

Simurg ecosystem: a zero-coding agent-driven infrastructure for quantitative pharmacology and MID3 applications

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Introduction

Pharmacometrics analyses typically require modelers to apply multiple methodologically distinct functions across diverse tools and environments, prompting substantial reformatting efforts and increasing both time costs and error risks – motivating the development of more integrative, user-friendly platforms [1,2]. The rapid evolution and growing accessibility of AI tools has opened a fundamentally new layer of opportunities for building such environments, spanning both scripted and graphical user interface (GUI)-based approaches [3,4].

Aim

In this work we present Simurg – an ecosystem for applied pharmacometrics that integrates three complementary interface paradigms: script-based workflows in R and Python, an application-driven infrastructure with a GUI, and local human-in-the-loop AI assistance.

Materials and Methods

The Simurg achieves a unique combination of capabilities through the integration of scripting, GUI and AI. It possesses two principal features:

- Applications (plugins) templates are engineered to be fully integrated to the ecosystem as separate entities on one side and to be developed via vibe coding by specialists with pharmacometrics background and no programming experience. All GUI building block and algorithms are available for plugins
- Simurg enables seamless workflow for data analysis at each step and having all tools close. GUI and scripting languages are synchronized to support convenience, speed and reproducibility

This design offers a unique opportunity for the broad community of pharmacometricians to integrate novel mathematical methods, models, and functionalities by building and deploying new applications and gradually expand the ecosystem.

Architecture

Simurg operates as a unified, governed ecosystem supporting both Linux/Windows desktop deployment and a web-based TypeScript application with a plugin architecture.

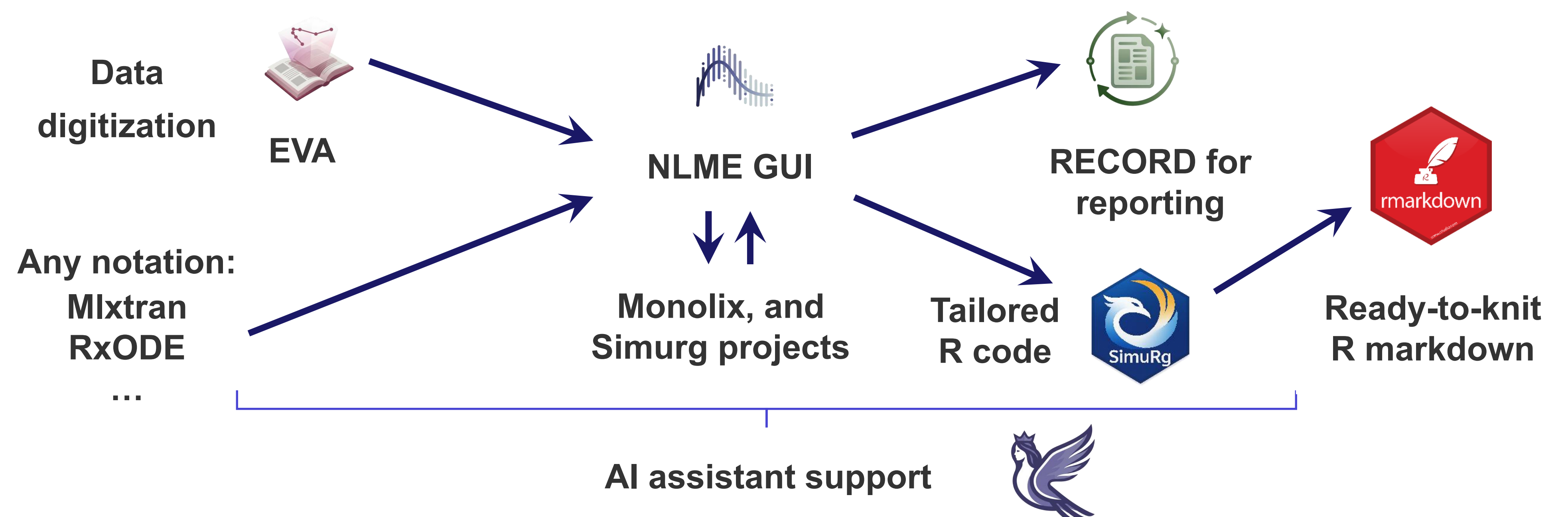
The backend is built with a Node.js server capable of interfacing with SQL databases, executing C++ algorithmic code, and orchestrating Docker containers to run R and Python scripts as well as RStudio Server.

