Quantifying information for a stochastic particle in a flow-field

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The question of how the information content of a particle in a flow-field can be quantified is addressed theoretically within the general framework of nonequilibrium statistical physics. It is observed that the rotational component of a flow-field, which characterizes the degree of irreversibility of the stochastic dynamics, does not explicitly appear in the equation that quantifies the rate of system entropy production. The residence time of a particle in an arbitrary neighborhood of a flow-field is characterized in terms of the flow properties. This information is important when the flow transports vital signaling molecules necessary for system function. These results shed light on how information can be measured and controlled in complex artificial and living flow-based systems.

There has been a great deal of progress in recent years regarding the question of how to quantify the information content in small fluctuating systems. This stems from the rigorous formulation of stochastic processes and thermodynamics of information and entropy production \cite{1–7}, together with the experimental detection and manipulation of these properties in various systems including colloids \cite{8,9}, active \cite{10,11} and living matter \cite{12–14}. These questions, however, have so far not been explored in the ubiquitous system of flow-fields in which stochastic particles are transported (see Fig. 1). Flows are present in diverse settings from microfluidic devices to solid-state systems. In living systems, flows can transport vital signaling particles necessary for the function of the system \cite{15,16}. For instance, complex flow patterns have been measured in the brain ventricles of mammals \cite{17}, which contain guidance molecules that cue the migration and development of young neurons \cite{18}. Therefore, it is natural to ask what information is carried by a small particle in a flow-field.

To answer this question, we develop a general expression for the rate of change of information content of a stochastic particle in a flow-field, which features contributions from the flow characteristics as well as the system fluctuations. We note that previous work on thermodynamics in flow-fields has focused on changes in local particle conformation \cite{19,20}. The joint effects of diffusion and advection have been studied for inertial particles or regular flows such as shear or strain \cite{21–24}. Here, we develop a formalism for generic flows applicable to complex fields or realistic scenarios. We find that the rotational component of a flow-field that controls the degree of irreversibility of the dynamics does not make an explicit contribution to the system entropy production.

To demonstrate the wide range of possible implementations of our formalism, we approximate the flow field in a local neighborhood. The formalism can be used to calculate the change in information content and residence time scale for various geometries and flow-fields. For instance, we uncover a mechanism for retaining a particle for a longer period of time than diffusion would typically permit. Our results provide a way to quantify the information and transport properties for generic flows, which can be applied in various contexts including experimentally measured fields.

We consider a particle with diffusion coefficient $D$ that undergoes stochastic motion in a $d$-dimensional position space under the influence of a flow-field $\mathbf{v}(x)$, and is characterized by the probability distribution $P(x,t)$. To analyze the information content, we use the system (Shannon) entropy $S = -\int d^d x P \ln P = \langle s \rangle$, where $s \equiv -\ln P$ is the stochastic entropy of the system from a given finite trajectory \cite{25}. This is an appropriate measure as it quantifies how spread out the distribution is: when the distribution is sharply peaked, the entropy is low as one can reliably locate the particle \cite{26,27}. Using the Helmholtz-Hodge decomposition, we can represent the vector field in terms of conservative and rotational components, namely, $\mathbf{v}(x) = -D \nabla \Phi + w(x)$, where $\nabla \cdot w = 0$.

By invoking the continuity equation $\dot{P} + \nabla \cdot J = 0$, where the flux is given as $J = \mathbf{v}(x) P(x,t) - D \nabla P(x,t)$, we find a closed-form expression for the rate of entropy production as (see Ref. \cite{28} for details)

$$\dot{S}(t) = -D \langle \nabla^2 m \rangle,$$

where $m \equiv \Phi + \ln P$ plays the role of a stochastic generalized chemical potential, as it is spatially uniform in equi-

![FIG. 1. What is the information content after time $t$ or particle residence time, for a stochastic particle in a complex flow? The answer is determined by an interplay between diffusion field.](image-url)
librium. We thus find that system entropy production exists only when the system is manifestly out of equilibrium with a non-zero Laplacian of \( m \). Remarkably, our result shows that the rotational component of the velocity, \( w \), which encodes the degree of the irreversibility of the flow-field, does not explicitly appear in the rate of system entropy production. Equation (1) can be written in an alternative form of
\[
\dot{S}(t) = \langle \nabla \cdot v \rangle + D(\langle (\nabla v)^2 \rangle),
\]
which highlights the positive definite entropic contribution to the entropy production rate as well as the dependence on the irrotational component of the flow-field, since \( w \) is divergence-free.

