

AI4Science series
November 4th, 2025

DEPLOYING AI INFERENCE SERVICES AT ALCF

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Team Lead
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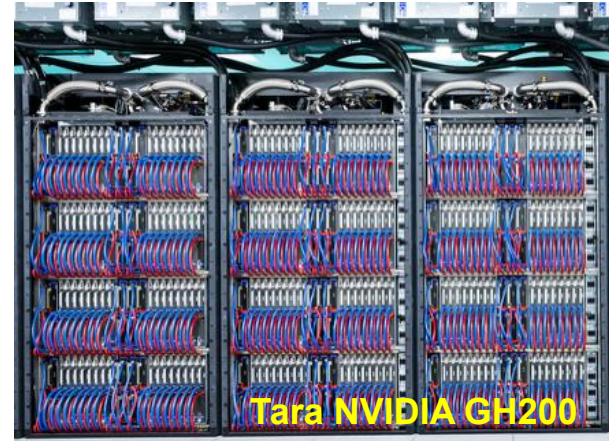


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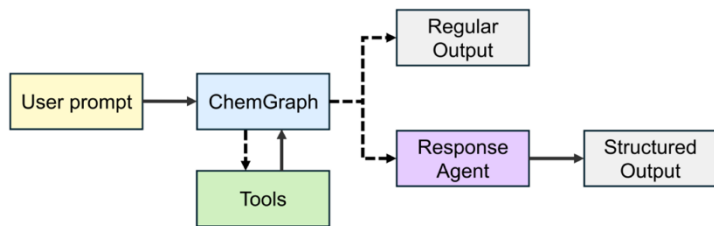
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NATIONAL LABORATORY

ALCF IS DEPLOYING DIVERSE INFERENCE SYSTEMS FOR SCIENCE



SOME INFERENCE SERVICE USE-CASES

ChemGraph – Thang et al. <https://www.arxiv.org/pdf/2506.06363>



Workflow and Cheminformatics

- LangGraph
- ASE
- RDKit
- PubChemPy

Simulation Backends

- | Semi-empirical | Ab initio | ML Potentials |
|----------------|-----------|---------------|
| - xTB | - NWChem | - MACE |
| - EMT | - ORCA | - UMA |

Largest usage is currently for generating synthetic data for science



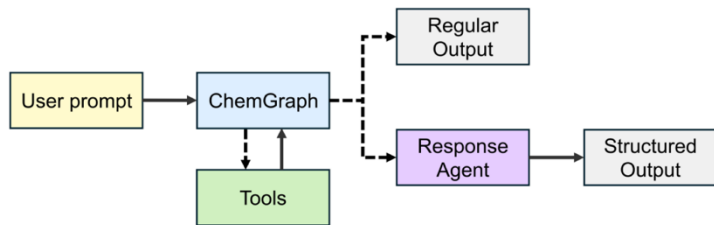
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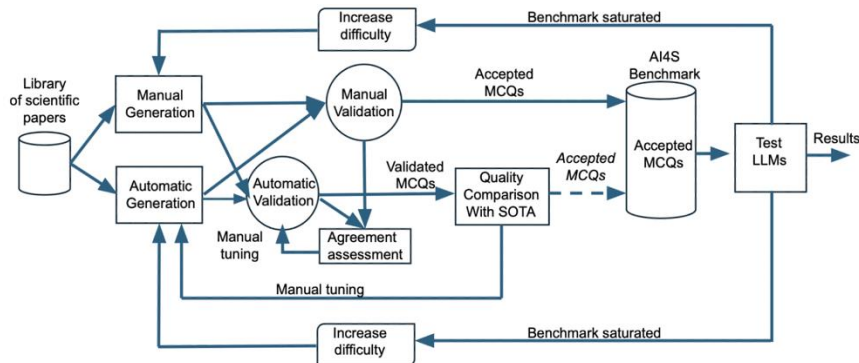
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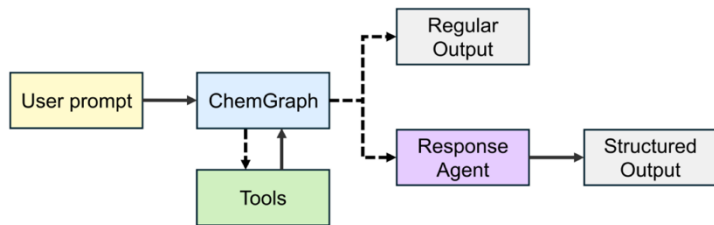
AuroraGPT-EAIRA – Capello et al. <https://arxiv.org/pdf/2502.20309>