The frontend is built with a Next.js and provides a development kit for GUI and for plugins. Everything done at the client side is provided with language translational system, UI components library and documentation.

Plugins are distributed as Webpack packages that can be installed or removed on demand; each exposes an intuitive GUI with component-level documentation powered by Storybook.

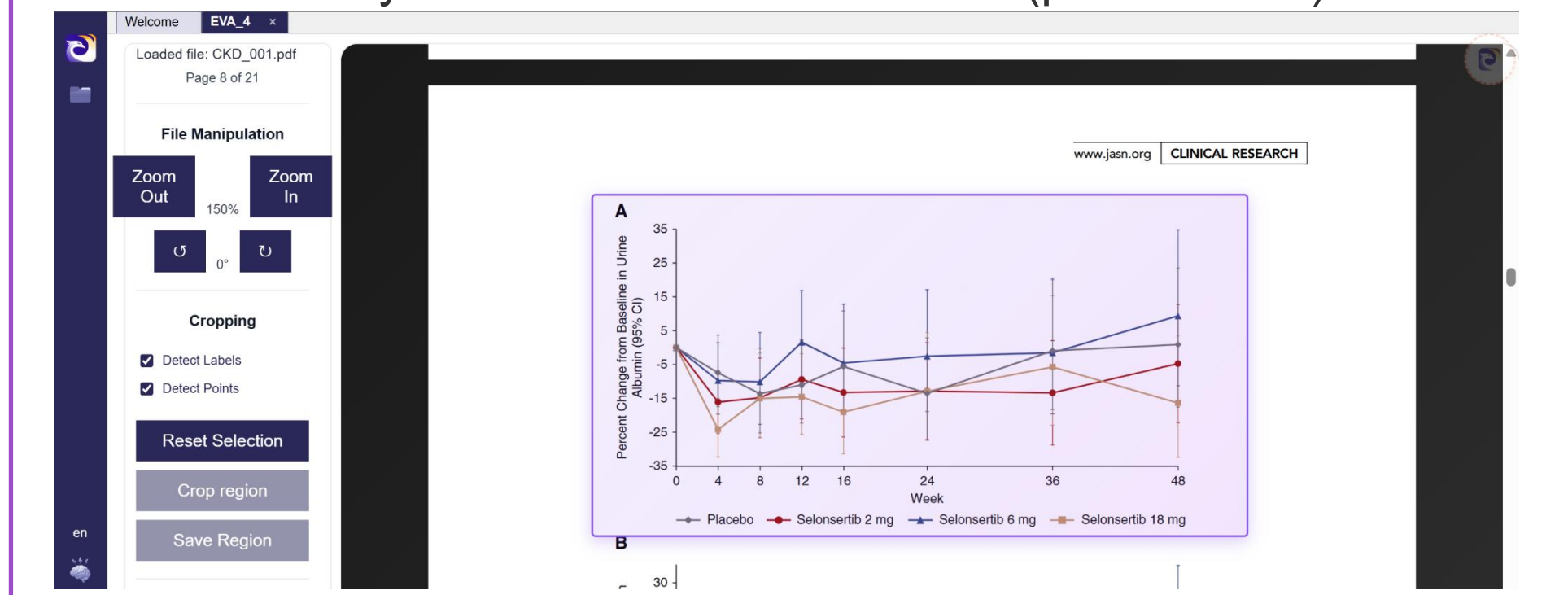
AI support is embedded through a locally deployable assistant, Sirin AI, which is composed of multiple large language models operating as a coordinated agent pipeline.

Ecosystem principle – seamless workflow



Applications

EVA enables automatic data extraction from time-series and scatter plots, and provides tools for evaluation, correction, and downstream analysis of the extracted results (poster S-10).



