AI4Science series
November 4th, 2025

DEPLOYING AI INFERENCE SERVICES AT ALCF

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U.S. DEPARTMENT of ENERGY
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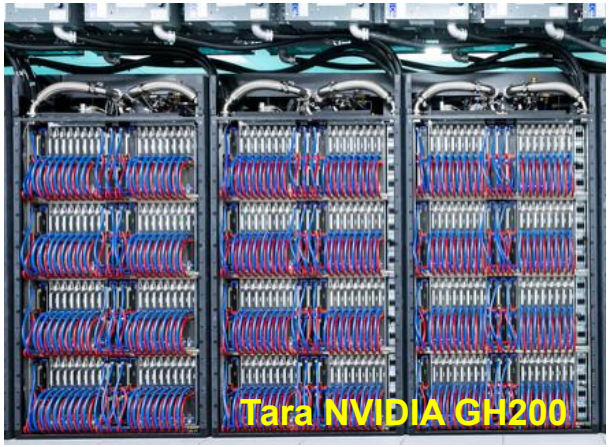
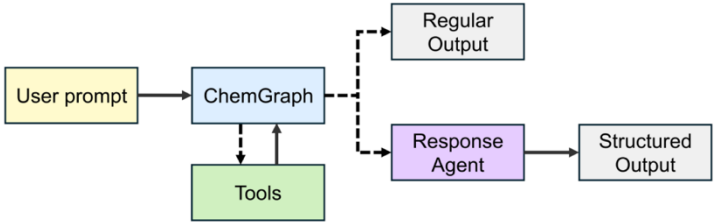
ALCF IS DEPLOYING DIVERSE INFERENCE SYSTEMS FOR SCIENCE



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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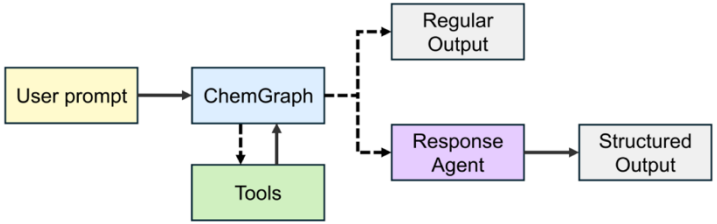

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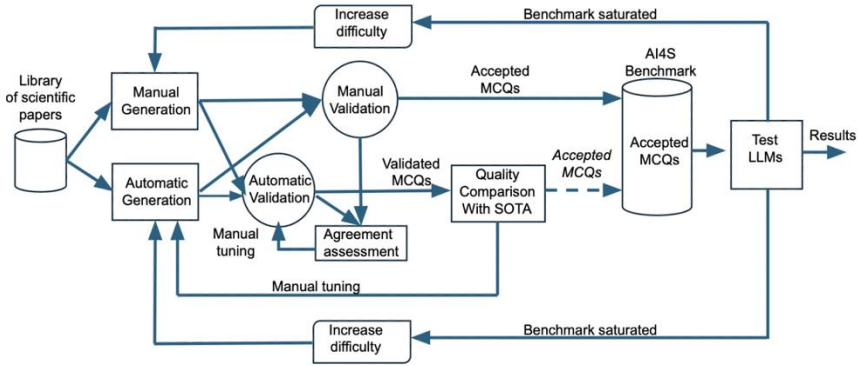

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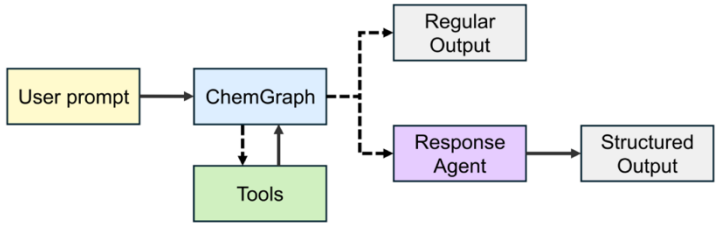

