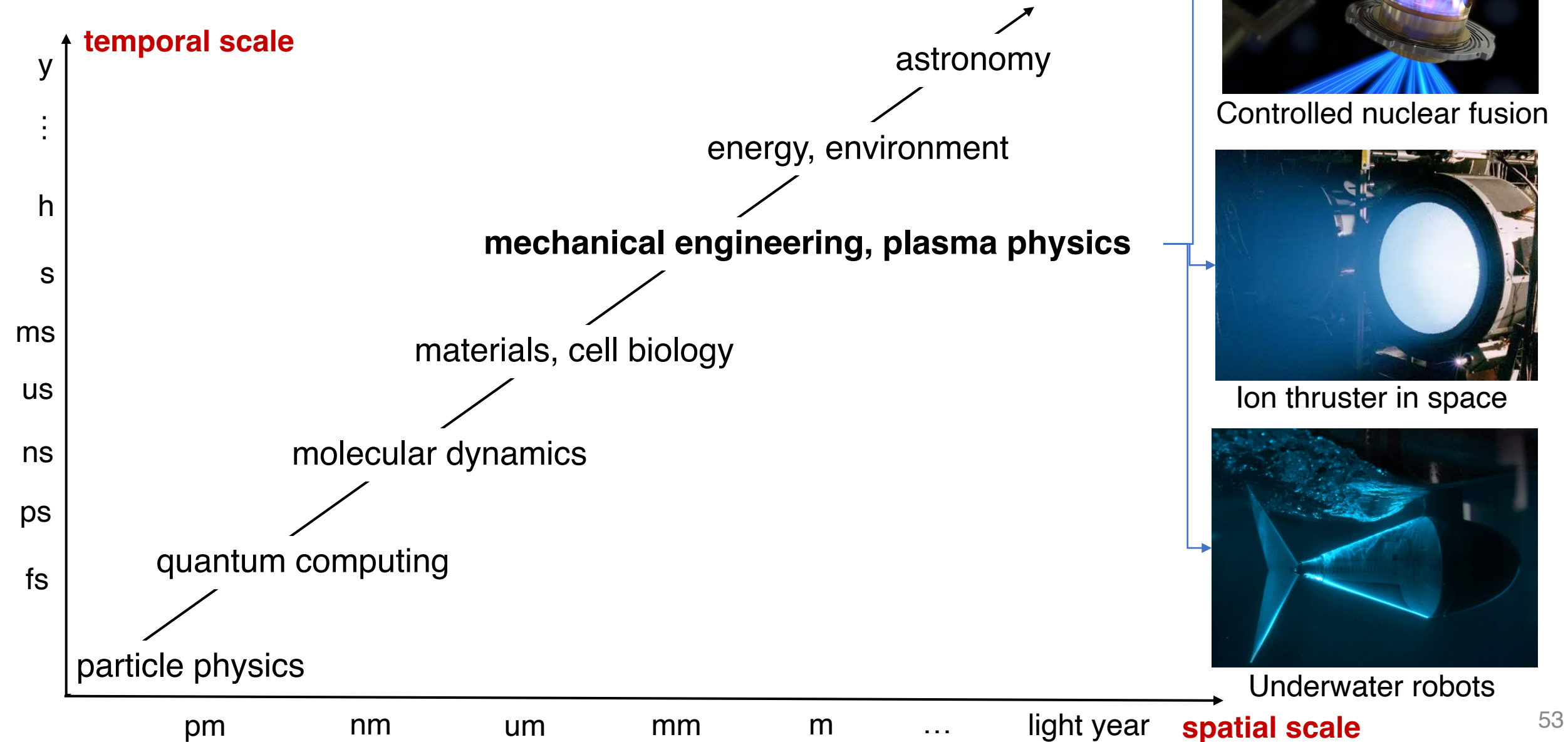


Material simulation & design

