



中國科學院高能物理研究所
Institute of High Energy Physics
Chinese Academy of Sciences

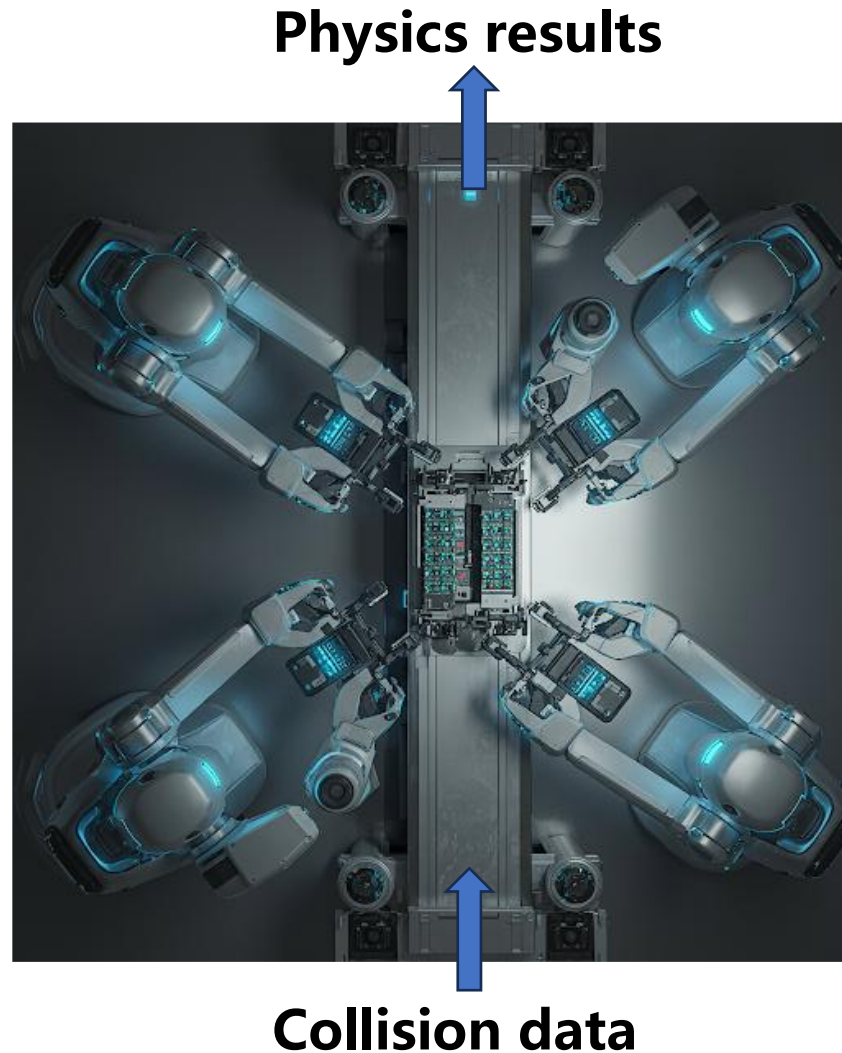
LLM-based AI assistant for HEP data analysis

Ke Li

on behalf of Dr. Sai working group

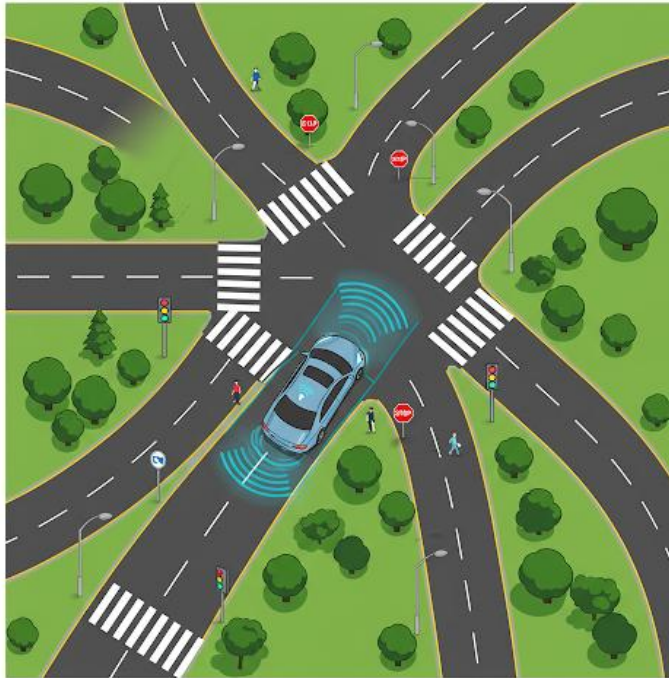
Outline

- Motivation
 - what is LLM
 - why we need LLM
- Dr. Sai project
 - architecture
 - training
- Results from beta version
- Summary and prospects

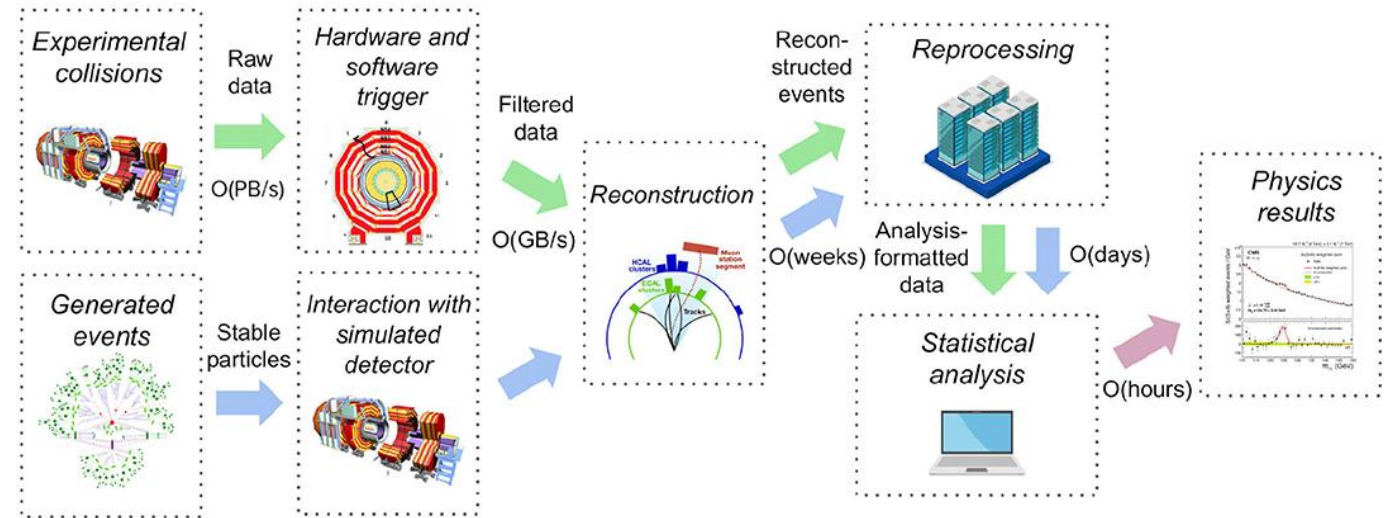


Goal:
A virtual
“robots” to
work on HEP
data analysis

Driving vs. HEP data analysis

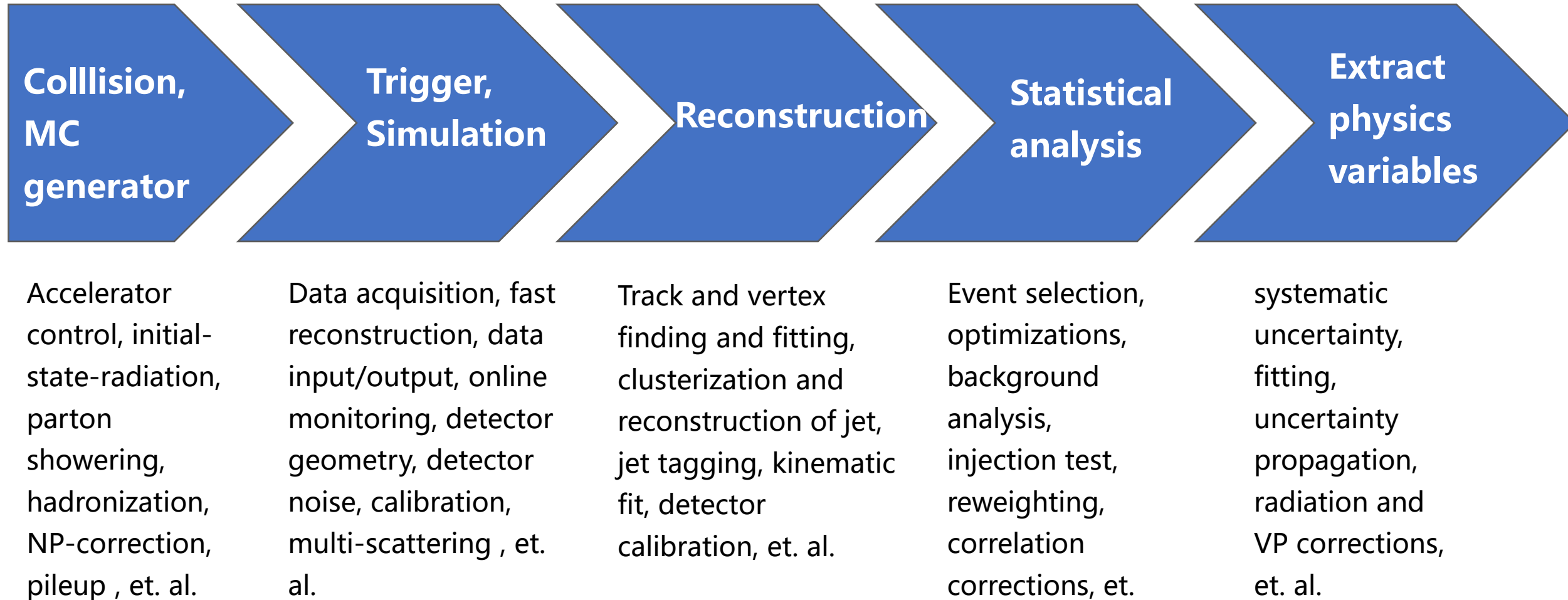


- Clear rules,
- Simple actions,
- Massive training data



- Complex rules, huge amount of degree-of-freedom
- Lots of sub-steps, need lots of HEP knowledge
- Only $\sim 10\text{k}$ experimental results delivered in 50 years

Data process workflow at HEP experiment



Too complicated, similar lines of code as windows/macOS

Data process workflow at HEP experiment



Accelerator

Data acquisition, fast

Track and vertex

Event selection

systematic

control

state-r

parton

shower

hadron

NP-correction,

pileup, et. al.

multi-scattering, et.

al.

calibration, et. al.

correlation

corrections, et.

