Programming Dynamic Self-Assembly: Theory and Simulations

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Motivation—Our goals are to: (1) Understand how living systems dynamically self-assemble, reconfigure, and disassemble materials. (2) Harness energy-consuming proteins, such as microtubules and directional motor proteins, outside of cells, as molecular self-assembly "construction crews." (3) Program these processes in non-cellular environments, to build hierarchical, dynamic materials.

Accomplishment—We have developed a set of stochastic simulations of microtubules (MTs) and kinesin motor proteins that illustrate several types of programmable dynamic self-assembly. The dynamic and statistical properties of the MT dynamic instability and kinesin transport along the MTs were matched to experimental behaviors.

The first simulation was designed to mimic the dynamic optical properties of melanophores (color-changing skin cells of fish and amphibians). We were seeking a minimal set of protein types that would enable repeatable, nano-scale pigment particle condensation (for transparent volumes) and dispersal (for opaque volumes). We succeeded using only MT-organizing centers, MTs, and pigment granules coated with two types of motor proteins: an inward-walking motor and a genetically engineered outward-walking motor that can be reversibly "locked" to prevent transport. Our engineered system requires far fewer protein types to achieve this optical control than the actual melanophore cells use. Simulation results, showing the system in the condensed and dispersed states, are shown in Fig. 1.

The second simulation was designed to illustrate sorting and patterning of mixtures of two nano-scale particle types. This was achieved by coating one particle type with only outward-walking motors and the other with only inward-walking motors before introducing them into the mixture. By controlling the placement of multiple MT-organizing centers, the simulation showed that we can create volumes that exclude one particle type and condense the second. In addition, if there is a boundary on the space that blocks MT growth, then that boundary is decorated with the single excluded particle type. See Fig. 2.

The third simulation (Fig. 3) was designed to illustrate selective harvesting of nano-particles from a mixture, then delivering the harvested particles at a controlled time to a destination labeled by MT stabilizers. This required genetically engineered switches for both inward- and outward-walking motors, selective coating of the particles to be harvested with both motors, and placement of MT-organizing centers in the mixture region.

Significance—These simulations demonstrate multiple ways in which disordered and mixed nano-particles can be ordered using energy-expending protein networks. An interesting aspect of these results is that we harness stochastic mechanisms to produce order in a reliable way, in imitation of biological self-assembly processes. Our stochastic simulation capability provides a testbed for predicting the structures and yields of dynamic self-assembly processes that can be realized experimentally. The results presented here represent key components of a much broader set of programmable self-assembly processes that we will explore in the future.

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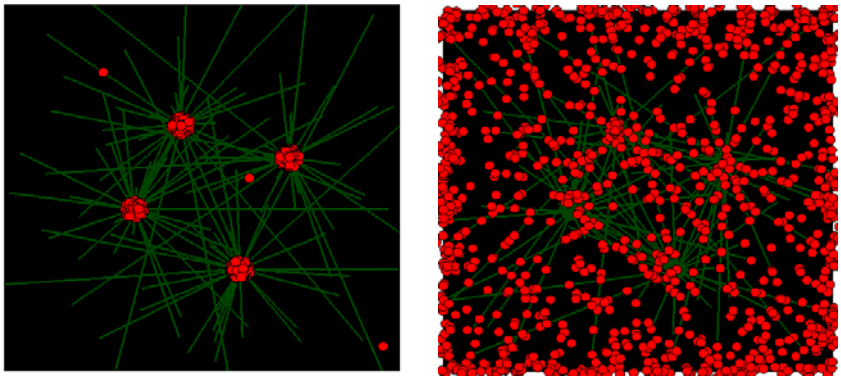

Figure 1. Results from melanophore simulation, showing condensed (left) and dispersed (right) states. Pigment granules are red, MTs are green.

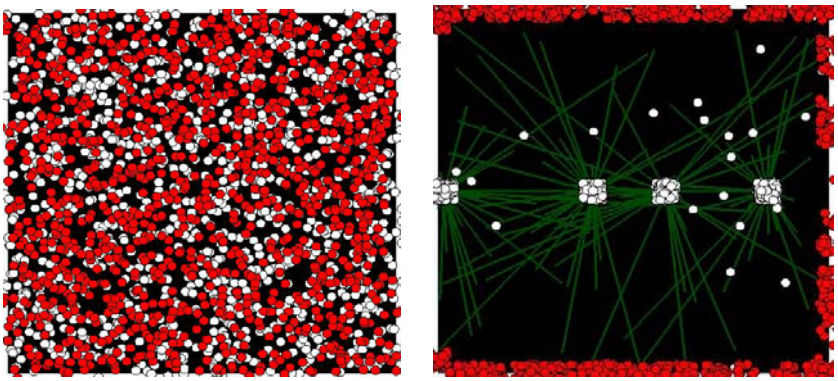

Figure 2. Initial disordered state (left). White (red) particles have inward-walking (outward-walking) motors. After ~10 minutes simulation time, red particles are excluded from the volume and decorate the boundary, while white particles are collected at the MT-organizing centers along the mid-line.

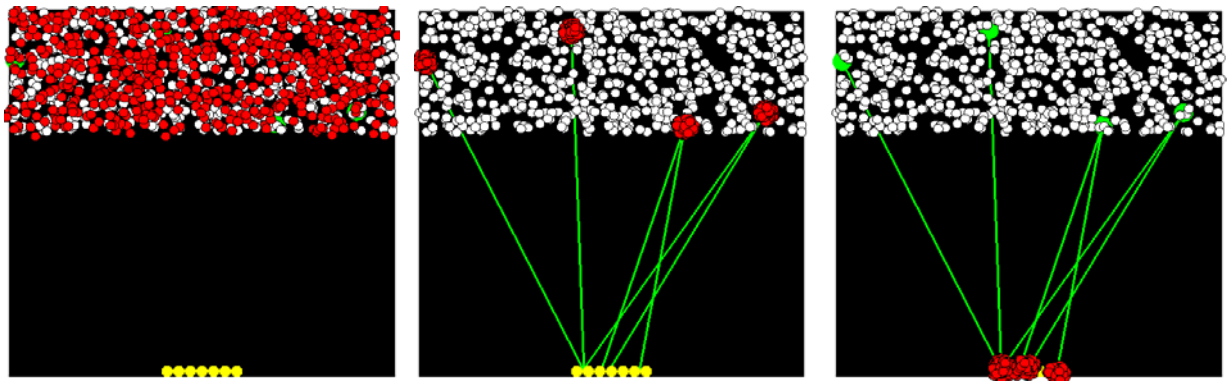

Figure 3. Initial state (left) with mixed particles (red and white) and MT-organizing centers (green) in upper portion of space, MT stabilizers (yellow) along the bottom. Red particles have lockable inward-and outward-walking motors; initially outward motors are locked. White particles have no motors. After ~7 minutes simulation time (center), red particles are harvested to the MT-organizing centers and MTs (green) grow a bridge to the stabilizers. Then, the harvested particles' outward motors are unlocked and inward motors are locked, so that the red particles are transported to their destination, at the MT stabilizers at the bottom (right).