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

Topical White Paper

Title: What follows is **Chapter 1**,
Self-organization only possible far from equilibrium—machines making machines 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,
NASA/CP-20205010493, March 2021,
Paul Chaikin, Compiler, New York University, New York City, New York; Noel Clark, University of Colorado Boulder, Boulder, Colorado; Sidney Nagel, University of Chicago, Chicago, Illinois.

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.

2.1 Self-Organization Only Possible Far from Equilibrium—Machines Making Machines

2.1.1 Self-Assembly

Equilibrium self-assembly, the growth of crystals, alloys, colloidal, and polymer structures, has been known for thousands of years and understood fundamentally over the past two centuries from the development of statistical mechanics. Potential energies and entropy together provide us with thermodynamic potentials that through diffusive motion, guide particles to configurations in which these thermodynamic potentials are minimized. The materials and structures formed can be programmed from the specific interactions of the particles and lead to static configurations.

Nonequilibrium self-assembly involves forces rather than potentials and there are as yet no general principles such as free-energy minimization that can be applied, just Newton's (or quantum mechanical) equations of motion. But the processes yield new ways of making not just static structures but active devices and dynamical systems that can move and morph, transform energy, and even perform the functions of life. The forces can derive not only from potentials but from chemical activity and flow like hydrodynamic interactions and motors. Understanding nonequilibrium phenomena is a fundamental undertaking of 21st-century science and technology. Modern material processing is predominantly far from equilibrium and new types of driven self-assembly allow the creation of materials and devices not previously possible.

2.1.2 Active Matter

Motility-induced phase separation (MIPS) (Cates and Tailleur, 2015) is a beautiful example of dynamic self-assembly. Active matter, fish, birds, bacteria, and artificial colloidal swimmers, can form dense clusters, flocks, and even crystals, not because they attract one another but because as they swim, they slow down when they are crowded together creating a net inward flux. In the past two decades, chemists, physicists, and material scientists have produced a wonderful collection of active particles including chemically fueled phoretic swimmers and spinners, magnetic swimmers and rollers, light activated and fueled particles, surface-tension driven Marangoni swimmers, electrical field-driven (induced-charge) electrokinetic, and Quincke spinners (that make use of spontaneous electrorotation of a dielectric sphere submerged in a conducive fluid exposed to a static electric field) (Gompper et al., 2020; Bricard et al., 2013).

Spinning particles can form a fluid with "odd" viscosity (Banerjee et al., 2017) where you shear the fluid and it densifies or ping it and you get a new type of sound. Rotating particles can create flows that trap one another in a dynamic motile cluster, again with no potential attraction (Driscoll et al., 2017). Externally driven systems also present opportunities. Sheared colloids self-assemble into a hyperuniform phase not permissible in equilibrium but with useful photonic properties (Wilken et al., 2020). Elongating particles spontaneously choose a handedness and circulate clockwise or counterclockwise (Wu et al., 2017). When you use internally or externally driven systems, you break all sorts of equilibrium theorems and untie many restrictions.

2.1.3 Prospects

We have seen some examples of what can be done with active particles that interact with simple forces: they self-assemble into more complex and interesting entities. They are micromachines making machines on a larger scale. This resembles what we find in living systems as, for example, molecular motors in organelles or cells in organisms. Every living thing is a self-assembled machine made out of machines (Needleman and Zvonimir, 2017). What we need are more and different kinds of interactions between our particles, communication, sensing, and responding. The communication can be chemical, optical, and acoustic. Some of these ideas have been demonstrated on a centimeter scale in miniature robotics where individual robots, kilobots, with simple instructions and some communication can assemble a myriad of dynamic structures (Rubenstein, Cornejo, and Nagpal, 2014).

We aim toward colloidal-scale active elements assembling into micromachines that are motile, communicating, shape shifting, and sensing and manipulating their environment. New types of catalysts, fluids with controllable rheology, self-replicating, evolving, and self-healing materials that can store, transform, and deliver energy that conceptually behave like hybrid artificial biological systems. Along with these new materials, we expect new types of phase transitions, new phenomena, and new science.