VP corrections,

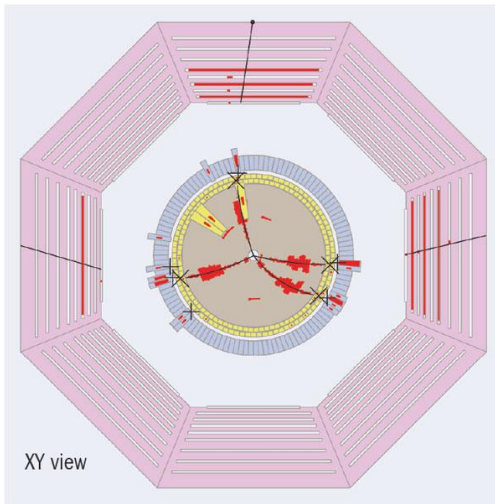
et. al.

**One small task needs : several people + several years !
we have to make it more efficient !**

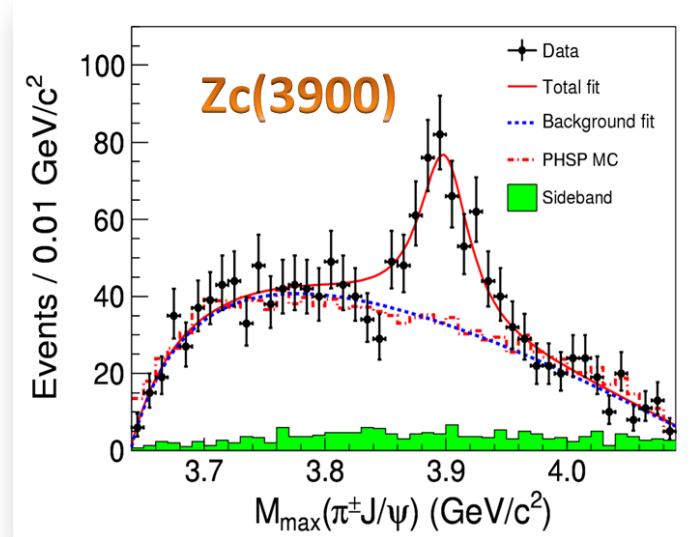
Too complicated, similar lines of code as windows/macOS

Focus on last two steps

Collision event



Physics result



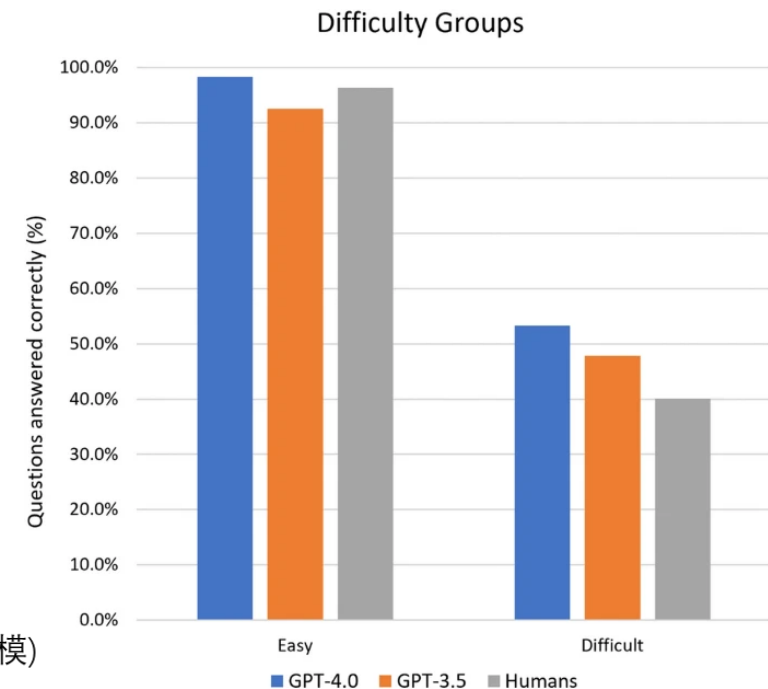
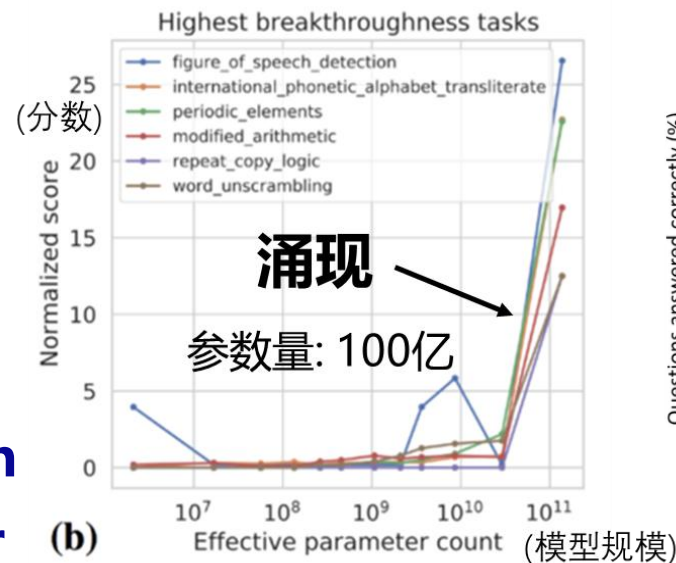
DAQ->Hits -> reconstruction -> selections and statistical analysis -> physics results extraction

Take BESIII as a starting point,
given the analysis at LHC is
much more complex

Can we use AI(LLM) to automate the workflow ?

What is Large Language Model (LLM)

- Large language models (LLMs), normally build on transformer architecture, has demonstrated impressive performance in **text/code generation**
 - GPT4o, Gemini, LLaMa3...
 - Could be used for HEP studies
 - Game changer
- A foundation model (large, computing intensive) + fine tuning for each task individually (smaller data set)
- **For us, open-source foundation model + higher level model for HEP + fine tuning for BESIII**



Why we need LLM

- Major effort in BESIII analysis is spent in writing/testing/updating code/text
 - **LLM is good at code/text generation !**
- Key problems for LLM at HEP
 - How LLM can understand and remember HEP **knowledge** better?
 - Logic, data structure, tools' guideline, validation and feedback ...
 - Current solutions:
 - **More accurate and good quality data for training**
 - **More tests and validations**
 - **More proper architecture**

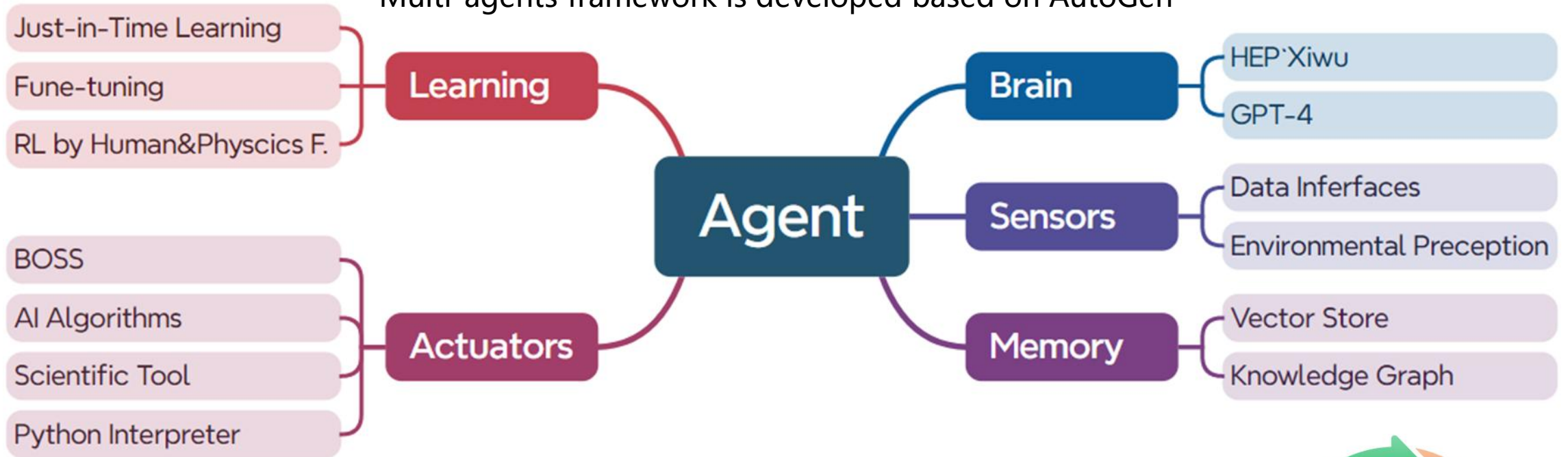
Dr. Sai (赛博士) project for BESIII/HEP

Short for Dr. Science and
Dr. Cyber in Chinese

- AI Agent: AI tools capable of autonomously performing complex tasks
 - LLM = brain -> AI agent = human
- AI agent based on **LLM** model (switchable: GPT/LLaMa/DeepSeek)
 - A demo: Xiwu model, based on Llama 3, trained with a part of BESIII internal data, e.g. memo/drafts, BOSS source code, Q-A during internal review
- One milestone: **AI assistant** (<https://drsai.ihep.ac.cn>)
 - Chatbot, MC generation, signal extraction, and a navigator inside BESIII
 - Capable of simple task
 - **Ready for BESIII internal test !**
- Final goal: **AI scientist**, it can analyze the collision data automatically
 - Developing new AI models, targeting at ~2027

Preliminary Dr. Sai

Multi-agents framework is developed based on AutoGen



Key of this project:

