Supporting Theory Simulations with Large Language Models

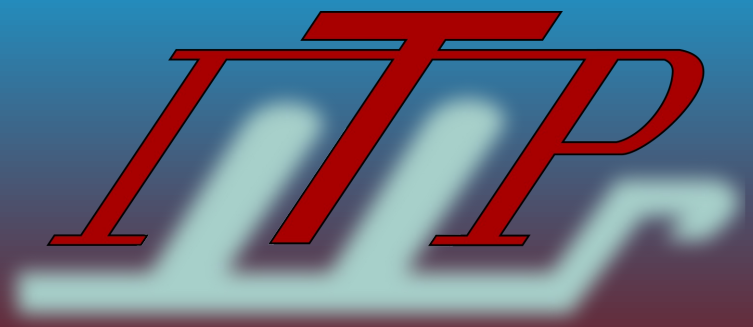
Daniel Schiller

15.05.2026, NPTwins, Trento

Based on **MadAgents** [arXiv:2601.21015]

With Tilman Plehn and Nikita Schmal



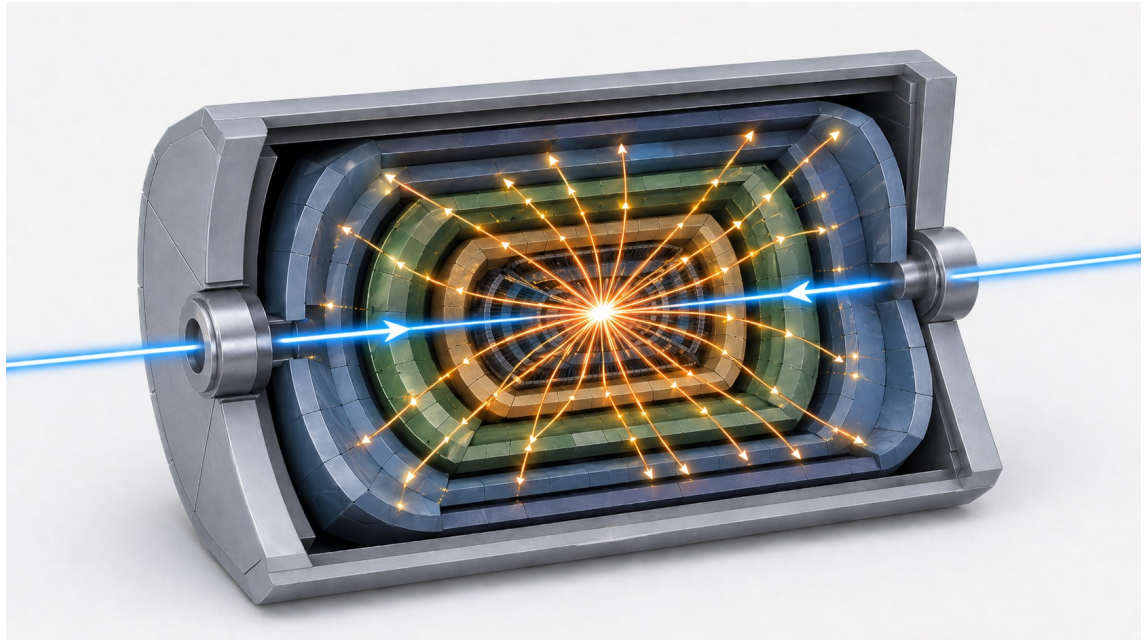




STRUCTURES
CLUSTER OF
EXCELLENCE

MadGraph

- Particle physics collider simulation
- Hard-scattering matrix-element generator
- Monte Carlo phase-space integrator



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- Hard-scattering matrix-element generator
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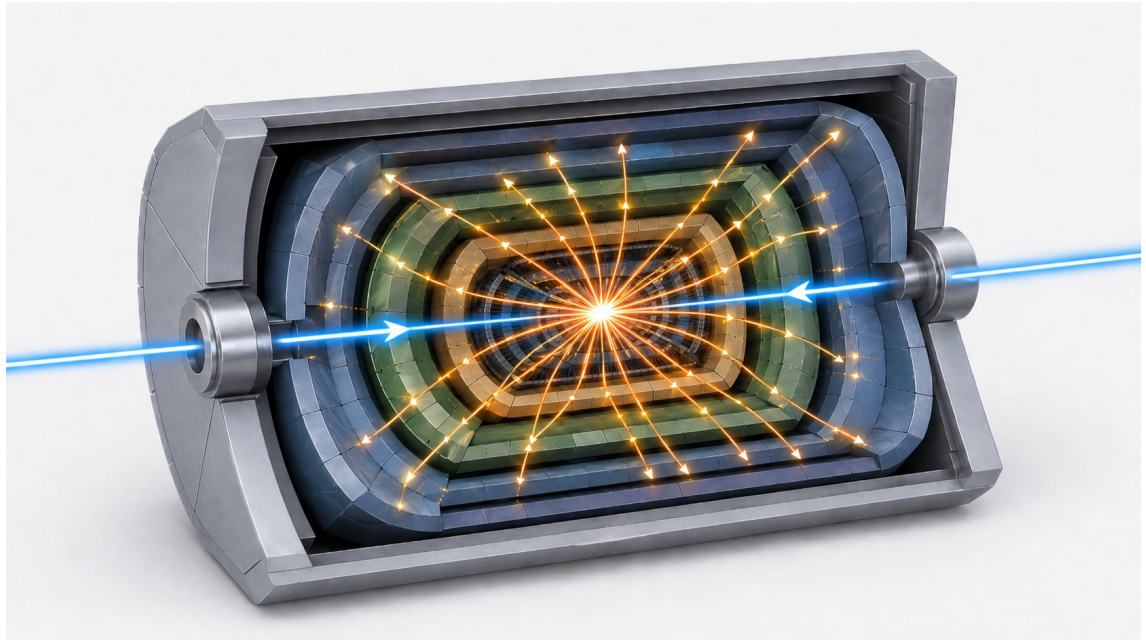
- Interfaces to
  - PDFs
  - Hadronization simulations
  - Detector simulations



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- Over 30 years of development
- AI plugins

MadGraph



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- High accuracy within well-understood approximations
- Over 30 years of development
- AI plugins
- **Powerful**, yet **challenging to use**…

```
Cross-section : nan +- nan pb
Number of events written: 0
```

```
./bin/madevent: line 123: gfortran: command not found
Error: Fortran compiler gfortran not found
```

The wall between two worlds

Developers:



Users:

The wall between two worlds

Developers:

- Add **advanced** capabilities



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- **Documentation** and **user interfaces** typically **limited**
- **Academic** development

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- **Use** MadGraph **for** their **research**
- Typically have **limited interest** in **technical details**

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MadAgents: Multi-Agent system as the **smart interface for MadGraph**

