Academy

Building Scalable Agentic Systems for Science

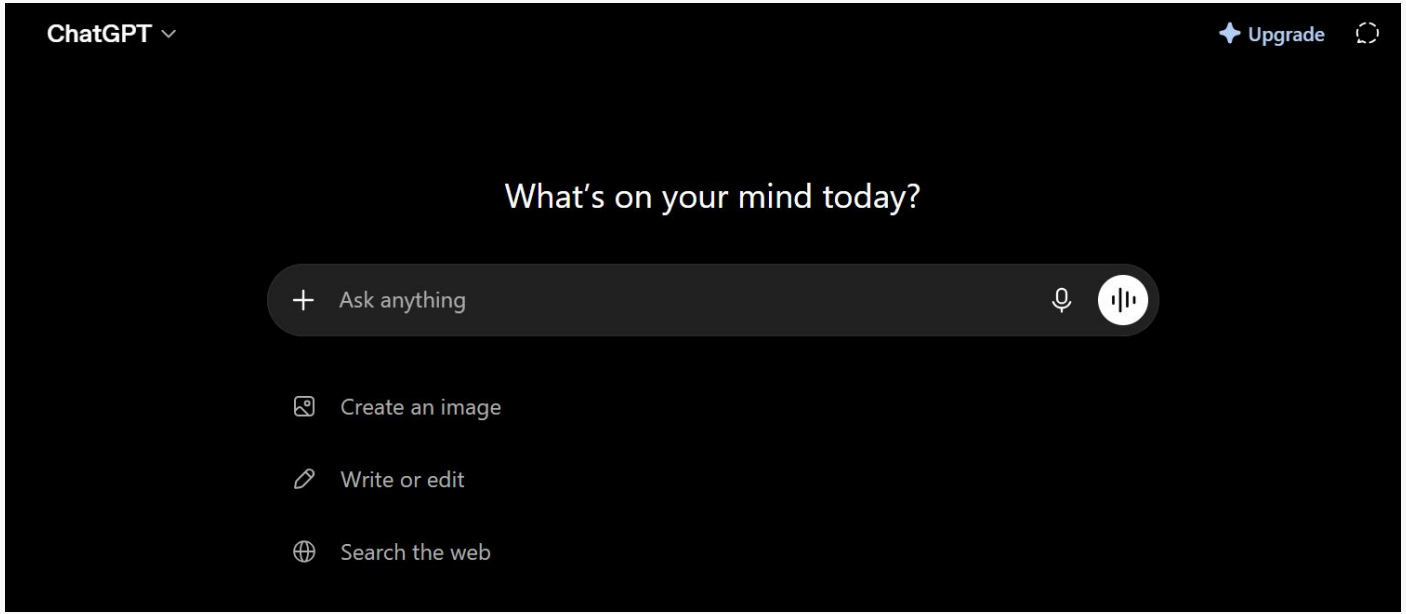
*Concepts, Architectures, and Hands-On with **Academy***

Kyle Chard
chard@uchicago.edu

github.com/academy-agents/academy-tutorial

Large language models

Traditionally an LLM call is stateless: one question → one answer



What is an “agent”?

- In artificial intelligence (AI), an “intelligent agent” is [Wikipedia] “**an entity that perceives its environment, takes actions autonomously to achieve goals, and may improve its performance through machine learning or by acquiring knowledge**”
  - An AI component, sensors, actuators, memory

→ Agents decide what to do next based on what they observe rather than what they were asked

- Reason across multiple steps, take actions, and respond to results

See also: https://gist.github.com/simonw/beaa5f90133b30724c5cc1c4008d0654

ReAct (Reason and Act) Agents

- An agent is given a question and a set of tools: *“Compute primes < 500”*
- It reasons about what to do: *"To answer this I need to call the* `compute_primes` *tool"*
- It acts: calls the tool and receives the result
- It reasons again: *"The result is 95, so my answer is 95 primes < 500"*
- This loop repeats until the agent decides it has enough information to answer
- Simple, effective, and the foundation of most LLM agent frameworks

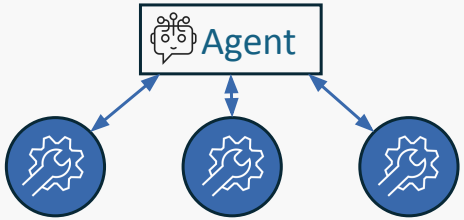
More general: the “sense-plan-act-learn” loop

- Initialize state and goals
- Repeat until termination:
  - **Sense**: Gather observations from environment
  - **Plan**: Evaluate goals and state, plan/select next action
  - **Act**: Execute chosen action on environment
  - **Learn**: Update internal state, memory, or model based on outcomes

Many agentic frameworks

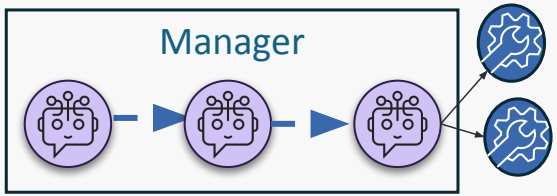
Common agentic patterns: **Coordinators**, **workflows**, **federated agent networks**

