OAK RIDGE National Laboratory

The Agentic Revolution: Lightning Sessions on Agentic Workflows

The (R)evolution of Scientific Workflows in the Agentic AI Era: Towards Autonomous Science

SC25 - WORKS25 Paper

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Workflows Community Talks

Woong Shin, Renan Souza, Daniel Rosendo, Frédéric Suter, Feiyi Wang, Prasanna Balaprakash, Rafael Ferreira da Silva

U.S. DEPARTMENT OF ENERGY

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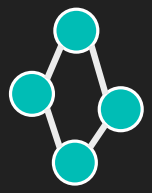
The Vision with Agentic AI in Workflows
"Autonomous Science"

Current State



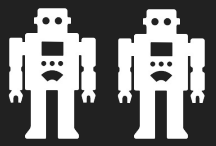
Static DAGs

Manual Coord.

Months per Cycle

Human Bottleneck

Future State



Intelligent Agents

Autonomous Coord.

Hours per Cycle

Continuous

10~100x Discovery Acceleration

How do we Get There?

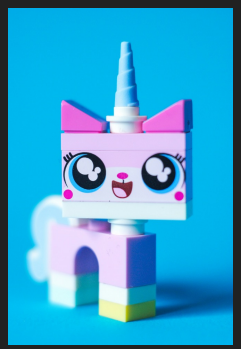
Scientific Workflows in the Agentic AI Era

How does AI interplay with existing workflows?

What about traditional machine learning techniques?

What are we supposed to do? Ditch the 20-year infrastructure?

Fatigue



Fiercely Optimistic

Fiercely Optimistic

But…

Workflows and AI Agents share the same DNA!

Agentic AI is merely an evolutionary extension!

We can do this!

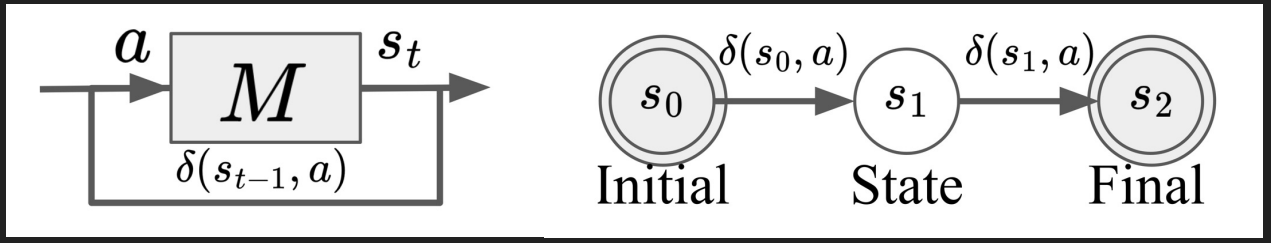
Fierce Optimism: Autonomous Science is an Evolution
Not a … *cough cough* … Revolution

Shared DNA: Computational Structure

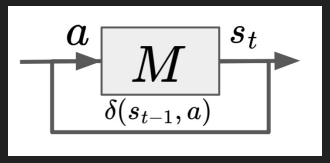
Scientific Workflows	AI Agents
States (task, data)	**States** (context, mem)
Transitions (deps.)	**Transitions** (actions)
Control **logic** (rules)	Decision **logic** (policy)