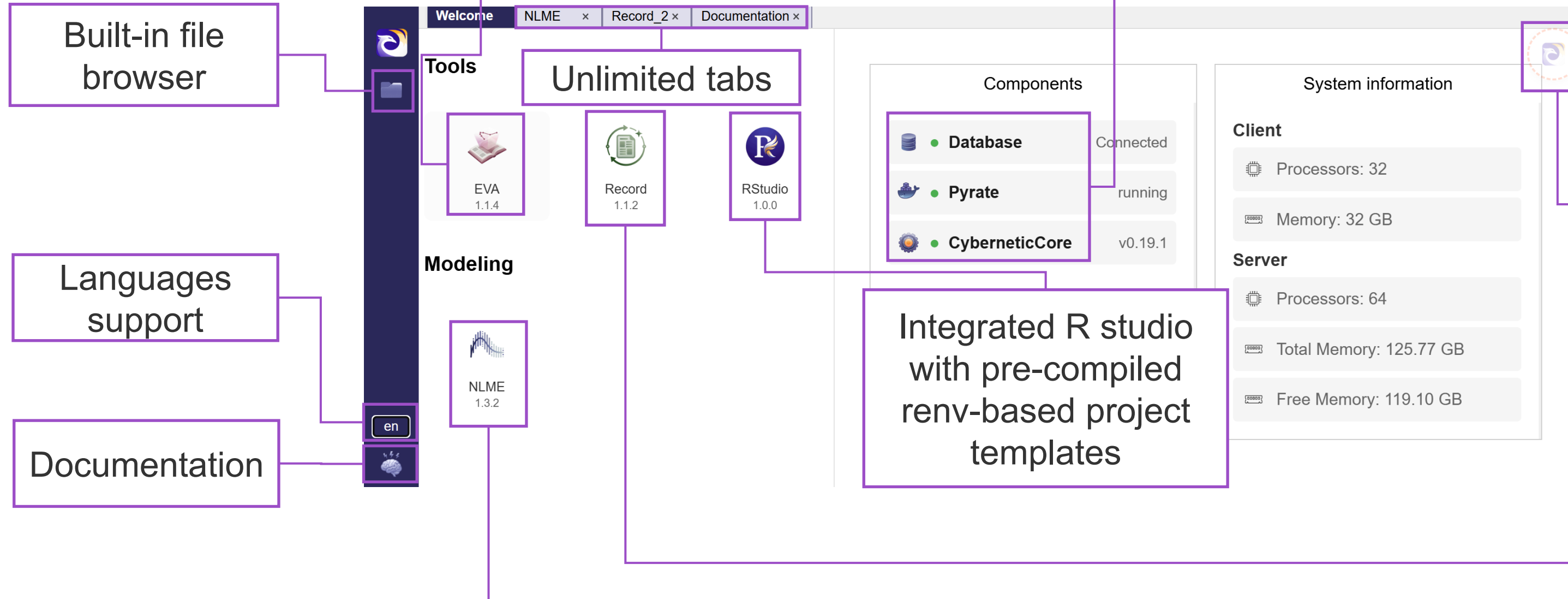
Natively WEB technology but supports Linux/Win deployment

Docker scripts in R, Python, Julia, ...