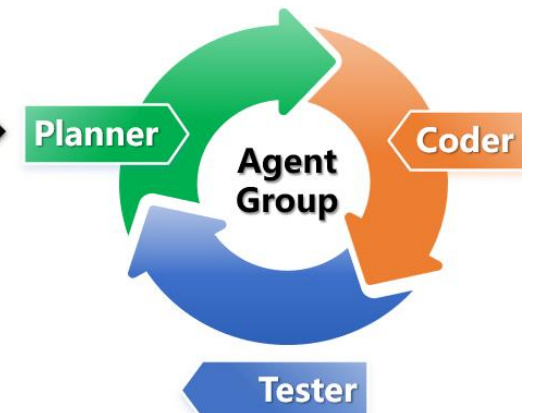
make the results from AI more reliable

- Good quality data
- In-the-fly validation and test
- Multi-agents architecture

Main Agents:

- Planner: Planning and tasks decomposition
- Coder: Write BOSS code
- Tester: Using scientific tools for testing

Scientist ↔

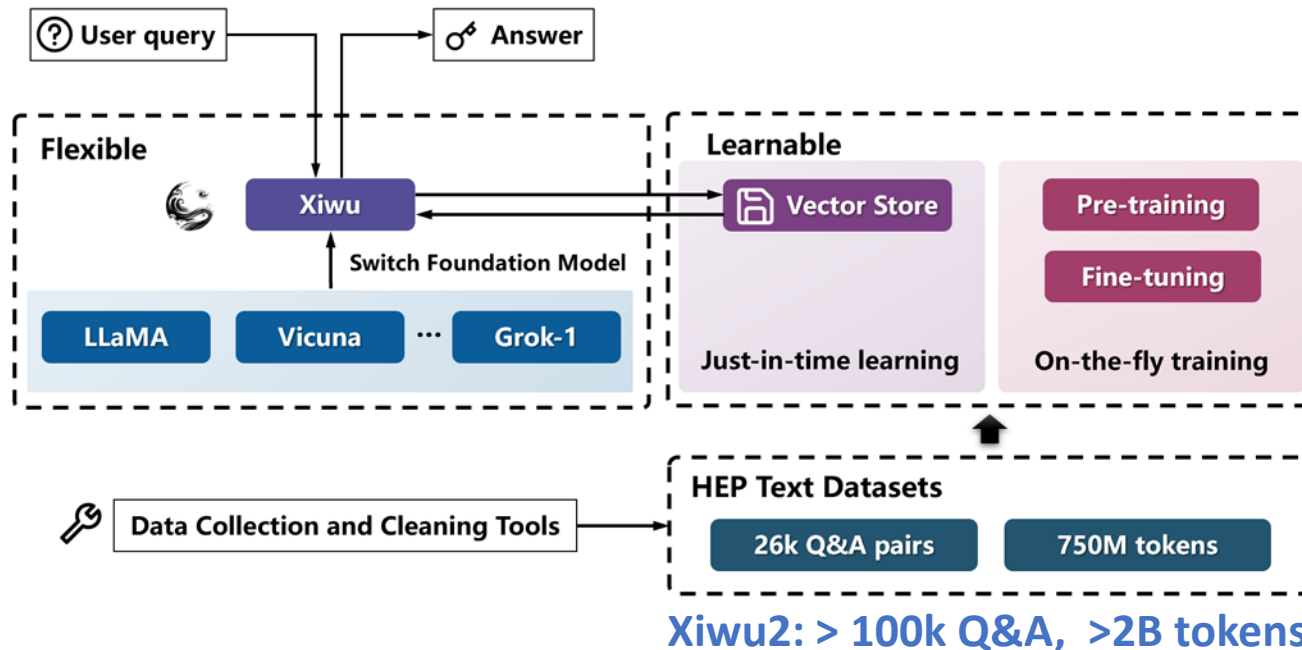


Current training data

- Recent papers on arXiv
 - PDF files parser: HaiNougat, advanced iteration of the Nougat model
- Good quality chat history from IHEP-AI platform
 - The data is cleaned by human or AI (GPT4)
 - 180k Question-Answer pairs in 3 months
- **BESIII internal data**
 - Internal memo/notes, parsed by HaiNougat
 - Question-Answer pairs from internal paper review
 - BESIII Offline Software System (BOSS) source code
 - BESIII public webpages and internal webpages
 - The data on indico will be used later
- All the BESIII internal data sets are stored in RAG or used in training and fine-tuning

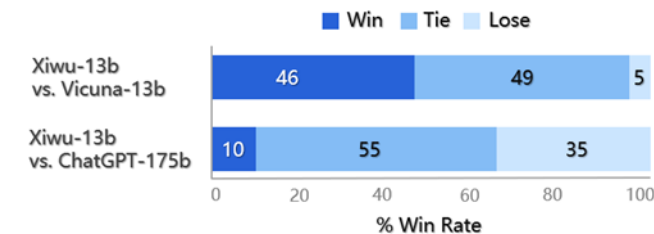
The brain of Dr. Sai - Xiwu (溪悟) model

- Xiwu: a basis flexible and learnable LLM for HEP
- First version release at April (refer to [arXiv:2404.08001](https://arxiv.org/abs/2404.08001) for more details)
 - High level model based on open-source foundational LLM, e.g. LLaMa
 - **First LLM for HEP, version 3 will base on DeepSeek-V3/R1**



Test Results

Size: 13B



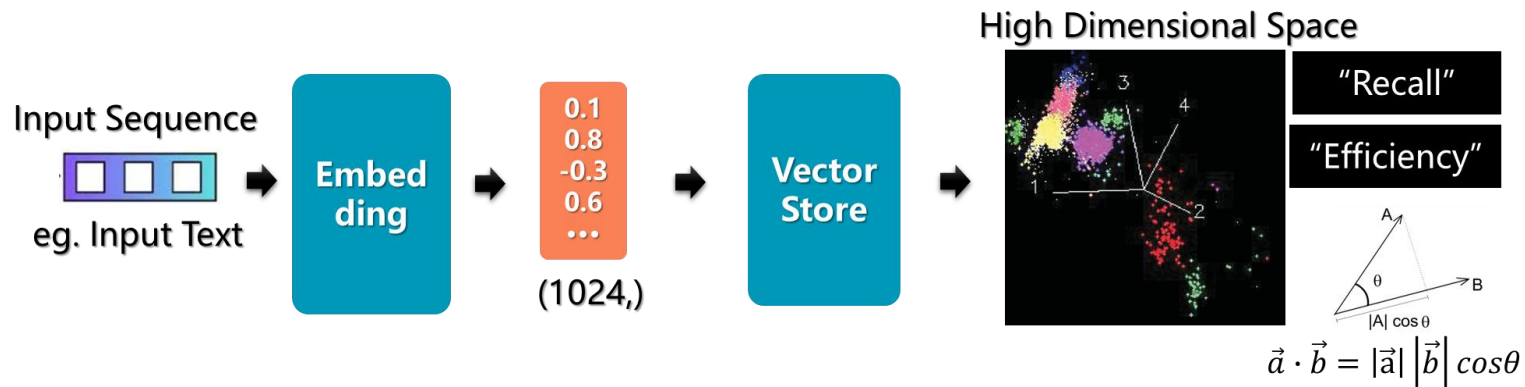
Xiwu 2.0 preliminary evaluation result

Model	MMLU_average	BoolQ	Humaneval	Hep_test
Baichuan2-7B-Chat	48.9	5.44	2.44	74.56
chatglm3-6b	51.82	72.6	61.59	71.52
vicuna-7b-v1.5-16k	33.03	45.81	17.07	62.67
Llama3-8b	58.34	83.61	21.34	76.94
Xiwu 1.0	41.66	0.8	12.2	48.06
Xiwu 2.0	58.23	83.55	19.51	78.06

- Xiwu 2.0: fine-tuned from LLaMa3-8B
 - Feasibility verified preliminarily
 - Improvements by introducing new domain data
 - Next: more smart way to represent and train the HEP data

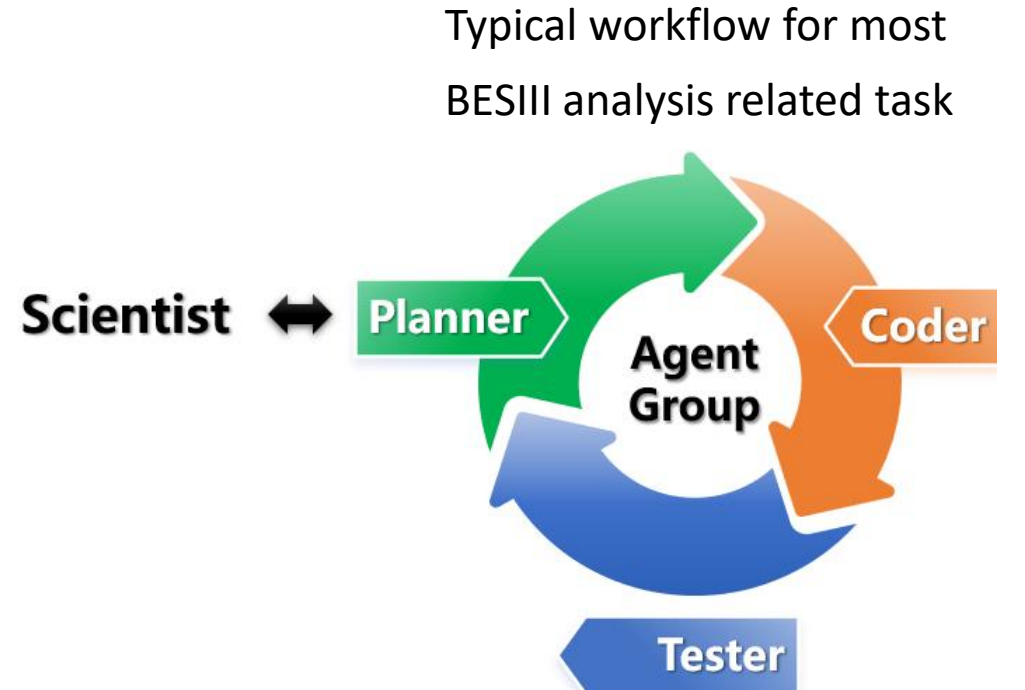
The Memory of Dr. Sai - RAG

- Retrieval-Augmented Generation (RAG)
 - Most promising solution to avoid hallucinations
 - Goal: store private data so no need for retraining
 - Current approach: vector store
 - Embeddings (BGE-M3 model):
 - Convert input data into vectors of a multidimensional space
- Usage: store BESIII internal data
 - user send BESIII related questions
 - RAG return question + BESIII internal data to LLM