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Large Language Model Agents

- LLMs can do more than answer questions. They can:
  - **reason** before providing an answer.
  - **inspect** images and PDF files.
  - **execute** tools, e.g. run bash commands, search the web, …
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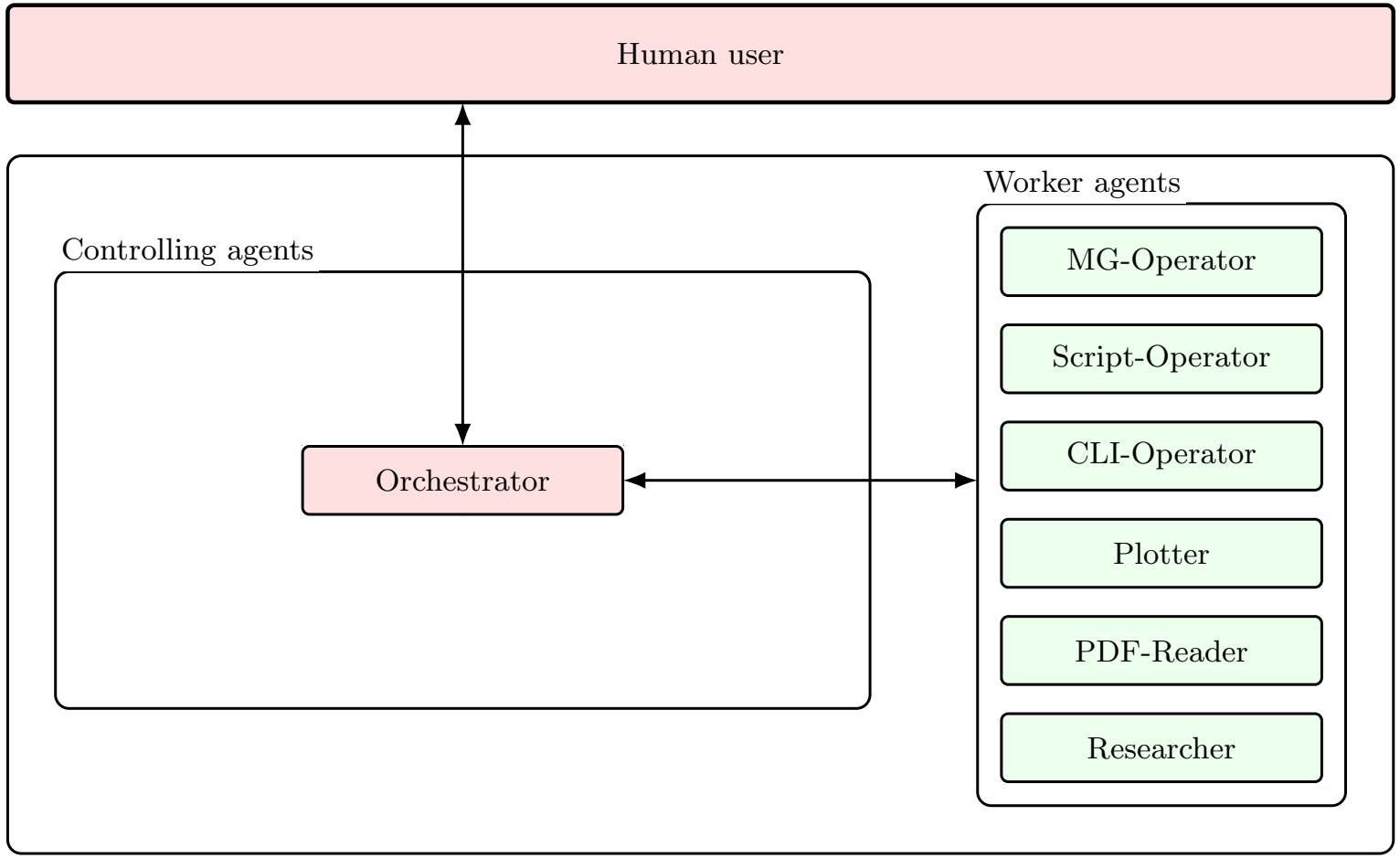
- **Specialized** = instructions, tools, …

MadAgents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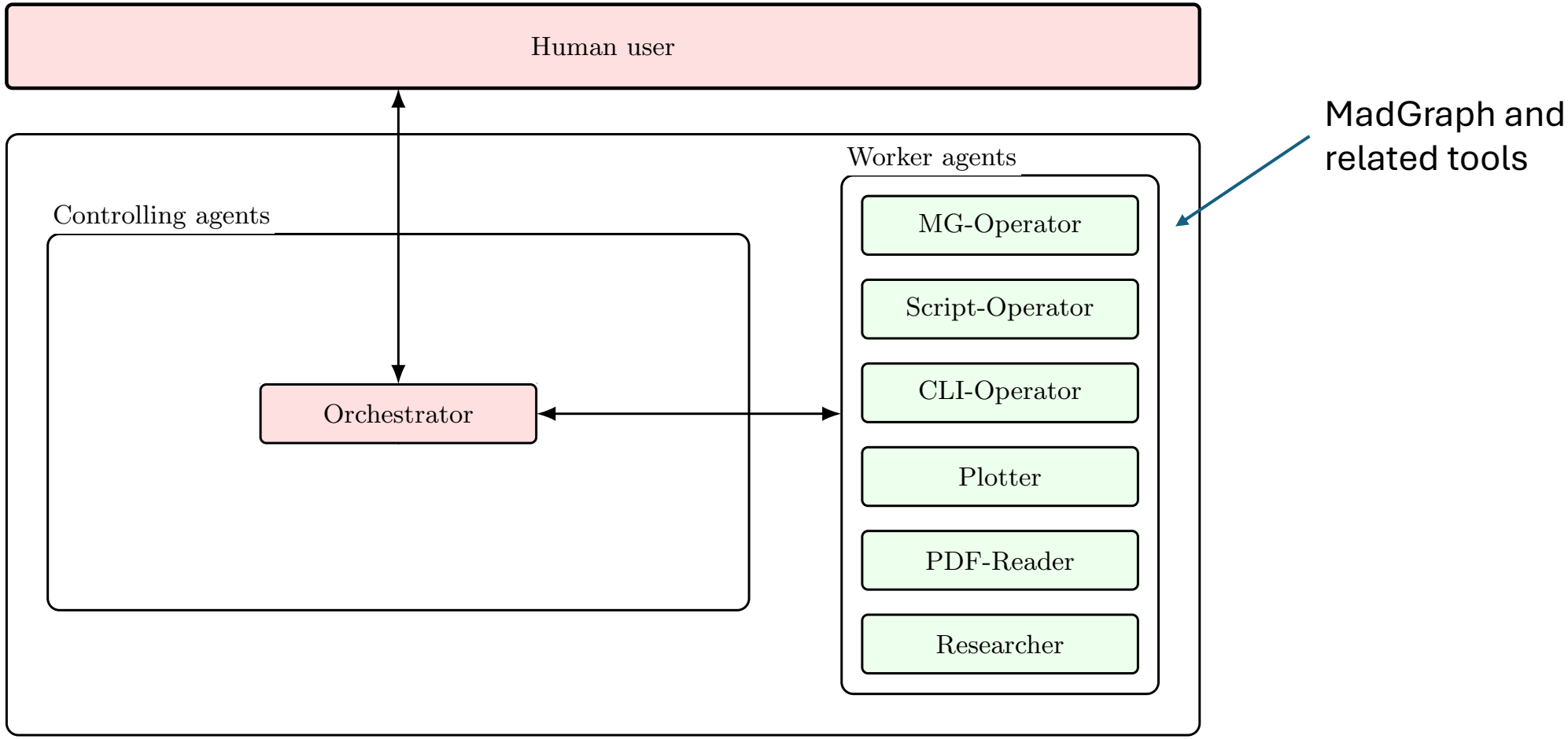
Worker agents
Controlling agents
MG-Operator
Script-Operator
CLI-Operator
Orchestrator
Plotter
PDF-Reader
Researcher

MadAgents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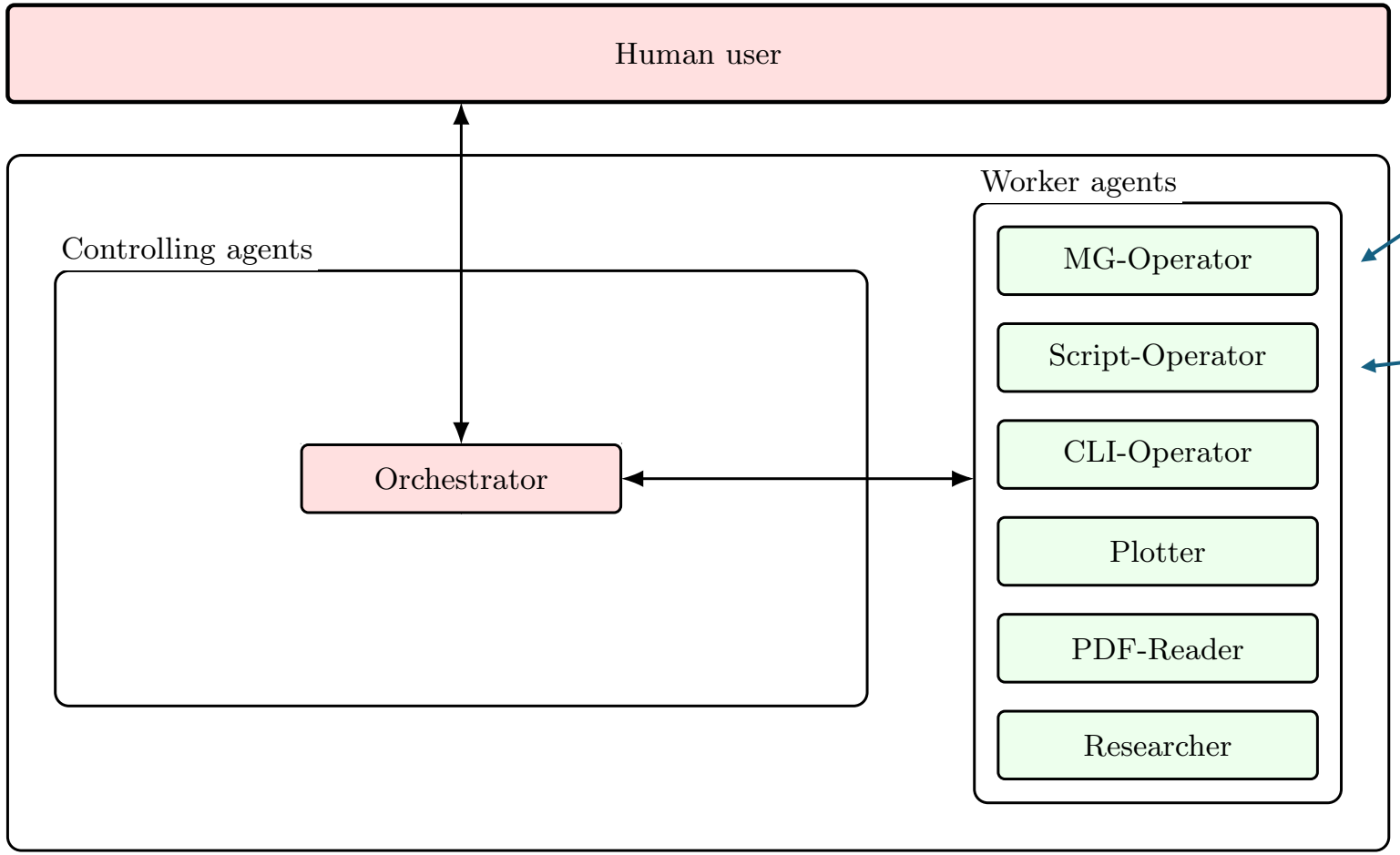

