

Convective heat transfer patterns in plane-layer Rayleigh-Bénard convection revealed by transient almost-invariant sets

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Horizontally extended plane-layer convection flows are characterized by characteristic patterns of turbulent heat transfer due to the convective fluid motion consisting of a nearly regular ridge network where hot fluid rises and cold fluid sinks. Here, we analyze this transport behavior by the so-called inflated generator framework, which identifies quasistationary families of almost-invariant sets, derived from leading inflated generator eigenvectors. We demonstrate the effectiveness of this data-driven analysis framework in three-dimensional turbulent flow, by extracting transient characteristic heat transfer patterns as families of almost-invariant sets subject to a gradual evolution, which contribute least to the convective heat transfer.

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I. INTRODUCTION

Turbulent convection phenomena are ubiquitous starting with heat and momentum transfer processes in stellar interiors [1] via vortex formation in planetary atmospheres to magnetic field generation by dynamo action in planetary cores [2] and heat exchanger and cooling devices in technology [3]. In the simplest setting buoyancy forces drive fluid motion, caused by the temperature dependence of the fluid density, in a planar fluid layer of height H that is uniformly heated from below ($z = 0$) and uniformly cooled from above ($z = H$) [4,5]. This is the fundamental Rayleigh-Bénard convection (RBC) case [6,7] in which the mass density is a linear function of the temperature deviation from a reference equilibrium state, the working fluid is incompressible, and the material parameters, such as thermal conductivity and kinematic viscosity, are constant across the fluid volume. For imposed temperature differences between top and bottom, which significantly exceed a critical threshold value, a (turbulent) fluid motion is initialized. Heat is transferred then by diffusion and dominantly by advection. This thermal driving is quantified by the dimensionless Rayleigh number Ra [4,5].

One central question in turbulent convection is the exact amount of heat that is transferred on average from the bottom to the top as a function of the imposed outer temperature difference (i.e., on Ra) and the material properties of the working fluid in the plane layer [7–9]. Depending on the horizontal extension (in x and y directions) of the fluid layer, this turbulent transport proceeds frequently in the form of regular and gradually evolving horizontal fluid flow patterns at scales that exceed the thickness H of the layer. These

patterns set a large-scale order, which exists despite the fact that the convection flow is fully turbulent on smaller scales; they are termed *turbulent superstructures* of convection [10–12]. Recently, it has been shown that these structures are rooted in a hierarchical (i.e., successively coarser) network of thermal plumes with increasing distance from the wall. These plumes are linearly unstable fragments of the thermal boundary layer that detach from the walls and rise into the bulk. This implies that turbulent superstructures are formed in a bottom-up process, starting with the smallest building blocks—the thermal plumes—from the walls [13]. In addition, it is found that the characteristic “mesh width” of this plume network follows a self-similar scaling with Rayleigh number, which scales with the Rayleigh number as $\sim Ra^{-1/3}$.

The large-scale patterns of plane-layer convection depend on the thermal boundary conditions [14]. For prescribed temperature at the top and bottom, the Dirichlet boundary condition case (which will be considered here), we observe a collection of circulation rolls with cross-roll modulations that fill the layer vertically from bottom to top. They exist as a single entity in closed cylindrical convection cells with aspect ratio near 1 and are termed here large-scale circulation [8,9,15].

In terms of the material transport in the turbulent fluid, i.e., from the perspective of the Lagrangian frame of reference, these convection cells can be considered as coherent sets [16]—regions that largely trap Lagrangian tracer particles for a transient period of time in their cores and thus essentially reduce the mixing and heat transfer from bottom to top in the convection case. This concept has been discussed in several other material transport problems in the atmosphere and ocean [16–19]. The complementary perspective is to detect and study the manifolds between the nearly coherent sets, which can serve as barriers to material transport [20–22]. Both frameworks stem from dynamical systems theory. Coherent sets were investigated in RBC in different ways, e.g., by various implementations of the dynamic Laplacian or dynamic clustering [23–27], their long-term behavior was described

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by a Markov model [28], the arising advective and diffusive transport barriers were analyzed [29], and so-called collective variables were calculated to model transitions between large-scale states [30].

