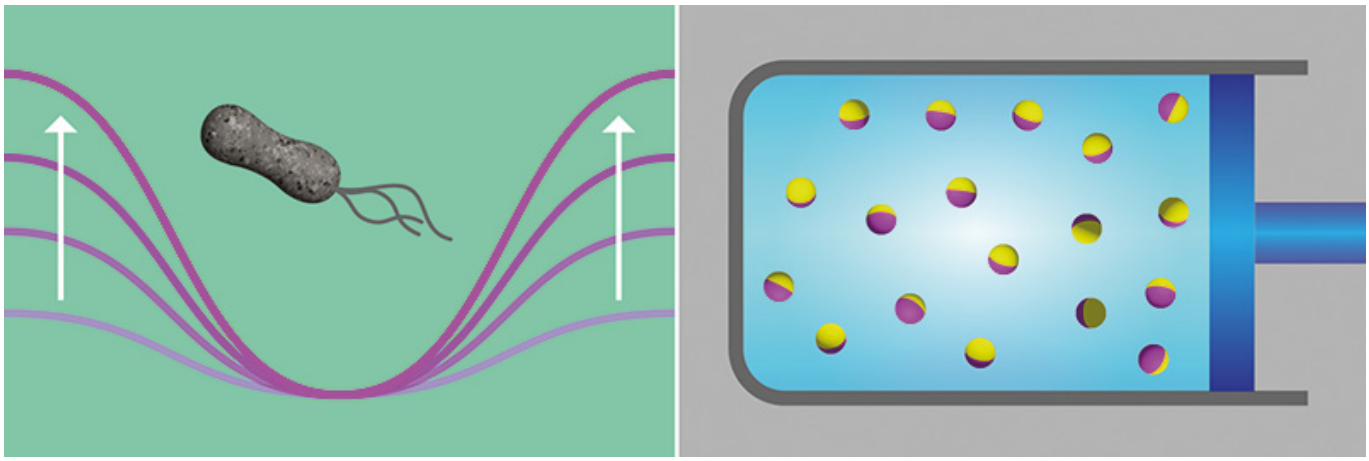

CONTROLLING ACTIVE MATTER: THE NEED FOR THERMODYNAMIC CONSISTENCY

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An outstanding challenge is to provide a comprehensive framework predicting how to control the collective states of active systems, and how to optimally switch between such states. This agenda requires extending the tools of equilibrium thermodynamics to properly capture and account for the nonequilibrium properties of active matter.

From empirical to optimal control

Active matter encompasses a large class of nonequilibrium systems where individual components convert some energy resources, naturally present in their environment, into mechanical work to produce a sustained dynamics. Such systems can be either biological (*e.g.*, bacterial swarms) or synthetic (*e.g.*, catalytic colloids in a fuel bath). The studies of active matter therefore lie at the interface between Physics, Chemistry and Biology, with many potential applications in material design and biomedicine.

Experimental techniques have demonstrated the ability to alter the collective dynamics of active systems with various types of external perturbations. In many cases, one can simply shine light on the system to specifically trigger activity in space and time. This strategy has been successfully deployed in bacterial swarms [1], where locally modulating density allows one to select target profiles [Fig. 1], and in biomimetic materials of cytoskeletal filaments and molecular motors [2], where promoting and driving topological defects allows one to regulate internal flows [Fig. 1].

In many experiments, the spatiotemporal control of activity is often optimized using system-specific procedures. In general, optimizing the perturbation of active systems to stabilize target patterns has largely remained an empirical effort so far. Then, motivated by recent experimental progress, there is a dire need for a systematic roadmap guiding experiments towards optimal control: how to determine the protocol which most efficiently changes the properties of active systems.

Energetic perspective on control cost

Optimizing control first requires choosing an appropriate cost function. Some theoretical works have defined this cost by penalizing the deviation from target patterns. This approach has led to elegant results on how to best reverse the circulation flow of active nematics [3] (*i.e.*, model for biomimetic materials [2]), and how to best deform an active drop [4] (*i.e.*, model for a single cell). Despite the success of this approach, its implementation largely remains system-specific, so that it is generally challenging to delineate any generic property of the corresponding optimal protocols.