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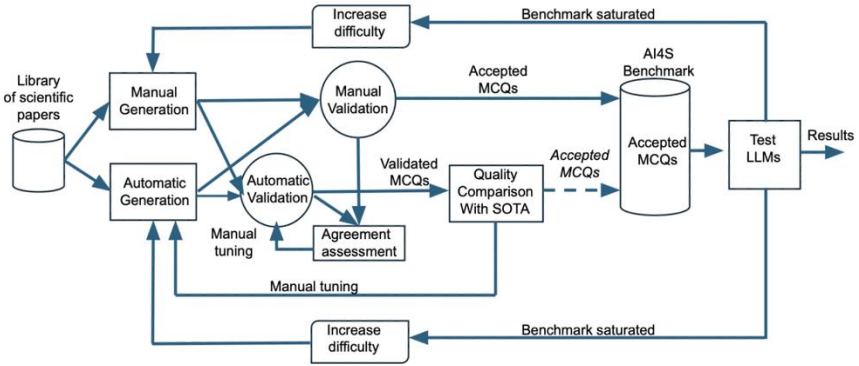

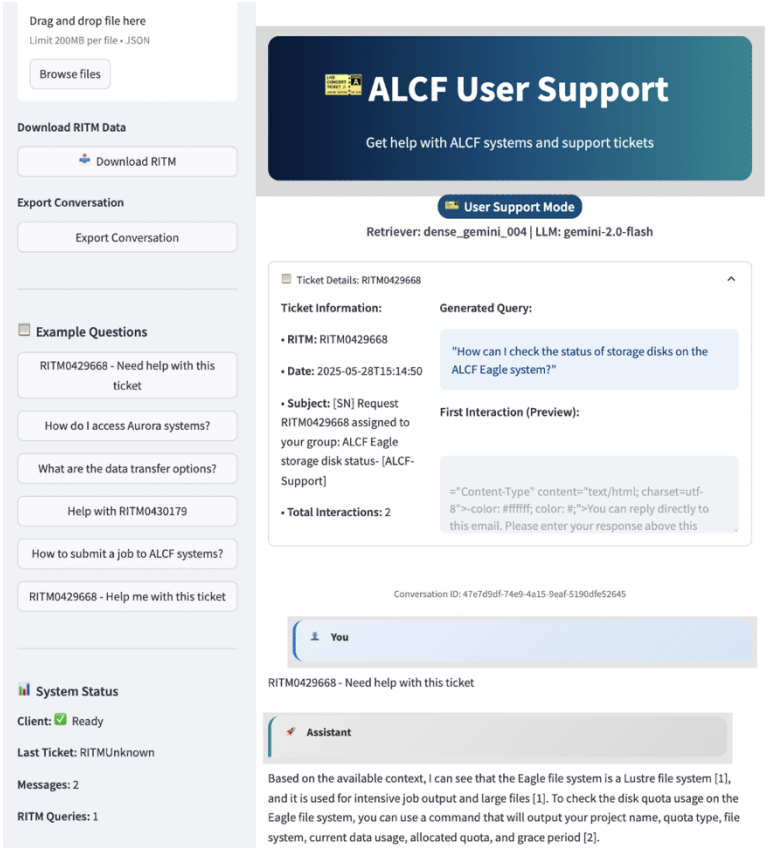

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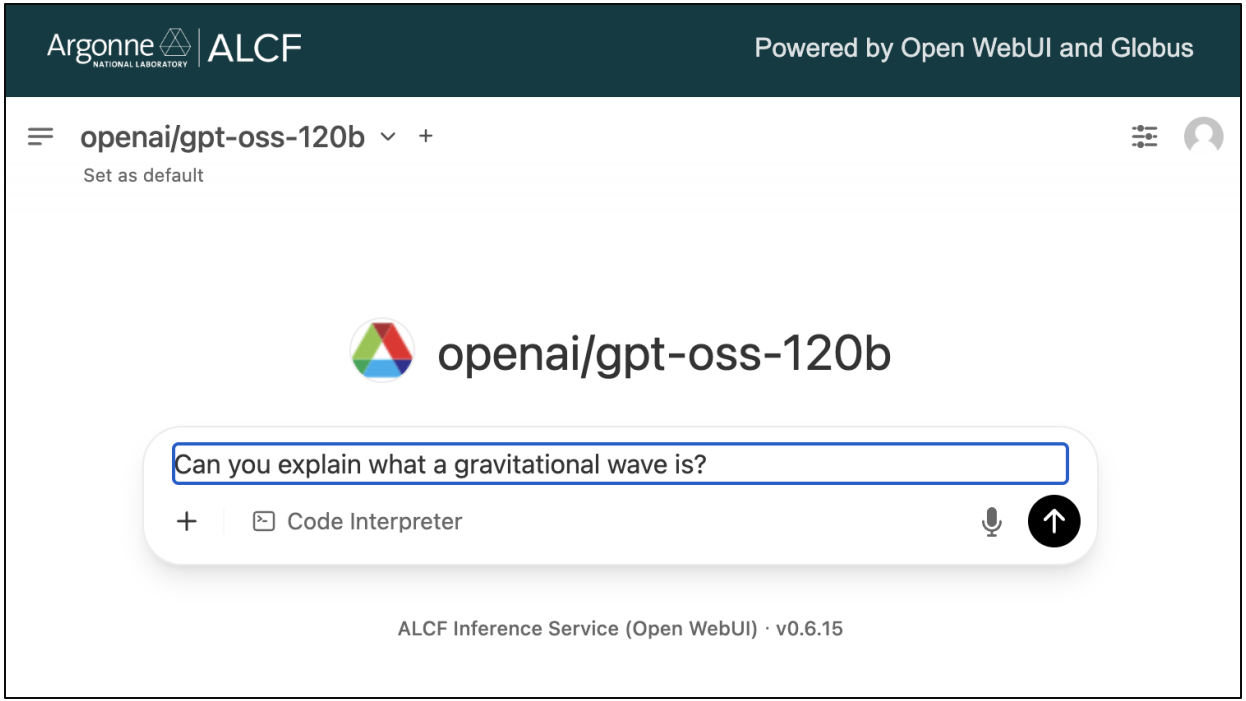