Despite turbulent convection flows being time-dependent, turbulent superstructures slowly form and only gradually change before fading away. While they exist, they are therefore almost-invariant sets [31]; i.e., they stay approximately fixed in space and only slowly leak fluid. Both coherent sets and almost-invariant sets trap fluid for times much longer than local characteristic mixing times. The key difference is that coherent sets may move rapidly in space (carrying fluid within them), while almost-invariant sets remain fixed in space while they exist. Due to the quasistationary-in-space property of the turbulent superstructures, we analyze the convective heat transfer (CHT) in a turbulent plane-layer RBC flow using almost-invariant sets rather than coherent sets. Such an approach will filter out coherent sets that are not associated with the turbulent superstructures and better target the superstructures. In contrast to standard almost-invariant set analysis, which can only detect almost-invariant sets that possess the almost-invariance property throughout the flow duration, here we study the flow over long duration in which we expect the birth and death of many superstructures. We seek quasistationary families of almost-invariant sets, namely, time-dependent fluid parcels that may appear, slowly evolve in a quasistationary-in-space manner, and ultimately disappear. Each such family represents a convection cell, as discussed above. We go beyond prior work by tracking the onset and decay of the convection cells and filtering out possibly spurious coherent sets that move rapidly in the fluid.

We employ a recent data-driven framework [32], built around the (time-varying) infinitesimal generators G_t , which generate the Perron-Frobenius or transfer operators, the operators that describe the evolution of the distribution of a (probability) measure in the phase space of a dynamical system for a positive time. We “inflate” (time-extend) the individual generators G_t from the spatial into the spatiotemporal domain of the time-dependent RBC flow in the plane layer to create an inflated generator $\mathcal{G}$. Through this special time extension, we are able to capture the almost-invariant character of the transport patterns, as well as their appearance, time evolution, and disappearance.

An eigenvector analysis of $\mathcal{G}$, which builds on the sparse eigenbasis approximation (SEBA) [33] technique, is subsequently used to identify quasistationary families of almost-invariant sets. Our analysis can extract the gradually evolving patterns in the bulk of the horizontally extended plane-layer turbulent convection flow; they can be successfully compared with the time-windowed Eulerian fields of the convective heat transfer, which correlates velocity and temperature and thus form the important transport pattern in the RBC flow [34]. We note that velocity data are used in the present framework to reproduce correlations between velocity and temperature. We thus provide a proof of concept to apply the framework from dynamical systems theory to reveal the spatiotemporal organization of convective heat transfer in horizontally extended plane-layer configurations, which are termed mesoscale convection flows [12], from reduced

information. The analysis will also allow one to analyze the correlation of the SEBA fields with u_z .

The outline of the manuscript is as follows. Section II introduces the convection flow with its parameters. Here, we also detail the convective heat transfer, the coupled field of velocity and temperature, which characterizes the turbulent heat transfer due to fluid motion. Section III summarizes the analysis methods for almost-invariant sets. Afterwards, in Sec. IV, we present the results of our data analysis before the final conclusions are drawn in Sec. V.

II. RAYLEIGH-BÉNARD CONVECTION MODEL

A. Boussinesq equations and parameters

The data for the analysis are generated by direct numerical simulations (DNS). To this end, we solve the three-dimensional Navier-Stokes equations in the Boussinesq approximation numerically. This couples velocity $\mathbf{u}(\mathbf{x}, t) = (u_x, u_y, u_z)$ and temperature $T(\mathbf{x}, t)$ fields with $\mathbf{x} = (x, y, z)$ [5,7]. The nondimensional form of the governing equations is given by

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + T \hat{\mathbf{z}} + \sqrt{\frac{\text{Pr}}{\text{Ra}}} \nabla^2 \mathbf{u}, \quad (1)$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \frac{1}{\sqrt{\text{PrRa}}} \nabla^2 T, \quad (2)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (3)$$

The equations are solved by the spectral element method (SEM) using the graphics processing unit (GPU)-accelerated SEM solver, nekRS [35]. The computational domain is a cuboidal cell of $\Gamma = L/H = 8$ with periodic boundary conditions along the horizontal directions, where L is the horizontal extension and H is the height. The horizontal coordinates are $x, y \in [-4, 4]$. The top and bottom walls are found at $z = 0$ and 1. The simulation domain is the volume $V = L^2 H$.

We set no-slip condition on the velocity field and prescribe uniform temperatures $T_{\text{top}} = 0$ and $T_{\text{bot}} = 1$, respectively. The two dimensionless parameters that characterize the convection flows (in addition to the aspect ratio Γ) are the Rayleigh number Ra and the Prandtl number Pr , which are given by

$$\text{Ra} = \frac{g \alpha \delta T H^3}{\nu \kappa} \quad \text{and} \quad \text{Pr} = \frac{\nu}{\kappa}, \quad (4)$$

where g is the acceleration due to gravity, $\delta T = T_{\text{bot}} - T_{\text{top}} > 0$ is the temperature difference between the hot and cold plates, α is the thermal expansion coefficient, κ is the thermal diffusivity, and ν is the kinematic viscosity. The present study uses one dataset at $\text{Ra} = 10^5$ and $\text{Pr} = 0.7$. The characteristic length, velocity, and temperature scales used to obtain the nondimensionalized Eqs. (1)–(3) are H , $U_f = \sqrt{g \alpha \delta T H}$, and δT , respectively, where U_f is the free-fall velocity of the thermal plumes.