Coordinator



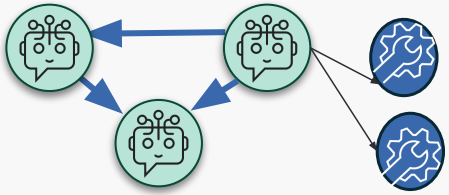
- One reasoning "brain" holds full context and decides the next action at each step
- Tools invoked on demand
- Control flow is decided dynamically based on intermediate results
- Simple to reason about

Workflows / chains



- Specialized agents/nodes, each with a defined role, connected via a DAG
- Control flow (mostly) defined in advance, with conditional edges for branching
- Enables parallelism and separation of concerns (planner, retriever, critic, etc.)

Federated Networks



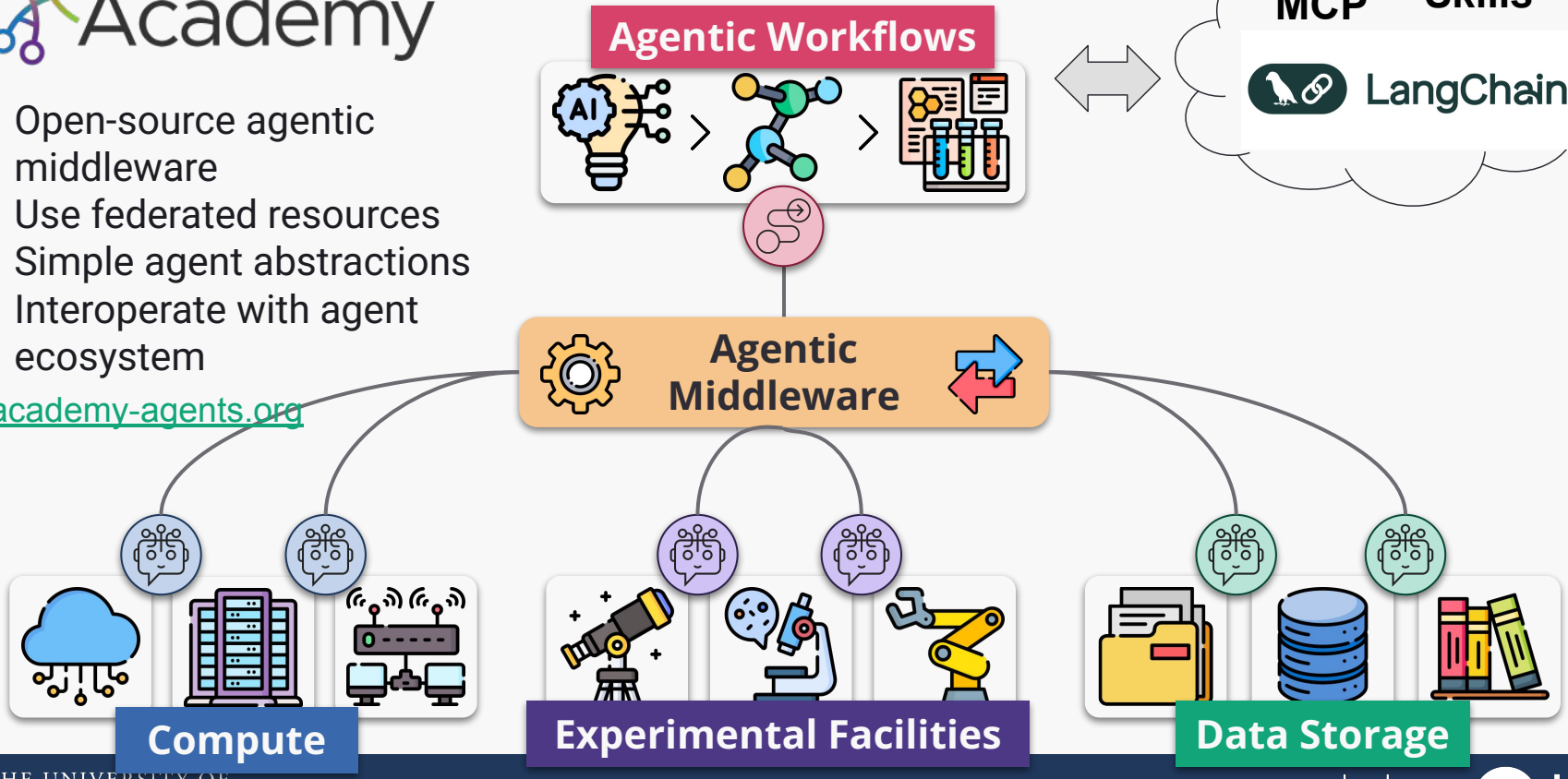
- Agents distributed across infrastructure domains
- Coordination via message-passing or shared protocols rather than a central scheduler
- Naturally fault-tolerant and scalable, but debugging and reproducibility

