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Entropy, complexity, and causality in direct and approximated fluid simulations

Curtis J. Saxton[1,2], Ajay Chandrarajan Jayalekshmi[2], Anna Guseva[1], Ben F. McMillan[2], Steven M. Tobias[1]

(1) Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, UK
(2) Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Information entropy measures the disorder or inherent difficulty of predicting spatial and temporal structures in a time-series or spatially in a high-dimensional dynamical system. Statistical complexity characterises departures from equilibrium distributions (even given a fixed entropy), and can distinguish deterministic from stochastic physics (chaos vs noise). Related measures of causality quantify the relative influence of time-irreversible and -reversible processes (or directionality spatially). Calculating these scores from direct numerical simulations can characterise the importance of coherent structures or turbulent transitions. It is also interesting to compare the scores for physically equivalent models calculated via approximate methods (e.g. generalised quasilinear models or data-driven codes). The entropic cost of any approximation scheme is objectively derivable. We consider diverse applications to (e.g.) fluid thermal convection, magneto-rotational turbulence, and gyrokinetic plasma turbulence.

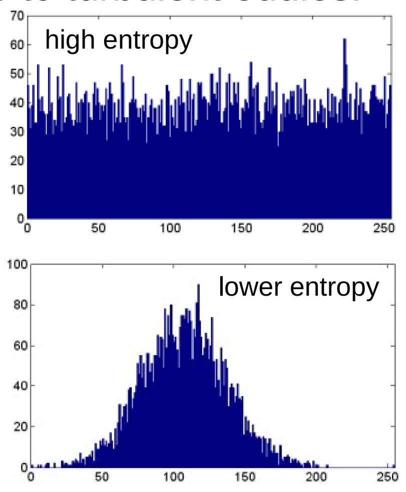
Information entropy = H

- Evolving systems show a distribution of **power in modes** or **probabilities of states**, described by **PDF**. Any conceivable system: from rolling dice to turbulent eddies.
- Given a PDF of states, how many **binary questions** do we need to identify the **present** state, in the **"game of twenty questions"**? $-\log_2(p_i)$
- **Information entropy** is the mean:
- A **uniform** PDF gives max entropy.

$$S = -\sum_i p_i \log_2(p_i)$$

$$H \equiv S/S_{\max}$$

$$S_{\max} = \log_2 N$$



Vazquez-Fernandez+ (2010)

- **FLAW:** H doesn't change if we shuffle the histogram bins. This "entropy" definition is blind to "**order**."

(e.g. Shannon 1949; Powell & Percival 1979; Xi & Gunton 1995; Miranda+ 2015)

Statistical complexity = C

- Measure **divergence** of PDF (P) from equilibrium (U).

$$J(P,U) = S\left(\frac{P+U}{2}\right) - \frac{S(P)}{2} - \frac{S(U)}{2}$$

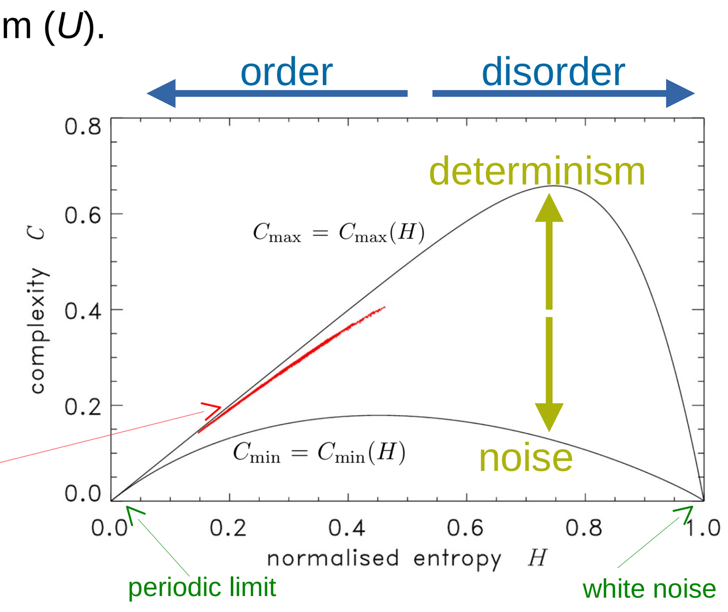
- Normalise disequilibrium: $Q = J / J_{\max}$
- **Complexity** = disequilibrium × unpredictability

$$C \equiv QH$$

(Martin+ 2006)

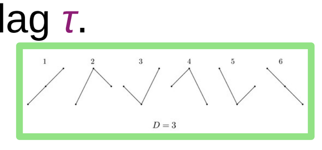
 - High $C \Rightarrow$ deterministic / fractals / **chaos**;
 - Low $C \Rightarrow$ stochastic / simple / **noise**.