Multi-agents managment system

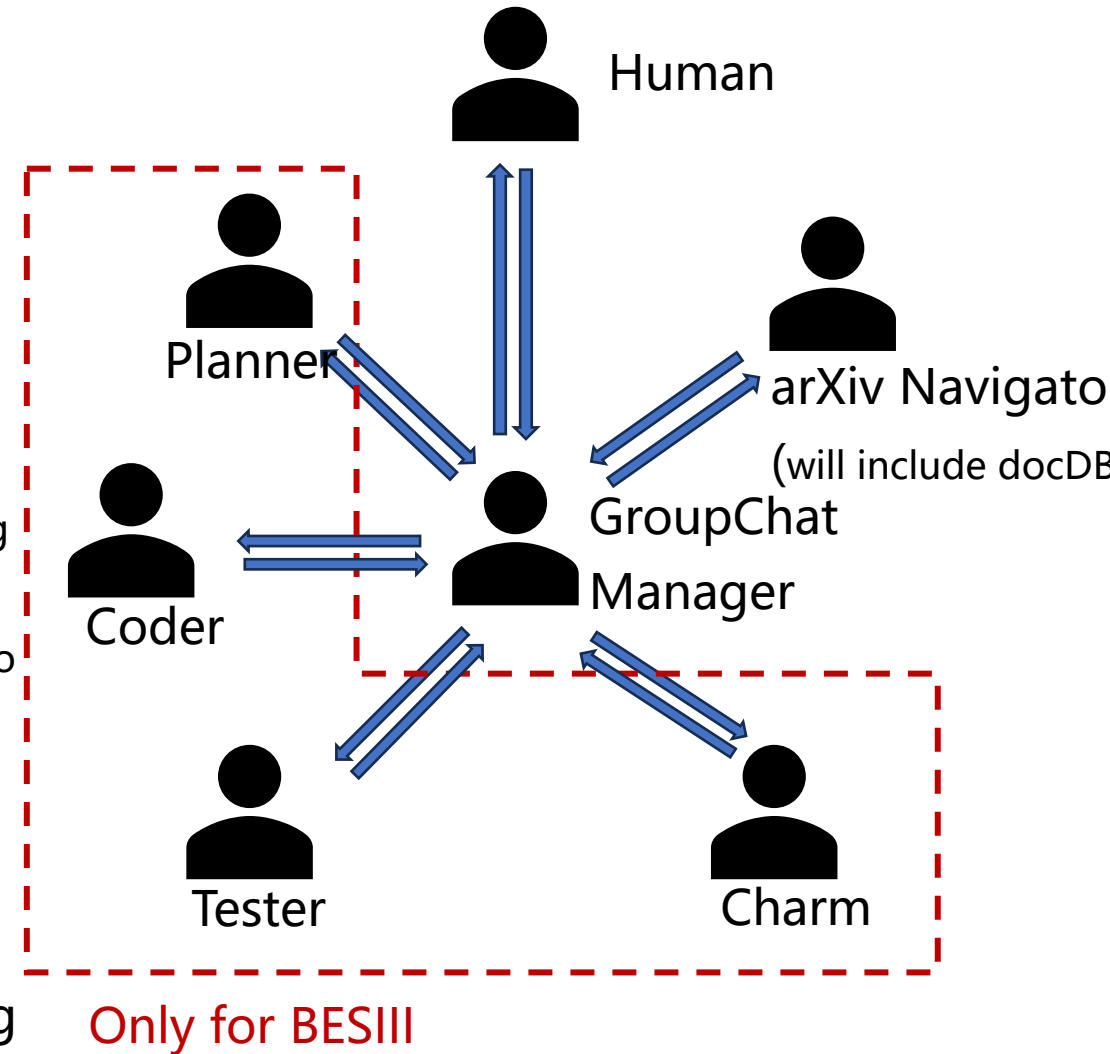
- Developed based on AutoGen framework
- Normally one agent is dedicated for one task, HEP data processing is very complicated, impossible for one agent
- Multi-Agents (foundation model is switchable):
 - **GroupChatManager**
 - **Planner**: Planning and tasks decomposition
 - **Coder**: Write C++/python/BOSS code
 - **Tester**: Using scientific tools for testing/execution
 - **Charm**: BESIII internal assistant
 - Common tools: arXiv navigator, plotting et.al.
- Human can interact via HumanProxy



- If test failed, the feedback will be used to improve the prompts at next iteration.
- For each task, we have multi-unittests

Groupchat for multi-agents

1. Human pass task to Dr. Sai by HumanProxy
2. GroupChatManager will select the proper speaker (agent)
 1. Human can correct the selection
 2. The task will be decomposed into subtasks in the beginning and can be revised later
 3. All the messages including the chat history will be passed to the next speaker
 4. If one task failed, error message will send to GroupChatManager then restart the task
3. If Tester need to execute a BESIII-related program, people have to set up a worker in BESIII computing environment first

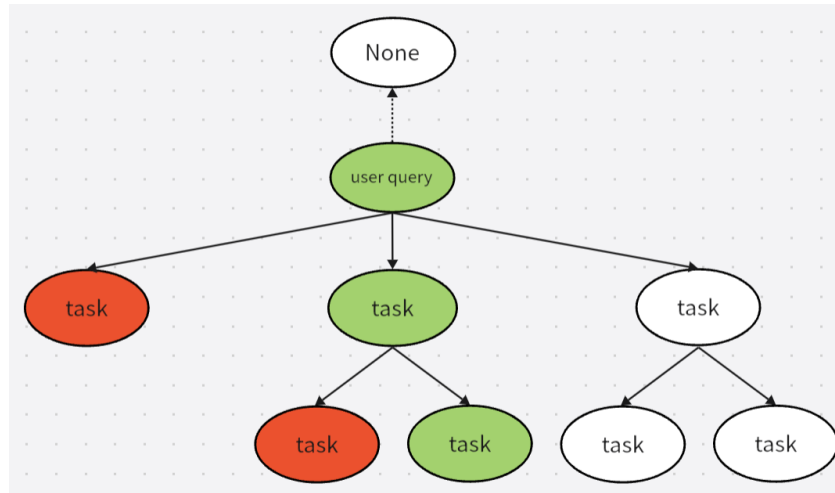


Status and prospects for Dr. Sai

- **First version is Ready** for BESIII members
 - webui: <https://drsai.ihep.ac.cn> (contact us if you can't access)
 - 3 main components
 - **Preliminary BESIII AI assistant**
 - automated data analysis : task decomposition, code/text generation, execution and test
 - Personal assistant
 - user can make their own vector store for personal data
 - Chatbot
 - switchable: GPT3.5/4, LLaMa3, Xiwu2 ...
 - can read PDF and image

Task decomposition

- One of the key part of Dr. Sai
 - Compose complex task into multiple small, simple, and well-defined sub-tasks
 - We will prepare more data to train the model again in future
- Sub-tasks will be executed in sequence
 - All sub-task succeed = task succeed



"Observation": "The user requests to decompose the task of searching for Zc(3900) from electron-positron collision data at a center-of-mass energy of 4.26 GeV.",

"Thoughts": "To decompose the task, we need to break down the process into manageable steps, including data collection, event selection, background suppression, signal extraction, and analysis.",

"Status": "CONTINUE",

"Plan": [

"(1) Data Collection: Gather the electron-positron collision data at a center-of-mass energy of 4.26 GeV from the BESIII experiment.",

"(2) Event Selection: Identify and select events that are likely to contain the Zc(3900) signal. This typically involves selecting events with the final state particles of interest, such as $\pi^\pm J/\psi$.",

"(3) Background Suppression: Apply criteria to reduce background events that can mimic the signal. This may involve using kinematic cuts, particle identification, and other techniques.",

"(4) Signal Extraction: Use invariant mass calculations and other methods to extract the Zc(3900) signal from the selected events. This involves plotting the invariant mass spectrum of the $\pi^\pm J/\psi$ system and identifying peaks corresponding to Zc(3900).",

"(5) Statistical Analysis: Perform a statistical analysis to determine the significance of the observed signal. This includes fitting the invariant mass spectrum and estimating the signal yield and background.",

"(6) Systematic Uncertainties: Evaluate and account for systematic uncertainties in the measurement. This may involve varying selection criteria, fitting methods, and other parameters.",

"(7) Results and Interpretation: Interpret the results in the context of theoretical models and previous measurements. Compare the observed properties of Zc(3900) with theoretical predictions and other experimental results.",

"(8) Documentation and Reporting: Document the analysis process, results, and conclusions. Prepare a report or publication to share the findings with the scientific community."

],

"Comment": "The task involves a detailed and systematic approach to search for the Zc(3900) particle in electron-positron collision data. Each step is crucial to ensure the accuracy and reliability of the results."

} •

Example: BESIII Internal Navigator

Dr. Sai can assist people to find the correct information, the prompt is "what is the path of inclusive MC sample produced at center-of-mass energy = 3.773 GeV. ".

what is the path of inclusive MC sample produced at center-of-mass energy = 3.773 GeV

Attention: auto-selected speaker 'Charm' is ready to handle the current task:
'what is the path of inclusive MC sample produced at center-of-mass energy = 3.773 GeV'.
Please give feedback if you have any comments (in 10 seconds).
1.'r' - Revise.
2.'c' or None - Continue.
3.'s' - Stop. ●

[ST]Ask human input for 10s[END]

No user input ●

To determine the path of the inclusive MC sample produced at a center-of-mass energy of 3.773 GeV, we need to identify the relevant information from the provided cases.
From the given cases, Case 3 provides specific information about the inclusive MC samples at 3.773 GeV:

```
Raw code
Sample Type
Sample Type,Ecm (GeV),RUNS,Luminosity(pb^-1) of DATA (not MC)
```

system tools

```
Sample Type
Sample Type,Ecm (GeV),RUNS,Luminosity(pb^-1) of DATA (not MC)
on-ψ(3770) (2010),3.773,11414-13988,2931.8+-0.2+-13.8 *
on-ψ(3770) (2010),3.773,14395-14604,2931.8+-0.2+-13.8 *
on-ψ(3770) (2011),3.773,20448-23454,2931.8+-0.2+-13.8 *
```

Additionally, Case 4 provides the location of the dst files for MC samples:

```
Raw code
Location of dst Files
Directories for the MC samples can be found at:
BESIII DOC-228 http://docbes3.ihep.ac.cn/cgi-bin/DocDB/ShowDocument?
docid=228
* Scripts were copied from
/panfs/panfs.ihep.ac.cn/home/data/bes3gen/workarea6XX/TestRelease/TestRelease-
00-00-XX/psipp/
/ihepbatch/bes/ambrose/workarea-
662/workarea/Reconstruction/QCMCFilterAlg/QCMCFilterAlg-00-00-
01/share/jobOptions_QCMCFilter_makedst.txt
/besfs/offline/data/661-1/psipp/c/4040/JobOptions/
```

Combining this information on the path for the inclusive MC sample produced at a center-of-mass energy of 3.773 GeV can be inferred as follows:

```
Raw code
/besfs/offline/data/661-1/psipp/mc/3770/JobOptions/
```

This path is derived from the general structure provided in Case 4, adapted for the specific energy level of 3.773 GeV mentioned in Case 3.

