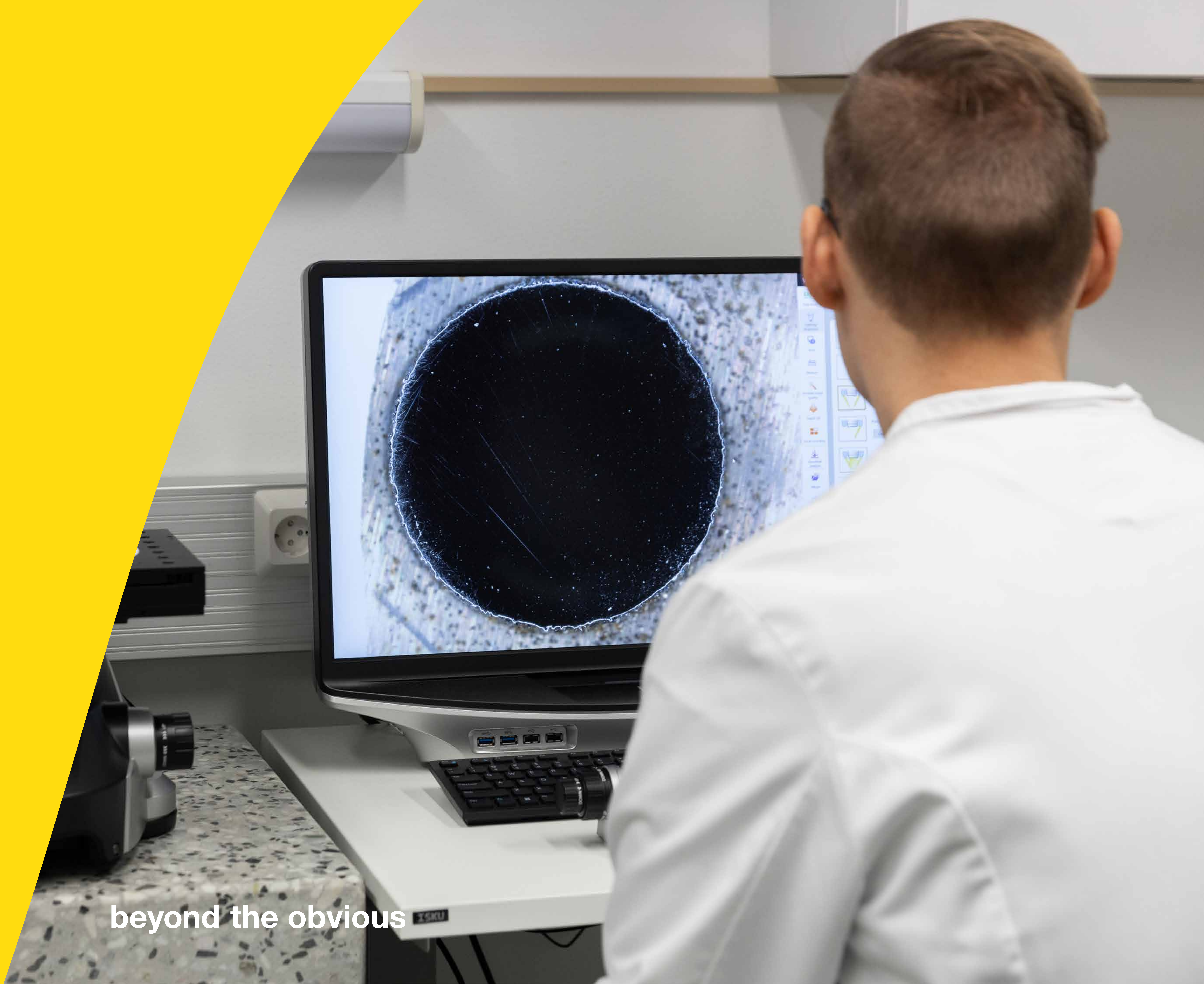
VTT

From ICME towards MAPs –

Unlocking new material innovations



beyond the obvious

Introduction

In today's world, the critical themes of sustainability, energy transition and resource scarcity are reshaping the landscape for material innovation. This confluence of factors emphasises the pressing need for advanced material solutions with improved functionalities and performance. The call is not just for progress, but for a transformative shift towards better performing, environmentally friendly and circular materials.

At the same time, the race to develop new solutions faster and more cost-effectively is getting tougher every day across all industries. Moreover, new regulations banning, for example, single-use plastics and non-recyclable packaging are being introduced around the world.

Navigating these new waters is made possible through accelerated material development fuelled by integrated computational material engineering (ICME). It allows us to explore novel materials, boost innovation and contribute to the development of more sustainable products. Using material modelling, you can predict the behaviour and properties of materials under different conditions in a fully virtual environment. By doing so, you can streamline the development process, minimise costs, optimise material performance and unlock the potential for revolutionary advancements in material science and technology.

In this publication, we will decipher what computational material modelling is and highlight the exceptional outcomes made possible by it. We'll walk you through how VTT ProperTune® material modelling is already being used to create extraordinary material innovations and introduce the next big thing: Materials Acceleration Platforms (MAPs). We'll wrap up with three powerful visions for the future.

Contents

1. Computational material modelling – what is it and what does it deliver?

Today, most material development is still done by iteratively creating a prototype based on an idea and testing it in the lab to see if it works as expected — a process that is both expensive and slow.

