

Preface

Automated design is emerging as a powerful concept in materials science. By combining computer algorithms, simulations, and experimental data, new techniques are being developed that start with high-level functional requirements and identify the ideal materials that achieve them. This represents a radically different picture of how materials become functional in which technological demand drives material discovery, rather than the other way around.

At the frontiers of this field, materials systems previously considered too complicated can start to be controlled and understood. Particularly promising are materials far from equilibrium. Material robustness, high strength, self-healing, and memory are properties displayed by several materials systems that are intrinsically out of equilibrium. These and other properties could be revolutionary, provided they can first be controlled.

This thesis conceptualizes and implements a framework for designing materials that are far from equilibrium. We show how, even in the absence of a complete physical theory, design from the top down is possible and lends itself to producing physical insight. As a prototype system, we work with granular materials: collections of athermal, macroscopic identical objects, since these materials function both as an essential component of industrial processes as well as a model system for many non-equilibrium states of matter. We show that by placing granular materials in the context of design, benefits emerge simultaneously for fundamental and applied interests.

As first steps, we use our framework to design granular aggregates with extreme properties like high stiffness and softness. We demonstrate control over nonlinear effects by producing exotic aggregates that stiffen under compression. Expanding on our framework, we conceptualize new ways of thinking about material design when automatic discovery is possible. We show how to build rules that link particle shapes to arbitrary granular packing density. We examine how the results of a design process are contingent upon operating conditions by studying which shapes dissipate energy fastest in a granular gas. We even move to create optimization algorithms for the expressed purpose of material design, by integrating them with

statistical mechanics. In all of these cases, we show that turning to machines puts a fresh perspective on materials far from equilibrium. By matching forms to functions, complexities become possibilities, motifs emerge that describe new physics, and the door opens to rational design.

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