To study the behavior of this expression in realistic flow-fields, we analyze the stochastic dynamics of a particle with trajectory \( r(t) \) in the presence of noise and advection due to a vector field \( v(r) \) (Fig. 1). Specifically, in the local neighborhood of the origin, \( r = 0 \), where the particle is located at \( t = 0 \), the flow-field can be approximated using a Taylor expansion. Up to the first order in the expansion, this gives the Langevin equation
\[
\frac{d\mathbf{r}}{dt} = \mathbf{v}(\mathbf{r}) + \mathbf{K} \mathbf{r} + \sqrt{2D} \xi
\]
where \( \xi(t) \) represents a white noise (Gaussian random variable of unit strength), and we denote \( v_i(0) = v_i \) and \( \partial_i v_j(0) = K_{ij} \). This description will allow us to study how the short-time stochastic dynamics of the particle depends on the local characteristics of the flow-field.

Using a path integral method \cite{29}, we find that the probability for the particle to be found at a distance \( x \) away after time \( t \) is (see Ref. \cite{28} for details)
\[
P(x, t) = \frac{\exp\left(-\frac{1}{2D} |x - r_d(t)|^2 M^{-1} |x - r_d(t)|\right)}{(4\pi D)^{d/2}(\det M)^{1/2}},
\]
where
\[
r_d(t) = (e^{Kt} - 1)K^{-1}v,
\]
\[
M(t) = \int_0^t dt_1 e^{K(t-t_1)}K^T(t-t_1).
\]
It is useful to decompose \( K \) into its symmetric and antisymmetric components: \( K = E - \Omega \). Note that \( E \equiv \frac{1}{2} [(\nabla v) + (\nabla v)^T] \) is the strain rate tensor and \( \Omega \equiv \frac{1}{2} [(\nabla v) - (\nabla v)^T] \) is the vorticity tensor.

We can now calculate the average stochastic entropy for this probability distribution and find that Eq. (1) gives the total entropy production as
\[
\dot{S}(t) = \nabla \cdot v + \frac{1}{2} \text{tr} (M^{-1}).
\]
Note that this result is independent of the diffusion coefficient \( D \).

![FIG. 2. Transport of a particle in a divergent flow field. (a) Examples of flow fields that secrete \( k > 0 \), and absorb \( k < 0 \) fluid within a region \( R \); the flow profiles are shown on the right. The particles start at the origin which is within \( R \). (b) The probability of observing the particle in a diffusion-limited range as a function of time. The absorbing field retains a particle for longer times (blue) compared to the baseline set by diffusion (green), while the converse is true for the secreting field (red). (c) The rate of change of the information content as a function of time. At the beginning, the rate of change of the information content is \( \dot{I}(t=0) = -\frac{1}{2} \nabla \cdot v \) so is positive, and hence more informative for the absorbing field (blue) as compared to diffusion (green), and vice-versa for the secreting field (red). At long times, the absorbing field saturates to \( \dot{I}(t) = 0 \), consistent with an effective steady-state distribution. Meanwhile, the secreting field saturates to \( \dot{I}(t) \to k \), describing a probability distribution that keeps spreading out. Clearly, this is only physical within the length-scale in which the linear expansion remains valid. All plots use \( D = 0.1, |k| = 0.5 \) and \( r_0 = 0.1 \times (1,1,1) \).]

We can examine the short time behavior of the result by using the series expansion
\[
M(t) = t \left( I + Et + \frac{1}{3} (2E^2 - [\Omega, E]) t^2 + O(t^3) \right),
\]
where \([\Omega, E] = \Omega E - E\Omega \) and \( I \) is the identity tensor. This yields
\[
\dot{S}(t) = \frac{d}{2t} + \frac{1}{2} \nabla \cdot v + \frac{t}{6} \text{tr} (E^2 + [\Omega, E]) + O(t^2).
\]
In comparison, for a purely diffusive particle with \( P_D(x, t) = \frac{1}{(4\pi D t)^{d/2}} \exp\left(-\frac{x^2}{4Dt}\right) \) this rate is given as \( \dot{S}_D(t) = \frac{d}{2t} \). Hence, the rate of change of the information content of the tracer particle in the flow-field relative to the case of pure diffusion can be obtained from their difference \( \dot{I}(t) = -\dot{S}(t) - \dot{S}_D(t) \). Therefore, we find
\[
\dot{I}(t) = -\frac{1}{2} \nabla \cdot v - \frac{t}{6} \text{tr} (E^2 + [\Omega, E]) + O(t^2),
\]
which determines how the local properties of a flow-field—divergence, strain rate, and vorticity—affect the
information content of tracer particles in any given region. Note that the short time expansion is consistent with our earlier expansion of the velocity field in a local neighborhood. Characterizing information by comparing differences in entropy across regions has been done in other contexts \cite{30, 31}, including information content in gene expression levels \cite{32–34}.