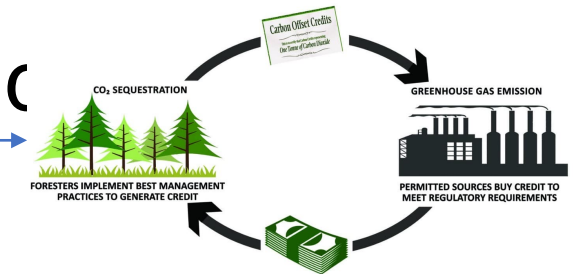
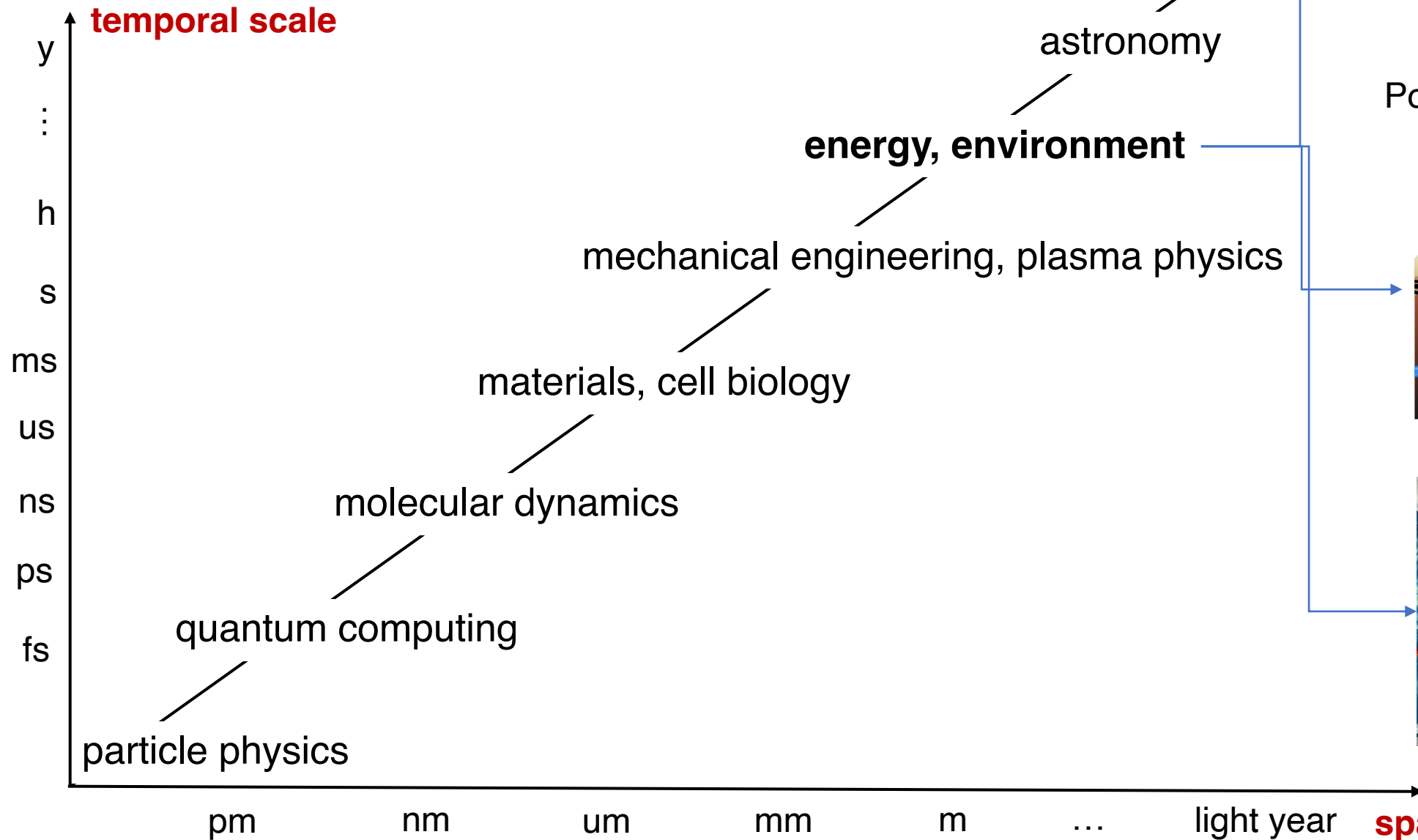