Deploying and managing agents across the computing continuum

Academy

- Open-source agentic middleware
- Use federated resources
- Simple agent abstractions
- Interoperate with agent ecosystem

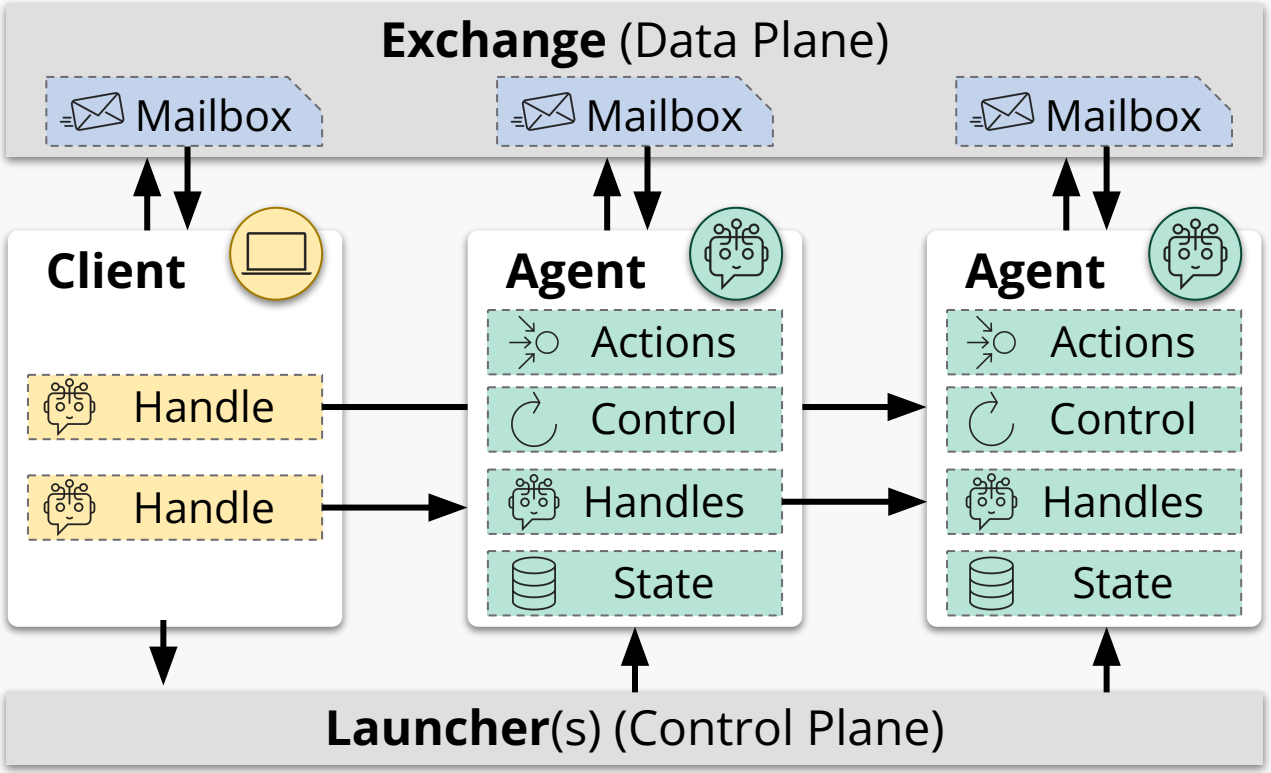
www.academy-agents.org



Focus 3: Coordinate async agent messaging

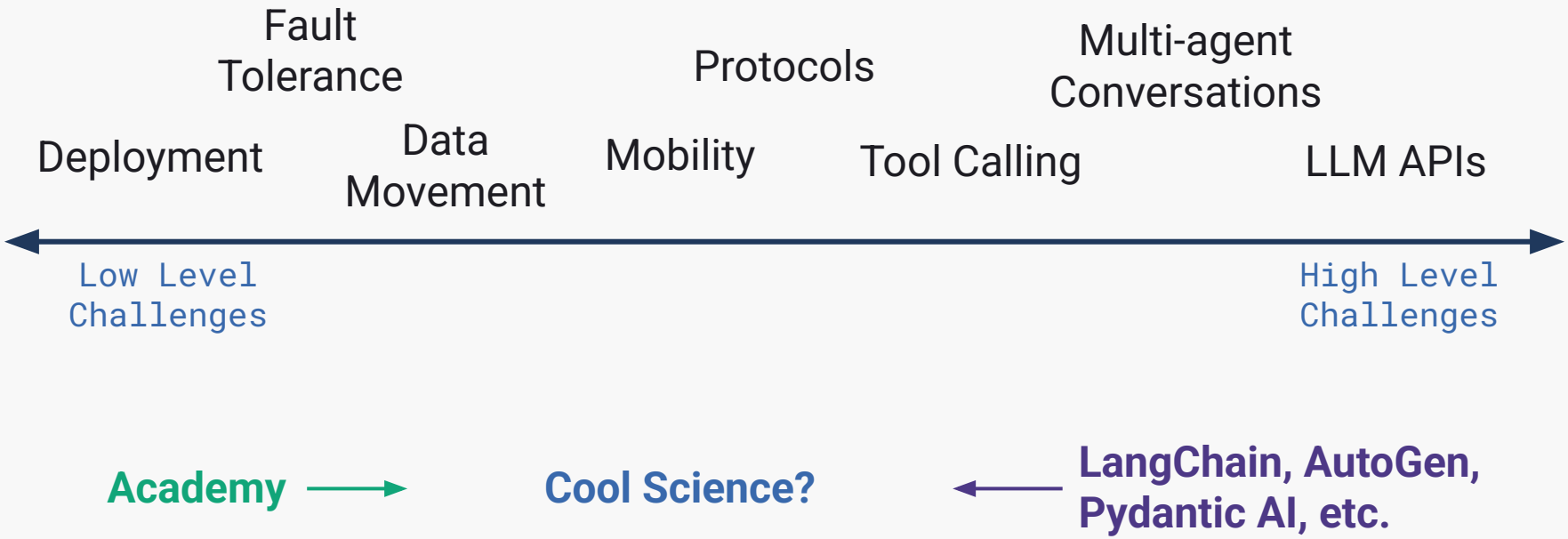
Focus 1: Program diverse agents and interactions