MadGraph and related tools

Generic bash and Python calls

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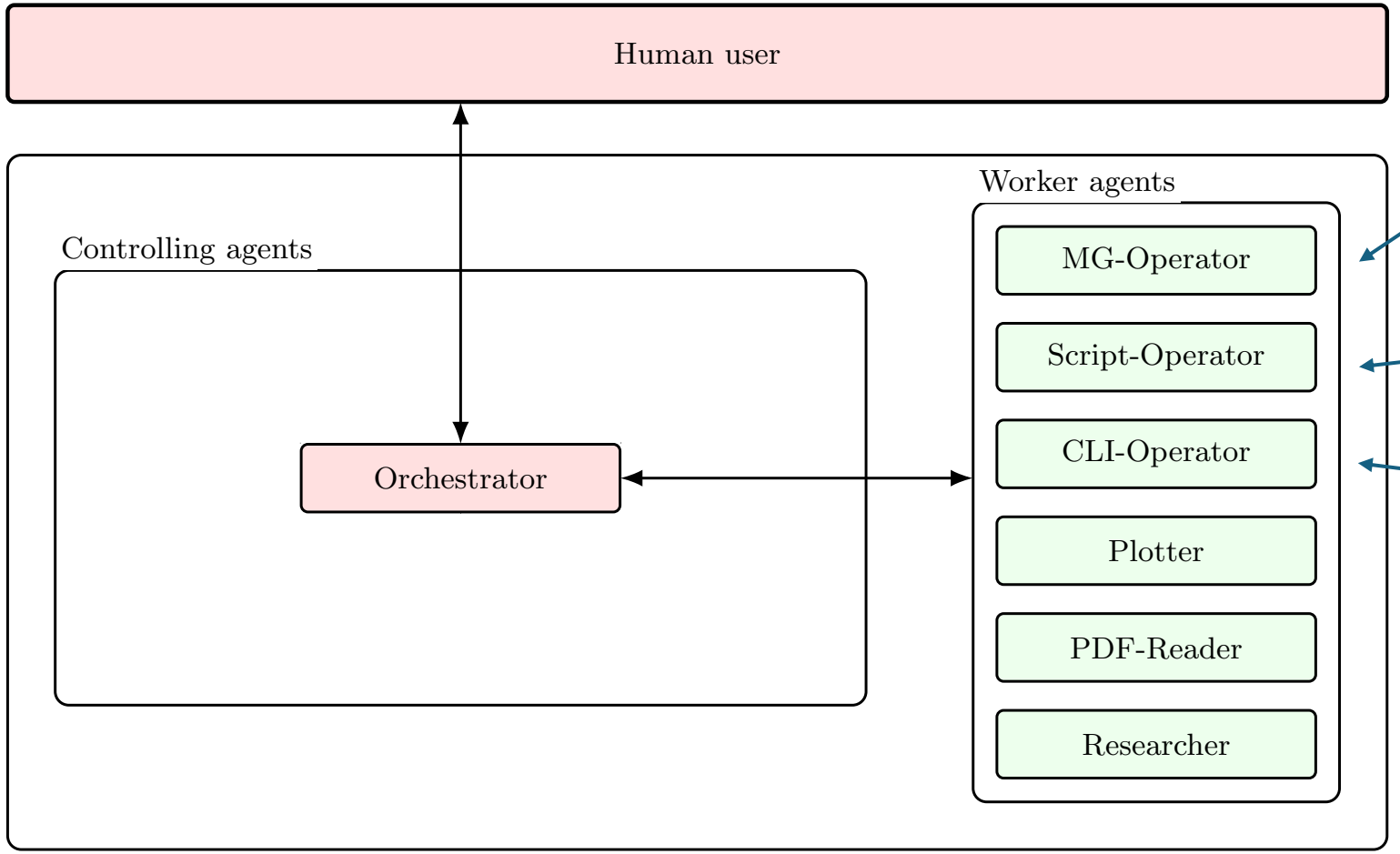