Small molecules & protein simulation

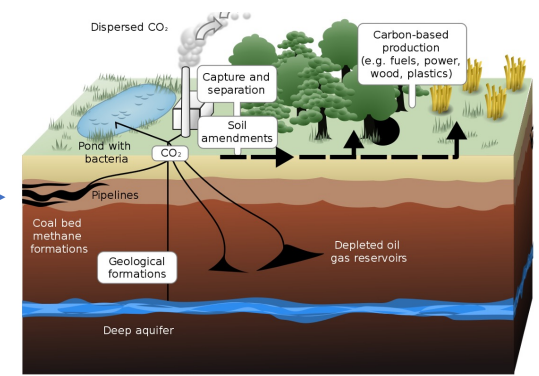
AI for Science: from microscopic to macroscopic



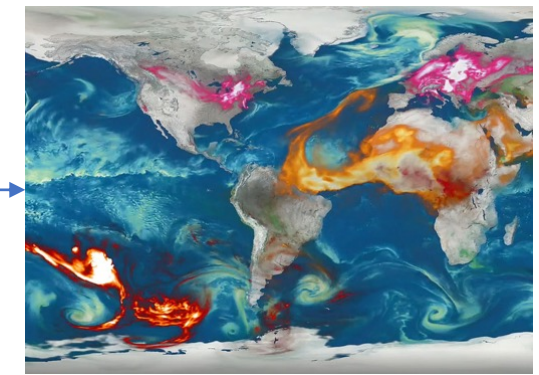
AI for Science: from microscopic to macroscopic



