New proposal:
R&D for the exa-scale computing environment

Team:

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Introduction

- This new proposal follows COMP_04 (and COMP-03) as its successor
- COMP_04:
  - “Evolution of the computing environment for high-energy and astro-particle experiments”
  - The project was led by Fabio Hernandez, Renaud Vernet, Sebastien Gadrat, and Tomoaki Nakamura from FY2019 to FY2024
  - The close collaboration between IN2P3 Computing Center (CC-IN2P3) and KEK Computing Research Center (KEK CRC) in computing

→ Let me report the achievements of COMP_04 in FY2024

CC-IN2P3 and KEK CRC

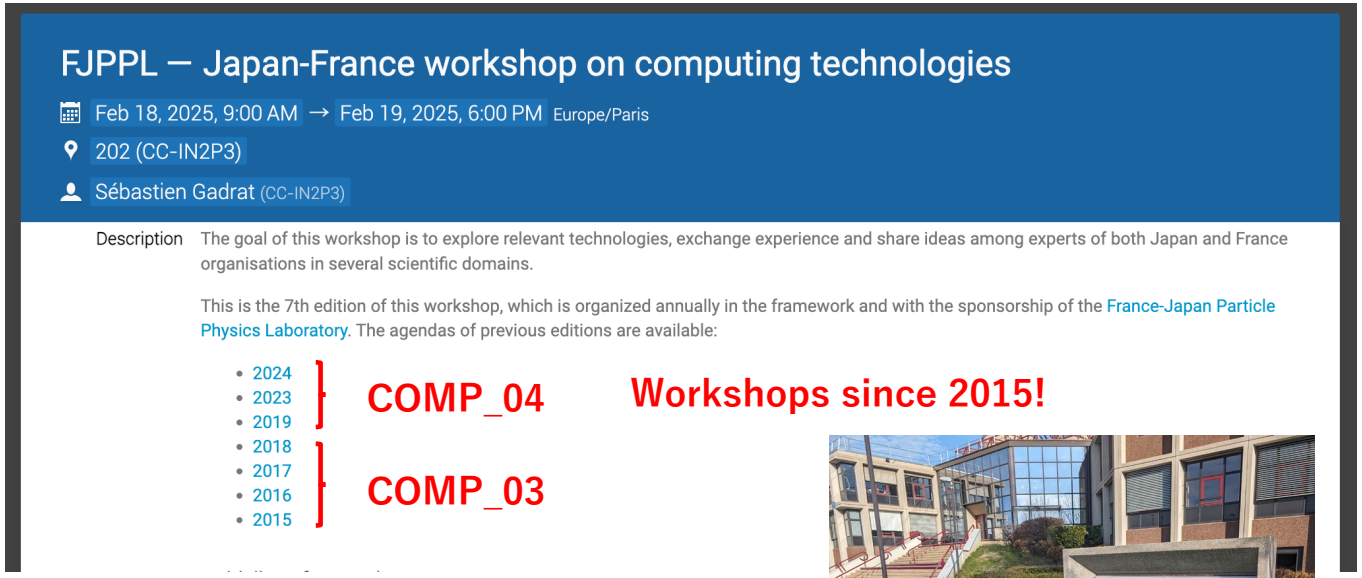
- CC-IN2P3 and KEK CRC support a wide range of experimental projects
  - Including BelleII, LHC, T2K, etc
- Many common challenges to overcome
  - Both hardware and software areas
- Shared interests regarding new technologies
  - Machine learning(ML), ID federation, etc

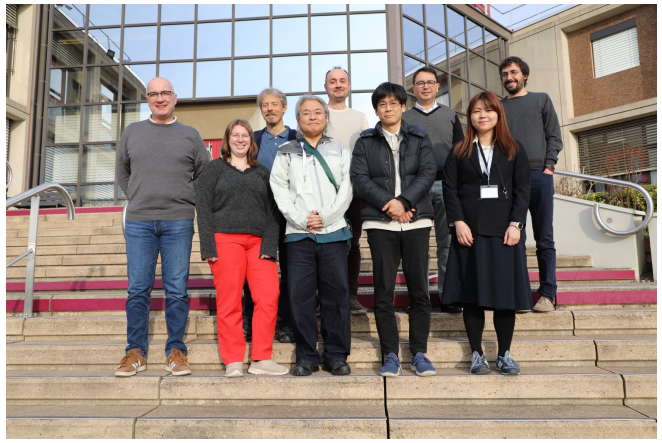
→ Exchange of experience, and know-how is quite essential !!

