

NanoSolveIT NanoInformatics Models and Tools for the Risk Assessment of Nanomaterials



EuroNanoForum 2019

Session 3.3 Open Science and Industry Commons
June 12-14, 2019, Bucharest, Romania

Antreas Afantitis PhD, MBA
afantitis@novamechanics.com

NovaMechanics Ltd
Cheminformatics & Nanoinformatics Excellence
www.novamechanics.com



This project has received funding from
the European Union's Horizon 2020
research and innovation programme
under grant agreement No 814572



Innovative **Nano**informatics models and tools: towards a **Solid, verified** and **Integrated Approach to Predictive (eco)Toxicology (NanoSolveIT)**

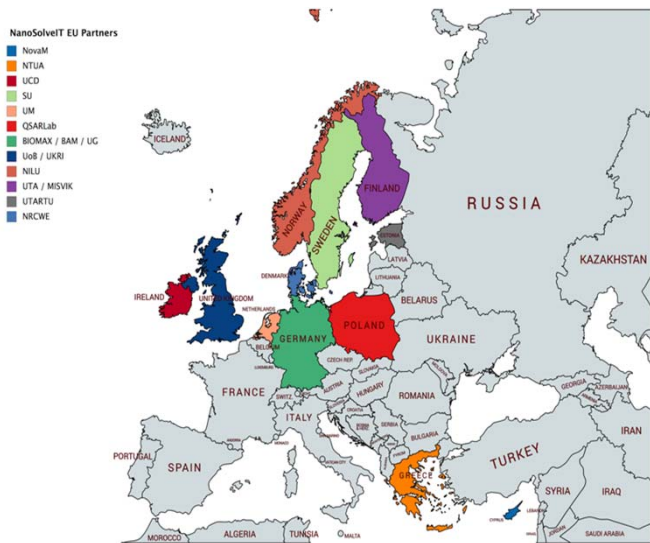
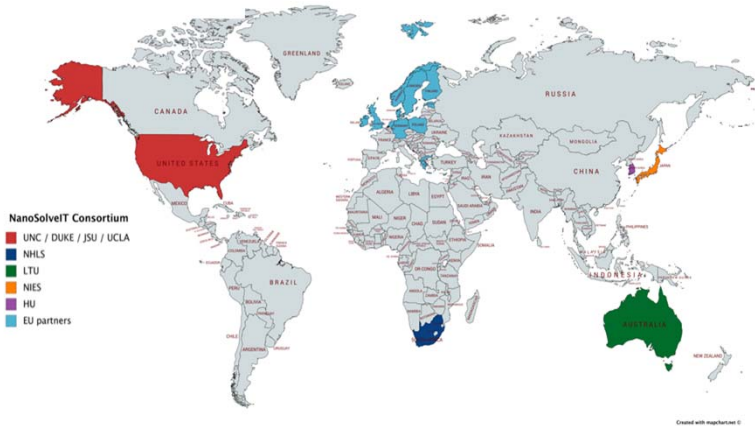
NanoSolveIT aspires:

- To introduce a ground-breaking in silico Integrated Approach to Testing and Assessment (IATA)
- Environmental health and safety of Nanomaterials
- Implemented through a decision support system packaged as both a stand-alone open software and via a Cloud platform.

NanoSolveIT consortium

24 Partners

16 European (12 Countries) -
8 International (5 Countries) Institutes



NanoSolveIT will develop and deliver:



a reliable user friendly knowledge-based infrastructure for data hosting, sharing and exploitation



NM fingerprints, sets of nanodescriptors and properties that can be predictively linked to NM functionality, exposure and hazard, thereby supporting NM grouping, safe-by-design (SbD) and regulatory risk assessment (RA)



innovative methodologies for NMs predictive (eco)toxicology underpinned by artificial intelligence (AI) and state-of-the-art in silico techniques