Policy design for carbon credit

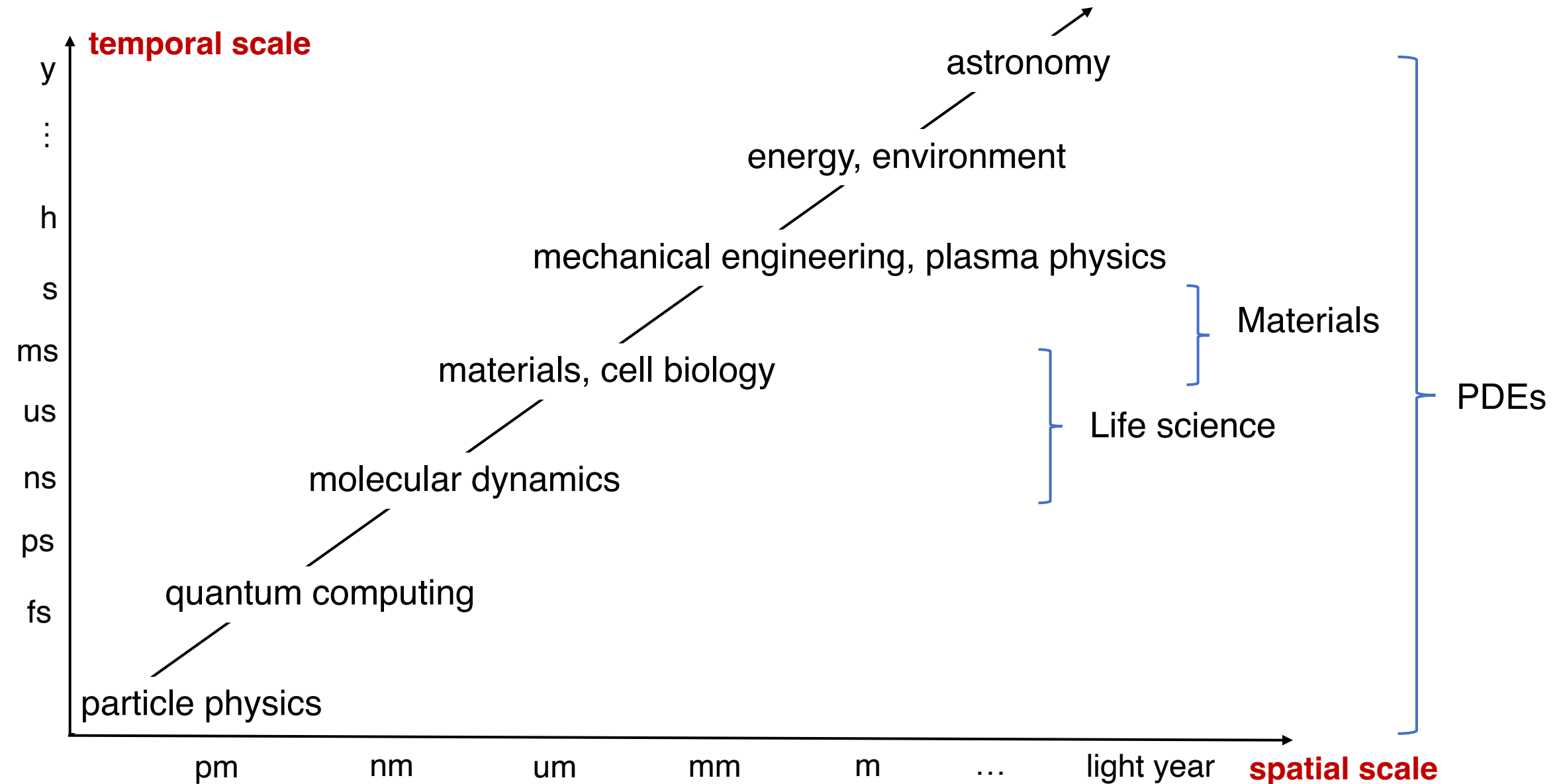


Carbon capture

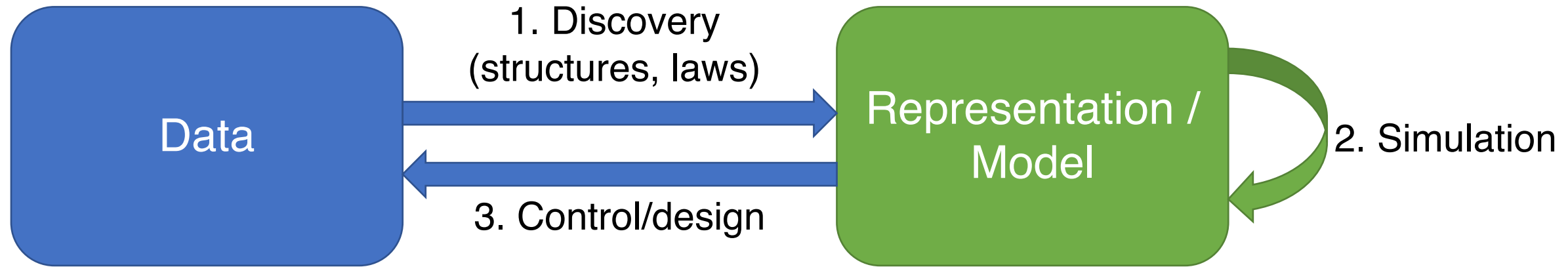


Weather forecasting

Application in AI for Science: from microscopic to macroscopic



AI for Science: universal tasks



These three tasks are fundamental in **science** and **engineering**

These three tasks are equally fundamental in **machine learning**

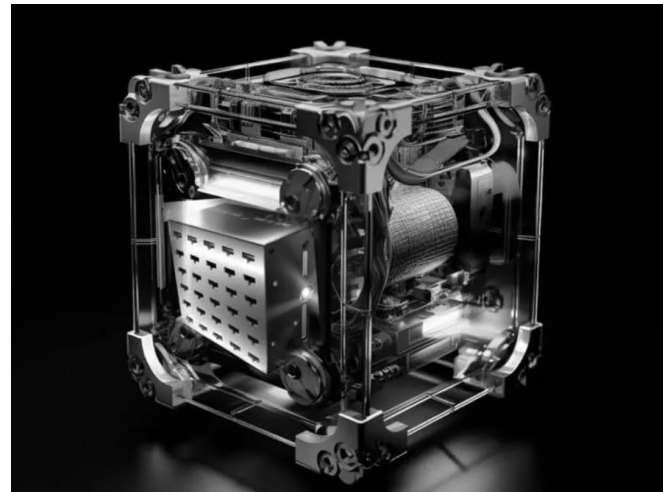
Application: Summary

Application	Area	Course #
Robotics	AI	6 (Tailin)
Self-driving	AI	7 (Kaicheng Yu)
AI + PDEs/scientific computing	AI for science	14 (Tailin Wu)
AI + Life sciences	AI for science	12 (Ziqing Li)

Trend 1: Integration of technologies

- **Aerospace + Controlled nuclear fusion:** a spacecraft could theoretically reach 1/10 the speed of light (30,000 km/s) [1], which is 1,700 times the current maximum spacecraft speed of 17 km/s.

[RocketStar](#) is developing the FireStar Drive thruster based on controlled nuclear fusion technology.