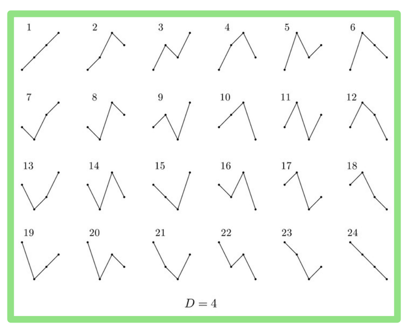
e.g. scatter-plot from gyrokinetic simulations of ion temperature gradient (ITG) driven turbulence



Ordinal statistics

- Given a long **time series** (or spatial pattern),
$$y = \{y_0, y_1, \ldots, y_{N-1}\}$$
- Select short **subseries** s_n of size D and lag τ.
$$s_n = \{y_n, y_{n+\tau}, \ldots, y_{n+(D-1)\tau}\}$$
- What is the **rank order** of elements?
$$\pi_n = \mathrm{sort}(s_n)$$
- Count PDF(π_n) of **pattern** frequencies.
- Find **ordinal entropy** and **complexity**.
- Results encode **order** but not **power**!
- **FLAW:** free scales D,τ ∴ not universal.

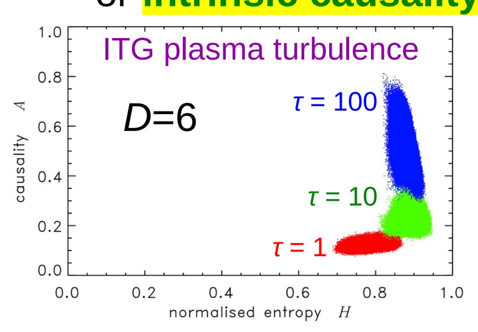




(see: Bandt & Pompe 2002; Zunino+ 2017)

Intrinsic causality = A

- Each pattern π has a **reversed** partner π'.
- Is one direction more frequent than the other? ⇒ **irreversibility** or **time asymmetry** or **intrinsic causality**.



Statistical divergence of **actual** PDF from **expected** distribution W is….
(Kullback & Leibler 1951)

