Experience and Lessons Learned From Transnational Access Activities for Nanosafety and Advanced Materials Stakeholders

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NanoCommons
Nano-Knowledge Community

Introduction

The Horizon 2020 (H2020) e-infrastructure project NanoCommons brings together a multidisciplinary group of experts covering the entirety of the nanosafety research data lifecycle (Figure 1, experimental planning, data management, data capture, processing and analysis, computational tools, databasing) to deliver a sustainable and openly accessible nanoinformatics framework for the risk assessment of nanomaterials. This framework (knowledgebase and integrated computational tools) is supported by expert advice, data interpretation and training from the NanoCommons consortium members. In this way, NanoCommons becomes a one-stop-shop offering the necessary skills to meet the expectations and needs of stakeholders (academia, industry, regulators) in the rapidly evolving, cross-disciplinary landscape of modern research.

Aims & Objectives

- To bring together the necessary expert skills, tools and services covering the entire data management lifecycle, with a focus on nanosafety data.
- To offer an accessible state-of-the-art expertise and services framework, free of charge, to all stakeholders involved in nanosafety research, commercialisation and regulation.
- The tools and services focus on:
  - the design and implementation of modern data management and semantic annotation services from the outset of experimental and computational workflows;
  - the use of image analysis tools for the extraction of dedicated nanodescriptors;
  - the development and implementation of modelling workflows.
- The Data Shepherd role has been introduced to oversee and facilitate communication between the data generators (experimentalists, analysts, modellers), the database managers and data customers (regulators, industry etc.) as shown in Figure 1.