Computational, performance-based material development is always based on knowledge – rather than just wild ideas. This shift takes us from an Edisonian approach to scientific discovery to an era of inverse design, where the desired properties of the material drive the solution. It allows us to predict the behaviour and properties of materials under different conditions in a fully virtual environment, eliminating the need for extensive physical testing and costly trial-and-error processes.

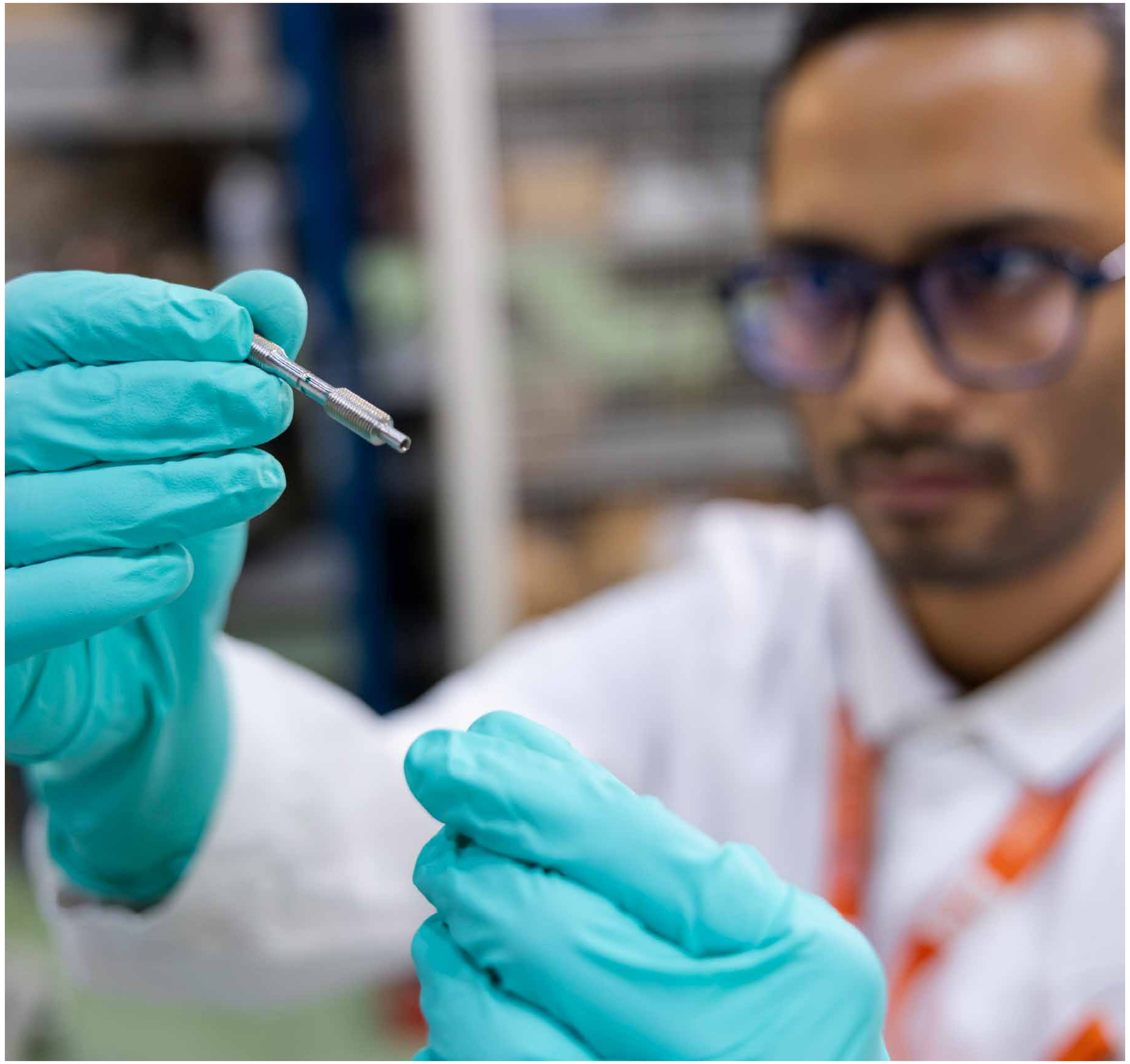
Experimental data and validation of computational material modelling

The development of all material models is based on understanding of physical phenomena. Experimental data is used to validate the accuracy and reliability of computational models. By comparing the model predictions with real-world experimental results, you can assess the model's effectiveness and make necessary adjustments. This interplay of experiments and modelling is critical for the overall success of computational material modelling.

Once the model has been built and validated, it can be used to run a near infinite number of what if scenarios. What if there were this much more of ingredient A? What if the manufacturing process used a higher temperature? Getting answers to these questions by creating accurate models in realistic conditions virtually eliminates the need for expensive, time-consuming testing and shortens the time to market.

VTT ProperTune® shortens the time-to-market for new products by 50%

VTT has been helping companies optimise material properties for over 20 years with a solution called VTT ProperTune®. It is an Integrated Computational Materials Engineering (ICME) concept that uses multiscale modelling for optimal computational material design. It allows us to model material behaviour from atomistic level properties to material manufacturing and real-life application in a fully virtual environment.



VTT ProperTune® can be used to optimise a wide variety of material properties, such as electrochemical properties (e.g. corrosion resistance, battery energy density) and mechanical properties (e.g. wear, fracture and fatigue) just to name a few. Accurate modelling can be applied to almost any material and coating ranging from biomaterials, metals and plastics to composite structures.

So far, we have described what can already be achieved with computational material modelling. However, the tale doesn't end here; we are on the brink of a transformative change. In the next chapter, you'll learn that the stage is set for a cut in the development time of new materials by 90%.

