HGS MathComp

IWR Interdisciplinary Center for Scientific Computing

UNIVERSITÄT HEIDELBERG
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IWR COLLOQUIUM · HGS MATHCOMP VON NEUMANN LECTURE

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Machine learning and Inverse design of soft materials

Predicting the emergent properties of a material from a microscopic description is a scientific challenge. Machine learning and reverse-engineering have opened new paradigms in the understanding and design of materials. However, the soft-matter field has lagged far behind in embracing this approach for materials design. The main difficulty stems from the importance of entropy, the ubiquity of multi-scale and many-body interactions, and the prevalence of non-equilibrium and active matter systems. The abundance of exotic soft-matter phases with (partial) orientation and positional order like liquid crystals, quasicrystals, plastic crystals, along with the omnipresent thermal noise, makes the classification of these states of matter using ML tools highly non-trivial. In this talk, I will address questions like: Can we use machine learning to autonomously identify local structures, detect phase transitions, classify phases and find the corresponding order parameters in soft-matter systems, can we identify the kinetic pathways for phase transformations, and can we use machine learning to coarse-grain our models? Finally, I will show how one can use machine learning to reverse-engineer the particle interactions to stabilize nature's impossible phase of matter, namely quasicrystals?

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