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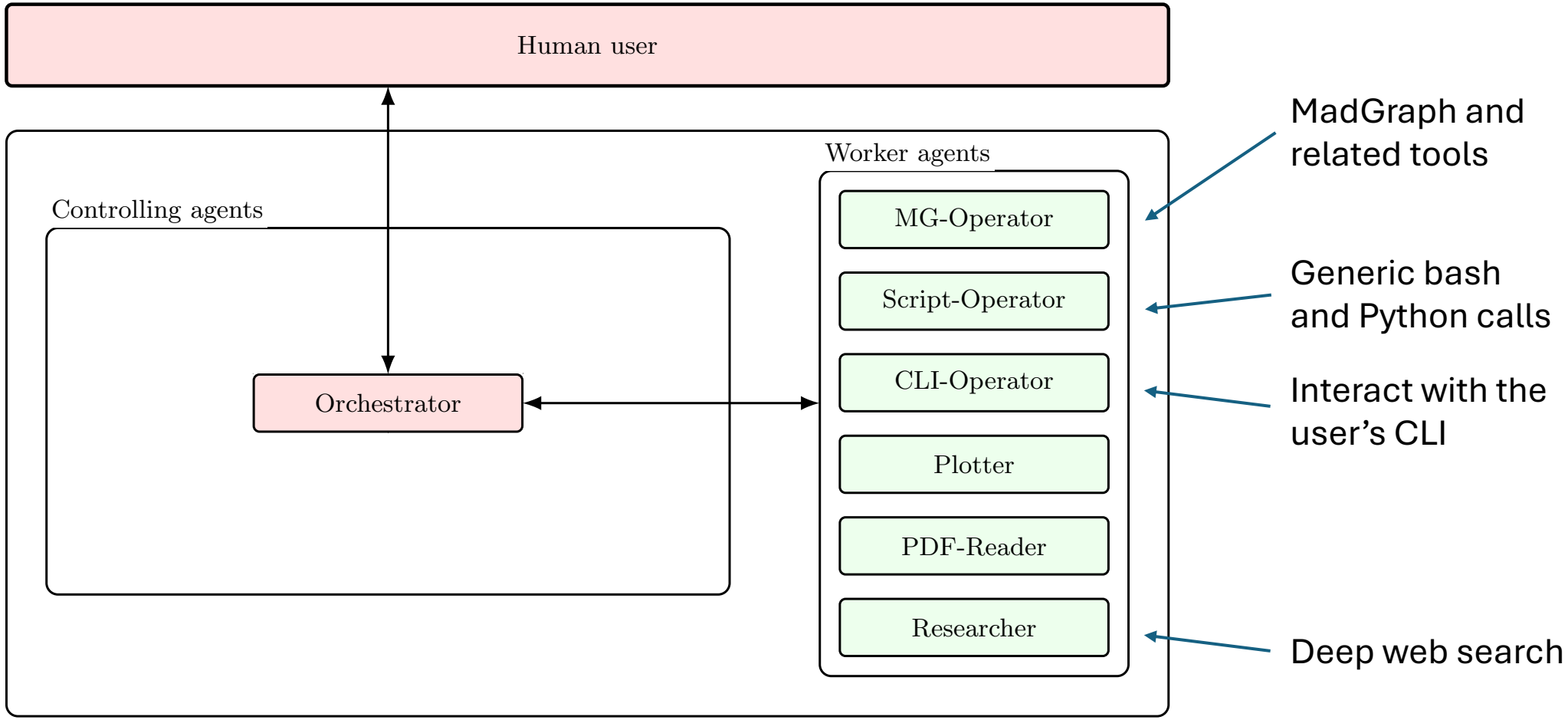
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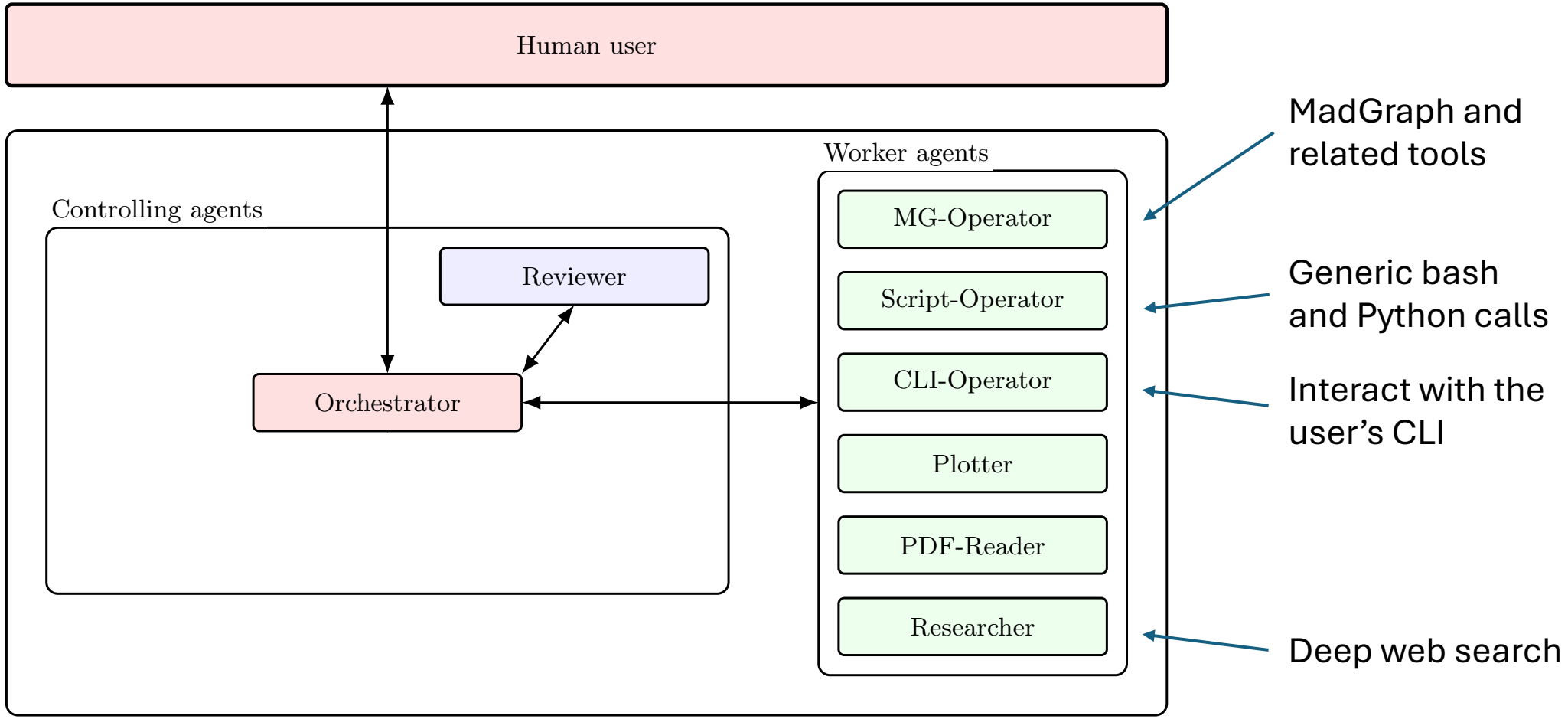
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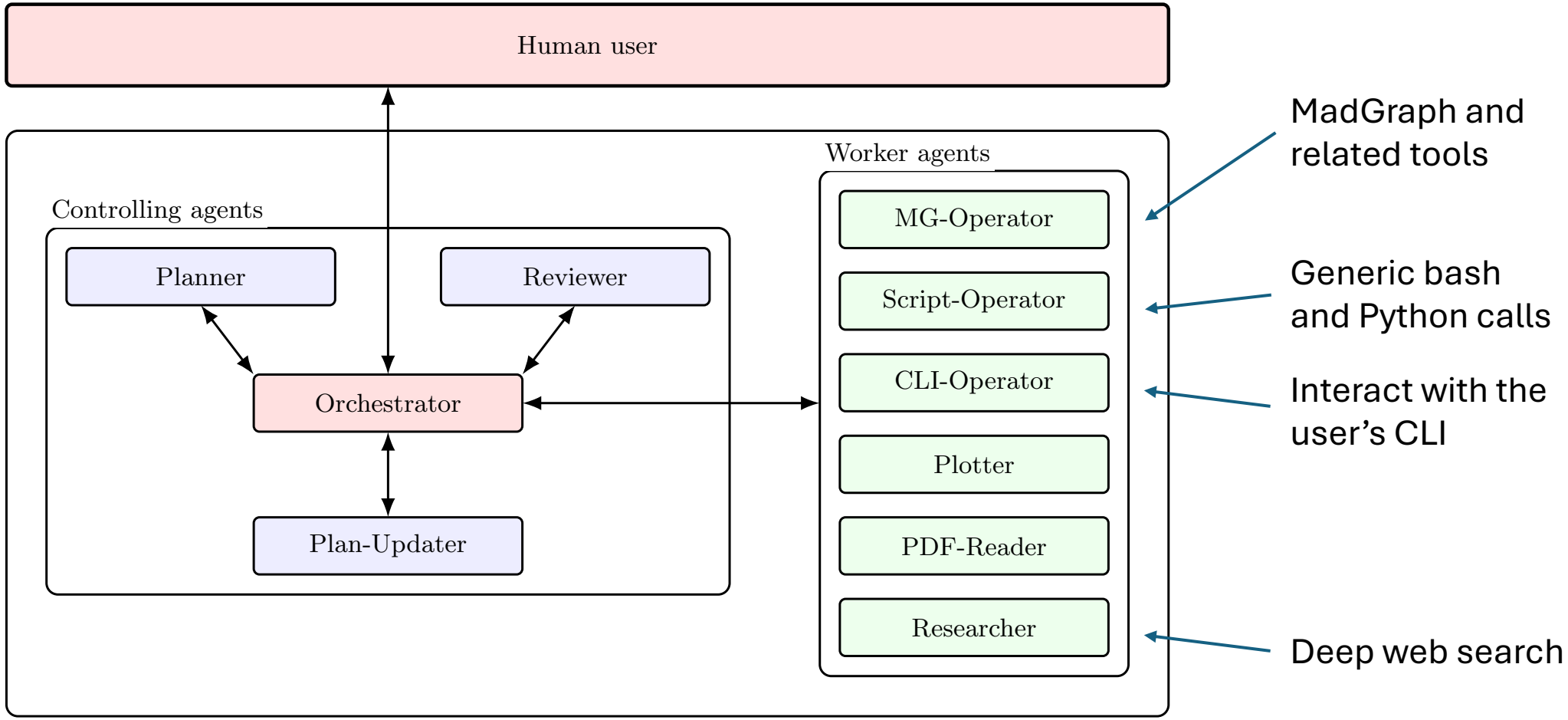
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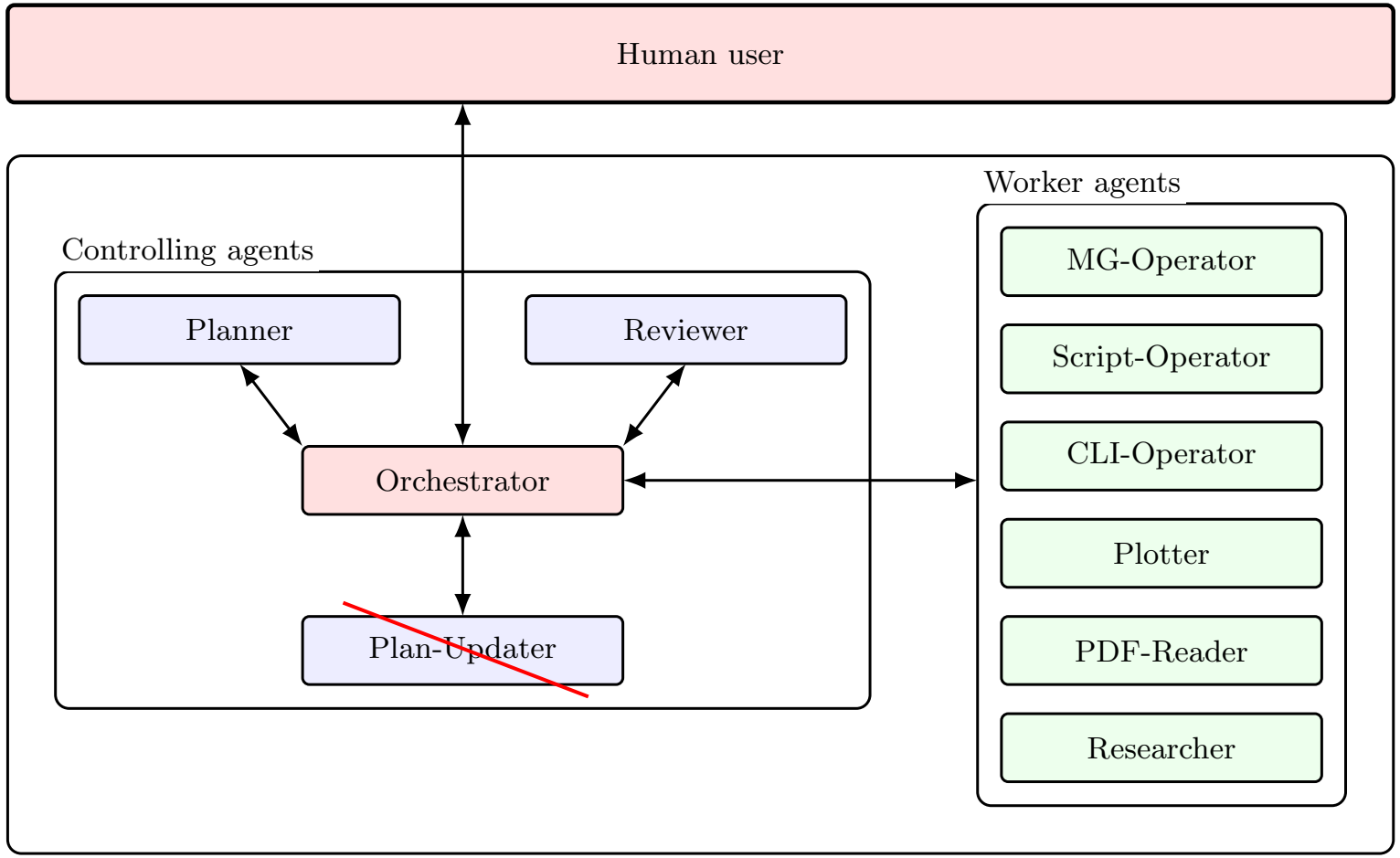

