THE NANOINFORMATIX PLATFORM

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Introduction and Objectives

In the EU Horizon 2020 NanoInformaTIX project we are developing a sustainable data management and multi-scale modelling framework to facilitate the (eco)toxicity and exposure assessment of engineered nanomaterials (ENMs). This framework will be implemented as a web-based platform specifically tailored to the needs of stakeholders from industry, regulatory bodies and academia. The platform can connect relevant databases to *in silico* models covering Materials, Exposure, Physiologically-Based Pharmacokinetics (PBPK), Quantitative-Structure-Activity Relationships (QSAR) and System Biology to support *in vitro-in vivo* extrapolations (IVIVE), grouping and read-across for regulatory risk assessment and safe by design purposes.

The platform has been specifically designed to: 1) enable user-friendly access to relevant databases and *in silico* models according to stakeholders' needs, 2) facilitate addition of new models or extending existing ones by defining additional input and output requirements, and 3) be interoperable enough to seamlessly connect to external data repositories and models that are currently not part of the platform.

Methods

The databases and models are linked to the platform by means of a common Application Programming Interface (API), while to establish interoperability between models and/or data repositories we have adopted the Modelling Data Elements (MODA) scheme of the European Materials Modelling Council. This enables the user to design chains of data sources and models corresponding to specific analyses of relevance for the safety assessment of ENMs (e.g. prediction of genotoxicity, dose-response assessment, IVIVE, grouping, read-across). Results of the analyses will be presented as both dynamic charts and textual reports.

The technical implementation of the platform is graphically described in Fig. 1. All the services described in Fig. 1 are running inside Docker containers.

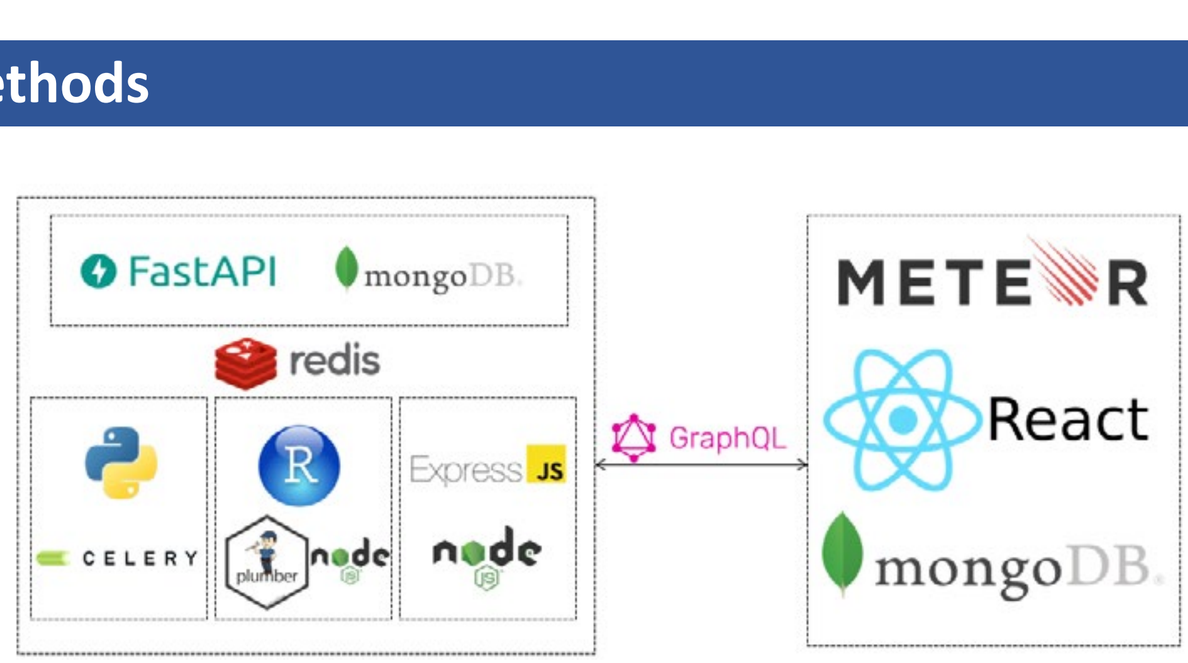

Fig. 1: Schematic overview of the technical implementation of the current version of the NanoInformaTIX platform. The frontend is based on Meteor and React, while the backend is based on FastAPI, and currently supports executing models programmed in R, Python or JavaScript. Data is stored in MongoDB.

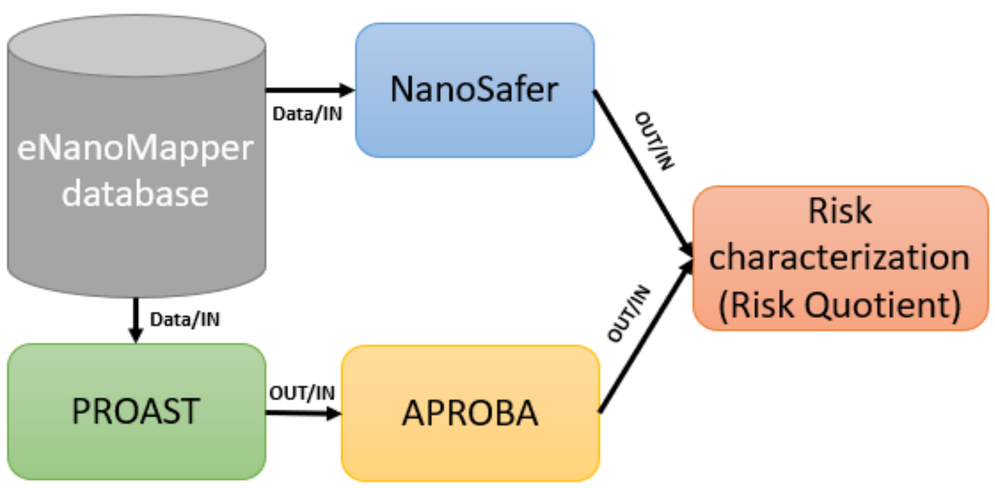

Fig. 2: An example of a chain of models (i.e. NanoSafer, PROAST, APROBA). This chain allows estimating risk for Human Health in an occupational scenario.

In the platform, each model is described by a Manifest file. The Manifest file is a JSON document which specifies the set of inputs (alongside with data type and domain) and the expected outputs of a model.

To be able to create a chain of models to perform a specific task, the models' inputs and outputs are matched to each other based on specified ontologies entries. An example of a chain of models for performing risk assessment is presented in Fig. 2.

To obtain optimal confidence in the use of the platform, the models, their inputs and outputs, their applicability domains, and the steps to create the model chains will be carefully documented according to established standards and Good Practices.

Conclusions

The NanoInformaTIX platform is currently under development. A first prototype of the platform will be available to project partners and stakeholders by the end of summer 2020, while the final version will be released in 2023.

Acknowledgments

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