Agentic-Al Assisted Research Workflow

Al for Scientific Discovery Participatory Design Workshop

Facilitated by
University of Washington
Scientific Software Engineering Center







Who we are



Niki Burggraf Senior RSE

Niki spent over 6 years at Amazon on its serverless compute offering, AWS Lambda, supporting several customer-facing feature launches by building and maintaining microservices on AWS.



Sarah Stone *Executive Director*

Sarah Stone is the Executive Director of the eScience Institute. Stone handles eScience operations and planning, develops research and training programs, participates in strategic planning, and serves as the primary contact for university and industry partners, funding agencies and the public.



Anant Mittal Senior RSE

Anant received his Ph.D. in Computer Science from UW focusing on Human-Computer Interaction, His dissertation work focused on designing and building systems for communication, collaboration, and coordination in complex settings like Accessibility and Health.



Don Setiawan *Principal RSE*

Don has been a research software engineer at UW for 8+ years contributing to open-source research software. Don has a background in Oceanography and Marine Technology. He is currently pursuing an MS in UW SET Tacoma.



Anshul Tambay *Technical PM*

Anshul brings experience in building infrastructure for research from his time as a Data Analyst at Northwestern University, where he studied community violence intervention programs.

Our Mission



eScience Institute empowers researchers and students in all fields to answer fundamental questions through the use of large, complex, and noisy data.



SSEC helps researchers create sustainable software solutions.

Stages of Data Science Lifecycle

Question

Defines research question



Discovery

Identify data source, extract, transform, load



Analysis

Investigate specific variables of interest

Sharing

Communicate results to community



Interpreting

Distill the results

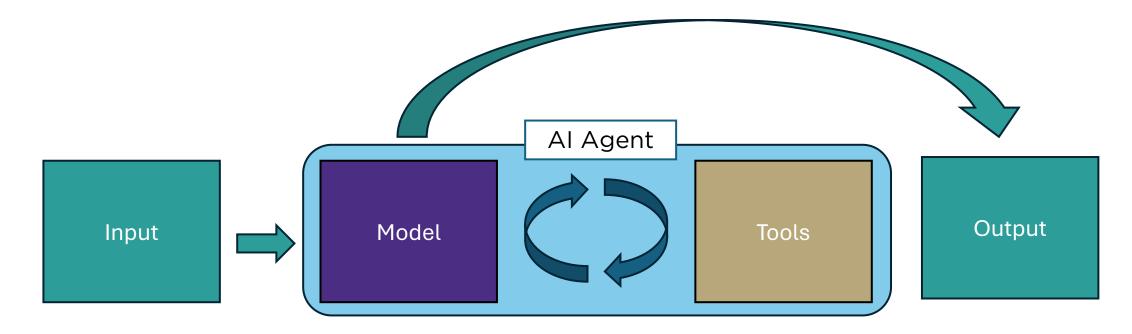


Modeling

Select, implements, and execute analytical tools

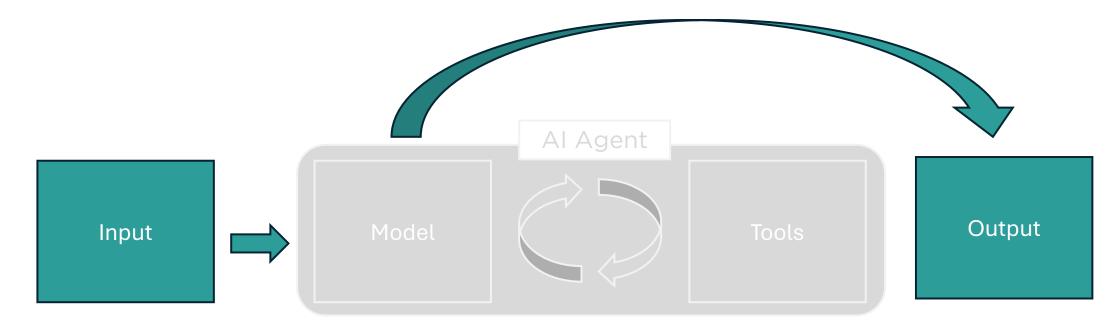
What is an Al Agent?