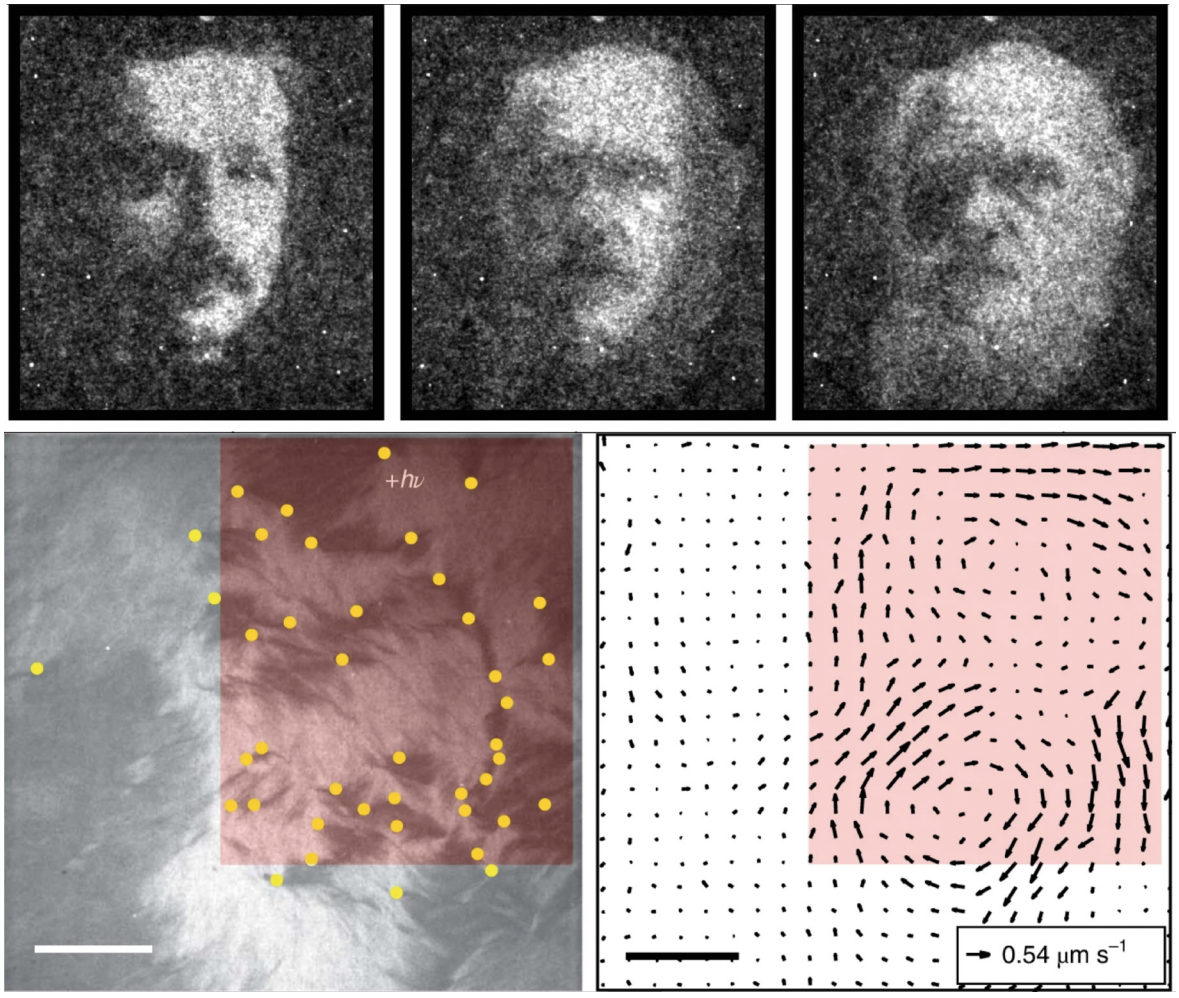
An alternative strategy for defining the control cost is to rely on energetic observables, such as work and heat, derived from generic thermodynamic principles. The work is the energy provided by the operator to enforce a given perturbation; it was actually considered as cost in [4]. The heat is the energy dissipated into the thermostat. In active systems where fluctuations cannot be neglected, one should build on stochastic thermodynamics to determine work and heat as stochastic observables: this was first developed in passive matter [5], and more recently extended to active matter [6].

