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On principles of emergent organization

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ABSTRACT

After more than a century of concerted effort, physics still lacks basic principles of spontaneous self-organization. To appreciate why, we first state the problem, outline historical approaches, and survey the present state of the physics of self-organization. This frames the particular challenges arising from mathematical intractability and the resulting need for computational approaches, as well as those arising from a chronic failure to define structure. Then, an overview of two modern mathematical formulations of organization—intrinsic computation and evolution operators—lays out a way to overcome these challenges. Additionally, we show how intrinsic computation and evolution operators combine to produce a general framework showing physical consistency between emergent behaviors and their underlying physics. This statistical mechanics of emergence provides a theoretical foundation for data-driven approaches to organization necessitated by analytic intractability. Taken all together, the result is a constructive path towards principles of organization that builds on the mathematical identification of structure.

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1. Genesis

Consider a fluid contained within a box. If isolated from its environment, the fluid will be in thermodynamic equilibrium, a state of maximal symmetry with uniform temperature and velocity fields unchanging in time.

Now, heat the box from below. When the temperature gradient is low, thermal energy is transported up through the fluid via conduction, and the fluid velocity remains everywhere zero. Symmetry is broken vertically, in the direction of heat flux, but maintained in the orthogonal directions. As the temperature gradient is further increased it will eventually reach a critical value and a moment of magic occurs. Symmetry now breaks in the orthogonal directions, in a spectacular manner. All of a sudden, and all at once, the fluid conspires to form convective columns in, for example, a hexagonal lattice, as convective heat transport becomes favored over conduction.

Spontaneous symmetry-breaking in the orthogonal directions signifies the onset of *pattern formation*, a special case of the more general phenomenon of *spontaneous self-organization* that is our topic of discussion.

The fluid-in-a-box scenario just described is known as the Bénard instability (sometimes Rayleigh-Bénard convection), first studied by Henri Bénard in 1900, initiating the formal study of pattern formation [1]. Over the following century it has become one of the most studied phenomena in physics, both theoretically and experimentally [2–6]. Despite the intense study, deep mysteries persist with this system and with self-organization more generally.

Self-organization is ubiquitous in natural systems, at essentially all scales—from patterning in quantum wave functions at sub-Planck-length scales [7] to biological morphogenesis [8] to the mass distribution at the largest scales of the universe [9–11]. For additional examples and phenomenology, see e.g. Refs. [12,13].

The myriad of self-organizing systems found throughout nature emphasizes a basic question—What actually *is* organization? Certainly a highly organized system will also be highly correlated, but organization is a property beyond correlation—something not quantifiable with a simple scalar value. We can recognize that the Great Red Spot of Jupiter has an intricate level of organization, a blend of randomness and regularity, but how do we specify this? How do we "write down" the Great Red Spot?

The fundamental question of formalizing organization, as a system characteristic, has largely been side-stepped in the study of the physical process of self-organization. For analytical tractability, historically much of the focus has been on exact symmetries and small perturbations from them. Only a small subset of this might we consider as directly addressing forms of organization. To understand how organization spontaneously arises, surely we first need a deeper understanding of what organization actually is.

2. Narrative and roadmap

We start our journey in Section 3 with an overview of pattern formation theory, which currently provides the best framework for the physics of self-organization. The present work addresses two shortcomings of pattern formations theory: (i) it is not a "thermodynamic" theory of self-organization and (ii) mathematical intractability prevents its application to complex forms of organization that emerge far from equilibrium. As we will show, only the latter is an actual shortcoming, the former only apparently so.

We examine thermodynamic considerations of self-organization in Sections 4 and 5. A continued distinction in contemporary literature between pattern formation theory and the theory of dissipative structures by Prigogine et al. suggests that pattern formation is generally not seen as a "thermodynamic" theory of self-organization. This despite the two theories sharing the same core goal: compute the exchange of stability of nonequilibrium steady states as a function of an external driving parameter. Since the theory of dissipative structures approaches this problem by constructing an entropy-based Lyapunov function, one must conclude that pattern formation theory is not considered a thermodynamic theory as it does not directly invoke entropy or any of its nonequilibrium generalizations.

Given the persistent confusion and conceptual difficulty surrounding entropy and its possible nonequilibrium generalizations, it is necessary in Section 4 to set the stage with an in-depth review of organization in thermodynamic equilibrium. We emphasize that entropy is not a measure of "disorder" and detail its information-theoretic interpretation. Section 5 then begins with a review of irreversible thermodynamics for local equilibrium field theories. While entropy and the 2nd Law provide a variational selection principle in equilibrium, as described in Section 4, Section 5 reviews the arguments and counterexamples against entropy production variational principles for nonequilibrium steady state selection. Such a selection principle, if one exists, would provide a base level understanding of pattern formation—a patterned state arises because it is the unique state that satisfies the selection principle.

While historically notable, dissipative structures must be relegated to history as a failed theory of self-organization. Section 5.4 recalls the arguments invalidating dissipative structures by showing the proposed "excess entropy production" is not a Lyapunov function and thus has no bearing on the stability of nonequilibrium steady states. Given more than four decades ago, these arguments disproving dissipative structures seem to be largely forgotten. Section 5.5 uses the subadditivity property of entropy to show that the differential entropy balance equation, key in the development of dissipative structures, cannot hold for organized systems. This provides theoretical insights into why dissipative structures does not hold in general.

In addition, Section 5.1 shows that the nonequilibrium generalizations of entropy and the 2nd Law are not necessary to derive the nonequilibrium transport equations used by pattern formation theory and dissipative structures. It is these equations that determine nonequilibrium steady states and their stability. Therefore, entropic quantities do not explicitly appear in pattern formation theory as they are simply not needed. One of our primary goals is to convey that pattern formation theory fully fills the role of a thermodynamic theory of self-organization as attempted by dissipative structures.

Having addressed the first shortcoming of pattern formation theory—by showing it is not actually a shortcoming—we then turn to address the limits of its applicability. Section 6 details how pattern formation theory fits into the reductionist paradigm of constructionism for explaining physical phenomena. In this, it is necessary to formulate mathematical equations to model the phenomenon of interest and then deduce physical consequences from the model. There are two main challenges hindering the extension of pattern formation theory beyond simplified systems near equilibrium.

First is the mathematical tractability of computing the stability of steady states (or time-dependent states) from more complicated sets of coupled partial differential equations with difficult boundary conditions. We review uncomputability and **P**-Completeness from the theory of computation, in the context of constructionism, to highlight formal limits on our ability to deduce physical consequences from complicated mathematical models. This places a fundamental restriction on the scope of phenomena that can be explained using the tools of pattern formation theory.

Second, analyzing a particular form of organization via pattern formation theory—think of the Great Red Spot—requires a way to "write it down" such that the organization can be substituted into the governing equations of motion and evolved. However, such complex organization eludes traditional representational bases like Fourier modes or wavelets. Any theory that aims to explain self-organization far from equilibrium, whether a direct extension of pattern formation theory or otherwise, must have some way to mathematically represent the complex organization that arises. This is the forefront of the physics of self-organization.

Section 7 addresses this frontier with a review of data-driven methods to formalize complex organization: evolution operators and intrinsic computation. Necessarily, these are outside the constructionist paradigm. Rather than attempt to write down organization in terms of pre-specified basis templates, intrinsic representations are learned directly from system behaviors. The section begins with general computation-theoretic motivations for learning representations of organization through compression—of representational resources, not of a gas by a piston, for example.

Evolution operators provide Hilbert space dynamics for classical field theories. Koopman operators evolve system observables, analogous to the Heisenberg picture of quantum mechanics; while Perron–Frobenius operators evolve densities, analogous to the Schrödinger picture. Eigenfunctions of these operators provide a natural representational basis of system behaviors that are intrinsic to the system's dynamical evolution. Compression is achieved by retaining a finite set of eigenfunctions—functions that capture any organization present in the system. The leading Koopman modes—projections onto Koopman eigenfunctions—provide a statistical notion of organization for time-independent systems.

Almost-invariant sets—leading eigenfunctions of Perron–Frobenius operators—and related coherent sets identify coherent structure and organization related to transport in time-dependent systems. Data-driven algorithms implementing the operators then provide rigorous approximations that can be deployed in practice on real-world systems.

In a complementary way, intrinsic computation achieves compression using the idea of predictive equivalence: if two past histories of system behaviors lead to the same possible set of future behaviors, those past histories are considered equivalent. And, they are grouped together as they give the same predictive information about the system's future.

For discrete statistical field theories, predictive equivalence provides the unique minimal model for optimal prediction of system behaviors. This model has a semigroup algebraic structure that generalizes exact symmetries and their group algebra. Intrinsic computation rigorously identifies structure and organization as generalized symmetries. It considers organization to be a predictive regularity. And, in so doing, it covers the full spectrum from the perfect regularity of exact symmetries to the absence of regularity for independent random events. Interesting organization, like Jupiter's Great Red Spot, is found somewhere in between, with a mixture of order and randomness.

For classical field theories, predictive equivalence of lightcones identifies coherent structures and organization through generalized spacetime symmetries and local deviations from them. We show there is a close relation, both conceptually and in data-driven approximation, between coherent structures identified through predictive equivalence and through evolution operator coherent sets.

Although we now have representations in hand for complex organization, these cannot be "plugged in" to governing equations, as would be done with pattern formation theory—evolution operators and intrinsic computation fall outside the constructionist paradigm. Data-driven scientific understanding of emergent behavior beyond constructionism is a large and ongoing endeavor. As such, it is not fully clear what "principles of organization" will ultimately look like in this new paradigm.

That said, Section 8 closes with an intriguing path forward, bringing together evolution operators and predictive equivalence to provide a statistical mechanics of emergence. While higher-level emergent behaviors cannot (generally) be deduced from their lower-level governing equations, our statistical mechanics provides the physical foundations for a complete and self-contained dynamics governing the emergent behaviors—dynamics that is consistent with the lower-level physics. Thus, evolution operators and intrinsic computation represent complex organization as emergent higher-level degrees of freedom while simultaneously providing the complete and consistent dynamical laws for their evolution. This again is all behavior-driven and so outside the constructionist paradigm: higher-level degrees of freedom cannot be written out analytically and their dynamics are not (generally) expressed by any closed-form equations of motion.

3. Nonlinear dynamics

Dynamical systems theory provides a geometric view of structures in a system's state space—structures that guide and constrain nonlinear behaviors, amplifying fluctuations and eventually attenuating them into macroscopic behaviors and patterns. A canonical example is fluid turbulence—a dynamical explanation for which occupied much of the '70s and '80s.

3.1. Structure in turbulence

Fluid turbulence was long recognized as the pre-eminent problem in thermodynamic self-organization; important too in nonlinear physics according to Heisenberg [14]—whose dissertation was on turbulence. Landau had introduced the idea that turbulent behavior consisted of a collection of incommensurate oscillators—a sufficient number of which could produce the experimentally-observed power spectra. This was superseded by the mathematical discovery in the 1950s of chaotic attractors and the 1970s conjecture that they were the state of turbulent flow [15]. This was experimentally verified only in the 1980s [16], overthrowing the Landau theory.

The implicated mechanism was one that amplified microscopic fluctuations exponentially-fast to macroscopic scale. As they reached observable scales they were guided by complex state–space structures, eventually condensing into complex spatial patterns as nonlinearities attenuated their growth. This understanding was eventually articulated in the subfield of pattern formation [8,12,13,17].

While describing and predicting the state–space structures that guide and constrain the behavior of complex systems is clearly an essential insight from dynamical systems, this too falls short of leading to a principle of emergent organization. Patterns emerge, but what exactly are they, and what complex behavior do they exhibit?

3.2. Pattern formation theory

Patterns are born out of conflict and compromise. Whenever patterns form (out of equilibrium) there are two competing forces at play: the inexorable pull towards thermodynamic equilibrium—dissipation due to the 2nd Law—and an external push away from equilibrium—drive given by gradients in intensive quantities and fluxes in extensive quantities. To monitor the competition, we define a dimensionless *bifurcation parameter R* that is the ratio of the competing forces:

$$R \propto \frac{\text{Drive}}{\text{Dissipation}} .$$

R can be thought of as a proxy for the distance from thermodynamic equilibrium.

To monitor the Bénard instability in fluid flow, one uses the Rayleigh number R which is proportional to $\Delta T/\nu\kappa$, where ΔT is the temperature difference across the fluid, ν is the kinematic viscosity, and κ the thermal diffusivity. (Additional constants are included to nondimensionalize R.) From R we see that driving and dissipation are crucial ingredients for nonequilibrium organization—a constant supply of energy, and potentially matter, must be continuously pumped into the system and simultaneously dissipated away to maintain nonequilibrium organization. We explore these thermodynamic considerations shortly.

We assume the system is governed at the macroscopic level by an effective field theory, given as a set of nonlinear partial differential equations [12]:

$$\partial_t X(\mathbf{r}, t) = F\big(X(\mathbf{r}, t), \partial_r X(\mathbf{r}, t), \ldots; R(\mathbf{r}, t)\big) . \tag{1}$$

The system state is given by X, which varies smoothly and continuously in space $\mathbf{r}$ and time t. Time evolution, as given by Eq. (1), is governed by internal dynamics with local interactions (finitely many spatial derivatives of X) that are applied uniformly in space and time; i.e., they do not have explicit space or time dependence. Additionally, the dynamics of the full system depends on external conditions as encapsulated by the bifurcation parameter $R(\mathbf{r}, t)$, which may in general vary over space and time. To avoid over-complication, for now we assume R is constant.

For fluid flows, these are the Navier–Stokes equations (or some approximation thereof), given as

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} + \nabla)\,\mathbf{u} = -\nabla p + \frac{1}{Re}\nabla^2 \mathbf{u} ,$$

for incompressible flows, where $\mathbf{u}(\mathbf{r}, t)$ is the fluid velocity field, $p(\mathbf{r}, t)$ is the pressure field, and Re is the Reynolds number. We consider Eq. (1) as a *macroscopic* description of the system due to the presence of dissipation in the form of R. Dissipation means that macroscopic state space volumes decrease over time. By contrast, a *microscopic* description—think of the collective state of the fluid's constituent molecules—obeys Liouville's theorem that says microstate state space volumes are preserved over time. Reconciliation of dissipative macroscopic dynamics arising from conservative microscopic dynamics—the thermodynamic arrow of time—has a long and storied history, starting with Boltzmann [18,19]; see e.g. Refs. [20,21] for modern reviews.

With fixed, gradient-free boundary conditions $R = 0$ and the system reaches thermodynamic equilibrium with X uniform in space and time. If the boundary conditions are fixed with nonzero gradients, R is nonzero and the system reaches a *nonequilibrium steady-state*. Close to equilibrium, with R small but nonzero, the nonequilibrium steady-state is known as the *base state*, which we denote as $\bar{X}$. The base state shares the symmetries of the boundary conditions. And so, if the boundary conditions are time-independent, then the base state will also be time independent:

$$\partial_t \bar{X}(\mathbf{r}, t) = 0 .$$

Below a critical R value R_c, the base state is stable. All infinitesimal perturbations—e.g., thermal fluctuations—exponentially decay as:

$$\delta X(\mathbf{r}, t) = A e^{\sigma t} e^{ik\cdot\mathbf{r}} .$$

For $R < R_c$, the growth rate $\mathrm{Re}(\sigma)$ of perturbations is negative. At R_c, though, the growth rate of a perturbation at wavenumber k_c becomes zero for the first time. Linear stability analysis shows that this critical mode begins to grow as the system moves through R_c. Perturbation theory (e.g., amplitude equations [12,22]) shows how this growing mode saturates just above R_c to create a patterned state. Which mode grows and how it saturates are dictated, in this close-to-equilibrium regime, by the geometry of the boundary conditions.

This simple exposition of Bénard convection illustrates the mathematics of *bifurcation theory*: The base "conduction" state becomes unstable at the critical Rayleigh number when convection takes over from heat conduction and saturates to form a patterned state. There is an exchange of stability, from the previously-stable base state to the now-stable patterned state, as R moves through R_c. Similar bifurcation-theoretic analyses have successfully predicted many similar pattern-forming phenomena that closely agree with experiment [12,17].[1]

So, are pattern formation and self-organization, more generally, "solved"? Clearly this note would not be necessary if this were the case. What mysteries remain then?

Bifurcation theory has been most successful in describing and predicting the near-equilibrium "primary bifurcation", as just described above with small R such that the base state going unstable during the bifurcation is the nonequilibrium steady-state closest to equilibrium. Continuing on, though, the patterned state that is the stable steady-state after the primary bifurcation may itself become unstable as R is increased and as the system is driven further from equilibrium.

[1] An analogous explanatory framework for some pattern formation phenomena falls under the rubric of "symmetry-breaking". As symmetry plays such a pivotal role in physics, the symmetry-breaking perspective is a fundamental one. Mathematically, though, it is a special case of dynamical system's bifurcation theory. And, in any case, this is a bit of a distraction, since organization is more than a collection of broken symmetries, as we will show.

Many important natural occurrences of self-organization exist in these far-from-equilibrium regimes. For example, hurricanes cannot be explained as finite-amplitude instabilities as bifurcation theory would attempt [23].

In short, today no general theory predicts what patterns and organization may emerge far from equilibrium. In contrast to equilibrium phase transitions and near-equilibrium bifurcations, there does not appear to be any notion of universality in the forms of organization that appear. As stated by Harry Swinney [24]:

> Far beyond the primary instability, each system behaves differently. Details matter... There is no universality ....

Or, from Philip Ball [25]:

> ... the patterns of a river network and of a retinal nerve are both the same and utterly different. It is not enough to call them both fractal, or even to calculate a fractal dimension. To explain a river network fully, we must take into account the complicated realities of sediment transport, of changing meteorological conditions, of the specific vagaries of the underlying bedrock geology–things that have nothing to do with nerve cells.

This is not to say that nothing is known about the behavior of systems far from equilibrium. Recent work with chemical reaction networks connects properties of the system to its nonequilibrium steady states and their stability. For example, chemical systems may organize out of equilibrium to "fine tune" to their environment so that they extremize forcing from the environment (dissipation is necessarily extremized as well, so that steady-state is maintained) [26]. It has also been shown that far-from-equilibrium dynamics of chemical reaction networks, including sequences of bifurcations as the system is driven further and further from equilibrium, are controlled both by dynamical properties, such as autocatalysis (nonlinearity in the dynamics), as well as structural properties like network sparsity [27]. While these insights point towards useful and interesting principles for out-of-equilibrium chemical reaction networks, they are not general principles that apply to other types of systems like kinetic gasses or fluid flows.

Compounding the challenge, even in the near-equilibrium regime, where bifurcation theory has been so successful, there are still mysteries. When the base state goes unstable, why should the newly-stable state exhibit any degree of organization, let alone organization not present in the base state? Is there a general *selection principle* that dictates the necessity of intricate organization in the system?

This question takes us to our next field of study, equilibrium statistical physics, where there *is* a general state selection principle in thermodynamics' 2nd Law. It also provides a framework that has been used to try to understand another mystery. The nonlinear dynamics analysis above addresses the macroscopic level, in terms of continuum field theories. However, we know this is only an approximation to the collective motion of an enormous number of discrete particles. How do the water particles conspire to organize together into convective columns in Bénard convection, for example? The macroscopic patterns that emerge live on a scale that is about one million times larger than the characteristic length scales of individual water molecules.

4. Equilibrium statistical physics

The phenomenology of pattern-forming systems like Bénard convection certainly has thermal aspects, as does the bifurcation analysis just described. The instability is thermally driven by a temperature gradient, and the bifurcation parameter was described in thermodynamic terms as a distance from equilibrium. Yet, most do not consider the nonlinear dynamics theory of pattern formation as a *thermodynamic theory*. The most likely reason it is not considered so is that it does not invoke the most central quantities of thermodynamics—energy and entropy—nor the cornerstone Laws governing thermal systems—the 1st Law and 2nd Law. While the dynamical framing of some forms of self-organization may involve variables and parameters that refer to energy and entropy or equations of motion that refer to thermodynamic laws, these are neither always necessary nor foundational to the dynamical analyses. In short, dynamical systems theory stands on its own without mention of entropy or the 2nd Law. Its purview is behavior arising in any state space governed by general dynamics—with energetics or not, inside or outside physics.

Bénard convection has been the guiding example thus far and, arguably, the 1st Law *is* central in this case. The equations of motion on which bifurcation analysis is carried out are derived based on energy and mass conservation. Further, Chandrasekhar analyzed the primary Bénard instability in terms of energy balance between viscosity and buoyancy; "Instability occurs at the minimum temperature gradient at which a balance can be steadily maintained between the kinetic energy dissipated by viscosity and the internal energy released by the buoyancy force" [3, pg. 34].

To stress the point here, though, there are pattern-forming real-world phenomena whose mathematical models are constructed with regard to neither energy nor entropy. One might imagine recent attempts to describe emergent social order [28–31], where energy is irrelevant and not defined, in any case. Consider an even simpler setting—the well-studied arena of cellular automata (CAs) [32–35]. Much of their investigation rather directly arose due to the wide range of intricate patterns that they readily generate. Pattern formation in CAs, though, does not occur through the kind of bifurcation considered here. Generally, there is no system invariant quantity that is the analog of energy to be conserved.

To make the distinctions clearer, the setup so far may be described as "physical pattern formation", particularly since the bifurcation parameter R has indeed been formulated in energetic terms. The nonphysical self-organizing examples serve to highlight that pattern formation arises more broadly in dynamical systems.

While energy is thus not necessary for pattern formation, the conservation of energy provides a simplification in analyzing physical dynamical systems, as well as a unified theoretical framework. All physical systems, from steam engines to motor proteins, obey the 1st Law. Similarly, all physical systems obey the venerated 2nd Law. This universality makes thermodynamics one of the most powerful and widely-employed theories in science. It is inevitable then, to wonder if there are thermodynamic principles of self-organization in physical systems given in terms of energy and entropy.

As we will now detail, much of the confusion surrounding self-organization, and our understanding of it, stems from the subtleties of entropy and the 2nd Law for equilibrium systems and from attempts to generalize these to out-of-equilibrium systems. The following first contends with entropy and the 2nd Law before moving to survey historical attempts at general nonequilibrium Laws and related attempts at thermodynamic theories of self-organization.

Particular emphasis is given to the theory of *dissipative structures*, often treated as synonymous with thermodynamics of self-organization. We recall the counterexamples and arguments invalidating the theory, which appear to have been largely forgotten. We then show that the generalizations of the 1st and 2nd Laws given by the classical theory of irreversible thermodynamics, the starting point of dissipative structures, simply yield the nonequilibrium transport equations of Eq. (1)—the starting point of dynamical systems pattern formation theory just reviewed.

4.1. Equilibrium formalism

Due to the subtleties of thermodynamics, both in equilibrium and particularly in attempts to generalize out of equilibrium, it is worth stepping back to firmly ground ourselves in its formalism and terminology. Equilibrium thermodynamics is a phenomenological theory that formalizes empirical observations of allowable manipulations for macroscopic systems. A thermodynamic *system* is characterized by a collection of relevant thermodynamic *properties*, some of which are *extensive* and scale linearly with system size—such as, volume and particle number—while others are *intensive* and are invariant to system size—such as temperature and pressure.

A *transformation* of a thermodynamic system is a change in its properties. Central to equilibrium thermodynamics is the notion of a *state variable*: a property whose changes do not depend on the particular transformations taken. State variables may be defined more precisely as properties with exact differentials [36], but the following does not require this level of detail. More loosely, the *state* of a thermodynamic system is uniquely specified by a set of properties, and an *equilibrium state* is one in which the system's intensive properties are uniform in space and all properties do not change over time. State variables are the necessary and sufficient properties for completely describing an equilibrium thermodynamic state.