agent ≈ model + tools, within a loop + environment



Input and Output

agent ≈ model + tools, within a loop + environment

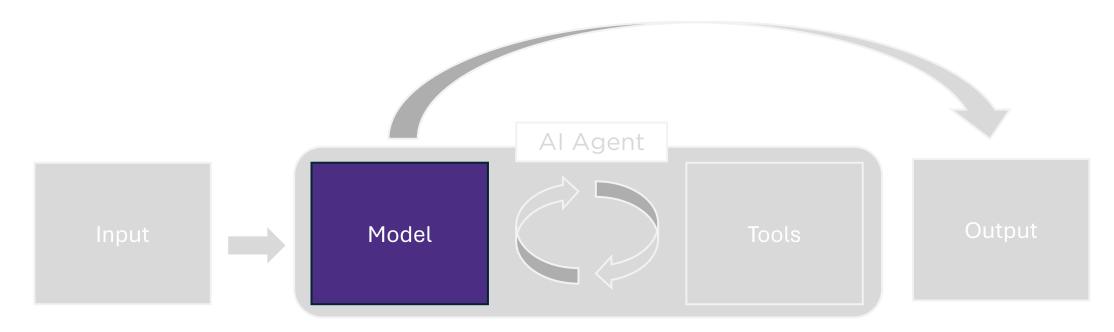


Input: The data input in the form of text, image, and/or videos, along with a set of instructions in natural language.

Output: The immutable results or outputs of the agent's work (e.g., a generated summary, a file, an image, or structured data)

Model (LLM)

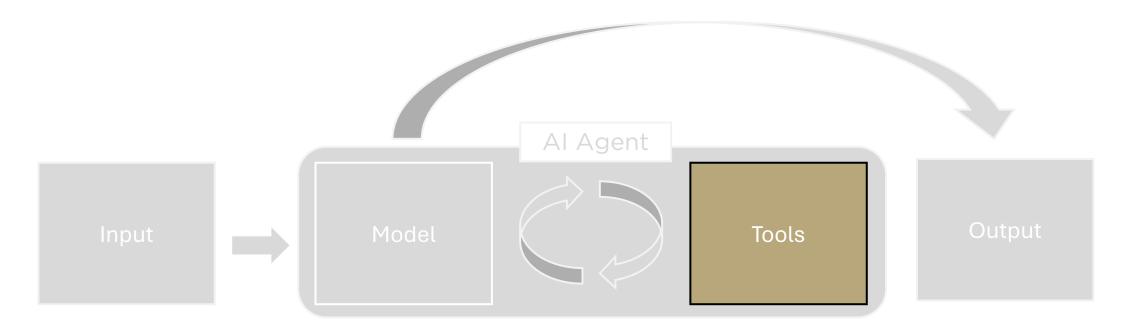
agent ≈ model + tools, within a loop + environment



Large Language Model is the brain of the whole system. **Examples: GPT-4.1, Claude Sonnet 4, Gemini 2.5 Pro, LLaMA 4, OLMo 2**.

Tools

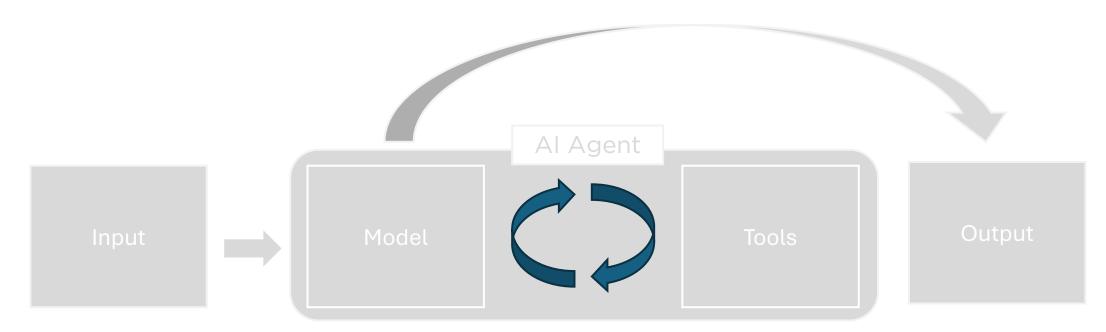
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All the software programs that an LLM can access and use. **Examples: Your data pipelines, "classic" ML models, database** access, and other web services.

