WORKSHOP

ALCF
Hands-on HPC Workshop

October 7-9, 2025
Argonne National Laboratory

U.S. DEPARTMENT of ENERGY

Argonne NATIONAL LABORATORY

Agentic Workflows at ALCF

Riccardo Balin, Thang Pham, Taylor Childers, Harikrishna Tummalapalli,
Aditya Tanikanti, Murat Keceli
Argonne National Laboratory

2025 ALCF Hands-On HPC Workshop
September 24, 2025

What are Agentic Workflows?

- AI-powered computational pipelines that can autonomously perform complex tasks, make decisions, and adapt in real-time based on intermediate results or user input
- Agentic workflows exhibit "agency/intelligence" – can reason, plan, and execute tasks based on new results with minimal human intervention
- Key characteristics:
  - Break down complex tasks into discrete steps, each step handled by an agent
  - Autonomous and real-time decision making
  - Adaptive execution

Agentic Workflows for Science

- LLMs can provide immense value to scientific research, but struggle on complex topics (hallucinations)

Human

Provide the SMILES string corresponding to this molecule: 9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine

** SMILES = Simplified Molecular Input Line Entry System

LLMs (with GPT-4o)

The molecule **9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine** has the following structure components:

- A **purine** core
- Substitution at position 9: a **(2,6-dichlorophenyl)methyl** group
- Substitution at position 6: an **amino group**
- That **amino group** is further substituted with a **furan-2-ylmethyl** group

Constructed SMILES:

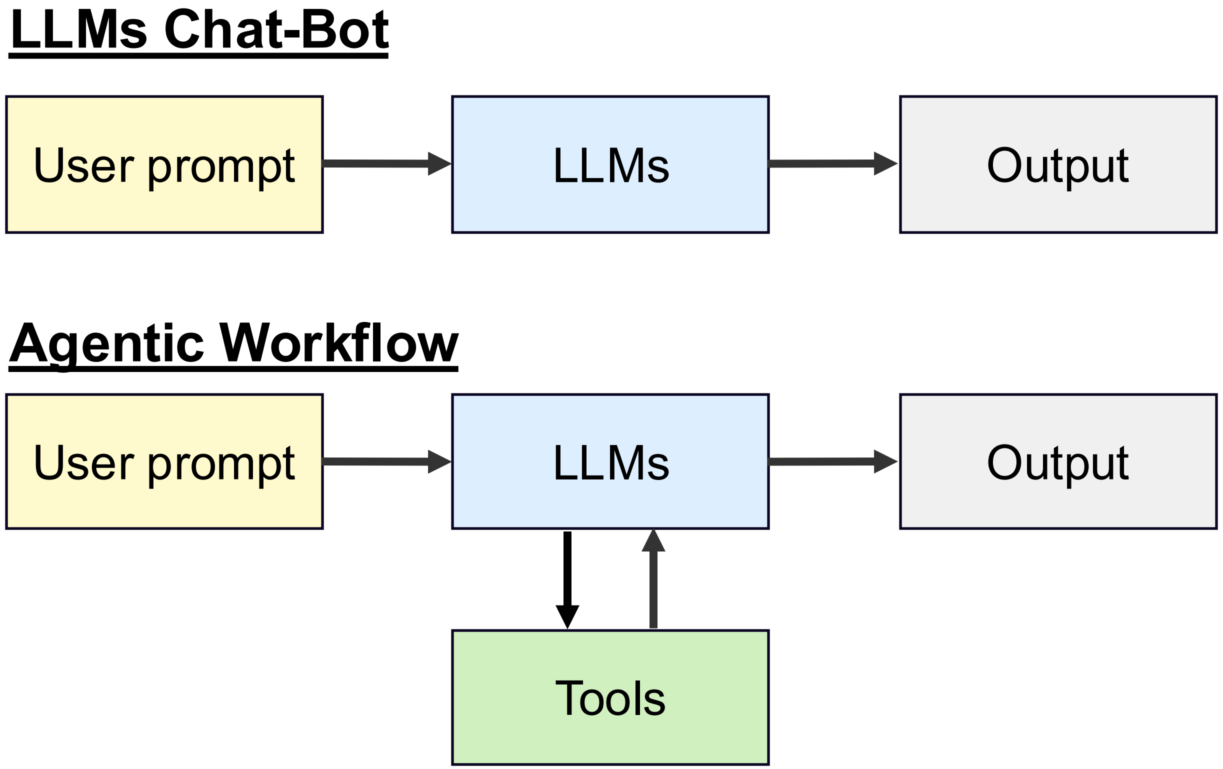
Clc1cccc(Cl)c1CN2c3nc(nc(NCC4=CC=CO4)c3nc2)N