A *path* is a continuous sequence of states through which the system passes, and a *process* specifies a path that maintains a particular relation among state variables—called an *equation of state*. For example, an isothermal process is a path along which the temperature does not change. A *quasistatic process* is one for which the system is instantaneously always in an equilibrium state, so that if external conditions are suddenly fixed the system is instantaneously in equilibrium at the current state. A *reversible process* is the limiting case of a quasistatic process in which the total entropy change vanishes. The direction along the path of a reversible process can change due to an infinitesimal change of external conditions. For example, heat flow between two systems with temperatures infinitesimally close is reversible since an infinitesimal change in temperature will change which system is hotter than the other. Note that reversible processes are quasistatic, but not all quasistatic processes are reversible. Finally, a *cycle* is a path that starts and ends in the same state. Since changes in state variables are path independent, they remain unchanged after a complete cycle.

To ground the formalism, consider two thermodynamic systems at different temperatures, T_1 and T_2, that only exchange thermal energy U between each other in the form of heat Q. It is observed that heat flows between the two systems, from high temperature to low temperature, until the two temperatures are equalized: $T_1 = T_2$. The equilibrium state for the composite system—which as a whole is an isolated system—is achieved when the intensive property of temperature is uniform; i.e., the two subsystems reach the same temperature. The net flux of the extensive property U vanishes.

Transformations between equilibrium states are governed by the First and Second Laws of Thermodynamics. The 1st Law formalizes the observation that energy is conserved in isolated systems—those that have no external interactions. In particular, the 1st Law is typically stated to show that thermal energy, in the form of heat Q, and mechanical energy, in the form of work W, may both contribute to changes in a system's internal energy U:

$$dU = đQ + đW \ . \tag{2}$$

The notation $đ$ indicates inexact differentials whose values are path-dependent. Since the internal energy U is a state variable, it has an exact differential and the difference $\Delta U = U_2 - U_1$ between two thermodynamic states does not depend on the particular path taken between them. Whereas, heat and work are not state variables and typically have inexact differentials. Therefore, their values $đQ$ and $đW$ generally do depend on the particular path taken between the two thermodynamic states.

Conservation of energy, the 1st Law of Thermodynamics, is one of the most powerful theories in physics and expresses a fundamental symmetry of nature. The 1st Law originated as a mathematical formulation of empirical observations of energy conservation, particularly Joule's (at the time surprising) results on "the mechanical equivalent of heat" [37]. The mathematical formulation in Eq. (2) necessitated the introduction of the *internal energy* property, a state variable, to express the observed conservation law.

The 1st Law expresses a symmetry through time and, thus, cannot indicate a preferred direction in a system's temporal evolution. If a process conserves energy in forward time, it must necessarily conserve energy in reverse time. In our simple composite-system heat exchange example, energy is conserved if the heat flowing out of one subsystem equals the heat flowing into the other. As far as the 1st Law is concerned, it does not matter whether heat flows from hot to cold or cold to hot. For macroscopic systems, it is empirically observed that in such scenarios, there *is* a preferred direction of heat flow. Heat flows "spontaneously" from hot to cold and never the other way around. Spontaneous here means there are no other sources of energy change, such as work, that may drive a heat flow from cold to hot; e.g., no refrigeration.

The 2nd Law was introduced as a means to formalize the empirical observation of thermodynamic processes that occur spontaneously in one direction but not the reverse, even though both directions conserve energy and thus satisfy the 1st Law. As the state variable of internal energy U was introduced to mathematically encode the 1st Law, a new state variable *entropy* S was introduced to formalize the 2nd Law. Building on the earlier work of Carnot [38], Clausius recognized the significance of the ratio $đQ/T$ in governing the direction of thermodynamic processes [39]. Using this ratio, he mathematically formulated his statement of the 2nd Law:

$$\oint \frac{đQ}{T} \leq 0 \ . \tag{3}$$

That is:

> *it is impossible to construct a device that operates in a cycle and whose sole effect is to transfer heat from a cooler body to a hotter body.*

Several other equivalent "impossibility statements" of the 2nd Law follow from the Clausius inequality, such as the impossibility of creating a perpetual-motion machine.

Equality in Eq. (3) is achieved if and only if the process is reversible, allowing for the introduction of the entropy state variable whose change is given by:

$$dS = \frac{đQ_r}{T} \ , \tag{4}$$

where $đQ_r$ is a reversible heat flow. The Clausius inequality Eq. (3) then takes its more familiar form:

$$dS \geq \frac{đQ}{T} \ , \tag{5}$$

for arbitrary heat flow $đQ$. The most common statement of the 2nd Law follows:

> *The entropy of an isolated system ($đQ = 0$) increases over time for irreversible processes or remains constant for reversible processes.*

The Clausius entropy in Eq. (4) is sometimes referred to as *physical entropy*, since reversible heat flow and temperature are quantities that can be measured in the lab. Strangely, while entropy was introduced to formalize the observed irreversibility of some thermodynamic processes, precise values of (changes in) entropy can only be calculated for reversible processes. Equilibrium thermodynamics is thus sometimes seen as a theory of reversible processes.

There is no paradox however, owing to the path-independence of state variables. Due to path-independence, the entropy change between two equilibrium states is the same for an irreversible path between those states as for a reversible path between them.

To avoid confusion, we emphasize that the Clausius inequality does *not* state that the entropy change is different for reversible and irreversible processes. It is the relationship between changes in entropy (path-independent) and heat flow (path-dependent) that differs between reversible and irreversible processes. This point will be clarified shortly.

The power of path-independence is also seen when combining the 1st Law and 2nd Law. Note that the statement of the 1st Law in Eq. (2) has a path-independent change in a state variable on the left hand side given in terms of path-dependent quantities of heat and work on the right hand side. For reversible processes, we can substitute the physical entropy along with $đW_r = -PdV$, where P is the pressure and V the volume, to get the fully path-independent relation:

$$dU = TdS - PdV \ . \tag{6}$$

Due to path-independence, this important relation is fully general for reversible and irreversible processes alike. It is only for reversible processes that the right hand terms are identified as heat and work.

There is an additional path-independent contribution to changes in internal energy that occurs due to exchange of particles, sometimes known as *chemical work* in analogy with the mechanical work $đW_r = -PdV$. Including this term gives one of the most important relations in classical thermodynamics, the *thermodynamic identity*:

$$dU = TdS - PdV + \sum_k \mu_k \, dN_k \ , \tag{7}$$

where μ_k is the intensive chemical potential and N_k the extensive number of particles of species k. Rearranging the identity, we see that the entropy of a thermodynamic system changes due to exchanges of internal energy (thermal interactions), volume (mechanical interactions), or particles (diffusive or chemical interactions). In this way, the thermodynamic state of a large class of systems (e.g., those without magnetic interactions) is fully specified by the three state variables (U, V, N).

4.2. Equilibrium organization

Entropy is one of the more subtle and apparently mysterious concepts in the physical sciences. While it may be convenient to side-step this subtlety by referring to entropy as a "measure of disorder", this does a great disservice, muddying key issues. After all, if entropy is disorder, then the 2nd Law states that disorder always increases. And, if self-organization is the spontaneous formation of order, is not the phenomenon at odds with the venerated 2nd Law?

Sadly, when Boris Belousov discovered an oscillating chemical reaction in the early 1950s he was unable to publish precisely due to this misconceived conflict; this despite his providing the recipe for others to reproduce his experiment [40]. It was perfectly acceptable for, say, clear chemical reagents to mix and turn to opaque homogeneity. It was thought impossible at the time, due to this misunderstanding of entropy and the 2nd Law, for these reagents to apparently unmix and the solution turn clear again, as happens with the "chemical clock" discovered by Belousov.

Today, the Belousov–Zhabotinsky (BZ) chemical reaction–diffusion system [41] has become a prime example of pattern formation, much like Bénard convection in hydrodynamics. There are two key reasons why spontaneous self-organization, like that observed by Belousov, does not exist in opposition to the 2nd Law. First, as hopefully made clear above in Section 3, self-organization in the BZ reaction and in Bénard convection occurs outside of equilibrium, where the 2nd Law does not apply. In the case of the BZ reaction, a chemical concentration gradient is the thermodynamic force maintaining the system out of equilibrium. Second, entropy is *not* strictly a measure of disorder. In point of fact, organization may emerge in equilibrium systems, such as strongly correlated electron materials [42–44] and nematic phases of superconductors [45]. More on this momentarily.

Self-organization in equilibrium systems occurs *due* to the 2nd Law, not in opposition to it. Consider, for example, the role of free energy in the Landau theory of phase transitions [46]. Analogous to the conflict and compromise of driving and dissipation out of equilibrium, there is conflict and compromise in balancing free energy between internal energy and entropy. The system evolves to minimize energy and reach its ground state, but is prevented doing so by thermal fluctuations. Self-organization in equilibrium systems is dictated by the 2nd Law, meaning that the organization which emerges represents the highest entropy state of the system commensurate with the given constraints.

As for the 2nd Law itself, it must be emphasized that it only applies to isolated systems in equilibrium. A subtlety arises when considering composite systems—the simplest case being a *system of interest* and an *environment* with which it interacts. The system is thus not isolated from the environment, but the environment is suitably defined such that the composite *system* + *environment* is isolated—it does not interact with anything else. The 2nd Law then states the total entropy of *system* + *environment* is nondecreasing. Yet, it cannot say anything specifically about the system itself. Moreover, it has nothing to say about the "order" that may or may not arise in the system of interest.

We can further clarify this point using the expression for entropy changes from classical irreversible thermodynamics [47,48]. For a system interacting with an environment in equilibrium, the change of system entropy S is:

$$dS = d_eS + d_iS \ . \tag{8}$$

Here, for simplicity, $d_eS = dQ/T$ denotes a change due to energy exchange (under fixed volume and no particle exchange) and $d_iS \geq 0$ are changes due to "irreversible processes". Eq. (8)'s decomposition nicely encapsulates many well-known properties of entropy changes under thermodynamic transformations:

- *Clausius inequality*:
  $dS \geq dQ/T$;
- *Reversible transformation*:
  $d_iS = 0 \Rightarrow dS = dQ/T$;
- *Reversible cycle*:
  $dS = 0$ and $d_iS = 0 \Rightarrow dQ/T = 0$;
- During an *irreversible cycle* the system dumps waste heat into environment:
  $dS = 0 \Rightarrow d_eS = -d_iS < 0 \Rightarrow dQ < 0$; and
- 2nd Law:
  For an isolated system $d_eS = 0 \Rightarrow dS \geq 0$.

Note that for general transformations, the entropy of a system interacting with an environment may increase or decrease: dS may be positive or negative depending on the balance of driving d_eS and dissipation d_iS. Thus, even if entropy *were* a measure of disorder, spontaneous self-organization (in equilibrium) would not be in conflict with the 2nd Law. Spontaneous "order" in a system is allowed, as long as it is duly paid for with a compensating increase in the environment's entropy.

4.3. *What* is *entropy?*

If entropy is not a measure of disorder, what is it and why is it so often conflated with disorder? In short, as Jaynes emphasized early on [49], entropy is a measure of uncertainty in a system's microscopic state, given the constraints specified by the macroscopic state. This uncertainty, applied too broadly to the *organization* of system configurations, is

the origin of entropy's disorderedness interpretation. A system we describe as "more ordered" on the macroscopic scale will often, but not always, provide more constraint on the microscopic state.

The prime example of this mismatch is a phase transition with the higher-entropy state coinciding with a more ordered configuration [50, pg. 56–57]. This occurs, for example, in the nematic transition of liquid crystals studied by Onsager [51]. Consider a collection of many cylindrical rods contained in a two-dimensional box. Now, vary the density of the rods by changing the box's size. At higher density the rods get jammed into random "disorderly" orientations. As the box's size increases and the rods are free to move around, they prefer to orient themselves into more "orderly" raft-like shapes. The decrease in orientational degrees of freedom is more than compensated for by the increase in translational degrees of freedom in the lower-density state. Therefore, the seemingly ordered state actually has higher entropy than the randomly-arranged disordered state. Similarly, gravitational systems may also evolve to ordered configurations of higher entropy [52].

While Jaynes' information-theoretic interpretation of entropy in statistical mechanics has been elaborated upon at length elsewhere [49,50,53], it is worth going into some detail here. Recall from above that classical equilibrium thermodynamics is a phenomenological theory introduced to explain, most broadly, empirical observations of irreversible processes. The theory applies to what we now call *macroscopic systems*. It was only later that a successful atomic theory was introduced and experimentally verified. In this, macroscopic systems are seen as being composed of a large number of universal microscopic "building blocks"—what we will simply call *particles*—that obey the laws of quantum mechanics. That noted, the classical laws of Newtonian mechanics will suffice for our purposes here.

The thermodynamic state is thus called the *macrostate* in the context of statistical mechanics, since state variables are macroscopic properties. Roughly, macroscopic properties are those we experience on the human scale, whereas microscopic properties—i.e., positions and momenta of constituent particles—we do not experience. For example, we feel heat flow when touching a surface at a different temperature from our skin, while we do not feel the collisions of individual particles from that surface.

Clausius, Maxwell, and Boltzmann were key contributors linking macroscopic thermodynamics to the microscopic kinetic behavior of particles [54], and it was Boltzmann who first made the connection between macroscopic entropy and microscopic kinetics [54,55]. His key observation was that typically there will be many different microstates that correspond to a single macrostate. That is, there may be many different collections of particle positions and momenta that give rise to the same total internal energy. For a given thermodynamic macrostate $(U, V, N, \ldots)$, the number of corresponding microstates is a state variable called the *multiplicity*, denoted as $\Omega(U, V, N, \ldots)$. Boltzmann's formulation of entropy as:

$$S = k \ln \Omega \tag{9}$$

follows from three key assumptions:

1. All (accessible) microstates are equally probable,
2. Entropy is a function of Ω, and
3. Entropy is *additive*.

Additivity means that when combining two systems 1 and 2 together, the entropy of the full composite system is equal to the sum of entropies of the two constituent systems: $S_{12} = S_1 + S_2$. Additivity in particular is a strong assumption that we examine in more detail shortly, as it has immediate implications for a thermodynamic theory of organization.

Our statement of the 2nd Law above is the most general form of the "impossibility" versions of the 2nd Law. It forbids thermodynamic processes that decrease entropy of an isolated system, such as heat flowing from a cold subsystem to a hot subsystem. However, there is an alternative, more constructive, perspective one can take of the 2nd Law that is most salient to thermodynamic theories of organization. As first formulated by Gibbs [56], the 2nd Law is seen as a variational selection principle:

> *For given fixed external conditions, the equilibrium state of a thermodynamic system is that which maximizes its entropy consistent with the external conditions.*

We elaborate on the Gibbs perspective and its connection to information theory momentarily, but let us first examine the Boltzmann entropy expression Eq. (9) in light of the 2nd Law as a variational selection principle.

As is standard in introductory statistical mechanics texts (e.g., Refs. [57,58]), the variational statement of the 2nd Law follows as a statistical argument from the Boltzmann entropy and the assumption of equally-probable microstates. Simply, the argument is that if all microstates are equally likely, then a macrostate with a multiplicity significantly larger than other macrostates will be observed with probability close to 1.0 due to the vast majority of microstates contributing to its multiplicity.

In statistical kinetic theory, macroscopic thermodynamic behavior is seen to arise in the *thermodynamic limit* of infinitely-large systems. In this limit, it is assumed that the multiplicity of a single macrostate does indeed dominate. The canonical toy example is flipping many fair coins, with each particular sequence of heads or tails being the microstate and the total number of heads being the macrostate. As the number of coin flips increases, the overwhelmingly most likely macrostate is that consisting of microstates each with equal number heads and tails. Shortly, we will see the information-theoretic justification for this assumption is the *asymptotic equipartition theorem*.

Table 1
Thermodynamic interactions and equilibria.

Interaction	Exchange (extensive)	Equilibration (intensive)	Formula
Thermal	U	T	$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_{V,N}$
Mechanical	V	P	$\frac{P}{T} = \left(\frac{\partial S}{\partial V}\right)_{U,N}$
Diffusive	N	μ	$\frac{\mu}{T} = -\left(\frac{\partial S}{\partial N}\right)_{U,V}$

Gibbs' ensemble approach is somewhat inverted from Boltzmann's, although they are ultimately closely related. Boltzmann starts with the assumption that all microstates are equally likely and that each microstate has an associated macrostate, with many microstates being associated to each macrostate. Then, in the thermodynamic limit, the unique equilibrium thermodynamic state is that with the (overwhelmingly) largest multiplicity. From the Boltzmann expression of entropy in Eq. (9), the 2nd Law naturally follows.

Gibbs takes the variational statement of the 2nd Law as the starting point. It is *not* assumed that all microstates are equally probable, and we emphasize microstates are associated with a thermodynamic system, perhaps in contact with other systems that have their own distinct microstates. Rather, particular parameterized families of microstate probability distributions, called *ensembles*, are determined as a function of the equilibrium thermodynamic macrostate. Thus, the 2nd Law determines the equilibrium macrostate, which then determines the microstate ensemble distribution.

In the Gibbs formulation, the entropy of a given microstate distribution is:

$$S = -k \sum_i p_i \ln p_i \ , \tag{10}$$

where p_i is the probability of microstate i. We assumed a countable number of accessible microstates to avoid measure-theoretic complications and make more direct connections to information theory. The equilibrium macrostate is that which maximizes the entropy in Eq. (10), subject to fixed external constraints. In modern use, the Gibbs approach is applied to find the microstate distribution for a given equilibrium macrostate. That is, the macrostate is taken as a given and used as the constraint. The notion of "external constraint" is not clearly specified and, as is typical with thermodynamics, careful bookkeeping is required.

4.4. Equilibrium selection principles

To further refine our appreciation of entropy, it is first helpful to clarify three distinct types of thermodynamic equilibrium. As described above in connection to the thermodynamic identity Eq. (7), the entropy can change due to thermal, mechanical, and diffusive interactions. Each form of thermodynamic interaction has an associated thermodynamic equilibrium. For two systems that exchange only internal energy as heat, they reach thermal equilibrium when they have the same temperature. Similarly, two mechanically interacting systems reach mechanical equilibrium when they have the same pressure, and diffusive equilibrium is reached when two systems have the same chemical potential. See Table 1, adapted from Ref. [58]. The extensive variables exchanged in these thermodynamic interactions fully specify the thermodynamic state in most cases. Thus, the thermodynamic state is typically given as (U, V, N).

Despite being directly related by Legendre transforms, one reason the extensive exchange variables are typically chosen over the intensive equilibration variables is that the extensive exchange variables remain well-defined on the microscopic level, whereas the intensive variables are not necessarily defined. In the Gibbs ensemble approach, these key macroscopic state variables are defined as ensemble averages over their microscopic counterparts:

$$U = \langle H \rangle = \sum_i p_i H(i) \tag{11}$$

$$V = \langle V \rangle = \sum_i p_i V(i) \tag{12}$$

$$N = \langle N \rangle = \sum_i p_i N(i) \ , \tag{13}$$

where $H(i)$ is the Hamiltonian, $V(i)$ is the volume, and $N(i)$ is the number of particles, of the ith microstate.

The standard maximum entropy derivation of the microstate ensemble distributions in the Gibbs approach proceeds as follows [49,50,59]. Each type of thermodynamic equilibrium, or combinations thereof, has an associated ensemble—a parameterized family of microstate distributions. The most common is the *canonical ensemble*, associated with only thermal interactions and equilibria. For the given ensemble, the corresponding extensive exchange variable is assumed known and its expectation value is then given as a constraint. In addition, the normalization condition:

$$\sum_i p_i = 1 \tag{14}$$

is always also given as a constraint. The microstate distribution $\{p_i\}$ is then determined by extremizing the entropy in Eq. (10), while maintaining the given constraints, using Lagrange multipliers. For example, the canonical ensemble is found by extremizing entropy subject to Eq. (11)'s and Eq. (14)'s constraints, resulting in:

$$p_i = \frac{1}{Z} e^{-\beta H(i)} \quad \text{(canonical)} \,, \tag{15}$$

with Lagrange multiplier $\beta = (kT)^{-1}$ and normalization given by the *partition function* $Z(\beta) = \sum_i e^{-\beta H(i)}$.

There are several points to expand upon. First, note that if a system does *not* have a particular thermodynamic interaction with its environment then the corresponding exchange variable is a fixed constant for the system, and the associated expectation value in Eqs. (11)–(13) is simply given by that constant value.

For example, if the system has an immovable physical boundary, it does not exchange volume with its environment and so its volume remains fixed at some value V_0. Thus, every microstate has the volume $V(i) = V_0$, for all i. The expectation value constraint in Eq. (12) then simply reduces to the normalization constraint in Eq. (14). In particular, if the system is isolated from its environment, it has *no* thermodynamic interactions and so exchanges none of the extensive quantities. The only constraint then is normalization, and extremizing the entropy subject to this constraint yields the *microcanonical ensemble* of Boltzmann with all microstates being equally probable:

$$p_i = \frac{1}{\Omega} \quad \text{(microcanonical)} \,, \tag{16}$$

with Ω the total number of microstates—i.e., the multiplicity.

Second, notice that in the example of the canonical ensemble the Lagrange multiplier β, which enforces the expectation value constraint of the exchanged extensive variable $\langle H \rangle = U$, is proportional to the associated intensive equilibration variable formula in Table 1, up to a Boltzmann factor $\beta = (kT)^{-1}$. This is of course no accident. The appropriate ensemble distributions are recovered only when the physically appropriate mathematical extremization constraints are used to express the thermodynamic "external constraints" describing the type of thermodynamic equilibrium. This point is critical to seeing the Gibbs version of the 2nd Law as a selection principle for the equilibrium thermodynamic state (U, V, N). In deriving the canonical ensemble, it appears as though we must specify the state variable U as a constraint. Note, though, that the resulting expression in Eq. (15) does not require the specific value of $\langle H \rangle = U$. Either U or the Lagrange multiplier β can act as the independent variable that determines the other.

The Gibbs 2nd Law is thus seen as a selection principle for the thermodynamic state in the following way. Consider a thermodynamic system interacting with its environment. First, the type(s) of thermodynamic interaction(s) must be specified, as determined by which of the extensive state variables are exchanged between the system and environment. Exchanged variables have an associated expectation value constraint Eqs. (11)–(13), and the entropy Eq. (10) is extremized subject to these constraints together with the normalization constraint Eq. (14). The result is a parameterized microstate distribution with either the expectation value(s) or Lagrange multiplier(s) as independent variables. Recall that the system and environment exchange extensive quantities until they reach the same value of the corresponding intensive quantity. Thus, the equilibrium state (U, V, N) is selected by specifying the Lagrange multiplier as the independent variable, whose value is given by this equilibrium condition. In the simplest case, the environment is a *reservoir* such that its intensive quantities remain unchanged through the interactions and so immediately specifies the equilibrium value for the system.

4.5. Principle of maximum entropy

The Gibbs entropy in Eq. (10) is identical in form to the Shannon entropy of information theory [60,61]. The Shannon entropy of a probability distribution provides a scalar measure of uncertainty represented by that distribution. The information-theoretic interpretation of the Gibbs entropy follows from viewing the extensive state variables as the independent parameter during constrained entropy maximization, as just described. The Gibbs entropy is then a measure of the uncertainty in the precise microstate, given the corresponding macrostate.

The connection between Gibbs and Shannon entropy was first elaborated upon by Jaynes [49], who additionally advocated for a deeper logical Principle of Maximum Entropy (PME) that states the distribution most logically consistent with known constraints is that which maximizes the Shannon entropy subject to those constraints. The argument, in brief, is that the PME procedure results in a distribution that is as uniform as possible while still satisfying the known constraints. This is interpreted as avoiding any bias in the distribution not justified by the constraints.