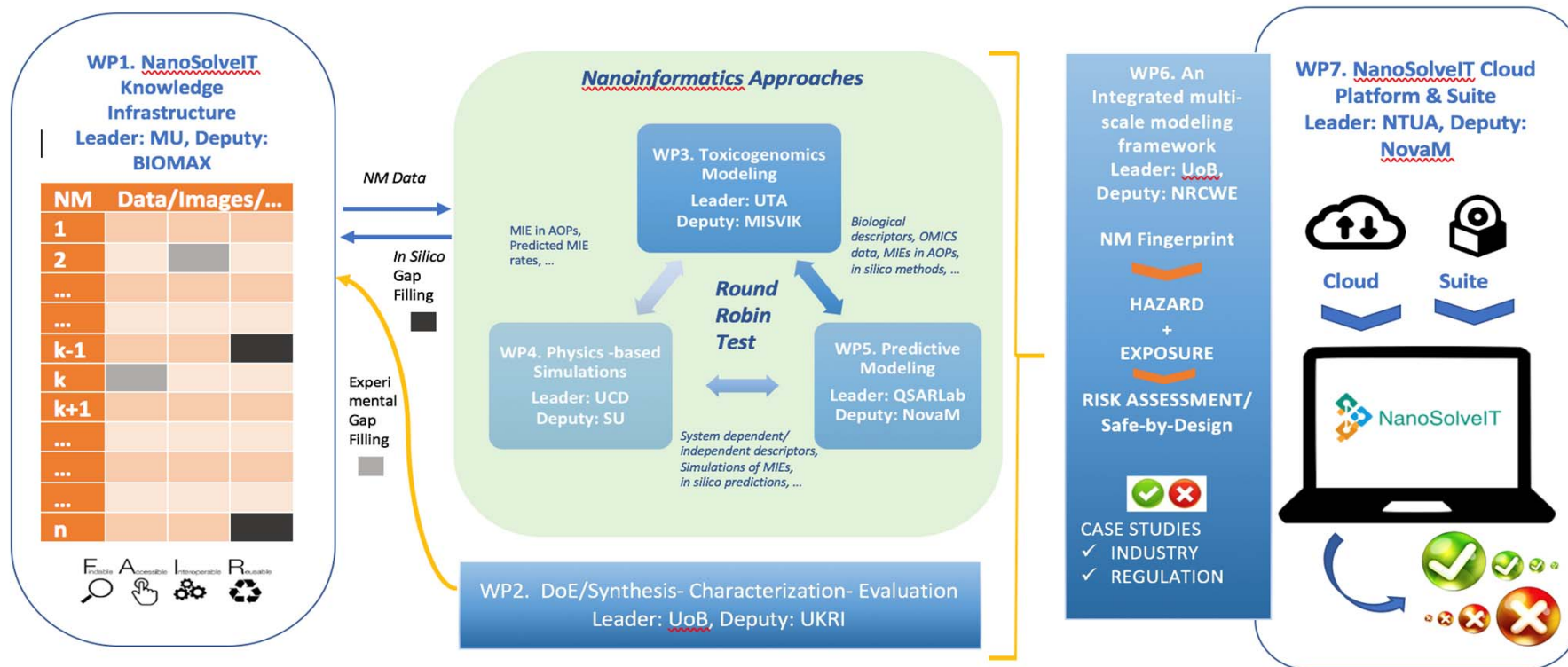


Integration with RA and governance frameworks developing in EU H2020 funded projects