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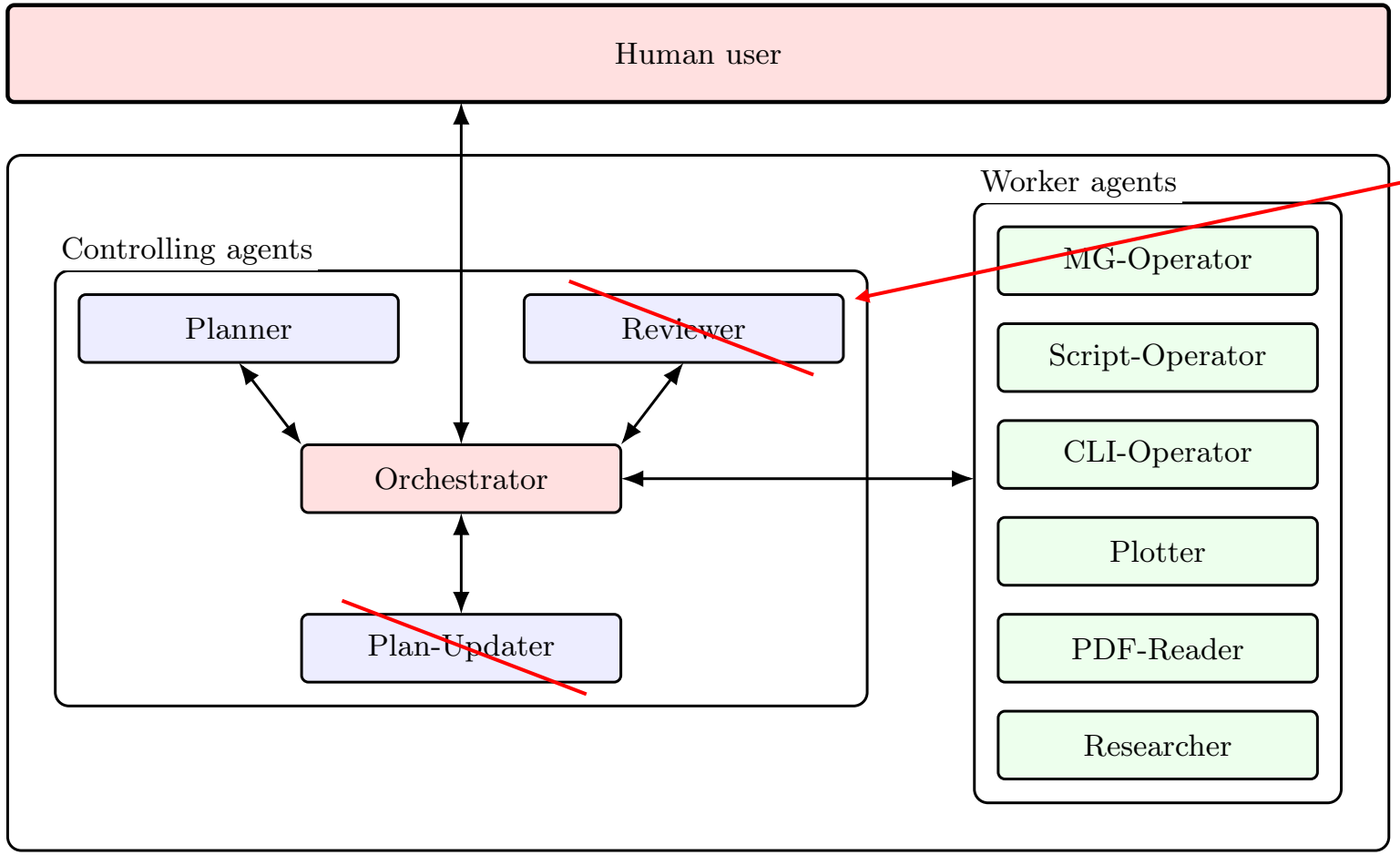

Specialized reviewers:

- Plan-Reviewer
- Verification-Reviewer
- Presentation-Reviewer

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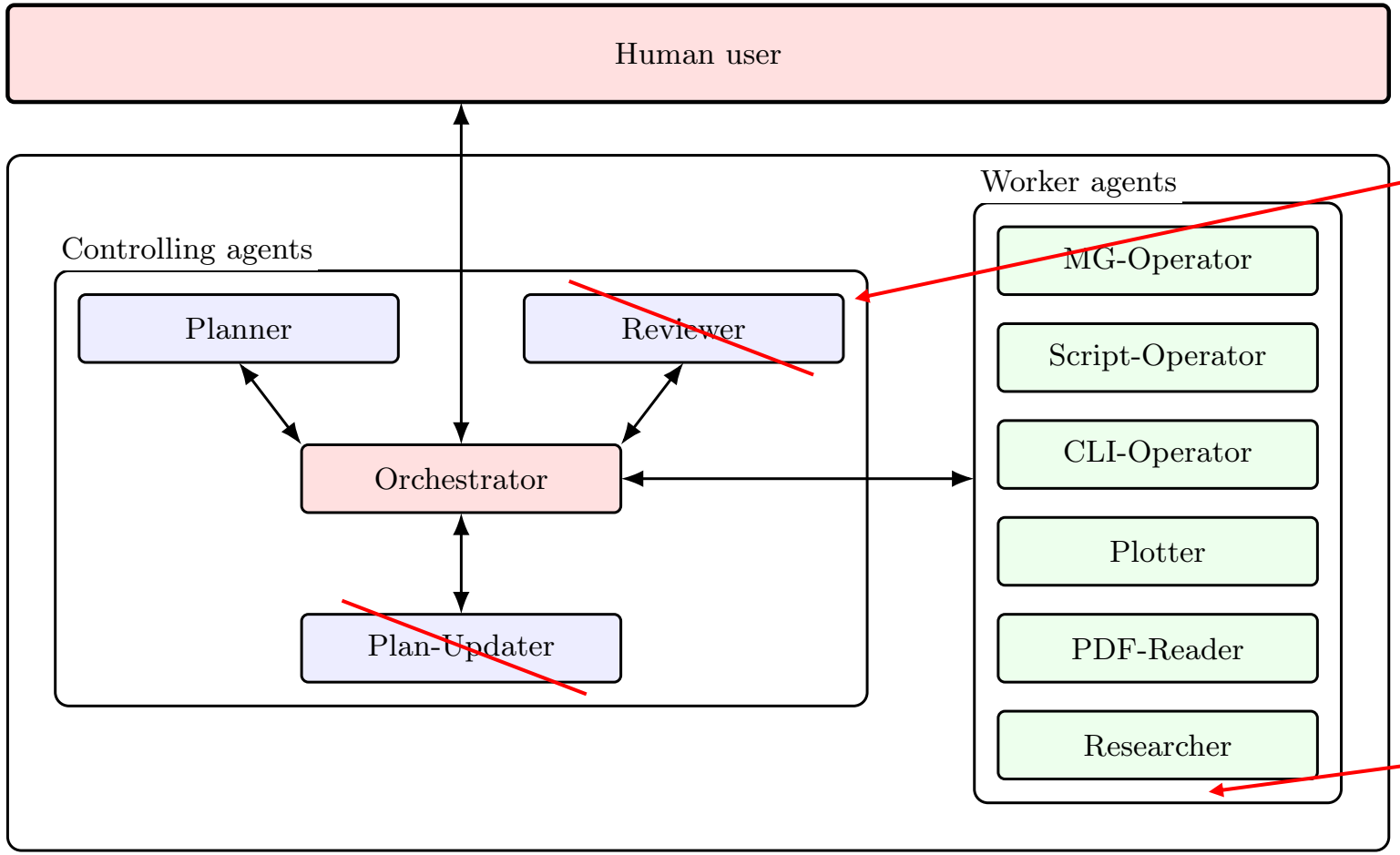