Note that the PME argument applied to thermodynamic equilibrium constraints is precisely the same as used above for the Gibbs 2nd Law [49]. Many contemporary practitioners are cautious of how foundational the PME may be for statistical mechanics. The standard objection is that including other constraints—such as, e.g., the second moment $\mathrm{Var}(H)$ of U—results in a distribution different from the desired ensemble. The correct ensemble results from the correct constraint, which appears to be applied in hindsight. This particular argument—that the correct ensemble results only from the correct constraints—applies to the Gibbs ensemble approach independent of the Jaynes PME. The same constraints Eqs. (11) and (14) are used in the standard statistical mechanics ensemble derivation of the canonical ensemble Eq. (15) [57, 3.2]. Similarly, the derivation of the canonical ensemble starting from a system + reservoir in a microcanonical ensemble—joint system+reservoir microstates are equally likely—the correct distribution Eq. (15) results only if just the linear term

is kept in the Taylor expansion of the (logarithm of the) reservoir multiplicity [57, 3.1]. Including the second-order term results in the same "incorrect" ensemble the PME arrives at with a nontrivial Var(H) constraint added.

We will return to the PME briefly below, to discuss its potential as a foundational approach to nonequilibrium statistical mechanics.

4.6. Asymptotic equipartition

Regardless of the PME's foundational status for statistical mechanics, it is universally recognized that the Gibbs entropy Eq. (10) of statistical mechanics is a Shannon information entropy. Mathematical results from information theory that apply to entropy of the form Eq. (10) provide useful results for statistical mechanics, in addition to conceptual insights provided by information theory.

The first such result we discuss here highlights the universality of the microcanonical ensemble (all microstates equally probable) and the Boltzmann entropy Eq. (9). Stated in statistical mechanics terms, the *asymptotic equipartition theorem* defines a *typical set*, denoted $\tilde{\Omega}$, such that for a large number of microstates x the probability of finding a microstate in the typical set is close to unity: $\Pr(x \in \tilde{\Omega}) > 1 - \epsilon$. Moreover, for a large number of microstates, the microstates in the typical set are nearly equiprobable [61, Theorem 3.1.2]. Both results follow from the weak law of large numbers.

Thus, for large systems—of order at least 10^{23} particles for the macroscopic systems considered in classical thermodynamics—the assumptions used for the microcanonical ensemble and Boltzmann entropy follow naturally when we consider the "accessible number of microstates" to be the size of the typical set for a given macrostate. (See also Ref. [50, 4.1] for a more in-depth discussion. The typical set is referred to there as the "high probability manifold".) In light of the asymptotic equipartition theorem, it is not surprising that the canonical ensemble limits to the microcanonical ensemble in the thermodynamic limit, a well-known result. The asymptotic equipartition theorem applies, however, to arbitrary microstate distributions, which also converge to the microcanonical ensemble in the limit of infinitely-many microstates.

4.7. Subadditivity

The most important mathematical property of the Gibbs entropy Eq. (10) for a thermodynamic theory of organization is *subadditivity* [59]. Classically, thermodynamic entropy is given as an extensive function of the extensive variables:

$$S(\lambda U, \lambda V, \lambda N) = \lambda S(U, V, N) \ .$$

(See, e.g., Ref. [62].) Practitioners commonly exchange extensivity for *additivity*.

Consider two interacting thermodynamic systems A and B. Entropy is additive if the entropy of the joint AB system is given as the sum of the entropies of the subsystems A and B: $S_{AB} = S_A + S_B$. While general expositions state the caveat that additivity applies for independent or "weakly interacting" systems, this conditional is often neglected in practice, as we will discuss below in Section 5. In general, entropy is *subadditive* [59] such that:

$$S_{AB} \leq S_A + S_B \ . \tag{17}$$

The equality—i.e., strictly additive case—is given in the limit of weakly-interacting or independent subsystems.

From the Boltzmann microcanonical perspective, entropy is additive when multiplicity is multiplicative:

$$S_{AB} = S_A + S_B \iff \Omega_{AB} = \Omega_A \Omega_B \ . \tag{18}$$

This is a statement of subsystem independence: microstate configurations of the subsystems do not affect each other. More generally from the Gibbs perspective, entropy is additive when microstate probabilities are multiplicative:

$$S_{AB} = S_A + S_B \iff \Pr(AB) = \Pr(A)\Pr(B) \ . \tag{19}$$

That is, additivity follows when the *joint* probability distribution $\Pr(AB)$ over microstates is given by the product of the *marginal* distributions of the subsystems, $\Pr(A)$ and $\Pr(B)$. Note that, again, the microcanonical condition in Eq. (18) follows as a special case when the joint and marginal microstate probabilities are uniformly distributed.

Subadditivity follows from the mathematical form of Gibbs entropy in Eq. (10). The information theory connection here, however, is conceptually very useful. For the simple two-subsystem case considered so far, the joint entropy decomposes as:

$$S_{AB} = S_A + S_B - I_{AB} \ . \tag{20}$$

The *mutual information* $I_{AB} \geq 0$ between subsystems A and B tracks the discrepancy between the true joint system entropy and the sum of subsystem marginal entropies. Thus, the mutual information is zero when A and B are independent, and so the mutual information quantifies the amount of information each subsystem contains about the other [61]. (I_{AB} is symmetric with respect to A and B.) In the context of statistical mechanics, I_{AB} quantifies the reduction in microstate uncertainty of one subsystem if the microstate of the other is known. Clearly, this quantity is zero if the subsystems are independent. Mutual information can be considered as an information-theoretic generalization of a correlation measure.

We cannot overemphasize the importance of entropy subadditivity in the context of the thermodynamics of organization. Entropy is only additive for independent subsystems. This is the antithesis of an organized collection of subsystems. As we discuss in more detail below in Section 5, irreversible thermodynamics considers equilibrium field theories such that the joint system is composed of infinitely-many subsystems. It additionally treats densities of extensive thermodynamic quantities as additive so that their joint full-system values are given by volume integrals. In particular, the full system entropy is $S = \int_V s(\mathbf{r})dV$. *Irreversible thermodynamics, at its very starting point, considers the systems' volume elements to be independent and therefore not organized.*

For an organized system like Bénard convection, the volume elements are clearly not independent. The fluid volumes move together in coherent motion to form the macroscopic convective patterns. Thus, it must be that $S < \int_V s(\mathbf{r})dV$. A useful multivariate generalization of mutual information is known as the *total correlation* C and is given by the difference between the full system joint entropy and the sum (integral) over the marginal entropies [63]. In our case, this is:

$$C = \int_V s(\mathbf{r})dV - S \ , \tag{21}$$

which can be seen as an *entropy of organization*. It quantifies the amount the true entropy of an organized system is overestimated if the system volume elements are considered independent and, hence, not organized.

Before moving on to nonequilibrium thermodynamics, there is a final point regarding entropy subadditivity in equilibrium statistical mechanics. Ref. [64] shows that the Clausius form of physical entropy differentials Eq. (4) is recovered from the entropy of statistical mechanics Eq. (10) only when the full joint distribution over microstates is considered. The Boltzmann approach that considers single-particle marginal distributions is insufficient for capturing thermodynamic properties that arise from interparticle forces—pressure, in the case shown in Ref. [64]. The Boltzmann approach neglects interparticle forces implicitly through the assumption of independence by using single-particle marginal probabilities—his famous *Stosszahlansatz* assumption of *molecular chaos* [65]. Thus, in very general physical circumstances, a proper accounting of the entropy contributions to organization is crucial to connect statistical mechanics entropy with physical entropy.

As a side note, Ref. [66] shows a related result connecting the Gibbs and Clausius entropies. In essence, this shows the expectation value constraints when maximizing the Gibbs entropy in statistical mechanics (i.e., using the PME) are the correct constraints to recover classical thermodynamics and Clausius entropy. The resulting microstate distributions are called generalized Boltzmann distributions there.

We emphasize, though, that the arguments in Ref. [64] should not be interpreted as saying that the "correct" physical entropy of Clausius is recovered from the more fundamental statistical mechanics entropy of Gibbs. Rather, it should be seen as a consistency between the two perspectives. Since physical entropy changes can be measured in a laboratory setting, by virtue of absolute temperature and heat exchanges being macroscopically measurable, it is seen as the more physically-grounded formulation of entropy.

It is important to remember that the relation between thermodynamic entropy, heat, and temperature were devised by Clausius with certain assumptions and limitations [39]. In a sense, Clausius' arguments have been lost in time, as they are not standard in modern thermodynamic developments. It is simply taken that Eq. (4) is *the* definition of physical entropy, without any qualification. This is not to say the Clausius definition Eq. (4) is wrong, although it is likely incomplete. The most obvious way it can be incomplete is that Clausius derived the expression without the consideration of particle exchange. Including diffusive interactions into Clausius' arguments, outlined in Ref. [39], results in a different physical entropy differential. This new form of physical entropy is just as physically grounded, but it is appropriate to physical circumstances not originally considered by Clausius.

The lengthy discussion on the foundations and assumptions of entropy is necessary as we move away from equilibrium systems. Thermodynamic theories of organization in out-of-equilibrium systems necessarily must be built on a foundation of nonequilibrium thermodynamics. Such a foundation is not at all well-established. It is not even clear where to start when formulating theories of nonequilibrium thermodynamics. In assessing proposed and potential theories, it is therefore essential to understand the starting points and assumptions going into the theory. For example, the presumed additivity of entropy in local equilibrium theories is immediately suspect as a foundation for a thermodynamic theory of organization.

5. Nonequilibrium statistical physics

The spontaneous patterns in Belousov's and Bénard's experiments emerge in systems that are manifestly out of equilibrium. As such, they cannot be described in terms of equilibrium transformations. Why? When the driving d_eS is removed during a quasistatic equilibrium transformation, the system response immediately halts. By assumption the system is always instantaneously at equilibrium, including at the moment when driving stops.

In contrast, the Belousov and Bénard patterns are the result of *nonequilibrium steady-state processes*. When driving is turned off, the processes do not immediately stop, but rather begin to relax to the equilibrium state determined by the now uniform and fixed boundary constraints. For example, convection in the Bénard experiment is driven by a temperature gradient. Thus, no-driving corresponds to zero gradient and there is a single boundary temperature that determines the subsequent equilibrium state. There is active heat transport in this nonequilibrium steady-state process, but no net transport in an equilibrium state.

The previous section recounted the central role entropy plays in equilibrium theory. When it comes to explaining pattern formation and self-organization, we said that a "thermodynamic theory" should be an entropic theory. In equilibrium, this holds. Although spontaneous self-organization in thermodynamic equilibrium at first blush appears at odds with the 2nd Law, we saw this is not the case. Organization in equilibrium is due to the 2nd Law, not in spite of it. From the perspective of the 2nd Law, entropy plays a crucial role as a selection principle: equilibrium states, including organized states, are those that maximize entropy consistent with environmental constraints.

Classical irreversible thermodynamics, and in particular the theory of dissipative structures built upon it, aims (in part) to provide a generalization of the 2nd Law as a selection principle for nonequilibrium steady-states. The *entropy production*, introduced shortly, is called upon to play a role out of equilibrium analogous to that of entropy in equilibrium. Historically, entropy production in classical irreversible thermodynamics is most notable for the various proposed extremum principles to determine nonequilibrium steady-states. As will be described in more detail, though, to date no entropy production extremum principle is generally accepted as a valid selection criterion for determining nonequilibrium steady-states.

To appreciate this, we first introduce the basics of entropy production (density) in the context of classical irreversible thermodynamics and argue that this quantity does not generally have a firm physical basis. Despite their claimed primacy, we show that entropy production and the entropy balance equation—that generalizes the 2nd Law—are, in fact, largely superfluous in classical irreversible thermodynamics. The main question raised in this Section is: What role, if any, does entropy (or an appropriate generalization) play in a "thermodynamic" theory of self-organization out of equilibrium?

5.1. Irreversible thermodynamics of local equilibrium

Equilibrium theory describes irreversible changes between equilibrium states, with calculations performed along idealized reversible paths. This assumes that the system is always *instantaneously* in equilibrium. In contrast, to describe dynamical transport processes, classical irreversible thermodynamics, pioneered by Onsager [67,68] and Prigogine [47], instead assumes *local equilibrium*.

In this, one considers a spatially-extended system in contact with an environment, such as the box of fluid in contact with two heat baths for Bénard convection. The system consists of many mesoscopic "elementary volume units" dV such that they are differential volume elements from the macroscopic perspective; i.e., the total volume is given as $V = \int dV$. However, from the microscopic perspective they contain sufficiently-many particles that their momenta follow a Maxwell distribution. Thus, local equilibrium assumes intensive quantities—e.g., temperature—become fields and extensive quantities are replaced by their densities, with all varying over time and space. For these quantities to be well-defined on the mesoscale, the thermodynamic identity Eq. (7) must hold locally in each volume element dV.

In the local equilibrium field theories of classical irreversible thermodynamics, the 1st Law and 2nd Law are given in the form of *balance equations* [48]. Following Ref. [69, Box 15.1], a general balance equation for an extensive quantity Y is derived as follows.

Let y be the density of Y and $\mathbf{J}_Y$ the current density of Y, and consider an arbitrary volume V. The change of Y in the volume due to the current flow is given by the surface flux $\int_{\partial V} \mathbf{J}_Y \cdot d\mathbf{n}$. Let $P[y]$ be the amount of Y produced or destroyed per unit volume per unit time. Hence, the change of Y in V due to internal changes is $\int_V P[y]dV$. (Consider, for example, molecular concentrations that may change internally due to chemical reactions.) The time rate of change of Y in the volume is given by the integral balance equation:

$$\int_V \left(\frac{\partial y}{\partial t}\right) dV = \int_V P[y]dV - \int_{\partial V} \mathbf{J}_Y \cdot d\mathbf{n} \ .$$

Using Gauss's divergence theorem, the surface flux integral can be changed to a volume integral, giving:

$$\int_V \left(\frac{\partial y}{\partial t}\right) dV = \int_V P[y]dV - \int_V (\nabla \cdot \mathbf{J}_Y) dV \ .$$

Since the volume V is arbitrary, the integrands on both sides must be equal, giving the differential balance equation:

$$\left(\frac{\partial y}{\partial t}\right) + (\nabla \cdot \mathbf{J}_Y) = P[y] \ . \tag{22}$$

Using the differential balance equation and the form of the 2nd Law in Eq. (8) we now review the derivation of the entropy balance equation [48,69]. We will then examine what role entropy balance and entropy production may, or may not, play in nonequilibrium theory.

First, we express the time derivatives of the terms in Eq. (8) by volume and flux integrals as:

$$\frac{dS}{dt} = \int_V \frac{\partial s}{\partial t} \, dV \tag{23}$$

$$\frac{d_e S}{dt} = -\int_{\partial V} \mathbf{J}_S \cdot d\mathbf{n} \tag{24}$$

$$\frac{d_i S}{dt} = \int_V \sigma \, dV \ . \tag{25}$$

Since entropy is an extensive quantity, it is assumed to have a well-defined density s that obeys the thermodynamic identity. Second, we recall that d_eS referred to the change of entropy due to energy and material transport, and so we express its time rate of change in terms of an *entropy current density* $\mathbf{J}_S$. Finally, the internal generation $P[s]$ of entropy is defined as the *entropy production* σ. Since we postulated that $d_iS \geq 0$ and recalling the volume V is arbitrary, it must be that $\sigma \geq 0$. That is, entropy may be internally generated, but not destroyed, during irreversible processes. The righthand terms in Eqs. (23)–(25) are those of an integral balance equation. The differential entropy balance equation is:

$$\frac{\partial s}{\partial t} + \nabla \cdot \mathbf{J}_S = \sigma \ . \tag{26}$$

Specific forms of entropy current density and entropy production are found using the local thermodynamic identity:

$$Tds = du + Pdv - \sum_k \mu_k dn_k \ , \tag{27}$$

along with balance equations for energy density u and chemical concentration n_k. It is found that entropy production has a general bilinear form [48,69]:

$$\sigma = \sum_i F_i \mathbf{J}_i \ , \tag{28}$$

with products of thermodynamic fluxes $\mathbf{J}$ and thermodynamic forces F.

This expression is in line with an intuition that thermodynamic force gradients in intensive quantities drive fluxes in extensive quantities during irreversible processes. For example, the force $\nabla(1/T)$ drives a heat flux $\mathbf{J}_u$ in Bénard convection. Analogous to the physical entropy of Clausius, thermodynamic forces and fluxes are macroscopic quantities that can be measured, and so the quantity σ in Eq. (28) can be computed for physical systems.

That said, the practical utility and physical significance of Eq. (28) is questionable. In particular, while the extremum of entropy provides a selection criterion for equilibrium states, Section 5.3 below will establish that nonequilibrium steady-states do not correspond to extrema of σ. More alarming, the usefulness of the entropy balance equation Eq. (26) itself is unclear! We show shortly that entropy balance is superfluous for deriving nonequilibrium transport equations—the central endeavor of classical irreversible thermodynamics. This is surprising, given that the entropy balance equation is the nonequilibrium generalization of the 2nd Law, the cornerstone of equilibrium theory.

As Ref. [48] points out, the balance equations for entropy, energy, and species concentration are insufficient to determine the time evolution of all relevant variables, even if the bilinear form of entropy production Eq. (28) is used. The missing relations between variables comes in the form of *phenomenological laws*, sometimes also called *constitutive relations*. These laws assume that thermodynamic fluxes are linear functions of thermodynamic forces, with a general form given as:

$$J_i = \sum_k L_{ik} F_k \ , \tag{29}$$

where the L_{ik} are known as the *phenomenological coefficients*.

Familiar transport phenomena like Fourier's heat law, Fick's law of diffusion, and Ohm's law of electrical conduction employ linear phenomenological laws. Additionally, Eq. (29) encompasses cross-effects in transport, such as the Seedbeck and Peltier thermoelectric effects [69,70]. The celebrated Onsager reciprocal relations [67,68] place symmetric or anti-symmetric constraints on cross coefficients $L_{ik} = \pm L_{ki}$. Inserting Eq. (29) into the bilinear form of entropy production Eq. (28) gives a nonnegative-definite constraint to the matrix of phenomenological coefficients. Relying on linear laws, classical irreversible thermodynamics is often called *linear nonequilibrium thermodynamics*.

5.1.1. Case study: heat conduction

To demonstrate the superfluousness of entropy balance in deriving transport equations, let us now examine the canonical example of heat conduction and Fourier's law. Start with the phenomenological law:

$$\mathbf{J}_u = L_{uu} \cdot \nabla\left(\frac{1}{T}\right) \ , \tag{30}$$

that takes the more familiar form:

$$\mathbf{J}_u = -\kappa \nabla T \ , \tag{31}$$

where $\kappa = L_{uu}/T^2$ is the conductivity coefficient or tensor for anisotropic systems. Relation Eq. (31) expresses the familiar observation that heat flows down a temperature gradient, from hot to cold. Next, consider the balance equation for internal energy. In integral form, this is:

$$\frac{d}{dt}\int_V u \, dV = -\int_{\partial V} \mathbf{J}_u \cdot \mathbf{n} \, dV \ ,$$

and in differential form:

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{J}_u = 0 \ . \tag{32}$$

Appealing to local equilibrium thermodynamics, the internal energy density is related to the temperature field through:

$$\partial u = c\rho \ \partial T \ , \tag{33}$$

where c is the specific heat and ρ the mass density. Combining relation Eq. (33) with internal energy balance Eq. (32) and the phenomenological law Eq. (31), we arrive at Fourier's heat law:

$$\frac{\partial T}{\partial t} = k\nabla^2 T \ , \tag{34}$$

with $k = \kappa/c\rho$.

We emphasize that entropy production and entropy balance were not necessary for deriving the self-contained equation of motion for the temperature field—or, equivalently, internal energy density. Notably, the two most widely-used textbooks on classical irreversible thermodynamics [48,69] both start their sections on heat conduction with the bilinear form of entropy production:

$$\sigma = -\frac{1}{T^2}\mathbf{J}_u \cdot \nabla T \ .$$

They then proceed, as we have above, without further reference to it. For a more complicated example of deriving nonequilibrium transport equations-of-motion Eq. (1) without entropy production or entropy balance, see Ref. [48, Chapter IV, Section 4]. It derives the equations of motion for a single chemical component isotropic fluid, which it calls "thermo-hydrodynamics".

5.2. Reprise

Let us pause to reflect on the status of entropy production and entropy balance. Recall that equilibrium thermodynamics introduces the entropy state function and the 2nd Law to formalize the observation that some processes occur spontaneously in only one direction, despite both directions being consistent with the 1st Law. The derivation of Fourier's heat law and other nonequilibrium transport laws demonstrates that entropic quantities are not necessary to produce a full set of equations-of-motion for nonequilibrium transport processes. Furthermore, entropy balance—the generalization of the 2nd Law—is not necessary to capture irreversibility, as this is already inherently contained within the resultant equations-of-motion. For these reasons, entropy production and entropy balance (as defined and used above) are superfluous in the general theory of classical nonequilibrium thermodynamics.

In the context of self-organization, this is exactly how the nonlinear dynamics approach to pattern formation proceeds. The governing local equilibrium transport equations Eq. (1) are derived (and, typically, simplified) and it is from these equations that the bifurcation analysis is performed. We emphasized that a "thermodynamic" theory generally implies an entropic theory. We now see why entropic quantities are not present in the nonlinear dynamics analysis—they are simply not needed.

No surprise then that entropy balance, in particular, is largely absent from contemporary work in nonequilibrium thermodynamics. A notable exception is the recent review of the 2nd Law for the climate system [71]. However, the authors note that the entropy balance equation "contains no additional information about the flow that is not already contained in the energy budget". Entropy balance is only used to provide nonnegative-definite constraints on entropy production.

Most contemporary research in nonequilibrium thermodynamics adopts the statistical approach and uses stochastic processes, such as Langevin dynamics [72,73]. Since the stochastic setting works with probability distributions, Shannon entropy is commonly employed. And, then, the time rate of change of Shannon information is often referred to as "entropy production". Paralleling equilibrium entropy, the terminology "entropy production" is overloaded and often leads to confusion.

5.3. Variational principles for nonequilibrium steady states

Beyond providing certain nonnegativity constraints, that may be useful in some situations, what is the utility of entropy production in classical irreversible thermodynamics? Historically, its most important appearances are in attempts to generalize the 2nd Law as a selection principle, where extrema of entropy production may determine nonequilibrium steady-states.

The first instance of a nonequilibrium variational principle is found in 1848, with Kirchhoff's study of current flow in electrical networks [74]. He identified the final network nonequilibrium steady state as that which minimized "dissipation": current distributes itself so as to dissipate the least possible heat for the given applied voltages. This predates by several decades Gibbs' variational statement of the 2nd Law for heterogeneous equilibrium [75] and Maxwell's principles of minimum heat [76, 407–408]. Helmholtz stated a minimum dissipation theorem for steady-state flow of

viscous fluids at low velocities [77]. Similar theories of minimum dissipation of energy were proposed by Rayleigh [78] and Lorentz [79].

To unify the known cases, Onsager [67,68] and Prigogine [47] both attempted to derive a general variational principle that determined near-equilibrium steady states. On the one hand, Onsager developed the *principle of least dissipation of energy*. Depending on the boundary constraints, he showed this principle can be cast as *maximizing entropy production*. (Note that Onsager clearly distinguished energy dissipation and entropy production.) Prigogine, on the other hand, advocated for the *principle of minimum entropy production*. Interestingly, it is not necessarily at odds with Onsager's maximum entropy production. Prigogine's principle can actually be derived from Onsager's, with additional restrictions. Refs. [80–84] and [50, Ch. 12] give in-depth accounts of nonequilibrium variational principles and their shortcomings. Helpfully, they include worked counterexamples demonstrating that well-known steady-states, such as heat conduction, cannot be extrema of entropy production.

