Decadal Survey on Biological and Physical Sciences Research in Space 2023-2032

Topical White Paper

Title: What follows is **Chapter 5**,
Mechanical metamaterials and topological soft matter: allostery and auxetics—distributed energetics and mutation upon deployment
from the Report from the APS Division of Soft Condensed Matter Physics
DSOFT, NASA sponsored Workshop on:
Grand Challenges in Soft Matter Science: Prospects for Microgravity Research,
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Executive Summary

The worldwide community of soft matter has grown rapidly in size, impact, and scope since the last NASA report in 2003 as evidenced by the organization of the new Division of Soft Matter (DSOFT) at the American Physical Society, and the arrival of a dedicated international journal "Soft Matter" published by the Royal Society of Chemistry. At the suggestion of NASA's Physical Science Research Program in the Space Life and Physical Science Research and Application Division[1] for an update of the 2003 report on the NASA Soft and Complex Condensed Matter Workshop, Paul Chaikin, Noel Clark, and Sidney Nagel, organized a focus session and workshop for the 2020 American Physical Society (APS) March meeting under the auspices of the DSOFT. Due to the COVID–19 pandemic, the March meeting was canceled and the workshop "Grand Challenges in Soft Matter and Opportunities for Microgravity Research" was reincarnated as a remote Zoom (Zoom Video Communications, Inc.) meeting convened Thursday, March 26, 2020, from 11:30 a.m. to 1:30 p.m. EST. After a brief introduction, the ~100 participants (mostly from the United States with several joining from the European Union) separated into eight breakout sessions on

1. Self-organization only possible far from equilibrium—machines making machines
2. Instrumentation—from neuromorphic computing to large-scale self-assembly
3. Suspensions, foams, emulsions, colloids, and granular materials—self-healing, tuning gravity, and life support for exploration
4. Packings, simulation, and big data—artificial intelligence emulation of soft matter
5. **Mechanical metamaterials and topological soft matter: allostery and auxetics—distributed energetics and mutation upon deployment**
6. Soft matter, bioscience, and biotechnology—evolution and the marginal stability of life
7. Active patterning and structure formation—self-limiting assembly, actuation, and integration
8. Fluids: liquid crystals—self-assembly of the superlarge and superweak active clothing

The participants then reassembled for a presentation of conclusions and general discussion. Three overarching themes emerged from this workshop and are presented with additional details:

- Machines made out of machines
- Scalable self-sustaining ecosystems
- Active materials and metamaterials

[1]Space Life and Physical Science Research and Application Division has moved to the Science Mission Directorate and is now the Biological and Physical Sciences Division.

2.5 Mechanical Metamaterials and Topological Soft Matter: Allostery and Auxetics

2.5.1 Metamaterials: Inverse Design and Additive Manufacturing

One area that has recently drawn the attention of soft matter scientists and engineers is the possibility of designing so called metamaterials that have their functions governed, not by the specific substance out of which the material is constructed, but rather by its microstructure. Illustrative examples of metamaterials are origami folded from a two-dimensional (2D) sheet or laser-cut out of rubber as shown in Figure 6. In such origami, the pattern of folds in the sheet governs how the sheet can fold into a desired 3D object (Bertoldi et al., 2017).

A vibrant research area is to map the possible reach of metamaterials functionalities. In the future, one could input into a computer (or experimental protocol) the desired property and have as an output the appropriate microstructure that would produce it. Such metamaterials could then be produced using additive manufacturing techniques. A natural question emerges: is there a way to create bulk quantities of folded or extremely deformable metamaterials without building them one piece at a time?

Another challenge is whether (meta)materials can be designed to have multiple functions encoded in their structure. This requires understanding what platforms for the underlying material would be amenable to this form of manufacture. For example, what material is best for 3D printing? It also requires understanding what types of functions can be programmed into a metamaterial. This problem would benefit from machine-learning techniques. Basic questions include (i) to what extent can multipotent metamaterials be designed so that they are capable of having multiple functions accessible upon deployment and (ii) is there a limit to how many functions can be encoded into a given structure.

More generally, in creating useful metamaterials, one typically starts with a goal and then tries to guess the structure able to accomplish it. What kinds of protocols can be used to solve this challenging inverse problem systematically? Making use of data as a learning algorithm is an enticing route to endow a material with a good protocol for generating desired functions.

2.5.2 Adaptable Materials

One tantalizing idea is that designed materials could be sufficiently adaptable to produce a desired outcome via training, that is, materials learning. In the area of network-based materials, pruning of specific bonds has been shown to be a viable strategy for imparting function (Goodrich, Liu, and Nagel, 2015). How can this be generalized? What other ways can we use to tune the properties of the resulting material? Certainly, one can think of adding other forms of complexity through structure, shape, interactions, and possibly activity that allow for an even broader range of functionalities.

If one departs from network materials, where all the bonds are specified at the outset, one arrives at a much more difficult problem. It is a big challenge to develop control over particulate systems where the particles are free to rearrange under an applied force. It is not clear, in that case, whether it is possible to even train functions in the same way as for the simpler case of networks. However, it is conceivable that the individual building blocks can have information built into them. For example, as in DNA-coated colloids, one can design specific interactions between particles of given types. One can generalize such adaptability to include more complicated information at each site.

One can also think of adaptable materials as a platform for some form of computation and memory formation (Keim et al., 2019). Thus, materials learn to distinguish between different classes of inputs imposed from the outside. This is machine learning where the machine is not a computer, but the physical material itself (Stern et al., 2020).