Yearly F2F workshop

https://indico.in2p3.fr/event/35206/

- F2F workshops are unique opportunity to discuss on-going work and new technology at both centers
- Topics of 2025 workshop@Lyon were:
  - Status report from CC-IN2P3 and KEK CRC
  - News from LSST experiment
  - Open access project at KEK
  - AI session ← Focus of this presentation





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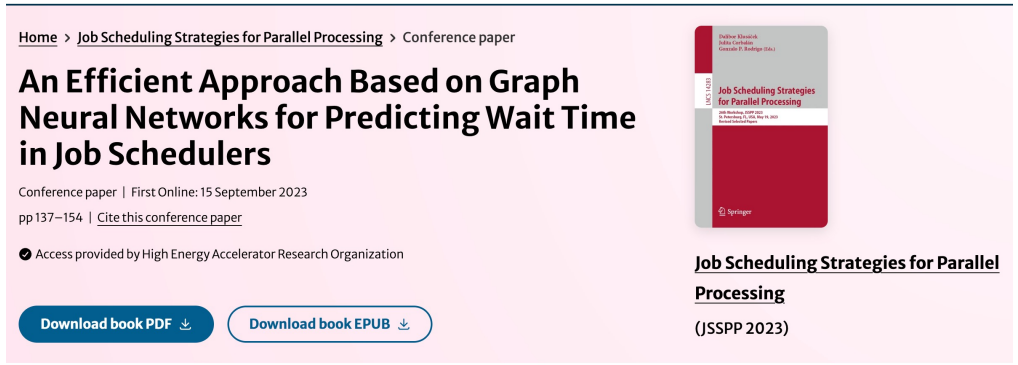
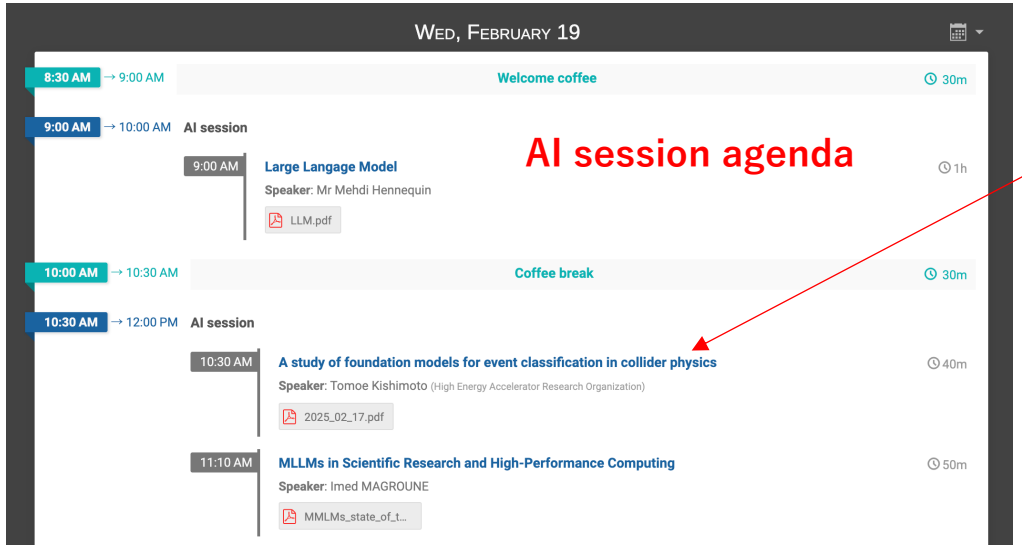
AI session