Having the necessary expressions in hand, it is instructive to reproduce the heat conduction counterexample here, as found in Refs. [82–84] and [50, Ch. 12]. For a one-dimensional rod of length L, the total entropy production is the integral of σ along the rod:

$$\begin{aligned}\frac{dS_i}{dt} &= \int_0^L \mathbf{J}_u \cdot \nabla\left(\frac{1}{T(x)}\right) dx \\ &= \int_0^L \frac{\kappa}{T^2(x)}\left(\frac{\partial T(x)}{\partial x}\right)^2 dx \,, \end{aligned} \tag{35}$$

using the linear phenomenological law Eq. (30) above. Recall that the derivation of Fourier's heat law does not require entropy production, and it is a self-contained equation-of-motion for the temperature field with steady-state solution:

$$T^*(x) = T_h - (T_h - T_c)\frac{x}{L} \,, \tag{36}$$

which solves Laplace's equation $\nabla^2 T(x) = 0$.

To recover the steady-state solution Eq. (36) as an extremum of entropy production in Eq. (35), a "near-equilibrium" approximation is required [48,69] such that $L_{uu} = \kappa T^2(x) \approx \kappa T_{avg}^2$. However, the extremum of Eq. (35) can be directly computed, without approximation, by the Euler–Lagrange equation [83]:

$$T\frac{\partial^2 T}{\partial x^2} = \left(\frac{\partial T}{\partial x}\right)^2 \,,$$

which has an exponential solution:

$$T_{ext}(x) = T_h e^{-a(x/L)}, \quad a = \ln(T_h/T_c) \,.$$

This exponential steady-state temperature distribution has not been observed in the lab. And so, the true steady-state cannot be an extremum of entropy production. Ref. [84] argues that the approximation used above to recover the true steady-state distribution is only valid in equilibrium, and so only equilibrium solutions are extrema of entropy production. Despite clear and numerous counterexamples, variational principles of entropy production, particularly minimum entropy production, are regularly invoked or referenced as valid.

As Ref. [81] points out, in the cases for which the steady-state solution is compatible with an extremum of entropy production—e.g., examples in Refs. [48,69]—the variational principle is redundant. This is because the final Euler–Lagrange equations reduce to the conservation and phenomenological laws; e.g., Laplace's equation for heat conduction, with the "near-equilibrium" approximation used. And, the latter was already valid before invoking a variational principle. This is not surprising, given that entropy balance is similarly redundant.

Finally, the nonlinear dynamics framework has shown that many systems exhibit multistability far from equilibrium. This means that multiple steady-state solutions become stable for a given value of R. Stability analysis alone then, in whichever form, cannot determine which of these stable states is realized in the system. As emphasized earlier in Section 3, which state is realized depends on the particular details and history of the system up to that point.

5.4. Dissipative structures

While the nonlinear dynamics approach to pattern formation may be rightly considered a thermodynamic theory, the notion of a thermodynamic theory of self-organization continues, regrettably, to be synonymous with Prigogine et al.'s theory of *dissipative structures*. Even more regrettable, it has become so synonymous that several contemporary authors continue to cite dissipative structures while lacking awareness of the many critiques and counterexamples that disprove the theory. Worse still, dissipative structures are sometimes cited without a basic understanding of the theory.

The theory of dissipative structures [69,85,86] attempted to create a "thermodynamic"—i.e., entropic—analysis paralleling the nonlinear dynamics' bifurcation theory. Both approaches center on the stability and exchange of stability between nonequilibrium steady-states. The nonlinear dynamics approach employs linear stability analysis—Lyapunov's

first method. Dissipative structures follows Lyapunov's second method, attempting to create entropic Lyapunov functions that determine the stability of nonequilibrium states.

The theory of dissipative structures proposes two nonequilibrium steady-state stability criteria, one for "near-equilibrium" and one "far-from-equilibrium"—both of which do not hold in general. Recall that Section 3 above introduced the bifurcation parameter R as a distance from equilibrium. Starting in equilibrium, we have $R = 0$. As R is slowly increased from $R = 0$ the system remains, for small R, in stable nonequilibrium steady-states until the first, or primary, bifurcation occurs, denoted $R = R_c$. The dissipative structure approach refers to the "near-equilibrium" values of $0 \leq R < R_c$ as the *thermodynamic branch*; see, for example, Ref. [69, Chapter 18]. (Above we referred to this as the base state.) Recall that a "near-equilibrium" assumption is necessary for an extremum of entropy production to coincide with the steady-state solution of the nonequilibrium transport equations. (As we have seen, though, these only coincide in general exactly at equilibrium.)

The dissipative structure approach uses the proposed principle of minimum entropy production to state that the thermodynamic branch is always stable "near-equilibrium". Recall though that nonequilibrium steady-states—states that are any nonzero distance from equilibrium—do *not* generally correspond to states of minimum entropy production.

5.5. Universal evolution criteria?

According to dissipative structures, minimum entropy production guarantees that steady-states "near equilibrium" are always stable (again, this is not true in general), and therefore pattern-forming instabilities must occur "far-from-equilibrium". In the far-from-equilibrium regime, the phenomenological laws may no longer be linear. To assess the stability of states arbitrarily-far from equilibrium, Prigogine and Glansdorf introduced the "universal evolution criterion" [85], based on the *excess entropy production* or *second variation of entropy* $\delta^2 S$. They showed that, as long as the local equilibrium assumption is valid, then $\delta^2 S < 0$. With this, to be a Lyapunov function, the time derivative of $\delta^2 S$ must additionally be positive for stable states and negative for unstable states. They found the time derivative takes a bilinear form:

$$\frac{d}{dt}\frac{\delta^2 S}{2} = \int_V \sum_i \delta F_i \delta J_i \, dV \ .$$

Similar to entropy production density in Eq. (25), this expresses excess entropy production in terms of (variations of) physical quantities that can be computed or measured.

Recall that essentially the entirety of classical irreversible thermodynamics was developed in the near-equilibrium linear regime. In this light, the universal evolution criterion was a hugely ambitious attempt to address arbitrarily-far-from-equilibrium states. Unfortunately, the universal evolution criterion does not hold in general and the excess entropy production is not a Lyapunov function. Following the theme here, the nonequilibrium transport equations-of-motion—that, again, do *not* require entropy production—are typically valid far from equilibrium (but may breakdown in extreme cases). And so, steady-states and their stability may be assessed independently of excess entropy production; i.e., using nonlinear dynamics bifurcation analysis.

In a series of back-and-forth letters to the *Proceedings of the National Academy of Sciences*, Keizer and Fox provided counterexamples for which the excess entropy production makes stability predictions that are counter to the established linear stability analysis of the transport equations-of-motion [87–91]. While Prigogine et al. initially attempted to respond, a final counterexample was given by Fox [91] for which there is no rebuttal. Anderson and Stein similarly concluded that the universal evolution criterion is nothing of the sort; "As far as we can see, in the few cases in which this idea can be given concrete meaning, it is simply incorrect" [92].

The latest version of Kondepudi and Prigogine's textbook softens the universal evolution criterion to provide "a necessary but not a sufficient condition for instability". And, it remarks more generally that "in the far-from-equilibrium nonlinear regime, there is no such general principle for determining the state of the system" [69, Chapter 18]. When providing examples of pattern-forming instabilities, this textbook and Ref. [93] both revert to the standard linear stability analysis, after introducing dissipative structures. Likely, this causes confusion, leading readers to associate the theory of dissipative structures with nonlinear dynamics' well-vetted bifurcation theory. We emphasize again, however, that the theory of dissipative structures is auxiliary to the nonlinear dynamics approach and does not provide a similar stability analysis since the excess entropy production is not a Lyapunov function.

Interestingly, in their back-and-fourth letters to PNAS, Keizer and Fox advocate for a competing entropic stability criterion [94]. We are not aware of similar counterexamples to their criterion, but it also does not appear that it has been widely adopted. That said, given that it takes a stochastic approach, based on fluctuation–dissipation relations, it is more in line with contemporary nonequilibrium thermodynamics and, thus, may be worthwhile revisiting. However, *any* successful entropic stability criterion adds nothing fundamentally new to the nonlinear dynamics analysis, as their goals are the same. Perhaps, optimistically, some stability calculations may be easier within an entropic stability theory.

One claimed advantage of an entropic stability criterion is to give "a physical meaning in terms of thermodynamic quantities of direct experimental interest to the otherwise abstract predictions of the qualitative theory of differential equations" [88]. However, given the ample success of matching nonlinear dynamics predictions with experiment, this is a dubious claim. (See the many examples described in Ref. [17].) Yet again, entropic considerations appear quite superfluous in nonequilibrium theories.

5.6. Entropy productions

Given the central role of entropy and the 2nd Law in equilibrium theory, it is quite surprising to find the generalizations of entropy production and entropy balance do not play a similar role in nonequilibrium theory. Perhaps shockingly, they appear to play almost no role at all in classical local equilibrium field theories! This is by no means a novel insight, but it is not something we have seen emphasized much in discussions of classical nonequilibrium thermodynamics.

By way of contrast, other terms called "entropy production" feature prominently in contemporary stochastic thermodynamics [73,95]. While various terms may share the title of "entropy production", the physical relationship between them is often unclear; particularly so between uses in stochastic thermodynamics and what we have introduced above in classical irreversible thermodynamics.

Section 4 gave a lengthy discussion on the nature of entropy in equilibrium theory. It concluded that the Shannon information interpretation of entropy is the best foundation available for understanding what entropy actually is. It also emphasized that from this perspective, an assumption of entropy additivity implies independence between components. Thus, taking volume integrals of entropy density in local equilibrium field theories implicitly assumes there are no interactions or correlations between mesoscopic volume elements. While in restricted settings this may be a reasonable assumption—as with, say, heat conduction through an isotropic material—from the outset it precludes describing organized systems.

Furthermore, recall that the derivation of the differential form of entropy balance Eq. (26) required the volume integrals in Eqs. (23)–(25). This makes the entropy balance equation suspect in the general case. For instance, the time rate of change of total entropy cannot equal the volume integral of the time rate of change of entropy density in Eq. (23) if total entropy is not equal to the volume integral of entropy density. Using the residual total correlation introduced above in Eq. (21), we have:

$$\frac{dS}{dt} = \int_V \frac{\partial s}{\partial t}\, dV - \frac{dC}{dt} \ .$$

The total correlation (degree of organization) term depends on the volume over which it is evaluated, and recall that independence from the arbitrary volume was necessary to go from integral balance equations to differential balance equations. An immediate consequence is that the differential entropy balance equation, on which dissipative structures is largely based, is not valid for organized systems. That is, dissipative structures was an attempt at a thermodynamic theory of self-organization, but was built on assumptions that do not hold for organized systems.

In the general subadditive case, it is not clear how to conceptualize an entropy production density σ. And, while it may seem intuitive that currents of matter and energy may "carry entropy", from an information-theoretic perspective such "flows of information" are difficult to properly define and interpret [96]. Overall, there is not a solid physical basis for assuming that information, and thus entropy, is locally conserved [50].

One can only conclude that (differential) entropy balance and entropy production density do not have a solid physical basis in the general subadditive case when organization is present in the system. In this light, it is rather fortunate that they are not needed to derive the full set of nonequilibrium transport equations Eq. (1).

This is not to say, however, that entropic quantities should be banished from nonequilibrium theories. Quite the opposite, in fact, as recent developments have recognized the significance of information as a thermodynamic resource [97]. Entropy is a subtle concept that must be invoked with care. While the information-theoretic approach is the most promising, high-dimensional information theory is in its infancy [98,99]. Contemporary work in stochastic thermodynamics typically concerns low-dimensional systems. And, with a few exceptions [100], there remains a disconnect between theoretical developments in stochastic thermodynamics and the physical phenomenon of self-organization.

5.7. Principle of Maximum Caliber

To close the discussion on thermodynamics, we briefly return to Jaynes' Principle of Maximum Entropy. Recall that this approach builds up equilibrium statistical mechanics starting from the perspective of information-theoretic entropy, along with the logic that unbiased distributions should maximize entropy subject to appropriate constraints. This foundation allows for a clear and rigorous path to nonequilibrium statistical mechanics. The *Principle of Maximum Caliber* (MaxCal), a generalization, creates time-dependent microstate distributions by maximizing uncertainty over space–time paths, consistent with the constraints of the macroscopic process [50,101–103].

MaxCal suffers from the same objections as the Principle of Maximum Entropy, though—that the resulting microstate distributions depend on the specific macroscopic constraints given. That noted, when using appropriate macroscopic constraints, MaxCal derives known phenomenological laws—e.g., Fick's and Fourier's laws—from first principles using linear perturbation theory [50]. Given the prominence of phenomenological laws in nonequilibrium theory, any potential derivation from first principles is worth consideration. Furthermore, numerical evidence suggest that bifurcations in fluid instabilities [104] and lasers [105,106] are consistent with MaxCal.

Ideally, MaxCal would offer a path to deriving as-yet undiscovered nonlinear constitutive relations for far-from-equilibrium systems. To date this has not been achieved, due to the intractability of the nonperturbative space–time path integrals. Conceptually, a nonequilibrium statistical mechanics, such as MaxCal, links microscopic dynamics with

the macroscopic field theories that nonlinear dynamics shows exhibit pattern-forming and self-organizing behavior. So, technically speaking, this provides one answer to "how" microscopic constituents organize into macroscopic patterns. However, nonequilibrium statistical mechanics so far falls short of providing a constructive and direct answer to this question due to the many layers of logic and complicated mathematical operations separating the macroscopic from the microscopic.

This separation and general intractability of nonequilibrium statistical mechanics and high-dimensional information theory lead us to an important interlude in the discussion of far-from-equilibrium thermodynamics and self-organization more generally. There is reason to believe these hurdles are not exceptional but rather typical for self-organization, in much the same way nonlinear dynamics is the norm and linear dynamics the exception in mechanics. This intractability is one likely reason why self-organization has stubbornly resisted our understanding for so long. However, there are others.

6. Intractability and limits of constructionism

From one perspective, at this point we reached our destination in the search for principles of emergent organization. Macroscopic equations of motion Eq. (1) are derived from conservation and phenomenological laws, without the need for entropic quantities or generalizations of the 2nd Law. Their range of validity away from equilibrium depends on the range of validity of the phenomenological laws. In many cases, those laws hold very far from equilibrium—e.g., the Navier–Stokes equations governing fluid flow. From such equations, emergent organization can be derived in principle from the bifurcation analysis of their nonlinear dynamics. In another sense, though, the journey has only just begun towards principles of organization. Much of the challenge ahead hides behind two simple words used above: *in principle*.

6.1. Constructionism

Quantitative science relied on and flourished due to the reductionist hypothesis—that the constituents of all systems, no matter how complicated, are governed by the same fundamental laws. This, however, came at the cost of an erroneous assumption—what the late Philip Anderson called *constructionism*—the ability to start from the fundamental laws and reconstruct the universe [107]. That is, although a macroscopic system of interest is, *in principle*, fully described by the Hamiltonian dynamics of its constituent particles, its macroscopic dynamics cannot always be constructed directly from the microscopic dynamics. Even though emergent organization may be derived from bifurcation theory in principle, there are intractability limits in practice. Reductionism and constructionism are effective tools for uncovering the fundamental laws of the universe, but "in principle" answers do not go far enough for understanding emergent phenomena.

Statistical mechanics traditionally considers a single bridge between two levels—"macroscopic" transport equations Eq. (1) are constructed from "microscopic" Hamiltonian particle dynamics [108]. Pattern formation theory of nonlinear dynamics is then seen as an additional bridge, with the "macroscopic" dynamics of Eq. (1) taken as the starting point, from which organization and patterns that emerge are constructed. To avoid confusion, let us refer to the "microscopic" description of system behavior, in terms of Hamiltonian dynamics of particles, as Level I. "Macroscopic" continuum dynamics will then be Level II, and emergent organization will be Level III. Traditional statistical mechanics bridges Level I to Level II[2], and pattern formation theory attempts to bridge Level II to Level III.

Note that for some purposes the Hamiltonian dynamics of particles is sufficient as the "lowest" Level. However, other purposes may require considering quantum fields or strings as lower Levels of description. Oppositely, higher Levels—relevant to, say, chemistry and biology—may be required.

Here, the term *Level* [111] delineates a *consistent* and *self-contained* mathematical formulation of a system's behavior [112]. There is nothing different about the physical system and its behavior when moving between Levels; what changes is how those behaviors are described. Consider properties of the air in the room you are sitting in as you read this. We typically think of the air as an "ideal gas", in the thermodynamic sense, with properties of temperature, pressure, and volume. These are the properties we experience on the human scale. Empirically, it was discovered that these properties are related to one another in a consistent and self-contained manner, encapsulated in what we now call the Ideal Gas Law. Another consistent and self-contained description of air in a room is given by the kinetic theory of gases, in which the air mass is seen as a collection of a huge number ($\sim 10^{23}$) of air molecules whizzing about and colliding with each other and with objects in the room. An early triumph of statistical mechanics was to derive, i.e. construct, the Level II Ideal Gas Law starting from the Level I kinetic description.

From Ref. [54, Ch. 1], "The kinetic derivation of the ideal gas law is still frequently cited as a paradigm of scientific explanation by teachers and philosophers, despite (or perhaps because of) the fact that it is hard to find such simple connections between microscopic models and macroscopic properties in modern physical science." Indeed, the derivation of Fourier's heat law reviewed above is entirely thermodynamic; i.e., it refers only to the macroscopic Level. Direct construction of Fourier's law from microscopic kinetics remains an open challenge [113]. For the remainder of this Section, we argue why such bridges between Levels are indeed quite hard to come by in the constructionist paradigm. The

[2] Historically, the tools of statistical mechanics are applied to construct Level II from Level I Hamiltonian physics, like the thermodynamics of gasses [54] or fluid flows [109], which is what we mean when we say "traditional" statistical mechanics. These tools, however, can be extended and generalized to apply to a wider array of systems in which the lower Level is not necessarily Hamiltonian dynamics, e.g. with biological systems [110].

failure of constructionism leaves a void necessitating a wholly new paradigm for studying the mechanisms of emergent organization.

To ground the discussion, let us return once again to Bénard convection and give an in-depth examination of a successful application of constructionism to emergent organization. This makes clear what is missing when constructionism cannot be relied upon.

For Bénard convection, Level I is the statistical description of particle motion given by the Boltzmann equation, Level II is the continuum field theory of the Navier–Stokes equations, and Level III describes the (in this case static) hexagonal Bénard cells that emerge. The construction of Level II from Level I for fluid systems has a long and storied history, including Hilbert's Sixth Problem—to extend mathematics' axiomatic methods to physics and beyond [109,114].

In the following, though, the construction of Level III from Level II is what concerns us. The derivation of the emergence of Bénard cells for the near-equilibrium primary bifurcation highlights the power of constructionism in explaining emergent organization—when it is successful. Different constitutive relations in the Level II equations represent *mechanistic hypotheses* that underlie the organization that emerges. The correct mechanism is found by identifying which Level II equations are able to *construct* the emergent organization that agrees with observation.

The linear stability analysis performed by Rayleigh [2] was the first theoretical attempt to explain the spontaneous self-organization observed by Bénard. However, his calculated value of the critical Rayleigh number that determines the exchange of stability from conduction to convection—the primary instability—did not agree well with Bénard's experimental value. Despite subsequent analyses and refined experiments, the disagreement persisted. It turned out that Rayleigh made an incorrect assumption about the underlying *physical mechanism* driving the instability. Bénard performed free-surface convection experiments, but Rayleigh assumed surface-tension effects would be negligible compared to buoyancy effects.

M. J. Block [115] later posited that surface-tension effects would dominate in free-surface convection, and this was subsequently confirmed by the calculations of J. R. A. Pearson [116]. He performed a linear stability analysis similar to Rayleigh, but with surface-tension rather than buoyancy effects, and this calculation agrees well with Bénard's and now other's free-surface experiments [117].

The competing mechanistic hypotheses are instantiated in various phenomenological laws that are then used as part of the Level II transport equations on which the linear stability analysis is performed. Rayleigh assumed that density varies linearly with temperature and that density variation is only significant in the buoyancy force. He included no surface tension effects. Pearson did the opposite, neglecting density variation while including surface tension and its dependence on temperature. Once the hypotheses were formulated into equations of motion, the same linear stability analysis is performed to construct the resulting physical phenomenon of interest—deducing the critical Rayleigh number at which convection sets in.

Discovering that surface-tension effects dominate the instability mechanism for free-surface convection is a triumph of constructionism. Not only is the onset of instability and pattern emergence predicted, but different physical mechanisms encapsulated in the phenomenological laws predict different onsets for free-surface and closed convection and these match experiment. We detailed constructionism's success in explaining the primary Bénard instability to raise a key question in the study of emergent organization: how do we explain emergent behaviors if we cannot construct Level III from Level II? As Anderson pointed out, and as we now detail, constructionism cannot always be relied upon. There are cases (perhaps many) where Level III simply cannot be deduced or derived or constructed directly from Level II.

Bifurcation theory's success in quantitatively predicting the primary Bénard instability was greatly facilitated by the problem's relative simplicity. And, this raises a critical challenge. How does the constructionist approach break down for more complex systems? Complicated boundary conditions and base states certainly make the analytical calculations more difficult, perhaps even intractable. However, these challenges can be (approximately) overcome using numerical solutions, as is commonly done now for many nonlinear systems.

A more fundamental issue arises that cannot be easily side-stepped through numerical solutions. In the convection example, it is possible to isolate a single mechanistic hypothesis (as given by a particular phenomenological law) and construct its emergent effect. For more complex systems, though, it may not be possible to isolate the effect of a single physical mechanism on the resulting behavior of interest within the tangle of nonlinear interactions and feedbacks [118].

In essence, successfully simulating a behavior does not mean we understand it. For example, we do not have a complete picture of the physical mechanisms underlying the formation and dynamics of hurricanes, despite being able to simulate them quite well with sophisticated general circulation models [119–121]. Similarly, turbulence remains one of the great mysteries of physics, despite decades of successful and exquisitely detailed numerical simulation [14].

For any given analysis that challenges us, is it really intractable or are we simply insufficiently clever? For certain problems, we know there is no clever solution to be found and that the problem is truly intractable in general. Such problems are known as *undecidable* or *uncomputable*—there is no algorithm or fixed procedure that yields an answer in finitely-many steps for all instances of the problem [122]. While some instances of an undecidable problem may be solvable, there is no single procedure that always gives an answer for all instances.

Equilibrium statistical mechanics is the quintessential example of a bridge between scales that computes Level II properties from the system's underlying, "fundamental", Level I description. Such a bridge does not always exist if Level $(i + 1)$ properties are uncomputable starting from Level i. Ref. [123] rigorously showed that for at least one case, the macroscopic properties of an Ising-like model are uncomputable from the underlying microscopic dynamics. There

are cases then when knowing the lower-Level theory really cannot reveal everything needed to know about emergent higher-Level phenomena, even if the lower-Level theory is a consistent description, in principle.

As an aside, if it seems strange that the theory of computation has something to say about our fundamental ability to understand physical phenomena, recall that uncomputability was first devised to answer a similarly fundamental question in the foundations of mathematics [124].

6.2. As simple as possible, but not simpler

It is illuminating to examine these issues in a markedly simpler setting than hydrodynamics. The setting of *cellular automata* (CA) models allows us to make rigorous statements about formally-difficult problems in understanding their behavior using the resource analyses provided by the theory of discrete computation [125–127].

A CA deterministically evolves a fully-discrete classical field: A spatial lattice whose sites take on values from a finite alphabet evolves in discrete time steps according to a simple spatially-local deterministic update rule—its *lookup table*. Unlike continuum models, no approximation scheme is required to numerically simulate CAs. Their numerical evolution is exact; effectively mapping one large integer (the spatial configuration) to a unique next integer. Therefore, there is nothing missing, nothing hiding, in CA simulations. This makes them ideal for studying how governing equations, given as the local update rule, produce particular temporal behaviors and spatial configurations.