Towards Dr. Sai V2/V3

- V2 (end of 2025)
 - Better knowledge representation: vector store -> **knowledge graph**
 - Better agents interaction logic
 - Modeling of experimental analysis procedure:
 - Reorganize the analysis framework to reduce the amount the code/text to be generated
 - Preliminary **DSL (domain specific languages)** for HEP analysis
 - Comprehensive evaluation system
- V3 (end of 2026)
 - Extract **chain-of-thoughts (CoT)** from all HEP papers
 - Extract the analysis procedures from all experimental papers to DSL
 - Align the DSL with domain code and CoTs, and perform reinforcement learning based on DSL, similar to deepseek-r1, and get the feedbacks from human experts

An extremely simplified example of CoT

Problem: We're looking for a hypothetical "dark photon" (A'), a particle that interacts with dark matter. One way to search for it is through its decay into an electron-positron pair (e^+e^-). We expect the dark photon to be relatively light.

Chain-of-Thought:

1. **Theoretical Prediction:** The dark photon (A') is predicted to decay into an e^+e^- pair.
2. **Data Collection:** We analyze data collected by the ATLAS detector. We look for events with two energetic electrons (e^+ and e^-).
3. **Reconstruction:** We measure the momentum and energy of the e^+ and e^- . We calculate the invariant mass of the e^+e^- pair. If the dark photon exists, the invariant mass of the e^+e^- pair should cluster around the mass of the A' .
4. **Observation:** We see a small "bump" or excess of events in the invariant mass distribution of e^+e^- at a specific low mass value.
5. **Inference:** The "bump" *might* suggest that a particle with that mass is decaying into e^+e^- .
6. **Simplest Decision:** If the mass of the "bump" is consistent with the predicted mass range for the dark photon, we say we *might* have seen evidence for it.

Lots of on-going activities, stay tune

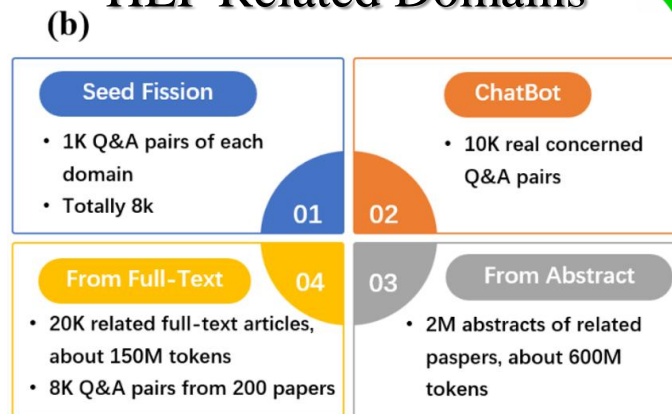
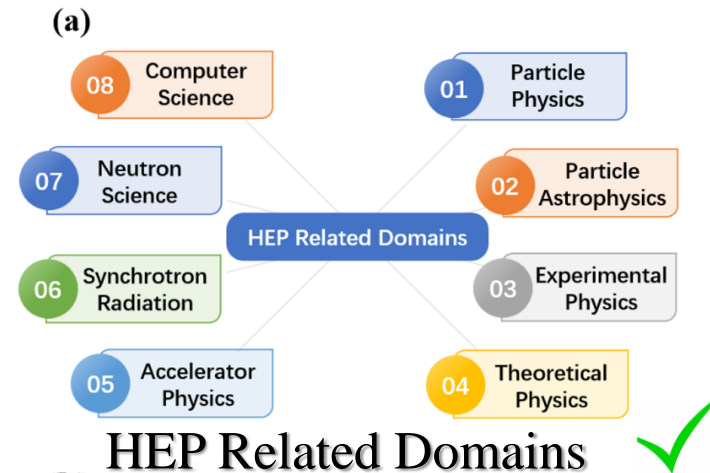
Summary

- **LLM could be useful for HEP**
 - Not just generate code/text preliminarily, but can be used to automate the analysis
- A demo: **AI agents system for HEP** - Dr. Sai
 - It can help people on data analysis (**good accuracy for small task**)
 - Many on-going studies to improve accuracy especially for complex task
 - Easy to port to other lepton collider experiments
 - Bottleneck: lack of **"data"**
 - Modeling of experimental analysis procedure and knowledge
 - Personpowers are more than welcome
 - Next Dr. Sai V2: more data, state-of-art AI technologies
- IHEP formed a **ML Collaboration** to work on AI4HEP
 - Lots of on-going activities, more details in the [kick-off meeting](#)
 - Welcome to join/collaborate/discuss AI for HEP ! Contact me (like@ihep.ac.cn)

back-up

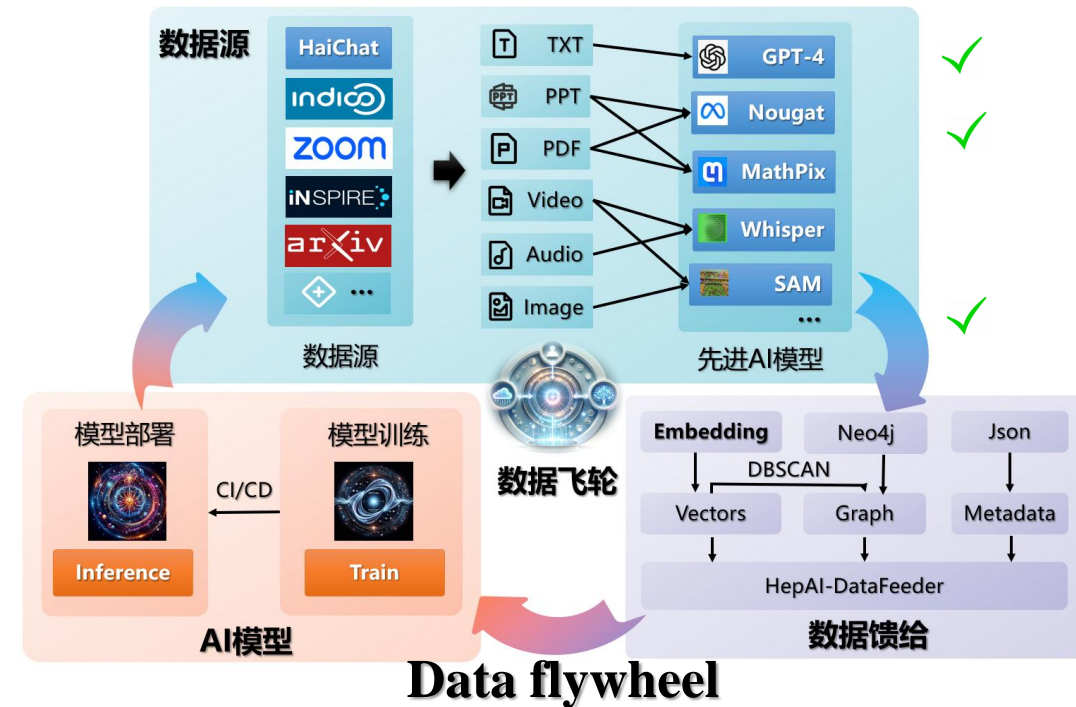
Sensors of Dr. Sai

Data flywheel enables **continuous iterative evolution of models**



Totally 26k Q&A pairs for fine-tuning, 750M tokens for pre-training.

Four ways to collect data



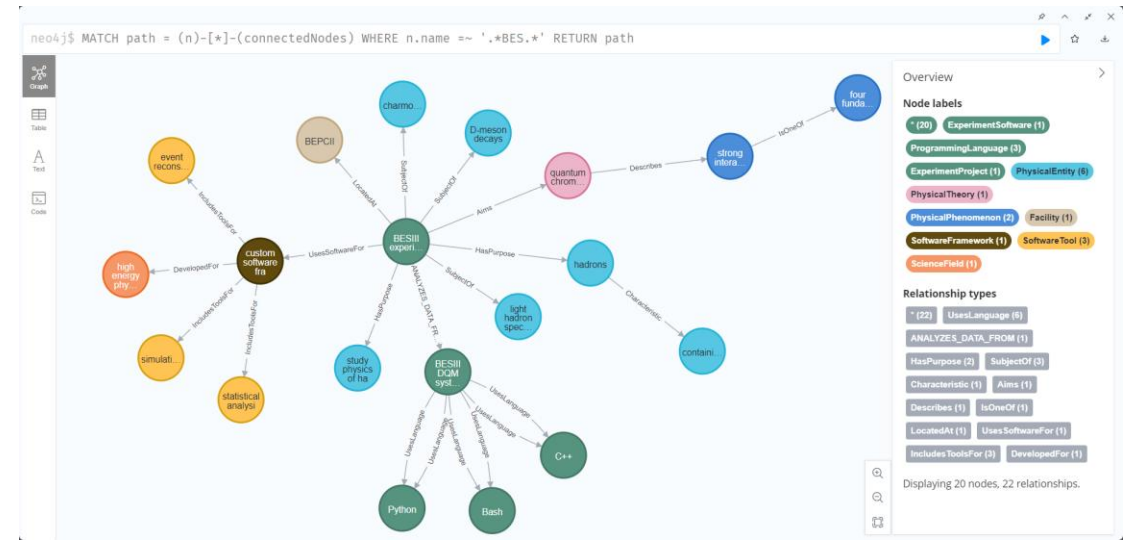
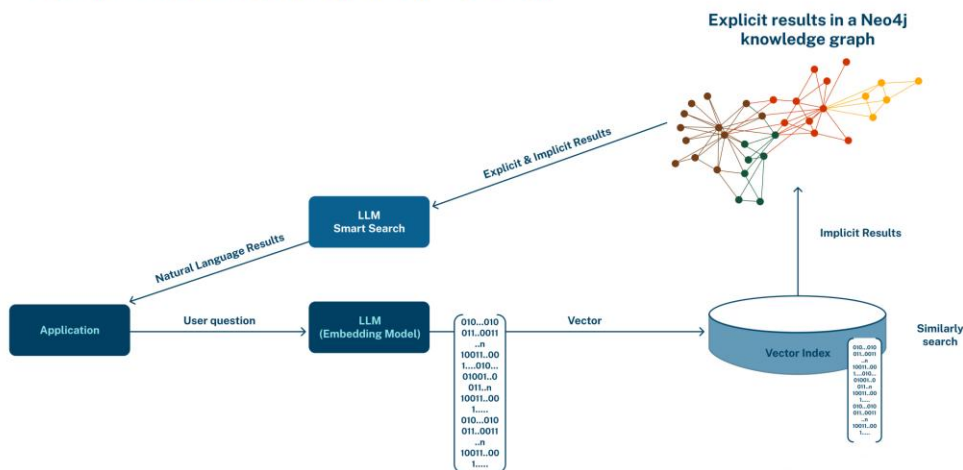
The "data-driven flywheel effect" improves the algorithm model by constructing a circular data path, attracting more users and generating more data during their use. The new data is then used to improve the algorithm model, forming a positive feedback loop.