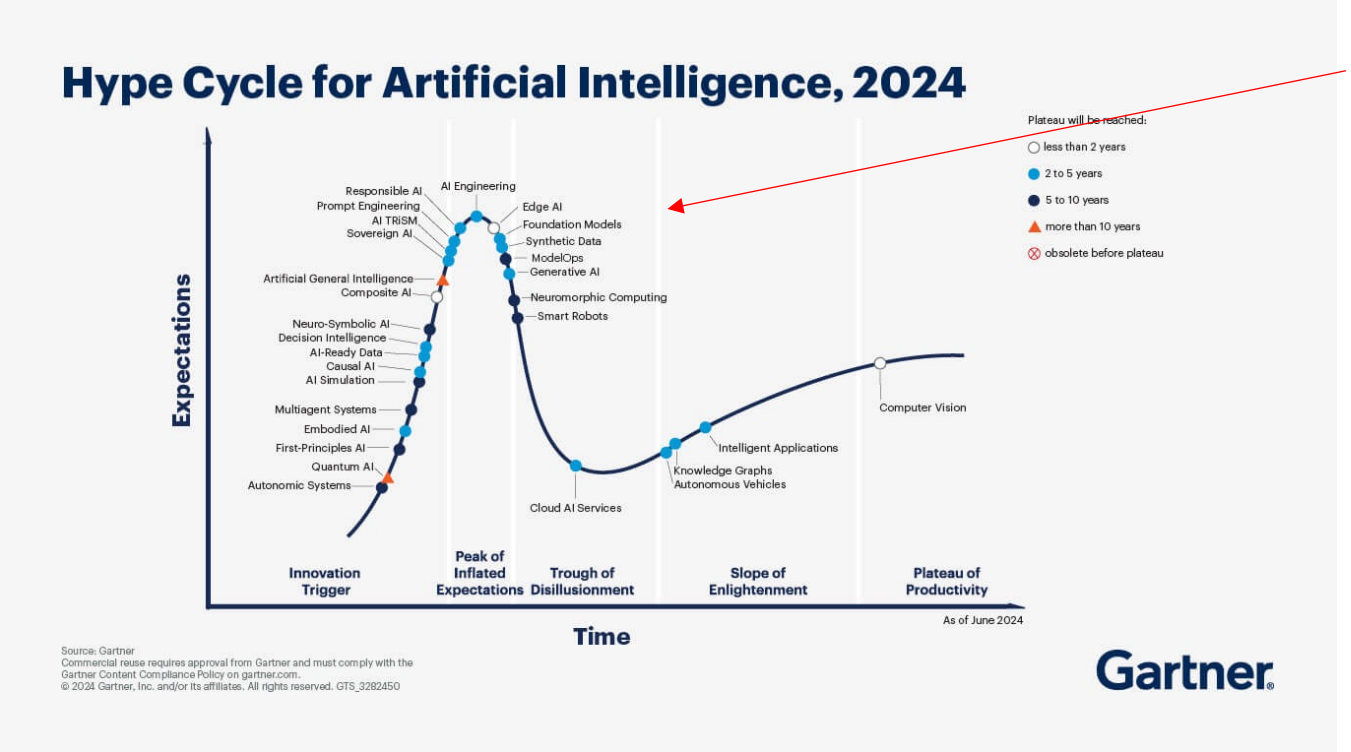


- ML has been a focus of joint collaborative efforts between CC-IN2P3 and KEK CRC
  - A successful application for estimating job waiting time in batch schedulers

  → **Published in Lecture Notes in Computer Science**

- New application has been investigated:
  - The idea is to apply the concept of foundation models to collider physics
  - A potential approach to reduce computing resource usage in future collider experiments

Foundation models



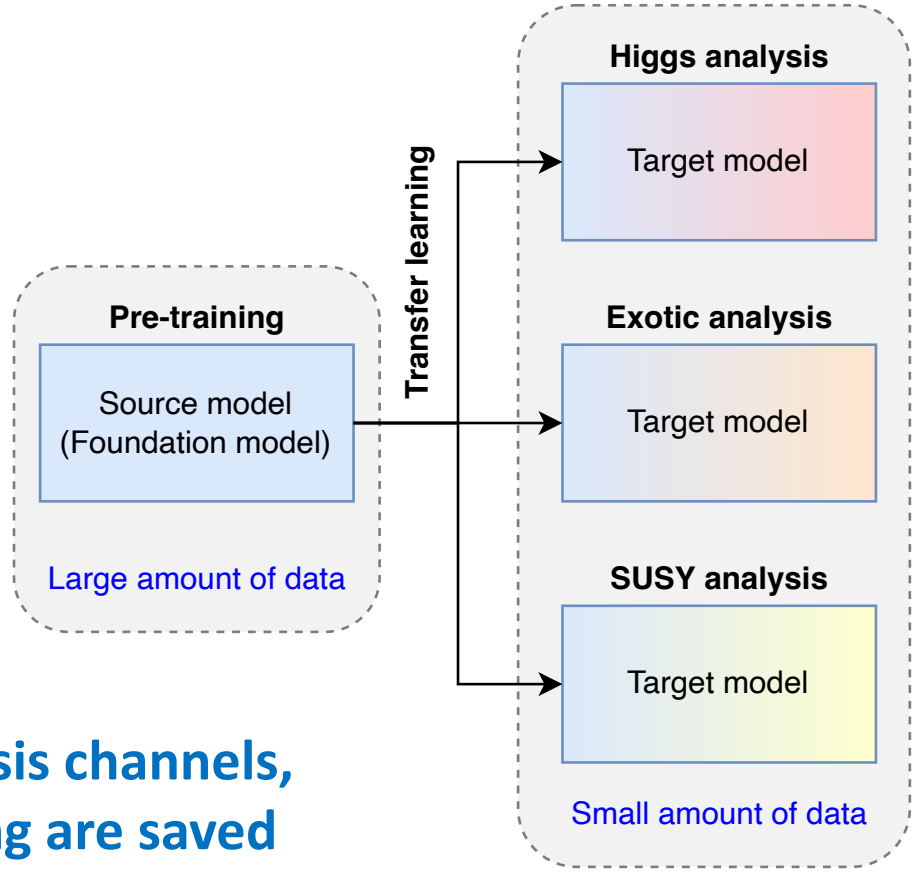
Gartner.com

- "Foundation models" is one of the keywords for AI
  - Pre-training using a larger amount of "unlabeled" data
  - Fine-tuning for a target application (transfer learning)

→ Q: Is the concept of foundation models beneficial to collider physics?

Use case of physics analysis

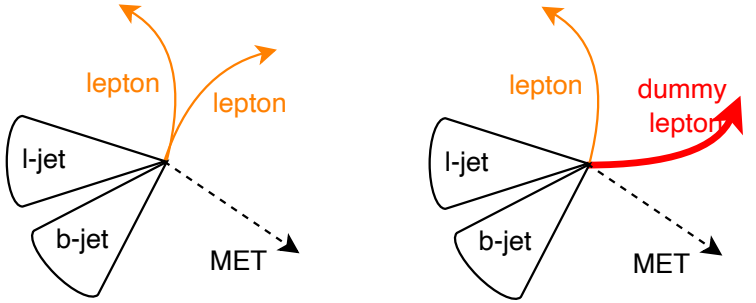
- Many analysis channels in collider physics
  - Higgs, Exotic, SUSY, etc
  - Dedicated Deep learning models are trained from scratch for each analysis channel
  - Large amount of training data (MC) for each channel



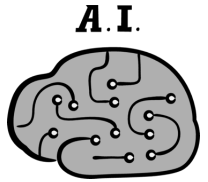
→ If transfer learning can be applied to different analysis channels, computing resources for MC simulations and DL training are saved

