AI for Nuclear Physics

FY 2024 - H1 Update

May 1, 2025

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Jefferson Lab

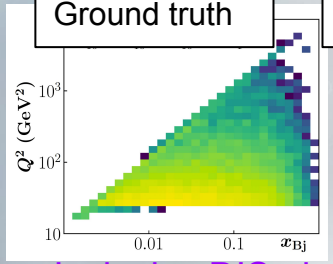
U.S. DEPARTMENT of ENERGY

Progress in Q2

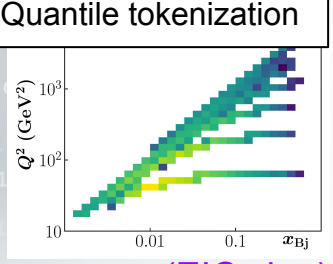
Revised work plan

Aims	Objective number	Milestone	FY25 H1	FY25 H2	FY26 H1	FY26 H2
1	LQCD Milestone 1	Collect data for PDF to Ioffe time transformations.				
	LQCD Milestone 2	Design suitable tokenization to support bi-directional PDF to Ioffe time transformer.				
	PDF Milestone 1	Collect all the data available at LHAPDF.				
	PDF Milestone 2	Generate PDF data for all the PDF sets using the LHAPDF interpolation software across a dense grid in x and Q2, along with their corresponding 1-sigma confidence bands.				
	JED Milestone 1	Simulate eP data using Pythia and generate a variety of phase space distributions.				
	JED Milestone 2	Design suitable tokenization scheme that integrates the simulated event-level data and the phase space distributions.				
	PDF/JED/LQCD Milestone 3	Design a suitable tokenization scheme that integrates the info file of the Ioffe time, PDF, and JED datasets.				
	PDF/JED/LQCD Milestone 4	Train and validate the embedding models using the tokenized Ioffe time, PDF, and JED data.				
1	Milestone 1	Explore language foundation models for hadronic physics inverse problems.				
2	Milestone 1	Train the base, open-source LLMs in an unsupervised manner using JLab-specific unlabeled data, specifically, the vector database developed in Aim 1.				
	Milestone 2	Carry out a systematic analysis of the latent space with existing tools.				
3	Milestone 1	For the three use cases, develop the questions for the task-specific fine-tuning.				
	Milestone 2	Tune the LLM and validate the data from Milestone 1.				
	Milestone 3	Evaluate the trained LLM from initial LLM and post-transfer learning. Evaluations will include accuracy, biases, training time, and generalizability.				

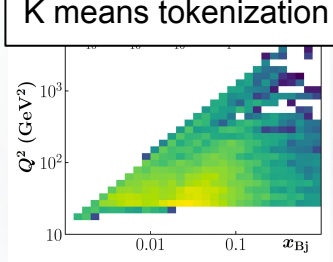
Ground truth



Quantile tokenization



K means tokenization



Inclusive DIS phase space (EIC sim.)

Overarching goal:

Integrate NP data (experimental events, simulations, LQCD, quantum correlation functions from global analysis, domain text) into LLMs.

The trained models with NP data is envisioned to provide variety of downstream application including solving inverse problems, classification and regeneration of data

Progress:

Collect and transform NP data into tokens to be assimilated by the LLM preserving fidelity in the inverse transform.

Particle events has been the most challenging and several tokenization schemes has been investigated. Currently finalizing VQA approach.

Project course:

Continue the R&D of tokenizing NP data and post-train open source LLMs

New opportunity: use agentic workflows to enable LLMs to leverage high-fidelity non-ML tools to orchestrate executions of downstream applications in NP (sames as before and more)

