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5 Using Ecology to Quantify Organization in Fluid Flows

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Summary. Numerous applications of variational principles derived from physical thermodynamics have been made to the description of development in living systems. While some have met with varying degrees of success, it appears none of the measures from classical thermodynamics adequately incorporates the roles of intrinsic system constraints into a robust description of biotic development. The flow network measure *ascendency*, therefore, has been formulated to express more explicitly the constraints immanent in ecosystem trophic exchanges. Ascendency has wide applicability and can be used as well to provide a measure of the overall degree of organization inherent in a purely physical flow field, such as rates of energy exchange. It can also be employed to pinpoint the bottlenecks that control the fluid flow field.

5.1 Introduction

The body of phenomenology known as thermodynamics derives almost entirely from observations on physical systems. It remains rich, however, in its implications for living systems. Of especial interest to biologists is the concept of entropy, and particularly the derivative variational principles of minimal and maximal entropy productions. For example, one encounters the Prigoginian notion of minimal entropy production applied to living systems (Zotin 1972). Conversely, the tendency towards maximal entropy production finds application in the physical realm (Paltridge 1975, 2001, this volume) as well as the biological (Swenson 1989; Kleidon and Fraedrich, this volume; Toniazzo et al., this volume).

The extrapolation from the physical realm to the biological is not without its difficulties, however. While physical constraints, such as conservation of energy and mass, clearly apply, there seems to be a tacit consensus that internal constraints play a proportionately larger role in biological behaviors than they do among physical processes. Some look for a way around this by reformatting the laws of thermodynamics in unitary fashion (Hatsopoulos and Keenan 1965; Kestin 1976). To capture biological directions, Schneider and Kay (1994) proposed a corollary to the unitary formulation, whereby living systems always act to degrade existing gradients in exergy (energy available for work) at the maximal rate possible (see also Schneider and Sagan 2004).

58 R.E. Ulanowicz and M.J. Zickel

For yet others, such reformulations do not incorporate sufficiently the informational constraints inherent in the processes that support life. Thus, Kauffman (1995) calls for a "Fourth Law of Thermodynamics" to fill the void. The utility of variational principles or goal functions as providing direction for the development of living systems was the subject of a recent symposium (Mueller and Leupelt 1998). The emerging consensus was that no single principle or goal function seems capable of adequately explaining the life process at all scales. Rather, each principle serves in its turn as an "orientor" that helps to guide, but not fully determine, the unfolding of living systems (Bossel 1998).

5.2 Constraint Among Biotic Processes

These limitations and inadequacies notwithstanding, a more effective quantification of the constraints intrinsic to biological systems appears desireable. It was, after all, Schroedinger's emphasis upon what he called "negentropy" that invigorated the search for ways by which biological constraints can be encoded in matter and which culminated in the discovery of DNA. "Negentropy", however, has been a difficult notion to quantify, and the limitations inherent in entropy as a state variable have circumscribed its possible role in the description of biotic processes.

Bearing these difficulties in mind, Ulanowicz (1980, 1986) made the decision to play down somewhat the energetic aspects of biology in order to highlight the role that emerging constraints play in organic development. He sought to develop a phenomenology of biological constraint by attempting to quantify the hidden agencies that channel biotic transfers along certain pathways. He remained confident that biotic constraints could be quantified, even in the absence of explicit knowledge about their constituent mechanisms – just as in thermodynamics it is possible to measure state variables without any concrete knowledge about microscopic details.

The system of interest for Ulanowicz was the flow network that depicts the transfers of material or energy between all pairs of predators and prey. He denotes the transfer of material or energy from prey (or donor) i to predator (or receptor) j as T_{ij} , where i and j range over all components of an nmember ecosystem. The total activity of the system is taken to be simply the sum of all system processes, $T_{..} = \sum_{i,j} T_{ij}$, or what is called the "total system

throughput" (A dot as a subscript is taken to mean summation over that particular index).

The constraints inherent in the flow network are assumed to arise in connection with the increase in the influence of autocatalytic feedbacks as the ecosystem develops (Ulanowicz 1986). Such unspecified constraints serve to channel flow ever more narrowly along those pathways that most effectively participate in the autocatalytic processes. Alternatively, constraints may be regarded as anything that causes certain flow events to occur more frequently than others. With frequency thus in mind, one supposes that constraint is somehow connected with the joint probability that a quantum of medium is *constrained* both to leave *i* and enter *j*. This probability may be estimated by the frequency $(T_{ij}/T_{..})$. One then notes that the *less constrained* probability that a quantum merely leaves *i* for an unspecified destination can be acquired by summing the joint probability over all possible destinations. Such frequency becomes $(T_{i.}/T_{..})$. Similarly, the unconstrained probability that a quantum enters *j* is estimated by $(T_{.j}/T_{..})$. Finally, one reckons the probability that a quantum could make its way by pure chance from *i* to *j*, without any constraint, as the product of the latter two frequencies, or $(T_{i.},T_{.i}/T^2)$.