Besides the information content of the distribution, it is also helpful to analyze the residence time of a tracer particle in a particular location before it is washed away by the flow-field. This can be characterized by the probability to observe the tracer particle in a region of $\sigma^d$ around the origin after time $t$, which can be defined as $P(\sigma, t) = \int d^d x \exp(-\frac{x^2}{2Dt})P(x, t)$. Using the solution (4), we find

$$P(\sigma, t) = \left(\frac{\sigma^2}{2D}\right)^{d/2} \exp\left(-\frac{1}{2\sigma^2} r_d(t)^T[M + \frac{\sigma^2}{2D} I]^{-1} r_d(t)\right) \frac{\det[M + \frac{\sigma^2}{2D} I]^{1/2}}{\det[M + \frac{\sigma^2}{2D} I]^{1/2}}.$$  

Performing a short time expansion and setting $\frac{\sigma^2}{2D} = \alpha > 0$ such that we can directly compare the behavior of the system to diffusion, we find $P(\sqrt{2Dt}, t) \approx \frac{1}{2\pi\tau} \exp\left(-\frac{1}{2} (\nabla \cdot v + \frac{\sigma^2}{2D}) t - \left(\frac{\sigma^2}{4D} + \frac{5}{36} \text{tr}(E^2)\right) t^2 + O(t^3)\right)$. Keeping only the lowest order term, we have

$$P(\sqrt{2Dt}, t) \approx \frac{1}{2^{d/2}} \exp\left(-\frac{t}{2\tau}\right),$$  

where

$$\tau^{-1} = \frac{1}{2} \left(\nabla \cdot v + \frac{\sigma^2}{2D}\right),$$  

which is controlled by the same residence time scale.

These expressions predict that a divergent field will play a role in the vicinity of the origin, i.e. $\sigma^2 \ll 2Dt$, then we obtain

$$P(\sigma \ll \sqrt{2Dt}, t) \approx \left(\frac{\sigma^2}{2Dt}\right)^{d/2} \exp\left(-\frac{t}{\tau}\right),$$  

where $\alpha > 0$. Hence, Eqs. (6) and (8) show that the probability for a secreting field becomes dispersed into the fluid and $P(\sqrt{2Dt}, t) \rightarrow 0$ (red line in Fig. 2b). Instead, for an absorbing field with $k < 0$, it saturates to a constant at long times as $M(t) \rightarrow \frac{\sigma^2}{2D} I$. Hence, the probability for this case approaches unity ($P(\sqrt{2Dt}, t) \rightarrow 1$) (blue line in Fig. 2b), which is a manifestation of the localization of the particle.

Using Eq. (8), we note that the change of information content has an initial value of $\dot{I}(0) = -\frac{1}{2} \nabla \cdot v$. This is positive for the absorbing field $k < 0$, which is more localized as compared to diffusion and hence more informative, and vice-versa for the secreting field (see Fig. 2c). At long times, $\frac{1}{3} \text{tr}(M^{-1})$ goes to 0 when $k < 0$ and to $|k|$ when $k > 0$. Hence, Eqs. (6) and (8) show that the absorbing field saturates to $I(t) = 0$, consistent with an effective steady-state distribution. However, the secreting field saturates to $\dot{I}(t) \rightarrow -k$, describing a probability distribution that spreads out at a faster rate than diffusion. Clearly, this is only physical within the length-scale in which the linear expansion remains valid, $l \sim \frac{|k|}{r_0}$, and within $t \sim 1 \ln \frac{1}{r_0}$ before boundary effects come into play.
The change of information content from Eq. (8) has no initial value since these fields are divergence-free. In the direction of the strain rate $\mathbf{E}$ field with pure vorticity $\mathbf{\Omega}$, we see oscillations with a period of $2\pi/c$ from the baseline value of diffusion (green). The probability distribution $P(x,y,t)$ is plotted at various time points within a period, showing oscillatory motion around the vortex center that decays due to diffusion. Fields with pure vorticity such as this one have no relative change in their information content as compared with diffusion. These plots again use $D = 0.1$, with $c = 1$ and $r_0 = (0.5, 0, 0)$.