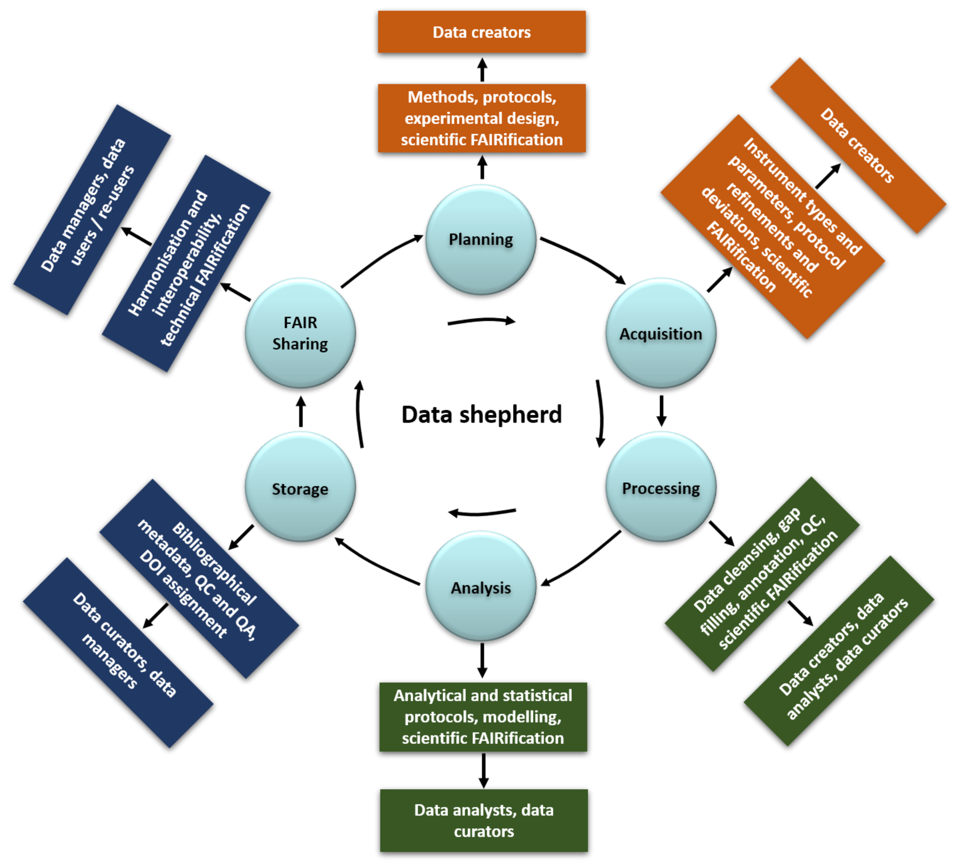
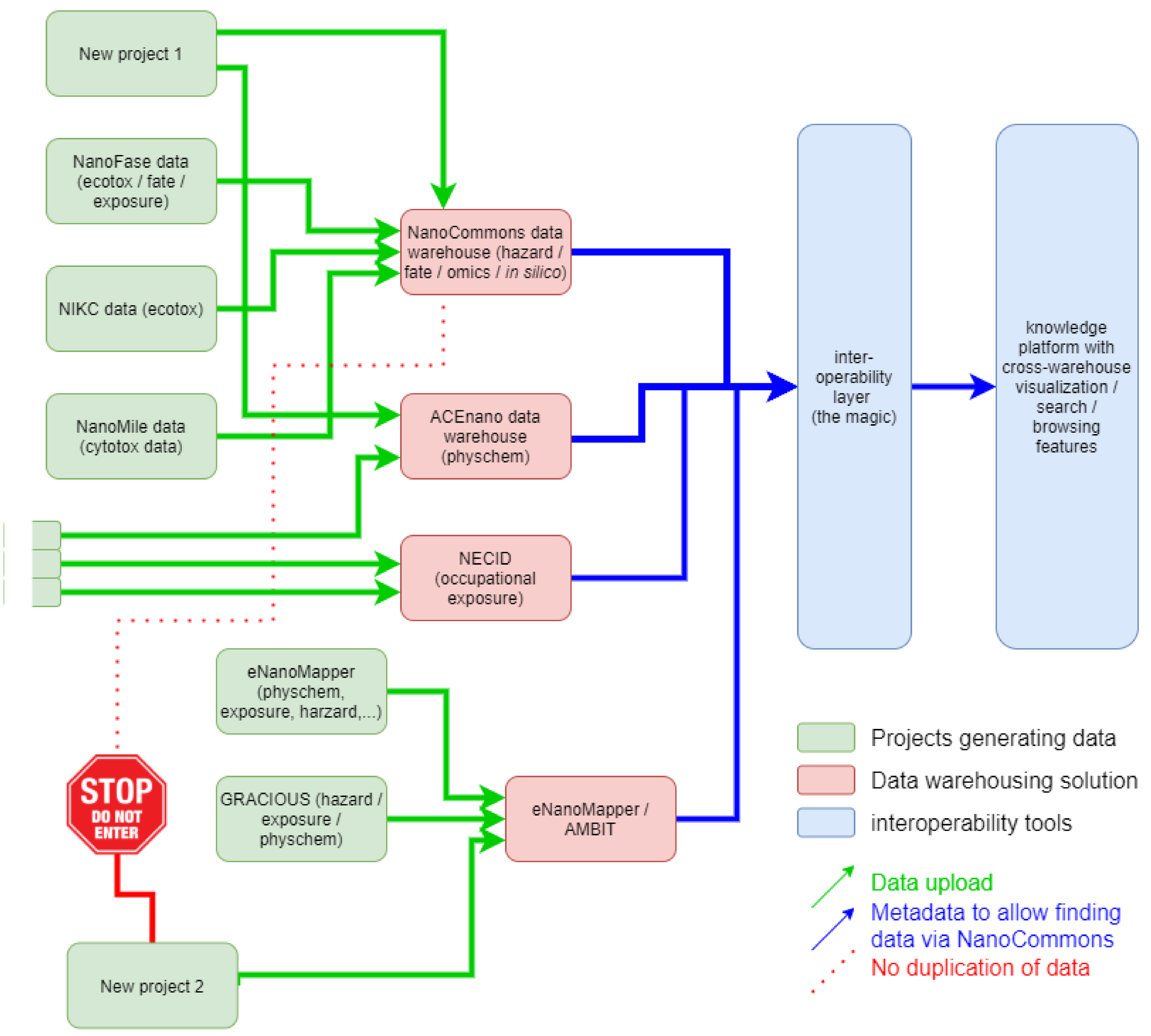
