Simulating, Understanding, and Exploring the Limits of the Physical World

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From soap bubbles to viscous paints and from beating human hearts to dexterous octopus tentacles, complex physical systems exist in every corner of the natural world. Understanding the mechanics and exploring the limits of these systems is key to making scientific discoveries and creating new designs in many areas. However, this process is notoriously challenging, due to both the inherent complexity of the processes and the infinite possible combinations of parameters in trial-and-error experiments. Most of the discoveries of new materials, structures, and mechanisms were made by intuition, abundant trials, and even partly by chance.

I develop computational approaches to automate the process of exploring complex physical systems. By combining predictive simulation, data-driven methods, and machine learning algorithms, I am pioneering the creation of fully automated computational frameworks to reveal fundamental mechanisms and probe the limits of a variety of physical systems. My goal is to devise novel simulation-based and data-driven approaches to further our understanding of the complex physical world. I have taken three particular steps in exploring these approaches. First, I have developed simulation tools to model physical systems that exhibit complex characteristics, which would be intractable to model otherwise. Second, I have built algorithms that map structures to functional properties and created approaches to efficiently explore the limits of these properties. Third, I have devised machine learning algorithms to unveil the intrinsic mechanisms and new patterns associated with the extremal properties. These three steps constitute a completely automated method to investigate physical systems and make scientific discoveries. Next, I highlight each of these steps.

CURRENT AND PAST RESEARCH

Physics Simulation. The beauty and complexity of our physical world are alluring. I create simulation tools to capture this beauty in a virtual world and investigate this complexity in a computational context. In particular, I develop novel numerical approaches to study physical problems that are connected to fundamental science, with practical significance, and that were previously infeasible to solve.

One of my main focuses is on devising computational infrastructures to simulate complex fluid phenomena. These phenomena exhibit vanishingly thin features (e.g., thin films and filaments) and complex dynamics (e.g., blowing and bursting bubbles) that attract attention from researchers in many different areas. However, it is challenging or even intractable for conventional methods to capture these features and model their evolutions. I have devised algorithms based on novel geometric data structures and discrete PDE solvers to address these challenges, which enable the simulations of a variety of complex fluids, such as bursting bubbles [1], viscous paints [2], milk crowns [3], and burning flames [4] (see Figure 1, left). For example, in my Ph.D. dissertation [5], I have established a unified computational framework based on non-manifold simplicial complexes to simulate fluids with codimensional features. My key philosophy is to use the tetrahedra, triangles, segments, and points of simplicial complexes as the natural discrete analogue of fluid volumes, sheets, filaments, and small droplets. This new geometric structure, in conjunction with the novel discrete Poisson solver, has been able to simulate, for the first time, a broad range of fluid phenomena observed in experimental settings, such as the "waterbell," the "fishbone," and the "caternoid." It furnishes researchers an effective computational tool to investigate these complex phenomena and solve new codimensional PDE-driven problems in different areas.

On another front, I have devised simulation tools to model a broad range of complex solid systems, aiming to address a diversity of challenges in 3D printing, medical education, and interactive design. For example, to bridge the gap between the current printing hardware and computational software, I have devised multi-scale and parallelized simulation tools to predict the behavior of complex soft bodies with remarkably high resolution [6] [7]. To address the difficulties in communicating the nature of dynamic systems in medical education, I have created a sketching interface enhanced by reduced and thus fast simulation to help surgeons illustrate various types of heart defects and surgical procedures [8]. To enable efficient design of customized drones [9] and CAD models [10], I have contributed to automating the processes of modeling, simulating, and optimizing various kinds of complex mechanical systems.

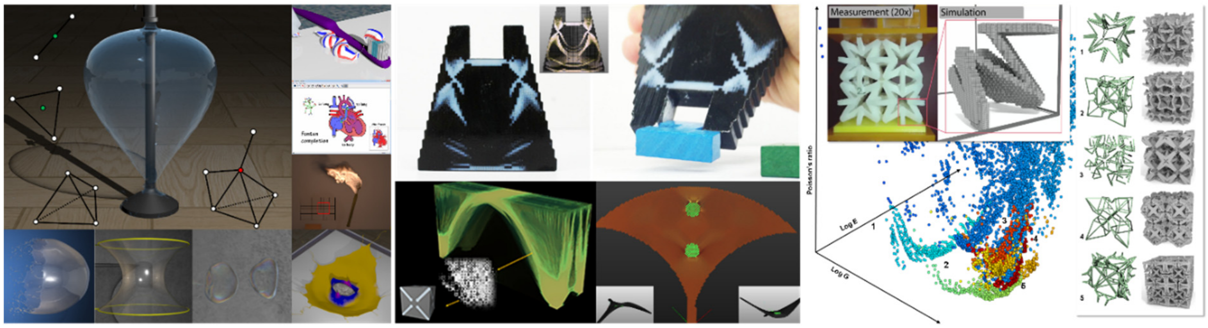
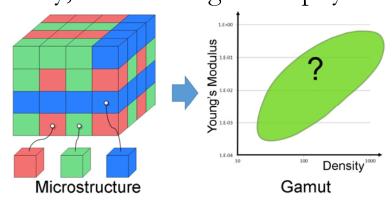


Figure 1 I develop computational approaches to explore complex physical systems. The three main stages consist of physics simulation (left), gamut exploration (middle), and automated pattern discovery (right).

