Scientists harness chemical dynamics for complex problem solving

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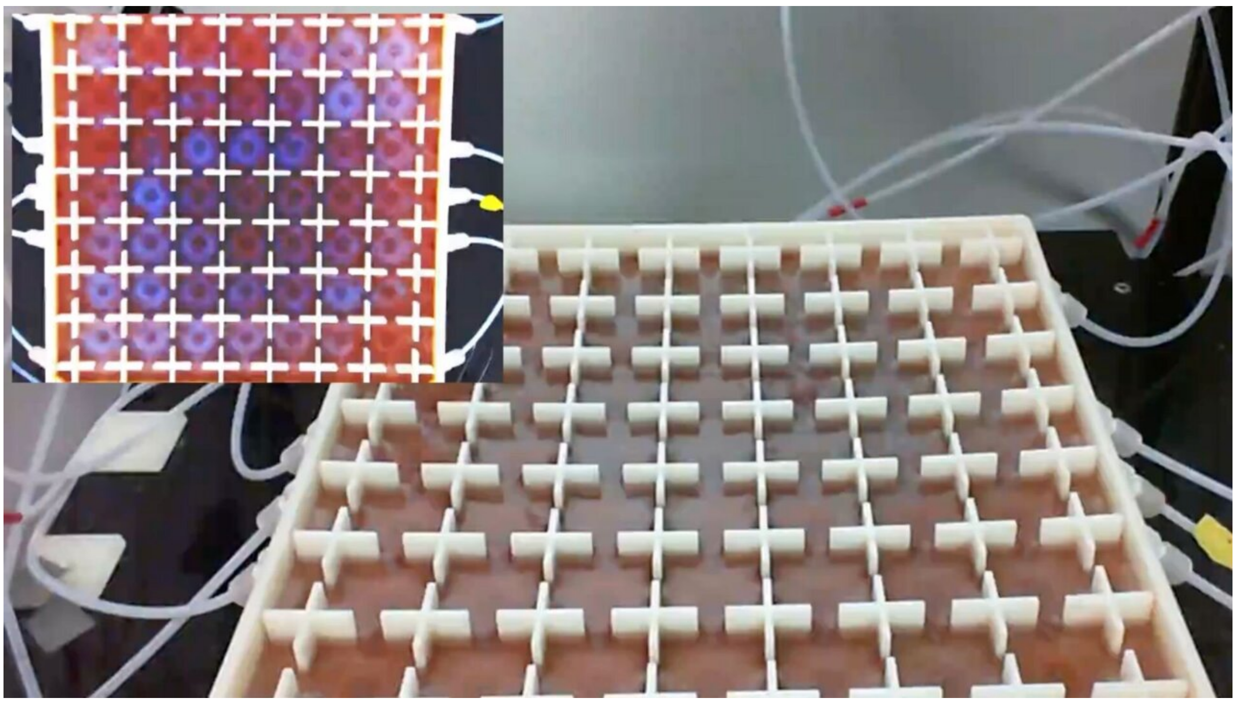

A closeup of the 3D printed reactor array with emerging chemical oscillation patterns. Credit: Digital Chemistry Lab, University of Glasgow, UK.

At the intersection of chemistry and computation, researchers from the University of Glasgow have developed a hybrid digital-chemical probabilistic computational system based on the Belousov-Zhabotinsky (BZ) reaction which can be used for solving combinatorial optimization problems.

By harnessing the inherent probabilistic nature of BZ reactions, the system demonstrates emergent behaviors like replication and competition seen in complex systems, reminiscent of living organisms. This could pave the way for novel approaches to computational tasks that are fazed by the limitations set by modern computation.

Combining electronic control and chemical dynamics offers a way to perform efficient computation, combining the best of both towards the development of adaptive, bio-inspired computing platforms with unparalleled efficiency and scalability.

The research led by Prof. Leroy Cronin, the Regius Chair of Chemistry at the University of Glasgow, was published in *Nature Communications*. Prof. Cronin spoke to Phys.org about their work and stated his motivation behind pursuing the same.

"I wanted to see if we could make a new type of chemical information processing system as I am inspired by how biology can process information in wet brains," he said.

Limitations of modern computing

Modern computing relies on transistors, the building blocks of electronic devices, that are used to create logic gates and memory cells, forming the basis of digital circuits. But, the need and demand for more computational power means that transistors are getting smaller and smaller.

The miniaturization of transistors has several limitations due to constraints set by fabrications and the laws of physics. The smaller the transistor, the harder it is to manufacture and requires more power, dissipating more heat and being less and less energy efficient.