Since CA description Levels do not map onto the Levels of fluid flows used above, we refer to the full CA system with dynamics governed by the lookup table as Level A and emergent organization in the spatial configurations and temporal behavior as Level B. The emergent Level B dynamics may be deterministic [35,128] or stochastic [32,129]. Ref. [123] showed that Level B dynamics that correspond to thermodynamic properties for an Ising-like CA are uncomputable from the Level A CA dynamics. We emphasize that while the Level B description cannot be directly constructed in general, specific instances are always realized through evolution—whether "simulated" by a computer or by hand—of the Level A dynamics. Uncomputability provides a hint of mystery for how Level B arises from Level A, but due to the exactness of discrete CAs we know for certain there is nothing extra-physical or magical in Level B that is not consistent with Level A.

Beyond the physically-motivated CA studied by Ref. [123], many CAs, such as Conway's Game of Life [130], are famously *Turing complete*. In a concrete sense, they are capable of producing arbitrarily complex behaviors. In general, for a given look-up table and initial condition, one cannot know whether a particular lattice configuration will ever be generated by a Turing-complete CA (due to a reduction of the halting problem) [131]. How can we deduce the relation between mechanistic hypotheses in the governing equations and resultant long-term behaviors if the latter are not computable from the former? Relatedly, dynamical systems with uncomputable long-time behavior represent a level of unpredictability above and beyond that presented by chaotic systems [132].

Recall though that uncomputability means there is no general algorithm or procedure that gives an answer (in finite time) for *all* instances of a problem. Also, it is the long-term CA behavior described above that is uncomputable. For particular instances of finite-time behaviors, we can always simulate a system's governing equations and observe what patterns and behaviors emerge. In addition to undecidability, many CAs pose another formal challenge that complicates mechanistic analysis for specific behaviors that arise in finite time. For example, determining the configuration (system state) of certain CAs from a given initial condition after t time steps is **P**-Complete [133,134]. Let us explain the consequences of this.

Although not formally established, it is widely believed that there is a class of "inherently sequential" problems that are in the computational complexity class **P** but not in **NC**. Problems in **P** can be solved in polynomial time on a serial computer, whereas problems in **NC** can be solved in polylogarithmic time on a parallel computer. For example, there is a class of "quasi-linear" CAs whose state prediction problem is in **NC** [135]. Algebraic properties of these CAs allow information from an initial condition to be split onto multiple processors, and then each processor performs a logarithmic-time computation on its own simplified problem. If, as widely believed, $\mathbf{NC} \neq \mathbf{P}$, the **P**-Complete CA prediction problem is inherently sequential. As a consequence, a prediction cannot be computed qualitatively faster than explicitly evolving each state from its proceeding state, in sequence—which is linear in time.

Cellular automata directly and concretely demonstrate that very simple rules, repetitively applied, can give rise to arbitrarily complicated behaviors. Moreover, they can be formally hard to analyze, confounding traditional constructionist methods. For many CAs deducing emergent Level B properties and long-term behaviors from Level A dynamics is uncomputable. For inherently sequential CAs, mechanistic hypotheses must be tracked through at each time from an initial condition to a behavior at a later time. The number of relevant interactions between initial and latter times (the lightcone) grows exponentially with time. Of the 256 "elementary" CAs—radius-1 interactions and binary alphabet—one, rule 110, is known to be Turing complete [128] and inherently sequential [134]. Both of these properties arise through emergent Level B organization that can be mapped to a model of universal computation. Why is it that the particular lookup table of rule 110 is the only Level A dynamics of elementary CAs that produces such complex Level B behaviors? This is not known.

Even though providing the bridge to explain Level B behavior from Level A is formally difficult for rule 110, something we can do is to formulate a complete and self-contained model for Level B behaviors. The computational properties of rule 110 (Turing completeness and being inherently sequential) are proven using these Level B behaviors. A complete and self-contained model for the Level B dynamics has also been shown for rule 54 [35], although these behaviors are not nearly as rich as for rule 110.

To summarize, most approaches to pattern formation theory seek to provide a bridge from the Level II theory provided by the nonequilibrium equations of motion to the Level III organization that may spontaneously emerge. In this, *principles* of organization attempt to address "how" and "why" questions: e.g., how does fluid in a box spontaneously form hexagonal convection cells, and why does it happen at different critical temperature gradients for open- and closed-top boundary conditions?

The previous section discussed how such questions are typically answered from a constructionist approach. Mechanistic hypotheses of the underlying physics are formulated as the Level II theory that then "explains" the observed Level III behavior if said behavior can be constructed from the Level II equations of motion. This constructionist paradigm breaks down if the construction becomes intractable. Cellular automata models rigorously show that constructing the higher Level (B) from the lower Level (A) can be uncomputable, and thus formally difficult. Even though there is no mystery in the microscopic constituent components and their interactions, there are cases where knowing these cannot help us understand higher-Level organization that emerges from the lower Level dynamics.

These observations force turning attention away from constructionism to an alternative approach to *principles* of organization. Although we cannot always bridge from one Level to the next, can we at least, as with rule 110, formulate a complete and self-contained theory of the higher-Level organization that emerges? The rigorous results of intractability in CAs suggests that constructing Level III from Level II in physical systems, like fluid flows, may be generally intractable. Can we, though, discover general principles common to Level III descriptions of these systems, for example analogous to conservation laws found in Level II descriptions? We will return to this question in the final Section 8.

While the computation-theoretic methods cannot be easily applied to continuum models, cellular automata provide examples of self-organizing systems that are provably difficult to study and for which simulation is very likely a requirement for their study. Taken together, the arguments here point to computation theory playing a central role in the study of self-organization and, thus, in the formulation of general principles of organization. This is in contrast to the typically analytically-oriented formulation of general principles in physics. This is perhaps historically why principles of organization have remained elusive there. The central contribution of computation theory in our diagnosis of the failures of constructionism is that intractability stems from the growth of the resources required to evolve organized configurations. This suggests a duality between emergent organization and the resources a system commandeers to evolve them. We now turn to modern formulations of emergent organization using concepts and constructions from the theory of computation.

7. Organization beyond constructionism

If we seek general principles of organization, surely we must first lay out what organization *actually is*. Bifurcation theory identifies organization with exact symmetries (and small deviations from them) using Fourier modes. Failing exact symmetries and their associated group algebra, how does one write down a mathematical expression for, say, a hurricane?

As a concrete example, consider the dynamics of vortices in free-decay two-dimensional turbulence. The Level II theory is the vorticity equation (derived from Navier–Stokes) and the Level III theory describes the behavior of the "vortex gas" that emerges from random initial conditions. In this, like-signed vortices may undergo a pairwise merger if certain geometric conditions are met [136], resulting in a power-law decay of the number of vortices over time. This behavior was discovered empirically, using a specialized algorithm to identify vortices based on vorticity thresholding and additional geometric considerations [137]. As a prerequisite to general principles of organization and moving away from relying on specialized approaches for specific systems, can we first identify general principles for mathematically identifying emergent organization?

In addition to solving nonlinear equations through numerical simulation, computation—in the guise of computation theory—points a way to answering this question, by providing a mathematical accounting of more general forms of organization in—what it calls—*formal languages*. This section outlines two modern approaches for formalizing organization beyond exact symmetries—approaches inspired by computation theory. The following section then discusses their relationship and how they fit into a statistical mechanics of emergence that gives a theoretical foundation for data-driven modeling of organized behaviors and their dynamics.

7.1. Organization through compression

One motivating intuition behind understanding organization is that of *compression*. Organized behaviors are higher-Level degrees of freedom that emerge from *collective motion* of lower-Level degrees of freedom. Bénard cells and more general vortices, for instance, involve the coordinated motion of many fluid parcels (differential volume elements). Since the fluid parcels evolve together, they need not be tracked separately. They may be considered equivalently and collectively as a single emergent degree of freedom. The collective degrees of freedom then provide a natural dimensionality reduction for a compressed representation of a system's behavior and configurations.

Another perspective on the importance of compression is more easily seen through the lens of "pattern". (For our immediate purposes "pattern" and "organization" are essentially synonymous.) One's typical mental image of a "pattern" is some exact symmetry; e.g., a repetitive tiling in two spatial dimensions. The Bénard cells that have been our guiding example form a symmetric hexagonal tiling, under the right circumstances. Such symmetries provide a predictive regularity—one region of Bénard cells "predicts" other parts. And, the regularity of exact symmetries can be predicted exactly.

As emphasized above, though, our goal is to articulate a more general notion of organization beyond exact symmetries. One path to this is to account for partial or noisy symmetries that describe approximate predictive regularities. Like exact regularities, these noisy regularities can also be leveraged to create a system's compressed representation. The latter will be constructed using semigroup algebra which generalizes the group algebra of exact symmetries to noisy symmetries. Before delving further into these two approaches—predictive regularity and dimensionality reduction—it is insightful to review several computation-theoretic ideas that motivated the use of compression in the first place.

Statistical mechanics' successful use of correlation functions, structure factors, order parameters, and symmetry groups to describe regularities in physical systems [138] has for some time inspired the search for mathematical descriptions of organization in the form of scalar quantities. Historically, what came to be called measures of "complexity" [139], we will consider here as measures of "degrees of organization".

The most notable complexity measure motivated by compression is that introduced by Kolmogorov and Chaitin. An object's Kolmogorov–Chaitin (KC) complexity is the length of the shortest universal Turing machine program that reproduces it [61,140–142]. KC complexity measures the minimum computational resources—information storage and computational operations—required to exactly describe an object. Intuitively, objects consisting of more complex patterns require more description and so are less compressible.

However, it is now well-appreciated that KC complexity is in fact a quantitative measure of randomness, rather than organizational complexity [143]. Related complexity measures—such as, *sophistication* and *logical depth* [144–148]—attempt to separate out the "meaningful" complexity from randomness. And, in any case, all approaches that rely on minimally compressed programs are nonconstructive—the task of determining minimal programs is uncomputable.

Although uncomputable, the true minimal program may be approximated in practice using practical compression algorithms. A popular choice is the Lempel–Ziv algorithm [149,150] used for zip and Unix compress. Here too, though, there are difficulties in separating organization from randomness. For instance, the Lempel–Ziv algorithm doubles the length of random strings when, being incompressible, they should be unchanged.

Another compression-based method relies on determining an object's *minimum description length* (MDL) by encoding descriptions of both model and residual error [151]. Using this information-theoretic criterion, the MDL principle selects the predictive model with the lowest generalization error from a given set of candidates. So, while useful for training in a parameterized model class—such as, autoencoder neural networks used for dimensionality reduction [152]—it does not provide a constructive basis for a first-principle approach to quantifying organization.

7.1.1. Compression in statistical mechanics

The original motivation for statistical mechanics was a means to tame the unwieldy dynamics of a huge number of particles. Analyzing the average behavior of particles, rather than all of their individual behaviors, signifies some form of compression. The physical consistency of this statistical compression comes from asymptotic equipartition and the typical set [153], as described above in Section 4. A recent extension of typicality gives a similar statistical compression and consistency to nonequilibrium processes [154].

For simple systems, the behavior on the typical set can be seen as an "averaging out" of the thermal fluctuations from the variations in individual particle motion. For more complicated behaviors, e.g. near a critical point, fluctuations across multiple scales can be systematically averaged out using the renormalization group [155]. The renormalization procedure of removing irrelevant degrees of freedom can similarly be viewed as a statistical compression.

Building on the computation-theoretic notions of compression given above, the compressions of system dynamics given below are in service of formulating mathematical representations of organization. In contrast, the compression in statistical mechanics is not necessarily associated with any organization at all, as with e.g. an ideal gas. It is employed to show how effective theories at higher Levels may emerge from lower Level physics. What is the relationship between these statistical and dynamical notions of compression?

Interestingly, the formulation of the renormalization group for time-dependent critical phenomena requires the use of evolution operators, introduced shortly. In particular, the effective Hamiltonian in equilibrium renormalization is replaced with the Perron-Frobenius operator (defined below) [156]. In this case, there is a close relation between the compression of renormalization and the "modes of organization" described next. Both cases examine the effect on a system's dynamics when certain modes, representing noise or fluctuations, are systematically removed.

In Section 8 we utilize intrinsic computation and evolution operators—first introduced to identify organization—to show physical consistency between emergent higher Level dynamics and the lower Level physics. This general framework does not require criticality, and degrees of freedom are not necessarily removed. It is thus more closely related to the information-theoretic approach given by Ref. [157] to show how effective theories emerge from lower Level physics through parameter space compression. That said, it is possible to systematically remove degrees of freedom in our statistical mechanics of emergence and thus compare with renormalization-type procedures. Making connections between these theories warrants further exploration.

7.2. Modes of organization

The structure of configurations generated by classical field theories is commonly approached in physics and engineering through the notion of compression via dimensionality reduction. Consider a (classical) spacetime field $X(\mathbf{r}, t)$ and assume

it can be decomposed through a linear superposition as:

$$X(\mathbf{r}, t) = \sum_{i=1}^{\infty} a_i \phi_i(\mathbf{r}, t) \ , \tag{37}$$

where $\mathbf{r}$ are spatial coordinates and t is time. In principle these coordinates are continuous, but in practice they are discretized for use with numerical methods. The spacetime components $\phi_i(\mathbf{r}, t)$ of the decomposition are referred to as *modes*.

If $X(\mathbf{r}, t)$ is structured—e.g., there is collective motion among its degrees of freedom through time—then this organization can be exploited to produce a compressed representation $\tilde{X}_n(\mathbf{r}, t)$ using only a finite number of n modes:

$$\begin{aligned} X(\mathbf{r}, t) &\approx \tilde{X}_n(\mathbf{r}, t) \\ &:= \sum_{i=1}^{n} a_i \phi_i(\mathbf{r}, t) \ . \end{aligned}$$

From the preceding discussion of organization through compression, the intuitive idea is that an optimal truncation that minimizes the reconstruction error $\|X(\mathbf{r}, t) - \tilde{X}(\mathbf{r}, t)\|$ leverages any organization present to create the modes $\phi_i(\mathbf{r}, t)$. The leading modes of an optimal truncation individually contribute more to the full system behavior if they contain collective, organized motion. (Though, not all modes describe collective behavior.) This motivates seeking specific constructions of $\{\phi_i(\mathbf{r}, t)\}_1^n$ as *modes of organization*.

As a first step, it is typical to separate the space and time dependencies, so that there are *spatial modes* $\phi_i(\mathbf{r})$ with time-varying coefficients $a_i(t)$:

$$X(\mathbf{r}, t) = \sum_i a_i(t) \phi_i(\mathbf{r}) \ . \tag{38}$$

That is, the spatial modes $\phi_i(\mathbf{r})$ form a complete basis to express a system's configurations—the spatial field $X(\mathbf{r}, t^*)$, at any (and every) time t^* using the coefficients $a_i(t^*)$. That said, there may not be a complete basis such that Eq. (38) holds. This is the case, for example, with turbulent fluid flows. There is a natural generalization to Eq. (38) for these cases given below.

The standard method to compute a finite set of spatial modes and their time-varying coefficients is *principal component analysis* (PCA), also known as *proper orthogonal decomposition* (POD), among other names [158]. In this, modes are computed using the singular value decomposition or, equivalently, an eigendecomposition of the data covariance matrix. From a statistical viewpoint, an organized system will have a high degree of correlation among its degrees of freedom due to their collective motion. POD computes modes that are linearly uncorrelated with each other, and so capture the majority of correlations in the system.

In this way, POD finds a change of coordinates to an orthonormal basis such that the first mode—the first dimension in the new coordinates—captures the majority of the system's variance, the second mode captures the majority of the remaining variance, and so on. From a physics point of view, POD provides an optimal finite decomposition since for any fixed number n of modes the reconstruction error $\|X(\mathbf{r}, t) - \tilde{X}(\mathbf{r}, t)\|$ is minimized by POD [159]. If the spacetime field is, for example, the velocity field of a fluid flow, POD is optimal in capturing the dominant energetic contributions [160].

A finite decomposition as in Eq. (38) can be used as a reduced model of the system dynamics. In this, the partial differential equation Eq. (1) for the evolution of $X(\mathbf{r}, t)$ is replaced by a finite set of ordinary differential equations that govern the evolution $\dot{a}_i(t)$ of the time-dependent coefficients. This can be achieved through a Galerkin projection of the PDE evolution operator onto the space spanned by the modes [161] or through data-driven forecasting of the coefficients [162,163]. Note that POD mode orthogonality is very useful in this.

7.3. Evolution operators

While POD has been an remarkably fruitful method for analyzing coherent structures in fluid flows, it is an ad hoc empirical method. Its use in investigating organization in fluid flows followed shortly after the notion of coherent structures emerged in the study of turbulence. Let us recall this history as a means to introduce a much richer and theoretically-grounded framework for formalizing coherent organization in classical field theories based on the Koopman and Perron–Frobenius *evolution operators* [164].

Statistical studies of turbulence in the latter half of the 20th century found a separation of scales in fluctuations about the mean flow. There are smaller scale "random" fluctuations on top of coherent periodic fluctuations. The *triple decomposition* [165,166] of the fluid velocity field formalizes this:

$$X(\mathbf{r}, t) = \bar{X}(\mathbf{r}) + X_p(\mathbf{r}, t) + X_c(\mathbf{r}, t) \ ,$$

where $\bar{X}(\mathbf{r})$ is the mean flow, $X_c(\mathbf{r}, t)$ is the chaotic component that generates the apparent small scale randomness, and $X_p(\mathbf{r}, t)$ is the coherent component consisting of spatial modes that evolve periodically in time as:

$$X_p(\mathbf{r}, t) = \sum_i e^{\omega_i t} \phi_i(\mathbf{r}) \ ,$$

with $\omega_i \in \mathbb{C}$. Spatial structures that evolve collectively at a single frequency, such as those in $X_p(\mathbf{r}, t)$, were first studied in the context of linear stability where they were identified as *global modes* [166,167].

7.3.1. Koopman operators

Motivated in this way, we now review a general and rigorous framework for modal decomposition of arbitrary dynamical systems using Koopman operators, as first introduced in Ref. [168]. Rather than analyze the system through the geometric viewpoint of the nonlinear evolution of $X(t) \in \Omega$, it is useful to analyze the linear dynamics of system observables given by Koopman operators [169].

An *observable* g is simply a scalar-valued function of the system state $g : \Omega \to \mathbb{R}$. Observables are elements of a function space $\mathcal{F}$. The parameterized (semi)group of *Koopman operators* $\mathcal{K}^\tau : \mathcal{F} \to \mathcal{F}$ are defined through composition with the dynamics Φ^τ:

$$\begin{aligned} \mathcal{K}^\tau g &:= g \circ \Phi^\tau \\ &= g\big(\Phi^\tau(X)\big) \ , \end{aligned} \tag{39}$$

where Φ^τ is the flow map defined by Eq. (1) such that $X(t_0 + \tau) = \Phi^\tau\big(X(t_0)\big)$.

Koopman operators define a dynamic in the space of observables generated by Φ^τ. That is, for an initial state $X(t_0)$ and observable g_0, the action of the Koopman operator $\mathcal{K}^\tau$ gives a new time-shifted observable function g_τ defined by:

$$[\mathcal{K}^\tau g_0]\big(X(t_0)\big) := g_\tau\big(X(t_0)\big) \tag{40}$$

$$= g_0\big(X(t_0 + \tau)\big) \ . \tag{41}$$

Considering discrete time steps for simplicity, Koopman operators give a flow through the space of observables for a given observable g_0 and initial system state $X_0 := X(t_0)$:

$$\begin{aligned} &\{g_0(X_0), \\ &g_1(X_0) = [\mathcal{K} g_0](X_0), \\ &g_2(X_0) = [\mathcal{K}^2 g_0](X_0), \\ &\ldots, \\ &g_i(X_0) = [\mathcal{K}^i g_0](X_0), \\ &\ldots\} \ . \end{aligned}$$

For dynamical consistency, the space of observables $\mathcal{F}$ must be closed under the action of all Koopman operators: $\mathcal{K}^\tau g_i \in \mathcal{F}$ for all τ and all $g_i \in \mathcal{F}$. For almost all nontrivial cases, this means $\mathcal{F}$ is uncountable and the Koopman operators $\mathcal{K}^\tau$ are infinite-dimensional [170]. If $\mathcal{F}$ is a vector space, as is typical, then $\mathcal{K}^\tau$ are linear, even if the original state–space dynamic Φ^τ is highly nonlinear. The Faustian bargain in this is to trade-away nonlinearity in low-dimensions for linearity in infinite dimensions.

It is common to take $\mathcal{F}$ to be a Hilbert subspace $\mathcal{F} \subseteq L^2(\Omega)$ of square-integrable functions. Another common choice is the space $L^\infty(\Omega)$ of essentially bounded functions. Note that since Koopman operators are defined through composition with the system dynamic, if the system state remains bounded over time—i.e., does not "blow up"—then the action of Koopman operators on bounded functions always returns another bounded function. This gives the requisite dynamical consistency.

With the operators in hand, let us consider the *Koopman mode decomposition* [168,171] and its use to define organization in time-independent dynamical systems. A Koopman eigenfunction φ_i is a scalar observable satisfying:

$$K^\tau \varphi_i(X) = e^{(\lambda_i \tau)} \varphi_i(X) \ ,$$

with eigenvalue λ_i. If the full set of eigenfunctions forms a complete basis of the function space $\mathcal{F}$, then an arbitrary scalar observable $g \in \mathcal{F}$ can be expanded as:

$$g(X) = \sum_i^\infty \nu_i \ \varphi_i(X) \ ,$$

with expansion coefficients ν_i. It is natural to consider vector-valued observables, each component of which can be expanded as above:

$$\mathbf{g}(X) = \begin{bmatrix} g_1(X) \\ g_2(X) \\ \vdots \\ g_m(X) \end{bmatrix}$$

$$= \sum_i^{\infty} \varphi_i(X) \begin{bmatrix} \nu_1 \\ \nu_2 \\ \vdots \\ \nu_m \end{bmatrix}$$

$$= \sum_i^{\infty} \varphi_i(X) \vec{\nu}_i \ .$$

The vector-valued coefficients $\vec{\nu}_i$ are known as the *Koopman modes* of the vector-valued observable $\mathbf{g}$. They are given as the projections of $\mathbf{g}$ onto the eigenfunctions:

$$\vec{\nu}_i = \begin{bmatrix} \langle \varphi_i, g_1 \rangle \\ \langle \varphi_i, g_2 \rangle \\ \vdots \\ \langle \varphi_i, g_m \rangle \end{bmatrix} \ .$$

Emergent organization here is associated with the Koopman modes of one vector-valued observable in particular—the *state identity* observable $\mathbf{g}_I(X) = X$. While Koopman operators (and Perron–Frobenius operators introduced shortly) are defined for arbitrary dynamical systems, we now consider the system state $X(\mathbf{r}, t)$ to have a spatial structure $\mathbf{r} \in \mathcal{D}$ over spatial domain $\mathcal{D}$. In this case, for fixed time, the system state $X(\mathbf{r})$ is a function from the spatial domain $\mathcal{D}$ to the reals. It gives the value of the field $X(\mathbf{r}^*) \in \mathbb{R}$ at each spatial location $\mathbf{r}^* \in \mathcal{D}$. The components of the state identity observable are parameterized by the spatial locations $\mathbf{r}$ in $\mathcal{D}$ and map from full spatial fields $X(\mathbf{r}) \in \mathbb{R}^{\mathcal{D}}$ to the value $X(\mathbf{r}^*) \in \mathbb{R}$ of the field at the specific location $\mathbf{r}^*$: $g_{r^*}\big(X(\mathbf{r})\big) = X(\mathbf{r}^*)$.