Gamut Exploration. Understanding what a physical system can and cannot do is essential in many design and manufacturing problems. With a set of predictive simulation tools at hand, I have devised new algorithms that automatically map a given design space to the space spanned by physical properties—a gamut. For example, I have been tackling a fundamental problem in additive manufacturing, namely, determining what physical properties can be obtained by combining multiple base materials in a small cube that is spatially repeatable (called a "microstructure"). My key idea is to calculate a continuous gamut and explore its possible coverage for microstructures in the space of material properties (e.g., stiffness, elastic modulus, and density). In the process, I have incrementally built discrete mappings from microstructures to their corresponding physical properties.



This new representation has two important benefits: first, engineers and scientists can select materials according to their properties (or tradeoffs between properties) in a completely continuous manner; second, complex objects can be designed automatically by only specifying their function (and not shape as with standard design processes). By coupling the material gamut with a novel multi-scale topology optimization framework, I have enabled the automatic emergence of complex soft object designs with millions of microstructures (amounting to trillions of printing voxels), which is five orders of magnitude higher than the state-of-the-art techniques [6]. This enables fully automated design on a volume of one cubic meter at a resolution of 100 microns (see Figure 1, middle). My technique allows full utilization of the current 3D printing hardware and removes scalability limitations from the conventional topology optimization algorithms (where, e.g., only a few cubic centimeters could be feasibly optimized). My technique paves the road to the automated design and manufacturing of new classes of objects that were previously infeasible, such as robots, drones, and tissue engineering scaffolds.

Pattern Discovery. Predictive simulation enables the automated generation of large datasets of designs and their corresponding properties. In my research, I focus on the discovery of intrinsic mechanisms hidden in this data. I develop computational approaches that will change the way scientific discoveries can be made. Currently, scientists and engineers develop new designs by years of training, domain expertise, or simply trial-and-error. Alternatively, they look to natural systems for inspiration (e.g., velcro is inspired by burr). The resulting mechanisms and objects very rarely have the optimal trade-offs between the corresponding physical properties.

By coupling simulation, large data sets, and machine learning, I have built a new computational process to automate the process of new material discovery [7]. My key assumption is that most of the optimal mechanisms and structures exist near the boundary of the gamut of physical properties. I first identify these low-dimensional regions by massive simulations and data samplings [6]. Further, I use unsupervised machine learning algorithms to uncover the underlying novel mechanics and patterns. In particular, I have devised a four-stage pipeline, consisting of gamut estimation, class identification, template fitting, and parameter reduction, to fully automate the process of uncovering families of microstructural materials with extremal properties in a simulated virtual environment. I have automatically discovered five new classes of microstructures and validated them in real mechanical experiments, with novel actuation mechanisms and extremal auxetic properties that have never been uncovered by human scientists (see Figure 1, right). This framework has reversed the traditional observation-to-design procedure and opens up new possibilities for computational scientific exploration.

FUTURE RESEARCH PLANS

The overarching theme of my future research will be to create computational methods to automate scientific discoveries. By coupling simulation and data science, I aim to devise novel computational tools to change the way scientists and engineers explore the complex physical world. In particular, I plan to replace the laborious experiments guided by intuition and trial-and-error with simulation, data generation, and machine learning.

Computational Material Discovery. Computational approaches coupling continuum mathematics, physics, numerics, and informatics are revolutionizing the way we discover new materials. Following my previous efforts on the creation of automated tools for simulating complex physical phenomena [5] and discovering novel materials [6] [7], I aim to build computational infrastructures to enable the exploration of next-generation complex materials for the future of the manufacturing industry. Materials that exhibit multi-scale and multi-physics characteristics will be one focus. On the one hand, I intend to devise efficient simulation and data sampling techniques to explore the limits of these materials' multi-faceted physical properties, including mechanical, thermal, acoustic, and electromagnetic attributes. On the other hand, I plan to design new algorithms to uncover the novel mechanisms hidden near the boundary of the gamut of functional properties and meanwhile explore the tradeoffs of the various possible combinations. I plan to computationally discover various kinds of functional materials, e.g., metamaterials with stable expansion rates under extreme thermal conditions, microstructural materials with both optimal mechanical and acoustic properties to control sound waves, and soft materials with specified electromagnetic bandwidths for novel soft antenna designs.

Automated Design of Cyber-Physical Systems. Computational approaches based on high-fidelity simulations have not yet realized their full potential in the context of designing and manufacturing complex cyber-physical systems. I plan to devise new algorithms to improve their applicability. One particular focus will be on the automated design of soft robotic systems. First, I aim to develop simulation methods based on novel geometric structures and numerical PDE solvers to explore the gamut of physical properties underpinning soft robots. These properties range from surface tension, adhesion [1], and viscosity [2] of fluids, to topology, geometry, and materials [6] of complex soft bodies, which allow robots to explore their limits in delivering complex behaviors. On another front, I intend to create numerical approaches to explore the boundary of the space of functional metrics of soft robots, such as walking efficiency, swimming agility, and manipulation maneuverability. These approaches will enable these robots to perform complicated interactions with people and their physical environment. My goal is to computationally connect these two spaces to enable fully automated discoveries of novel geometries, topologies, materials, and actuation mechanisms for optimal performance. The target applications include the automated design of fast soft walkers, agile drones, efficient underwater swimmers, and dexterous surgical graspers.

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