

A Domain-Specific Chatbot for atomistic simulations: Enhancing Accessibility and Productivity Using LLMs and RAG

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Large Language Models (LLMs) have shown enormous potential in the computational materials science field[1,2], paving the way for smarter and more accessible simulation environments[3-5]. In this preliminary work, we experiment with integrating Large Language Models (LLMs) with Retrieval-Augmented Generation (RAG) frameworks[6] to design a domain-specific chatbot that eases and streamlines user interactions with the Abinit software ecosystem[7]. This system aims at answering user queries by retrieving fact-based information from diverse Abinit resources, including documentation, tutorials, codebase, and related tools like AbiPy. We describe the chatbot's architecture and validate its performance through an automatically built dataset of questions and answers, generated from Abinit resources and validated by expert users. Results highlight improvements in response accuracy when using the RAG framework compared to naive methods, as well as the potential of identifying gaps in existing documentation. We believe that this tool will facilitate the navigation of the extensive Abinit knowledge base, thereby both lowering the initial learning curve for new users and optimizing productivity for experts. Finally, we discuss its potential use as an automatic responder to questions in the Abinit's forum and as part of a broader AI-automated system, such as recent projects like LangSim[4] and LLaMP[5].

References

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Figures

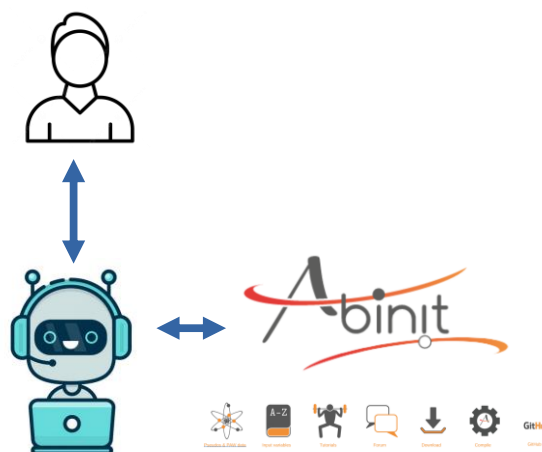


Figure 1. AbiBot: Retrieval-Augmented Generation (RAG) frameworks that streamlines user interactions within the Abinit software ecosystem.