Pre-training strategy

- Only low-level features of each object (4-vector+chargte) are used as inputs
- Real collision data (CMS open data) are used in pre-training
  - Self-supervised learning is employed to handle the unlabeled data
- Pre-training strategy
  - An object is randomly replaced with a dummy object when preparing mini-batch



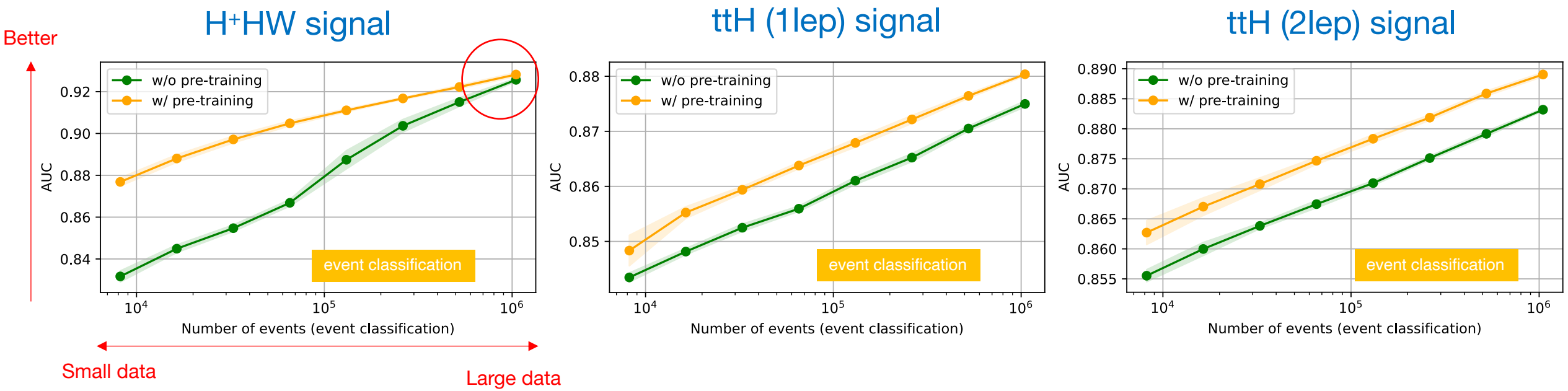
→ DL model is trained to predict what type of object was replaced



…lepton is dummy(?)

AUC of event classification

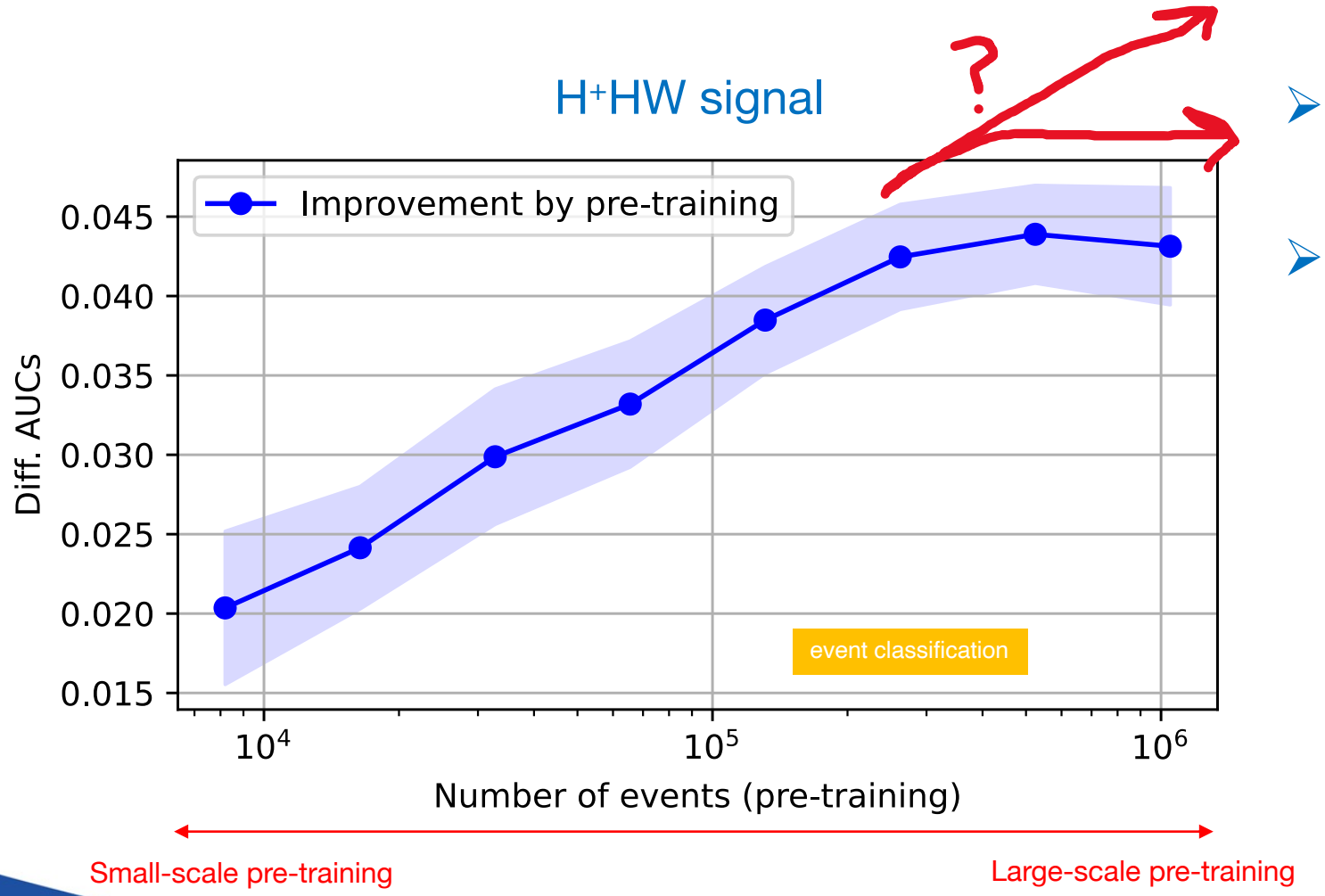
- The concept is examined using “Event classification” problem：signal vs background