The ultimate aim of these studies is to find the organizational principles of driven dynamical systems, and we have made some headway. We now know that random collisions under shear strain can lead to exploration of new configurations until the particles no longer collide, they stop, creating an organized absorbing state (Corte et al., 2008). Likewise, topological and symmetry constraints lead to new forms of organization and new types of excitations (Kane and Lubensky, 2014; Bertoldi et al., 2017). However, many of the basic problems remain. Thermodynamic systems tend toward equilibrium. In contrast, driven dynamical systems can tend toward steady state, time periodic, or chaotic constantly evolving states. As the number of degrees of freedom increases and the forces become more complex and different, it becomes harder to avoid chaotic behavior. Familiar properties like entropy and ergodicity become harder to define and measure and their utility in describing phenomena is questionable. Machine learning may prove useful in unraveling the phenomena and even in directing the relevant experiments. There will always be new discoveries as new fuels and materials are discovered. Nonetheless, progress has been made in rational design including spatiotemporal control. Advances are needed in the measurement of active forces and stresses. We would, for instance, like to predict rheology from measurements of the microscopic interactions. New imaging probes and modern microscopy coupled with high-speed cameras can provide an enormous amount of data. Coupled with the data produced by evermore-sophisticated simulations, there is the need for different types of data analysis and the incorporation of artificial intelligence perhaps embedded in both simulation and experiments.

2.1.4 Microgravity

Most of the active systems we have studied so far are microscopic, colloidal, or suspensions of particles in fluids. They are difficult to density match and, in a terrestrial environment, they sediment, which restricts the experiments to two dimensions. Opening the 3D world with microgravity allows a much greater variety of phenomena, types of organization, and different materials and processing. Further, in terrestrial gravity the driving temperature, concentration, and magnetic (see Figure 1), electric, and light fields create density gradients and produce flows that interfere with the basic phenomena we wish to study. Microgravity allows us to isolate the fundamental interactions and dissect the phenomena. Further, it may be possible to take the particles out of the suspending fluids, as in dusty plasmas (Shukla and Mamun, 2015), and enter a new world where inertia plays an important role and the systems are no longer overdamped. Material processing, such as additive manufacturing, relies heavily on gravity in Earth-bound implementation. In microgravity, new formulations of pastes and slurries are possible. Since future space missions will require fabrication of replacement and spare parts, techniques such as additive manufacturing will be needed. Better understanding of material processing will result from studies both with and without gravity.

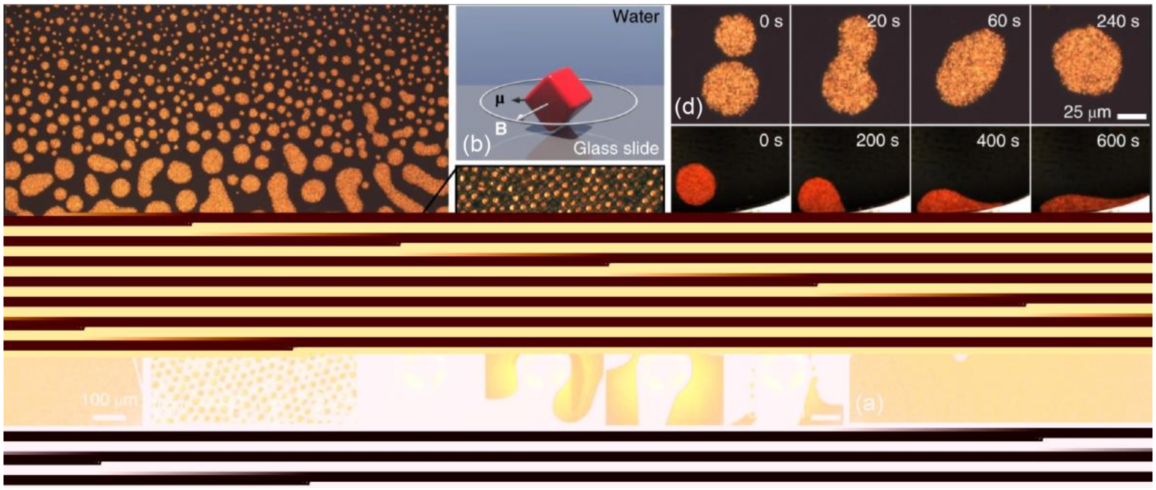

Figure 1.—Chiral fluid of spinning colloidal magnets. (a) An optical micrograph of colloidal magnets in bulk, after few minutes of spinning. (b) Schematic diagram of one colloidal particle. The ~1.6 µm haematite colloidal cubes have permanent magnetic moment (µ, black arrow). They are suspended in water, sedimented onto glass slide, and spun by rotating magnetic field (B, white arrow tracing the white circle). (c) An optical micrograph of colloidal magnets in bulk at increased magnification. Particles attract and form cohesive material with an apparent surface tension that over timescales from minutes to hours, behaves like fluid: (d) clusters coalesce and (e) spread like liquid droplets when sedimented against hard wall; (f) void bubbles collapse; and (g) when driven past an obstacle, fluid flows around it, thinning and eventually revealing an instability to droplet formation. All images were taken through crossed polarizers. Adapted from Soni et al., 2019.

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.