The behavior of $\mathbf{M}(t)$ also depends on the antisymmetric term $\mathbf{\Omega}$ (Eq. (7)). We can examine the effect of vorticity, while retaining linear flow profiles and parameters similar to the previous examples (see Fig. 3a), by using the following flow-field

$$
\mathbf{v}(r) = \alpha [(z - z_0)\mathbf{\hat{e}}_x + (x - x_0)\mathbf{\hat{e}}_y + (y - y_0)\mathbf{\hat{e}}_z].
$$

(14)

Here we see that these fields show a shorter residence time compared to diffusion (see Fig. 3b). The cases with positive and negative values of $\alpha$ have very similar features, although there is a slightly faster drop-off depending on the direction of the strain rate $\mathbf{E}$.

The change of information content from Eq. (8) has no initial value since these fields are divergence-free. Instead, the leading term is linear and negative, $\dot{I}(t) \sim -\frac{\alpha^2}{2}t$, so these fields become increasingly delocalized with time as compared to diffusion (see Fig. 3c). At long times, this expression saturates in the same way to $-|\alpha|$ for both fields, since $\frac{1}{2} \text{tr} \left( \mathbf{M}^{-1} \right) = \alpha \frac{2 - \cosh(\alpha t)}{\sinh(\alpha t)}$, which is even with respect to $\alpha$ (the orange and purple plots in Fig. 3c lie on top of each other). Similarly to the previous case of a secreting field, $\dot{I}(t) < 0$ only makes sense within the time- and length-scale of validity for the linear expansion.

The analysis of $\mathbf{M}(t)$ in Eq. (5) shows us that for a field with pure vorticity $\mathbf{\Omega} \neq 0$ and no symmetric contribution $\mathbf{E} = 0$, $\mathbf{M}(t)$ will not depend on $\mathbf{\Omega}$. This can be inferred directly from the expansion of $\mathbf{M}(t)$ in Eq. (7), where only the commutator $[\mathbf{\Omega}, \mathbf{E}]$ appears and not $\mathbf{\Omega}$ on its own. Hence, when $[\mathbf{\Omega}, \mathbf{E}] = 0$, which is trivially true in the case of $\mathbf{E} = 0$, the $\mathbf{\Omega}$ terms cancel in the evaluation of $\mathbf{M}(t)$. To demonstrate this point, we study a flow-field with pure vorticity and $\mathbf{E} = 0$ (Fig. 4a):

$$
\mathbf{v}(r) = -c\mathbf{\hat{e}}_x \times (r - r_0).
$$

(15)

While $\mathbf{M}(t)$ no longer depends on $\mathbf{\Omega}$, we note that $r_d$ and hence the exponential term in the probability expression still depends on $\mathbf{\Omega}$, as can be seen from Eq. (3). In fact, vorticity $\mathbf{\Omega} \neq 0$ results in $e^{Kt}$ having complex roots and hence oscillations. We can see this in the plot of the probability in Fig. 4b. At the origin $(x,y) = (0,0,0)$ (the blue cross in Fig. 4a), the particle rotates around the vortex center and hence the probability in that region decreases before returning to the baseline set by diffusion after a full period $2\pi/c$ (the blue plot in Fig. 4b). The probability density around the vortex is plotted at various times within a period to show the oscillatory motion, which simultaneously decays due to diffusion (Fig. 4c). Note that the rate of change of information content here is 0, i.e. no different from that of a diffusive particle, since $\mathbf{M}(t)$ does not depend on $\mathbf{\Omega}$ and we have $\nabla \cdot \mathbf{v} = 0$ and $\mathbf{E} = 0$ (see Eqs. (6) and (8)).

We derive analytical expressions for the rate of change of information content that explicitly illustrate its out-of-equilibrium character. We find that the leading contribution in time stems from the field divergence, and that the rotational component only makes a subleading contribution. We use this to study the information content and particle transport for a stochastic particle in a flow-field.

As our formalism is applicable in the local neighborhood of a generic flow, it can be applied to various scenarios including more complex flow patterns (see Fig. S1). It can also be used for experimentally-measured flow-fields in each local neighborhood, and hence within complex geometries such as those in biological tissues. The rich transport behavior is further characterized through an expression for the particle residence time, through which we identify a mechanism to retain a particle for longer times compared to diffusion. Intriguingly, vorticity only contributes to the change of information content when there is an additional symmetric field component, but produces oscillations in the probability density.

This work opens many new directions as our analysis can be extended to include the presence of different chemical species and gradients, or non-conserved particle densities. It would also be of great interest to probe how information can create feedback loops or time-dependent control of the flow field, as well as the possibility of learning from the available information. Overall, such work will inform the transmission of information in diverse scenarios, that are relevant for a range of vital chemical and mechanical processes.

We thank Babak Nasouri and Andrej Vifar for helpful discussions.
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