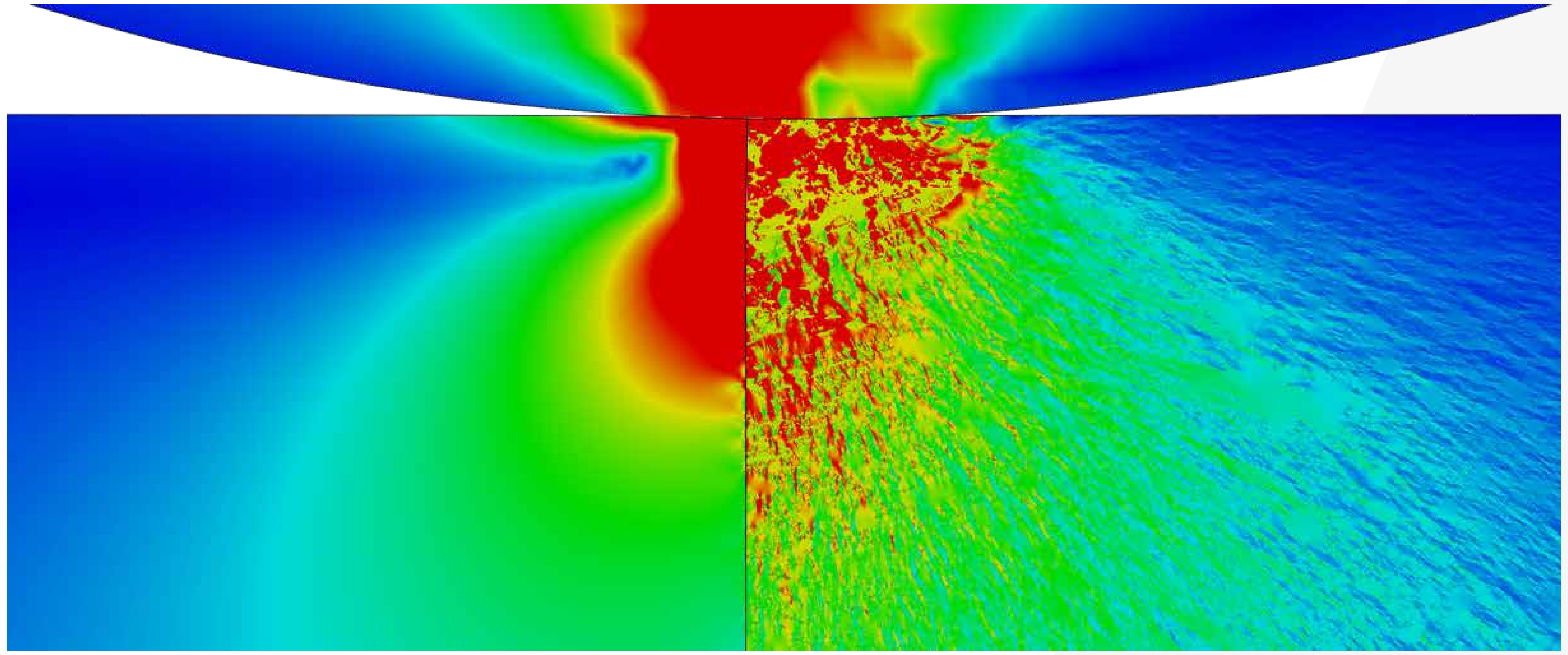
SUCCESS STORY:
ArcelorMittal – Discovery and design of new steel grades, performance improved by ~200–250%.

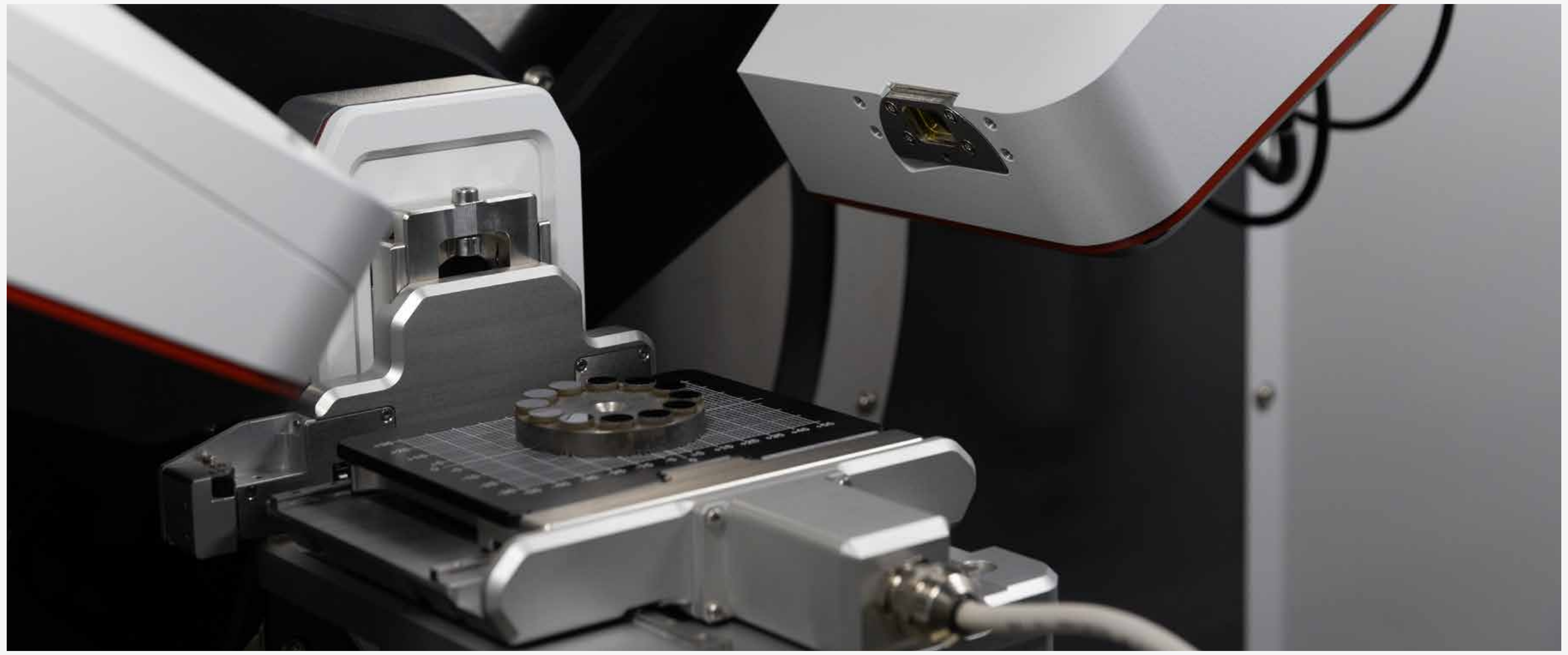
ArcelorMittal is the leading steel producer in the world, supplying quality steel to all major steel markets including automotive, construction, household appliances and packaging.

