The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators (NanoCommons)

Reporting

Project Information

NanoCommons

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Coordinated by
THE UNIVERSITY OF BIRMINGHAM
United Kingdom

Periodic Reporting for period 3 - NanoCommons (The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators (NanoCommons))

Reporting period: 2021-01-01 to 2022-06-30

Summary of the context and overall objectives of the project

NanoCommons brings together academia, industry and regulators to facilitate pooling and harmonising of methods and data for modelling, safe-by-design product development and regulatory approval purposes, thereby driving best practice and ensuring maximum access to data and tools.

NanoCommons's objectives were as follows:
(1) To develop an integrated data and methods capture, management and nanoinformatics platform to enhance the accessibility and reusability of nano-related data and associated protocols (JRA).
(2) To provide funded and expert-supported Access to a range of data / knowledge management tools and nanoinformatics services to the widest possible range of stakeholders (TA).
(3) To continuously assess community needs in terms of services required, and align training offers, tools integrated into the TA portfolio and demonstration case studies to address these needs (NA).

Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far

The final 18 months focused on (1) expanding the range of tools, models and data integrated into the NanoCommons Knowledge Infrastructure; (2) maximising community uptake of the tools, services and best-practice, through an extensive training programme and the demonstration cases; (3) delivery of the TA programme through in depth engagement with potential users; and (4) delivery of the NanoCommons Final conference and Nano-Week as an in-person event for the nanosafety community.

NanoCommons' mission was to move data management to the experimental design, planning and implementation phases,and to provide users with tools to support data and metadata capture into templates that are tagged with relevant ontology terms to direct databases on how to organise the data to allow it to be easily searched, organised, integrated with other data, and utilised in the development of predictive models for exposure, hazard and risk assessment. A key concept developed in NanoCommons, and already being taken up into other projects, is data shepherds who "herd" data from conception through to deposition in a long-term FAIR (Open) repository with all necessary metadata to allow its re-use by all stakeholders. JRA focussed on integrating existing models and tools, and bringing in approaches developed elsewhere: integration via Jaqpot computational workflows, KNIME nodes and the Enalos computational platform and NanoCommons KnowledgeBase which provides data to the models, and captures the resulting computational results, enriching the experimental data.

More than 30 TA projects provided services spanning four areas "Experimental Workflows Design & Implementation", "Data Processing & Analysis", "Data Visualisation & Predictive Toxicity", and "Data Storage & Online Accessibility". The networking & Training activities were central to supporting researchers in their transition to better nanosafety data management. The FAIRification prize, awarded at the the final NanoCommons conference in June 2022 was an important demonstration of

the community commitment to FAIR and Open science and data. The demonstration case studies addressed concepts and challenges that are “too big” for standard research grants and are used to demonstrate why research infrastructures are needed to advance communities towards maturity and self-sufficiency.

Access to all the services and approaches developed within NanoCommons, and the corresponding training materials is via: (i) NanoCommons Knowledge Base [1], (ii) NanoCommons User Guidance Handbook [2], (iii) NanoCommons tools/services [3], and (iv) NanoCommons training materials [4]. Maintenance of these four key outputs, and their use to support knowledge exchange, future reuse of the data and tools and updating with the evolving state of the art is guaranteed by project partners for the next 5 years at least.

This 3rd periodic report presents the summary and detailed results are reported in the accompanying Deliverable reports.

[1] https://ssl.biomax.de/nanocommons/cgi/login_bioxm_portal.cgi
[2] https://nanocommons.github.io/user-handbook/
[3] https://infrastructure.nanocommons.eu/
[4] https://nanocommons.github.io/user-handbook/training-courses/

Progress beyond the state of the art and expected potential impact (including the socio-economic impact and the wider societal implications of the project so far)

NanoCommons results have already begun to achieve impact as demonstrated by strong uptake of the concepts and solutions into different research projects, the increased availability of FAIR and open (nanosafety) data, the increased efficiency and effectiveness of nanosafety assessment by data reuse, and speeding up development of enabling and emerging technologies by increasing the level of digitisation in individual labs.

NanoCommons built a support system of data stewards and shepherds and a training environment, and strengthened awareness of the (commercial) value of high-quality data and its reuse, establishing data as the scientific currency. This was fostered by on-the-fly data management to generate structured, harmonised and FAIRer datasets, and tool access via application programming interfaces (API), supporting workflow management tools like KNIME, model hosting on Jaqpot and service deployment in EOSC.