INTERFACING WITH THE INFERENCE SERVICE

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



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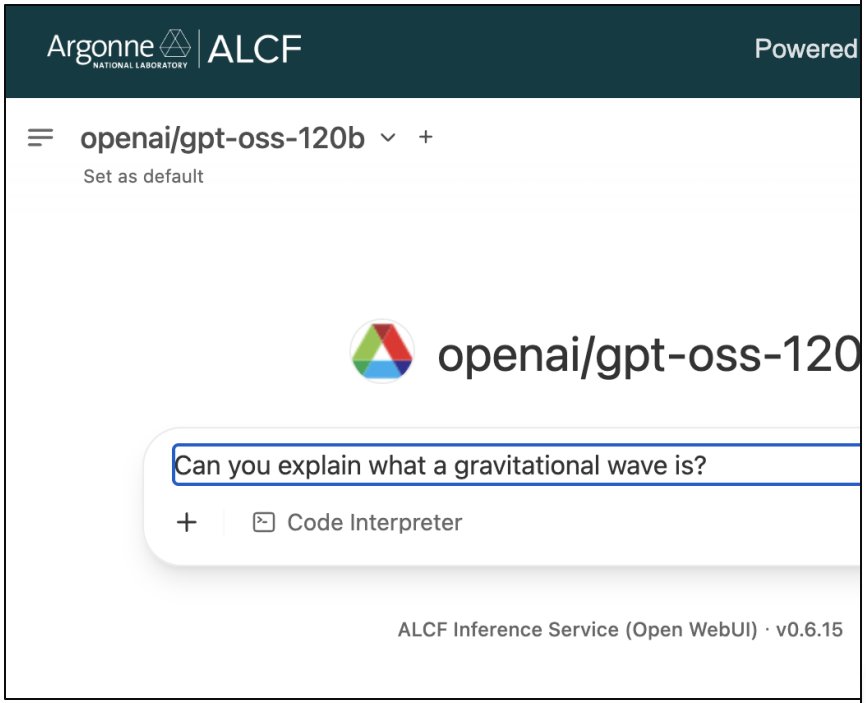