The company needed to develop a high-performance steel grade that was more wear-resistant than any of their previous steel grades. The parameters for the development project were very strict: the factory's manufacturing process could not be modified, and costs could not increase.

Using VTT ProperTune®, VTT created three new steel formulations that, as predicted by the models, more than doubled the wear resistance. ArcelorMittal produced the steel grades based on the formulations and confirmed in real-world conditions that they did indeed last up to 2.5 times longer than any of their previous steel grades. Moreover, the new steel recipes were finalised in less than half the time typically experienced by the customer.

Through computational material modelling, we were able to take an unconventional idea, model it at the microstructure level and determine what in the application is more durable.





2. The next big thing: Materials Accelerator Platform (MAP)

MAPs, or Materials Acceleration Platforms, are comprehensive research and development systems that combine computational and experimental tools like multiscale materials modelling, artificial intelligence (AI), high-throughput sample manufacturing and characterisation and testing. This integrated approach aims to expedite the material design process, ultimately cutting down costs and time involved in the material development.

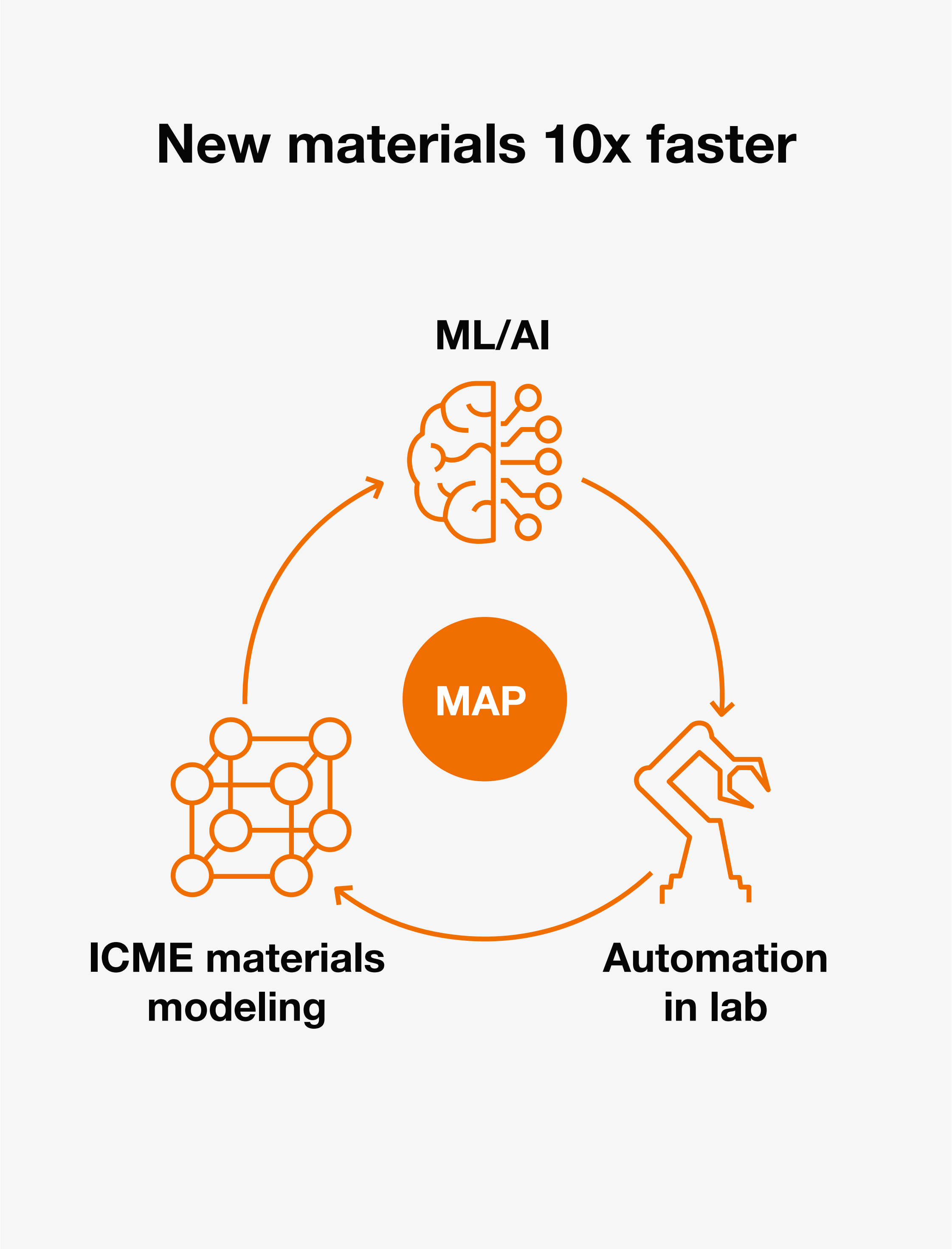
The success of MAPs hinges not on any single technology, but on the synergy of diverse capabilities working together to achieve outcomes greater than the sum of their parts. MAPs are not only about optimisation of existing materials but about discovering novel materials and solutions and creating market disruption: Used right, they can reduce development time by 90%.