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Physics-Expert

Flexible Orchestration

- No hard-coded series of agent calls – the Orchestrator decides
- Flexible user interaction

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- Flexible user interaction
- MadAgents can support users at different stages, e.g.:
  - **Installation**
  - **Teaching inexperienced users**
  - **Advanced user-support**
  - **Autonomous execution**

Highlights

with GPT-5.1

MadGraph Installation

- **Task**: Install MadGraph+ Pythia8 + Delphes and compile ROOT

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MadGraph Installation

- **Task**: Install MadGraph+ Pythia8 + Delphes and compile ROOT
- **Problem**: MadGraph did not find the ROOT executable
- MadAgents:
  - Inspected the MadGraph source code
  - Understood that MadGraph wanted a ROOT executable ending with “.exe”
  - Created a symbolic link

Tailored Tutorials

- **Task**: Create tutorials for a beginner worker on Simulation Based Inference

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- **Outcome**: 6-step tutorial:
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  5. BSM sim.
  6. SBI datasets

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MadAgents act as a **teacher**:

- Offer explanations
- Provide hints
- Help users on the fly

Adaptive, real-time teaching

Dataset Documentation

- Generated $t\bar{t}$ events with at
  - LO and NLO with the SM.
  - LO with a BSM model.
- Applied K-factor reweighting
- **Task**: Create a detailed documentation

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3.2 Top-quark parameters

From the param cards (`Cards/param_card.dat`):

- **SM LO and NLO samples**
  - Top mass: $m_t = 173\,\mathrm{GeV}$.
  - Yukawa: $y_t = 173\,\mathrm{GeV}$ (in SM convention).
  - Width: $\Gamma_t \approx 1.49\,\mathrm{GeV}$.
- **EFT UFO sample**
  - Top mass: $m_t = 172\,\mathrm{GeV}$.
  - Yukawa: $y_t = 172\,\mathrm{GeV}$.
  - Width: $\Gamma_t \approx 1.51\,\mathrm{GeV}$.
  - DIM6 block (excerpt): the EFT scale parameter is set to $\lambda = 1\,\mathrm{TeV}$, and among the listed Wilson coefficients only c_{tG} is non-zero; all other entries in that block are set to zero.

This introduces a small mismatch between the SM reference samples and the EFT UFO sample in m_t and Γ_t, which is acceptable for many use cases but should be kept in mind for precision studies.

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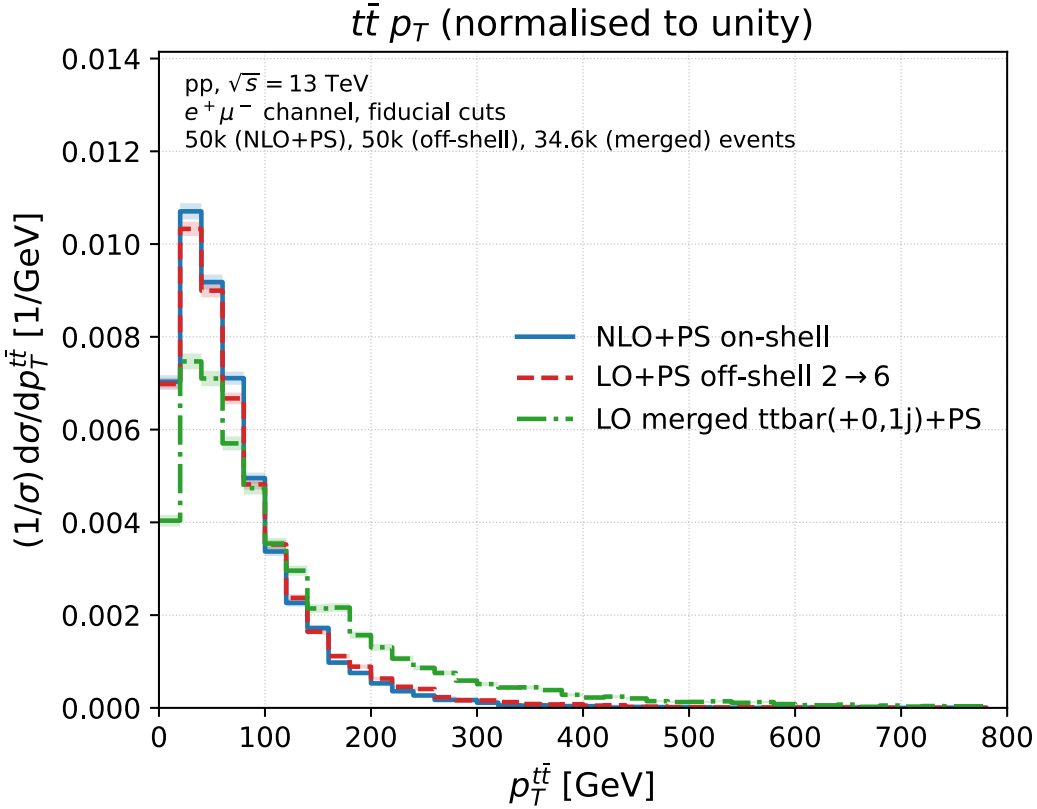
- Creates a plot to visualize the effects



Autonomous Event Generation

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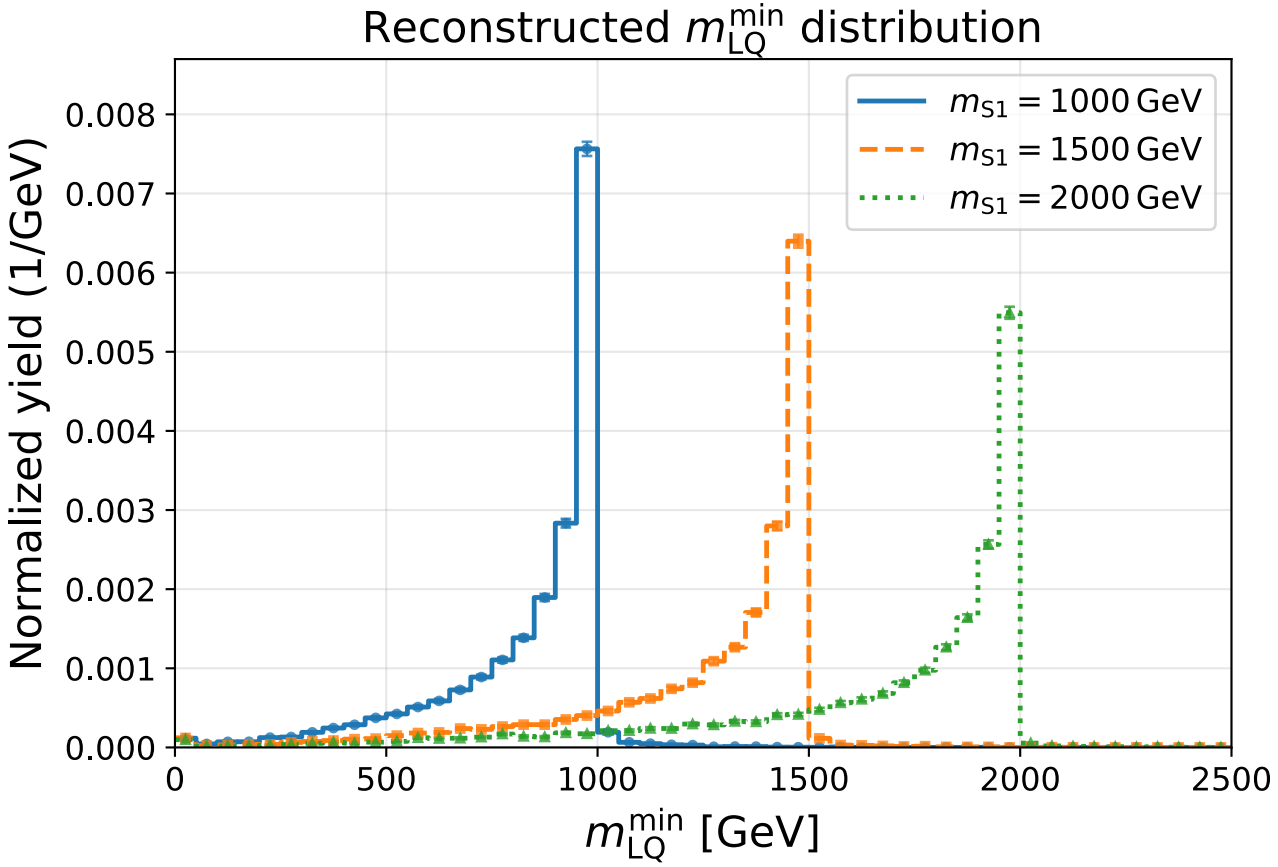