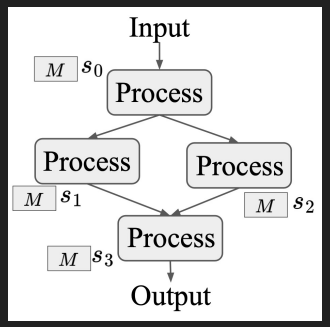
Common denominator – the State Machine

$$M = (S, \Sigma, \delta, s_0, F)$$



Shared DNA: Computational Structure



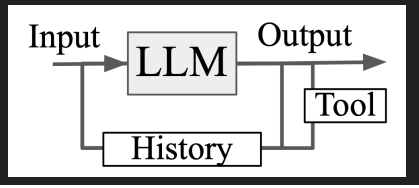


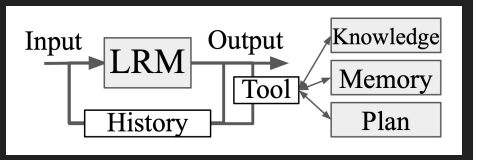
Scientific Workflows

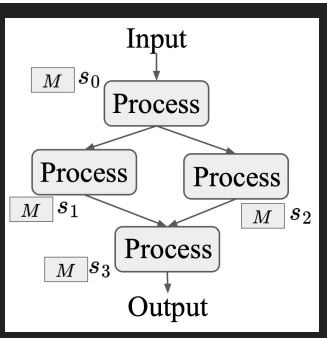
States (task, data)
Transitions (deps.)
Control **logic** (rules)

AI Agents

States (context, mem)
Transitions (actions)
Decision **logic** (policy)







Common denominator – the State Machine

Shared DNA: Computational Structure

Scientific Workflows

AI Agents

Shared foundation enabling systematic characterization of the evolution:

Dimension 1

Intelligence

How "smart" are the transitions?

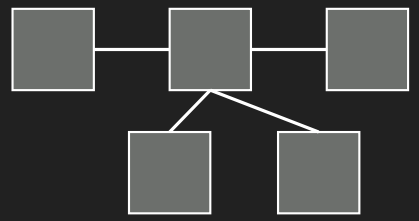
Dimension 2

Composition

How do they work together?

$$M = (S, \Sigma, \delta, s_0, F)$$

State Input **Transition** Initial Final



Evolution Framework

Shared foundation enabling systematic characterization of the evolution:

Progressive sophistication of the transition function

Intelligence

Static	Adaptive	Learning	Optimizing	Intelligent
$\delta : S \times \Sigma \to S$	$\delta : S \times \Sigma \times O \to S$	$\delta_{t+1} = L(\delta_t, H)$	$\delta^* = \arg\min_\delta J(\delta)$	$M' = \Omega(M, C, G)$

Progressive sophistication of coordination between entities

Composition

Single	Pipeline	Hierarchical	Mesh	Swarm
M	$M_1 \circ M_2 \circ \ldots \circ M_n$	$M_{mgr.}(M_1, M_2, \ldots, M_n)$	$\forall i, j : M_i \leftrightarrow M_j$	$M = \Phi(\{m_1, m_2, \ldots, m_n\})$

Evolution Framework

Shared foundation enabling systematic characterization of the evolution:

Intelligence

Composition

Details of each dimension in Table 1 & Table 2 in our paper

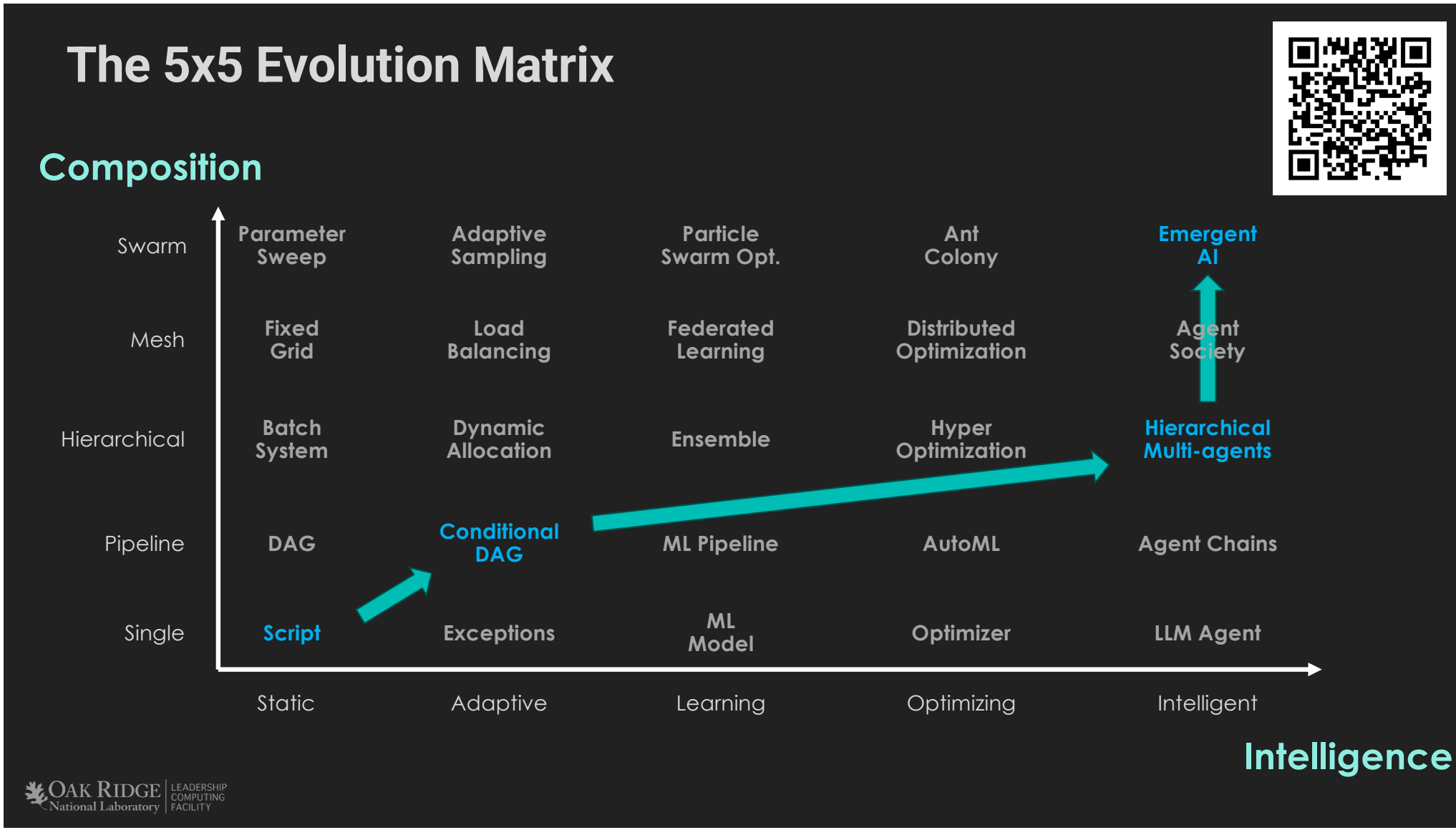
Table 1: The intelligence dimension

Dimension	Description
Static: $\delta : S \times \Sigma \to S$	Transition function depends solely on current state and input, implementing predetermined execution paths
Adaptive: $\delta : S \times \Sigma \times O \to S$	Extended with observations/feedback signals O enabling runtime adjustments and conditional branching
Learning: $\delta_{t+1} = L(\delta_t, H)$	Incorporates history through learning function L that updates transitions based on experience H
Optimizing: $\delta^* = \arg\min_\delta J(\delta)$	Seeks optimal behavior via cost function J, balancing exploration and exploitation
Intelligent: $M' = \Omega(M, C, G)$	Meta-optimization through operator Ω that can redefine states, transitions, and goals based on context