Incorrect

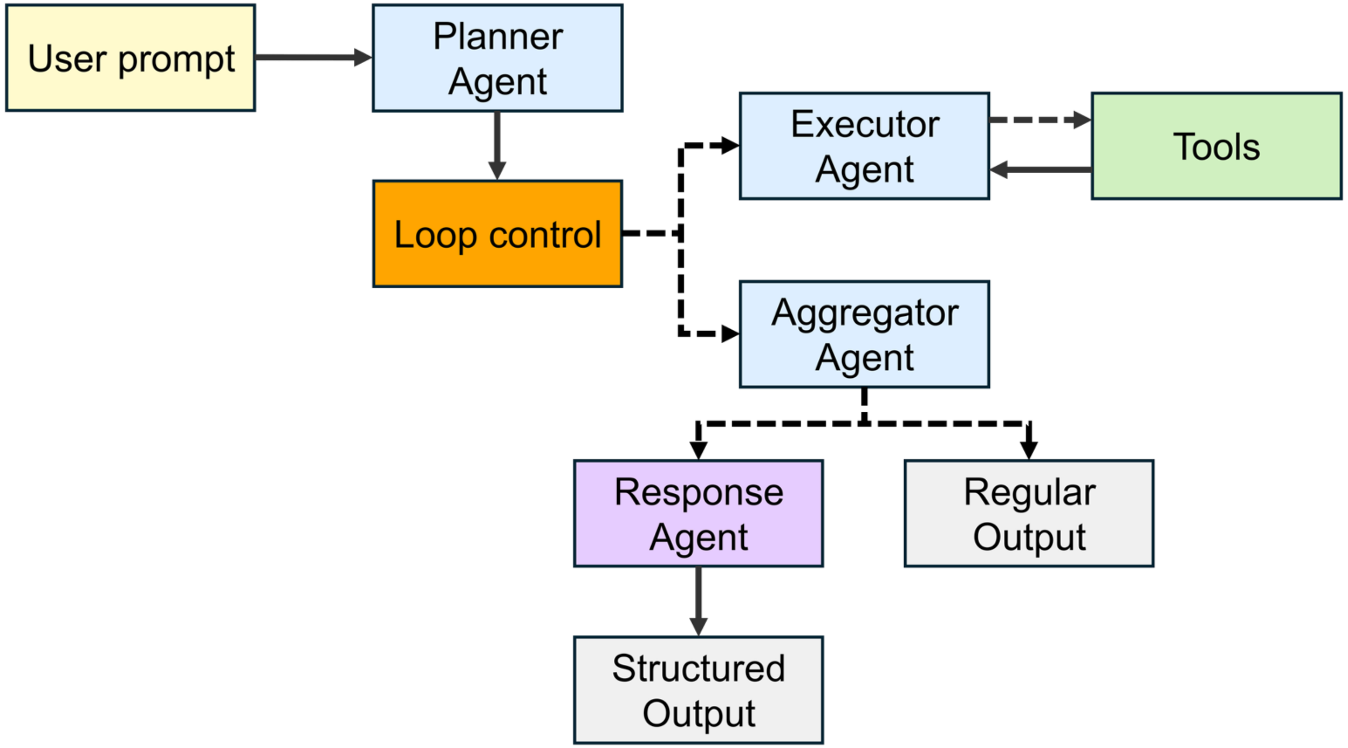
[…]

Agentic Workflows for Science

- Agentic workflows allow scientists to go beyond the "chat-bot" use of LLMs for question and answer
- They combine the power of gen-AI with computational science tools, research databases and HPC



ChemGraph: An Agentic Framework for Computational Chemistry Workflows



Software suite

ASE, RDKit (Open-Source Cheminformatics and Machine Learning), PubChem, xTB, NWCHEM (HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE), mace, FAIR Chemistry V2