Memory of Dr. Sai : knowledge graph

Association relationship retrieval based on knowledge graph

- Building BESIII Knowledge Graph:
 - Entity Relationship Construction → Eliminating Ambiguity → Adding Attributes and Labels → Storage
- Search:
 - User's question → Question Embedding → Search for Top K nodes → Obtain node information
- Progress: Built a BESIII knowledge graph demo based on 500 Q&A pairs

Grounding LLM Responses with Implicit and Explicit Search Through Neo4j's Knowledge Graph



- Next step: Test knowledge retrieval and inference performance, develop KG's API to serve Dr Sai

Memory of Dr. Sai

- Hepai worker+llama index+qdrant



Collections

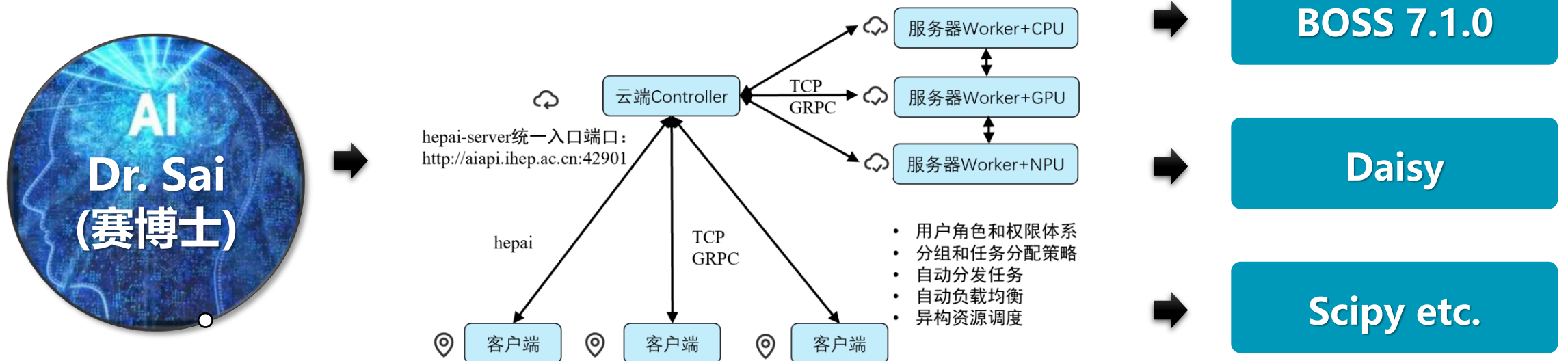
<input type="text" value="Search Collection"/>	
BESMEMO	DELETE
DoSai-coder	DELETE
DrSai-admin	DELETE
DrSai-anonymous	DELETE
DrSai-charm	DELETE
DrSai-coder	DELETE



Actuators of Dr. Sai

Based on HepAI DDF, it is easy to expand Dr Sai's actuator component.

The Distributed Deployment Framework (HepAI-DDF)



Example: fitting

Prompt:

"I want to do two things:

1. generate a fitting script to fit a Gaussian distribution from the output file 'fake_data.root'. There is a TH1F name 'h_gaus' in the file.
2. use Tester to execute this code."

Example: BESIII assistant

Prompt:

"what is the path of inclusive MC sample produced at center-of-mass energy = 3.773 GeV."

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Raw code

Sample Type

Sample Type,Ecm (GeV),RUNS,Luminosity(pb⁻¹) of DATA (not MC)

system tools

Please refer to Pan's talk for more details

Sample Type

Sample Type,Ecm (GeV),RUNS,Luminosity(pb⁻¹) of DATA (not MC)

on-ψ(3770) (2010),3.773,11414-13988,2931.8+0.2+-13.8 *

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Raw code

Location of dst Files

Directories for the MC samples can be found at:
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* Scripts were copied from
/panfs/panfs.ihep.ac.cn/home/data/bes3gen/workarea6XX/TestRelease/TestRelease-00-00-XX/psipp/
/ihepbatch/bes/ambrose/workarea-662/workarea/Reconstruction/QCMCFilterAlg/QCMCFilterAlg-00-00-01/share/jobOptions_QCMCFilter_makedst.txt
/besfs/offline/data/661-1/psipp/mc/4040/JobOptions/

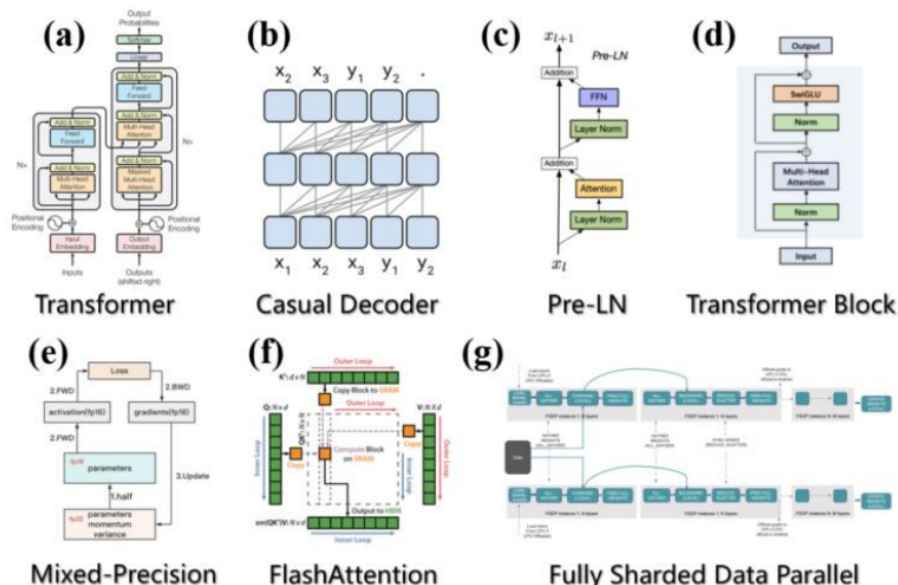
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Raw code

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Xiwu 2.0: Training techniques

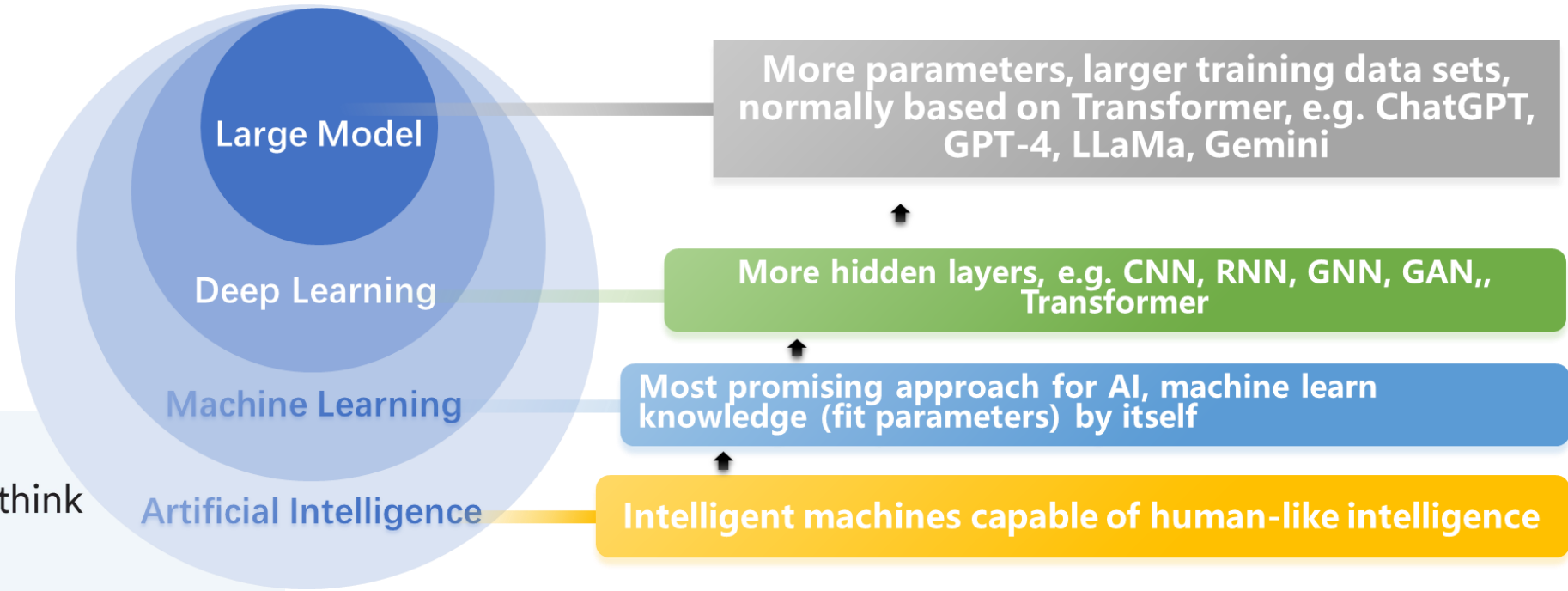


Reduce computational cost and training time, while improving model's performance

Frequently used techniques in LLM training

- **Mixed-precision Training**
reduce memory usage and improve computational throughput without sacrificing model accuracy
- **FlashAttention**
enhance floating-point operations per second (Flops)
- **Fully Sharded Data Parallelism (FSDP)**
parallel training across multiple devices
- **CPU-Offload**
offload certain computations from GPU to the CPU
- **Torchrun Parallelism**
Training on single node with Multi-GPU
- **Bitsandbytes**
vector quantization and mixed-precision decomposition
- **Deepspeed**
utilize mixed precision, gradient checkpointing, and offloading memory to the host CPU
- **ZeRO Series (ZeRO-2, ZeRO-3, ZeRO-offload)**
memory optimization strategies, such as activation checkpointing and optimizer state partitioning
- **Low-Rank Adaptive (LoRA)**
Approximate the weight matrices with low-rank factors while preserving the model's representational capacity