- The improvements are confirmed for different signal events

→ The pre-trained model (foundation model) generalizes well

Scaling raw



- The scaling behavior with respect to the number of events in pre-training
- Future works:
  - Need to check with larger models and larger data
  - Investigate new data augmentation approach
  - Explainability of AI: what kind of knowledge is learned during pre-training and utilized in downstream tasks…?

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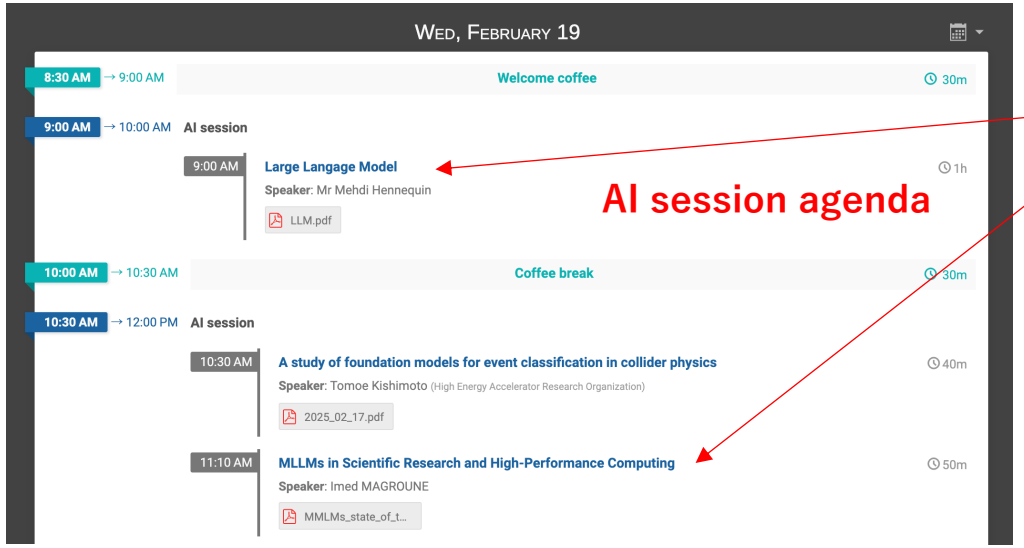
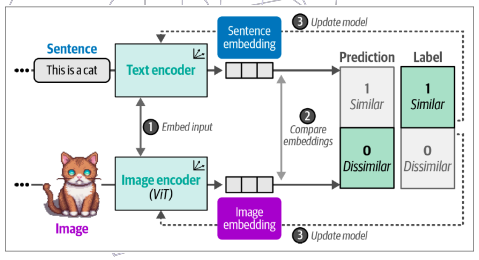
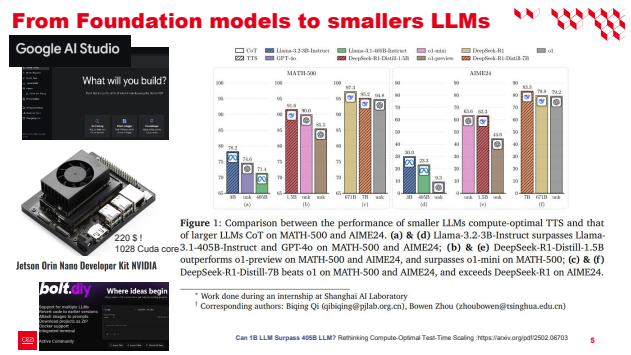
Large Language Models



How Can CLIP Generate embeddings to drive the generation of images





- We also discussed Large Language Models (LLM) and their applications in our fields during the workshop@Lyon
- User support for the efficient use of computing resources is a key challenge shared by CC-IN2P3 and KEK CRC
  - Distributed computing, HPC cluster, containerized workflow, Networks, etc