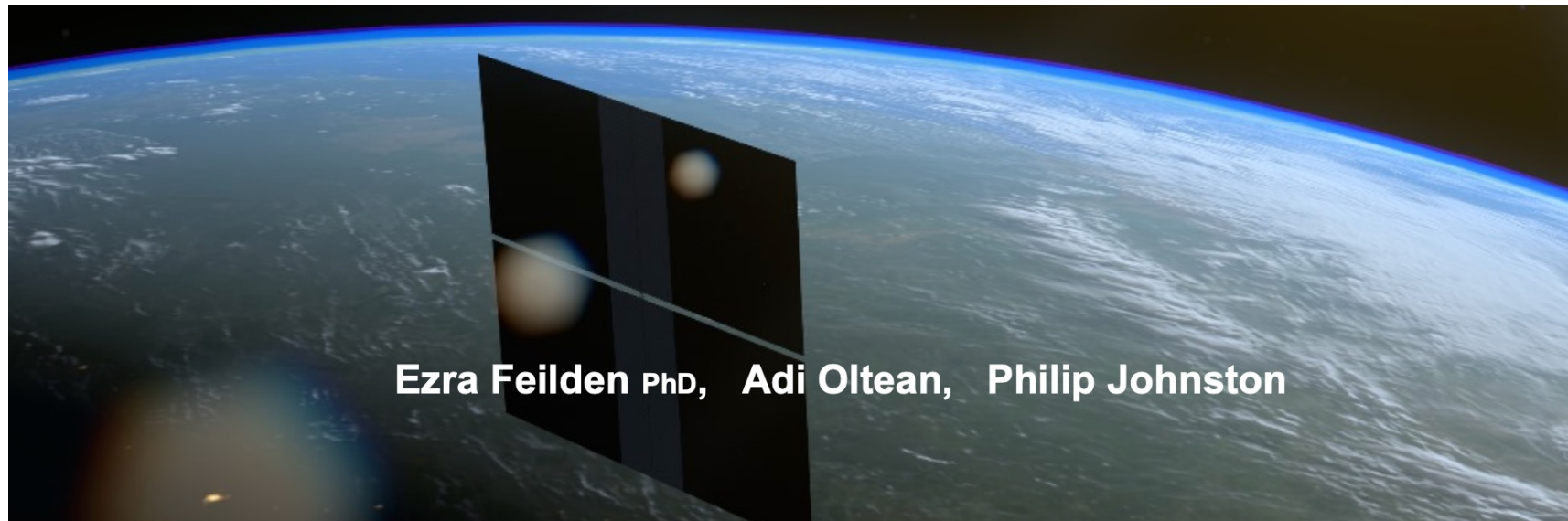


[1] 吴从军, 火箭推进速度上限的估算, 中国物理学会期刊网

Trend 1: Integration of technologies

- **Aerospace + GPU + Embodied AI:** Build GPU cluster in space

Lumen Orbit is planning to build the first GPU cluster in space [1].