Table 2: The composition dimension

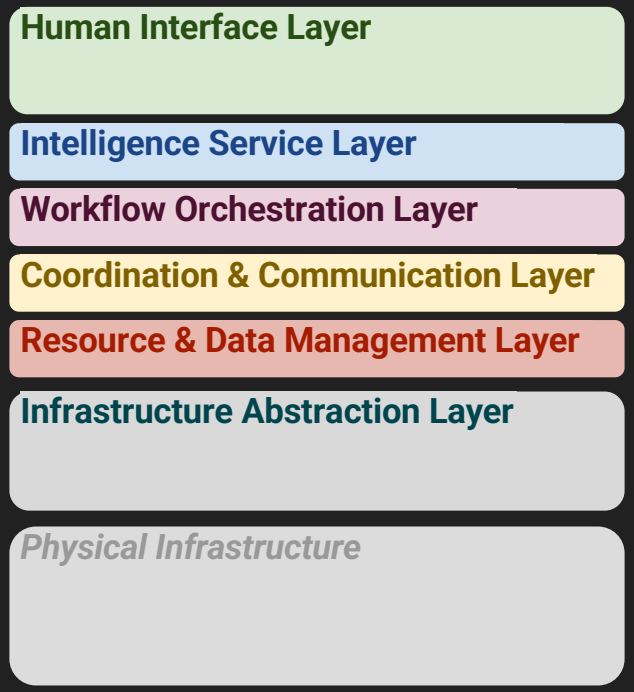
Dimension	Description
Single: M	One isolated machine with no coordination
Pipeline: $M_1 \circ M_2 \circ \ldots \circ M_n$	Sequential composition with unidirectional dataflow, enabling staged processing with clear dependencies
Hierarchical: $M_{mgr}.(M_1, M_2, \ldots, M_n)$	Manager structure implementing delegation and supervision with centralized control
Mesh: $\forall i, j : M_i \leftrightarrow M_j$	Full connectivity enabling peer-to-peer communication and collaborative problem-solving
Swarm: $M = \Phi(\{m_1, m_2, \ldots, m_n\})$	Emergent behavior through emergence operator Φ transforming local interactions into global behavior