ChemGraph: An Agentic Framework for Computational Chemistry Workflows. (2025)
Pham, T. D.; Tanikanti, A.; Keçeli, M. Under review. https://arxiv.org/abs/2506.06363

ChemGraph: Providing Accurate SMILES strings

Human

Provide the SMILES string corresponding to this molecule: 9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine

LLMs (with GPT-4o)

The molecule **9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine** has the following structure components:

- A **purine** core
- Substitution at position 9: a **(2,6-dichlorophenyl)methyl** group
- Substitution at position 6: an **amino group**
- That **amino group** is further substituted with a **furan-2-ylmethyl** group

Constructed SMILES:

Clc1cccc(Cl)c1CN2c3nc(nc(NCC4=CC=CO4)c3nc2)N

Incorrect

[…]

ChemGraph (with GPT-4o-mini)

Tool Call:

Tool name: molecule_name_to_smiles

Args: 9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine

Output:

"C1=CC(=C(C(=C1)Cl)CN2C=NC3=C(N=CN=C32)NCC4=CC=CO4)Cl”

The SMILES string corresponding to the molecule "9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine" is

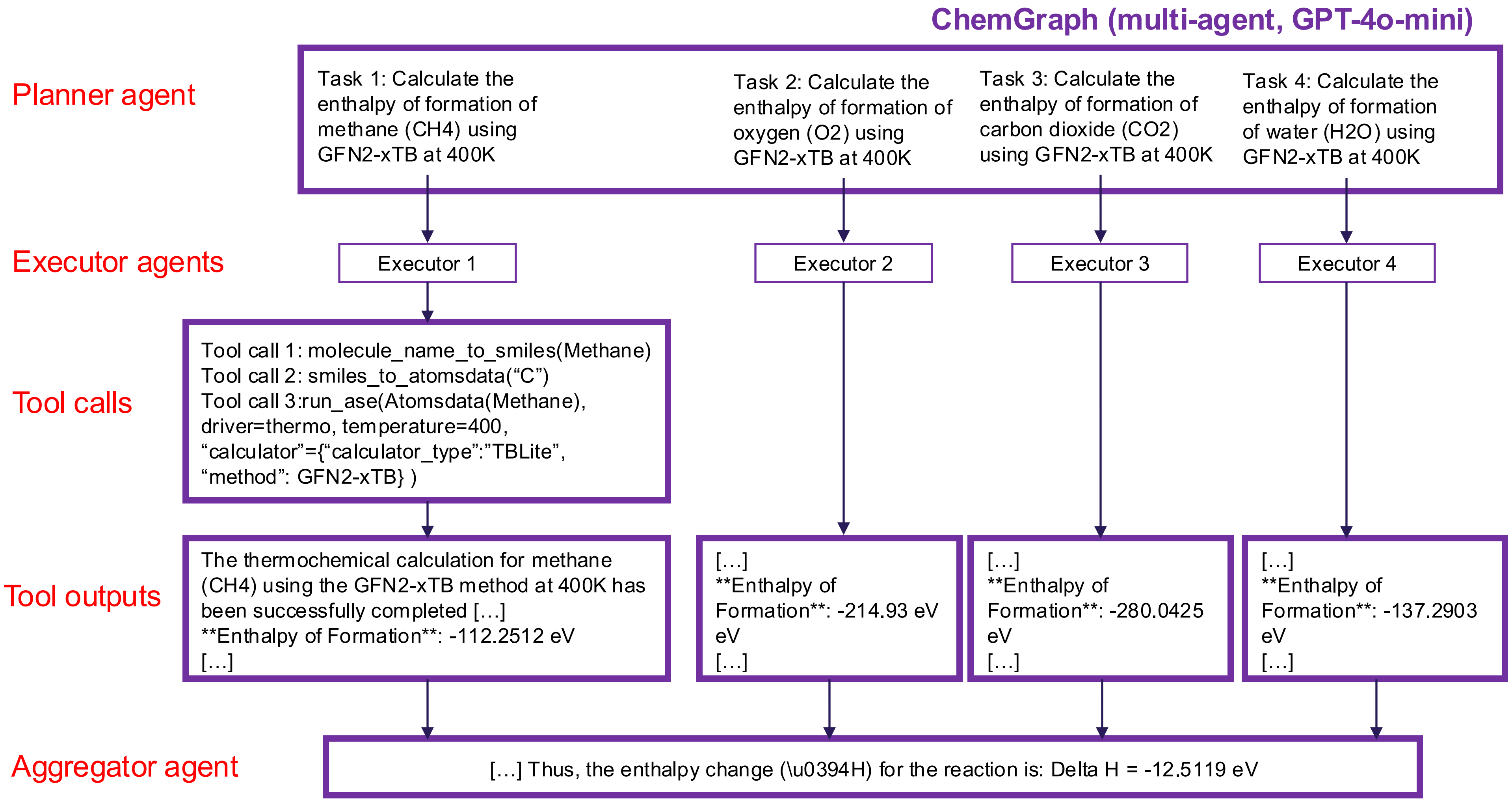
C1=CC(=C(C(=C1)Cl)CN2C=NC3=C(N=CN=C32)NCC4=CC=CO4)Cl