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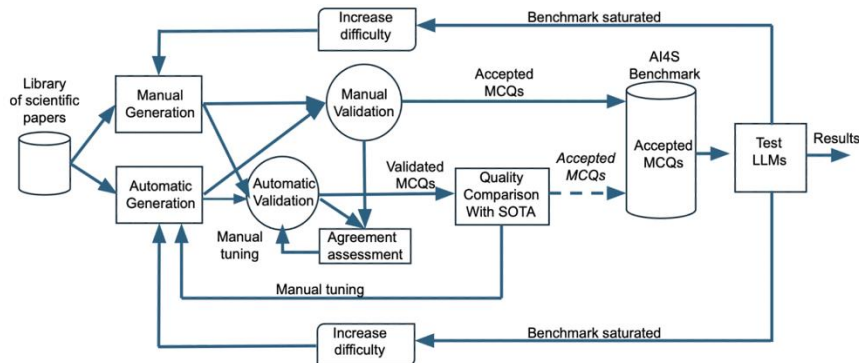
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Drag and drop file here
Limit 200MB per file • JSON

Browse files

Download RITM Data

Download RITM

Export Conversation

Export Conversation

Example Questions

RITM0429668 - Need help with this ticket

How do I access Aurora systems?

What are the data transfer options?

Help with RITM0430179

How to submit a job to ALCF systems?

RITM0429668 - Help me with this ticket

System Status

Client: Ready

Last Ticket: RITMUnknown

Messages: 2

RITM Queries: 1

ALCF User Support

Get help with ALCF systems and support tickets

User Support Mode

Retriever: dense_gemini_004 | LLM: gemini-2.0-flash

Ticket Details: RITM0429668

Ticket Information:

- RITM: RITM0429668
- Date: 2025-05-28T15:14:50
- Subject: [SN] Request RITM0429668 assigned to your group: ALCF Eagle storage disk status- [ALCF-Support]
- Total Interactions: 2

Generated Query:

"How can I check the status of storage disks on the ALCF Eagle system?"

First Interaction (Preview):

"Content-Type" content="text/html; charset=utf-8"> color: #ffffff; color: #; "> You can reply directly to this email. Please enter your response above this

Conversation ID: 47e7d9df-74e9-4a15-9eaf-5190dfe52645

You

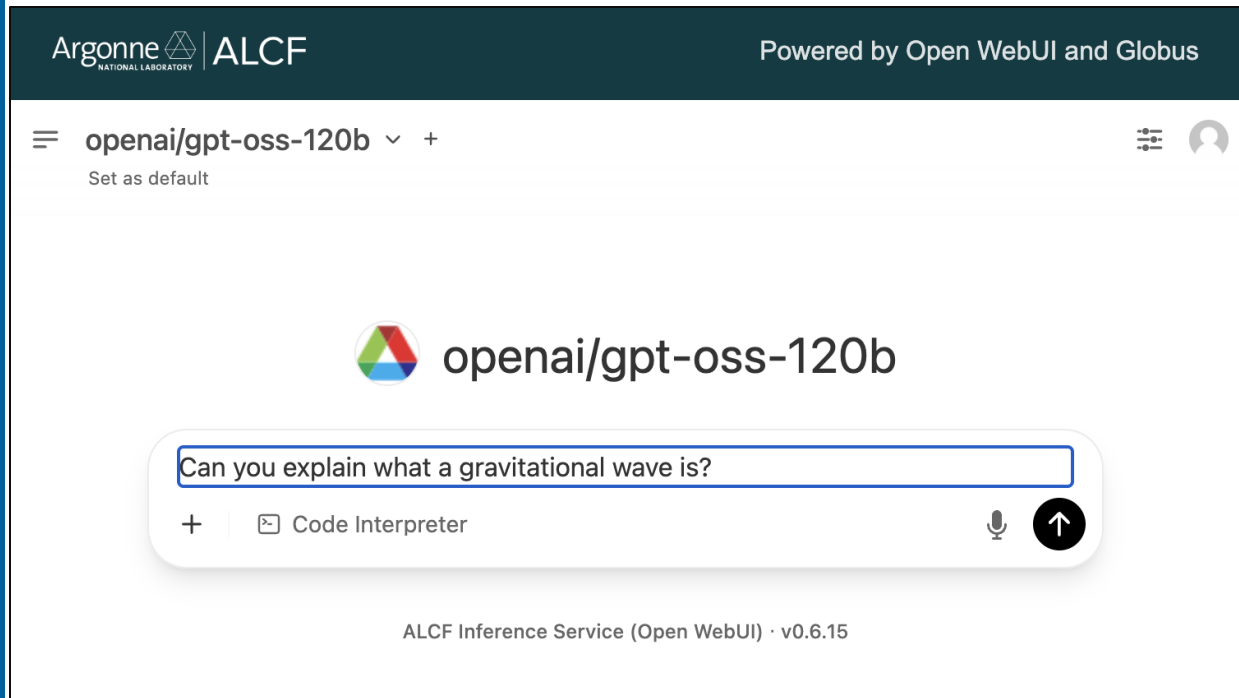
RITM0429668 - Need help with this ticket