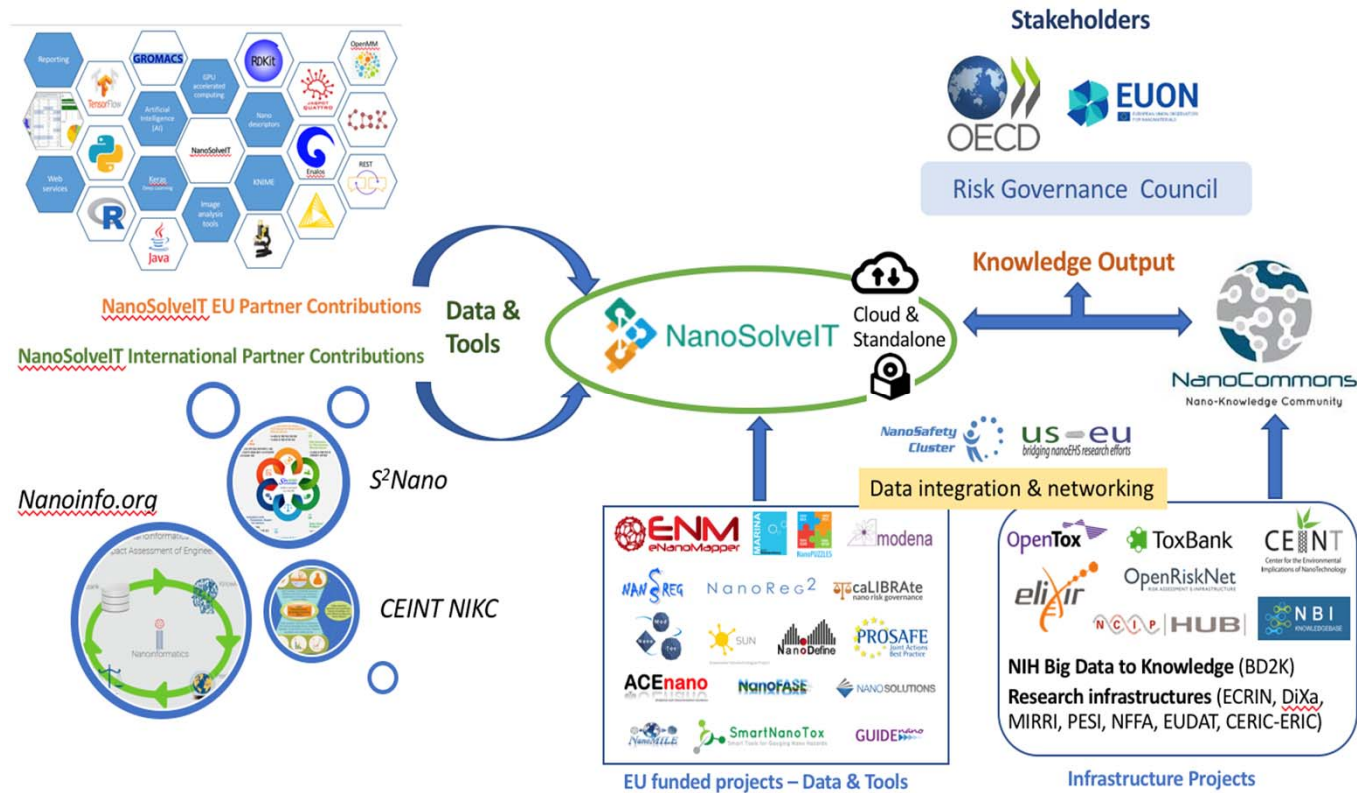
A validated, sustainable, multi-scale nanoinformatics IATA, tested and demonstrated at TLR6 via OECD-style case studies, to serve the needs of diverse stakeholders at each stage of the NMs value chain, for assessment of potential adverse effects of NM on human health and the environment.

NanoSolveIT Overview WPs Interlinkages



TRL 3-4 → TRL 5-6 → TRL 6-7

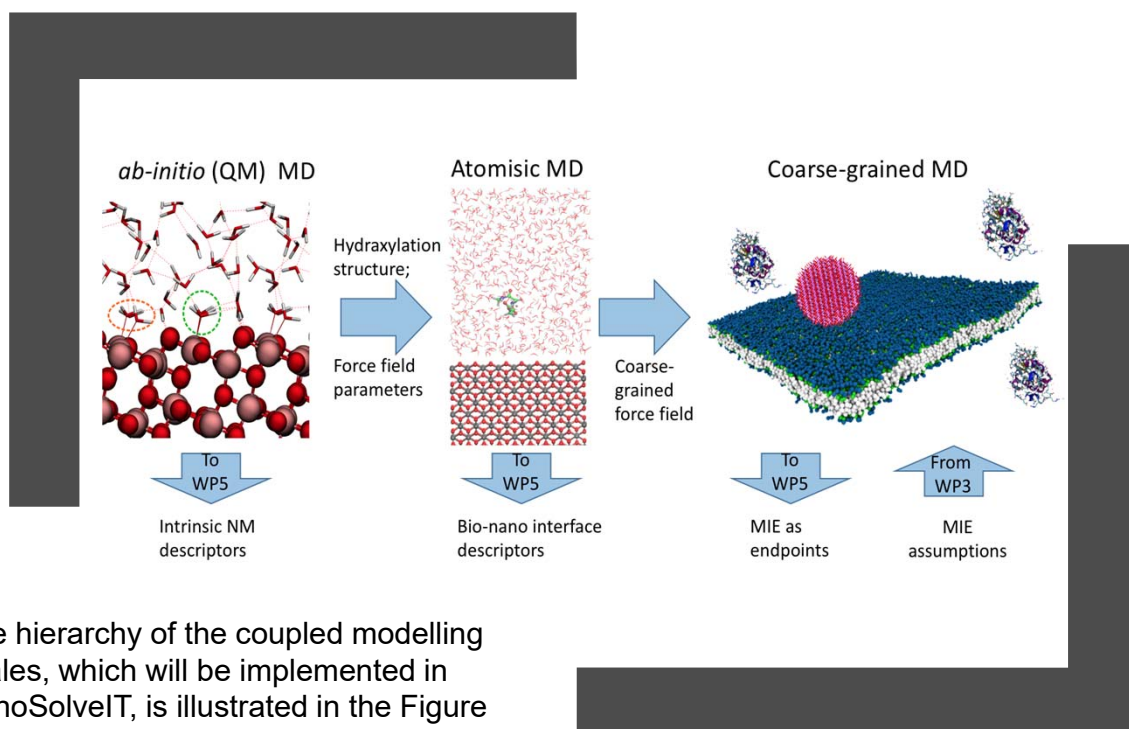
NanoSolveIT's positioning and liaison with other initiatives