When Tribus and McIrvine (1971) defined information as "anything that causes a change in probability assignment", they essentially were equating information with constraint. Information theory, then, could provide the format for how one might quantify constraint. Strangely, however, information theory does not address information (constraint) directly. Rather it starts with a measure of the rareness of an event, as first postulated by Boltzmann (1872) to be $-k \log p$, where p is the normalized probability ($0 \le p \le 1$) of the given event happening, and k is a scalar constant that imparts dimensions to the measure. One notices how for rare events ($p \approx 0$), Boltzmann's measure is very large; whilst for very common events ($p \approx 1$), it is vanishingly small.

Because the constraints that act to channel flows act to make certain things happen more frequently in a particular way, one expects that, on average, the probability of such constrained events would be greater than those of corresponding unconstrained events. The rarer (unconstrained or unguided) circumstance that a quantum leaves i and accidentally makes its way to jcan be quantified by applying the Bolzmann formula to the last probability defined above, i.e., $-k \log (T_{i.} T_{.j}/T_{..}^2)$. The more frequent condition that a quantum is constrained both to leave i and enter j would give rise under Boltzmann's assumption to $-k \log(T_{ij}/T_{..})$. Subtracting the latter quantity from the former and combining the logarithms yields a measure of the information inherent in the hidden constraints that channel the flow from i to j, i.e., $k \log(T_{ij}T_{..}/T_{i.}T_{.j})$.

Finally, to quantify the average constraint at work in the system as a whole, one weights each such pair-wise measure by the corresponding joint probability of constrained flow from i to j and then sums over all combinations of i and j (Abramson 1963). That is,

$$AMC = k \sum_{i,j} \left(\frac{T_{ij}}{T_{..}}\right) \log\left(\frac{T_{ij}T_{..}}{T_{i.}T_{.j}}\right)$$
(5.1)

where AMC is the "average mutual constraint" (known in information theory as the average mutual information.)



Fig. 5.1. a The most equivocal distribution of 96 units of transfer among four system components. b A more constrained distribution of the same total flow. c The maximally constrained pattern of 96 units of transfer involving all four components

To illustrate how an increase in AMC actually tracks augmented constraint, the reader is referred to the three hypothetical configurations shown in Fig. 5.1. In configuration (a) where medium from any one compartment will next flow is maximally indeterminate. AMC is identically zero. The possibilities in network (b) are somewhat more constrained. Flow exiting any compartment can proceed to only two other compartments, and the AMCrises accordingly. Finally, flow in schema (c) is maximally constrained, and the AMC assumes its maximal value for a network of dimension 4.

One notes in the formula for AMC that the scalar constant, k, has been retained. Tribus and McIrvine (1971) suggested that k be used to impart physical dimensions to an otherwise dimensionless information measure. Accordingly, the measure of constraint can be scaled by the total activity of exchange (T..) to yield a "quasi-power" function called the system *ascendency* A, where

$$A = \sum_{i,j} T_{ij} \log \left(\frac{T_{ij} T_{..}}{T_{i.} T_{.j}} \right)$$
(5.2)

In his seminal paper, "The strategy of ecosystem development", Eugene Odum (1969) identified 24 attributes that characterize more mature ecosys-

tems. These can be grouped into categories labeled species richness, dietary specificity, recycling and containment. All other things being equal, a rise in any of these four attributes also serves to augment the system ascendency (Ulanowicz 1986). It follows as a phenomenological principle that "in the absence of major perturbations, ecosystems have a propensity to increase in ascendency."

5.3 Quantifying Constraint in Fluid Flow

It is well and good that ecologists now have at their disposal a convenient measure of the level of constraint inherent in an ecosystem, seeing as how constraint appears to be a prominent aspect of living systems that heretofore had been insufficiently incorporated into conventional thermodynamic measures. The question of greater interest to the reader, however, is what relevance, if any, does this measure have to the disciplines of fluid flow, meteorology and climatology? (In the event a connection can be made, it would constitute an unusual "man bites dog" example of a concept first developed in the biotic sciences and then applied to the purely physical realm.)