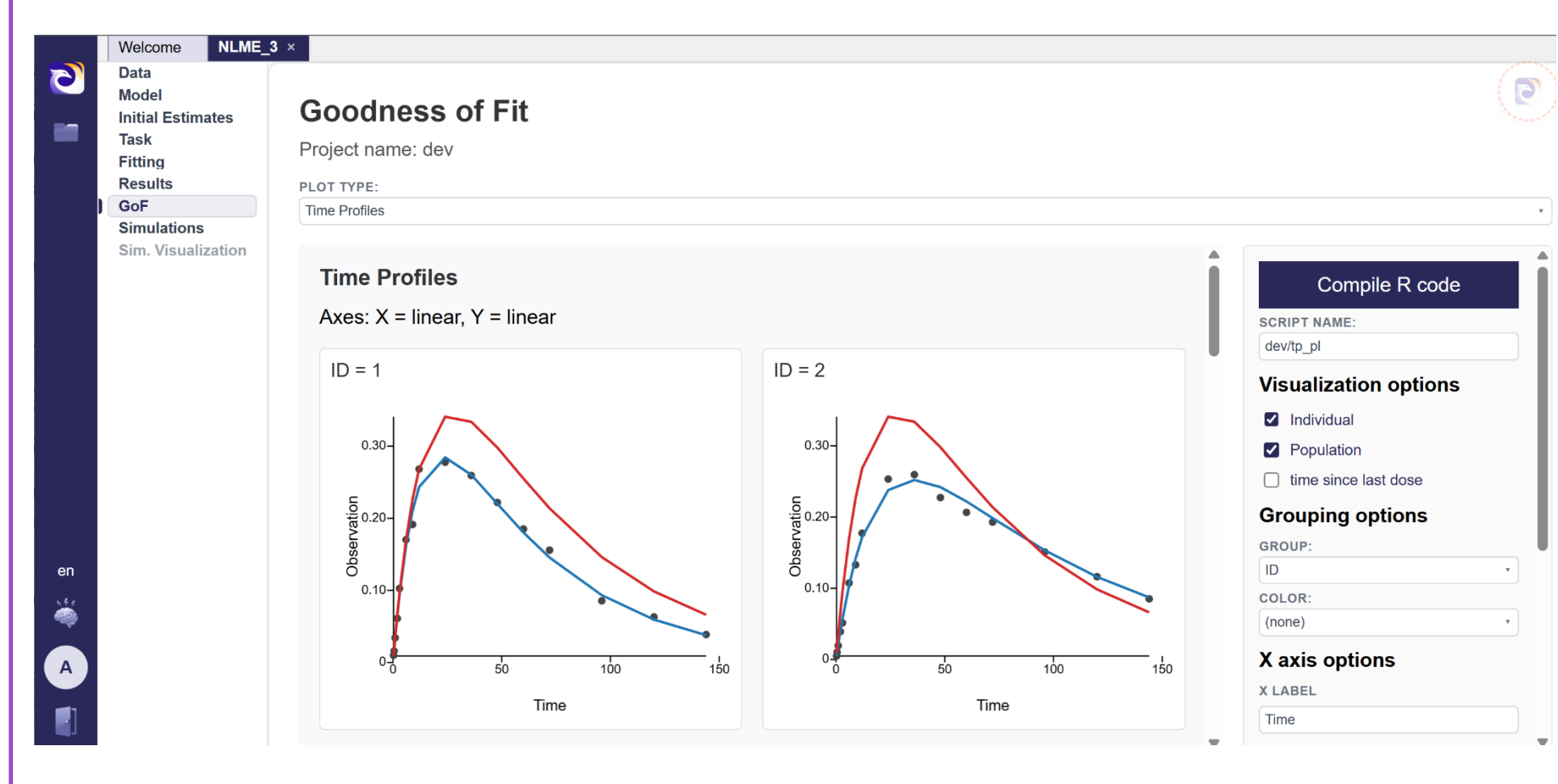
Simurg supports systems status:

- Authentication system with protected database
- Docker container responsible for scripts running
- C++ driven algorithms for performance related features

