SUCCESS STORY

IC-MPPE
Integrated Computational Materials Process and Product Engineering.

Programme: COMET – Competence Centers for Excellent Technologies

Programme line: COMET-K2 Centre

Type of project: Hybrid20, 01/2022-12/2026, strategic

Image: Tara Winstead on Pexels

USE OF PROBABILISTIC PROGRAMMING LANGUAGES FOR MATERIAL MODELS

RESEARCHERS AT MCL AND TU WIEN USE NEW PROGRAMMING LANGUAGES TO MAKE MATERIAL MODELS MORE MEANINGFUL

Scientists have always used mathematical models to answer research questions. Known relationships are often formulated in equations and used to conduct virtual experiments. One aspect of this is the consideration of uncertainties. For example, an input variable of the model can fluctuate due to measurement errors and one would like to understand how this fluctuation affects the result. The reverse question is also often asked: Assuming the final result is known, with what certainty can we infer the values of the input variables?

Although the theory for this type of problem exists (probabilistic models), there has been a lack of practical possibilities for programming and numerical solution algorithms in the past. In recent years, however, specialized programming languages for probabilistic models, PPLs for short, have made great progress. Researchers at Materials Center Leoben (MCL) have joined forces with colleagues from the Faculty of Computer Science at the Vienna University of Technology to apply probabilistic programming languages to material science problems. On the one hand, open research questions of materials scientists are being addressed, but on the other hand, the question of how probabilistic programming languages can be further developed is also being investigated. Particular attention is paid to additional capabilities of the programming environments. For example, the visualization of probabilistic models or new possibilities for debugging. Prof. Jürgen Cito says: "PPLs have developed rapidly. Now it is time to create

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additional tools to enable people to use them effectively."

Impact and effects

A well-described and executable probabilistic model is a powerful tool for many research tasks. For example, for experimental design. A probabilistic model can help to plan targeted experiments that provide the maximum amount of information, thereby reducing the cost of experiments. Another benefit is the better identification of statements that can already be made with a high degree of reliability based on the current state of knowledge. This facilitates the transfer of research results into practice while further research is carried out on open questions.

The involved researchers, image composition: MCL

At MCL, the new models are used in the rapid development of new materials (alloys) supported by artificial intelligence (AI), where small deviations in the composition have very high effects on the material properties.

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- Montanuniversität Leoben, Austria
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IC-MPPE is a COMET Centre within the COMET – Competence Centers for Excellent Technologies Programme and funded by BMK, BMAW, and the federal states of Styria, Upper Austria and Tyrol. COMET is managed by FFG.