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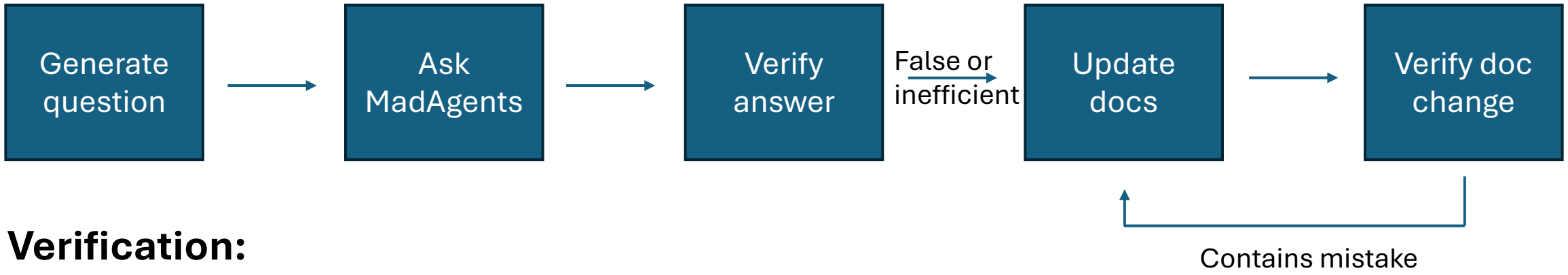

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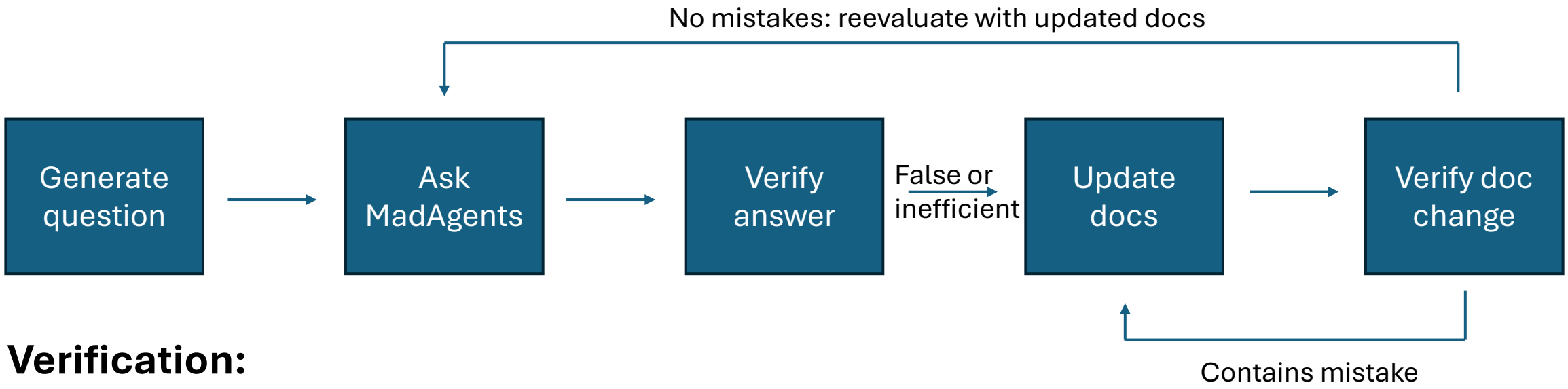

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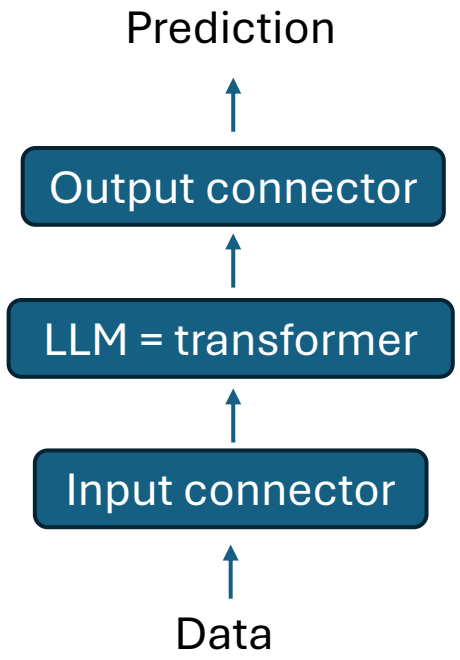

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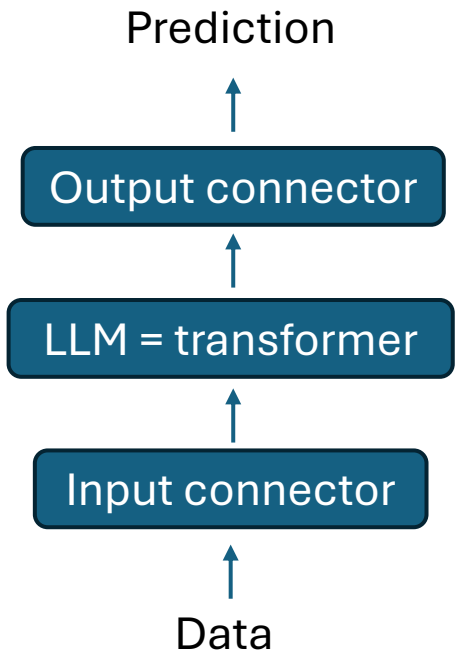

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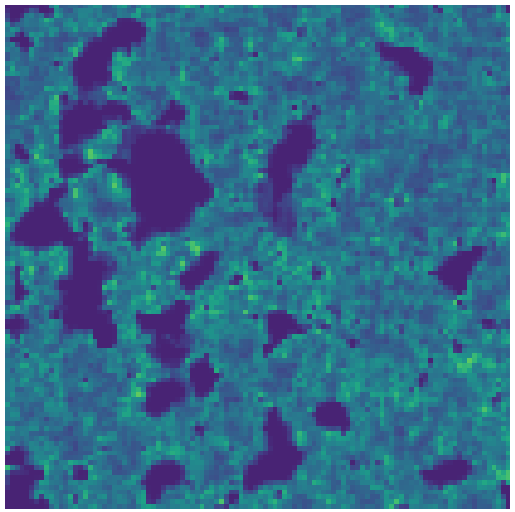

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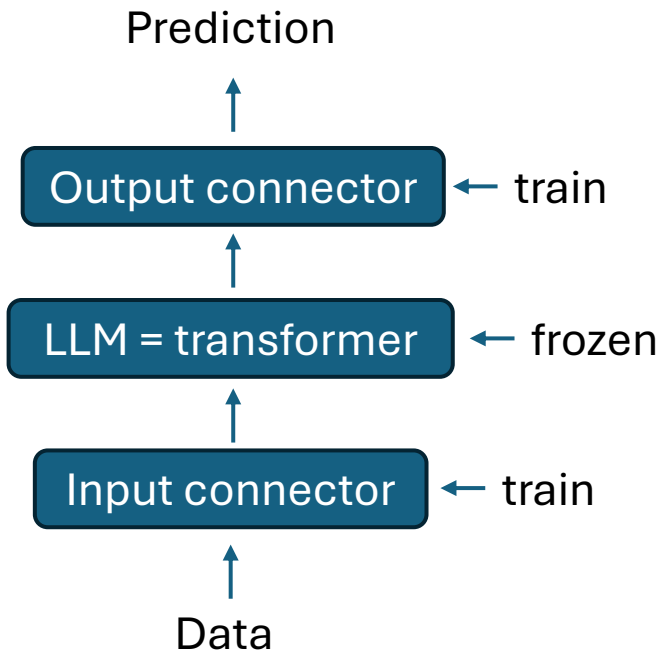