2.1. Key features of MAPs

Experimental and computational integration: In MAPs, there is a shift towards integrating experimental and modelling techniques seamlessly, feeding and orchestrating information exchange between the two as concurrently as possible. This includes efficiently generating required experimental data with high-throughput methods. In addition to using experimental data to support the construction of models and formulation of modelling hypotheses, it is simultaneously used to validate the model's accuracy and functionality. The data generated through modelling feeds into the design of targeted experimental work.

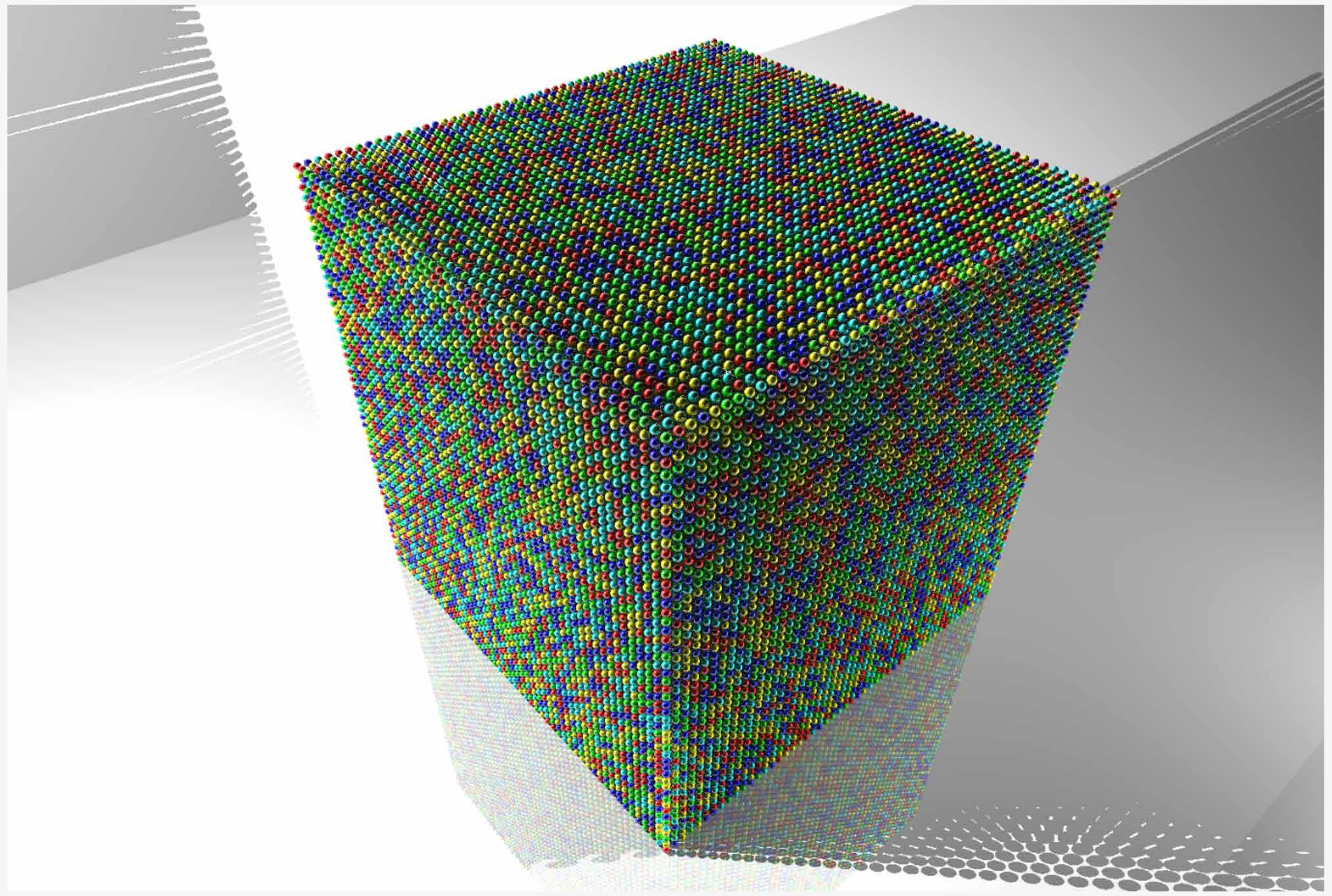
Multiscale modelling: Multiscale modelling facilitates the study of behaviours and properties of materials across multiple scales simultaneously. By moving between atomic, microstructural and macroscopic scales, you can examine how the desired outcomes can be achieved across scales exploiting hierarchical features of materials in the most cost-effective way.

