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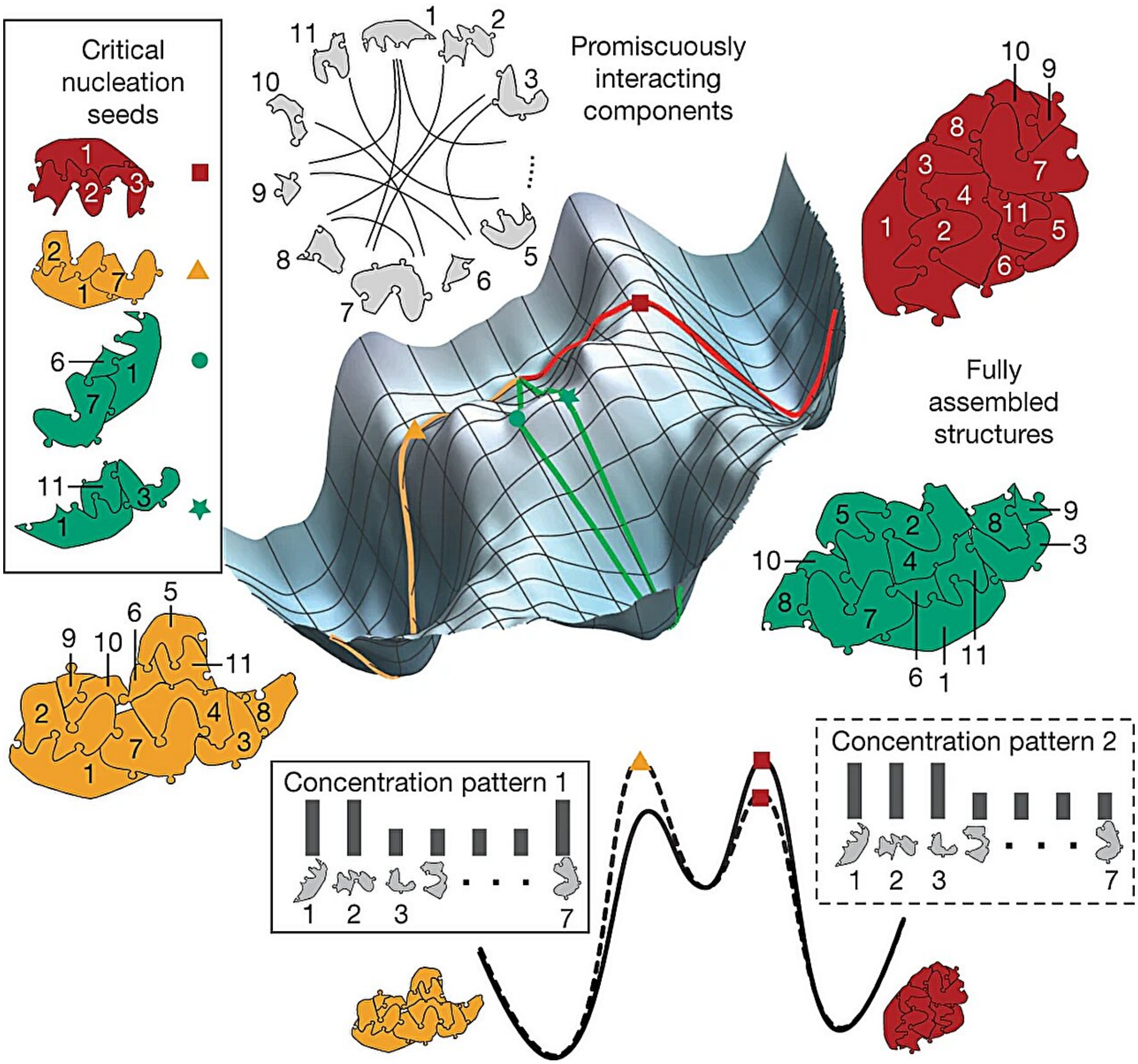
Study suggests that physical processes can have hidden neural network-like abilities

January 18 2024



Conceptual framework for pattern recognition by nucleation. When one set of molecules can potentially assemble multiple distinct structures, the nucleation process that selects between outcomes is responsive to high-dimensional concentration patterns. Assembly pathways can be depicted on an energy landscape (schematic shown) as paths from a basin for unassembled components that proceed through critical nucleation seeds (barriers) to a basin for each possible final structure. Seeds that colocalize high-concentration components will lower the nucleation barrier for corresponding assembly pathways. The resulting selectivity of nucleation in high-dimensional self-assembly is sufficiently expressive to perform complex pattern recognition in a manner analogous to neural computation. Credit: *Nature* (2024). DOI: 10.1038/s41586-023-06890-z

We tend to separate the brain and the muscle—the brain does the thinking; the muscle does the doing. The brain takes in complex information about the world and makes decisions, and the muscle merely executes. This has also shaped how we think about a single cell; some molecules within cells are seen as 'thinkers' that take in information about the chemical environment and decide what the cell needs to do for survival; separately, other molecules are seen as the 'muscle,' building structures needed for survival.