Correct

ChemGraph: Calculating Reaction Enthalpy

Human

You are given a chemical reaction: 1 (Methane) + 2 (Oxygen) -> 1 (Carbon dioxide) + 2 (Water). Calculate the enthalpy change for this reaction using GFN2-xTB at 400K.



ChemGraph (multi-agent, GPT-4o-mini)

Planner agent

Task 1: Calculate the enthalpy of formation of methane (CH4) using GFN2-xTB at 400K

Task 2: Calculate the enthalpy of formation of oxygen (O2) using GFN2-xTB at 400K

Task 3: Calculate the enthalpy of formation of carbon dioxide (CO2) using GFN2-xTB at 400K

Task 4: Calculate the enthalpy of formation of water (H2O) using GFN2-xTB at 400K

Executor agents

Executor 1

Executor 2

Executor 3

Executor 4

Tool calls

Tool call 1: molecule_name_to_smiles(Methane)
Tool call 2: smiles_to_atomsdata(“C”)
Tool call 3:run_ase(Atomsdata(Methane), driver=thermo, temperature=400, “calculator”={“calculator_type”:”TBLite”, “method”: GFN2-xTB})

Tool outputs

The thermochemical calculation for methane (CH4) using the GFN2-xTB method at 400K has been successfully completed […]
Enthalpy of Formation: -112.2512 eV
[…]

[…]
Enthalpy of Formation: -214.93 eV
[…]

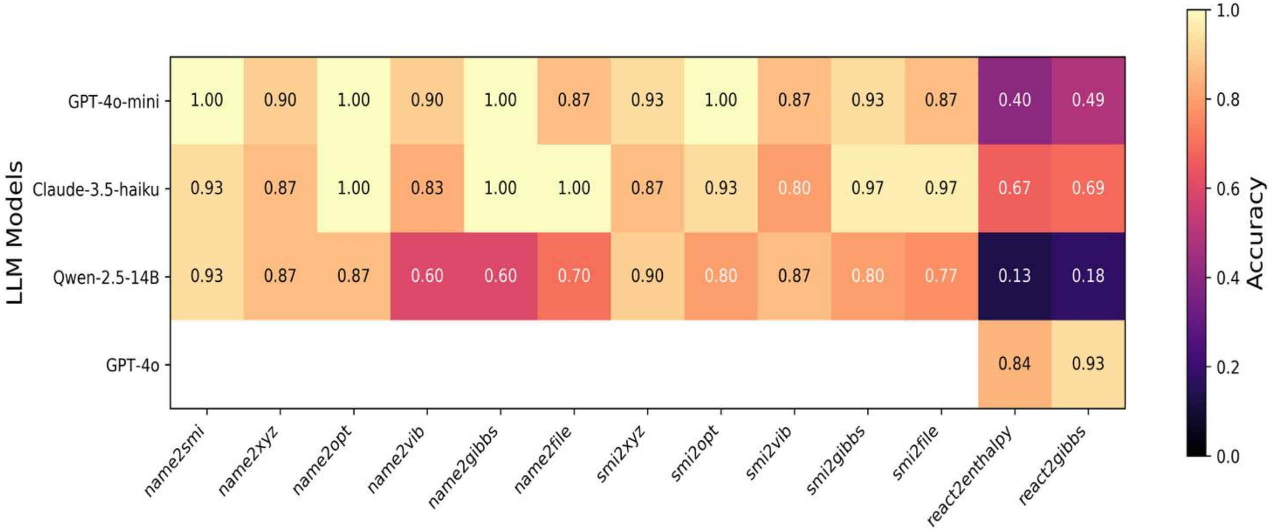
[…]
Enthalpy of Formation: -280.0425 eV
[…]