Loop (MCP)

agent ≈ model + tools, within a loop + environment

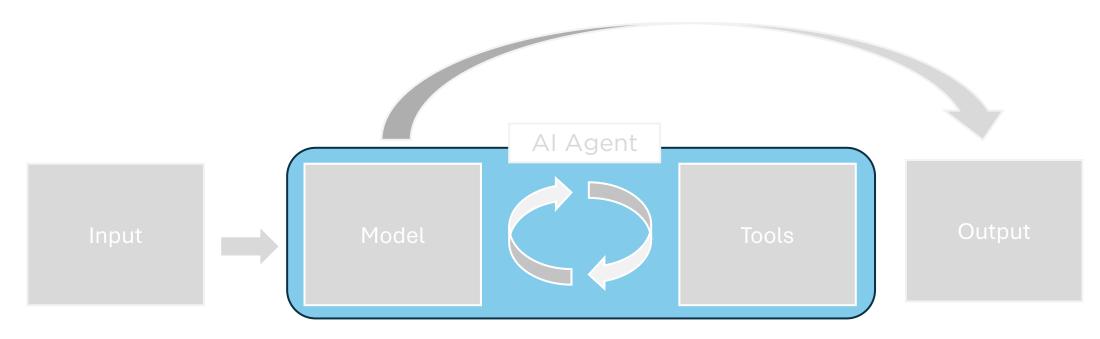


This is the action-and-feedback exchange between LLM and Tool usage. The LLM dynamically follow their own process and tool usage.

Example: The most common protocol for this communication is Model Context Protocol (MCP). https://modelcontextprotocol.io/.

Environment

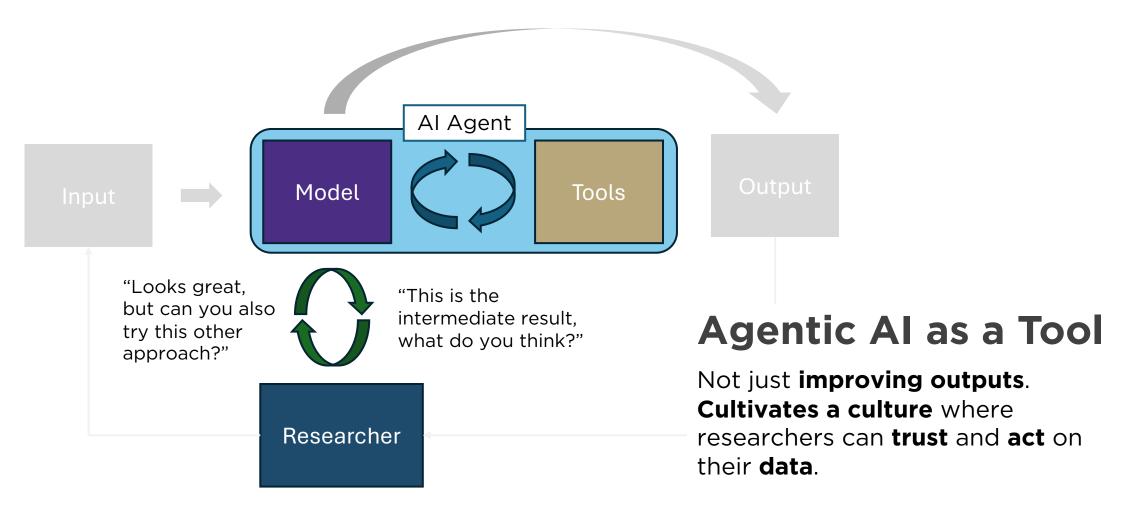
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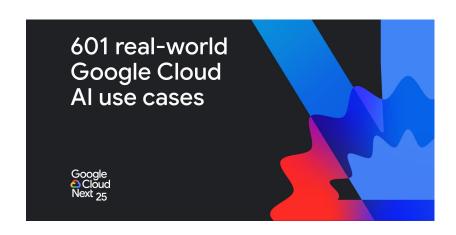
The runtime environment that supports the agent's operations.

Examples: Deployment Environment (Cloud vs On-premises), Security, Observability, Memory, Data Sources, Physical Environment, etc.

Our Goal: A balance of autonomy and human-in-the-loop



Agentic AI as a Tool How do we achieve this?



https://cloud.google.com/transform/1 01-real-world-generative-ai-usecases-from-industry-leaders



https://blogs.microsoft.com/blog/ 2025/04/22/https-blogs-microsoftcom-blog-2024-11-12-how-realworld-businesses-aretransforming-with-ai/

Agentic AI as a Tool How do we achieve this?

2025 Real-World
Agentic Al for
Science Use Cases



Where can we leverage Al Agent(s)?



Defines research question



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Source: https://ethos.academicdatascience.org/stages/

Some nuggets of wisdom

"Every **brilliant experiment**, like every great work of art, **starts** with an **act of imagination**."

Jonah Lehrer

"If you **want** to have **good ideas**, you must **have many ideas**." *Linus Pauling*

"Nothing in life is to be feared, it is only to be understood. Now is the time to understand more, so that we may fear less."

Marie Curie