Assistant

Based on the available context, I can see that the Eagle file system is a Lustre file system [1], and it is used for intensive job output and large files [1]. To check the disk quota usage on the Eagle file system, you can use a command that will output your project name, quota type, file system, current data usage, allocated quota, and grace period [2].


INTERFACING WITH THE INFERENCE SERVICE

Open WebUI interface
<https://inference.alcf.anl.gov>





INTERFACING WITH THE INFERENCE SERVICE


Open WebUI interface
<https://inference.alcf.anl.gov>

 **ALCF**


Powered

 **openai/gpt-oss-120b** ▾ +
Set as default



 **openai/gpt-oss-120b**

+  Code Interpreter

ALCF Inference Service (Open WebUI) · v0.6.15

 **ALCF**

Powered by Open WebUI and Globus

  **openai/gpt-oss-120b** ▾ +

2. How Gravitational Waves Are Produced

Gravitational waves are generated whenever **mass-energy accelerates asymmetrically**. The strongest astrophysical sources are:

SOURCE	TYPICAL FREQUENCY (HZ)	TYPICAL STRAIN (H) AT EARTH
Binary Black Hole (BH–BH) Merger	10–500	$10^{-21} - 10^{-22}$
Binary Neutron Star (NS–NS) Merger	10–2000	$10^{-21} - 10^{-23}$
Supernova Core Collapse	~100–1000	$10^{-23} - 10^{-24}$
Rapidly Rotating Neutron Stars (mountains)	~10–1000	$10^{-26} - 10^{-28}$
Stochastic Background (early universe)	$10^{-9} - 10^3$	Extremely tiny, model-dependent

Key points:


Quadrupole Moment: The dominant contribution to gravitational radiation comes from the second time derivative of the mass quadrupole moment Q_{ij} . A changing monopole (total mass) or dipole (center-of-mass motion) does **not** radiate in GR.

Energy Loss: As a system radiates, it loses orbital energy, causing binary components to spiral inward (the “chirp” observed by detectors).

3. What a Gravitational Wave Does to Space

When a GW passes, it **stretches** space in one direction while **compressing** it in the perpendicular direction, then swaps the roles as the wave oscillates. For a wave traveling along the z -axis, the metric perturbation in TT (transverse–traceless) gauge looks like:

$$ds^2 = -c^2 dt^2 + [1 + h_+(t - z/c)] dx^2 + [1 - h_+(t - z/c)] dy^2 + dz^2,$$

+  Code Interpreter



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INTERFACING WITH THE INFERENCE SERVICE

OpenAI API (including batch)

<https://docs.alcf.anl.gov/services/inference-endpoints>

cURL Python (OpenAI SDK)


```
#!/bin/bash

# Get your access token
access_token=$(python inference_auth_token.py get_access_token)

curl -X POST "https://inference-api.alcf.anl.gov/resource_server/sophia/vllm/v1/chat/completions" \
  -H "Authorization: Bearer ${access_token}" \
  -H "Content-Type: application/json" \
  -d '{
    "model": "meta-llama/Meta-Llama-3.1-8B-Instruct",
    "messages": [{ "role": "user", "content": "Explain quantum computing in simple terms." }]
  }'
```