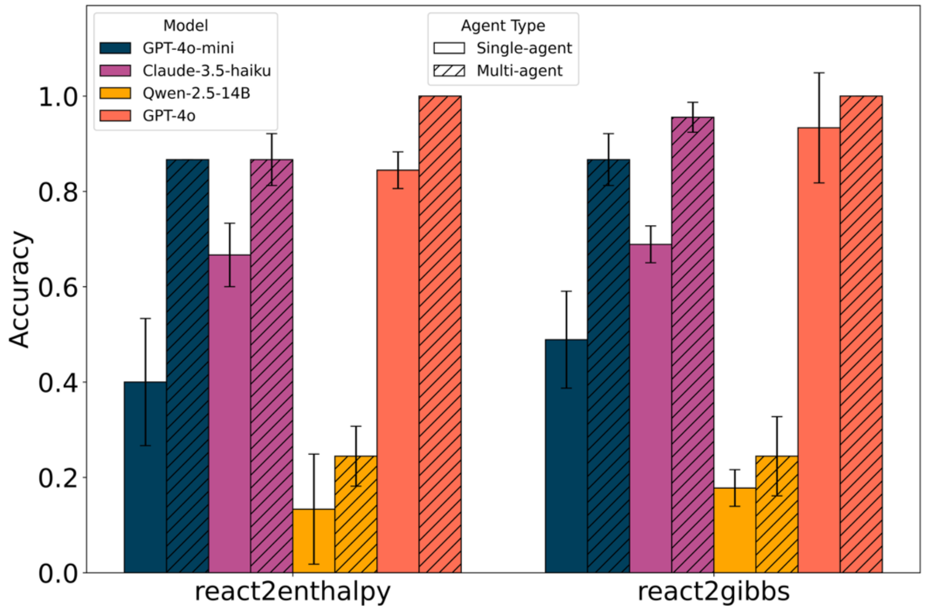
[…]
Enthalpy of Formation: -137.2903 eV
[…]

Aggregator agent

[…] Thus, the enthalpy change (\u0394H) for the reaction is: Delta H = -12.5119 eV

ChemGraph: Performance Across Task Complexity





Evaluation done on 13 different tasks, covering 360 instances and 200+ different molecules.

- Small language models (LLMs) are highly effective for simple, well-defined tasks.
- However, single-agent performance declines as task complexity increases.
- Multi-agent enables reaching higher accuracy even with small LLMs.

- ChemGraph UI provides a chatbot-style interface, where you can visualize results, molecular structures, vibrational modes, IR spectra, etc.
- You can run ChemGraph locally or on ALCF supercomputers.
- ChemGraph is open-source and available on GitHub

https://github.com/argonne-lcf/ChemGraph

Agentic Workflows at ALCF

- Users can leverage ALCF systems to accelerate scientific agentic workflows with our HPC resources
- Public GitHub with examples: https://github.com/argonne-lcf/alcf-agentics-workflow

Multi-system (Remote) Workflows

- Agents run and launch components on various ALCF or local systems
- LLMs served remotely (e.g., ALCF Inference Service)
- Pros:
    - Lower implementation complexity
    - Can leverage ALCF services
    - Target specific system with each computational component (efficient use of allocation)
    - Better support for long-running workflows (agents can run on local system)
- Cons:
    - Higher latency between tasks
    - Subject to scheduler when launching tasks

Single-system (Local) Workflows

- All agents and components of the workflow run on the same system, even within same batch job
- LLMs served locally on system nodes
- Pros:
    - Lower latency between tasks
    - Not subject to scheduler when running tasks
- Cons:
    - Higher implementation complexity
    - Subject to queue limitations (e.g., max. run time)
    - May consume allocation inefficiently