

Deploying Conversational Agents in Virtual Research Environments: Approaches and Lessons Learned

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Abstract. The rapid progress of conversational artificial intelligence and Large Language Models (LLMs) has opened new opportunities to enhance user interaction, support, and accessibility in Virtual Research Environments (VREs). This poster presents the approaches, challenges, and lessons learned from a multi-year effort to design, develop, and deploy conversational agents within the D4Science infrastructure. Through three successive implementation cycles—Janet, D4Science AI Agent, and DAVE—the poster traces a process of iterative refinement aimed at improving flexibility, extensibility, usability, and integration with existing VRE services. Janet, the first prototype, explored modular NLP components but revealed limitations in adaptability and feedback integration. The second approach, based on the Cheshire Cat framework, improved modularity and LLM interoperability but remained constrained by a single-agent design. The latest solution, DAVE (D4Science Assistant for Virtual research Environments), introduces a multi-agent architecture built with Google's Agent Development Kit, enabling secure and context-aware interaction with multiple D4Science services. DAVE combines specialized agents for tasks such as document analysis, catalogue navigation, social interaction summarization, and algorithm deployment within D4Science's computational platform. Integrated feedback mechanisms and a Retrieval-Augmented Generation (RAG) knowledge base further enhance its learning and personalization capabilities. The findings demonstrate that conversational agents can lower barriers to VRE adoption, streamline workflows, and foster user engagement by offering intuitive, natural language interfaces. Lessons learned from this evolution suggest key design principles for future research infrastructure agents, emphasizing modularity, interoperability, and data security. Future work will involve usability evaluations, the integration of user-driven feedback, and experimentation with locally-hosted LLMs to strengthen privacy and operational sustainability.

#LLM, #NLP, #RAG

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The Challenge

The emergence and rapid progress of conversational artificial intelligence and Large Language Models (LLMs) have opened new opportunities to enhance user interaction, support, and accessibility across various digital contexts, including Research Infrastructures, Science Gateways, and Virtual Research Environments.

Embedding conversational agents in an infrastructure like D4Science presents unique challenges including (a) *complexity and diversity*—VREs combine heterogeneous services and data; (b) *flexibility and extensibility*—AI technologies evolve; (c) *user-centricity*—the system must assist users without adding friction and biases; (d) *security and trust*—respect data privacy.

The InfraScience laboratory is actively addressing these challenges by exploring a range of innovative conversational agent designs. Our approach focuses on seamless integration with the D4Science infrastructure, leveraging modular architectures for scalability and adaptability. We prioritize the adoption of the D4Science authentication system across all layers to ensure robust security, while maintaining user-centricity and minimizing potential biases or friction.

The D4Science Journey: from Janet to DAVE

JANET: the modular NLP Prototype (2023)

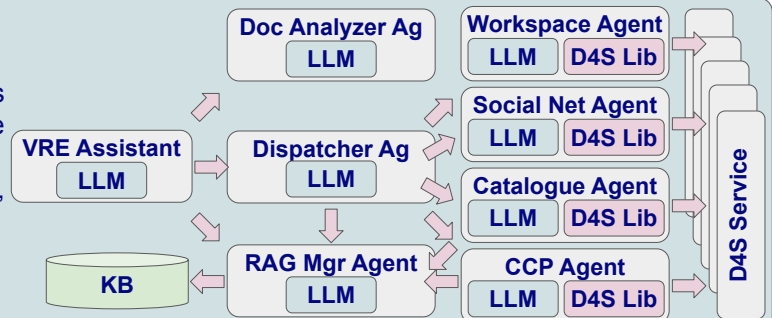
- Designed as a *pipeline of fine-tuned NLP components* (intent classifier, entity extractor, retriever, generator).
- Explored automated support for question answering and content retrieval.
- *Limitations*: Rigid pipeline, limited adaptability, and no real-time feedback integration.

D4Science AI Agent: the Single-Agent Framework (2024)

- Built using the Cheshire Cat framework for modularity and LLM flexibility.
- Integrated with D4Science APIs through Python plugins; supported RAG-based memory.
- *Lessons learned*: Improved flexibility but constrained by a single-agent architecture, with limited support for multi-user and collaborative settings.

DAVE: the Multi-Agent evolution (2025)

- Implemented with Google's Agent Development Kit (ADK).
- Features a central orchestrator and specialized sub-agents (for document analysis, social summarization, catalogue navigation, and algorithm deployment).
- Includes feedback collection, RAG-based knowledge base, and configurable LLM bindings per agent.
- *Outcome*: Enhanced modularity, interoperability, security, and user experience.



WHAT'S NEXT: (a) adopt a co-creation approach by engaging users in refining the agent; (b) assess usability and effectiveness through both quantitative metrics and qualitative feedback from real scenarios; (c) explore the possibility of including a locally-hosted LLM, so to keep all processing on-site and strengthen data protection and confidentiality.

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