While problems often present themselves at a macro level, such as a product or a component needing specific capabilities to withstand certain conditions, the process of resolving the problem commonly takes place at a completely different modelling level. At the microstructural level, you can examine, for example, the effects arising from the elemental composition of the material or the parameters influenced by the manufacturing process, i.e. the temperature, pressure or manufacturing method that will produce feasible material characteristics.



AI-accelerated development: There are several ways AI accelerates material development, common examples in the following.

- **Faster screening and inverse design:** Physics-based models can only create and screen a limited solution space due to computational constraints. To expand possibilities, machine learning methods such as surrogate models are employed to efficiently navigate the solution space, uncovering and discovering the most potential designs.
- **Leveraging generative and agent driven AI for creating novel structures:** Generative AI offers a solution when the desired material properties are known but, for example, the exact structure to achieve them isn't. Generative AI can suggest novel structures based on the required properties and the databases provided. This capability not only accelerates the materials discovery process but also opens up possibilities for designing advanced materials with tailored characteristics and functionalities that were previously inaccessible through traditional methods.
- **Automation:** With AI, you can automate and significantly speed up the experimental processes. Machine learning models can be, for instance, fed with substantial SEM image data, enabling them to learn to identify and analyse key features such as cracks, pits, corrosion-induced cracks, crystal structure distribution and more, replicating the observations and insights typically made by a human analyst. Or then simply always improve experimental design of experiments. This automation optimises the modelling workflow, enabling faster insights and distillation of knowledge.



CASE:
MAP in action – Development of a Materials Acceleration Platform (MAP) for high entropy alloys (HEA)

VTT has developed a SOLID-MAP platform for high throughput alloy development by combining computational materials engineering, artificial intelligence, high throughput sample processing and testing.

In a use case, we used active learning-based surrogate modelling and CALPHAD simulation to screen suitable chemical compositions for high entropy alloys. This was followed by further thermodynamic screening and first-principles density functional theory simulations to select a group of HEAs based on their mechanical properties. Samples of these novel alloys were then fabricated with high throughput direct energy deposition (DED) from elemental powders by on-line alloying and using optimised process parameters.

Finally, the SOLID-MAP process was completed by characterisation of processed HEA candidates by using automated x-ray diffraction, scanning electron microscopy (SEM) characterisation and automated analyses of these measurements using AI based models.

The goal was to establish a seamless MAP chain: First, combining physics-based modelling and AI to screen the most promising solutions. Then, speeding up sample generation and testing significantly using high throughput automated workflows that allow for the creation and testing of multiple samples swiftly.

With the current setup, the DED device is capable of automatically producing 4 times 12 sample pallets of varying compositions within 24 hours, which results in substantial advancements in time saved. A similar HEA metal alloy project using traditional means would take significantly longer.

3. Materials of tomorrow

The goal of performance-based material development and MAPs is simple: to unlock new material innovations that meet the demands of tomorrow. Let's explore a few examples of the types of materials we are striving towards.

3.1. Innovations in material behaviour modification

In demanding operating environments, such as high-temperature or corrosive environments, materials face significant challenges.

By altering the properties of materials, you can influence how the materials behave and react to these conditions. For instance, in a crusher crushing hard rocks, enhanced material properties can reduce the crusher's wear and tear. Similarly, you can modify the coating of wind turbine blades to resist abrasion from water, ice or sand to enhance durability.

The possibility to fine-tune the characteristics of materials by adjusting their composition and microstructure offers flexibility, making these materials suitable for various applications in challenging operating conditions.

For instance, advanced materials such as high entropy alloys (HEAs) exhibit promising attributes including strength, ductility, corrosion resistance and thermal stability while offering an extensive space for modification and development.

Development of sustainable bio-based materials

The world needs new sustainable alternatives to replace critical raw materials and fossil-based materials, ensuring the well-being of the planet and its inhabitants.

Bio-based materials are one way to address the need. They are inspired by nature and comply with nature's circular principles generating no waste.

When customised for specific applications, bio-based materials do not need to match fossil-based materials in all properties – only those essential for their intended use. For instance, wood-like bio-composite could be see-through, opening the door to a variety of new applications.

To bio-design future sustainable materials effectively, understanding the relationship between, for example, structure, properties and interactions in composite systems is essential. With computational material modelling and MAPs integrating the workflows of biotechnology and material sciences and engineering that can be achieved.

Novel soft materials with synthetic biology

Synthetic biology offers unparalleled flexibility in manufacturing raw materials, including various chemicals, polymers and proteins. This flexibility brings about a vast array of raw materials to explore, enabling the selection of materials suited for specific purposes. To expedite this process, ICME, synthetic biology and AI can be combined to form a MAP and be harnessed to create a comprehensive framework for uncovering novel soft materials. These materials can be leveraged to produce bio-based structural components like plastics and composites, as well as solvents, adhesives and alternative food products such as meat substitutes.

Novel functional materials

Functional materials are a fast-developing application area for MAPs. With MAPs, you can find new compositions and manufacturing processes to create novel functional materials that have customised magnetic, optical or electrical properties, use less critical raw materials and are more sustainable to process.