MULTI-AGENT FRAMEWORKS

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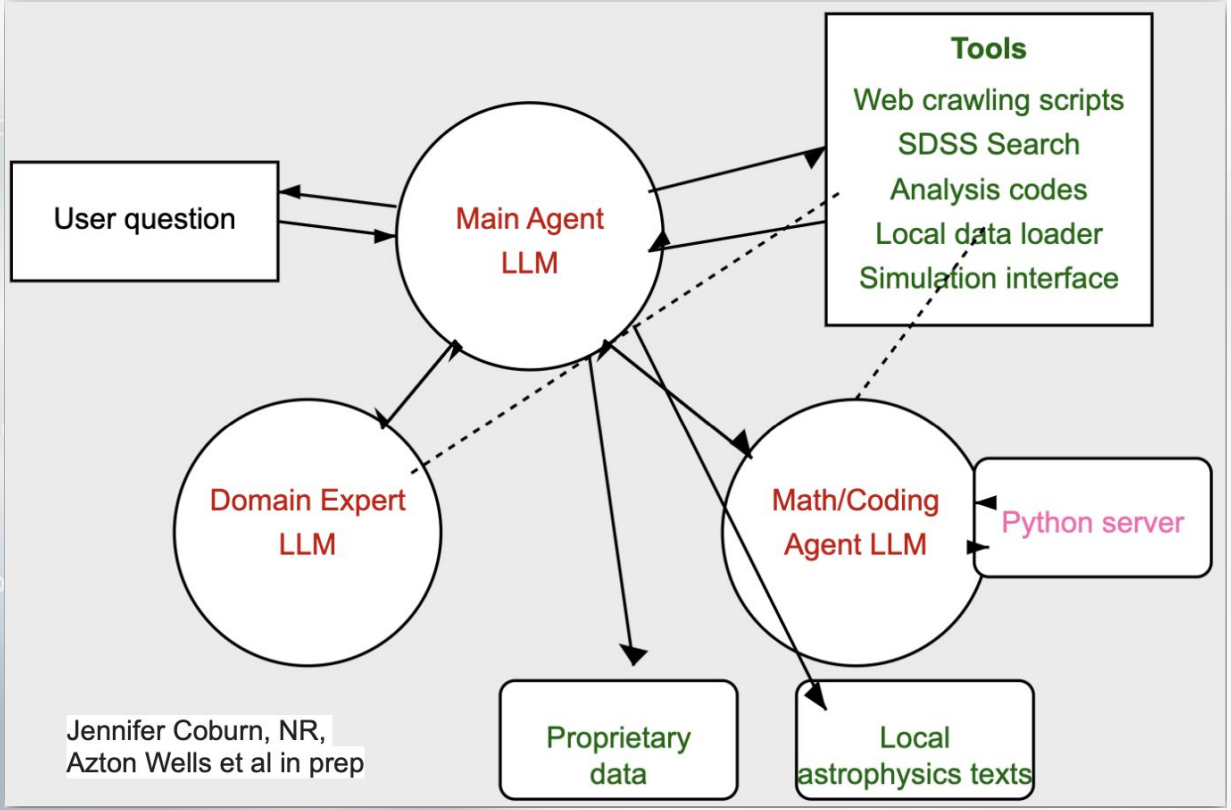

Ingredients: tools, servers, and databases

- LLMs or Reasoning models with tool access (web search, data base reading)
- Multiple expert interactions (Roles: Manager, domain-expert, coding expert, critic)
- Local datasets (texts and numerical data) access
  - Recent datasets, codes, publications
  - Proprietary data
- Local simulation interface access.
- Python server to run codes, feed results back to LLMs

Talk by N. Ramachandra (ANL) link

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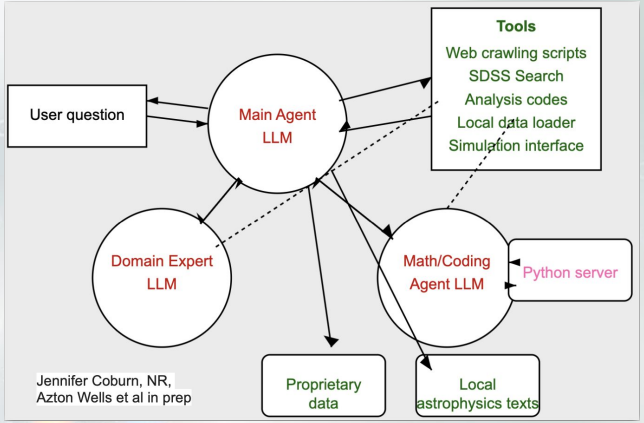


DA MACS

Multi-Agent Collaborative System for Astronomy & Cosmology

New run

What is the average brightness of galaxies with stellar mass between 10^10 and 10^12 solar masses and within the redshift range 0.1<z<0.2?