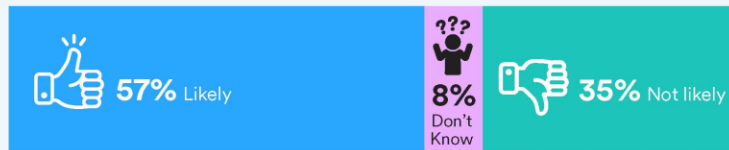
Machine learning and AI



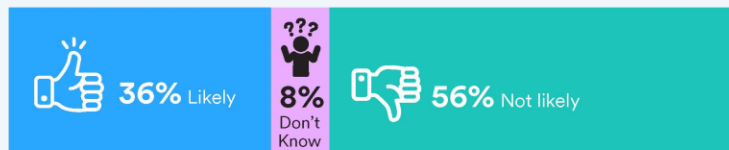
Global opinions: How people think AI will affect jobs, 2023

Source: Ipsos, 2023 | Chart: 2024 AI Index report

AI will change how you do your current job in the next 5 years



AI will replace your current job in the next 5 years



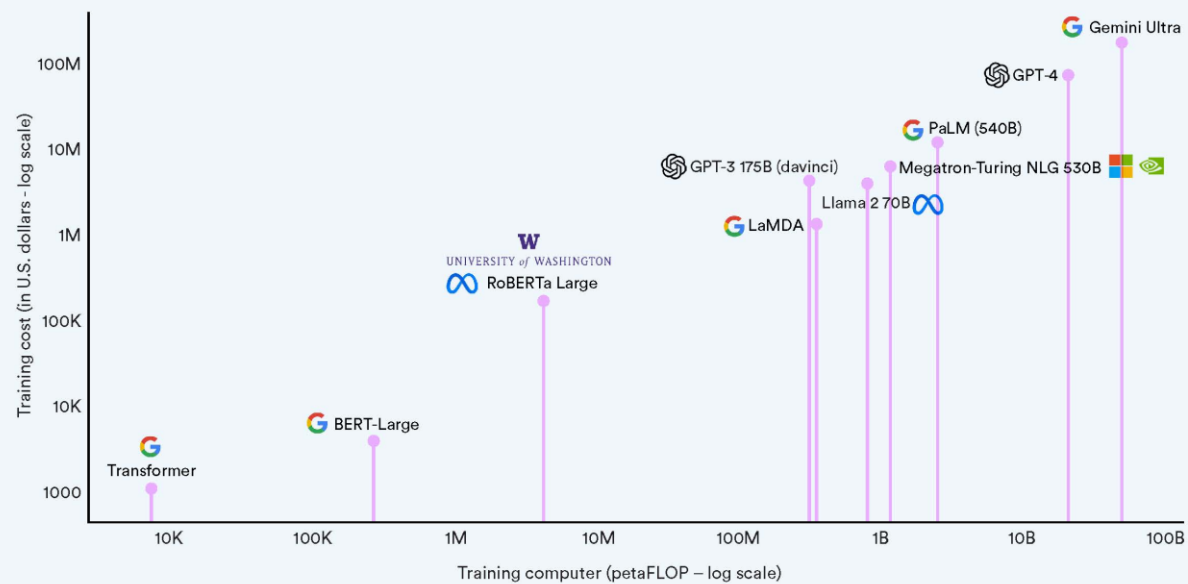
2024 AI index report

the next industrial revolution

AI+HEP in East Asia, Daejeon, Korea

Estimated training cost and compute of select AI models

Source: Epoch, 2023 | Chart: 2024 AI Index report



This is a C++ code for a class called 'Gam4pikp' which is used to analyze data from the BaBar experiment. The class contains several methods for filtering and sorting data, as well as outputting results.

This is a C++ code for a data analysis algorithm called Gam4pikp. The algorithm is designed to analyze data from high-energy particle collisions and identify specific patterns of particles. The code appears to be a part of a larger program that is used to analyze data from the Large Hadron Collider (LHC) at CERN.

This is the implementation of a ROOT-based algorithm called 'Gam4pikp' which is used to analyze particle physics data. The algorithm is designed to identify and reconstruct events containing four-pion (4π) and four-kaon ($4K$) resonances, and to perform various calculations and data analysis tasks.

This is a C++ code for a particle physics analysis tool, specifically a program that analyzes data from the Belle II experiment at the SuperKEKB collider. The code is designed to identify and reconstruct particles produced in high-energy collisions, and to study the properties of these particles.

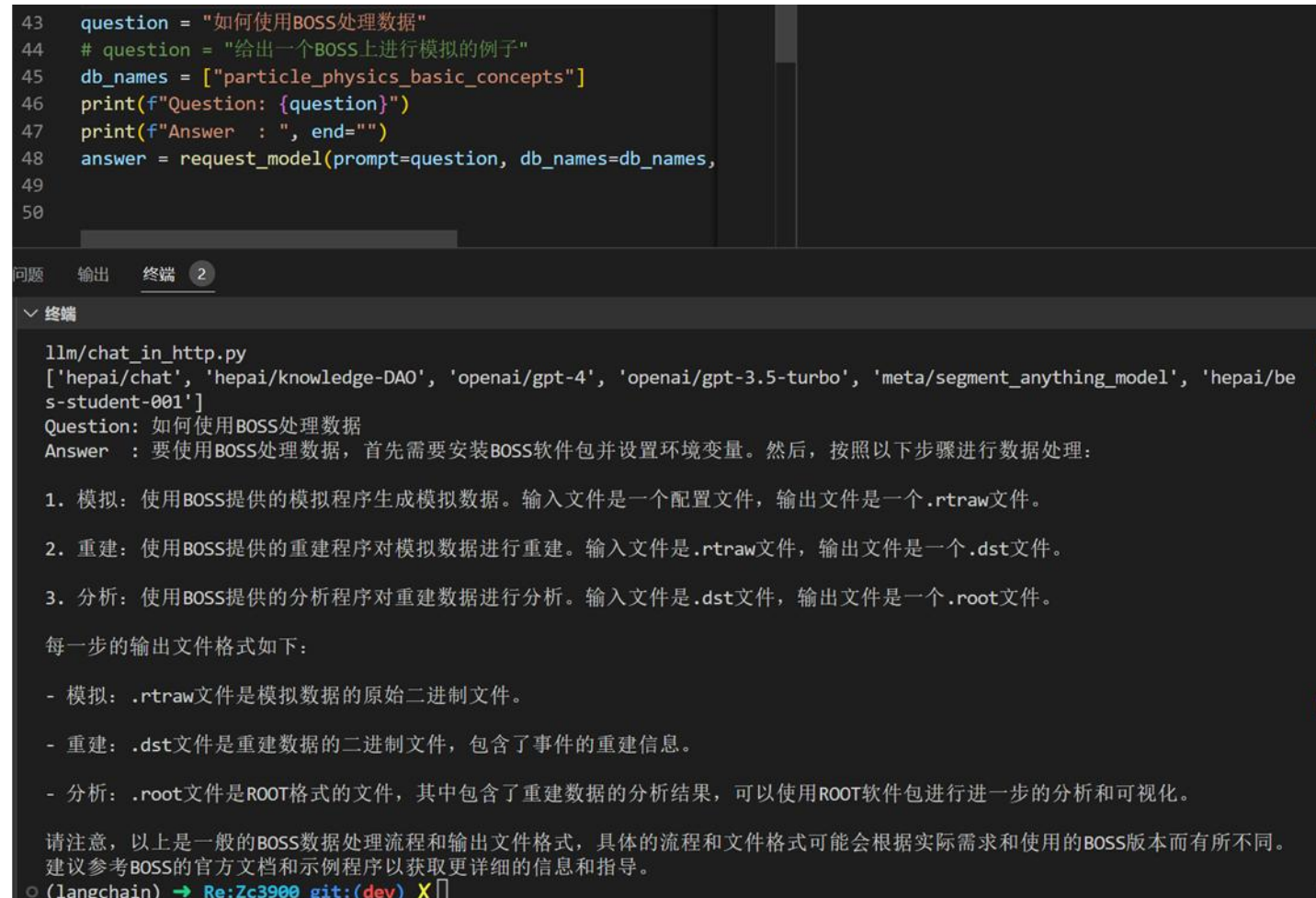
Simple test: Dr. Sai vs GPT4

As expected, better performance in HEP

Q: 如何使用BOSS处理数据？

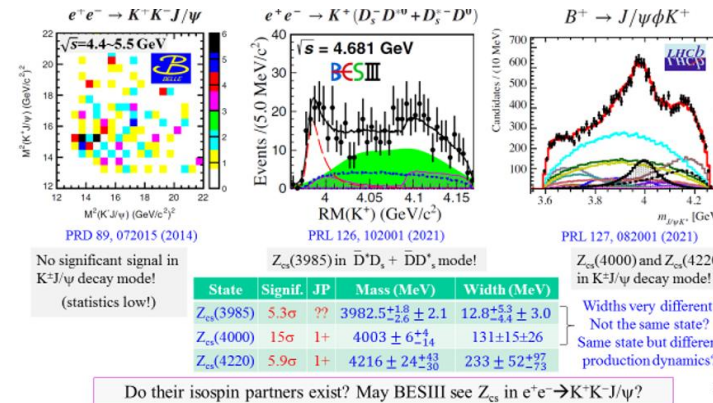
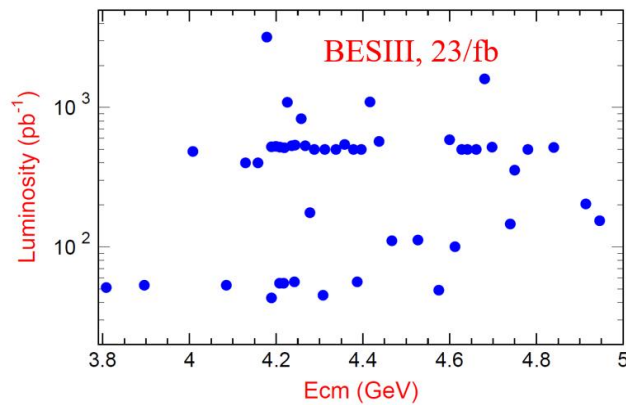
Answer from Dr.
Sai

