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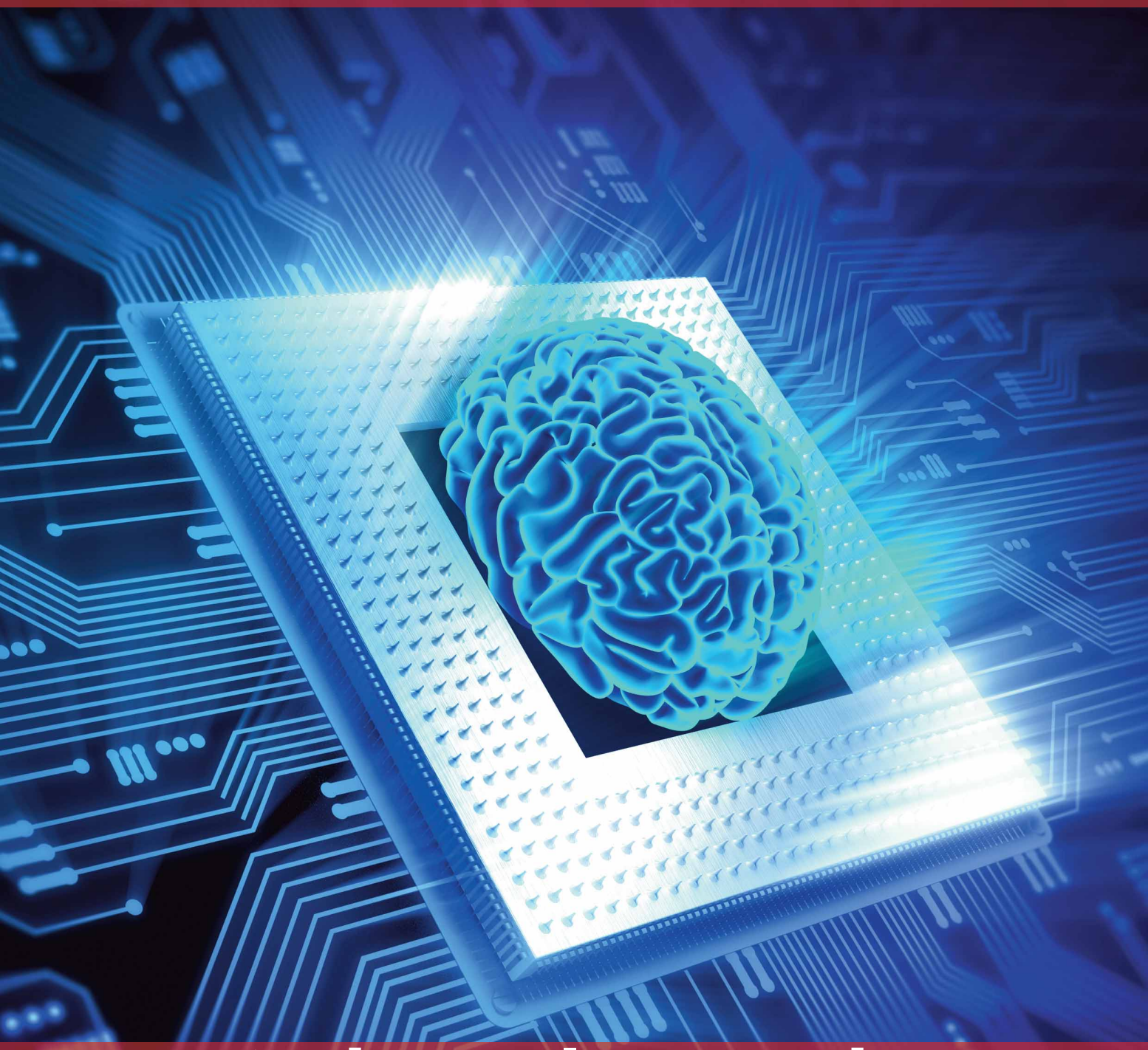

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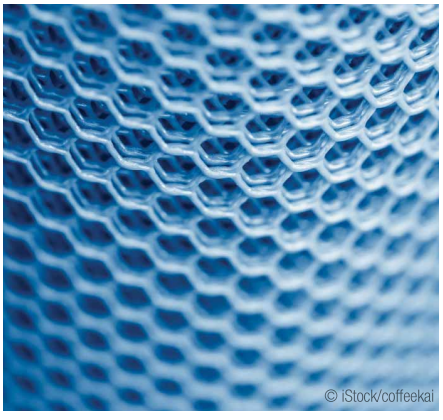
Driving the nanoinformatics wave

The NanoCommons research e-infrastructure and NanoSolveIT projects are developing the knowledge management and nanoinformatics tools to support *in silico* nanosafety assessment

The sheer range of different nanomaterial compositions available, spanning most of the periodic table of elements, and with extensive variation possible in terms of size, shape, surface functionalisation etc. means that there are over 20,000 different nanomaterials being developed in labs around the world. Assessing the safety of these (and all chemicals) is a costly and time-consuming process, requiring extensive characterisation and an increasing suite of *in vitro* (cellular) and *in vivo* (animal) tests as the production volume increases. One of the most significant challenges at present is understanding how different one nanomaterial needs to be from another in terms of its size, shape, and surface chemistry in order to be classified, from a regulatory perspective, as a distinct nanoform that requires separate hazard and risk evaluation.