Focus 2: Deploy agents on federated resources



https://docs.academy-agents.org/latest/concepts/

Agentic Middleware: Scope & Challenges

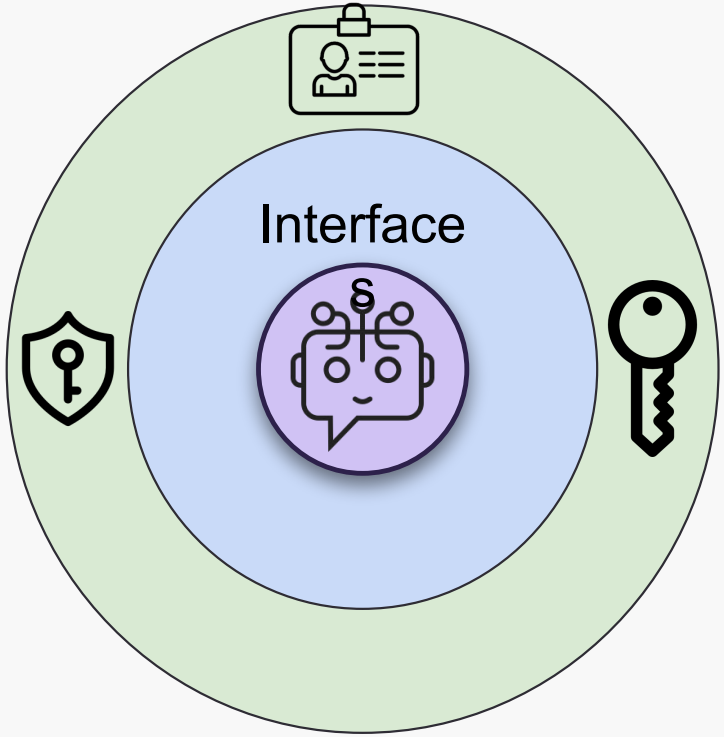


Anatomy of an Academy agent

Core agent code (local or remote LLM, interface to prompt, interpret responses)

Wrapped with a set of interfaces that enable deployment, lifecycle management, communication, etc…

Wrapped with a unique identity and permissions/tokens to perform a set of authorized actions



https://github.com/academy-agents/atpesc-tutorial

Hands-on Tutorial

Checkout the tutorial repo

```
$ git clone https://github.com/academy-agents/atpesc-tutorial
$ cd atpesc-tutorial
```

Install dependencies in a virtual environment

Native

```
$ python -m venv venv
$ source venv/bin/activate
```

Conda

```
$ conda create -n academy python=3.13
$ conda activate academy
```

UV

```
$ uv venv --python 3.13
$ source .venv/bin/activate
```

Start Jupyter

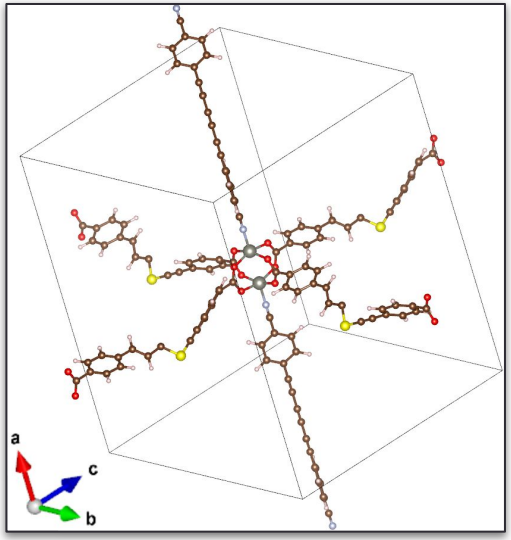
```
$ pip install jupyter
$ jupyter lab
```