$$\mathscr{D}(P,W) \equiv \sum_i p_i \log_2(p_i/w_i)$$

Hypothesis: time-reversible PDFs

$$M = (P + P')/2$$

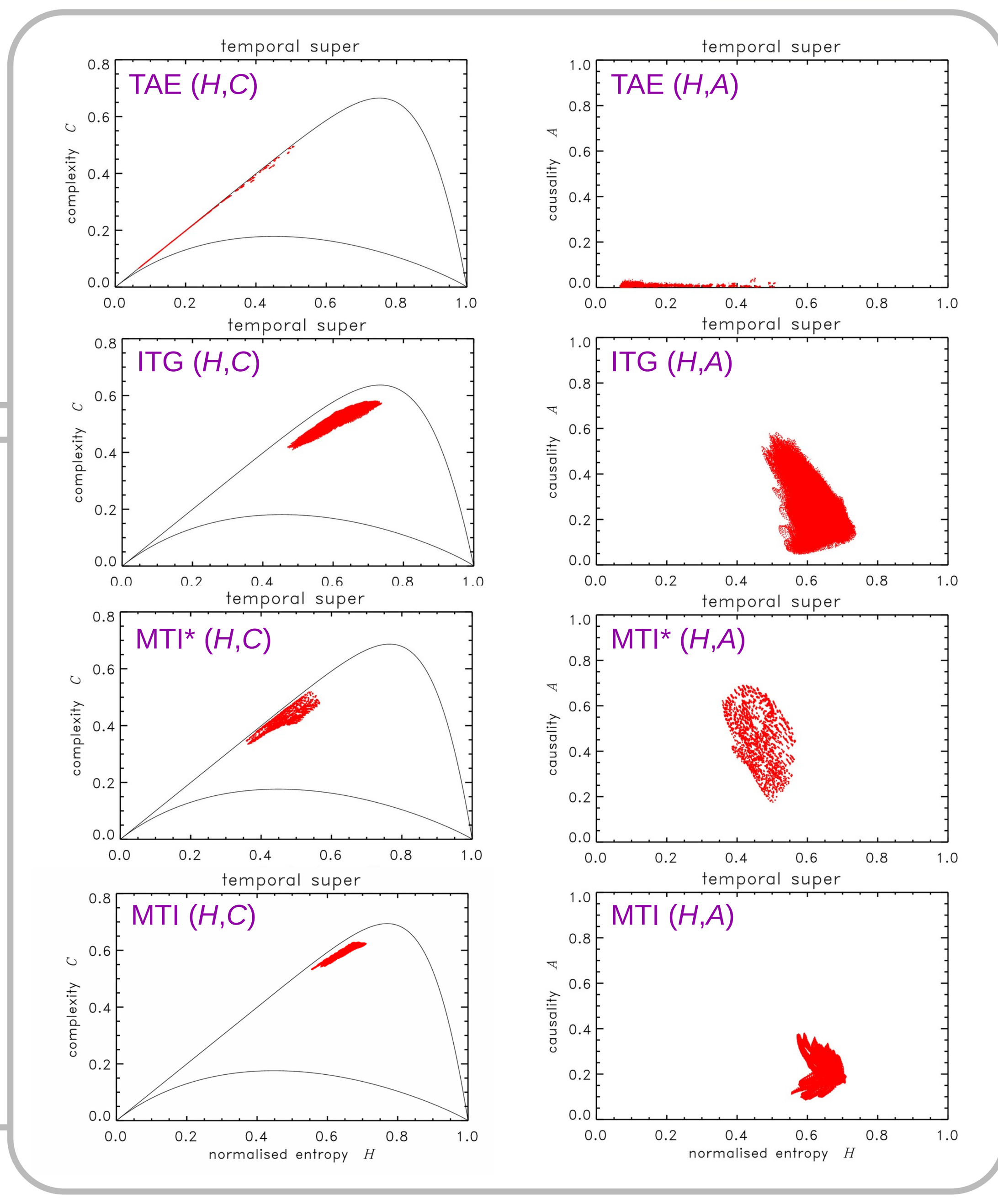
irreversibility / causality measure:

$$A = \frac{1}{2}\mathscr{D}(P,M) + \frac{1}{2}\mathscr{D}(P',M)$$

e.g. Martinez+ (2018, 2023)

Fourier × ordinal statistics? ✓

- Obtain the Fourier **power** a_i at frequencies f_i
- Reample time-series at intervals ~$1/f_i$ again separately for each i.
- Count **pattern** frequencies π_i and normalise by total power a_i.
- 2-parameter PDF(f_i,π_i) gives a more universal **super (H, C, A)**



Gyrokinetic turbulence

Magnetically contained plasma in a **tokamak** fusion reactor has low collisionality but particles gyrate tightly around magnetic field lines, reducing a 6D (***x***,***v***) phase-space problem to 5D. Fluctuating phase-space densities and electromagnetic fields mediate various forms of **turbulence**. We illustrate entropic properties of the || magnetic potential, in **GENE gyrokinetic** simulations. The box domain surrounds a local **flux tube**, with periodic boundaries including "twist-and-shift" coordinates. Each red dot in the scatter-plots is calculated from the evolution at one spatial point. Entropic characterisation might (perhaps) help interpret phenomena in real machines where **diagnostic** measurements are sparse and indirect.

- **TAE** = "toroidal Alfven eigenmodes" are periodic patterns analogous to fluid acoustic modes. At any point (x,y,z) the temporal variability is highly deterministic ($C≈H$) and time-reversible ($A≈0$).
- **ITG** = "ion temperature gradient" driven turbulence. Temporal entropy and complexity are high in the chaotic range, but variability is time-irreversible up to A≈0.6.
- **MTI*** = "microtearing instability", where some magnetic flux surfaces connect to their own tails, affecting current distributions, driving turbulence. This simulation (denoted *) develops **bursts** of heat transport between lulls. Overall entropy is moderate, complexity is high, and causality A is high.
- **MTI** = MTI again but without bursting; steadier turbulence. The (H,C) are higher, but causality A is lower.