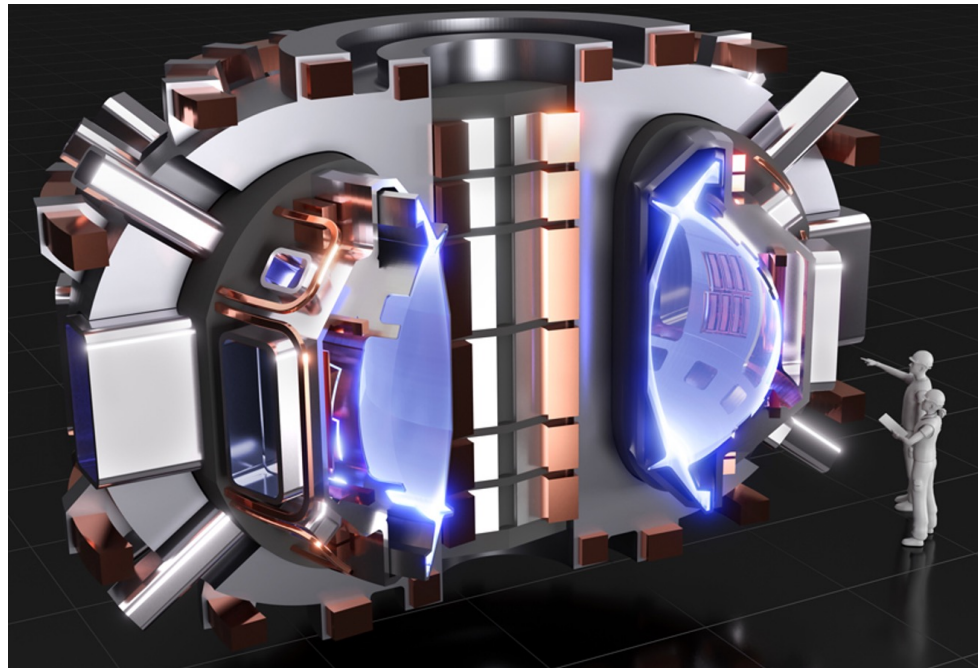
Trend 1: Integration of technologies

- **Aerospace + Mechanical engineering:** Gravity Jet Suit by gravity industries



Trend 1: Integration of technologies

- **Controlled nuclear fusion + materials:** The realization of high-temperature superconductors or room-temperature superconductors could significantly reduce the size of tokamaks.



China's National policy 国家政策

《国家空间科学中长期发展规划》中国科学院 国家航天局 中国载人航天工程办公室

第二阶段，2028—2035年，通过第一阶段任务实施取得位居世界前列的原创成果。运营中国空间站，论证实施载人月球探测、月球科研站、太阳系边际探测、巨行星系统探测、金星大气采样返回等科学任务。

第三阶段，2036—2050年，我国空间科学重要领域达到世界领先水平。论证实施大型任务5~6项，以及25项左右中小型和机遇型任务。

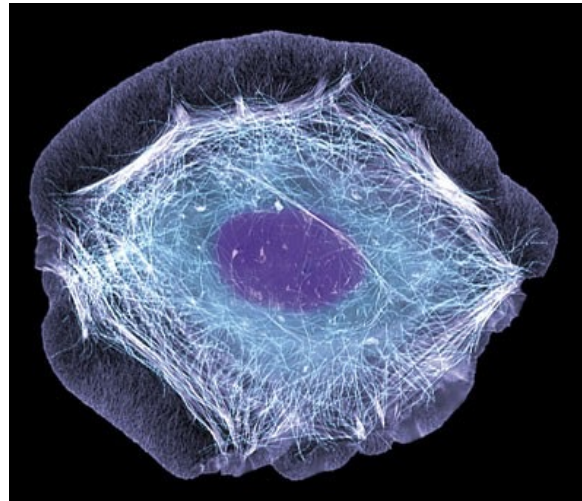
《通用航空装备创新应用实施方案（2024—2030年）》（工业和信息化部、科学技术部、财政部、中国民用航空局印发），提出到2030年，推动低空经济形成万亿级市场规模

Trend 2: Improvement of measurement technology

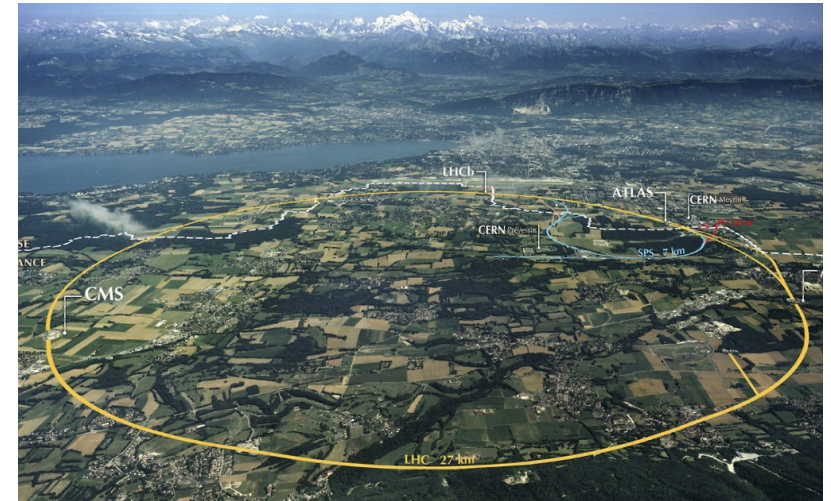
- **Better science needs better measurement**
 - Astronomy observation: New satellites and more accurate telescopes
 - Life science observation: Better single cell measurements
 - Particle collision measurement: Higher energy and better reconstruction