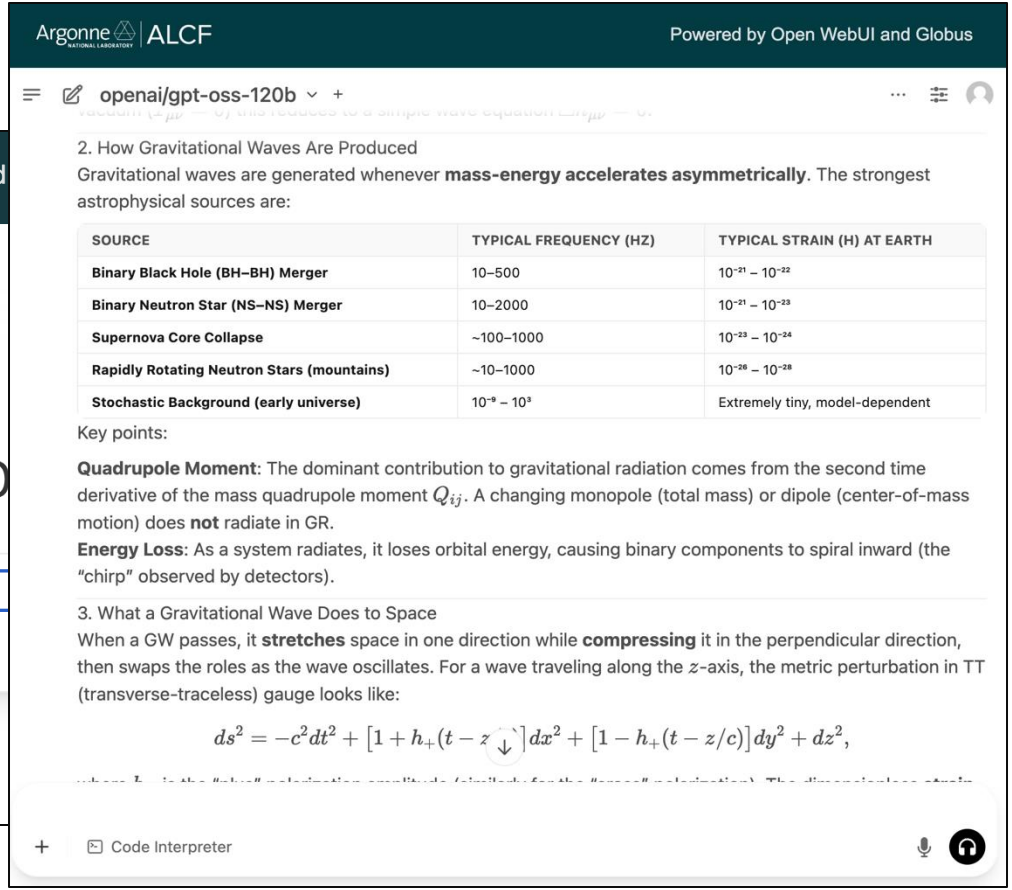

INTERFACING WITH THE INFERENCE SERVICE

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 ¶

Querying Endpoint Status

Querying Endpoint Status ›

Chat Completions

Chat Completions ›

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         }'
```

API Usage Examples ¶

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**Regul
ar Computers:**\n\nRegular computers use \"bits\" to store and process information. Bits ar
e like light switches that can be either ON (1) or OFF (0). When you combine these bits, yo
u 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 regula
r 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 affect
s the other qubits, no matter how far apart they are. This allows quantum computers to perf
orm calculations on multiple qubits simultaneously, making them incredibly powerful.\n\n**H
ow Quantum Computing Works:**\n\nImagine you have a combination lock with 10 numbers. A reg
ular computer would try each number one by one, taking a long time to find the correct comb
ination. A quantum computer, on the other hand, can try all 10 numbers simultaneously, than
ks to the power of qubits and entanglement. This makes quantum computing incredibly fast fo
r certain tasks, such as:\n\n1. **Cryptography:** Breaking complex codes and encryption met
hods.\n2. **Optimization:** Finding the best solution for complex problems, like logistics
and supply chain management.\n3. **Simulation:** Simulating complex systems, like weather p
atterns 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. **E
rror correction:** Qubits are prone to errors, which can affect the accuracy of calculation
s.\n2. **Scalability:** Currently, quantum computers are small and can only perform a limit
ed number of calculations.\n3. **Noise:** Quantum computers are sensitive to external noise
, which can disrupt calculations.\n\n**Conclusion:**\n\nQuantum computing is a revolutionar
y 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, re
searchers 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
```

