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1. Introduction

A new level of scientific progress would be possible if the challenge of enabling collaboration across two communities can be fast tracked. The Computational or Generative ML based Sciences have contributed to significant progress using AI/ Computational Sciences. Similarly, the experimental scientists have been contributed enormous progress using experimental lab facilities. If collaboration across these communities can be facilitated and even accelerated, it could lead to significant breakthrough.

The challenge:

To accelerate collaboration across communities



This works explores a solution by tapping into Multi Agent Al Explore an approach to address the challenge: Generative side collaborators

Generative
computational side collaborators

Wet
experiments
Wet
experiments

Figure 1: The challenge: How to enable collaboration across different scientific communities?

2. AID for Collaboration across communities

The challenge of bringing together Computational Sciences and Experimental Perspectives is addressed in this work with an innovative Multi Agent AI based approach. Inspired by the evolution of the internet, we propose GEM-AID, a federated composition of intelligence across the web, with a collection of intelligent agents (Figure 3). Each intelligent agent is itself an LLM-based intelligent system. A federation of such agents works together to move the wave of GEM-AID very effectively innovative thinking. illustrated via the graphical abstract (Figure 2). As illustrated in the graphic abstract, each lobe here in GEM-AID consists of an AI agent. GEM-AID is an Agentic AI-based Discovery that accelerates the Generative and Experimental Modelling of Molecules. GEM-AID is a Multi-Agent AI-based Federated Intelligence across the cloud of the web to bring together research communities from many fronts: The ML community, computational quantum sciences researchers, and experimental scientists.

Inspired by Nobel Prize for Chemistry 2024 for AlphaFold that creatively employed AI to accelerate science, we explore the new paradigm of the creative use of AI Agents to accelerate scientific discovery. How do we enable the Generative and Experimental communities to partner together at the speed of light?

To demonstrate this new paradigm of AI agents-aided Molecular Design, we develop AI Agents to assist researchers. Any interested researcher can use AID as a virtual research collaborator to perform any type of scientific task.

The graphical abstract (Fig 2) shows how different types of specializations can be brought under a federated brain or an umbrella intelligence to facilitate AI-facilitated research collaboration across different research communities (ML/bio generative lab, theoretical, computational lab, wet lab).

GEM-AID essentially democratizes access and means to execute scientific tasks. By simply instructing in plain English, a bioscientist can employ a virtual bioML scientist (an AID agent) and simply provide instructions in natural language. In the traditional paradigm, a bioscientist will need to learn ML/python skills to run AI experiments (Fig 5). In the new proposed paradigm, the bioscientist can simply use natural English to conceive, design and run AI experiments without any python/ML coding. This is because Multi-Agent AI based GEM-AID automatically understands natural simple English sentences, and automatically generates ML/python source code and also automatically runs AI experiments. The AI even interprets the computational results for the scientist, thus enables scientist in chemistry/bio wet lab facilities to run AI/Quantum Sciences computations.

For advanced collaboration, the virtual agent will consult in turn with a relevant human experts. Such a combination of virtual scientific agents with differentiation specializations can be created by the respective community (Fig 4). We have also enabled AID-GEM to run across the internet, so the collaboration can be at an internet scale across continents, allowing for inclusive access to researchers from different labs in different countries. To explore further and for the benefit of community, the project is being hosted online with open-source at <u>https://sites.google.com/view/gem-aid</u>

We demonstrate this proposed idea with an implementation. prototype open-source The implementation demonstrates the feasibility of this approach to solve the challenge. The prototype opensource implementation shows how accelerated collaboration can be enabled for GEM. In this prototype, the researcher guides the LLM-based AI agent, while the AI agent utilizes various problemspecific scientific tools. AID prototype integrates four frameworks/tools: chemical latent space-based dynamic generation of novel molecules using Variational AutoEncoder, BuildAMol library, dynamic generation of Python code for DFT studies with pyscf and DM21, and grounded literature retrieval from the web.

Project: https://sites.google.com/view/gem-aid

AID FOR COLLABORATIVE DISCOVERY: Ai agents links generative and experiment teams

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Figure 3: Implementation of the proposed solution (analogy : world wide web)



Figure 4: Comparison of benefits