→ We are planning to start a research project on chatbots for user support

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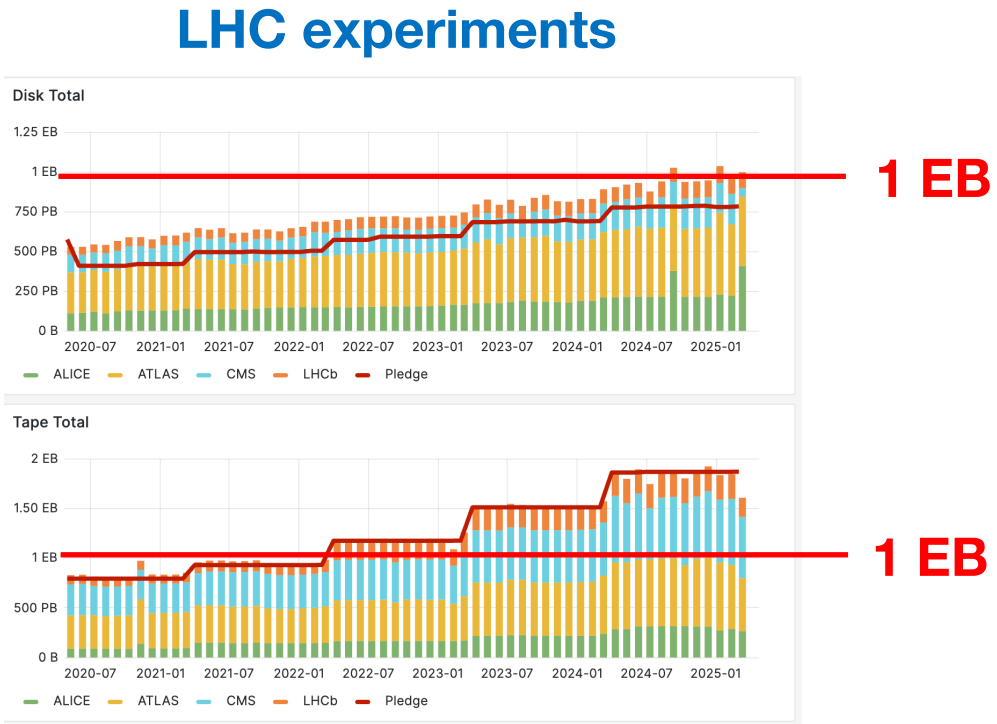
New proposal

- Multiple approaches for introducing brand-new technologies are necessary for the evolution toward the exa-scale computing environment
- Refine and extend the knowledge gained from COMP_04
- 3 topics selected for this year:

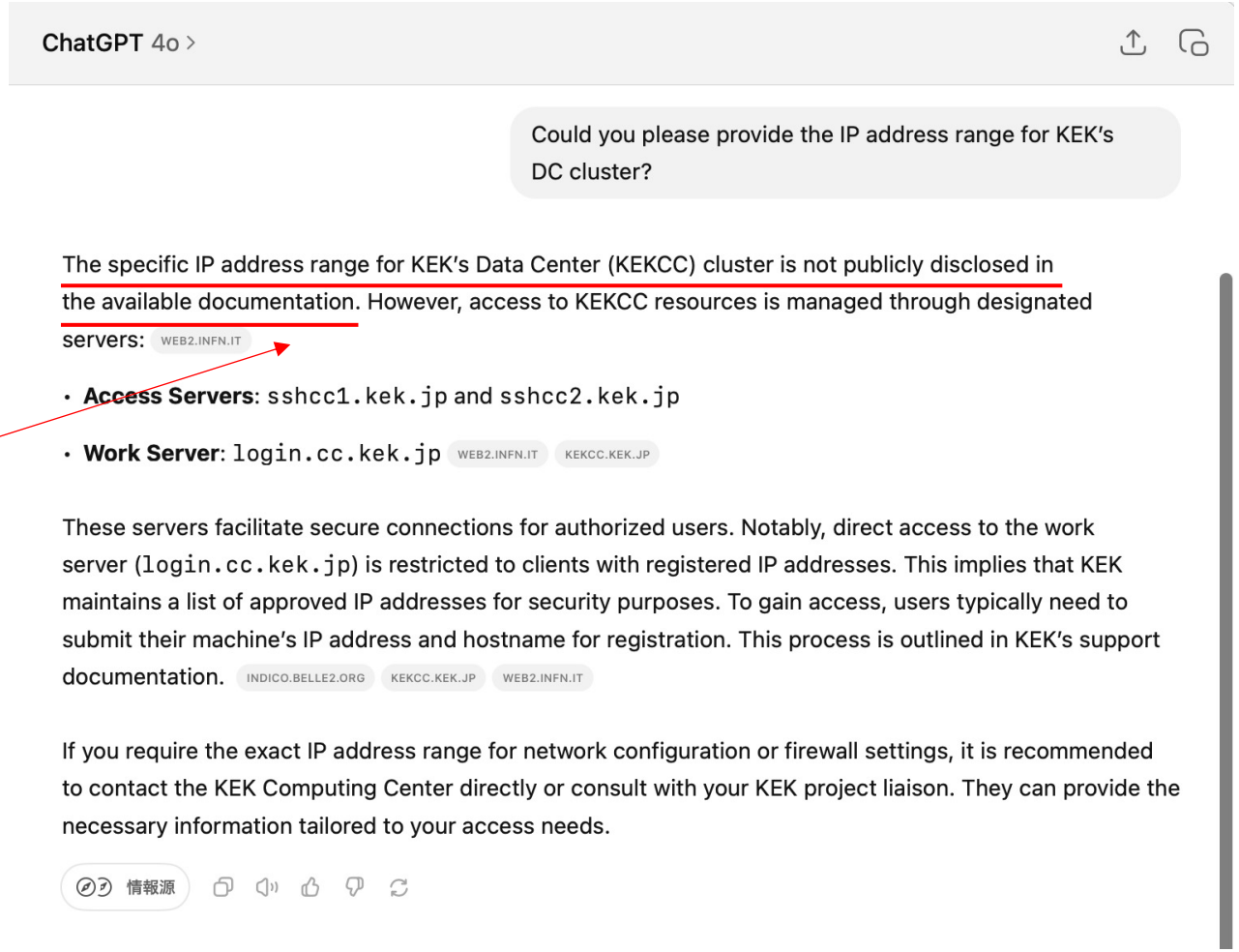


1. **Study of foundation models for event classification in collider physics**
   → This topic has been discussed in previous slides
2. **Research and application of chatbots (based on LLMs) in High Energy Physics**
3. **Research on enhancing the convenience of IT services based on identity federation**

Chatbots in HEP

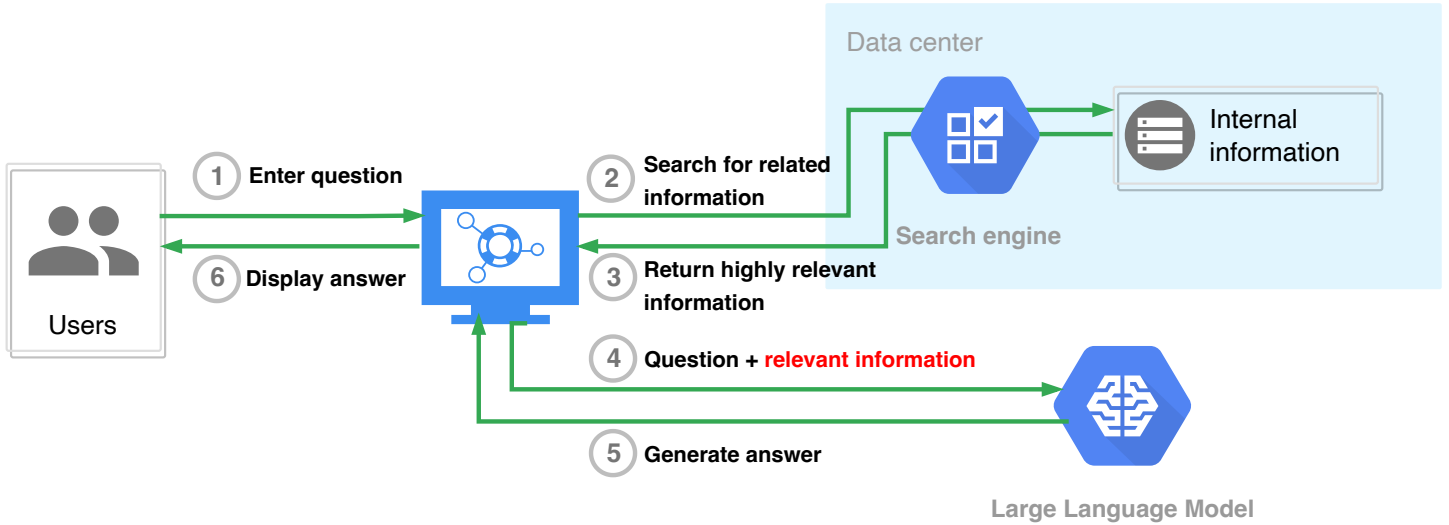
- User support in data center operations requires access to internal information
  - System configuration, Past tickets, etc
- Normal chatbots can't answer such questions (of course!)

→ Retrieval-Augmented Generation (RAG) is a promising approach



RAG

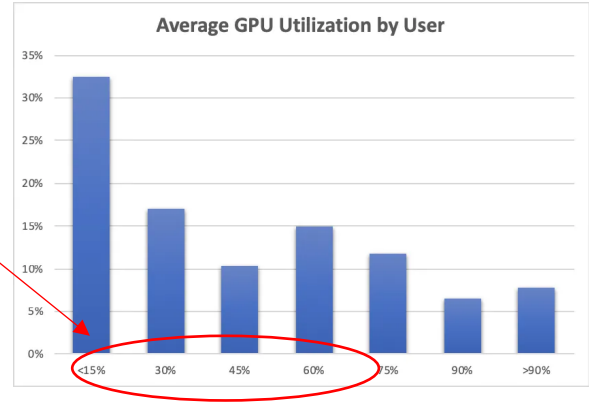
- Relevant information is retrieved and fed into LLMs for processing
  - Official documents, past ticket, e-mails, etc



→ Develop a chatbot for user support, including code generation optimized for our computing infrastructure

- Related research topics:
  - Methods for searching relevant information efficiently
  - Methods for fine-tuning or distillation to enable on-premise deployment of LLMs

Code optimization is necessary, but it heavily depends on the system



Link to article

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ID federation

- ID federation plays a crucial role in the efficient deployment of IT services (including chatbot)
  - Users are able to use services provided by other institutions with the credentials from their home institution

→ Reduce the effort required for account management

- Academic ID federation:
  - European ID federation → eduGAIN
  - Japanese ID federation → GakuNin
  - GakuNin can federate with eduGAIN

→ Plan to deploy a test service for verifying authentication and the exchange of user attributes

Migration: X.509 to Token

- ID federation is particularly critical for "Grid computing"
- The Grid authentication infrastructure is migrating from X.509 certificates to token-based authentication
  - KEK CRC is deploying a token issuer service (INDIGO IAM) for BelleII experiment
  - But, a user registration procedure for INDIGO IAM is no established yet…

→ Managing user identities and accounts for all collaborators with the security level required by Grid computing (*) is a significant challenge

→ We need ID federation!