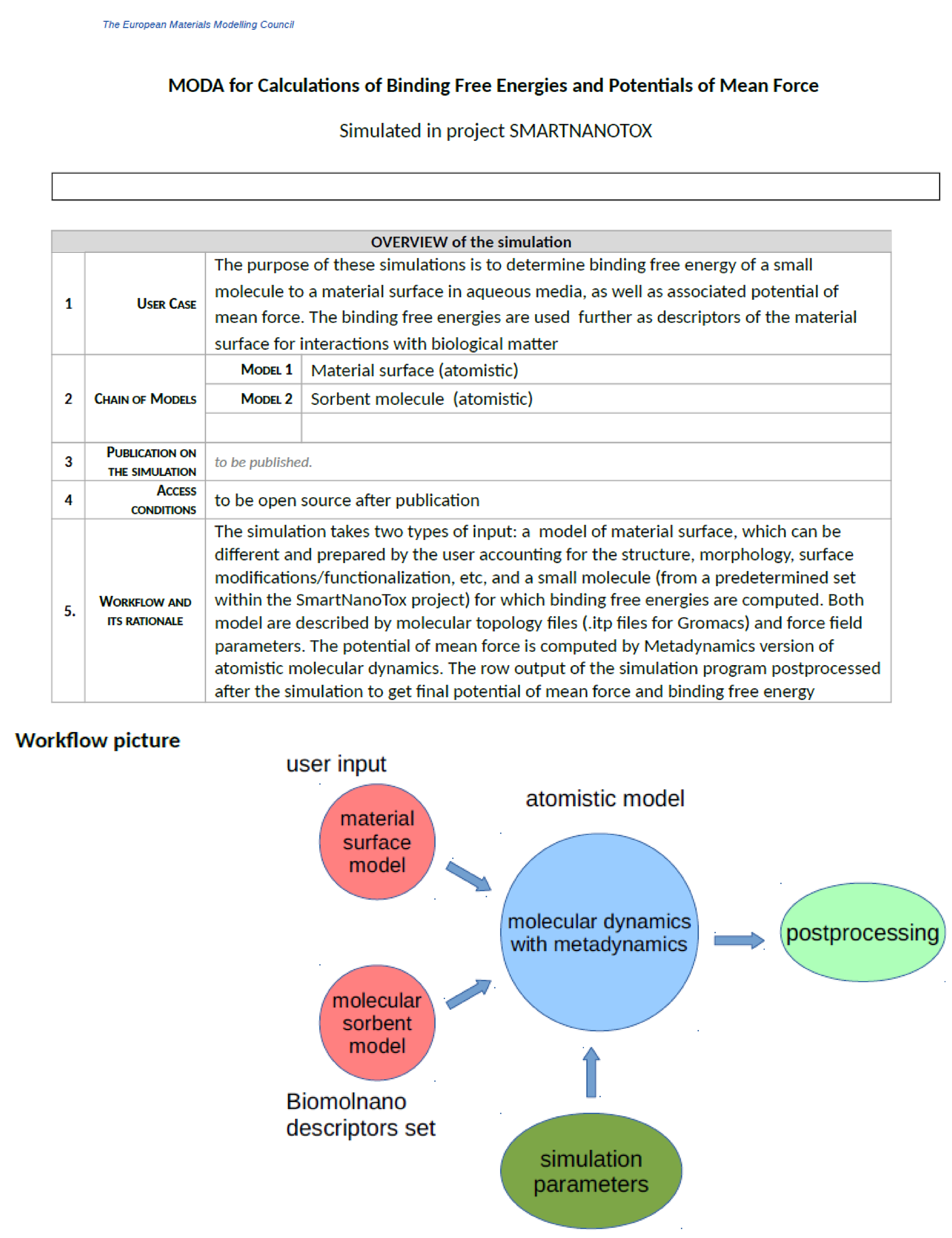