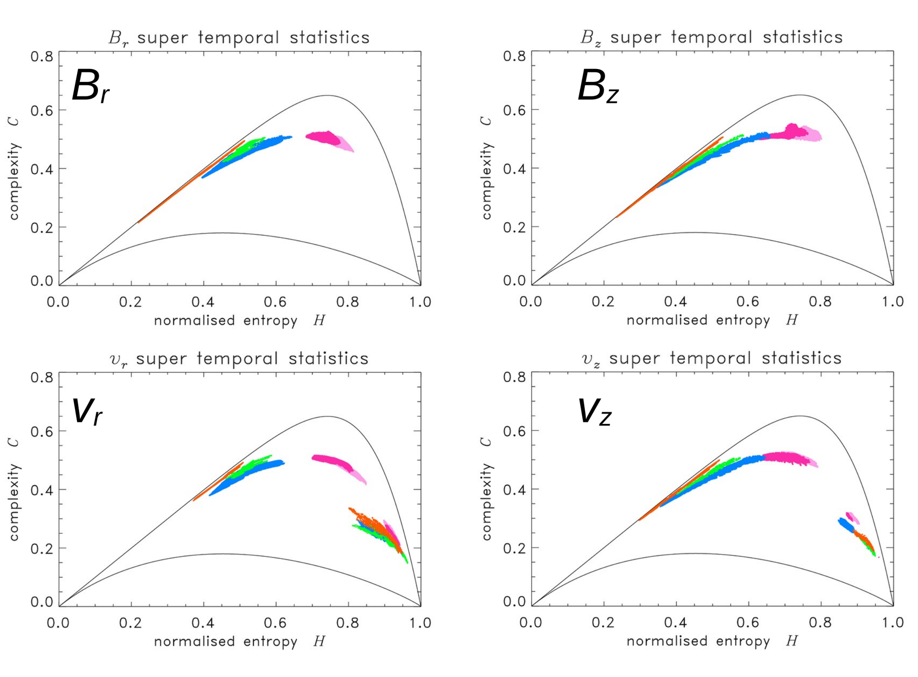
(see: Beer+ 1995; Goerler 2009; Ajay C.J. 2023; further simulations in progress ….)

Magnetorotational instability

art: © Mark A. Garlick

- Astrophysical **accretion discs** need effective viscosity to shed angular momentum and feed radial **mass inflow**.
- **MRI = magnetorotational instability:** orbital velocity shear winds up ***B***, while magnetic torques drive turbulence, enabling viscous inflow. (Velikhov 1959; Balbus & Hawley 1991)
- MRI can occur in **magnetic Taylor-Couette** experiments with conductive fluid sheared between differentially **rotating cylinders**, $r_i < r < r_o$ (e.g. Hollerbach & Rüdiger 2005; Hung+ 2019)
- Simulations find various oscillatory states and spatial modal structures near the onset of chaos. We reanalyse five cases for entropy/complexity (Guseva+2017; Guseva & Tobias 2023).
- Fix $\mathcal{R}e$=250; vary field strength $\mathcal{H}a \equiv B_0\,(r_o-r_i)\,/\,(\sigma/\rho\nu)^{1/2}$ → regimes of torque fluctuations:

$\mathcal{H}a$=100 very chaotic → $\mathcal{H}a$=120 chaotic
→ $\mathcal{H}a$=140 two periods → $\mathcal{H}a$=145 one period
→ $\mathcal{H}a$=149 standing wave