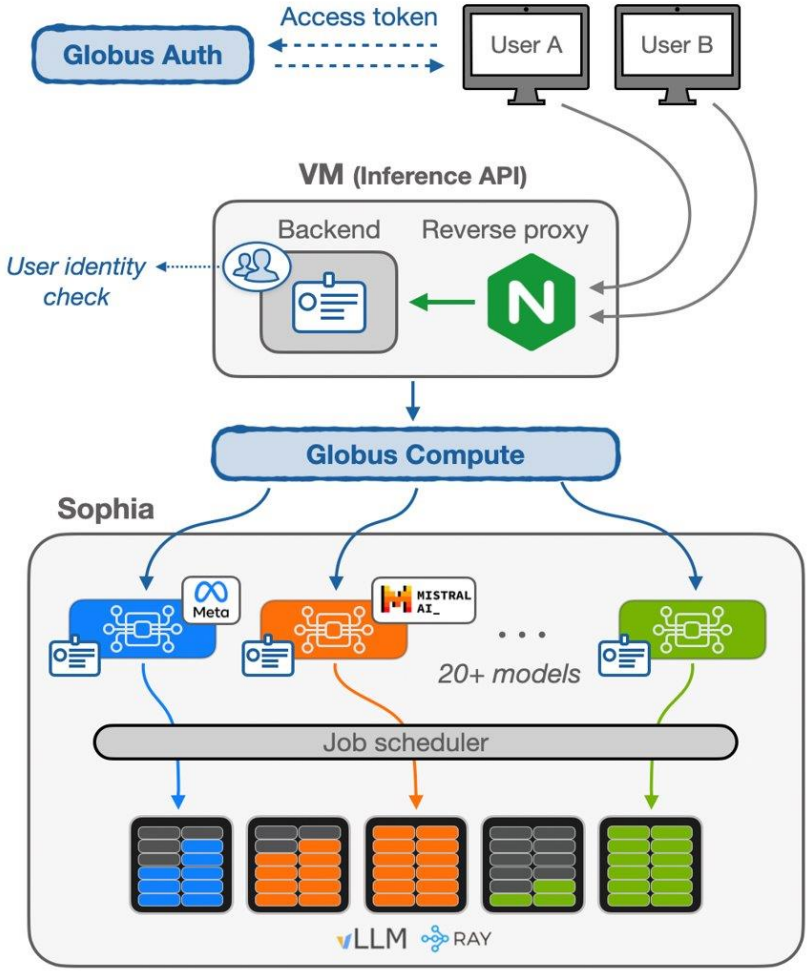
SYSTEM OVERVIEW

- 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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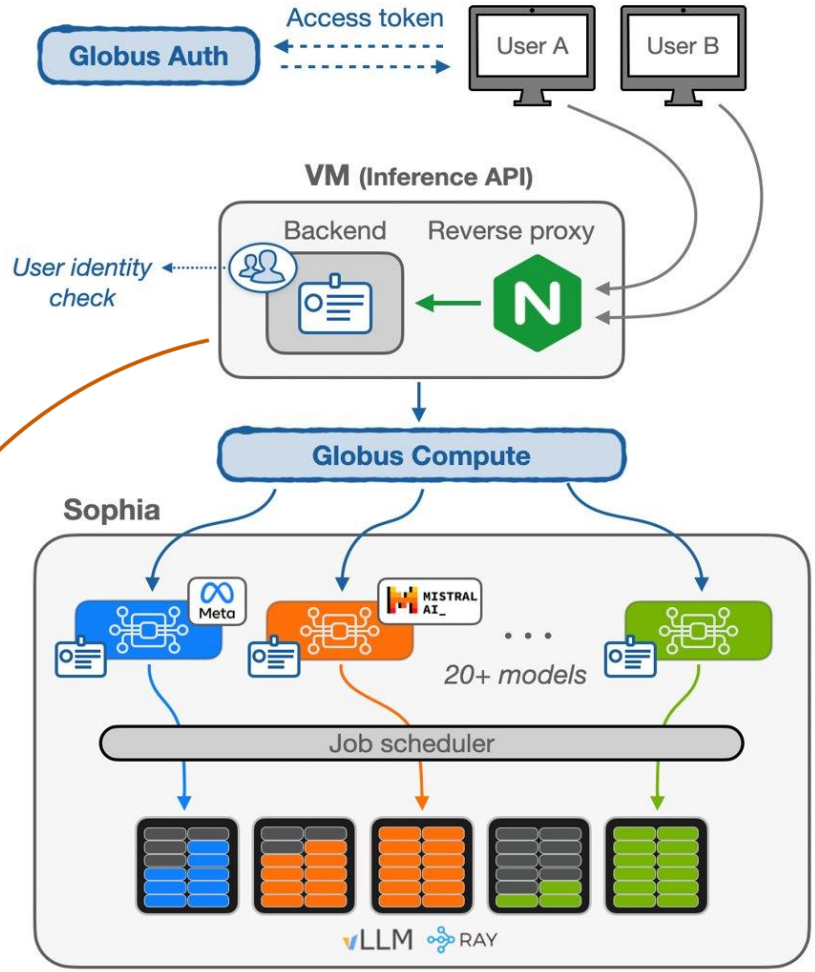

