How basic physics and chemistry constrain cellular functions in primitive and modern cells

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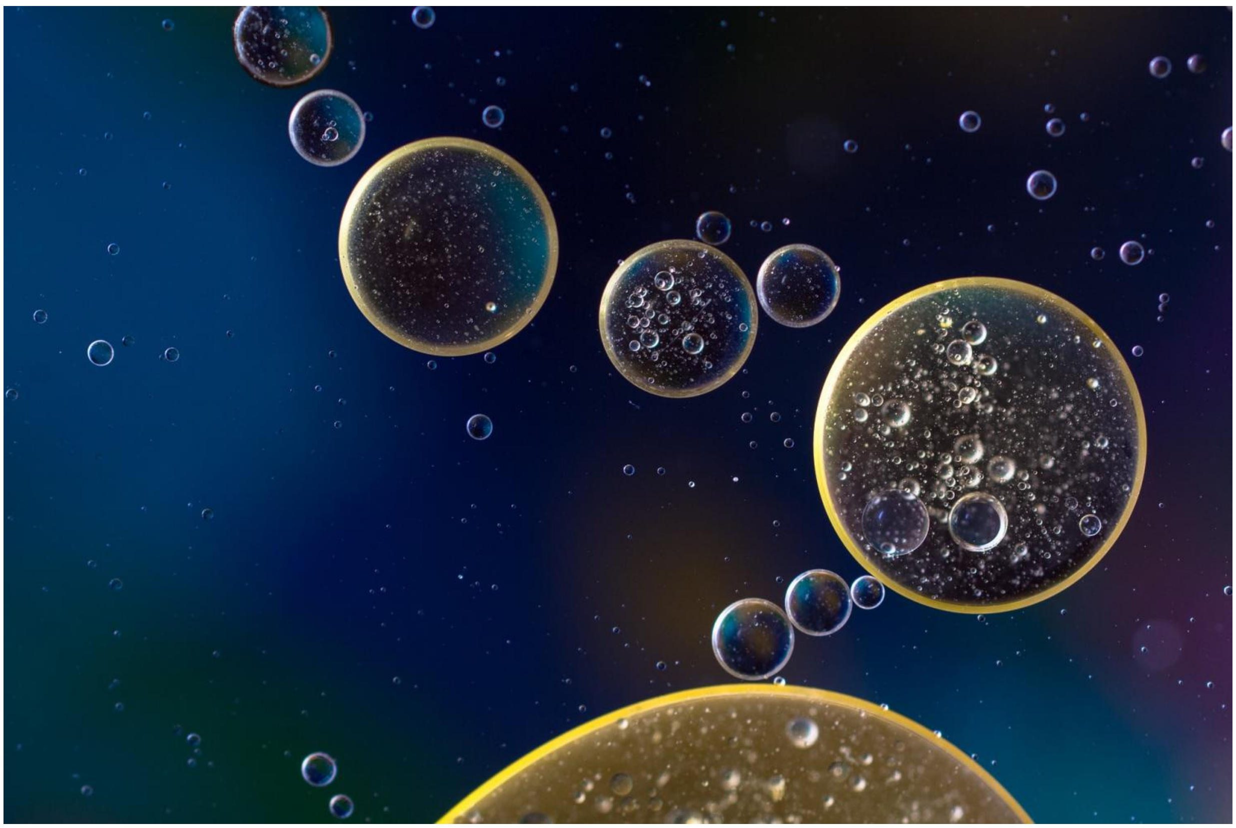

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A longstanding basic question in biology relates to how life satisfies the fundamental constraints put on it by physics and chemistry. Darwin's warm pond hypothesis for the origin of primordial cells is a familiar one. Advances have been made in mapping out the organic molecules that likely existed on the early Earth, and recently candidate prototypic pathways in early cells have been formulated. But how did these candidates' early biochemistry actually function as a system on which subsequent cellular life is based?

A team of bioengineers at the Novo Nordisk Foundation Center for Biosustainability, DTU, has now defined ten overarching classes of constraints on early metabolic networks dictated by basic chemistry and physics. These constraints concern fundamental aspects of chemical processes, such as thermodynamics, electroneutrality, osmotic pressure, and pH. These are abiotic constraints (called ABCs given their fundamental nature) that all living systems have to abide by.

The challenge has been to simultaneously reconcile all these complex constraints to define allowable operating conditions for living cells. This problem is a challenge in computational biology, a challenge that the team has resolved, the results having been published in *Nature Communications*.

"The computations are challenging because of the nonlinearity of governing equations and nonconvexity of solution spaces, which required special optimization techniques tailored to the geometric structure of the problem," says Dr. Amir Akbari, the lead author of the study.

"We worked hard on the formulation of the algorithms that eventually gave the solution and thus the conditions under which fundamental biochemical processes can operate."

The investigators analyzed how these constraints operate on basic energy metabolism in bacteria. The results demonstrated, among other things, the fundamental role of thermodynamic constraints in the evolution of alternative transport systems.

"The computations are consistent with published metabolomic data," says Bernhard Palsson, CEO and Professor at The Novo Nordisk Foundation Center for Biosustainability at Technical University of Denmark.

"The study also revealed how basic stress response mechanisms, such as those for osmotic pressure and reactive oxygen species (ROS) have to work and be regulated. Remarkably, the behavior of modern bacteria reflects the computational predictions."

Overall, this advancement helps to understand systems biology at a fundamental level and how the basis for the process of life shapes possible early evolutionary trajectories. The next step for the scientists is to apply this computational framework to gain insight into candidate abiotic organic chemical processes and the possible forms of initial metabolic networks.

"These processes have to form homeostatic states that are sufficiently stable to provide the environment for the evolution of more complex cellular functions," says Professor Palsson.

More information: Amir Akbari et al, The quantitative metabolome is shaped by abiotic constraints, *Nature Communications* (2021). DOI: 10.1038/s41467-021-23214-9

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