Promoting Open Science - Common data structures

- NanoSolveIT Knowledge Infrastructure will be developed to collect, FAIR-ify, and share data on NMs characteristics, biological interactions, and adverse outcomes.
- The infrastructure will be based on the NanoCommons / eNanoMapper platform and ontology concepts and will use a clear Open Science approach to ensure sustainability.
- All available information will be fully exploited through Open Access and Open Data Access policies and will align the activities with EU-US Nanoinformatics 2030 Roadmap, ELIXIR, eNanoMapper and EMMO ontologies, and ISA-NANO format for data logging.
- Cutting-edge research data management approaches
- Maximize International Synergies
- Novel data-gap filling approaches.
- Development of NanoSolveIT e-platform.

Promote and support the development of safe by design approaches



- Predictions without the need for any experimental input
- Utilizing only knowledge of system structure and composition
- NanoSolveIT IATA will enable NMs developers to screen NMs *in silico* before actually producing them
- Ensuring that the properties of concern are reduced or eliminated, which would make the NMs safe by design (SbD).

Promote and support the development of safe by design approaches



Advances in accessibility of the model platforms and underpinning datasets



Novel nanodescriptors based on ground-breaking *in silico* techniques developed for NMs



Read-across considering the multi-perspective characterisation of NMs.



Towards an Alternative Testing Strategy. Development of NanoSolveIT e-platform

Biokinetics



An application of pharmacokinetics to determine the relationship between the systemic exposure of a compound and its toxicity. It is used primarily for establishing relationships between exposures in toxicology experiments in animals and the corresponding exposures in humans.

[Launch Application](#)

Models Database



Predictive modeling uses statistics to predict outcomes. Most often the event one wants to predict is in the future, but predictive modelling can be applied to any type of unknown event, regardless of when it occurred.

[Launch Application](#)

NanoSolveIT Cloud Platform

Exposure Modeling



Mathematical exposure modeling is an indirect method of determining exposure, particularly for human exposure to environmental contaminants. It is useful when direct measurement of pollutant concentration is not feasible because direct measurement sometimes requires skilled professionals and complex, expensive laboratory equipment.

[Launch Application](#)

Predictive Modeling



Predictive modeling uses statistics to predict outcomes. Most often the event one wants to predict is in the future, but predictive modelling can be applied to any type of unknown event, regardless of when it occurred. For example, predictive models are often used to detect crimes and identify suspects, after the crime has taken place.

[Launch Application](#)

Predictive Modeling

Predictive modeling uses statistics to predict outcomes. Most often the event one wants to predict is in the future, but predictive modelling can be applied to any type of unknown event, regardless of when it occurred. For example, predictive models are often used to detect crimes and identify suspects, after the crime has taken place.

[Launch Application](#)



NanoSolveIT
H2020 Nanoinformatics Project

CONTACT US!



www.nanosolveit.eu



nanosolveit@novamechanics.com

FOLLOW US!



[@NanoSolveIT](https://twitter.com/NanoSolveIT)



Project
NanoSolveIT



NanoSolveIT



<https://github.com/NanoSolveIT>



[Home](#) [Overview](#) [Resources](#) [Communication](#) [Contact](#)



NanoSolveIT

Innovative Nanoinformatics Models and Tools



The project



Consortium



Tools



Library



Contact



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814572

Thank for your attention

www.novamechanics.com
afantitis@novamechanics.com



NovaMechanics