Given the inherent distribution in particle size, shape, and likely surface chemistry in a single batch, determining the thresholds or cut-offs for distinct nanoforms is a challenge. The Horizon 2020-funded projects NanoCommons and NanoSolveIT are thus developing a suite of nanoinformatics tools to address this challenge, as well as to replace costly animal experiments with predictive *in silico* testing that leverages existing datasets to predict the properties and effects of new nanomaterials.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The consortia

NanoCommons, a research infrastructure project which started on 1 January 2018 and which will run for 48 months, brings together 12 European and two US partners, providing a critical mass of internationally-recognised researchers and bioinformatics specialists with complementary skills and a proven ability to deliver knowledge-related services for the community and its wide stakeholder base.

Importantly, expertise from all of the related fields including chemistry and materials science, engineering, physical, mathematical, statistical, environmental and biological sciences is represented from the experimental side, and is complemented with expertise in bioinformatics, Big Data, computational sciences, software, hardware and ontology development.

NanoSolveIT, a research and development project which started on 1 January 2019 and will run for 50 months, brings together 16 partners from EU and associated countries and eight international partners from the USA, Australia, South Africa, Japan and South Korea. These European and international teams have individually or in small groups developed the current state of the art in nanoinformatics. Through each of its partners, NanoSolveIT inherits invaluable knowledge from previous projects and initiatives including

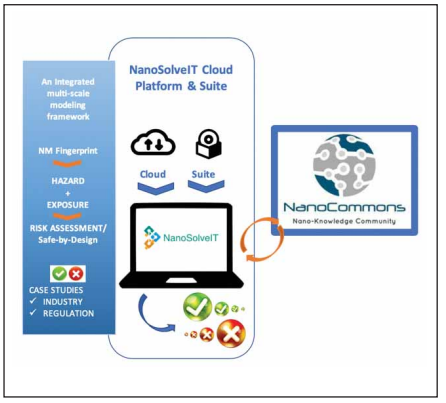

Fig. 1 Illustration of the NanoSolveIT nanoinformatics platform

nanomaterials characterisation, (eco)toxicology, environmental and human exposure data, Standard Operating Procedures (SOPs) and benchmarking, predictive modelling, and software applications interlinked with Application Programming Interfaces, thus providing an important leap forward for nanoinformatics deployment and acceptance.

NanoCommons solutions

To address the challenge of assessing the human and environmental safety of the enormous variety of nanomaterials reaching the market, NanoCommons is working to integrate the existing disparate and poorly accessible datasets on nanomaterials' environmental fate and toxicity by annotating them to the community-developed ontology and by semantically mapping them to support their interrogation, with the overall goal of making them findable, accessible, interoperable and re-usable (FAIR).

In addition, NanoCommons is developing approaches to move the curation of nanosafety

datasets to earlier in the data lifecycle, from being something that is done at the end of a project to being integral to the experimental planning and data collection steps. This is being achieved through the development of electronic notebooks linked to the NanoCommons database and ontology, allowing data capture templates to be set up as part of the experimental design and ensuring that data is collected in the optimal format for subsequent searching, mining, and use in model development and risk assessment.

As part of its services to the nanosafety community, NanoCommons is offering fully funded access to its tools and services via six-monthly calls for nanosafety data management and nanoinformatics projects.

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NanoSolveIT solutions

NanoSolveIT's approach to accelerating the assessment of the safety testing of nanomaterials is to introduce a ground-breaking *in silico* (a computer-based approach whereby existing data is used to train predictive computer models) approaches, and to link these into a tiered approach of increasing complexity, leading to an Integrated Approach to Testing and Assessment (IATA) for the environmental health and safety of Nanomaterials (see Fig. 1).

The resulting *in silico* approach will be implemented through a decision support system packaged as both a Cloud platform and as a stand-alone open software for industry users concerned about their proprietary data. Key innovations being developed in NanoSolveIT include:

- The concept of 'nanomaterials fingerprints', sets of nanodescriptors and properties that can be predictively linked to a nanomaterial's functionality, exposure, and hazard, thereby supporting the grouping and categorisation of nanomaterials, safe-by-design approaches, and regulatory risk assessment
- Innovative methodologies for the predictive (eco)toxicology of nanomaterials, underpinned by artificial intelligence (AI) and state-of-the-art *in silico* techniques

The resulting computational toolbox will dramatically reduce the need for the animal testing of nanomaterials in the future by utilising existing data to validate the predictive power of the machine learning and *in silico* approaches, thus reducing the cost and time required for assessing the safety of nanomaterials.

NanoSolveIT

NanoCommons
Nano-Knowledge Community

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