API Usage Examples 1

Querying Endpoint Status

 Querying Endpoint Status



Chat Completions

 Chat Completions



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```
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```

```
-d '{
```

```
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```

```
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```

```
}]'
```

API Usage Examples 1

Querying Endpoint Status

Querying Endpoint Status

Chat Completions

Chat Completions

```
{
  "id": "chatcmpl-68de443dde8b46659b4c34",
  "object": "chat.completion",
  "created": 1755114580,
  "model": "meta-llama/Meta-Llama-3.1-8B",
  "choices": [
    {
      "index": 0,
      "message": {
        "role": "assistant",
        "content": "Quantum computing is a new way of processing information that's
```

different from the way regular computers work. Here's a simplified explanation:\n\n**Regular Computers:**\n\nRegular computers use "bits" to store and process information. Bits are like light switches that can be either ON (1) or OFF (0). When you combine these bits, you get numbers, letters, and other data.\n\n**Quantum Computers:**\n\nQuantum computers use "qubits" (quantum bits) to store and process information. Qubits are special because they can be both ON and OFF at the same time, which is called a "superposition." This means a qubit can process multiple possibilities simultaneously, making it much faster than regular computers for certain tasks.\n\n**Another Key Concept: Entanglement**\n\nQubits can also be "entangled," which means that when something happens to one qubit, it instantly affects the other qubits, no matter how far apart they are. This allows quantum computers to perform calculations on multiple qubits simultaneously, making them incredibly powerful.\n\n**How Quantum Computing Works:**\n\nImagine you have a combination lock with 10 numbers. A regular computer would try each number one by one, taking a long time to find the correct combination. A quantum computer, on the other hand, can try all 10 numbers simultaneously, thanks to the power of qubits and entanglement. This makes quantum computing incredibly fast for certain tasks, such as:\n\n1. **Cryptography:** Breaking complex codes and encryption methods.\n\n2. **Optimization:** Finding the best solution for complex problems, like logistics and supply chain management.\n\n3. **Simulation:** Simulating complex systems, like weather patterns and molecular interactions.\n\n**Challenges and Limitations:**\n\nQuantum computing is still a developing field, and there are many challenges to overcome, such as:\n\n1. **Error correction:** Qubits are prone to errors, which can affect the accuracy of calculations.\n\n2. **Scalability:** Currently, quantum computers are small and can only perform a limited number of calculations.\n\n3. **Noise:** Quantum computers are sensitive to external noise, which can disrupt calculations.\n\n**Conclusion:**\n\nQuantum computing is a revolutionary technology that has the potential to solve complex problems that are currently unsolvable or take too long to solve with regular computers. While it's still in its early stages, researchers and companies are working to overcome the challenges and limitations, and we can expect to see significant advancements in the coming years."

```
"usage": {
  "prompt_tokens": 43,
  "total_tokens": 436,
  "completion_tokens": 393,
  "prompt_tokens_details": null
},
"prompt_logprobs": null,
"kv_transfer_params": null,
"response_time": 3.179178237915039,
"throughput_tokens_per_second": 137.14235798428732
```