Answer from
GPT-4

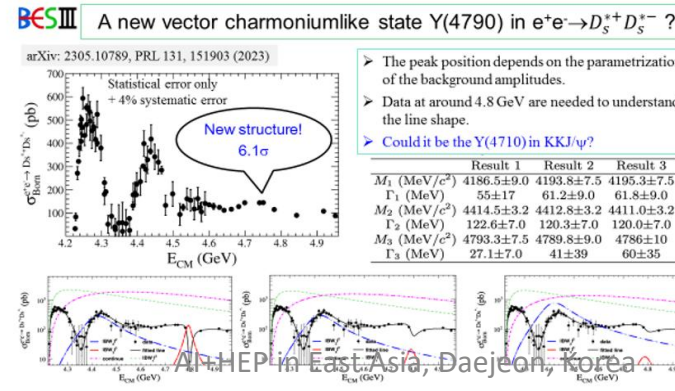
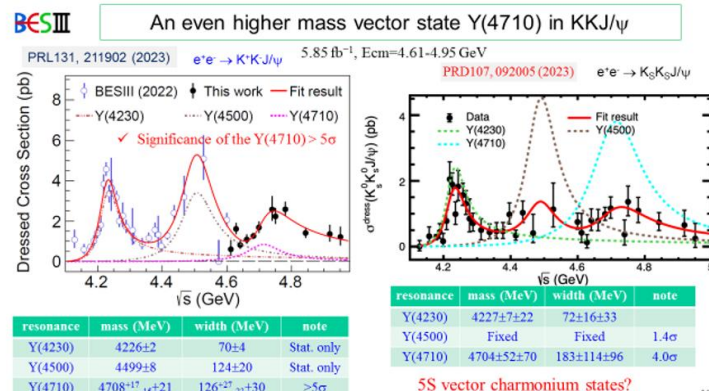


Status and prospects for Dr. Sai

- XYZ studies at BESIII:
 - Many (intermediate) resonants, many decay channels -> interferences
 - Difficult to retrieve useful information correctly

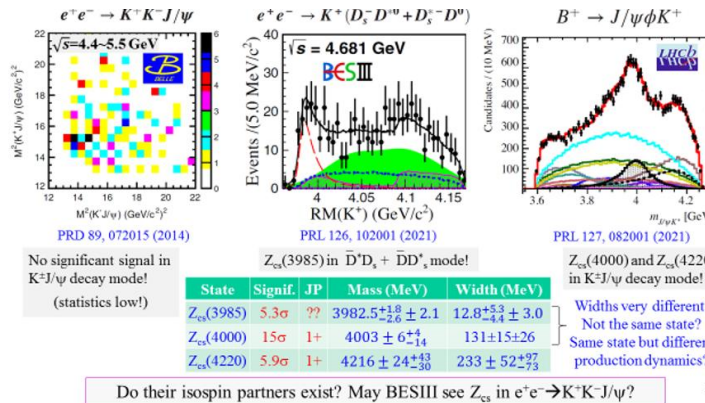
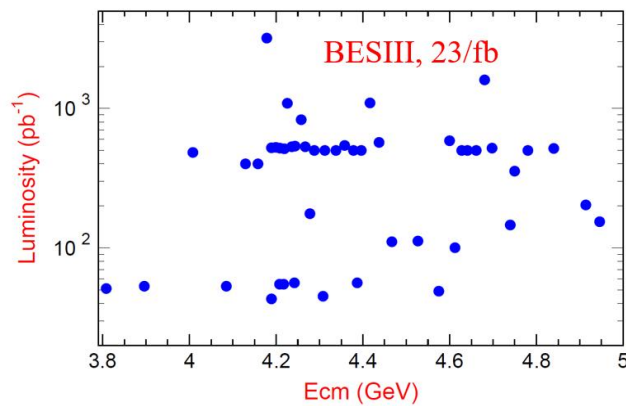


How to understand them? what is the physics behind them?



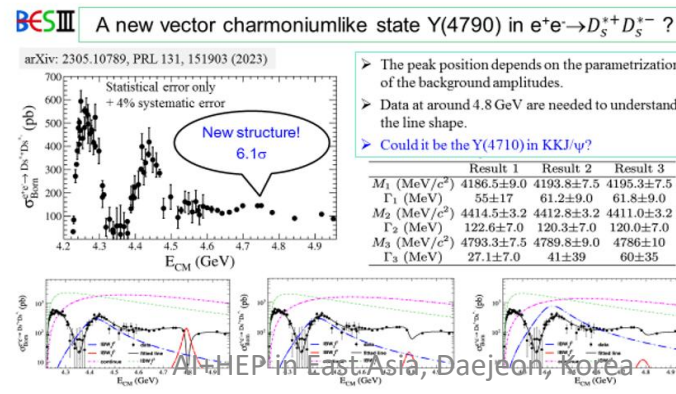
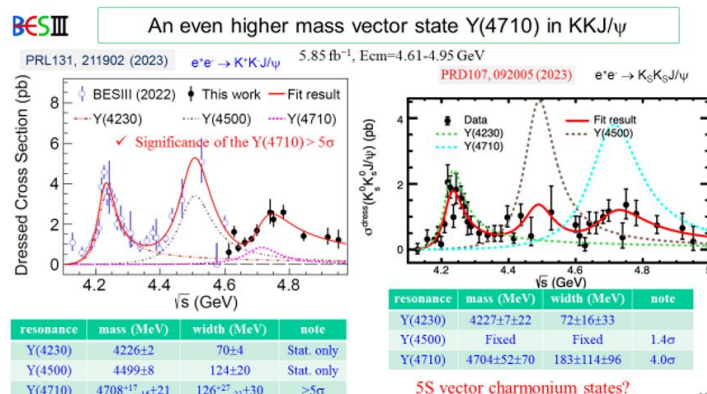
Status and prospects for Dr. Sai

- XYZ studies at BESIII:
 - Many (intermediate) resonants, many decay channels -> interferences
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How to understand them? what is the physics behind them ?

As a experimental people, I don't know.



But the cross section measurements of ALL channels should be one necessary condition.

how many papers published from BESIII



The number of papers published by the BESIII collaboration can vary over time as new research is conducted and published. As of my knowledge cutoff date in October 2023, I don't have the exact count of papers published by BESIII.

To get the most up-to-date and accurate information, you can:

1. **Visit the BESIII Collaboration Website:** The official website of the BESIII collaboration may have a list of their publications or a link to their recent papers.
2. **Check Scientific Databases:** Use databases like the INSPIRE HEP (High Energy Physics) database, the arXiv preprint service, or journal publishers' websites to search for papers published by the BESIII collaboration.
3. **Contact the Collaboration Directly:** You can reach out to the BESIII collaboration or one of its representatives for detailed information on their publications.

These methods should provide the latest count and specifics of the academic papers published by the BESIII collaboration.

tion has published over 1,200 papers in peer-reviewed journals. This number is constantly growing as new data is

iment at the Beijing Electron Positron Collider (BEPC) in studying the properties of exotic hadrons and other aspects. The collaboration is one of the largest in the world, with over 1,000 institutions in 20 countries.

cover a wide range of topics, including the properties of states, the search for new physics beyond the Standard Model, and various particle reactions and processes.

Summary:

- **Production Channel:**

- e^+e^- collisions with ISR: ($e^+ e^- \rightarrow \gamma \pi^\pm X(3872)$)

- **Decay Channels:**


- Predominantly hadronic decays like ($X^\pm(3872) \rightarrow \pi^\pm J/\psi$)
- Radiative decays like ($X^\pm(3872) \rightarrow \gamma \pi^\pm J/\psi$)
- Multi-body decays where the final state includes charmonium.


By focusing on these channels, you can efficiently search for the charged partner of $X(3872)$ at BESIII.

Data preparation: HaiNougat

- During the data clean for Xiwu LLM system, we found it is hard to obtain correct information from PDF, especially for Math equations and Tables
- For HEP-related papers, 20% more formulas per pages and 27% longer formulas than typical academic documents (computer science, chemics ...)
- Develop a model for HEP (HaiNougat) from the Visual Transformer model Nougat. Also an important part for dataset preparation from Xiwu LLM system!
- A demo accessible via <https://ai.ihep.ac.cn/m/hai-nougat>
- More details in <https://github.com/ai4hep/hai-nougat>

Data preparation: HaiNougat




 HaiNougat, the advanced iteration of the Nougat model, specializes in transforming PDFs into Mathpix Markdown, facilitating the extraction of complex information from high-energy physics documents. On this platform, you can experience HaiNougat's capabilities, upload PDFs, obtain Mathpix Markdown versions, visualize the results in an editor and preview area, and download the processed output.


You can drop a PDF here:

Choose a PDF

10.pdf

 Upload to HaiNougat

File processed successfully

 Download

as

$$\begin{aligned} \eta &= \frac{1}{2} M_D^\dagger (M^\dagger)^{-1} M^{-1} M_D \\ &= \frac{1}{2} m_D^\dagger (M_\Sigma^\dagger)^{-1} \left[\mathbb{I}_3 + \mu^* (M_\Sigma^\dagger)^{-1} (M_\Sigma^\dagger)^{-1} \mu \right] M_\Sigma^{-1} m_D \\ &\approx \frac{1}{2} m_D^\dagger (M_\Sigma^\dagger)^{-1} M_\Sigma^{-1} m_D. \end{aligned} \tag{33}$$

$$\Gamma(Z \rightarrow \ell^+ \ell^-) = \frac{m_Z^3}{12\pi v^2} \left[|(g_{\chi Z}^V)_\ell|^2 + |(g_{\chi Z}^A)_\ell|^2 \right], \tag{34}$$

$$\Gamma(h \rightarrow \ell^+ \ell^-) = \frac{m_h}{8\pi} \left[|(g_{\chi h}^L)_\ell|^2 + |(g_{\chi h}^R)_\ell|^2 \right], \tag{35}$$