The 5x5 Evolution Matrix

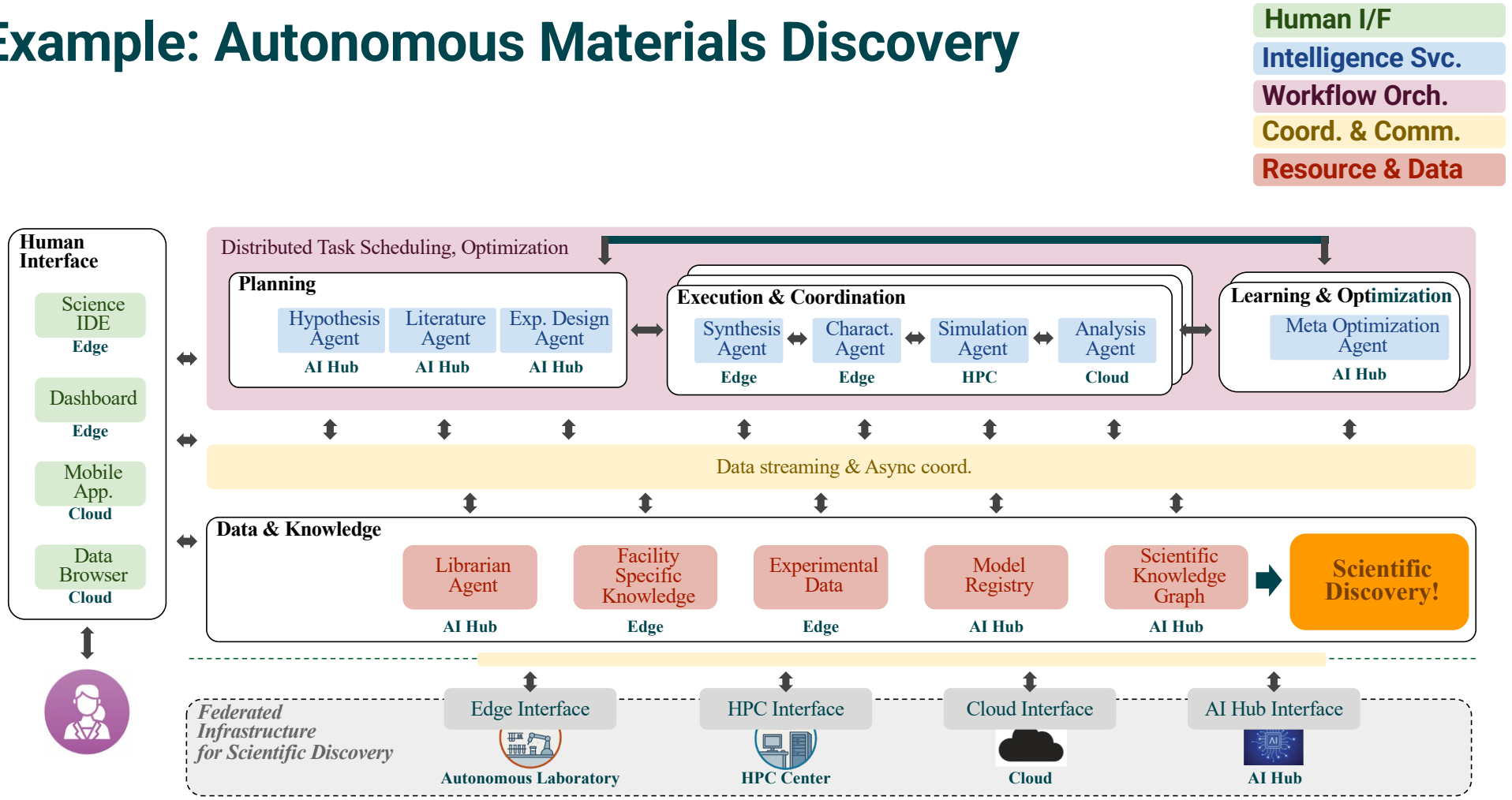


The 5x5 Evolution Matrix

Architectural Blueprint of this Evolutionary Path



Example: Autonomous Materials Discovery



Autonomous Science

The Revolution is Evolutionary

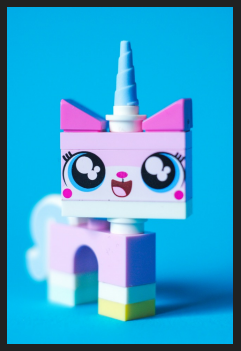
Autonomous Science

The Revolution is Evolutionary

Scientific Workflows

Fatigue

AI Agents



Fiercely Optimistic

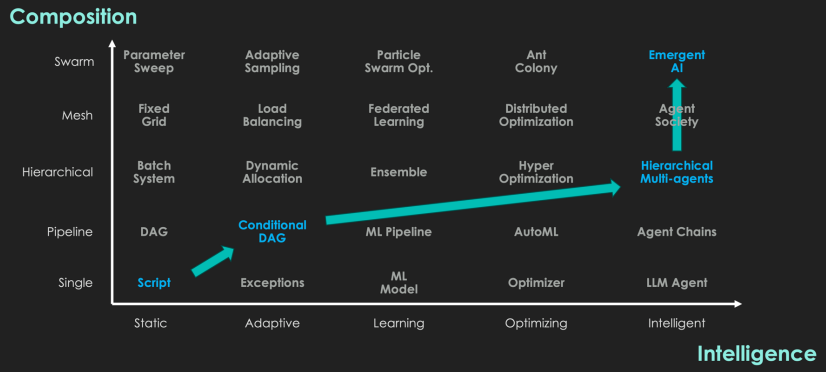
Autonomous Science

The Revolution is Evolutionary

Scientific Workflows

AI Agents

The 5x5 Evolution Matrix



Autonomous Science

The Revolution is Evolutionary

Scientific Workflows

Agentic AI

Nearer than we think!

Autonomous Science

The Revolution is Evolutionary

Scientific Workflows

Agentic AI

We are "the community" that can make this come true!

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Scientific Workflows

Agentic AI

Modularity, Communication, FAIR Partnership, Scientific Leadership +20 years of excellence

Autonomous Science

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Scientific Workflows

Agentic AI

Let's work together!

Autonomous Science

The Revolution is Evolutionary

Let’s work together!

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