New telescopes



Single cell measurement

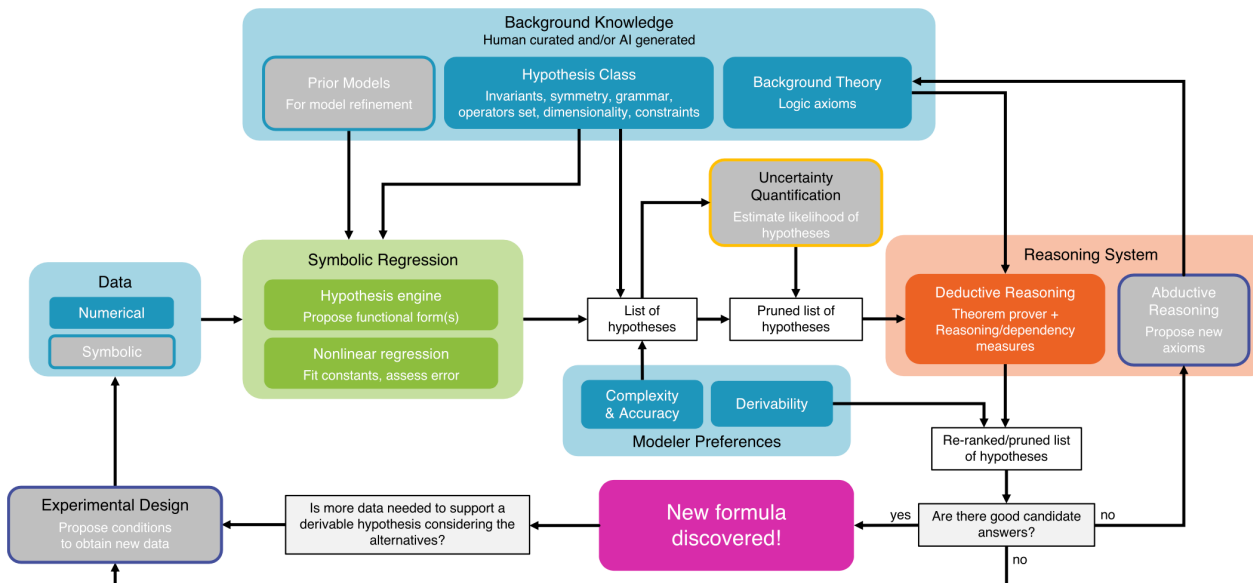


Large Hadron Collider (LHC)

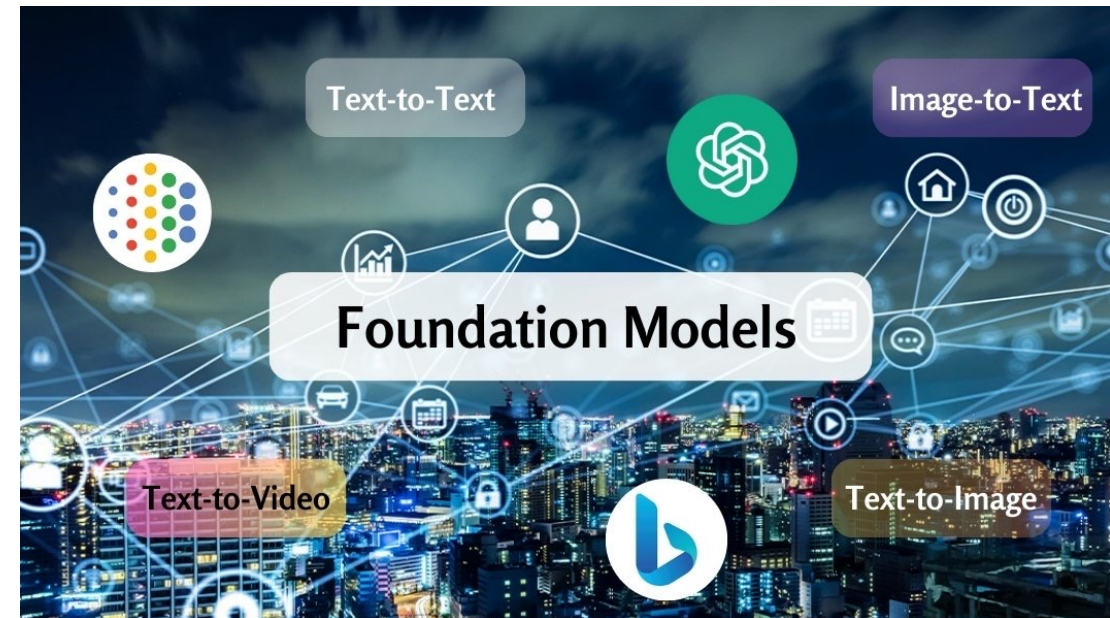
Trend 3: Foundation models

[1]Cornelio, Cristina, et al. "Combining data and theory for derivable scientific discovery with AI-Descartes." *Nature Communications* 14.1 (2023): 1777.