To demonstrate the utility of ascendency to fluid mechanics, one begins with an arbitrary flow field of interest that is finite, continuous and can be divided into a countable number of finite elements that cover the field entirely and are contiguous with each other. Without loss of generality, it may be assumed that the flow field is rectangular and is divided by a rectilinear grid. The flow field can be one, two or three dimensional, for it is easily demonstrated that only a single index is necessary to uniquely identify any element in any finite spatial domain. For example, if the flow field is twodimensional, one may divide the field into m rows of n cells each and number the cells consecutively $1,2,3,\ldots m, m+1, m+2,\ldots, (mn-2), (mn-1), mn$. A similar scheme can be used to enumerate a three-dimensional field. Again, without loss of generality, further consideration will be limited to a twodimensional $(m \times n)$ flow field.

It is assumed that a quantitative description of a fluid flow field, v(x, y), can be provided either by some analytical means or a numerical process, and the values of v(x, y) at any location (x, y) (and at the boundaries) are available with sufficient precision. (The dynamical case, v(x, y, t) is considered below.)

Under these premises, the translation of the physical flow field v(x, y) into an abstract flow network of dimensions $(mn \times mn)$ becomes straightforward. One begins by defining f_{ij} to be the total amount of fluid that passes from cell *i* to cell *j* during a unit of time. Only positive flows will be considered; that is, if a flow from *i* to *j* is calculated to be negative, then the absolute magnitude of the transfer is added to f_{ii} , instead of to f_{ij} .

Attention is now focused upon an arbitrary element k within the flow field. It exchanges fluid with elements (k-1) and (k+1) in the horizontal direction and with (k - n) and (k + n) in the vertical. For the moment

62 R.E. Ulanowicz and M.J. Zickel

attention is further narrowed upon the vertical line that separates spatial element k from element (k-1). The amount of fluid passing this interface can be calculated as $\int_{k,(k-1)} v_x dy$, where v_x is the horizontal component of the velocity, and k, (k-1) denotes a line integral over the vertical segment in question. Whenever this integral is positive, the calculated amount is added to the network element $f_{(k-1),k}$. If it is negative, the amount is added to $f_{k,(k-1)}$.

One can treat vertical transfers in similar manner: Over the horizontal boundary separating k from (k - n), one calculates the line integral $\int_{(k-n),k} v_y dx$. As before, if the result is positive, the magnitude is added to $f_{k,(k-n)}$; if it is negative, to $f_{(k-n),k}$.

By applying the first method to the interface between k and k + 1 and the second to that separating k from k + n, one accounts for all exchanges involving element k. Obviously, one wishes to avoid any double counting of transfers, which can be accomplished by iterating over all internal boundaries (rather than the elements themselves), visiting each edge once and only once. Should the external boundary conditions happen to be impermeable, that is "no-flow", then the conversion to a network description of the fluid flow field is now complete. Whenever the boundary conditions are "wrap-around" (e.g., the right-hand side of element 2 n is assumed to abut the left-hand side of element [n + 1], then the flows across these boundaries can be treated exactly like the internal boundaries. For more general boundary conditions, it will be necessary to increase the dimension of the flow matrix by at least one to (mn+1) to be able to accommodate the external world. Accounting for boundary flows would then entail the calculation of elements like $f_{3n,(mn+1)}$ or $f_{(mn+1),(5n+1)}$, etc. The resulting flow matrix is likely to have high dimension and to be very sparse. (By "sparse" is meant that most matrix entries are zero)

Having effected the conversion of a continuous (or approximately continuous) flow field into a discrete flow network, it is now but a formality to calculate the information indices that describe the status of ecosystem flow networks (Rutledge et al. 1976; Ulanowicz 1986; Ulanowicz and Norden 1990). As with the ecosystem trophic exchanges treated earlier, a dot is used as shorthand for summation over a subscript index.

The diversity of the flow field ${\cal H}$ can be defined using the familiar Shannon formula as

$$H = -\sum_{i,j} \left(\frac{f_{ij}}{f_{..}}\right) \log\left(\frac{f_{ij}}{f_{..}}\right)$$
(5.3)

This diversity, or complexity, encompasses both structured (constrained) and stochastic elements. Using Bayesian information theory, it becomes possible to parse out exactly how much of the calculated diversity can be characterized as structured from that which remains stochastic. As developed in the previous section, the amount of H which constitutes coherent (constrained) flow structure is assessed by the average mutual constraint as 5 Using Ecology to Quantify Organization in Fluid Flows 63

$$AMC = \sum_{i,j} \left(\frac{f_{ij}}{f_{..}}\right) \log\left(\frac{f_{ij}f_{..}}{f_{i.}f_{.j}}\right)$$
(5.4)

That is, AMC becomes an index of the organization inherent in the flow field. Presumably, the AMC will also corrolate strongly with one or more of the scalar metrics pertaining to the fluid flow correlation tensor.