Figure 1: The data lifecycle and the newly found role of the data shepherd.

Selected Case Studies



Case Study 1: The NanoCommons Knowledgebase points the user to data offerings, similar to how an app store is proposing apps based on the users need for a specific application. This is achieved by indexing metadata from the different databases and making it searchable via a common interface. The user is transferred to the respective data warehouse for data accessibility. The NanoCommons KnoweldgeBase can be accessed at https://ssl.biomax.de/nanocommons/cgi/login_bioxm_portal.cgi



The European Materials Modelling Council

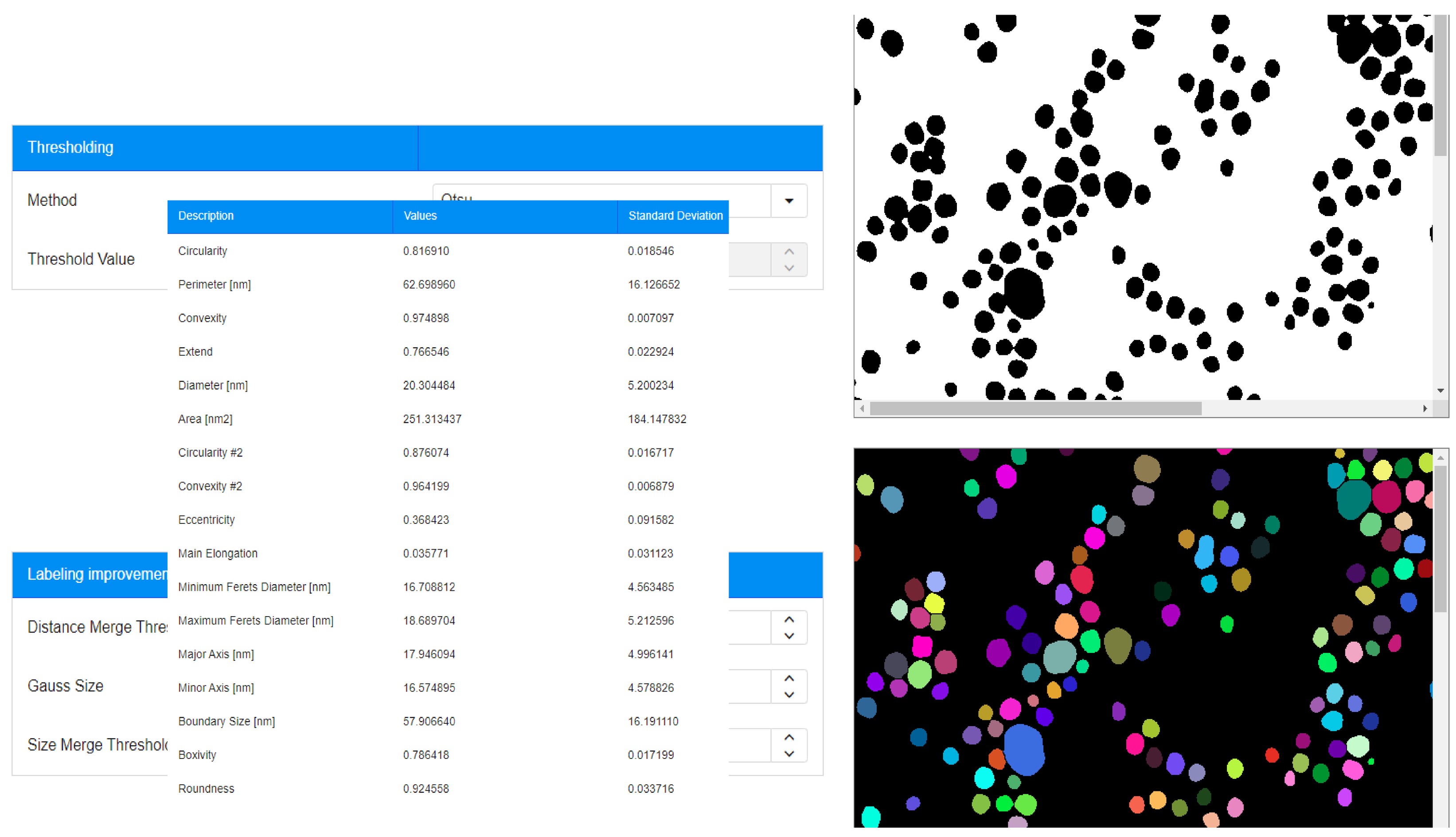
MODA for Calculations of Binding Free Energies and Potentials of Mean Force