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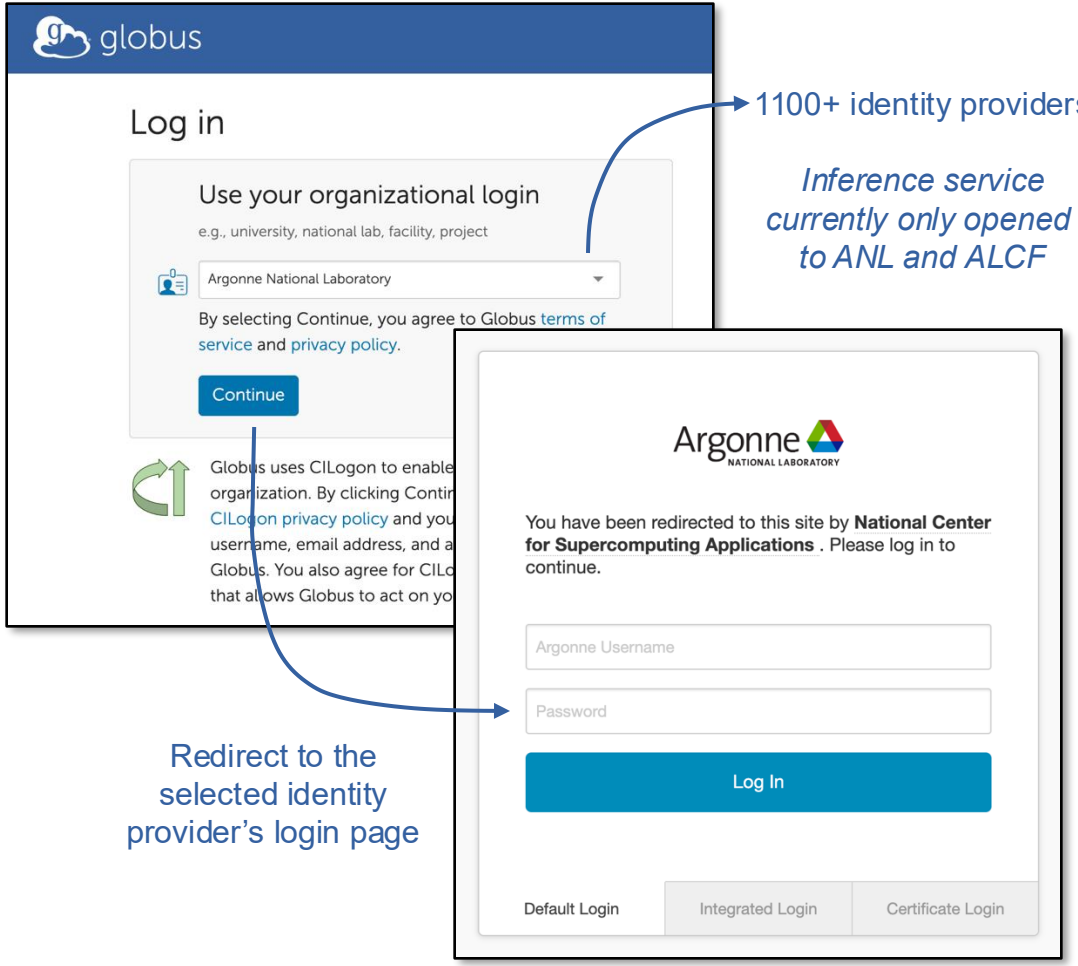
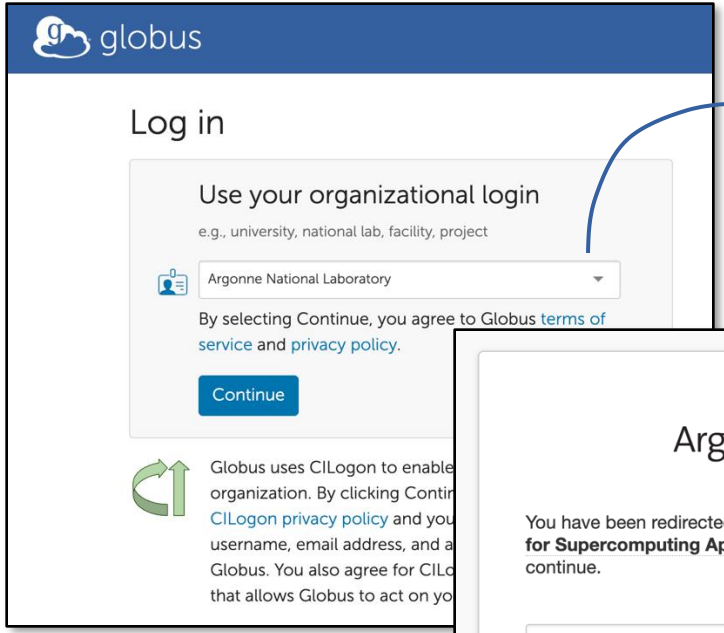
GLOBUS AUTH