The vector-valued Koopman modes have a component for each component of their vector-valued observables. The vector-valued (or field-valued) state identity variable has components indexed by the spatial locations $r \in \mathcal{D}$. And so, the Koopman modes also have components indexed by spatial locations. Said differently, the Koopman modes are themselves spatial fields. We can thus write the expansion of $\mathbf{g}_I$ as:

$$\mathbf{g}_I\big(X(\mathbf{r})\big) = \sum_i^{\infty} \varphi_i\big(X(\mathbf{r})\big)\ \vec{\nu}_i(\mathbf{r}) \ . \tag{42}$$

Using the definition of Koopman eigenfunctions, the evolution of $\mathbf{g}_I$ in the expansion takes the simple form:

$$\mathbf{g}_I\big(X(\mathbf{r}, t_0 + \tau)\big) = \sum_i^{\infty} \varphi_i\big(X(\mathbf{r}, t_0)\big)\ e^{(\lambda_i \tau)} \vec{\nu}_i(\mathbf{r}) \ . \tag{43}$$

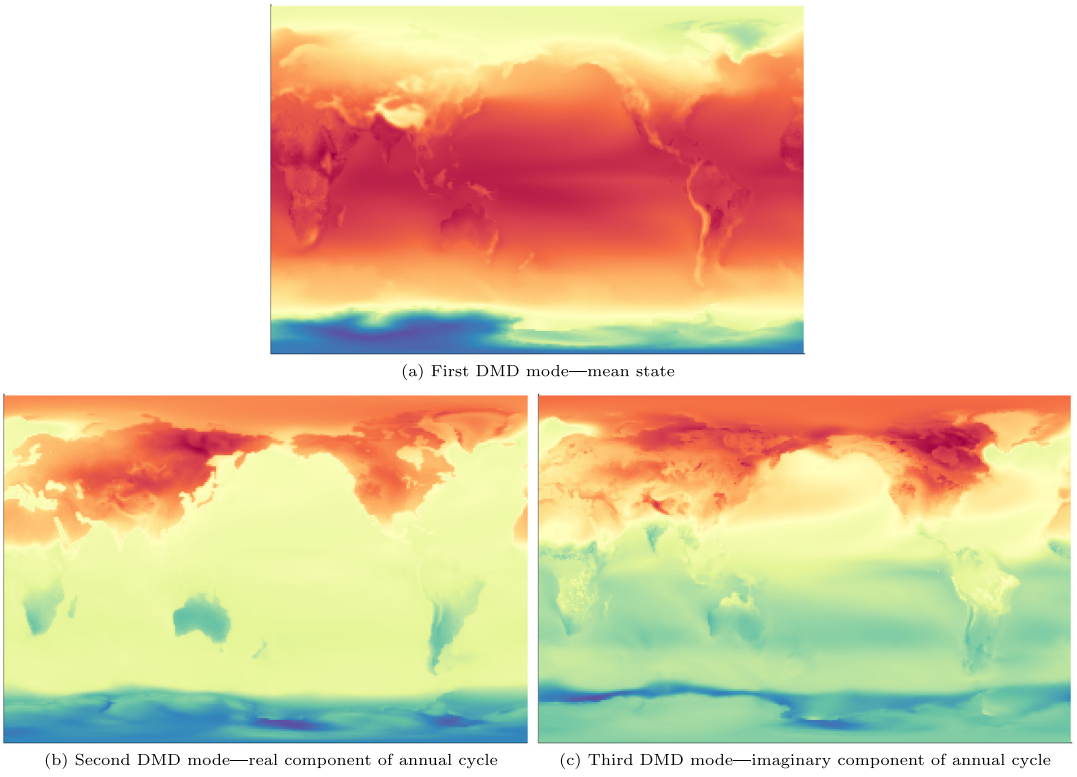
In this view, Koopman eigenfunctions are a complete basis of $\mathcal{F}$ that are intrinsic to the dynamics. And, importantly, Koopman modes are fields that express the flow in this intrinsic basis evolving in time at a single frequency—determined by λ_i. Therefore, they generalize the notion of global modes, introduced for turbulent flows, to any classical field theory.

Note that *all* Koopman eigenfunctions, by definition, evolve at a fixed frequency determined by their associated eigenvalue. When the eigenfunctions are a complete basis—e.g., Hamiltonian (conservative) system dynamics—the dynamics can be fully decomposed into Koopman modes. *Koopman modes distill a particular notion of organization in the system by decomposing the dynamics into components that evolve at single frequencies in time*. The decomposition applies to all field theories, whose behaviors can range between coherent collective motion and chaotic "random" motion.

As with the generic and POD modal expansions described above, the sum in Eq. (43) may be well approximated with a finite sum; adding an important level of constructiveness to the formalism. Consonant with this, the leading Koopman modes of this truncation are considered as coherent spatial structures in the flow, if any are present. In particular, system dynamics in the Koopman basis, Eq. (43), is given simply by the exponential $e^{(\lambda_i \tau)}$, and so $\mathrm{Re}(\lambda_i) \leq 0$ gives the temporal decay rate of the contribution from the eigenfunction ϕ_i and Koopman mode ν_i. The leading Koopman eigenfunctions and modes are those with largest $\mathrm{Re}(\lambda_i)$—i.e., closest to 0. These modes damp out the slowest and so dominate the system dynamics at later times when other modes have decayed away.

The popular *dynamic mode decomposition* (DMD) algorithm provides a practical and efficient method for approximating leading Koopman modes [171–173]. In this, a best-fit linear dynamic is found directly from a system's observed or measured behaviors. The eigenvectors of the best-fit matrix are the dynamic modes that approximate Koopman modes. The DMD modes are linear combinations of POD modes that evolve coherently with single frequencies. Said simply, DMD is a POD spatial model combined with a Fourier temporal model.

Koopman modes and DMD have proven useful for organization in Earth's climate, typically treated as the statistical behavior of the Earth system [174]. Example DMD modes for the temperature field of a 1-degree resolution Community Earth System Model run are shown in Fig. 1. The first mode, shown in (a), has eigenvalue $\approx$1.0 and so approximates the invariant climatological mean field. The next leading mode is imaginary with an imaginary eigenvalue corresponding to oscillations with a 12 month period, and so is associated with the annual cycle. The real and imaginary components of this mode are shown in (b) and (c), respectively. The climatological mean and annual cycle are the primary statistical



(a) First DMD mode—mean state

(b) Second DMD mode—real component of annual cycle

(c) Third DMD mode—imaginary component of annual cycle

Fig. 1. The first three DMD modes of the temperature field from a Community Earth System Model run. The first mode (a) has eigenvalue ≈ 1.0 and approximates the invariant field and corresponds to the climatological mean state. The next two modes (b) and (c) are the real and imaginary components, respectively, of the mode with an imaginary eigenvalue that corresponds to oscillations with a 12 month period, and so correspond to the annual cycle.

features that climate analysis is built upon. Dynamic Mode Decomposition is able to approximate Koopman modes that provide spatial fields associated with these statistical features.

To complete the discussion of Koopman operators, we now examine the case when the eigenfunctions do *not* form a complete basis. Vector-valued observables may still be fully decomposed, however the spectrum of Koopman operators will have a continuous component in addition to the discrete point spectrum of eigenvalues above. Using *spectral measures* of Koopman operators, we can expand the state identity observable as:

$$\begin{aligned}\mathbf{g}_I\big(X(\mathbf{r}, t_0+\tau)\big) = &\sum_j^{\infty} \varphi_j\big(X(\mathbf{r}, t_0)\big)\; e^{(\lambda_j \tau)} \vec{v}_j(\mathbf{r}) \\ &+ \int_{-\pi}^{\pi} e^{i\tau\omega} \tilde{\varphi}_\omega\big(X(\mathbf{r}, t_0)\big) d\omega \;, \end{aligned} \tag{44}$$

where $\tilde{\varphi}_\omega$ can be thought of as continuously-parameterized eigenfunctions. See Refs. [171,175] for more information on spectral measures of Koopman operators.

If we separate out the mean value of the field from $\mathbf{g}_I$, then Eq. (44) gives the generalization of the triple decomposition to arbitrary classical field theories [166]. The field dynamics are given by (i) the mean, (ii) a term representing "global modes" that evolve at single frequencies, and (iii) a chaotic component given by the continuous part of the spectrum. Complex dynamics typically contain an amalgam of regularity and randomness. And so, at its roots, extracting organization requires disentangling the randomness from the regularity. In doing so, the Koopman spectral decomposition shares a conceptual similarity with the intrinsic computation approach described below.

Finally, we note that the spectral measure with respect to an observable g is the Fourier transform of the dynamical autocorrelations $\langle \mathcal{K}^\tau g, g \rangle$ [171,175]. Intuitively, systems with high levels of organization should be highly correlated. While simple scalar quantities like two-point (auto)correlations do not directly capture the notion of organization we seek, the above results show organization can be reconstructed from the totality of dynamical multivariate autocorrelations using Koopman spectral measures.

7.3.2. Organization beyond Koopman modes

The Koopman mode decomposition, as just described, is best seen as describing organization statistically. Recall that the Koopman mode decomposition assumes a space and time separation of variables, given by Eq. (38). Thus, each Koopman mode, which captures potential organization, is a function of space only, and not time. Koopman modes then can only represent organization that is time-independent and spatially global, as exemplified by the climate modes in Fig. 1. Therefore, Koopman modes are best suited to statistical organization in autonomous systems whose dynamics do not have explicit time dependence. Any modal decomposition with a space and time separation, like Koopman modes, is, by definition, incapable of representing spatially-local organization that evolves through time.

Beyond the primary bifurcation, more complex and complicated organization may emerge that cannot be adequately described in the statistical sense of the Koopman mode decomposition. In particular, *coherent structures* [176] may form that are localized in space, dynamic over time, and ephemeral with finite lifetimes. Consider, for example, individual weather systems such as hurricanes and atmospheric rivers. For fluid systems, the Koopman mode decomposition is an Eulerian approach, whereas the Lagrangian framework is better suited to capture coherent structures [177]. Similarly, it is conceptually advantageous to utilize Perron–Frobenius operators, which are dual to Koopman operators. Because the evolution operators are dual to one another, they ultimately contain the same information about the system. However, one may be more convenient than the other for certain tasks [173], and for coherent structures in time-dependent flows Perron–Frobenius operators are more convenient than Koopman operators.

7.3.3. Perron–Frobenius operators

In contrast to Koopman operators evolving system observables, *Perron–Frobenius operators* $\mathcal{P}^\tau$ evolve probability distributions over the system states. For a probability measure μ, the probability distribution given by μ evolves in time according to Perron–Frobenius operators via:

$$\begin{aligned}\mu_\tau &:= \mathcal{P}^\tau \mu \\ &:= \mu \circ \Phi^{-\tau} \ ,\end{aligned} \tag{45}$$

where $\Phi^{-\tau}(A) := \{X \in \Omega \ : \ \Phi^\tau(X) \in A\}$ is the preimage of a measurable set A under the flow Φ^τ.

Comparing Eq. (45) to Eq. (39), Perron–Frobenius operators are adjoint to Koopman operators in appropriately defined spaces:

$$\langle \mathcal{P}^\tau f, g \rangle = \langle f, \mathcal{K}^\tau g \rangle \ .$$

They provide classical dynamics on Hilbert spaces, analogous to quantum mechanics. Perron–Frobenius operators are the classical equivalent of the Schrodinger picture, and Koopman operators of the Heisenberg picture.

Since Perron–Frobenius operators evolve probability distributions, they historically have a closer association to statistical mechanics than Koopman operators [20,178]. The most immediate connection is to notice that an eigenfunction of Perron–Frobenius operators with eigenvalue one is an *invariant distribution* μ^*, such that:

$$\mathcal{P}^\tau \mu^* = \mu^* \ .$$

Invariant distributions are abstractions of equilibrium and nonequilibrium steady-state distributions from statistical mechanics. For ergodic dynamics, there is a unique invariant distribution [20, Theorem 4.5]. For Hamiltonian dynamics, Perron–Frobenius operators reduce to the familiar Liouville operators of statistical mechanics [20].

Let us now detail how Perron–Frobenius operators complement the Koopman mode decomposition for analyzing structure and organization in time-dependent systems. We consider a Lagrangian flow in which fluid parcels evolve according to the time-dependent flow map

$$\mathbf{y}(t; t_0, \mathbf{y}_0) := F^t_{t_0}(\mathbf{y}_0) \ , \tag{46}$$

where $\mathbf{y}$ is a fluid parcel or tracer, as opposed to a full spatial field. The time-dependent dynamics $F^t_{t_0}$ define time-dependent evolution operators, $\mathcal{K}^t_{t_0}$ and $\mathcal{P}^t_{t_0}$, that depend on the initial time t_0 in addition to the evolution time t. Each initial time t_0 thus has its own Koopman mode decomposition. (The latter may or may not be unique; i.e., two different times may generate the same decomposition.)

For Lagrangian flows, the (now time-dependent) Koopman modes are no longer spatial fields, so their interpretation is not as clear. However, Perron–Frobenius operators evolve distributions over the state space, which for Lagrangian flow is the spatial domain. Recall, for analyzing statistical organization through the Koopman mode decomposition above, we considered the Koopman modes for a particular observable—the state identity observable. Now, we do a similar development in which we consider the time-dependent evolution of uniform distributions over smooth contiguous regions in the flow domain, known as *material surfaces*. The Lagrangian flow evolves all the points on this surface, and so the action of the Perron–Frobenius operator $\mathcal{P}^t_{t_0}$ gives the dynamics and deformation of these material surfaces.

Given that Koopman and Perron–Frobenius operators are adjoint, they share the same spectrum. In both the time-independent and time-dependent cases, the spectral decomposition of the evolution operators separates regular motion from chaotic motion in the system. However, regular—i.e., not chaotic—motion does not necessarily imply coherent

collective motion. The interpretation of Perron–Frobenius operators evolving material surfaces in Lagrangian flows allows for a more precise definition of coherent structures, or more generally *coherent sets*, that emerge.

The invariant distribution is one that does not change over time and is given as an eigenfunction of Perron–Frobenius operators with eigenvalue one. For Lagrangian flows, such an eigenfunction is a material surface that does not change with the flow. All of the fluid parcels originally in the surface, and only those, remain in the surface over time. This is the case of perfect collective motion, but is an idealization that is not realized in most physical scenarios of interest. Vortices in turbulent flows, for example, remain coherent, with a high degree of collective motion, but it cannot be expected that *all* parcels remain in the vortices forever.

Such behavior, of interest to real-world systems, is captured by eigenfunctions of Perron–Frobenius operators with eigenvalue close, but not equal, to unity—known as *almost-invariant sets* [179,180]. These correspond to *metastable states* in statistical mechanics [181,182]. Since the associated eigenvalues are not exactly one, they are not asymptotically-invariant. However, since they are close to one, a system tends to spend a long time in each before escaping. The simplest example is found in overdamped Langevin dynamics in a double-well potential [173]. The asymptotic distribution is evenly split between the wells. Before the asymptotic limit however, the system tends to spend a long time in each well individually before leaving. Thus, distributions concentrated in each individual well are metastable states. A more complicated example is given by protein configurations [182].

Returning to the Lagrangian flow case, recall that the Perron–Frobenius operators evolve sets on the flow domain. The dynamic and ephemeral coherent structures that interest us—as particular forms of emergent organization—present several complications to the simple notion of almost-invariant sets as eigenfunctions of Perron–Frobenius operators with eigenvalues near one. First, they may move through space over time while remaining coherent. Thus, the set will move over the flow domain and mostly not return to itself. In this case, we can formulate *coherent pairs* such that the probability of Perron–Frobenius operators evolving the first set in the pair to the second is close to one [183,184]. Fluid parcels in the initial configuration and location of a material surface are likely to end up in the later configuration and location if that surface is a coherent set. Finally, it has recently been shown how to extend the formulation of coherent sets using time-dependent Perron–Frobenius operators to capture the "birth" and "death" of ephemeral structures with finite lifetimes [185].

An example of coherent sets is shown in Fig. 2, reproduced from Ref. [186]. Dominant ocean gyres are identified from Lagrangian flow trajectories as coherent sets, reconstructed using a reproducing kernel Hilbert space approximation of evolution operators. The approximated coherent sets, corresponding to the ocean gyres, are shown in Fig. 2 (d). Lagrangian evolution of sample tracers are shown in (e), with colors corresponding to the coherent set they are assigned to at the initial time t_0. As expected from the definition of coherent sets, the trajectories in (e) largely stay contained within their original coherent set. However, there are some crossovers, for example between the red and green sets near the southern tip of South America.

A note on terminology: Almost-invariant sets and coherent sets are closely-related mathematical constructions, both based on the Perron–Frobenius operator. Data-driven approximation of these provide tools that help identify coherent structures in physical systems. In the above example, the ocean gyres are coherent structures—physical organization in the real ocean that we are interested in—and the coherent sets shown in (d) are data-driven tools that approximately identify the gyres.

7.3.4. Recap

Koopman and Perron–Frobenius evolution operators provide an alternative description of dynamical systems in terms of the evolution of system observables and probability distributions. Their spectral decompositions provide a means of mathematically identifying organization in classical field theories (and dynamical systems more generally). The continuous portion of their spectra is associated with chaotic, apparently random, motion. For time-independent systems, the eigenfunctions associated with the discrete spectrum (eigenvalues) evolve at single frequencies and their Koopman modes represent statistical organization of the system. For time-dependent field theories, coherent structures associated with localized collective motion are identified through eigenfunctions of time-dependent Perron–Frobenius operators defined from the Lagrangian flow map. In all cases, a finite set of eigenvalues, eigenfunctions, and their coefficients (modes) provide a compressed representation of the system and its dynamics, and hence its organization.

It is important to emphasize again, though, that Koopman and Perron-Frobenius operators are dual to one another on appropriately defined function spaces, and so they ultimately provide the same information. Both operators can be applied to any dynamical system. However, depending on the type of data available and the questions being asked, one or the other evolution operator may be more immediately useful [173]. Koopman modes are particularly useful for time-independent Eulerian flows, and Perron-Frobenius operators and their coherent sets are more convenient for time-dependent Lagrangian flows. But it is certainly possible to analyze time-dependent Koopman modes of Lagrangian flows and almost-invariant sets of time-independent Eulerian flows.

From their origins in the study of turbulence, today modal decompositions are the standard approach to coherent structure analysis. They are commonly employed in the fields of fluid mechanics [166,187,188], climate science [186,189–191], and computational chemistry [181,182], among others. This is due to the solid theoretical foundations based on Koopman and Perron–Frobenius operators outlined here, as well as the availability of effective algorithms to approximate them directly from data [172,173,192,193].

It is important to emphasize that, despite the rigor and their representational power, the evolution operators do not lead to a direct definition of what organization is. They are essential tools in this endeavor, but they skirt the definitional challenge. Addressing the latter requires taking a different view of the computation-theoretic concepts introduced above.

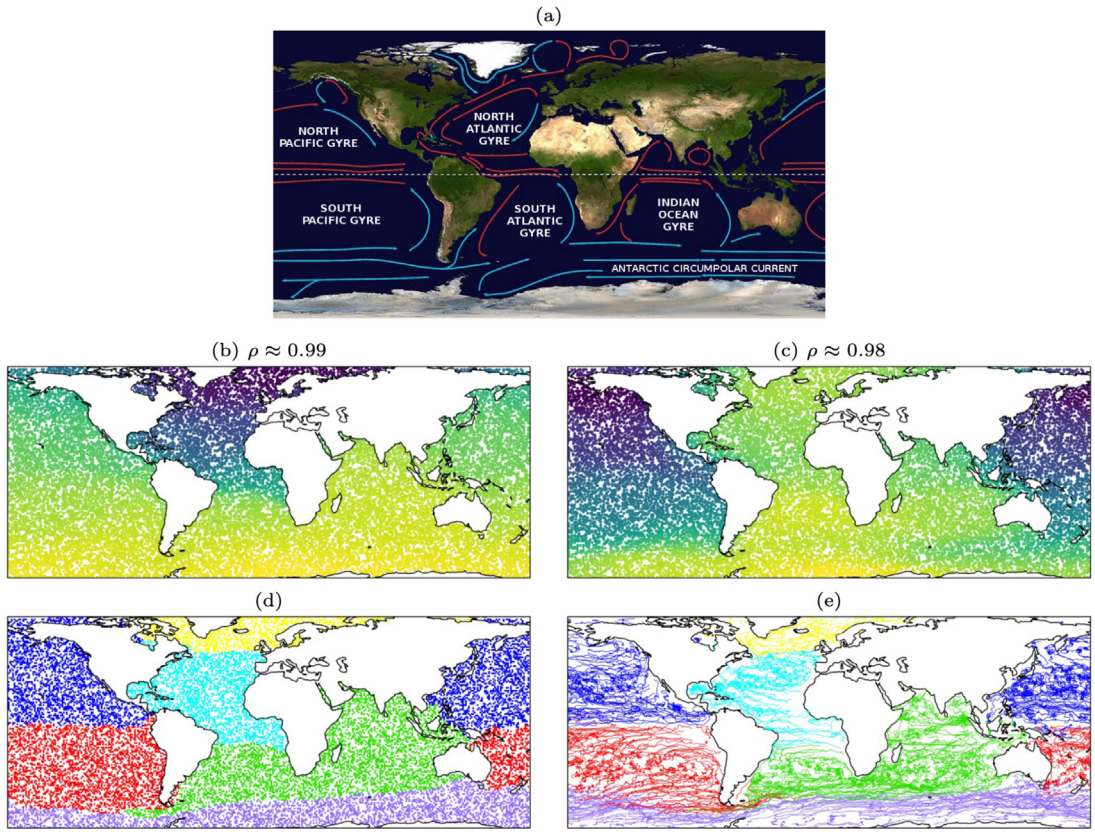


Fig. 2. (a) Illustration of the major ocean gyres (courtesy of NOAA). (b) First and (c) second eigenfunction. (d) k-means clustering of the first six eigenfunctions into six coherent sets. (e) Subset of the trajectories colored according to the coherent sets.
Source: Reproduced, with permission, from Ref. [186].

7.4. Intrinsic computation

The computation- and information-theoretic foundations and practical shortcomings of the approaches to organization through compression described above in Section 7 A led historically to the development of our second framework for formalizing organization. Founded on the idea that pattern and organization are predictive regularities, *computational mechanics* directly constructs optimally-predictive compressed descriptions that represent a system's *intrinsic computation*—how a system stores and transforms information [194]. The following briefly reviews this framework and its arguments for formalizing organization through intrinsic computation, emphasizing organization as generalized symmetries.

Due to its origins in computation and information theory, we start in the simplified setting of fully-discrete one-dimensional field theories. The systems considered here are collections of indexed sequences of symbols from a finite *alphabet* $\mathbb{A}$; e.g., binary strings with $\mathbb{A} = \{0, 1\}$. Indices may correspond to locations in time or space. Shifts in indices, given by the *shift operator* σ, correspond to translations in time or space. Shift-invariant collections of symbol sequences are called *shift spaces*, denoted $\mathcal{X}$. To connect to statistical mechanics, they may be thought of as *topological ensembles*.

For example, we may choose a binary alphabet of $\mathbb{A} = \{-1, 1\}$. The field here represents an abstraction of lattices of two-state spins—up versus down, say. In contrast to statistical mechanics, there is no probability distribution over symbol sequences. For a given shift space (topological ensemble), we are interested in mathematical representations of pattern and organization present in that system.

7.4.1. Organization in symbolic dynamics

The study of shift spaces is a rich subfield of nonlinear dynamics called *symbolic dynamics* [195]. It has a long and venerable history [196] with origins that overlap with early studies in dynamical systems [197], computability [198], decidability [199], and the logical foundations of mathematics [200,201].

An important distinction from statistical field theories is that the shift operator provides a dynamical relation between the elements of a shift space. The translations provided by the shift operator allow us to formalize symmetries, and their generalizations, in shift spaces. Since shift spaces are shift-invariant, equivalently they can be thought of as collections of

individual indexed-sequences related through the shift operator or as a single bi-infinite sequence with σ simply shifting the sequence indices.