Measuring work is usually straightforward, since it requires tracking only the degrees of freedom (DOF) of the external perturbation. In contrast, quantifying heat is more involved, since it needs tracking *all* the DOF dissipating energy. This task is generally challenging in active systems, since they include many DOF which are hardly accessible in experiments; typically, chemical DOF converting energy fuel into mechanical work. Remarkably, even from a theoretical perspective, many active models deliberately discard these underlying DOF, thus neglecting important contributions to the total dissipated heat.

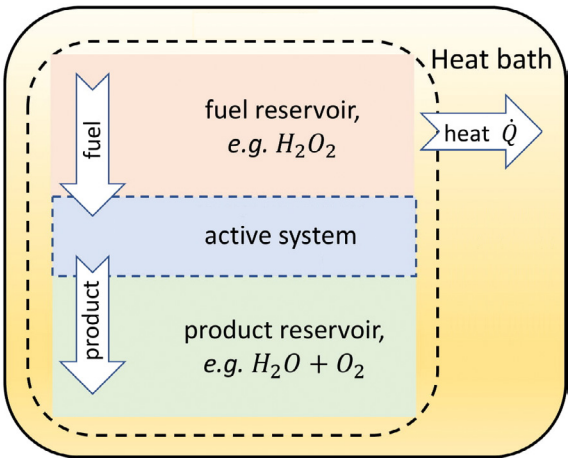
Thermodynamically consistent models

Most active models have been primarily designed to reproduce patterns, as observed experimentally, with only little care given to their energetic interpretation. Ongoing effort strives to build a novel generation of thermodynamically consistent (TC) models which provide an unambiguous quantification of heat by properly accounting for all sources of dissipation [7, 8, 9]. To this end, the main idea is to explicitly describe how the system couples with the external reservoirs fueling the activity of individual components [Fig. 2].

A remarkable by-product of TC models is that they are amenable to consistently evaluating heat at various levels of descriptions, from particles to fields. • • •



◂ **FIG. 1:** (Top) Controlling the local activity of bacterial swarms with external light allows one to switch density patterns: from Einstein's to Darwin's portrait, respectively in left and right panels; adapted from [1]. (Bottom) Illuminating a mixture of filaments and molecular motors (light shed only on red area) favors the formation of defects (yellow points) and enhances velocity flows (black arrows); scale bar 20 μm, adapted from [2].



▲ **FIG. 2:** Schematics of an active system in contact with a thermostat (heat bath) and two chemostats (fuel and product); adapted from [8]. Fixing the chemical potential difference between fuel and product sustains chemical reactions in the active system, which in turn maintains its components out of equilibrium. TC models explicitly account for the dissipation stemming from these reactions.

• • • Indeed, when models are formulated in terms of particles, the emerging collective states are often best analyzed at the hydrodynamic level. Yet, coarse-graining the dynamics typically involves some approximate closures which discard some fields, thus leading to underestimate the hydrodynamic heat. Recent methods have shown how to circumvent this issue with TC models [9, 10]: they allow one to directly evaluate heat from the field dynamics without any discrepancy with respect to its particle-based counterpart.

In practice, although TC models clearly provide the relevant platform to quantify and optimize heat, only a few of such models have been developed in active matter so far. The challenge is to reformulate existing active models, whose energetics is often ambiguous, to enforce a proper thermodynamic consistency while maintaining their rich phenomenology intact.