For example, tailored nanostructures can be used for many novel applications, such as electronics, biomedicine and energy storage. Self-healing materials can autonomously recover from mechanical stress or damage. They enable more durable, safe and sustainable products. These materials can be used in applications such as energy storage to increase lifespans.

4. Three visions for the future

With the help of MAPs, you can test even the wildest ideas quickly and cost-effectively. With the ability to virtually model and utilise machine learning algorithms, the process of screening potential solutions becomes significantly easier. Here's what we envision for the future:

4.1. Quantum technology integration paving the way for rapid material innovations

Most quantum experts believe we are going to reach quantum advantage within the next 5 years. For materials development, this means quantum computers could take on the high-intensity computational tasks within advanced modelling and simulations, thus ushering in a new era of rapid material innovation.

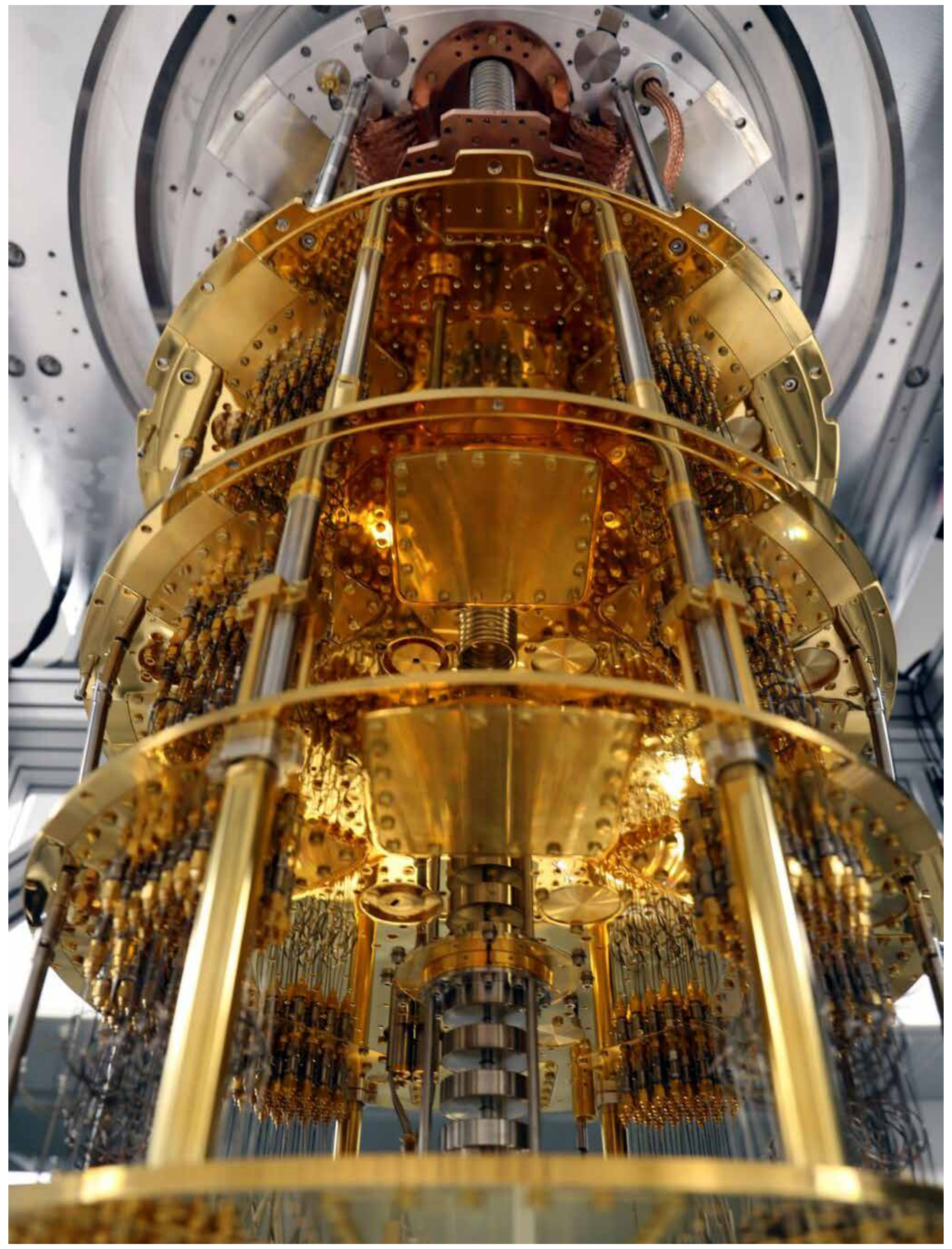
Quantum computers offer the potential to calculate previously unattainable tasks. As the scales and system sizes to study increase, the computational demands grow exponentially. With quantum computers, you can model complex interactions at the atomic and molecular resolutions deciphering how they subsequently influence higher-level behaviour and material properties. This advancement enables more precise predictions and opens new possibilities for understanding and designing complex material behaviours currently out of our reach.

4.2. Next-generation metamaterials: Reshaping materials development

Metamaterials are human-invented, artificial materials with greater capabilities than any naturally occurring material. By manipulating the structure and hierarchies of the materials across the scales, you can produce materials that don't exist in nature and achieve a wide range of advancements and capabilities. For example, functional smart materials with robotic-like reprogrammable functionalities can be enabled by mechanical metamaterials with inverse-designed nonlinear dynamic responses.

4.3. The breakthrough of data-driven generative AI

Currently, efforts are underway to harmonise and expand the availability of materials data produced within European research projects. As the repository of open material data grows, it morphs into a vast resource for advanced AI techniques. This progression will unlock the potential for creating tailored foundational and generative AI models specifically for materials. These models will be enriched by a mounting reserve and case specific high-throughput production of experimental and synthetic data, poised to autonomously propose innovative new material solutions.