Use Case: **MOF Discovery**

Metal Organic Frameworks (MOF)

- ➔ Composed of organic molecules (ligands) and inorganic metals (nodes)
- ➔ The sponges of materials science!
- ➔ Porous structures that adsorb and store gases
- ➔ Topologies can be optimized for targeted gas storage → **Carbon Capture**

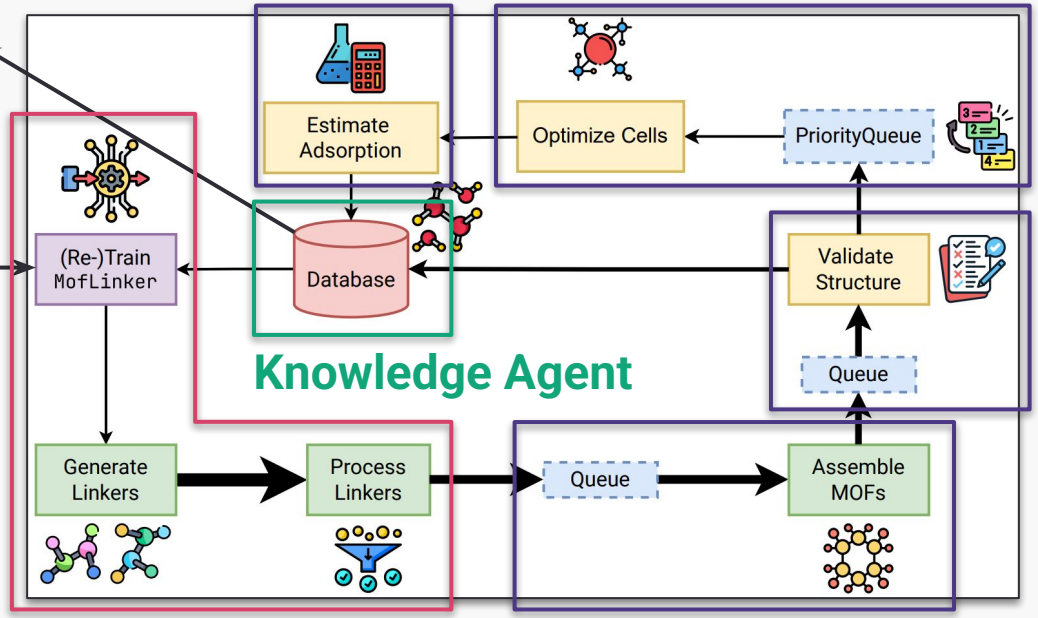
How to efficiently discover MOFs with desirable properties for target applications?