This has led scientists to explore other types of computing, such as quantum computing, which while being extremely powerful at solving problems classical computers can't suffer from scalability issues due to error correction.

On the other hand, computation based on physical processes, such as chemical reactions, uses a mixture of systems such as digital, chemical, and optical. This opens up new avenues for unconventional computing architectures with capabilities beyond traditional digital systems.

The BZ reaction

The BZ reaction is a classic example of a chemical oscillator, with the reactant and product concentrations undergoing periodic changes. It is observed in many chemical systems, such as laboratory settings and biological systems.

The BZ reaction's ability to exhibit complex, nonlinear dynamics makes it an attractive choice for studying emergent phenomena and unconventional computing paradigms.

In this research, the BZ reaction serves as the foundation for a hybrid computational system due to its inherent oscillatory behavior, adaptability, and responsiveness to external stimuli. By harnessing the dynamics of BZ reactions, researchers can emulate complex behaviors seen in natural systems, providing a versatile platform for computation.

The concentrations can serve as binary information (with 0 being low concentrations and 1 for high concentrations) and the oscillating concentrations can serve as time-dependent variables. Additionally, information can propagate between individual cells having BZ reactions through processes like diffusion.

Prof. Cronin further explained, "The reaction has two states on and off and each box [or cell] in the network can be flashing independently, in sync, or after communication. This is the process by which the system can be programmed to compute a problem which is then read out by the camera."

A hybrid programmable information processor

The core of the information processor is a 3D-printed grid of interconnected reactors. Each reactor or cell hosts the BZ reaction, making it an array of BZ reactions.

The input to this array is electronic and is controlled by magnetic stirrers capable of manipulating the reaction within these cells. There are also interfacial stirrers capable of facilitating interactions between coupled cells (via diffusion), this helps to synchronize the oscillations.

The researchers observed that the oscillations of the reactant and product concentrations occur as forced-damped oscillations, with the stirrers playing a crucial role in controlling them.

This behavior is a characteristic feature of BZ reactions, where chemical species undergo periodic changes in concentration over time. These changes are noticed by the changes in the color of the liquids.

The output processing involves two key components: a convolutional neural network (CNN) and a recognition finite state machine (rfsm). These components analyze the reactant and product concentrations within the BZ reaction, which are captured using video cameras.

The CNN classifies the concentrations into discrete chemical states, while the rfsm determines the corresponding chemical state based on this classification.

In simple terms, the discrete chemical states are classified and determined based on the concentrations of reactants and products within the BZ reaction, which are themselves probabilistic due to the nature of the reactions.

The probabilistic nature arises because the BZ reaction is non-linear, resulting in complex interactions between chemical species that exhibit inherent variability and unpredictability in their behavior over time.

The entire system operates smoothly and continuously based on a feedback loop based on the changing colors of the liquid. When the concentrations are oscillating the system is "on" indicated by blue colors and when there is a lack of oscillations, the liquids are red, meaning that the system is "off."

This loop manipulates the stirrers based on the colors, ensuring that the process is continuous with the help of "forced" or external control.

Chemical cellular automata and solving optimization problems

The researchers used the hybrid processor to showcase its computational capability by implementing chemical cellular automata (CCA) in 1D and 2D.

These are mathematical models to simulate complex systems composed of simple components interacting locally with each other according to predefined rules.

This leads to emergent behaviors such as replication and competition exhibited by "Chemits," which are multicellular entities defined by patterns of chemical concentrations within the grid of interconnected reactors hosting the BZ reaction.

These behaviors resemble those observed in living organisms and contribute to the complexity and adaptability of the computational system.

Moreover, the researchers demonstrate that their computational approach, which incorporates both electronic and chemical components, can efficiently tackle combinatorial optimization challenges, like the traveling salesman problem.

On the application side of things, hybrid systems like these could be very useful for deep learning tasks that require non-linear behavior. Chemical systems inherently offer such characteristics, making hybrid-computation architectures resource-efficient for specific problems where non-linearities and probabilistic behavior are vital.

Prof. Cornin added, "I see that a solid-state version could replace artificial intelligence hardware and be trained much easier."

In the future, he wishes to explore the miniaturization of this technology and increase the size of the grid to solve truly large problems.

More information: Abhishek Sharma et al, A programmable hybrid digital chemical information processor based on the Belousov-Zhabotinsky reaction, *Nature Communications* (2024). DOI: 10.1038/s41467-024-45896-7.