2.5.3 Active and Self-Sensing Biosoft Metamaterials

The microscopic constituents of a material or metamaterial, be it particles, bonds, or hinges, can be activated, that is, they can have their own source of energy as it occurs, for example, in biological tissues and filaments with motors. In addition, synthetic materials that use biological components give rise to novel collective phenomena and responses (Sanchez, 2012). Self-sensing metamaterials built out of robotic components (Y. Chen et al., 2020), like the active metabeam in Figure 7, displays feedback between local deformations and activity leading to new “odd” elastic moduli associated with distributed

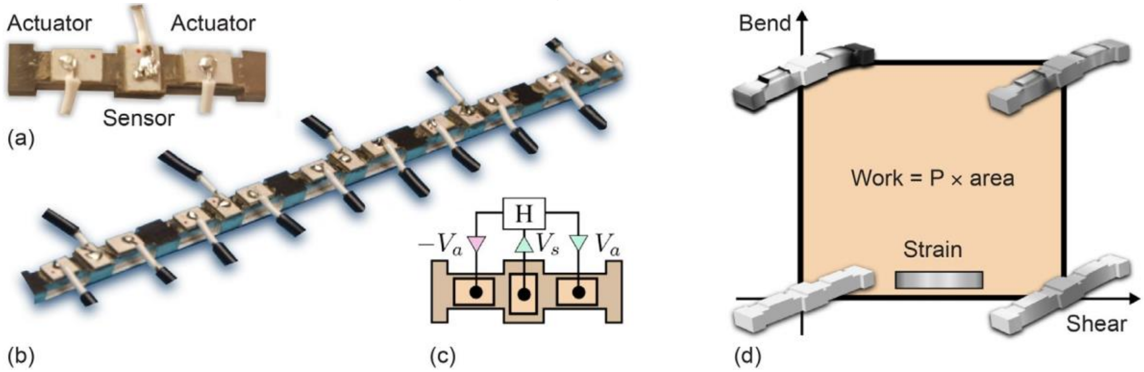

Figure 7.—Self-sensing metabeam utilizing minimal onboard computation. (a) Single unit. (b) Multiple units connected together. (c) Each unit cell consists of steel host beam equipped with three piezoelectric patches: central patch senses deformation and sends an electrical signal to outer patches, which actuate forces. (d) Feed-forward electromechanical results in an emergent odd elastic modulus P that cannot be derived from potential energy. Odd modulus is proportionality constant between area enclosed in deformation space and work extracted during mechanical cycles involving shear and bend. Figure adapted from Y. Chen et al., 2020.

energy cycles (Scheibner et al., 2020) Similarly, grains and colloids with motors can flow and transmit sound in unprecedented ways and exhibit exotic hydrodynamics (Marchetti et al., 2013) and phase transitions (Fruchart et al., 2020).

If we think of making active materials useful for biological implants, we must face the challenge of using biocompatible materials in additive manufacturing (e.g., 3D printing). Biophysical systems are inherently active matter. Molecular folding of proteins, tissues, and chromatin are key examples. A 20-year goal could be to create adenosine-triphosphate- (ATP-) driven molecular systems with spatiotemporally controlled activity. Such systems would involve chemistry-based nanoscale building blocks with controllable activated processes. A further goal would be to formulate topological design principles that protect the desired functionalities against noise and manufacturing imperfections (Shankar et al., 2020).

2.5.4 Integration of Computers and Materials

Information is physical. In his famous lectures on computation (Feynman and Hey, 2000), Feynman illustrates this mantra by means of thought experiments of computing with biological components. Soft biosystems are gradually emerging as viable platform for information processing and computation. However, we still think of materials, computers, and machines as distinct. The materials of the future will no doubt blur these boundary lines. Tasks such as autonomous information processing, microscopic energy transduction, and reconfigurability will need to be incorporated into materials design without recourse to external batteries or computers. There is, in fact, a deep connection between information and thermodynamics. A material platform that processes information autonomously in a cyclic manner must necessarily be active. Even if all sources of dissipation were to be minimized down to theoretical limit, erasing information upon resetting memory would always entail an energy cost (Plenio and Vitelli, 2001). The comprehensive integration between material design and computation required to create autonomous computing materials will entail a deeper theoretical understanding of the interplay between information science, material synthesis, and the physics of active matter.

2.5.5 Microgravity

Extreme soft matter mechanics: microgravity is the realm of the superweak, and potentially of the self-assembly of the superlarge. A famous example is the ISS-based diffusion-limited aggregation of submicron-sized colloidal particles into ultraweak fractal clusters of centimeter dimension (Lu et al., 2008), which would otherwise be crushed by 1g. But now we are pushing the limits of the directed self-assembly of structures to larger length scales and more complex structures, processes demanding microgravity. It is possible that there are many liquids, including water, that are actually ultrasoft solids, but are pushed beyond their elastic limits everywhere on Earth by the combination of gravity with self-assembly of structures to larger length scales and more complex structures, processes demanding microgravity. It is possible that there are many liquids, including water, that are actually ultrasoft solids, but are pushed beyond their elastic limits everywhere on Earth by the combination of gravity with geothermal dynamism, convection, and thermal activity due to solar heating.

References

Extensive references are provided for NASA/CP-20205010493, pp. 26-29, at https://ntrs.nasa.gov/api/citations/20205010493/downloads/CP-20205010493%20Final.pdf.