Intractable search space of ligand, node, & geometry combinations

MOFA: Online learning + GenAI + Simulation

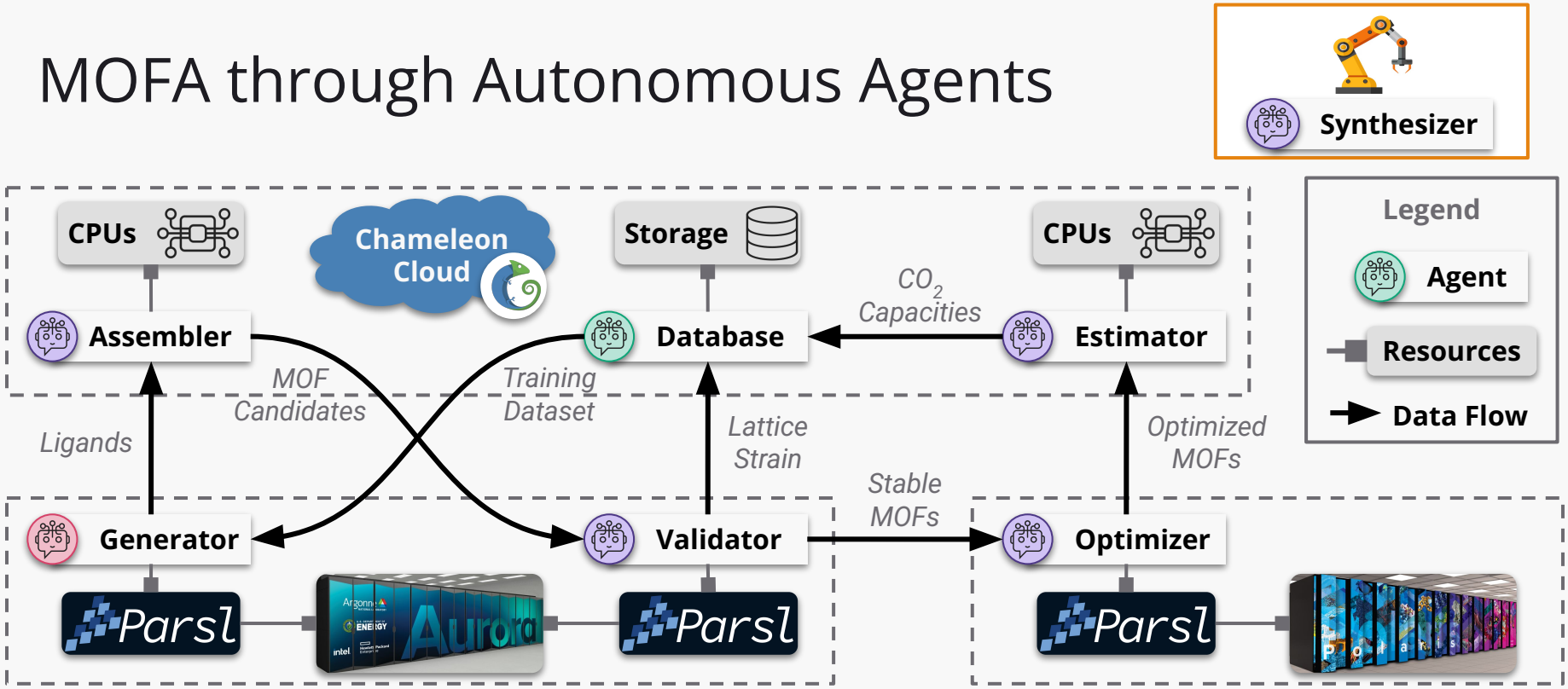
Embodied Agents*



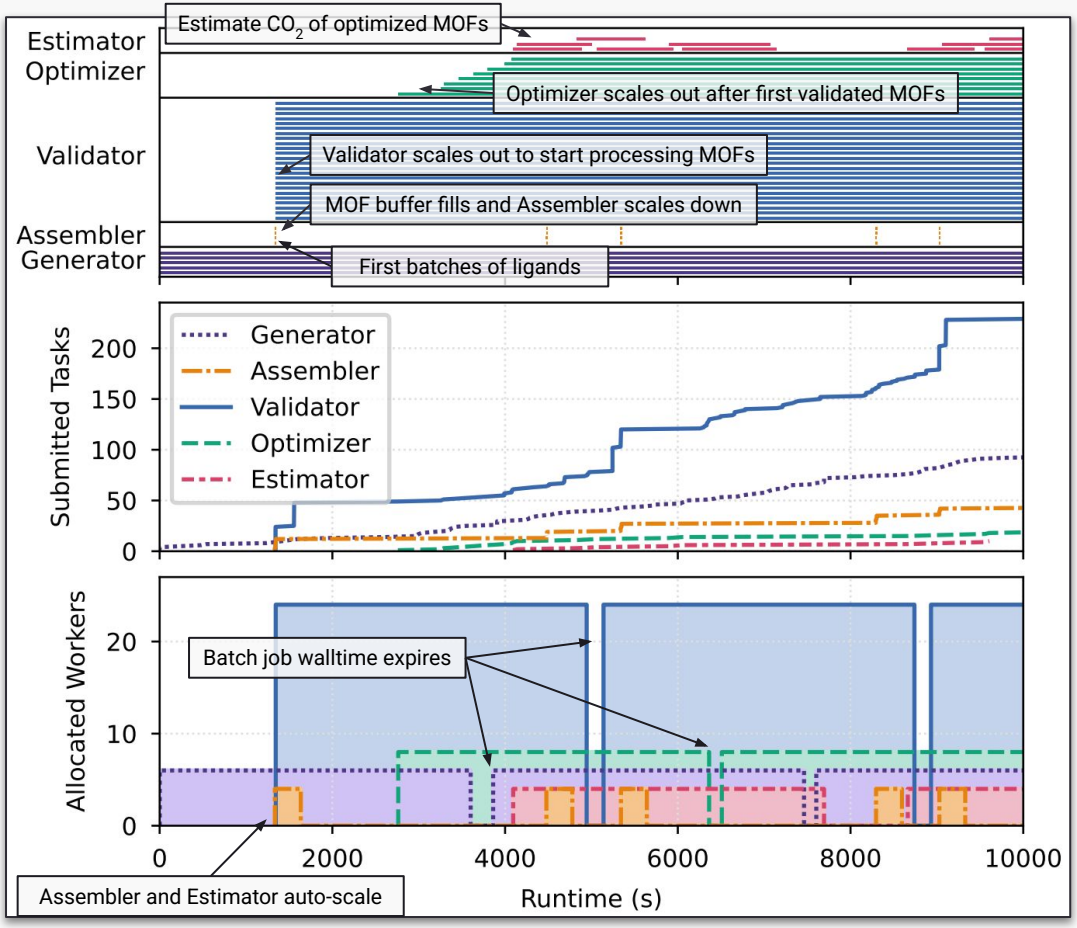
Computational Agents

Yan et al., "**MOFA: Discovering Materials for Carbon Capture with a GenAI- and Simulation-Based Workflow**" (Under Review)