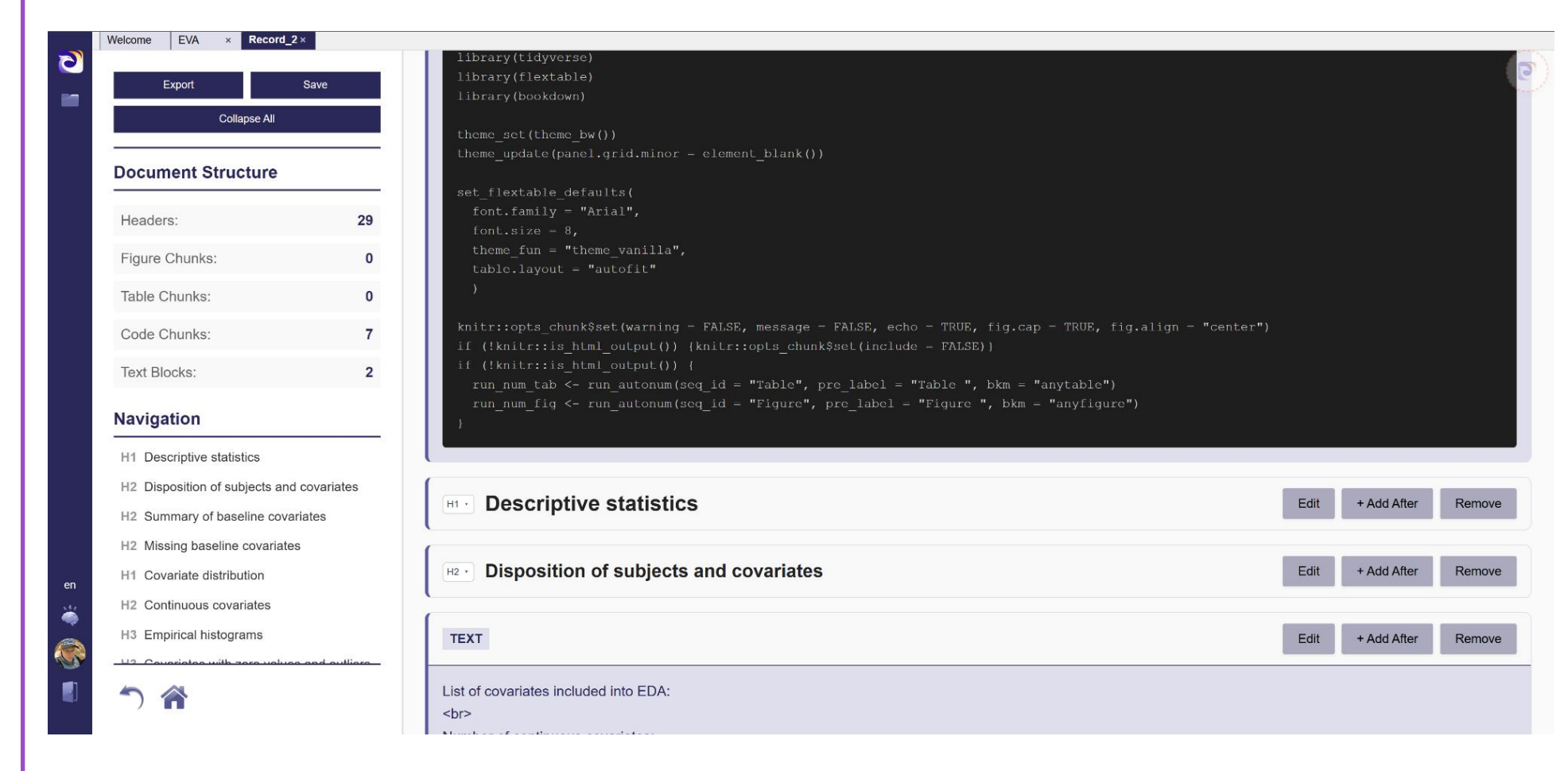
Local LLM assistant Sirin AI enables rapid onboarding, code linting and modification, as well as contextual support through natural-language interaction



Software-agnostic NLME tool that serves as a unified API for conventional population modeling tools while also incorporating its own C++ core for ODE solving and parameter estimation



RECORD streamlines the preparation of reproducible modeling reports in key formats including R Markdown, DOCX, and PPTX.



AI assistant

Local AI assistant is aligned with regulatory principles for AI in drug development – including explicit context of use, risk-based oversight, data governance, lifecycle management, and transparency [5,6] – and is further augmented by an internal knowledge base.

SimuRg

Model development conducted within the ecosystem can be readily exported to R scripts, allowing full reproduction of the workflow. The whole pipeline could be done using both the GUI and the **SimuRg** (poster I-102) package with same results and outputs.

Plugin templates and scripts

- For plugin development Simurg exposes templates that can be easily refined to cover expert knowledge with vibe coding procedure
- Scripts (R and Python) can be reused for plugin development with Docker containers with specific environments

Conclusions

Simurg is an ecosystem for pharmacometricians that unifies three paradigms – script-based workflows, an application-driven GUI infrastructure, and local human-in-the-loop AI assistance – into a coherent environment for executing end-to-end modeling workflows. Future directions include development of a more specialized AI agent capable of directly invoking ecosystem functions, expansion of no-code tooling for custom plugin creation, and integration of additional intelligent modules to further support analysts across the modeling lifecycle.

References

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