On one extreme, a sequence may possess an exact translational symmetry; e.g., {. . . 00100100100 . . .}. Such symmetries are described via a *group algebra*. If the symmetry's "pattern" is known—i.e., the group relations, and the current phase, or group element is known—then the configuration at any other location in the sequence can be exactly predicted. Exact symmetries represent full predictive regularity. On the other extreme, if the sequence is entirely random—e.g., generated by flips of a fair coin—then the symbols at other locations cannot be predicted at all. There is no pattern or organization present to leverage for any predictive regularity. It is commonly accepted that these two extremes—fully predictable and fully random—represent the "boundary conditions" of vanishing complexity. That is, they represent null organization [139,202].

Most shift spaces lie somewhere between these extremes. They are neither exactly predictable nor fully unpredictable. A generic sequence will possess some limited or partial predictability, some nonzero degree of organization and some nonzero amount of randomness.

As we seek to formalize organization as a generalization of exact symmetries, we restrict to the class of *sofic shifts*, which are shift spaces generated by finite semigroups [203]. Importantly, all sofic shifts can be *presented* by a certain class of finite-state machines [204]. These finite-state machines, called *semiautomata* [205], are given as a finite collection of *internal states* and *symbol-labeled transitions* between these states. Symbol sequences are generated from semiautomata by following transition paths between the internal states and recording the associated symbol for each transition. A semiautomaton is a *presentation* of a sofic shift if each sequence generated by the automaton is in the shift space and if all sequences of the space can be generated by the automaton.

Fig. 3(a) shows a semiautomaton presentation of the *even shift*—the set of binary sequences such that there can only be even-length blocks of 1s enclosed by 0s. Note the combination of randomness and regularity; transitions from internal state A can emit 0 or 1, while transitions from state B must emit a 1. The partial predictive regularity is given by the constraint, already noted, that blocks of 1s bounded by 0s must be an even number in length.

For every sofic shift there is a *unique* minimal presenting semiautomata, which we will define shortly. Crucially, every symbol sequence with a finite translation symmetry (i.e. periodic) is a sofic shift [206]. Moreover, the group algebra of the translation symmetry is equivalent to the permutation symmetry group of the minimal presenting semiautomaton of the sofic shift. Similarly, fully "random" sequences without regularity are also sofic shifts. Since sofic shifts encompass this full range of patterns, from no regularity to full regularity, we argue that the *minimal semiautomata presentations are the mathematical representation of the organization contained in symbol sequences.* Ref. [206] gives the details and proofs behind this position.

We emphasize again the hypothesized duality between organization and computation. Motivated by generalizing fully-symmetric sequences into a spectrum of partially-predictable sequences, the mathematical representation we found that does this is the class of models of discrete computation—the finite-state machines of elementary computation theory [125–127].

7.4.2. Organization through predictive equivalence

While viewing pattern and organization as generalized symmetries can be made rigorous in the discrete one-dimensional setting of sofic shifts, the central definition and construction of minimal presenting semiautomata—*predictive equivalence*—is fully generalizable to most cases of interest for self-organizing systems. These include higher dimensions and continuous and statistical field theories. We now give the simplest definition, for fully-discrete one-dimensional topological and statistical ensembles. Spatially-extended and continuous versions are given later. Ultimately, we will find predictive equivalence to be the most central concept to date for principles of organization.

First, it is helpful to consider sequence indices as corresponding to time. With this, a shift space represents a set of fully-discrete time series. The internal states of semiautomata (and finite-state machines more generally) are then defined as *equivalent histories*. This idea, dating back to the early physics of computation [207] and logical machines [208], provides the definition for the unique minimal semiautomata presenting a sofic shift, as well as the means to a statistical mechanics generalization.

For every sequence $x \in \mathcal{X}$ in a given shift space, let index t represent the *present* time. The semi-infinite sequence $\overleftarrow{x}_t = \{x_t, x_{t-1}, x_{t-2}, \ldots\}$ with indices less than or equal to t is the *past* of the sequence at time t and the *future* $\overrightarrow{x}_t = \{x_{t+1}, x_{t+2}, \ldots\}$ of the sequence at time t is then the complement—the semi-infinite sequence with indices greater than t.

For a given shift space $\mathcal{X}$, the *follower set* $F_{\mathcal{X}}(\overleftarrow{x})$ of a past configuration $\overleftarrow{x}$ is the set of all future configurations $\{\overrightarrow{x}\}$ such that the full sequence $x = \overleftarrow{x}\,\overrightarrow{x}$—the concatenation of $\overleftarrow{x}$ and $\overrightarrow{x}$—is an element of the shift space: $x \in \mathcal{X}$. Two pasts are considered *equivalent*—i.e., they are equivalent histories—if they have the same follower set. The central idea is that equivalence classes of unique follower sets $F_{\mathcal{X}}$ are the internal states for the unique minimal semiautomaton that presents the sofic shift $\mathcal{X}$.

Second, generalizing from topological to statistical ensembles of sequences is straightforward. We consider two pasts to be *predictively equivalent* if they not only have the same follower set, but if they have the same *predictive distribution* $\Pr(\overrightarrow{X} \mid \overleftarrow{x})$ over the follower set. (Note that the support of a predictive distribution is a follower set.) Predictive equivalence defines the unique minimal *hidden Markov chain* representation for the sequence ensemble [209]. Fig. 3(b) displays the

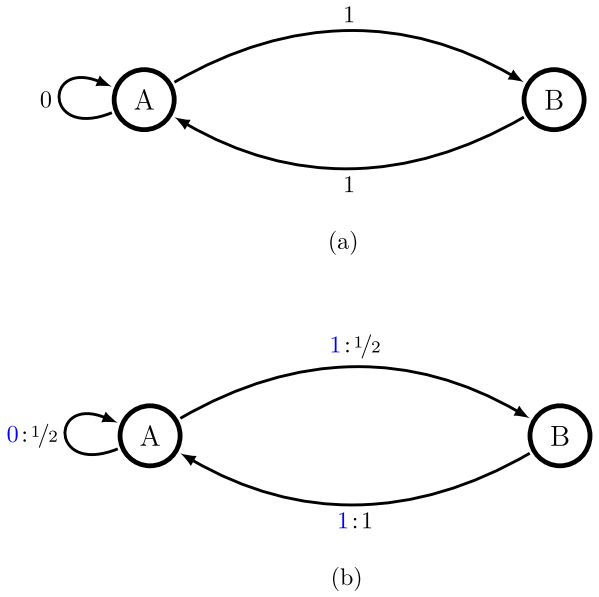


Fig. 3. (a) Semiautomaton presentation of the Even Shift with internal states $\{A, B\}$ and state-to-state transitions labeled with symbols from $\mathbb{A} = \{0, 1\}$. (b) Hidden Markov chain presentation of the uniform Even Process. Each transition leaving state A has probability $1/2$ of occurring. That returning to A emits a 0 and that going to B emits a 1. The transition leaving B is taken with probability 1 and emits a 1.

stochastic generalization of the semiautomaton in Fig. 3(a). The hidden states of this minimal hidden Markov chain—the predictive equivalence classes—are known as *causal states* [194].

In the temporal setting, where indices correspond to time, these ensembles of sequences are fully-discrete stochastic processes. And, the causal-state hidden Markov chain is the unique model that optimally predicts the given process with minimal computational resources [209]. Predictive equivalence ensures the dynamic over causal states is Markovian: the transition to the next causal state depends only on the immediately preceding causal state.

Importantly, the internal-state dynamic is *unifilar*: For each causal state S_i there is at most one causal state S_j to which S_i transitions for each symbol $a \in \mathbb{A}$. That is, there is at most one S_j such that $S_{t+1} = S_j$ given $S_t = S_i$ and $x_{t+1} = a$. Unifilarity ensures a one-to-one correspondence between sequences of symbols (realizations of the stochastic process) and the corresponding sequence of causal states. Summing over such symbol-labeled transitions gives a semigroup of Markov transition operators M_ϵ that governs the evolution of distributions over causal states:

$$\Pr(S_t) = M_\epsilon^t \Pr(S_0) \ , \tag{47}$$

with $M_\epsilon^{t_1}(M_\epsilon^{t_2} \Pr(S_0)) = M_\epsilon^{t_1+t_2} \Pr(S_0)$.

Computational mechanics merges the computation-theoretic tools of symbolic dynamics with statistical mechanics. Its hidden causal-state Markov chain—the *ϵ-machine*—provides an explicit mathematical representation of the temporal organization in fully-discrete processes. (However, shortly we will describe how this generalizes to continuous field theories.) The hidden Markov chain structure captures both organization as a generalized symmetry, as well as organization quantitatively as the intrinsic computational resources used by the system to convey the past to the future through the present [210]. It has been successfully applied to analyze the organization and information processes in a wide range of complex systems [194].

7.4.3. Local causal states in spatial field theories

To adapt organization as intrinsic computation to the spatially-extended systems of interest (classical field theories) [211], we use *lightcones* as local notions of pasts and futures. Recall that Eq. (1) imposed spatially-local interactions through finitely-many spatial derivatives. Due to this, information propagates at a finite speed c through the system. For a spacetime point $(\mathbf{r}, t)$ in a spacetime field $X(\mathbf{r}, t)$, the *past lightcone* of $(\mathbf{r}, t)$ is the set of all points at preceding times that could possibly have influenced $(\mathbf{r}, t)$ through the local interactions:

$$\mathrm{L}^- = \{(\mathbf{r}', t') : t' \leq t, \|\mathbf{r}' - \mathbf{r}\| \leq c(t' - t)\} \ .$$

Similarly, the *future lightcone* of $(\mathbf{r}, t)$ is the set of all points at later times that $(\mathbf{r}, t)$ could itself possibly influence through the local interactions:

$$\mathrm{L}^+ = \{(\mathbf{r}', t') : t' > t, \|\mathbf{r}' - \mathbf{r}\| \leq c(t' - t)\} \ .$$

The *local causal states* are then defined as the equivalence classes of the *local predictive equivalence relation*:

$$\ell_i^- \sim_\epsilon \ell_j^- \iff \Pr(\mathrm{L}^+|\ell_j^-) = \Pr(\mathrm{L}^+|\ell_i^-)\,, \tag{48}$$

where $\ell^\pm$ are specific lightcone configurations or realizations of lightcone random variables $\mathrm{L}^\pm$. Mirroring the one-dimensional case, local causal states are sets of past lightcones with the same conditional distributions over future lightcones. It is useful to state this equivalently in terms of the ϵ-*function* that maps from past lightcones to their associated local causal state:

$$\ell_i^- \sim_\epsilon \ell_j^- \iff \epsilon(\ell_j^-) = \epsilon(\ell_i^-)\,.$$

Since each point $X(\mathbf{r}, t)$ in spacetime has a unique past lightcone and this past lightcone has a unique local predictive distribution $\Pr\big(\mathrm{L}^+(\mathbf{r}, t)|\ell^-(\mathbf{r}, t)\big)$, each point also has a unique local causal state, denoted $S(\mathbf{r}, t) = \epsilon\big(X(\mathbf{r}, t)\big)$. For a full spacetime field X, we apply the ϵ-function to all its spacetime points $X(\mathbf{r}, t)$ to create a corresponding *local causal state field* with spacetime points $S(\mathbf{r}, t) = \epsilon\big(X(\mathbf{r}, t)\big)$.

Since the local causal state field is created through the pointwise ϵ-function, it shares the same spacetime coordinate geometry as the original field X. Therefore, characteristics of the field X can be analyzed through various properties of the associated local causal state field $S = \epsilon(X)$.

In particular, organized *coherent structures* are identified as *localized deviations from generalized spacetime symmetries* in X, which are given as exact symmetries in S [212,213].

Clustering algorithms may be employed to approximate local causal states in continuum field theories, such as those used to model fluid flows [211,214]. The local causal states can identify individual vortices in two-dimensional free-decay turbulence and recover their power-law decay behavior, as well as identify and track individual extreme weather events like hurricanes and atmospheric rivers in high-resolution climate data [211].

Recall that the Lagrangian perspective is useful for identifying complex organization in time-dependent fluid flows. In this case, *Lagrangian lightcones* may be used, which are collections of Lagrangian trajectories that can possibly lead to or from the present point; see Fig. 4. That is, the past Lagrangian lightcone is the set of all points at prior times that could possibly reach the present point through Lagrangian advection. Similarly, the future Lagrangian lightcone is the set of all points at later times that can be reached from the present point by advection.

Ref. [214] demonstrates that local causal states identify coherent structures in complex flows that agree well with structures identified by specialized geometric Lagrangian methods [177]. In particular, structures identified as coherent sets using Perron–Frobenius operators produce characteristic signatures in Lagrangian lightcones that then give rise to unique local causal states corresponding to the coherent sets (coherent trajectories create coherent lightcones). Similarly, the boundaries of coherent sets are associated with repelling structures that act as transport barriers [184], which Ref. [214] also demonstrated for local causal states. Transport barriers create distinct signatures in Lagrangian lightcones on either side of the barrier, giving two separate local causal states on either side with their boundary lying on the barrier. Note though that the dynamics of localized structures moving through space over time, as well as finite lifespans of structures, are naturally encapsulated by local causal states without special modification.

An example of identifying hurricanes in high-resolution climate data using local causal states is shown in Fig. 5, reproduced from Ref. [211]. The local causal states are approximated from the integrated vapor transport field (IVT), which measures water vapor flux and is often used by climate scientists for extreme weather analysis. The local causal states approximated from the IVT field are shown in (a) and, as highlighted in (b), there is a subset of local causal states that correspond to hurricanes. The water vapor field is shown in (c) with spacetime points assigned to the subset of hurricane local causal states highlighted in red. Ref. [211] demonstrates the hurricanes identified in this way by local causal states agree with the specialized heuristics currently used by climate scientists to identify hurricanes.

7.4.4. Recap

Intrinsic computation decomposes dynamical processes into their minimal causal components. These components—causal states—are defined as equivalence classes of past trajectories that produce the same conditional distributions over future trajectories. It has been shown that the causal states and their internal transitions—the ϵ-machines—are the unique minimal optimal predictors of discrete stochastic processes [209]. That is, they uniquely represent the most compressed representation that is still fully faithful to the original process. As a further argument for organization through intrinsic computation, it has also been shown that ϵ-machines identify patterns that algebraically generalize exact symmetries [206].

Recent progress extends intrinsic computation and predictive equivalence to continuous-time processes [215,216] and spatially-extended systems [211,212]. The straightforward definition through predictive equivalence makes intrinsic computation actionable in practice through approximation or Bayesian inference [217]. Thus, organization can now be identified and analyzed in a wide array of systems through intrinsic computation.

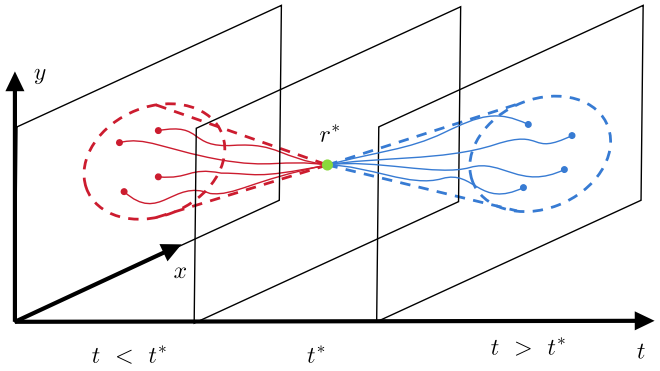


Fig. 4. Co-occurring past (red) and future (blue) Lagrangian lightcones at spacetime point (r^*, t^*) shown with dashed lines. All possible Lagrangian trajectories (examples shown by solid lines) leading to and emanating from (r^*, t^*) are contained within the lightcones.

7.5. Outlook on organization

Having completed our review of modern mathematical approaches to organization, let us ask again—what *is* organization? Is it identified through spectral decomposition of evolution operators or through equivalence classes of predictive equivalence relations? In short, the existence of a universal theory of organization remains an open question. Evolution operators and intrinsic computation represent distinct but overlapping characterizations of organization. For one, their domains of applicability do not fully overlap, with evolution operators strictly defined for dynamical systems (deterministic and stochastic), whereas predictive equivalence was originally defined for discrete stochastic processes.

That said, the extension of predictive equivalence to continuous field theories brings connections with evolution operators. This is particularly the case with coherent structures identified from Lagrangian flows, as just described. Coherent structures are key forms of organization, and the agreement on their identification between local causal states and evolution operators is encouraging. Further connections remain to be worked out; for example, between spectral measures of evolution operators [175] and spectra of ϵ-machines [218,219]. A key similarity is the ability of both approaches to separate randomness from regularity. It may be that predictive equivalence and evolution operators provide different views to the same underlying notion of organization.

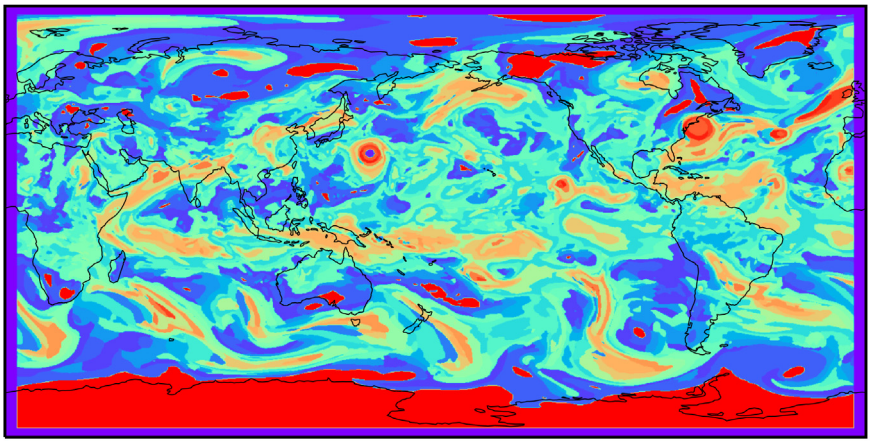
An important similarity between both approaches must be emphasized: They both fall outside the constructionist paradigm. Evolution operators and their spectral decompositions, as well as predictive equivalence classes and their transitions, are not directly constructible apart from a handful of idealized systems [164,220]. To be clear on this, one cannot start with the Navier–Stokes equations and write down the time-dependent Perron–Frobenius operators generated by the Lagrangian flow map for some specified boundary conditions, nor can one start with the predictive equivalence classes of Lagrangian lightcones. However, as emphasized, evolution operators and predictive equivalence provide a rigorous theoretical scaffolding on which to build data-driven algorithms that can discover emergent organization from the behaviors of complex systems.

With the concept of organization now addressed, what about principles? Since the modern formulations of organization lie outside the constructionist paradigm and the classical notions of "principles" are constructionist in nature, we are largely in uncharted territory. General formulations of scientific principles beyond constructionism is an enormous and ongoing endeavor that is beyond our scope here. However, we will conclude by returning to the concept of emergence—which, as we noted at the beginning, highlights phenomena that thwart constructionist principles of organization.

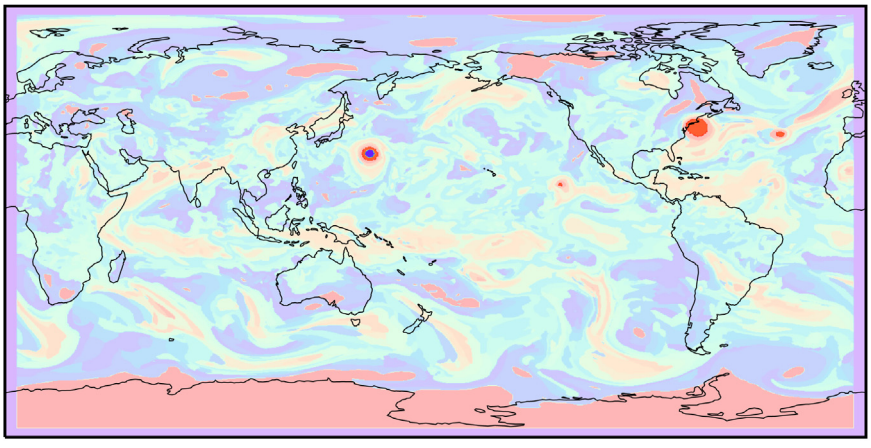
8. A statistical mechanics of emergence

Organization *emerges* as a higher-Level description that cannot be constructed from a system's lower Level dynamics. The seemingly stochastic vortex gas of two-dimensional turbulence [137] and the "particle dynamics" of elementary cellular automata [35] come immediately to mind. It is natural to ask *how* and *why* new organization appears. Constructionism is the standard paradigm for answering "how" and "why" questions in physics. A key mandate of equilibrium statistical mechanics is to show that higher-Level thermodynamics is consistent with lower-Level particle kinetics. It does so by directly constructing thermodynamic relations, like the ideal gas law, from the statistical behavior of kinetic particles. As we have argued, it is exceedingly rare that higher-Level behaviors can be directly constructed in this way from lower-Level dynamics.

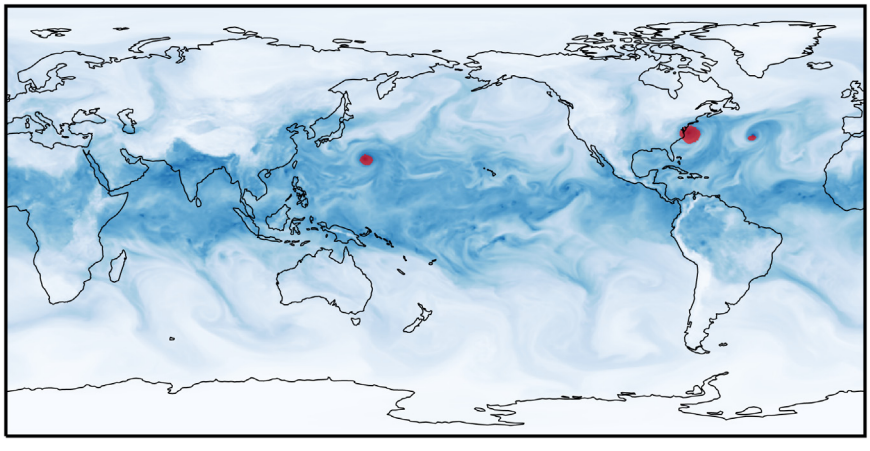
While in line with colloquial uses of the term, here we use *emergent* to emphasize organization that cannot be directly constructed. There is, at this time, no satisfactory paradigm to answer "how" and "why" questions in the absence of constructionism. Arguably, a central task of complexity science is to lay the foundations for this new paradigm [221].



(a) Local causal state segmentation of IVT field



(b) `hurricane` local causal states highlighted



(c) `hurricane` states overlaid on top of water vapor field

Fig. 5. Identification of hurricanes in high-resolution climate data using local causal states.
Source: Reproduced from Ref. [211].

As such, it is too big a task for us to conquer here. We can say, however, that this new paradigm will be intrinsically computational and data-driven, at least in part.

Rather than address theories of how and why organization may spontaneously emerge, we instead close with a universal theory to formulate complete and self-contained dynamics for higher-Level organization (and behaviors more generally) that is consistent with the lower-Level from which it emerges. This universal theory is, in fact, given by the causal states and their Markovian dynamics.

Generally, our *abstracted* statistical mechanics cannot, of course, analytically construct the dynamics of higher-Level organization from the lower-Level dynamics. However, we will show how to define the causal states and their dynamics in terms of Koopman and Perron–Frobenius evolution operators. This provides the requisite physical consistency between Levels.

This Section introduces a physical foundation to data-driven dynamics of emergent behaviors. These insights show how it is possible for data-driven methods like dynamic mode decomposition [172] or reservoir computers [222] to build models of a system's higher-Level dynamics without reference to, or even knowledge of, the system's lower-Level physics. As hopefully established by this point, intrinsic-computational and data-driven approaches are and will continue to be indispensable in the study of emergent organization. However, data-driven methods are often seen as "black box" and potentially not physically-grounded. The following shows that the causal states and their dynamics are the physical underpinnings of a complete, consistent, and self-contained dynamics of emergent organization. Here, the "self-contained" qualifier emphasizes that the emergent dynamics can be consistently approximated directly from data. For example, Refs. [223,224] use the statistical mechanics of emergence for data-driven reconstruction of long-term behaviors that emerge from short-term movements of simple organisms.

