M2i2 - Multiscale Materials Informatics & Innovation

TOWARDS A NEXT-GENERATION COMPUTATIONAL FRAMEWORK FOR PREDICTIVE MULTISCALE MATERIALS DESIGN, MANUFACTURING AND OPTIMISATION

white paper

This white paper presents a vision for a transformative multiscale materials modelling framework that enables predictive materials design, manufacturing process optimisation, and in-service performance simulation. Building upon the foundational principles of global initiatives such as Integrated Computational Materials Engineering (ICME), the Materials Genome Initiative (MGI), and Materials Genome Engineering (MGE), we propose a dynamic and integrated approach to connect material behaviour across spatial and temporal scales. Our proposed effort will establish a predictive modelling ecosystem that integrates high-fidelity simulations, virtual characterisation, and artificial intelligence (AI) tools. This initiative will deliver rapid, physics-based solutions to accelerate materials discovery, optimise manufacturing processes, and enhance the reliability of components in critical applications, including aerospace, nuclear energy, and high-value manufacturing.

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VISION: NEXT-GENERATION INTEGRATED COMPUTATIONAL MATERIALS SCIENCE

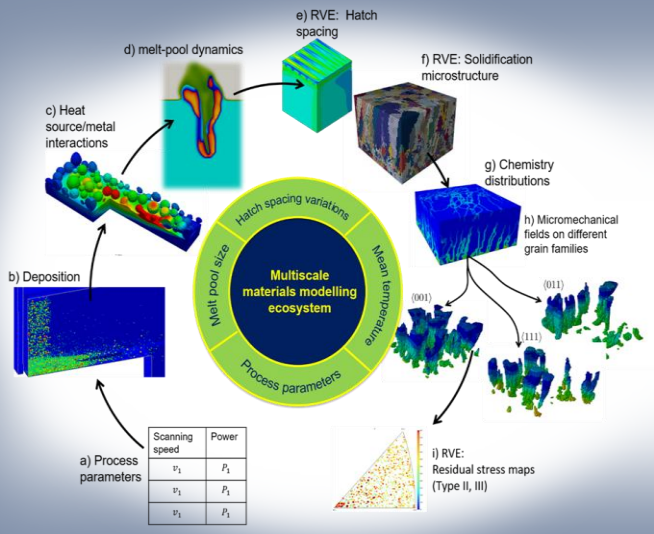
Materials innovation is central to technological competitiveness across aerospace, nuclear, automotive, and advanced manufacturing industries. Predictive materials modelling is no longer optional—it is essential for:

- Accelerating materials discovery by predicting new compositions and microstructures.
- Enhancing manufacturing process design by modelling process-structure-property relationships.
- Simulating in-service performance under complex operational conditions, such as fatigue, creep, and radiation damage.

However, unlocking these capabilities demands robust multiscale materials modelling that explicitly connects chemistry, structure, processing, and performance across length and time scales. Core capabilities of the framework:

- High-fidelity, physics-based simulations such as dislocation dynamics, cellular automata crystal plasticity linked to process models. z
- Advanced virtual characterisation techniques that can probe digital material representations under realistic service conditions.
- Artificial intelligence (AI) and machine learning (ML) tools for accelerating data analysis, extracting key features, and developing surrogate models.

The M2i2 framework integrates multiple modelling approaches to computationally derive process-structure-property relationships. For example, modelling additive manufacturing (AM) of engineering alloys, M2i2 workflows span powder deposition, melt pool dynamics, thermal history, microstructure evolution, and mechanical performance. AI models trained on these digital datasets can uncover optimal process parameters (e.g., laser power, scanning speed) to tailor microstructural features like grain size, texture, and defect density—enabling location-specific property control in 3D-printed components. These predictive capabilities for AM have received international recognition by winning the NIST AMBench 2018 and AMBench2022 challenges.



Multiscale material process model workflow for additive manufacture.

MATERIALS DIGITAL THREADS: BRIDGING SCALES AND SYSTEMS

At the heart of our vision is the creation of Materials Digital Threads—continuous, bidirectional data streams linking experiments, simulations, and operational platforms. These threads enable real-time integration of sensor data from manufacturing processes and in-service environments with physics-based simulations, allowing direct refinement of microstructural models and property predictions.

This approach empowers materials design not just for performance, but also for manufacturability and durability, facilitating the transition from materials development to certified deployment.

GENERATIVE AI CHATBOT FOR MATERIALS MODELLING

We propose to develop a new generative AI chatbot, HookGPT, designed to revolutionise materials simulation.

Currently, simulation tools in materials engineering pose a significant barrier to entry, requiring users to master partial differential equations, finite element methods, numerical analysis, and have deep expertise in multiscale materials physics. HookGPT will break down these barriers—dramatically reducing both production time and cost—by translating natural language prompts directly into ready-to-run code on M2I2's modelling platform.

By embedding materials-specific knowledge, thermal modelling, and computational mechanics, HookGPT will empower users to specify alloy composition, part geometry, and mechanical targets in plain language, and instantly receive the code needed to simulate the manufacturing process. With HookGPT, automated, prompt-driven simulation will become the new industry standard.

To achieve this, we will fine-tune open-source large language models using proprietary data and expertise gathered by M2I2 through years of consulting with industry partners. This valuable knowledge base, unique to M2I2, will be at the core of HookGPT's capabilities.

M2I2 AT THE FOREFRONT OF DIGITAL MATERIALS

By integrating advanced multiscale physics, AI-driven data analytics, and digital thread technologies, M2i2 offers a disruptive pathway toward predictive, adaptive, and rapid materials design.

Our vision enables not only materials discovery and process optimization, but also robust simulation of in-service performance for critical components—bridging the gap from lab-scale innovation to full industrial deployment.