Simulated in project SMARTNANOTOX

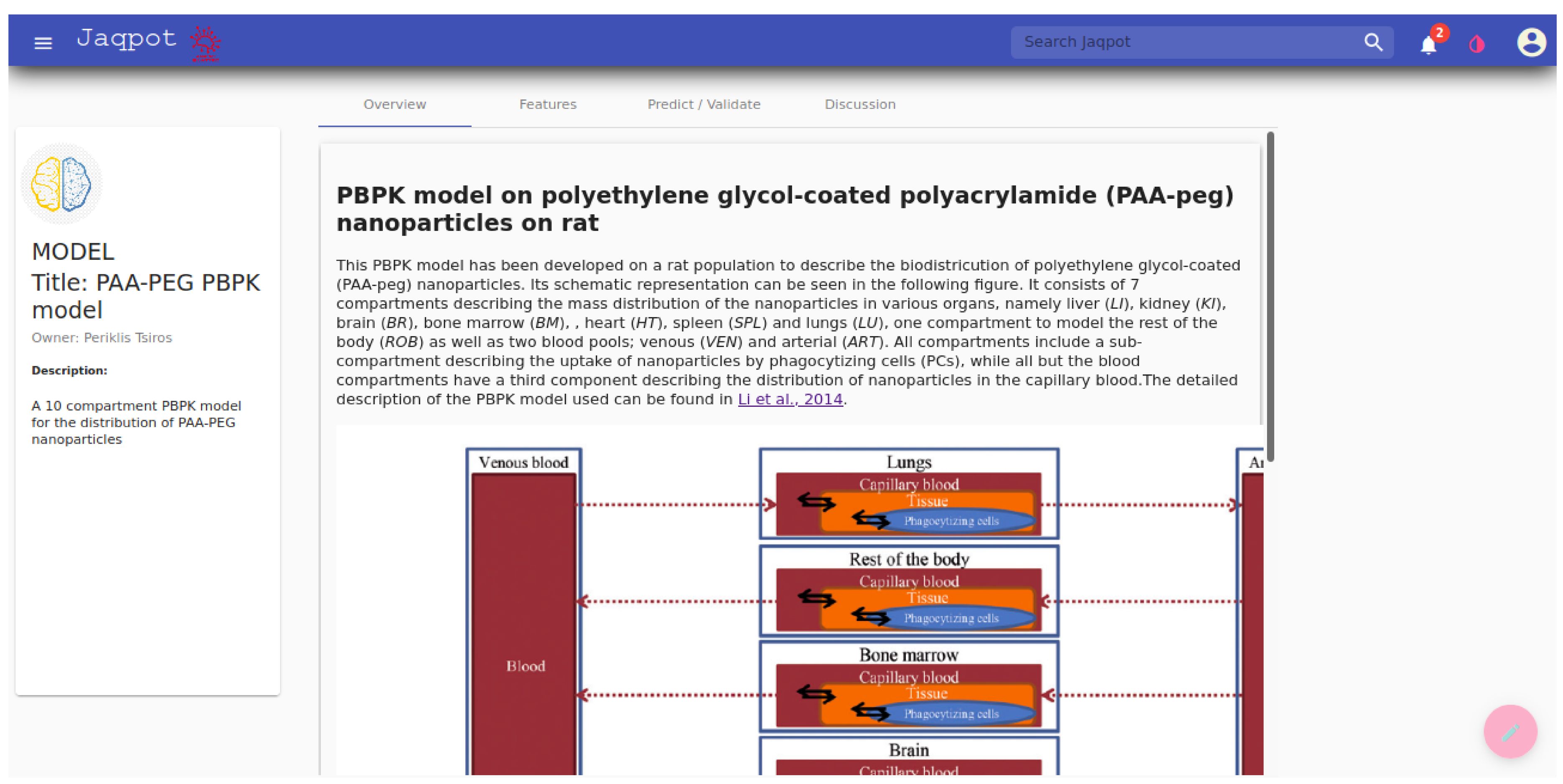
OVERVIEW of the simulation			
1	User Case	The purpose of these simulations is to determine binding free energy of a small molecule to a material surface in aqueous media, as well as associated potential of mean force. The binding free energies are used further as descriptors of the material surface for interactions with biological matter	
2	Chain of Models	Model 1	Material surface (atomistic)
		Model 2	Sorbent molecule (atomistic)
3	Publication on the simulation	*to be published.*	
4	Access conditions	to be open source after publication	
5.	Workflow and its rationale	The simulation takes two types of input: a model of material surface, which can be different and prepared by the user accounting for the structure, morphology, surface modifications/functionalization, etc, and a small molecule (from a predetermined set within the SmartNanoTox project) for which binding free energies are computed. Both model are described by molecular topology files (.itp files for Gromacs) and force field parameters. The potential of mean force is computed by Metadynamics version of atomistic molecular dynamics. The row output of the simulation program postprocessed after the simulation to get final potential of mean force and binding free energy	

Workflow picture

Case study 2: Implementation of a Modelling Data Capturing Template (MODA) developed in collaboration with the H2020 SmartNanoTox project. The purpose of the current model is the study nanomaterial interaction with biological matter. This is achieved through the determination of the binding free energy of a small molecule to an nanomaterial surface in aqueous media, as well as the associated potential of the mean force. NanoCommons is working closely with SmartNanoTox for the curation of all experimental and computational data (via TA).



Case study 3: Calculation of TEM image nanodescriptors for spherical Ag nanomaterials using the NanoXtract tool: Nanoparticles Image Analysis Tool Powered by Enalos Cloud Platform. The tool can generate a set of 18 image descriptors that greatly enhance and enrich the information extracted from images and which can be explored using predictive modelling to identify those descriptors most predictive of nanomaterials behaviour and/or biological effects. Collaboration with NanoSolveIT project. The tool is available at http://enaloscloud.novamechanics.com/EnalosWebApps/NanoXtract/



Case study 4: Physiologically-based pharmacokinetic (PBPK) modelling is used for predicting the biokinetics of a substance in an organism, and has recently been extended and successfully applied for describing nanomaterial's biokinetics. A web service for hosting PBPK models (https://app.jaqpot.org) was established, bridging the gap between PBPK developers and end-users. The Li et al. PBPK model was deployed on Jaqpot as part of NanoCommons TA activities, to increase model visibility and allow simulation and testing of biodistribution scenarios by users. Li et al. 2014, https://doi.org/10.3109/17435390.2013.863406

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HORIZON 2020

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