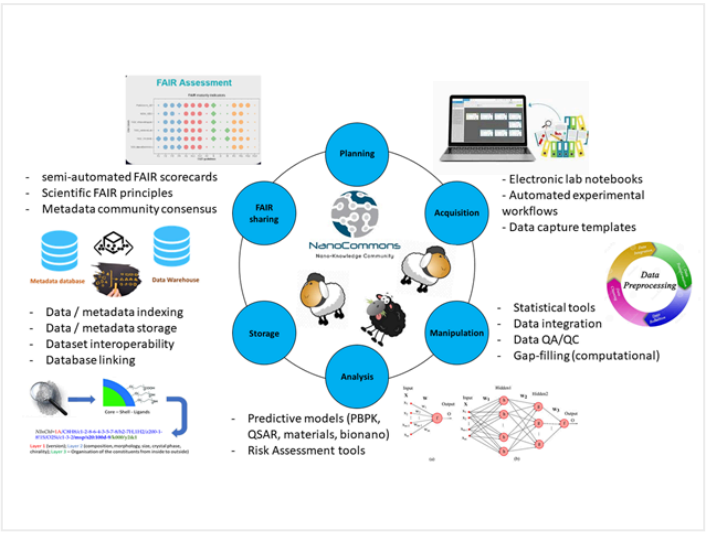
Nanomaterials (NMs) and advanced materials are defined by complex, multi-component structures, which need to be described by characteristics like core composition (possibly multi-layered); surface topography; surface coatings or functionalization. An additional complication is the dynamic nature of their properties that are influenced by the environment. As toxicity of NMs is largely due to their structure and surface properties, it is essential that detailed characterisation of the produced material and its fate is provided with each dataset to clearly specify the material under investigation and to

evaluate if it is the same material or similar to materials used in other studies. A computer-readable representation based on the IUPAC International Chemical Identifier (InChI) was used as the basis for developing the nanomaterial representation, the NInChI. The first prototype encodes chemical composition, size, morphology, crystallinity and chirality and allows complex core-shell structures, and is being transformed into a first version of the reporting standard.

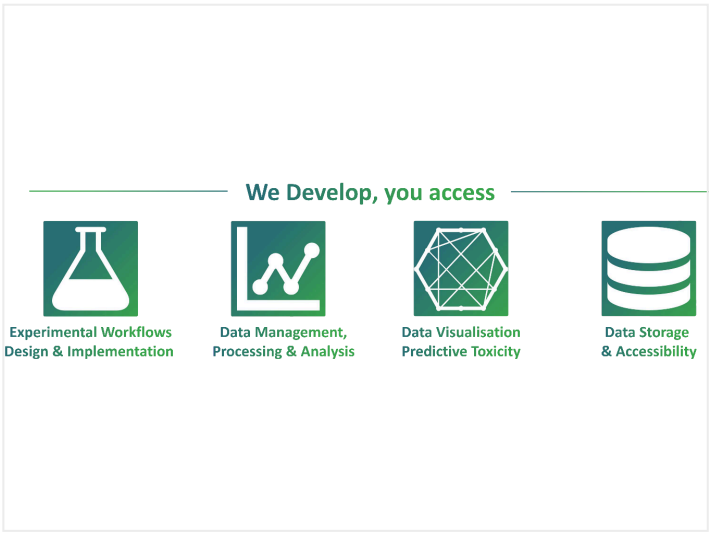
The most important changes to community practice driven by NanoCommons are:
1. On-the-fly data management, where data is reported as it is produced in a structured and harmonised manner. For this to become fully embedded into experimetnal workshlows, standardised data reporting formats, like the NANoREG and NanoFASE templates or the MODA/CHADA standards, need to be provided as data input tools independent of a specific database solution and must be usable for internal & external sharing.
2. Physics-based and data-driven models are documented in a standardized format (QMRF, MODA) and provided in a standard form, e.g. within the Jaqpot platform or/and as a web-services via Enalos Cloud Platform.
3. Interoperability between software and platforms (KnowledgeBase, Jaqpt and Enalos) supported by harmonised APIs & by integration into workflow management tools like KNIME allowing direct access to data and tools.
4. Knowledge exchange and dissemination of new concepts, approaches, tools and services using the NanoCommons User Guidance Handbook and the NanoCommons Service listing.