8.1. Consistency of emergent behaviors

We are interested in the interplay between two levels: emergent behaviors (Level B) and their underlying deterministic dynamics (Level A). Consider a system with a Level A description given as a deterministic dynamical system:

$$a_{t+1} = \Phi(a_t) \ . \tag{49}$$

For simplicity, we work in discrete time, but generalizing to continuous time is straightforward. This Level A description can correspond to, for example, the lookup table dynamics of cellular automata, or the nonequilibrium transport equations given by Eq. (1) (previously called Level II when we were interested in three Levels).

We now want to define an emergent Level B description that is physically *consistent* with the Level A description. To do so, we simply define Level B through *partial observations* of the Level A description. At each time, the system state at Level B is given by a *noninvertible* function of the Level A system state, so that $b_t = B(a_t)$. The noninvertibility of $B(\cdot)$ is crucial for identifying Level B as emergent, since the system state at the Level A description cannot be directly recovered from the Level B state description.

Furthermore, here we are interested in B Levels that describe the dynamics of emergent organization. For the formalism that follows to apply to organized structures, it is crucially important to have a function $B(\cdot)$ that identifies such organization. The methods outlined above in Section 7 do exactly this. That is, we may think of $B(\cdot)$ as being a set of local causal states defined from $\epsilon(\cdot)$, or $B(\cdot)$ may be a collection of finite-time coherent sets and the like.

As a guiding example in what follows, consider Level A as being (numerical simulations of) the two-dimensional vorticity equation and Level B as the dynamics of emergent vortices. Again, the function $B(\cdot)$ may be defined, e.g., using $\epsilon(\cdot)$ and the local causal states it induces [211]—as shown in Fig. 6—or coherent structures that arise in some Lagrangian method [177]. The collection of emergent vortices b_t at any given time is insufficient to determine the full vorticity field a_t, so $B(\cdot)$ is not invertible.

Our task is to define what it means to have a dynamical description that is fully *self-contained* at Level B, while also being physically consistent with the dynamics given by Level A. Following our emergent vortices example, we want a formulation of the evolution of the vortices $\{b_t, b_{t+1}, b_{t+2}, \ldots\}$ that is self-contained, without direct reference to the vorticity fields $\{a_t, a_{t+1}, a_{t+2}, \ldots\}$. However, the Level B vortex evolution must still be physically consistent with the Level A vorticity equation, such that there exists a sequence of vorticity fields—satisfying the vorticity equation—that gives $\{b_t = B(a_t), b_{t+1} = B(a_{t+1}), \ldots\}$. We will find that the Level B evolution is in general stochastic and is defined in terms of predictive distributions. Conditions for convergence to a deterministic Level B evolution, analogous to a thermodynamic limit, can then be given.

The starting point is to observe that $B(\cdot)$ is a vector-valued system observable, in the technical sense given above, and so it is evolved by Koopman operators. A unit-step of the dynamics at Level B is given by:

$$b_{t+1} = [\mathcal{K}B](a_t) \ . \tag{50}$$

Note though, this requires the initial Level A state a_t. Knowing only b_t on Level B at time t means the system at the Level A description could be in many states a_t that are consistent with the Level B observation: $b_t = B(a_t)$. Therefore, given b_t, many b_{t+1} may follow that are consistent with the Level A description:

$$\{b_{t+1} = [\mathcal{K}B](a_t) \ \text{ for all } a_t \in B^{-1}(b_t)\} \ , \tag{51}$$

where $B^{-1}(b_t) = \{a_t : b_t = B(a_t)\}$ is the pre-image of $B(\cdot)$.

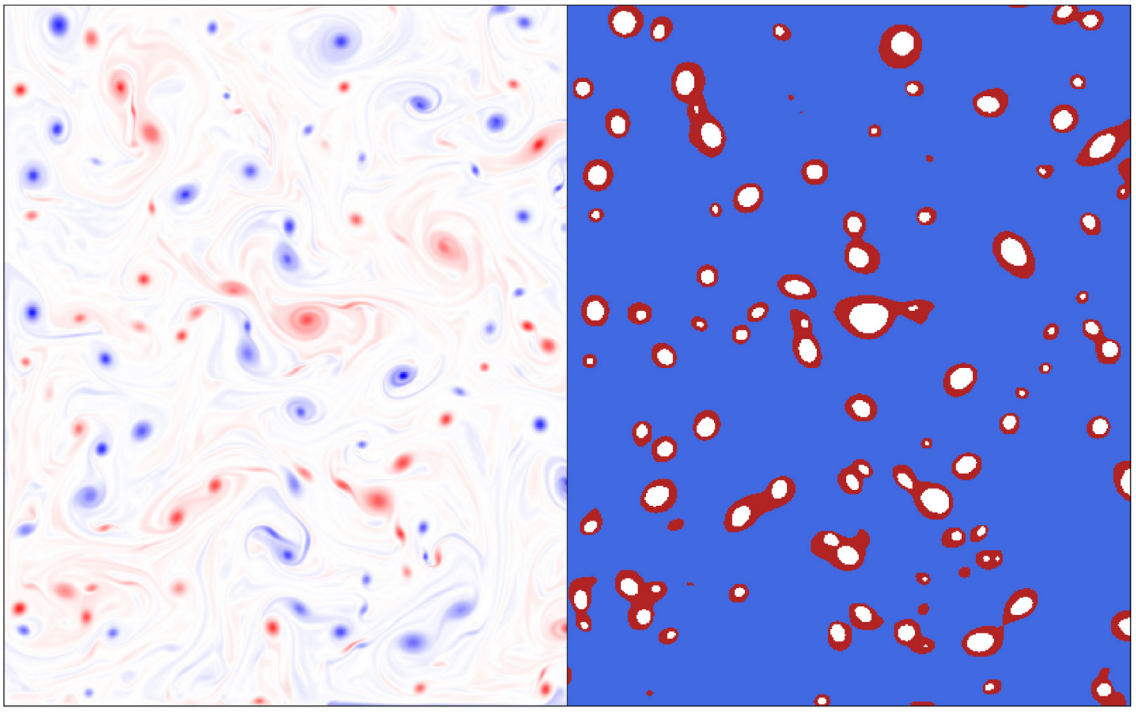


Fig. 6. A vorticity field a_t (left) from two-dimensional turbulence and its local causal state field $S_t = \epsilon(a_t)$ (right). Taking only the white vortex-core local causal states gives an example of higher-Level emergent organization $b_t = B(a_t)$.

Therefore, the *instantaneous dynamics* on Level B are stochastic:

$$\Pr(b_{t+1}) = M_0 \Pr(b_t) \,, \tag{52}$$

with some Markov operator M_0. The set in Eq. (51) can be seen as the support of a conditional probability distribution $\Pr(b_{t+1}|b_t)$. This is the *instantaneous predictive distribution* that captures the maximal information available about the next value b_{t+1} given a specific observed value b_t.

Under the Level A dynamics, knowledge of state a_t at any given time is sufficient to fully determine the Level A state at later times. Clearly, this is not the case for the Level B dynamics. There, state b_t is associated with a distribution over consistent future Level A states—the instantaneous predictive distribution. A notable consequence is that prior observations b_{t-k} contain relevant additional information for predicting future values.

This follows from the *Mori–Zwanzig equation* or generalized Langevin equation:

$$b_{t+1} = M_0(b_t) + \sum_{k=1}^{t} M_k(b_{t-k}) + \xi_{t+1}(a_0) \,. \tag{53}$$

This gives the *exact* Level B evolution for a given evolution at Level A and is equivalent to:

$$b_{t+1} = [\mathcal{K}^{t+1} B](a_0)$$

via the Dyson expansion of $\mathcal{K}^{t+1}$ using projection operators; see Refs. [225,226] for the full derivation.

The Mori–Zwanzig equation, originally developed as a first-principles theory of nonequilibrium transport [227], expresses as much of the Level B dynamics as possible in terms of Level B states. The first term M_0 is referred to as the *Markov* term, as it gives the dependence of b_{t+1} on its single prior value b_t. As discussed above, this is insufficient to fully determine b_{t+1}. There is an additional temporal dependence, given by the middle term. The M_k are known as *memory kernels*, and they capture how information is propagated and dissipated between the A and B Levels. The last term $\xi_{t+1}(a_t)$ is called the *orthogonal component* and it captures the remaining dependence on the initial unknown Level A state a_0 that cannot be accounted for by the memory contributions.

In our framing of emergent organization, Level A states are not accessible, and so we cannot include the orthogonal component $\xi_{t+1}(a_0)$. If this term is nonzero, it is required to recover the exact deterministic Level B evolution. And so, a self-contained and consistent Level B dynamics must be stochastic in this case.

At this point, changing perspective to consider trajectories or paths, as central entities, rather than instantaneous states is helpful. This is a common strategy in nonequilibrium statistical mechanics. Denoting the collection of current and prior

values of b_t as its *past* $\overleftarrow{b}_t = \{b_{t'}\}, t' < t$, we can directly subsume the memory dependence of the Mori–Zwanzig equation into a dependence on the past:

$$b_{t+1} = \overleftarrow{M}(\overleftarrow{b_t}) + \Xi(a_0) \ . \tag{54}$$

In this, the Markov and memory effects are combined to give a single contribution from the past $\overleftarrow{b}_t$. This procedure is formally carried out using Wiener projections of the Koopman operator onto pasts of partial observations [228,229].

Since Eq. (54) is equivalent to the Mori–Zwanzig equation in Eq. (53), the exact deterministic dynamics of b_t requires a dependence on its past and may exhibit a residual dependence $\Xi(a_0)$ on the initial A state. As above, a self-contained Level B dynamics cannot include $\Xi(a_0)$ since information about Level A is taken to be unavailable. The trajectory-oriented perspective compactly expresses the self-contained B dynamics as $\overleftarrow{M}(\overleftarrow{b_t})$—a Wiener projection of the action of the Koopman operator. The optimal projection takes the form of a conditional expectation:

$$\overleftarrow{M}(\overleftarrow{b_t}) = \mathbb{E}[b_{t+1}|\overleftarrow{b}_t] \ . \tag{55}$$

This has the form of an expectation over a *history-dependent predictive distribution*.

Appealing to the Maximum Caliber approach to nonequilibrium statistical mechanics, we can fully specify the predictive distributions, rather than only their expectations. In the absence of Level A and $\Xi(a_0)$, these predictive distributions give *all* of the possible future Level B trajectories that are physically consistent with the Level A dynamics and their relative likelihoods.

Note that the MZ equation, in either form, is exact only when the dependence on the initial Level A state a_0 is included. When the orthogonal term $\Xi(a_0)$ is not included, the conditional expectation $\overleftarrow{M}(\overleftarrow{b_t}) = \mathbb{E}[b_{t+1}|\overleftarrow{b}_t]$ taken over consistent trajectories may itself not be consistent with the Level A dynamics. Thus, using the full predictive distributions themselves, rather than their expectations, is crucial to maintain physical consistency between Levels. We now detail these predictive distributions and how they maintain consistency. This then leads us naturally to the causal states and their stochastic dynamics.

Returning to the example of vortex dynamics in two-dimensional turbulence, assume we observe a trajectory of evolving vortices without details of the vorticity field or knowledge of the vorticity equation. Many future trajectories will be physically consistent. In this case, this means vortices undergo pairwise mergers such that the total number of vortices decay over time as a power law [137]. Averaging over such trajectories may produce the correct power-law decay in the total vortex number, but it may not display the proper pairwise-merger mechanism generating the decay.

8.2. Consistent predictive distributions and causal states of partially-observed processes

Recall that the pre-image $B^{-1}(b_t)$ of a single instantaneous observation b_t gives the set of all a_t consistent with $b_t = B(a_t)$. With a subsequent observation b_{t+1}, it is not necessarily the case that the dynamics of all a_t in B^{-1} are consistent with the new observation. That is, there may be an $a_t^* \in B^{-1}$ such that $B\big(\Phi(a_t^*)\big) \neq b_{t+1}$. Therefore, new observations of the Level B dynamics may constrain the set of possible initial conditions on Level A that are consistent with the Level B dynamics. For a past $\overleftarrow{b}_t^k$ at time t of length k, let $\overleftarrow{B}_t^k$ denote the set of initial A states consistent with all B observations in $\overleftarrow{b}_t^k$.

Furthermore, recall that the action of the Koopman operator $\mathcal{K}^l$ on the set $B^{-1}(b_t)$ of initial Level A states consistent with the instantaneous Level B observation b_t provides the set of all possible future Level B observations b_{t+l} that are consistent with the initial observation b_t. From the above, a past history of observations $\overleftarrow{b}_t^k$ constrains the set of consistent initial Level A states. And, this also constrains the set of consistent future Level B observations b_{t+l}. Building on the original Mori–Zwanzig framework, this perspective again underscores the importance of past histories in formulating self-contained dynamics of emergent organization—dynamics that is consistent with the underlying physics. If the full history is not taken into account, the reconstructed self-contained dynamics may not be physically consistent.

To achieve an exact deterministic dynamics that is self-contained on Level B it is sufficient that $\overleftarrow{B}_t^k$ contains one and only one initial Level A state a_{t-k} for all times t (with k potentially limiting to ∞). Then there will always be one and only one:

$$b_{t+1} = [\mathcal{K}^{t+k+1}B](a_{t-k} = \overleftarrow{B}_t^k) \ .$$

This is analogous to a thermodynamic limit where fluctuations about the mean vanish in the limit. See Ref. [230] for further details.

It cannot be guaranteed that the residual dependence $\Xi(a_0) = 0$ in general, even if we take the $k \to \infty$ limit of infinite memory. In this case we can still give a complete and self-contained dynamic for Level B. It will simply be stochastic rather than deterministic. This complete and self-contained dynamic for Level B is given by the causal states and their Markov transitions.

Thus far, we showed that the set of future Level B observations consistent with a past history of Level B observations is given by the action of the Koopman operator:

$$\{b_{t+l} = [\mathcal{K}^l B](a_t) \text{ for all } a_t \in \overleftarrow{B}_t\} \ , \tag{56}$$

which holds for all distances l into the future. Since history dependence may persist arbitrarily far in the past and we can use the Koopman operators to evolve arbitrarily far into the future, we can use the above to define the support sets for *predictive distributions* $\Pr(\overrightarrow{b}_t|\overleftarrow{b}_t)$ in full generality, with semi-infinite pasts and futures.

We can go further and add a natural probability distribution that directly specifies these predictive distributions. Following Maximum Caliber, we assign a uniform distribution to the Level A states $a_t \in \overleftarrow{B}_t$ that are consistent with the observed Level B history $\overleftarrow{b}_t$ and assign zero probability to Level A states not in $\overleftarrow{B}_t$—i.e., those not consistent with the observed B history. This distribution is then evolved forward by Perron–Frobenius operators and pushed forward through the observation map $B(\cdot)$ to give the predictive distribution $\Pr(\overrightarrow{b}_t|\overleftarrow{b}_t)$; see Fig. 7.

With the predictive distributions in hand, it is straightforward to define causal states in the same way as above in Section 7—as sets of past histories with the same predictive distributions. We can also define the Markov operator M_ϵ for the stochastic dynamics over causal states using Perron–Frobenius operators, given that the ϵ-function is measurable. The full measure-theoretic details are left for the future.

Having established the continuous versions of causal states and their Markov chain dynamics for the emergent dynamics of Level B, it follows from the definition of predictive (causal) equivalence that this is an optimal self-contained predictive model [209, Theorem 1] of the Level B dynamics consistent with the physics of Level A. Here, we showed explicitly how predictive distributions, and hence causal states, encapsulate the full dynamical information self-contained on Level B that is consistent with Level A.

It is an important practical note that, while we can write down the general form of predictive distributions, unsurprisingly we cannot directly construct them in closed form in specific instances. However, as described above in Section 7, the causal states and their dynamics may be consistently approximated from data using predictive equivalence. This makes the information contained in predictive distributions actionable in practice.

We can now also import the tools and interpretations of intrinsic computation to this continuous setting of emergent dynamics. The asymptotic degree of temporal organization is given by the *statistical complexity* [194]—the entropy of the steady-state distribution over causal states. In other words, the statistical complexity is the amount of historical information a system stores. And, if there are uncountably-many causal states, the divergence rate of that stored information is given by the *statistical complexity dimension* [219].

In this way, the causal states provide a complete and self-contained description for general emergent behaviors. From their definition in terms of Koopman and Perron–Frobenius evolution operators, they are fully consistent with lower-Level descriptions of the system dynamics. At the same time, they decompose the dynamics into its (temporal) organizational structure. Recall from above in Section 7.4 that the causal states capture patterns as generalized symmetries through their semigroup algebra.

By combining evolution operators, nonequilibrium statistical mechanics (MaxCal), and predictive equivalence, we arrived at a universal framework for defining consistent and self-contained emergent dynamics in terms of causal states and their Markov transitions. Thus, the approach simultaneously presents emergent dynamics in terms of its structural organization.

9. Conclusion and looking forward

Historically, *principles of organization* are given in the *constructionist* paradigm. Paraphrasing Feynman [231], what we now call constructionism is described as: "We look for a new law [principle] by the following process. First, we guess it. Then, we compute the consequences of the guess ... to see what it would imply. Then we compare the computation results with experiment or observations". The nonlinear dynamics bifurcation-theoretic derivation of the critical Rayleigh number that predicts the first onset of Bénard convection cells is a prototypical example that follows Feynman's dictum. There are limits, however, to constructionism, and so general principles of organization require a new paradigm of understanding for complex systems with emergent behaviors.

For equilibrium, we outlined how the 2nd Law provides a variational organization principle: equilibrium thermodynamic states, including organized states, are those that maximize entropy subject to system constraints. We described Classical Irreversible Thermodynamics as an attempt to generalize the First and Second Laws of equilibrium thermodynamics to nonequilibrium field theories. However, we showed that the entropy production density and its associated balance equation—the nonequilibrium generalizations of entropy and the 2nd Law—are superfluous at best and, at worst, not physically justified. Indeed, extrema of entropy production do *not* determine nonequilibrium steady-states, analogous to extrema of entropy determining equilibrium states. Ultimately, empirically-derived phenomenological laws and energy balance—the nonequilibrium generalization of the 1st Law—are used to derive the nonequilibrium transport equations used by nonlinear dynamics' pattern formation theory.

Prigogine et al.'s theory of *dissipative structures* claimed to be a thermodynamic theory of pattern formation and self-organization. After reviewing prior arguments and counterexamples that disproved dissipative structures, we went further to show that certain foundational assumptions from classical irreversible thermodynamics—on which dissipative structures theory is built—are not valid for interacting systems with nonzero levels of organization. Therefore, dissipative structures cannot be a theory of self-organization, as it purported to be. The thermodynamics of pattern formation and spontaneous self-organization thus *remains an open problem*.

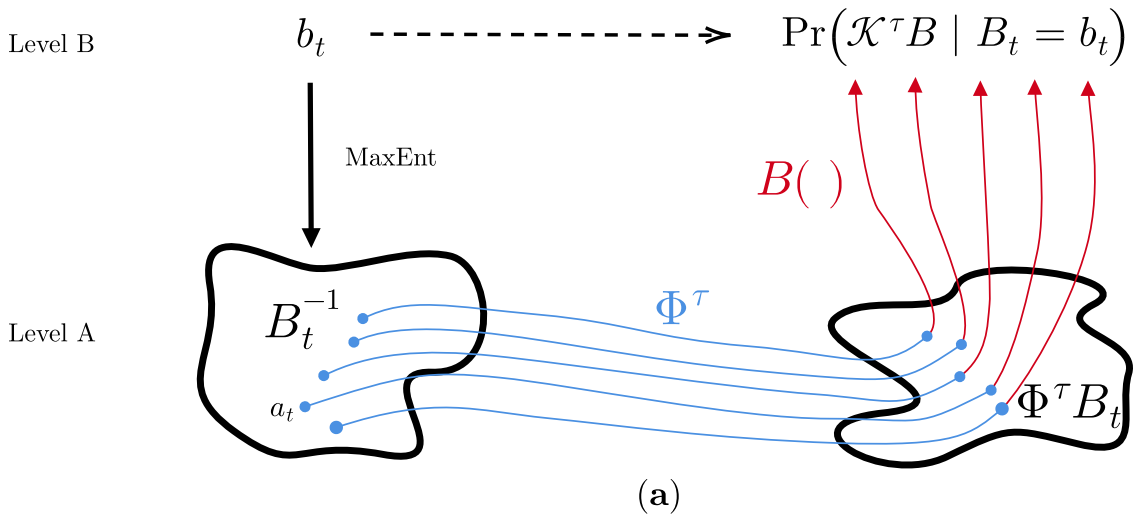


Fig. 7. Consistent predictive distributions: (a) Instantaneous case of a single Level B observation. (b) History-dependent case of a trajectory of Level B observations. MaxEnt (MaxCal) is used to infer the consistent set B_t^{-1} ($\overleftarrow{B}_t^k$) of Level A states from the Level B observation b_t ($\overleftarrow{b}_t^k$) in the instantaneous (history-dependent) case. The set of consistent Level A states will generally be smaller for more observations at Level B, leading to more accurate self-contained Level B predictions.

What might a future theory, or principles, of organization look like? We argued that the standard constructionist paradigm can fail for systems with *emergent* behavior. Since the intricate organization that forms in far-from-equilibrium systems is emergent, it is no wonder that universal principles of organization have remained elusive within the constructionist paradigm. Analytic intractability and even uncomputability thwart our ability to "compute the consequences" of a proposed mechanistic hypothesis.

A key step forward is to mathematically *identify* organization. Implicitly, this implies moving beyond simple notions of exact symmetries (and small deviations from them) and beyond subjectively selecting function bases for representational "dictionaries".

We reviewed two modern approaches to this challenge—evolution operators and intrinsic computation. Both lie outside constructionism, as neither can be analytically computed in general. However, they provide a theoretical framework for *data-driven* discovery of pattern and organization. Koopman and Perron–Frobenius evolution operators evolve system observables and probability distributions, respectively. Their spectral decompositions can identify statistical organization in time-independent systems, as well as coherent structures that heavily dictate transport in time-dependent systems.

In a complementary way, intrinsic computation decomposes a system into its minimal causal components using predictive equivalence. The semigroup algebra of intrinsic computation identifies organization by generalizing exact symmetries, and its extension to field theories using lightcones can also identify coherent structures.

Completing the relation between evolution operators and intrinsic computation is a challenge currently. It is encouraging that they both converge on their identification of coherent structures. At this time, though, it is not clear whether these two represent two pieces of a larger, universal theory of organization. Whether or not such a universal theory of organization even exists is an open question.

A tantalizing path forward is offered by combining evolution operators with predictive equivalence to formulate a statistical mechanics of emergence. Emergence is what has stymied efforts to develop constructionist principles of organization. The new mathematical tools that directly identify complex forms of organization also come together in a universal theory that provides complete and self-contained dynamics for a higher-Level emergent description of a system that is physically consistent with its lower-Level description. While not analytically constructible in practice, this theory provides a rigorous foundation for data-driven approximation of emergent dynamics through predictive equivalence.

We close with a brief remark on *causal mechanism* discovery. While nonequilibrium equations Eq. (1) govern transport of energy and matter, different equations—specifically those derived from different phenomenological laws—represent distinct, but equally important mechanisms governing system dynamics. To address emergent behaviors in such broader classes of complex system, the added importance of *information transport* [96,232,233] and related *causal mechanisms* [234] is increasingly appreciated. Identifying causal mechanisms directly from system behaviors is an active and ongoing area of research [235–237]. We once again see the data-driven paradigm to scientific discovery filling the void left by the shortcomings of constructionism for complex systems with emergent behaviors.

CRediT authorship contribution statement

Adam Rupe: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **James P. Crutchfield:** Conceptualization, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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