(*) Identity Assurance Level2 must be referred to F2F meeting or human resource DB

Summary

- Information exchange is highly valuable for both centers
- In the new proposal, we plan to focus on the application of AI technologies and ID federation
  - Milestones for FY2025: Development of an initial chatbot prototype and deployment of a test service for ID federation
- To strengthen the partnership, we request funding for:
  - **IN2P3-CC → KEK-CRC visit in Autumn** to discuss and jointly work on AI-related activities (AI hackathon)
  - **KEK-CRC → IN2P3-CC visit in Spring** to exchange information on computing technologies (annual workshop)

A new initiative

Backup

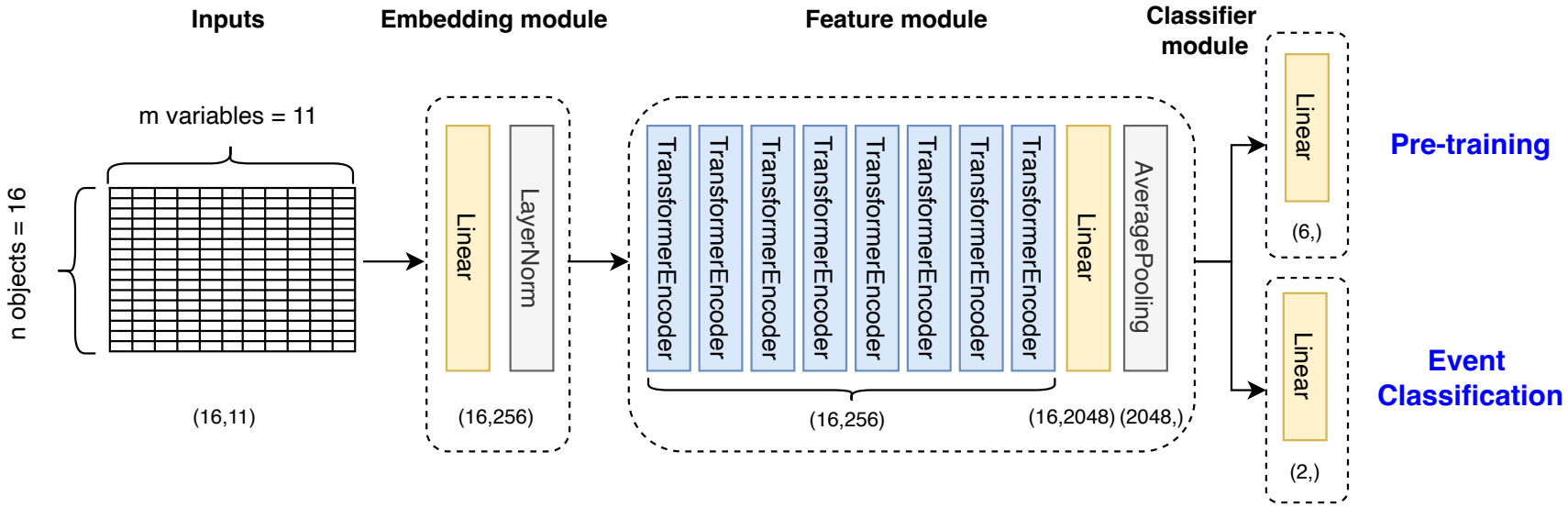
Datasets (CMS Opendata)

		Selections	# of events
Pre-training →	Collision data	lepton ≥ 1 + jets ≥ 2 + bjets ≥ 1	~10^6
Event classification	H^+tb[ref.] vs ttbar+jets	lepton ≥ 1 + jets ≥ 4 + bjets ≥ 1	~10^6
	H^+HW[ref.] vs ttbar+jets	lepton ≥ 1 + tau≥ 1 + jets ≥ 3 + bjets ≥ 1	~10^6
	ttH[ref.] vs ttbar+jets	lepton ≥ 1 + jets ≥ 4 + bjets ≥ 2	~10^6
	ttH[ref.] vs ttbar+jets	lepton ≥ 2 + jets ≥ 2 + bjets ≥ 1	~10^6

- Pre-training is performed using collision data (unlabelled data) based on the foundation model concept
  - ~10^7 events are available after the selection, but only ~10^6 events are used
  - NVIDIA A100: ~10^4 events/sec (10^7 events /10^4 x 500 epochs = 138 hours)

DL model

- Transformer encoder is employed:
  - ~11M trainable parameters



→ Weight parameters of embedding and feature modules are transferred and fine-tuned
→ Classifier module is always trained from scratch