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SYSTEM OVERVIEW

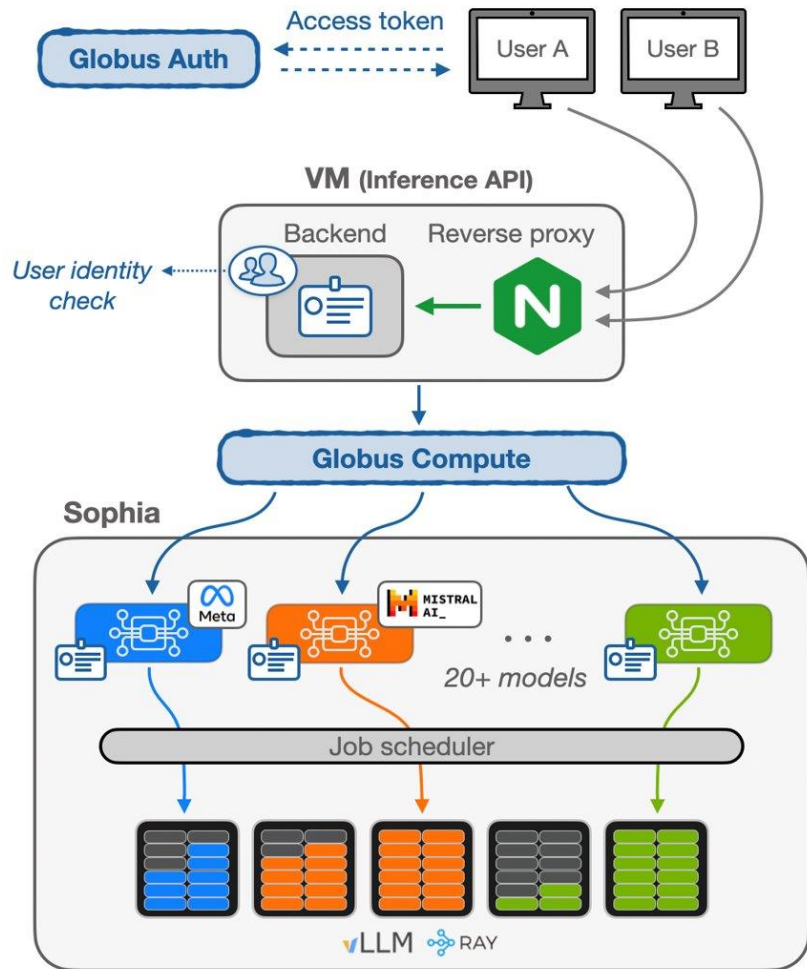
- Inference Service leverages ALCF computing resources to serve requests to a growing set of models
- Authentication via Globus Auth and orchestration using Globus Compute
- Combination of “in-memory/active” models and on-demand schedulable models
- Usage metrics are curated to understand and improve the service



Minerva (NVIDIA B200)



Metis (SambaNova SN40L)



<https://arxiv.org/abs/2510.13724>



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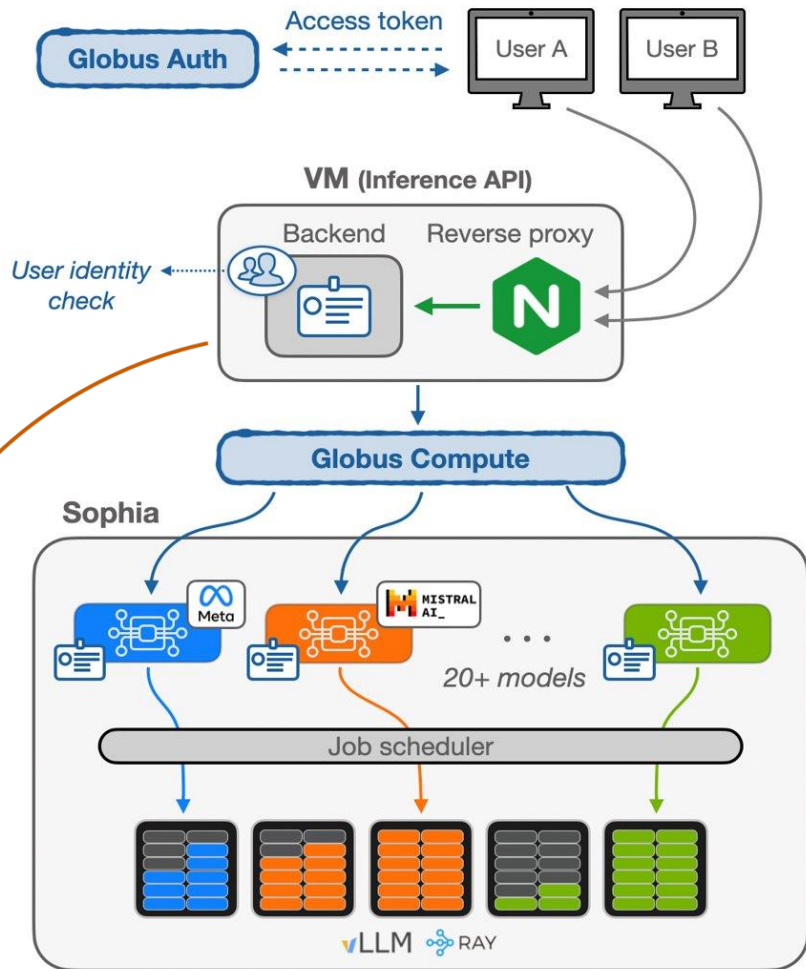
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GLOBUS AUTH

- Authentication and authorization platform (OAuth2/OpenID compliant)
- Federated identity provider integrating with different institutions worldwide

globus


Log in

Use your organizational login
e.g., university, national lab, facility, project

 Argonne National Laboratory

By selecting Continue, you agree to Globus [terms of service](#) and [privacy policy](#).