MOFA through Autonomous Agents



Agents executed remotely via Globus Compute



MOFA Agents Trace

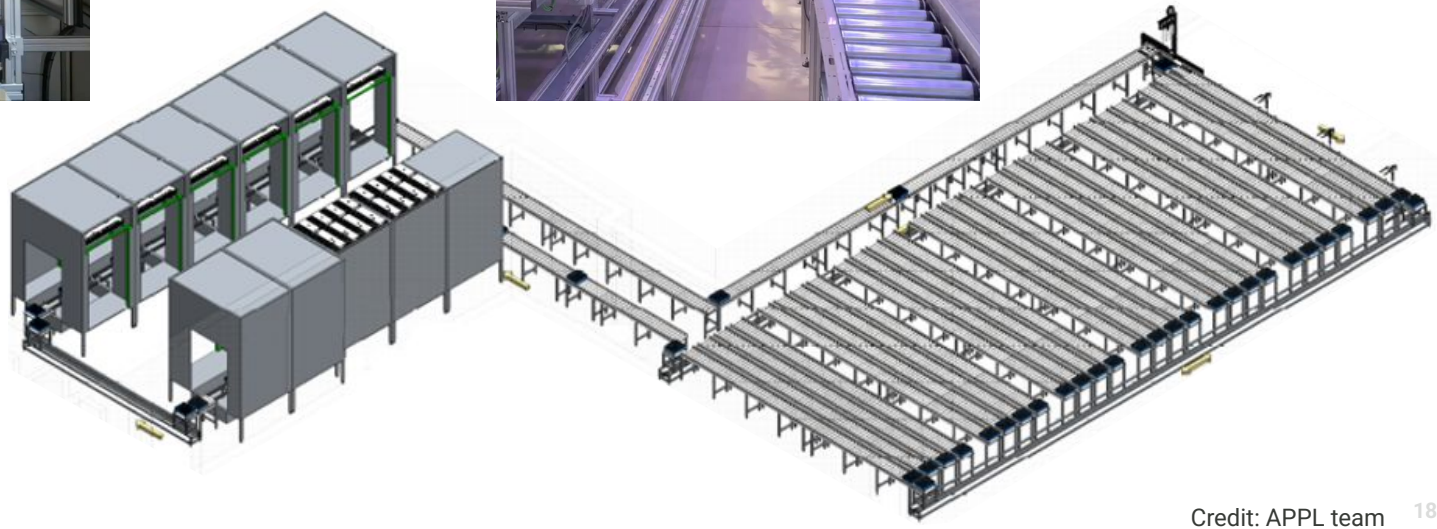
Why is this agentic model better?

- ➔ **Placement:** Move agents to resources
- ➔ **Separation of concerns:** Resource acquisition and scaling based on local workload
- ➔ **Loose coupling:** Swap agents or integrate new agents (e.g., SDL)
- ➔ **Shared agents:** Multiple workflows can share agents (microservice-like)

APPL is an automated 520-tray conveyor system that continually monitors plants using multimodal imaging.