But a new study shows how the molecules that build structures, i.e., the muscle, can themselves do both the thinking and the doing. The study, by scientists with the University of Chicago, California Institute of Technology, and Maynooth University, was published in *Nature* and may suggest avenues for new ways to think about computation using the principles of physics.

"We show that a natural molecular process—nucleation—that has been studied as a 'muscle' for a long time can do complex calculations that rival a simple neural network," said UChicago Assoc. Prof. Arvind Murugan, one of the two senior co-authors of the paper. "It's an ability hidden in plain sight—the 'doing' molecules can also do the 'thinking.'

Evolution can exploit this fact in cells to get more done with fewer parts, with less energy and greater robustness."

Thinking using physics

To survive, cells need to recognize the environment they are in and respond accordingly. For example, some combinations of molecules might indicate a time of stress that requires hunkering down, while other combinations of molecules might indicate a time of plenty. However, the difference between these molecular signals can be subtle—different environments might involve the same molecules but in different proportions.

Constantine Evans, the lead author of the study, explained that it is a bit like walking into a house and smelling freshly baked cookies versus smelling burning rubber. "Your brain would alter your behavior depending on you sensing different combinations of odorful chemicals," he said. "We set out to ask if just the physics of a molecular system can do the same, despite not having a brain of any kind."

The traditional view has been that cells might be able to sense and respond in this way using molecular circuits that conceptually resemble the electronic circuits in your laptop; some molecules sense the amount of salt and acid in the environment, other molecules make a decision on what to do, and finally 'muscle' molecules might carry out an action in response, like building an internal protective structure or a pump to remove unwanted molecules.

Murugan and his colleagues wanted to explore an alternative idea: that all of these tasks—sensing, decision making, response—can be accomplished in one step by the physics inherent to the 'muscle' molecules that build a structure.

They did so by working with the principle of "phase transitions." Think of a glass of water freezing when it hits 32F; first, a little fragment of ice 'nucleates,' and then grows out until the whole glass of water is frozen.

On the face of it, these initial steps in the act of freezing—called 'nucleation' in physics—does not resemble 'thinking'. But the new study shows that the act of freezing can "recognize" subtly different chemical combinations—e.g., the smell of oatmeal raisin cookies versus chocolate chip—and build different molecular structures in response.

Robustness in experiments

The scientists tested the robustness of 'phase transitions'–based decision-making using DNA nanotechnology, a field that Erik Winfree (BS'91) helped pioneer. They showed that a mixture of molecules would form one of three structures depending on what concentrations of molecules were present in the beaker.

"In each case, the molecules came together to build different nanometer-scale structures in response to different chemical patterns—except the act of building the structure in itself made the decision on what to build," Winfree said.

The experiment revealed that this 'muscle'-based decision making was surprisingly robust and scalable. With relatively simple experiments, the researchers could solve pattern recognition problems involving about a thousand kinds of molecules—nearly a 10-fold larger problem than had been done previously using other approaches that separated 'brain' and 'muscle' components.

The work points at a new view of computation that does not involve designing circuits, but rather designing what physicists call a phase diagram. For example, for water, a phase diagram might describe the temperature and pressure conditions in which liquid water will freeze or boil, which are 'muscle'-like material properties. But this work shows that the phase diagram can also encode 'thinking' in addition to 'doing,' when scaled up to complex systems with many different kinds of components.

"Physicists have traditionally studied things like a glass of water, which has many molecules, but all of them are identical. But a living cell is full of many different kinds of molecules that interact with each other in complex ways," said co-author Jackson O'Brien (Ph.D.'21), who was involved in the study as a UChicago graduate student in physics. "This results in distinct emergent capabilities of multi-component systems."

The theory in this work drew mathematical analogies between such multi-component systems and the theory of neural networks; the experiments pointed to how these multi-component systems can learn the right computational properties through a physical process, much like the brain learns to associate different smells with different actions.

While the experiments here involved DNA molecules in a test tube, the underlying concepts—nucleation in systems with many kinds of components—applies broadly to many other molecular and physical systems, the authors said.

"DNA lets us experimentally study complex mixtures of thousands of kinds of molecules, and systematically understand the impact of how many kinds of molecules there are and the kinds of interactions they have, but the theory is general and should apply to any kind of molecule," explained Winfree.

"We hope this work will spur work to uncover hidden 'thinking' abilities in other multi-component systems that currently appear to merely be 'muscles,'" said Murugan.

More information: Constantine Glen Evans et al, Pattern recognition in the nucleation kinetics of non-equilibrium self-assembly, *Nature* (2024). DOI: 10.1038/s41586-023-06890-z

Provided by University of Chicago

Citation: Study suggests that physical processes can have hidden neural network-like abilities (2024, January 18) retrieved 27 April 2024 from https://phys.org/news/2024-01-physical-hidden-neural-network-abilities.html