5. VTT – your partner in solving even the toughest material challenges

With over two decades of experience, we have honed our expertise in computational material modelling. Our track record boasts successful collaborations with some of the world's most prestigious companies, positioning us as a leading global player renowned for our comprehensive capabilities.

We invest heavily in developing our quantum technology infrastructure, featuring an in-house quantum computer. Our investments also encompass diverse experimental infrastructure and capabilities.

By partnering with us, you get the benefits of:

- VTT ProperTune® – Integrated Computational Materials Engineering (ICME) concept that shortens the time-to-market for new products by 50%
- VTT's versatile experimental materials performance capabilities ranging from lab to pilot scale
- Our AI for materials (AI4M) expertise:
  - VTT's quantum computers and access to LUMI, one of the world's most powerful supercomputers
  - Our vast expertise across diverse material applications
- A multidisciplinary team of experts and a unique combination of modelling, testing and piloting, all under one roof.

Whether you are you looking to gain a competitive edge in materials innovation or seek to replace fossil-based materials with bio-based solutions, we can help you solve your material challenge.

Want to find out more?
Get in touch!

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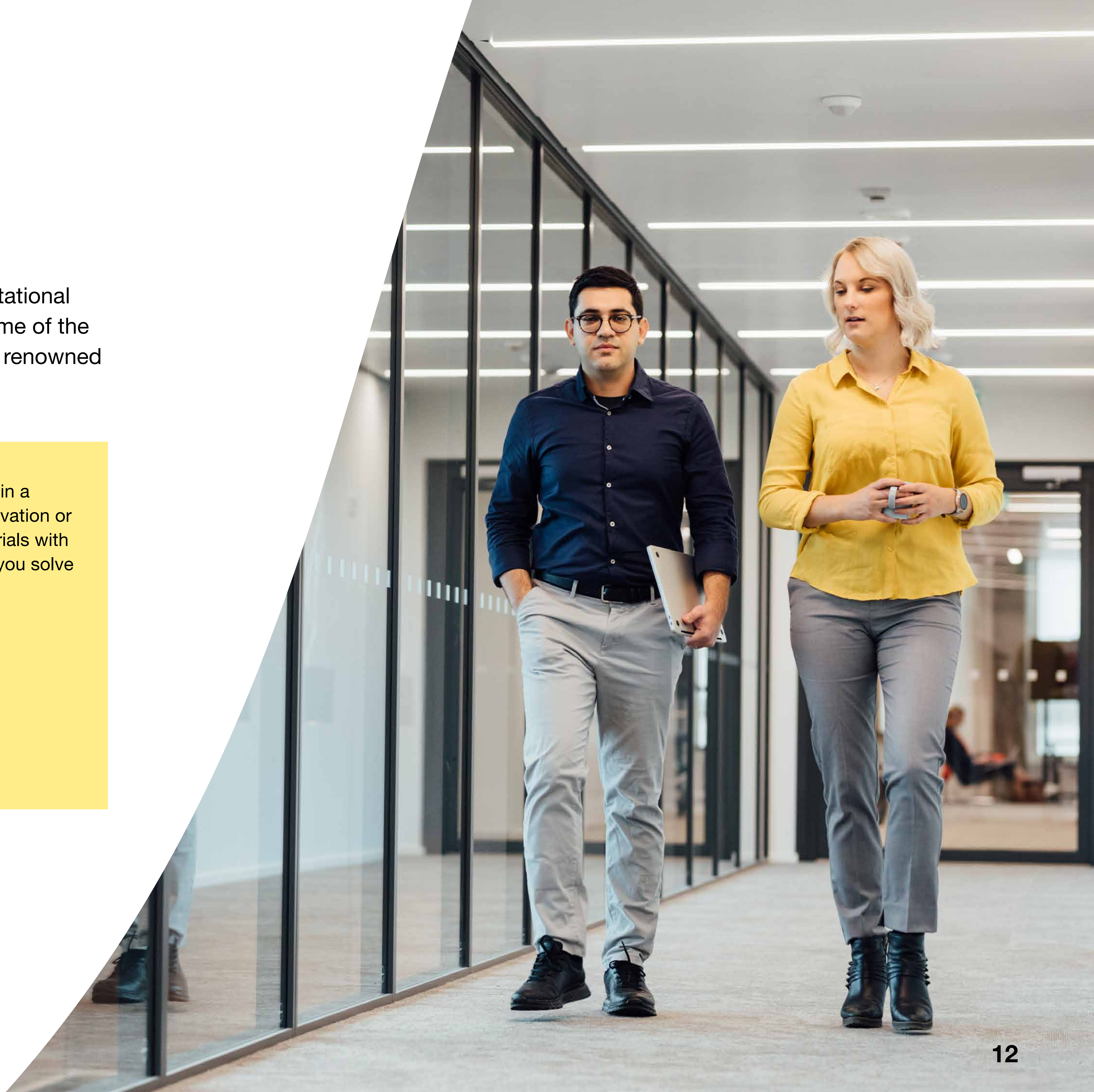

VTT

beyond the obvious

VTT is one of the leading technical research organisations in Europe, and we have over 80 years of experience in cutting-edge research and science-based results. Our more than 2,000 professionals work to develop systemic and technological solutions that can bring about fundamental transformation.

We promise to always think beyond the obvious.

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