Continue

 Globus uses CILogon to enable organization. By clicking Continue, you agree to the [CILogon privacy policy](#) and you authorize Globus to use your username, email address, and other information to act on your behalf.

1100+ identity providers

Inference service currently only opened to ANL and ALCF

Argonne
NATIONAL LABORATORY

You have been redirected to this site by **National Center for Supercomputing Applications**. Please log in to continue.

Argonne Username

Password

Log In

Default Login Integrated Login Certificate Login

Redirect to the selected identity provider's login page



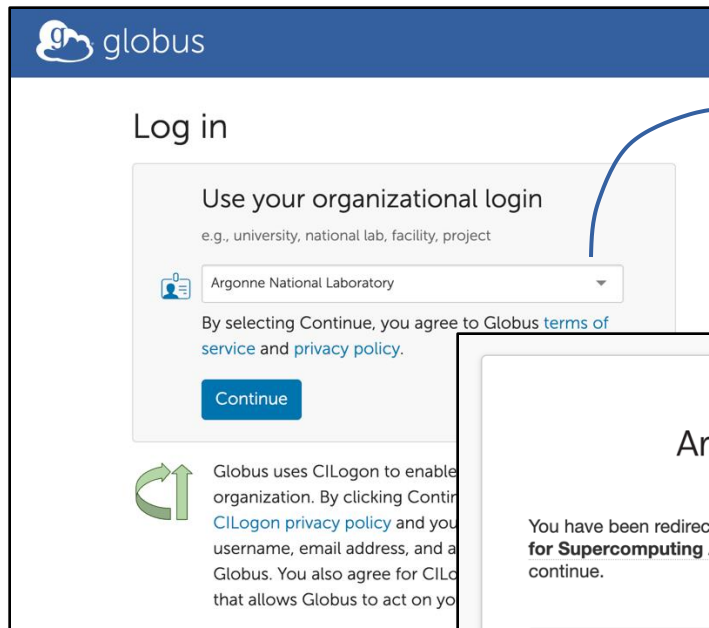
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GLOBUS AUTH

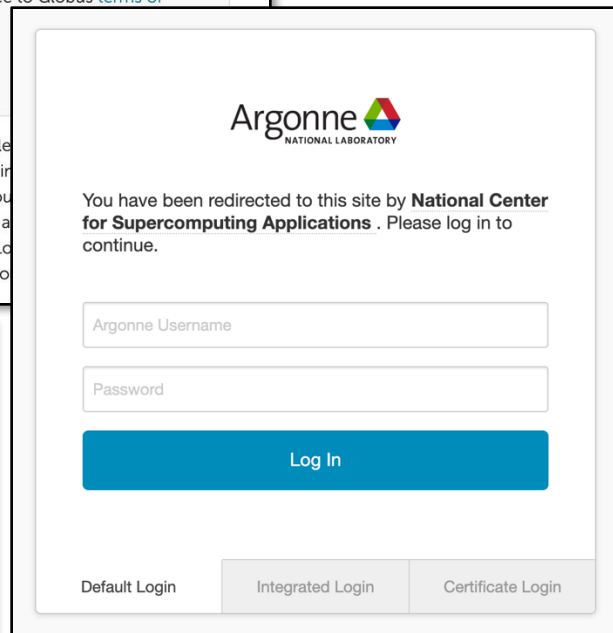
- Authentication and authorization platform (OAuth2/OpenID compliant)
- Federated identity provider integrating with different institutions worldwide
- From a user's perspective:
 - Globus Auth generates a token
 - The token is passed to our inference service as an API key



1100+ identity providers

*Inference service
currently only opened
to ANL and ALCF*

```
client = OpenAI(  
    api_key=access_token,  
    base_url="https://inference-api.alcf.anl.gov/resource_server/sophia/v1llm/v1"  
)  
  
response = client.chat.completions.create(  
    model="meta-llama/Meta-Llama-3.1-8B-Instruct",  
    messages=[{"role": "user", "content": "What are the symptoms of diabetes?"}]  
)
```