Optimal control from response theory

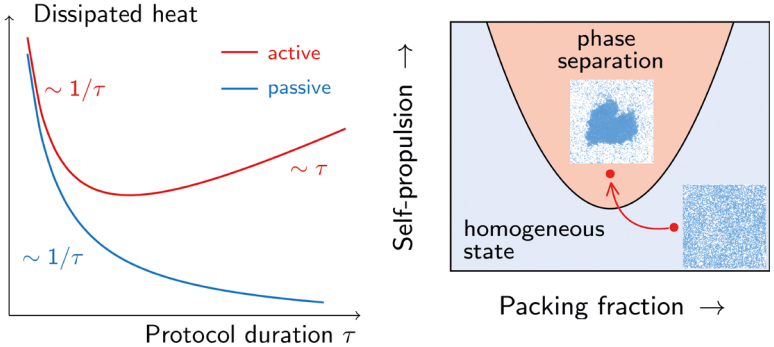
The main challenge in controlling active matter is to properly rationalize the interplay between (i) how activity shapes collective behaviors, and (ii) how the system relaxes as a response to perturbations. To this end, a useful strategy consists in considering as a reference the quasistatic protocol (QP), which slowly drives the system through steady states, and examining the effect of weak deviations. This response-based (RB) approach allows one to build the functional dependence of heat on the protocol by measuring some appropriate correlations in the unperturbed dynamics. The optimal protocol then follow from a standard minimization of the corresponding functional.

In passive systems, the QP always achieves the least dissipated heat, as expected from equilibrium thermodynamics; for a finite protocol duration, the optimal protocol follows the geodesics of some thermodynamic metrics [11]. In contrast, active systems dissipate energy at a constant rate even at rest (*i.e.*, in the absence of perturbation) to sustain their dynamics out of equilibrium, so that the QP is no longer optimal. Instead, the heat is now minimal for a finite protocol duration: it achieves the best trade-off between the dissipation stemming from internal activity (predominant for long duration) and that due to external perturbation (predominant for short duration) [Fig. 3]. The optimal protocol is no longer given by geodesics, but can still be deduced from a straightforward variational principle [12].

The main advantage of the RB approach is its versatility: it provides a systematic roadmap which can be deployed in a large variety of systems. In passive matter, it was shown useful both in experiments (*e.g.*, folding DNA hairpins [13]) and in theoretical models (*e.g.*, flipping the magnetization of spin systems [14]). In active matter, it was only used in minimal models so far, for a harmonically confined particle and for an assembly of repulsive particles [12]. Since many experiments have already shown how to accurately measure the response of active systems, the RB approach has the potential to foster future experimental studies on optimal control.

Remarkably, this framework can be straightforwardly adapted to other cost functions than heat and work. In practice, choosing any cost which is time-extensive in the unperturbed dynamics (*e.g.*, currents in active matter) will yield the same non-monotonic behavior as how heat varies with protocol duration. Importantly, despite being clearly versatile and easily adaptable, the RB approach remains inherently limited by assuming smooth protocols, which discards any abrupt change potentially yielding lower cost, and long protocol duration, which always drives the system slower than its typical relaxation.

▼ **FIG. 3:** (Left) The RB approach predicts that the dissipated heat decays like the inverse of the protocol duration when controlling passive matter, whereas it has instead a non-monotonic behavior when controlling active matter. (Right) A typical protocol to switch the collective state of active particles consists in controlling their self-propulsion and packing fraction. For instance, it can lead to induce transitions between homogeneous and phase-separated states.



Control of active phase transitions

The ability to optimally control active matter opens unprecedented perspectives for material design. Specifically, it offers the tools to craft systems which not only feature exotic phases, but which can now also optimally switch between such phases [Fig. 3]. In that respect, optimal control is the relevant framework to guide the design of active actuators which selectively change their properties according to specific perturbation. Efficiently switching actuators then requires predicting the optimal protocol driving active systems through phase transitions.

Using the RB approach for this agenda entails several challenges. Indeed, crossing phase boundaries typically involves exploring states with long relaxation times, which requires even longer protocol duration to ensure slow driving. Moreover, for discontinuous transitions with noise-activated events (*e.g.*, density nucleation in phase separation), the cost function usually no longer depends smoothly on control parameters, which conflicts with some assumptions of the RB framework. To overcome these difficulties, one could rely on spatially dependent control [14], for instance to reliably shape phase interfaces, and also gain further insights from some recent machine-learning methods [15]. ■

About the Author

Étienne Fodor is an ATTRACT Fellow (Fonds National de la Recherche, grant 14389168) at the University of Luxembourg. He was an Oppenheimer Research Fellow at the University of Cambridge, and obtained his PhD at Université Paris Diderot.

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