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



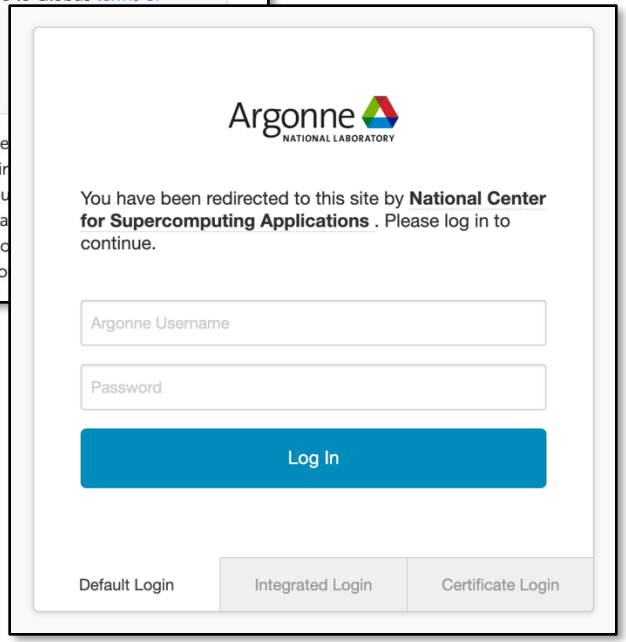
GLOBUS AUTH

- 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/vllm/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?"}]
)
```

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^{BTH}, Meta-Llama-3.1-8B-Instruct^{BTH}, Meta-Llama-3.1-405B-Instruct^{BT}, Llama-3.3-70B-Instruct^{BT}, Llama-4-Scout-17B-16E-Instruct^{BTH}, Llama-4-Maverick-17B-128E-Instruct^{T}
OpenAI	gpt-oss-20b^{BRTH}, gpt-oss-120b^{BRTH}
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^{BTH}, 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

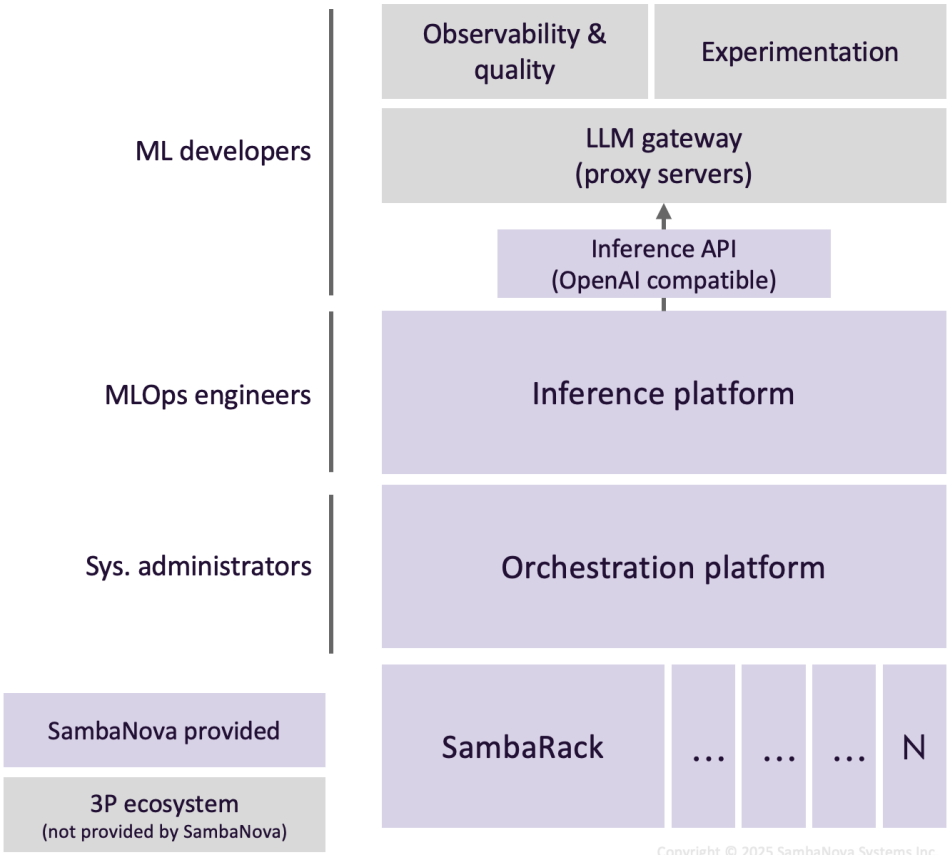
sambanova

SN40L: Accelerating AI

Reconfigurable Dataflow Unit (RDU)
Native multi-tenancy support with fast model switching
Ideal for production inference, multi-tenancy, agentic workflows

- 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



OpenAI compatible APIs allows integration with LLMOps platforms (e.g. LiteLLM) for service such as key management, RBAC, rate limits, playgrounds, chargeback, federated clustering…

OpenAI compatible inference API easy adoption, pluggable into upstream tools, frameworks & apps

Features and optimizations for efficient serving of inference requests from a cluster of nodes.
Exposes end-user facing functionality via APIs

K8s based deployment of services to serve inference requests over a cluster of nodes.

SambaRack SN40L-16 nodes new or software upgrade path for installed SambaNova Suite

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.

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