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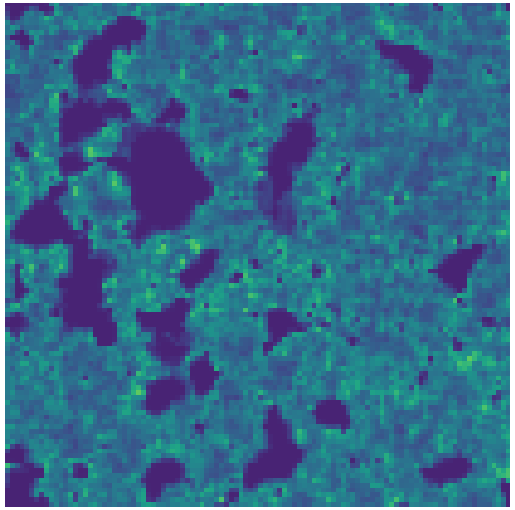

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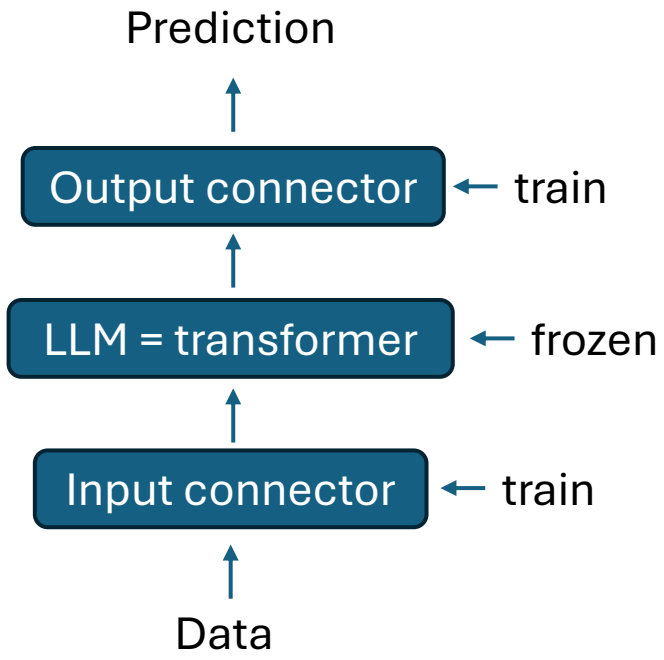

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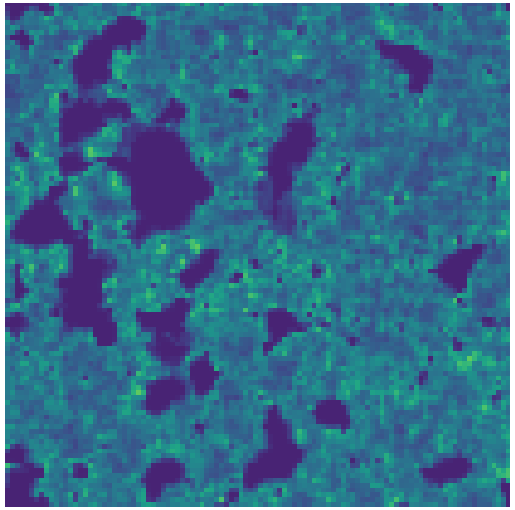

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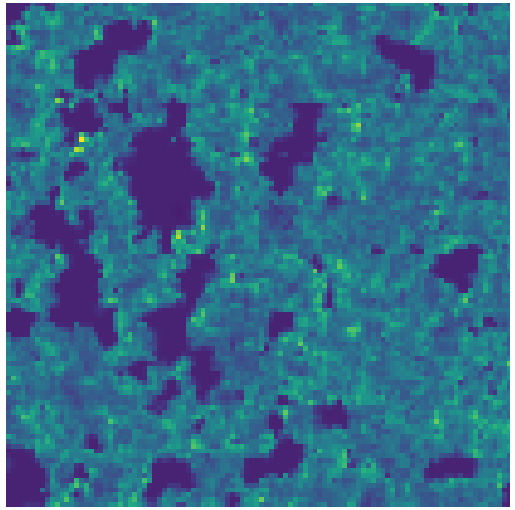

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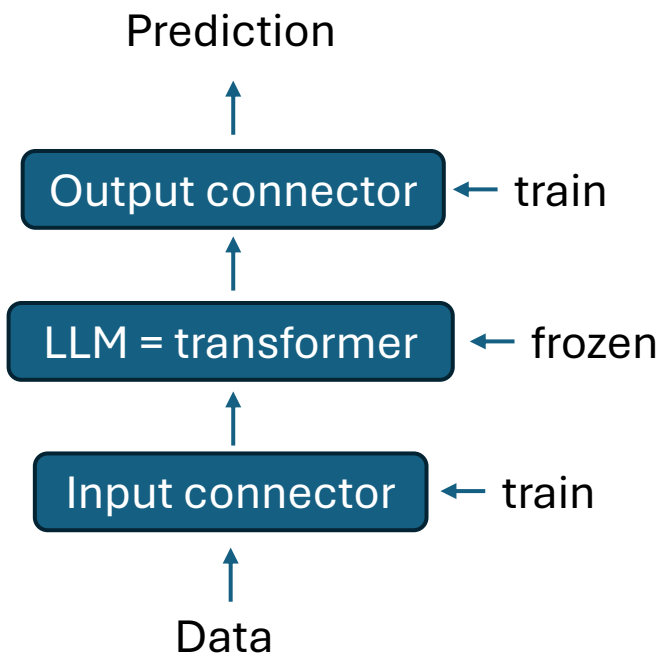

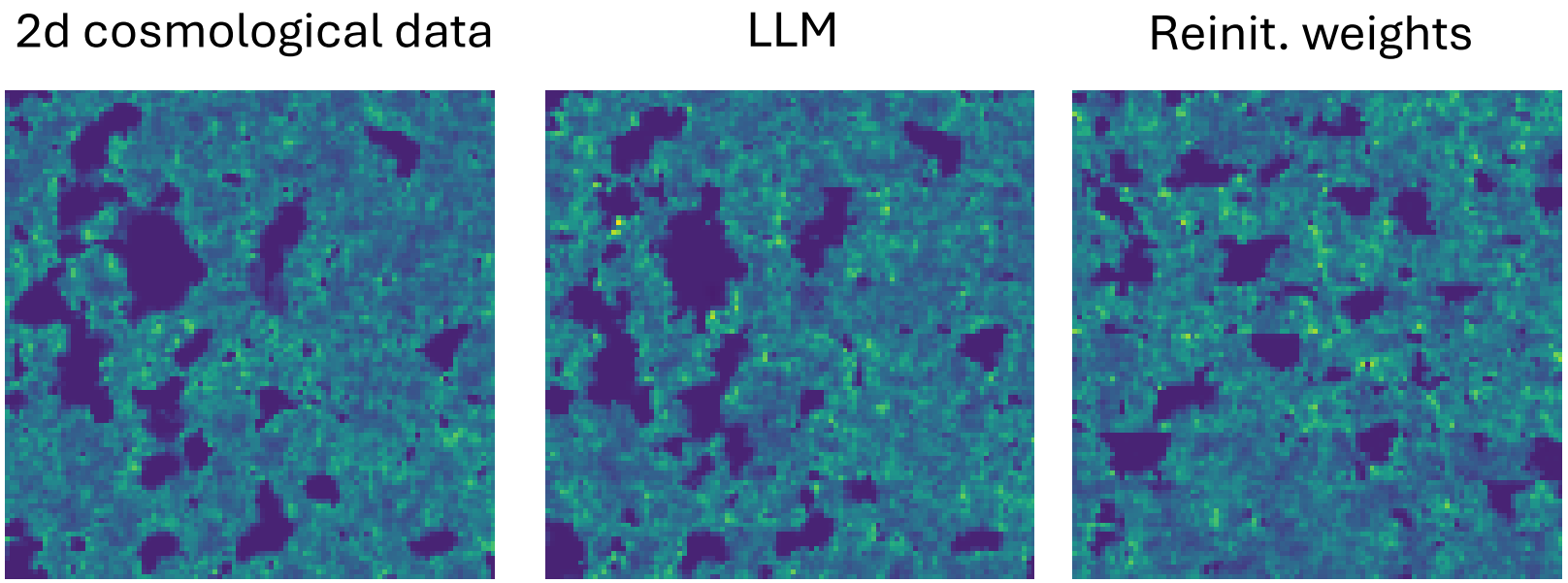

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Paper: arXiv:2601.21015
Code Repo: github.com/MadGraphTeam/MadAgents
A **Claude Code** implementation exists!
Soon: **CERN** integration