Buffer

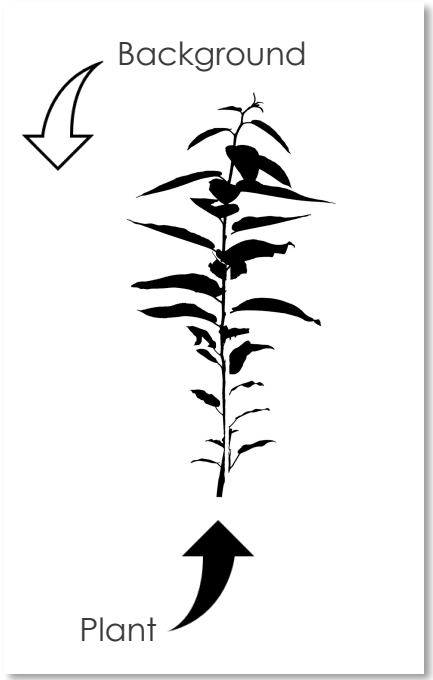
Imaging loop

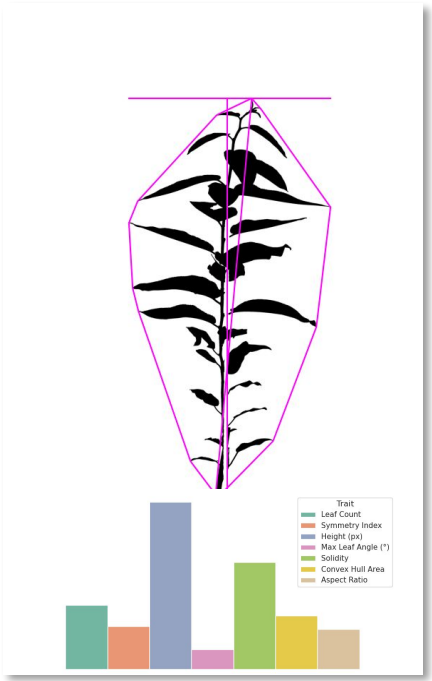


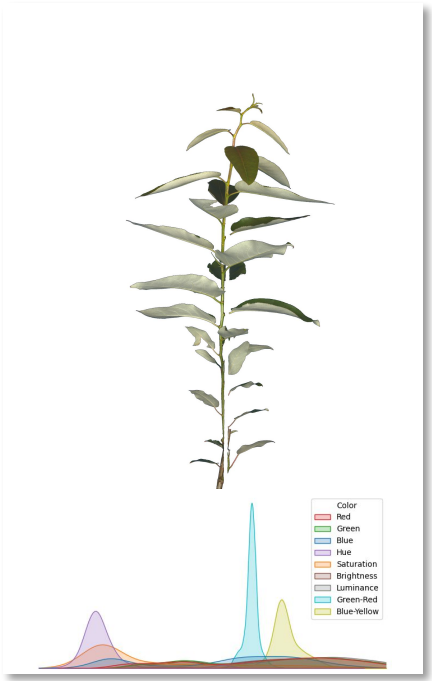
Credit: APPL team

Accurate image segmentation enables prediction of complex plant phenotypes

Original → Segmentation → Morphology → Spectral traits







Credit: APPL team

Daniel Rosendo

Renan Souza

Scientist

Genesis Mission
Platform Deployment for OPAL

Cloud

Model Services
Model Catalog

Intelligent Int.
LiteLLM Inference

i2 Auth
Globus / Google

Metadata Services
Data lakehouse

S3M

Co-pilot Agent
Academy

Chat UI
Chainlit

Provenance Service
Flowcept

Kubernetes cluster

aws

OLCF

ViT inference
Parsl

Compute Agent
Academy

Compute node

Login node

Lustre filesystem

APPL

Plant images + experiment metadata

Platform

Legend

APPL components

Frontier

AmSC services

AWS services

Demo video
https://www.youtube.com/watch?v=7szA15ncDx0

Credit: APPL team

AI-Enabled Integrated Enabled Intelligence System for the WHO African Region

World Health Organization
REGIONAL OFFICE FOR Africa

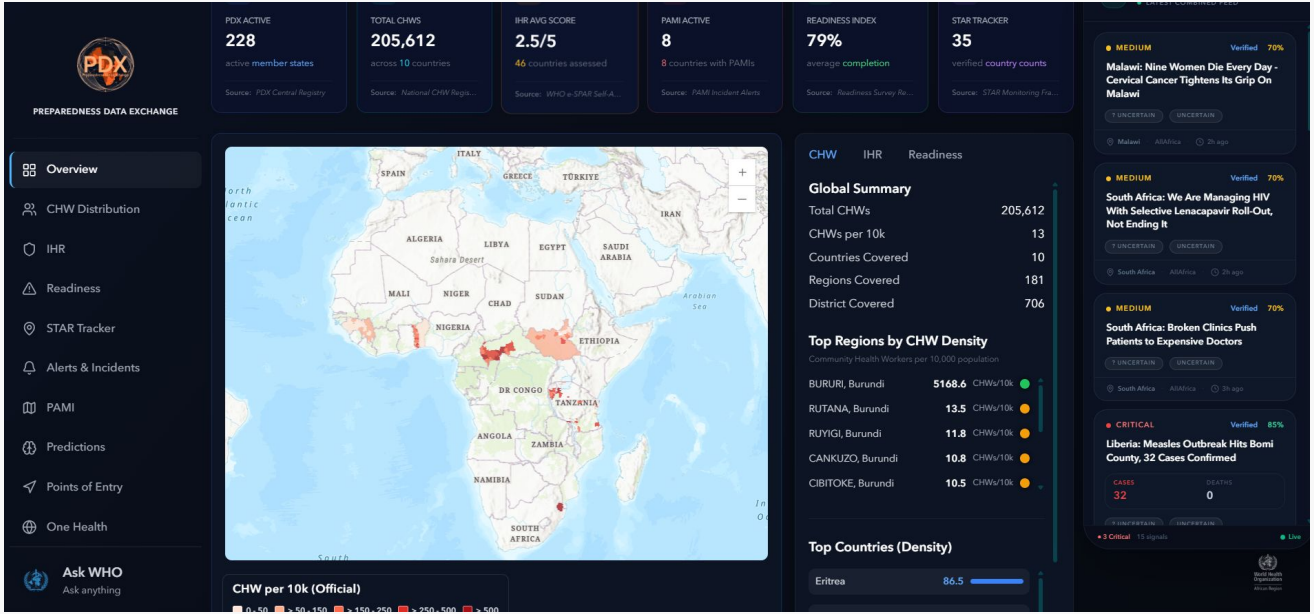
Credit: Isaias Fernandes

Preparedness data exchange aggregates and monitors regional data sources in near real time

Academy agents continuously analyze signals and triggers actions (e.g., notifications to public health workers, policymakers, WHO)

Enables **proactive response and coordination** through automated insights and alerts

Supports **local deployment** to ensure compliance with data sovereignty and governance requirements



The Future? The Scientific Method through Agents

Pauloski, Chard and Foster, "Agentic Discovery: Closing the Loop With Cooperative Agents," in *Computer*,. 2025, doi: 10.1109/MC.2025.3575029.

Questions?