The NanoCommons User Guidance is important to transition the NanoCommons infrastructure project into the community-driven NanoCommons infrastructure.

nanocommons-logo.jpg



nanocommons-data-lifecycle-and-tools.png



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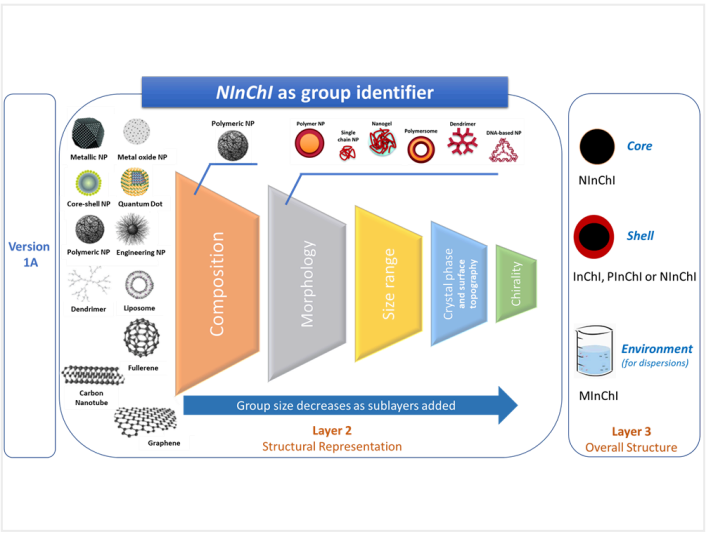

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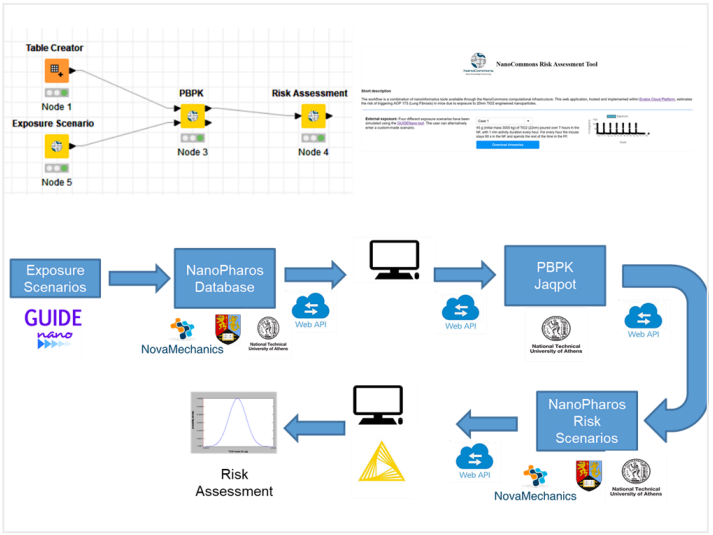

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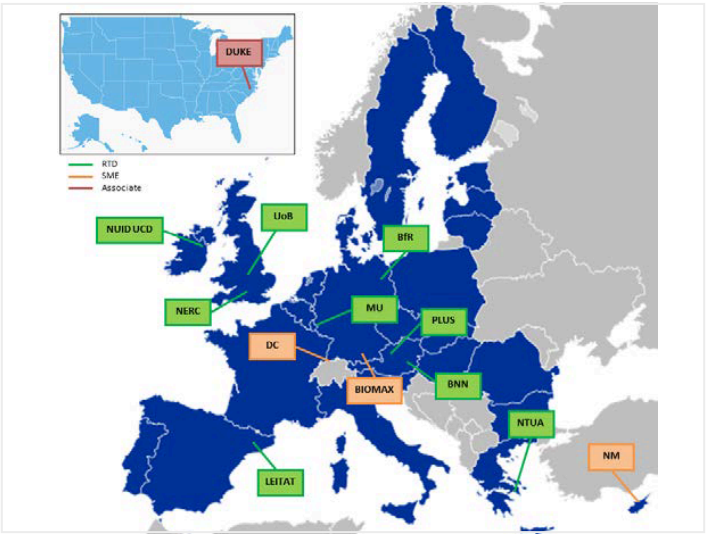

nanocommons-partner-map.png

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