HfApiModel - Qwen/Qwen2.5-Coder-32B-Instruct

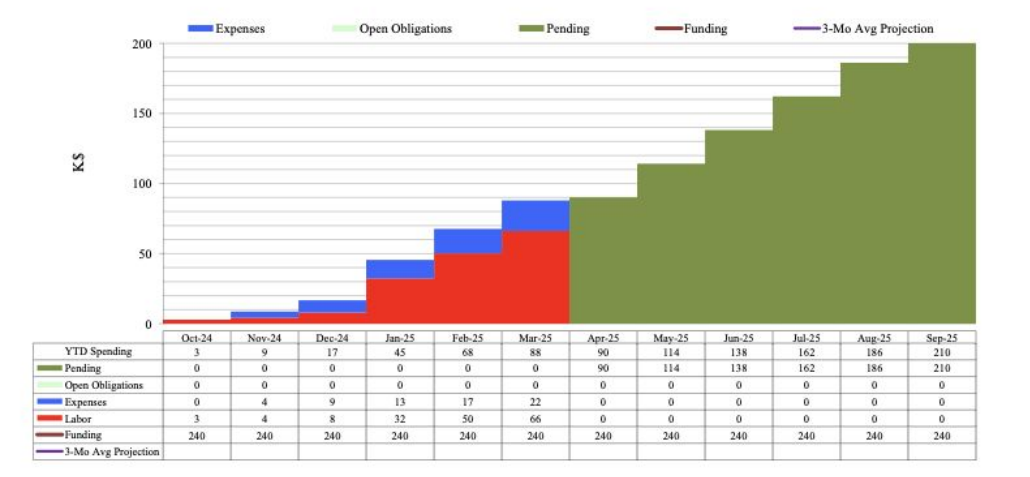
```
Press Enter to execute, or type 'no' to abort:
✅ Proceeding with execution.
 - Executing parsed code:
  final_answer(average_brightness)

Out - Final answer: -21.1615320371003
```

Final Answer from Main Agent in <1.5 minutes, with full logs of the reasoning steps, codes, issues and notes

Talk by N. Ramachandra (ANL)

Budget



	Oct-24	Nov-24	Dec-24	Jan-25	Feb-25	Mar-25	Apr-25	May-25	Jun-25	Jul-25	Aug-25	Sep-25
YTD Spending	3	9	17	45	68	88	90	114	138	162	186	210
Pending	0	0	0	0	0	0	90	114	138	162	186	210
Open Obligations	0	0	0	0	0	0	0	0	0	0	0	0
Expenses	0	4	9	13	17	22	0	0	0	0	0	0
Labor	3	4	8	32	50	66	0	0	0	0	0	0
Funding	240	240	240	240	240	240	240	240	240	240	240	240
3-Mo Avg Projection												

Agentic workflow expert for FY26 DS

Status

Steady spending invested on DS and NP researchers with dedicated weekly meetings. Will continue the planned work for the remaining of the year (**project is on track**).

This project is consistent with the Lab AI strategic planning and has the potential to revolutionize with the power of AI the R&D in Lab's strategic direction of ***"femtoscale imaging"***.

Plans for FY26

Continue the initial work plan of the project until the end of the project.

New opportunity on "agentic workflows": Need to invest in this growing area of research. Is a unique opportunity consistent with the scope of the LDRD. Will position the Lab as leader in the AI/ML within NP and create a track record in future NOFOs. We need to collaborate with ANL as they are leading this area in astrophysics.

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QUESTIONS?

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