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AVAILABLE MODELS ON SOPHIA (31 TOTAL)

B - Batch enabled
T - Tool calling enabled
R - Reasoning enabled
H - Always hot

Family	Models
Meta Llama	Meta-Llama-3.1-70B-Instruct ^{BT^H} , Meta-Llama-3.1-8B-Instruct ^{BT^H} , Meta-Llama-3.1-405B-Instruct ^{BT} , Llama-3.3-70B-Instruct ^{BT} , Llama-4-Scout-17B-16E-Instruct ^{BT^H} , Llama-4-Maverick-17B-128E-Instruct ^T
OpenAI	gpt-oss-20b ^{BRT^H} , gpt-oss-120b ^{BRT^H}
Mistral	Mistral-Large-Instruct-2407, Mixtral-8x22B-Instruct-v0.1
Aurora GPT	AuroraGPT-IT-v4-0125 ^B , AuroraGPT-Tulu3-SFT-0125 ^B , AuroraGPT-DPO-UFB-0225 ^B , AuroraGPT-7B-OI ^B
Other Models	Allenai/Llama-3.1-Tulu-3-405B, google/gemma-3-27b-it ^{BT^H} , mgoin/Nemotron-4-340B-Instruct-hf
Vision (VLM)	meta-llama/Llama-3.2-90B-Vision-Instruct
Embedding	Salesforce/SFR-Embedding-Mistral, mistralai/Mistral-7B-Instruct-v0.3-embed

METIS – SN40L INFERENCE CLUSTER

SambaNova SN40L



- 2x SN40L nodes each with 16x SN40 RDU (32 SN40L Accelerators)
- 1.5TB per RDU – 48TB in aggregate
- Highly optimized for inference

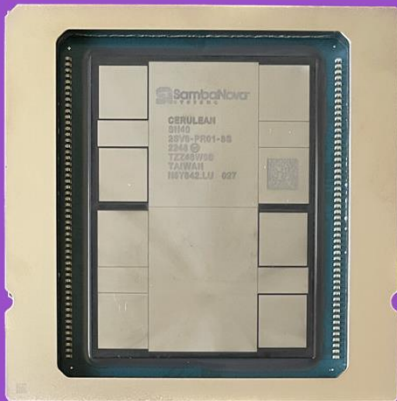
SN40L: Accelerating AI

Reconfigurable Dataflow Unit (RDU)