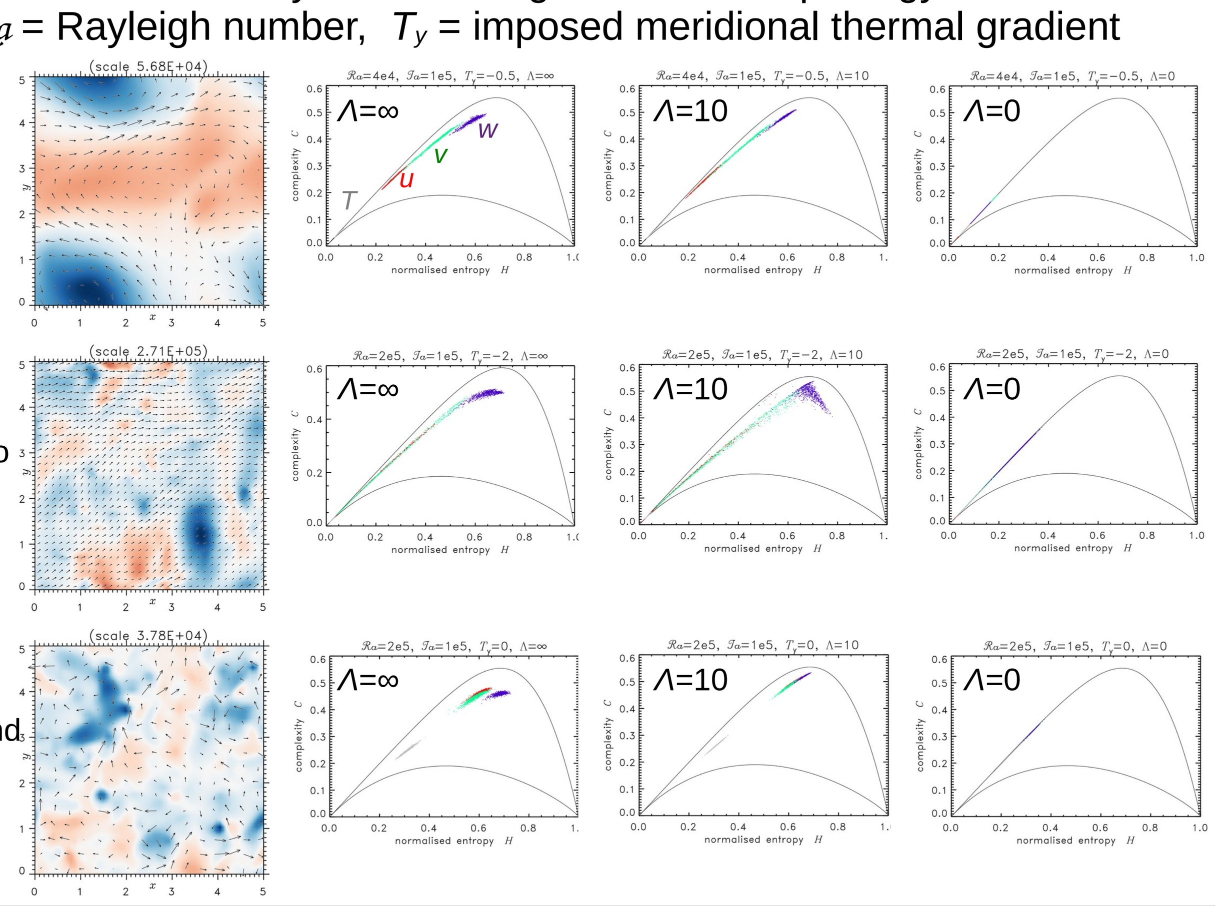


- **Spatially** $0.2 \lesssim H \lesssim 0.4$ for chaotic cases; $0.1 \lesssim H \lesssim 0.2$ for periodic cases. All deterministic, $C \gtrsim 0.98H$.
- **Temporal** (H,C,A) of ***B*** and ***v*** :
 - States occur at distinct (H,C).
 - Chaos is impure with **noise**.
 - B_θ, v_θ are trivial, $C≈H≈0.4$.
 - v_r, v_z are **bimodal** due to high-H, low-C, low-A boundary patches.
 - **Causality** is *weaker* in chaos; *stronger* for periodic cases. For B_z field, $A \lesssim 0.04$, 0.04, 0.25, 0.53, 0.52.

Rotating thermal convection

- **Rayleigh–Bénard convection** between hot and cold surfaces, in a periodic box subject to 45° global **rotation**, like a local section of atmosphere. (Hathaway & Somerville 1986; Currie 2014)
- **GQL** = **generalised quasilinear approximation** divides (k_x,k_y) space into "low" and "high" modes (background vs fluctuations), at a wavenumber cutoff Λ. (Saxton+ 2023)
- **Fourier spatial** (H,C) measure visually subtle changes to flow morphology at different Λ. input parameters: $\mathcal{R}a$ = Rayleigh number, T_y = imposed meridional thermal gradient

- **($\mathcal{R}a$,T_y)=(4x10⁴,-0.5) forms a giant vortex.** Distributions of u,v,w,T straighten and rise in C, for Λ=10. Λ=0 locks everything onto $C_{\max}$ curve at low H (quasiperiodic).
- **($\mathcal{R}a$,T_y)=(2x10⁵,-2) bursting cyclic winds.** Λ=10 raises H and cuts C to an edge in u,v,w,T distributions. Λ=0 locks everything to spatial QPO.
- **($\mathcal{R}a$,T_y)=(2x10⁵,0) turbulence uniform in *x*,*y*** Λ=10 flattens C variation and brings u,v,w together. Λ=0 locks everything to spatial QPO.



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