The amount of H that does not appear as structured flow, (H - AMC), represents the residual incoherency Φ :

$$\Phi = -\sum_{i,j} \left(\frac{f_{ij}}{f_{..}}\right) \log\left(\frac{f_{ij}^2}{f_{i.}f_{.j}}\right)$$
(5.5)

That is, Φ should be an index of how stochastic or turbulent the flow field appears under the network representation. One notes that $H \ge 0$, $AMC \ge 0$, and $\Phi \ge 0$.

The working hypothesis now being investigated by the authors is that whenever a flow field undergoes a transition from laminar (highly organized) to turbulent flow, AMC will decrease dramatically and Φ will abruptly increase. Conversely, if an organized flow suddenly displaces a stochastic one (as in the sudden appearance of Bernard or Langumir cells), AMC should rise abruptly and Φ should fall correspondingly. A related example of how AMC can be applied to a field of migratory animals is provided in Ulanowicz (2000), who showed, for example, how the ascendency of a uniform rectilinear migration field increased when a barrier was introduced into the middle of the migrating animals. He also demonstrated how the ascendency of a field of random migrations was negligible in comparison with one where migrations were directed and distinct. Such differences almost certainly will appear in analogous fluid flow fields.

The conversion of dynamical flow fields, v(x, y, t), into three-dimensional flow networks is rather straightforward: Instead of considering the four lines bounding the square grid, one treats the six sides of the cube that envelops k. It remains, then, only to define the expanded information measures that can be invoked to quantify the resulting 3-D network. As before, one defines f_{ijk} as the transfer from spatial element i to neighboring element j during time interval k. Again, the dot shorthand for index summation is employed. Pahl-Wostl (1995) showed how several coherencies are aggregated within the measure I_t which she calls the temporal information:

$$I_t = \sum_{i,j,k} f_{ijk} \log\left(\frac{f_{ijk}^2 f_{...}}{f_{ij.} f_{i.k} f_{.jk}}\right)$$
(5.6)

This index I_t can be decomposed into several components, each of which quantifies a different aspect of coherency, such as when a system begins to oscillate in response to a frequency in an imposed forcing function (Ulanowicz 1991).

5.4 Identifying Flow Bottlenecks

Because the information measures just introduced appear to parallel the metrics associated with the conventional correlation tensor, one might understand why the reader might want to question whether another set of seemingly redundant measures is really necessary? It should be pointed out, therefore, that the information calculus affords some very convenient mathematical properties not shared by the more conventional measures. In particular, the information format allows for the immediate calculation of a field of sensitivity indicators.

For example, above it was shown how scaling the AMC by the total system throughput yields a function called the system "ascendency" A:

$$A = f..AMC \tag{5.7}$$

or

$$A = \sum_{i,j} (f_{ij}) \log\left(\frac{f_{ij}f_{..}}{f_{i.}f_{.j}}\right)$$
(5.8)

It happens that the ascendency as it appears in (5.8) is an Euler function, so that one can immediately write the sensitivity of the ascendency with respect to any arbitrary flow, say f_{pq} as

$$\frac{\partial A}{\partial f_{pq}} = \log\left(\frac{f_{pq}f_{..}}{f_{p.}f_{.q}}\right) \tag{5.9}$$

One can then search this matrix of sensitivities for local maxima, which should indicate "hotspots' where the flow field as a whole is most sensitive to the particular transfer in question.

Ulanowicz and Baird (1999) used this formal scheme to appraise nutrient transfers in ecosystems. They had estimated parallel networks for the seasonal flows of carbon, nitrogen and phosphorus among the principal taxa of the Chesapeake ecosystem. Using those networks, they applied the sensitivity indices calculated from the last formula, to uncover the rate-limiting flows in the system. After the fact, they were able to demonstrate analytically that the maximal sensitivities indicated those elements that were rate-limiting in the sense of Justus von Liebig (1854). By analogy, it becomes possible to entertain the hypothesis that the maxima of the indicated sensitivities provide a convenient way of identifying the "bottlenecks" or control points in a fluid flow field.

5.5 Conclusion

One may hypothesize different levels of organization at the microscale, as characterized by different values of ascendency, should result in differing macroscopic states of the fluid flow field with contrasting rates of entropy production. Furthermore, the behavior of the ascendency index could provide additional insights about the organization of flow when MEP does not apply (e.g., smaller scales, departures from steady state). Using the ecological concept of ascendency could provide new and valuable contributions to the microscopic analysis of fluid flows and might also find fecund application to the related fields of meteorology and climatology.

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