Native multi-tenancy support with fast model switching

Ideal for production inference, multi-tenancy, agentic workflows

 sambanova
SN40L RDU



3-tier Dataflow Memory

520 MB On-Chip
SRAM Memory

Very fast memory for high speed
inference with caching

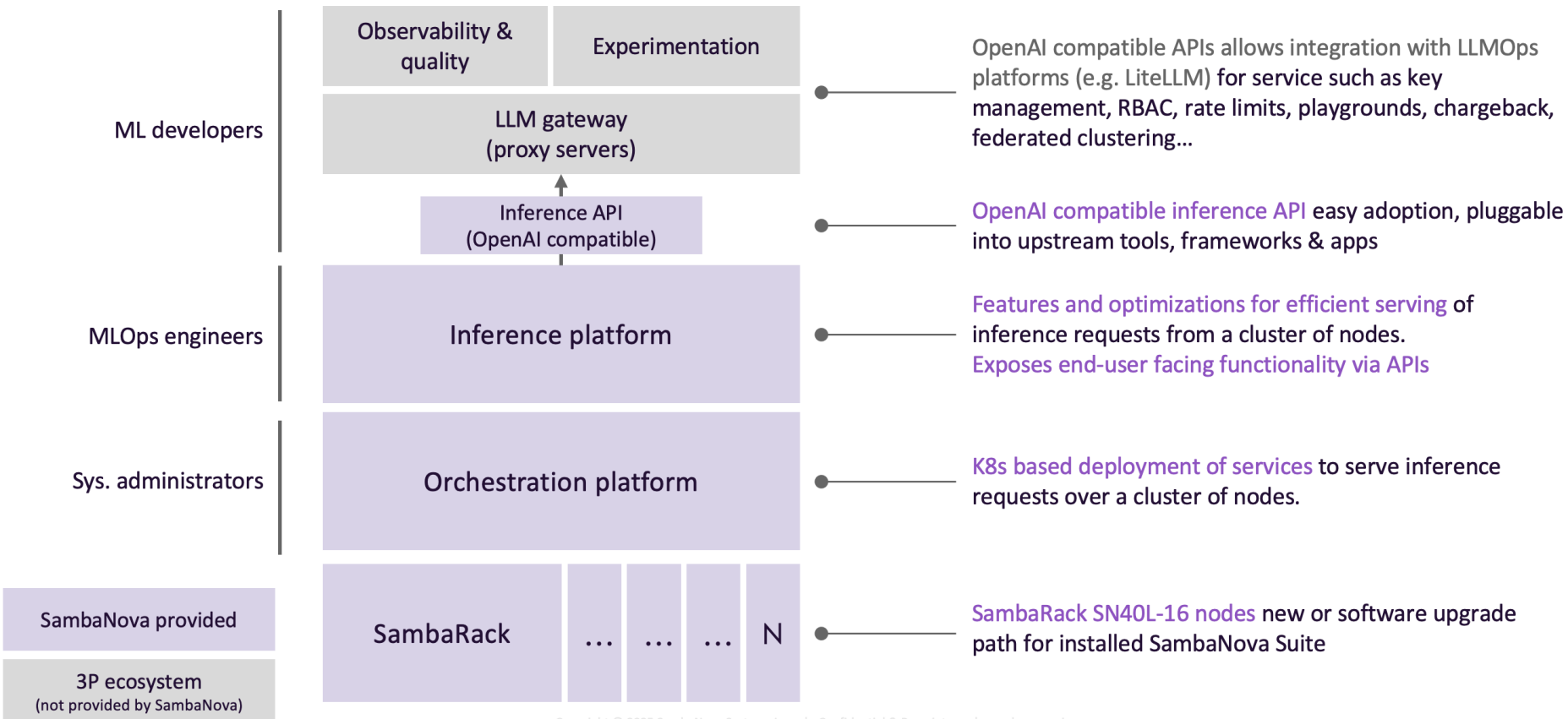
64 GB High
Bandwidth Memory

Switch between models in as
little as 2 milliseconds

1.5 TB High Capacity
DDR Memory

Hold large number of
models in memory

SambaStack Software Layers & User Personas



AVAILABLE MODELS ON METIS (2 TOTAL)

B - Batch enabled
T - Tool calling enabled
R - Reasoning enabled
H - Always hot

Chat Language Models

gpt-oss-120b-131072^{RH}

Llama-4-Maverick-17B-128E-Instruct^H

While Metis currently host less models than Sophia, our Gateway API has a direct connection to its models (i.e. does not rely on Globus Compute). This significantly reduces latency and improves the user experience on our web chat interface.



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FUTURE WORK

- Tool calling integration
- Working towards centralized logs and monitoring
- Host Gateway API on Kubernetes
- Implement model failure resiliency
- Integrate with local scheduler API to query job status and delete jobs
- Improve federated routing to offload requests to multiple clusters
- More dedicated resources (including Tara and Minerva from NVIDIA)
- Implement Globus-Flow base batch system for users outside of ALCF



LARGE COLLABORATION

Ryan Chard, Nick Saint, Tom Uram, Thang Pham, Murat Keceli, Rajeev Thakur, Ken Raffenetti, Le Chen, Yanfei Guo, Krishna Chetty, Murali Emani, Khalid Hossain, Nathan Nichols, Rachana Ananthakrishnan, Anthony Avarca, Bill Allcock, Tommie Jackson, Ian Foster, Mike Papka, Rick Stevens, ALCF and CELS Operations, Globus Labs, and many more.

Joint collaboration with Globus

CONCLUSION

ALCF Inference Endpoints democratize LLM access for scientific research by:

- Providing seamless access to 30+ cutting-edge models
- Supporting diverse use cases: chat, vision, embeddings, agents, and batch processing
- Integrating with multiple HPC backends for optimal performance
- Auto scaling based on request workload

Web Interface: <https://inference.alcf.anl.gov/>

Documentation (usage examples): <https://docs.alcf.anl.gov/services/inference-endpoints/>

Contact: support@alcf.anl.gov

See our paper: <https://arxiv.org/abs/2510.13724>

THANK YOU



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