- **AI Scientist** for *automatic and high-throughput* experiments
- **Foundation model** for solving diverse problems with a single model



AI-Descartes pipeline [1]



Foundation models

Course introduction: Summary

Tasks

- Classification/regression
- Simulation
- Inverse design/inverse problem
- Control/planning

×

Neural architecture

- Multilayer perceptron
- Graph Neural Networks
- Convolutional Neural Networks
- Transformers

×

Learning paradigm

- Supervised learning
- Generative modeling
- Foundation models
- Reinforcement learning
- Evolutionary and multi-objective optimization

Application (AI & Science)

- Robotics
- Games (e.g., Go, atari)

- Autonomous Driving
- PDEs

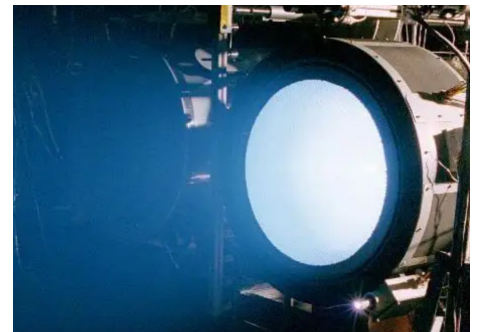
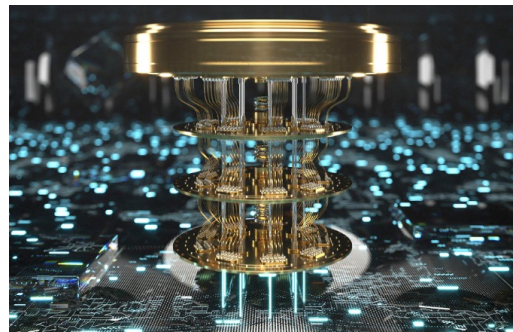
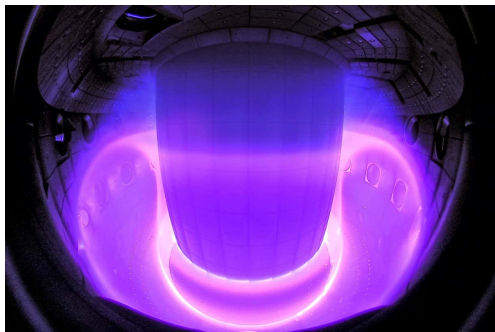
- Life science
- Materials science

Useful materials to get started in deep learning

- Learn PyTorch in 1h: https://pytorch.org/tutorials/beginner/introyt/introyt1_tutorial.html
- Book: Deep Learning book (<https://www.deeplearningbook.org/>)

我问DeepSeek：未来50年，人类最大的机会是什么？

DeepSeek: 未来五十年，人类最大的机会在于**利用技术革命与跨学科协作，系统性解决文明存续与发展的根本性挑战**：通过可控核聚变、高效储能和可再生能源网络实现能源自由，打破资源稀缺的桎梏；借助量子计算与人工智能的融合，突破药物研发、材料科学的认知边界；结合基因编辑、脑机接口与抗衰老技术重构人类生命形态；同步推进太空工业化与小行星资源开发，建立多行星生存能力。这一系列突破的**关键**在于打破学科壁垒，将能源技术、信息技术、生物技术、空间技术深度融合，同时在伦理框架下实现技术普惠——这不仅是科技跃迁，更是人类从“被动适应自然”向“主动设计文明”的范式转变。但最大的**挑战**并非技术本身，而在于建立与之匹配的**全球治理体系，避免技术垄断加剧不平等，让文明升级真正成为全体人类的共同机遇。**



Hope you all learn useful techniques to help your research!

Questions?