We follow the same workflow as in Samuel *et al.* [36]. Consequently, we ensure that the meshes are fine enough to resolve the boundary layers. The simulations are initialized with the diffusive equilibrium state of RBC for which the fluid is at rest and the temperature drops linearly from the bottom to the top. This equilibrium state is infinitesimally perturbed and develops into a turbulent convection flow for a transient

period. The turbulent state is statistically stationary; i.e., statistical moments and correlations are time-independent. Time averages, indicated by $\langle \cdot \rangle_t$, are taken in the following always as an arithmetic average over a sequence of statistically independent snapshot realizations of the turbulent fluid flow. We obtain such series of realizations from one long trajectory (in other words, a single very long DNS run). The time interval between the snapshots is one free-fall time T_f (which will be defined further below), sufficiently large such that the small-scale temporal correlations of the temperature and velocity fields have decayed. These time averages are combined with averages over the horizontal cross section plane $A = L^2$ or the simulation domain $V = AH$ and denoted by $\langle \cdot \rangle_{A,t}$ and $\langle \cdot \rangle_{V,t}$, respectively. Error bars are then standard deviation from this statistical analysis.

We determined Nusselt number, Nu , and Reynolds number, Re , which are the global measures of heat and momentum transport, respectively. To this end, we compute Nu from the nondimensionalized temperature gradient at the bottom wall, whereas Re is calculated from the volume-averaged root mean square (rms) velocity [see also Eq. (4)]

$$Nu = -\frac{\partial \langle T \rangle_{A,t}}{\partial z} \Big|_{z=0}, \quad Re = U_{rms} \sqrt{\frac{Ra}{Pr}}. \quad (5)$$

The dimensionless root mean square velocity U_{rms} in Eq. (5) is computed for the volume V , $U_{rms} = \langle |\mathbf{u}|^2 \rangle_{V,t}^{1/2}$. Recall that velocities are given in units of U_f .

To solve the system of Eqs. (1)–(3) using SEM, we discretize the domain into $N_e = 300 \times 300 \times 64$ elements. Each element is further discretized into Gauss-Lobatto-Legendre nodes from fifth-order ($p = 5$) Legendre polynomials along each direction, yielding a total of $N_e \times p^3 = 720$ million collocation points.

Each snapshot generated from DNS contains velocity, pressure, and temperature data at all collocation points. We obtained 150 such snapshots within steady state, separated by unit T_f , where $T_f = H/U_f$ is the free-fall time used to nondimensionalize time, covering a total of $150 T_f$ (resulting in 3.6 TB of data). The free-fall time T_f is a characteristic time that estimates how long cold dense fluid falls across a distance H under the action of buoyancy forces. To ensure a statistically steady state, data were sampled after an initial period of $2000 T_f$. Note that although the DNS is performed at sufficiently high spectral resolution—necessary to accurately calculate the temporal evolution of the velocity and temperature fields—the datasets are subsequently downsampled for the detection of the quasistationary almost-invariant sets.

Averaging over a sequence of statistically independent snapshots in the statistically stationary regime, we obtain the Nusselt number from our DNS to be $Nu = 4.264 \pm 0.058$, and the Reynolds number is $Re = 92.66 \pm 1.03$. These values are consistent with those obtained by Samuel *et al.* [36]. The slightly reduced value of Re is also consistent with the observations made for larger aspect ratios as shown for $Ra = 10^9$ in the same work.

B. Convective heat transfer field

While the global heat transport is quantified in nondimensional units using the Nusselt number, a local measure can be

obtained the CHT field, which is given by

$$H_c(\mathbf{x}, t) = u_z(\mathbf{x}, t)\theta(\mathbf{x}, t), \quad (6)$$

where $u_z(\mathbf{x}, t)$ is the component of the velocity field along the vertical z direction, and

$$\theta(\mathbf{x}, t) = T(\mathbf{x}, t) - \langle T \rangle_{A,t}(z) \quad (7)$$

the temperature fluctuation, obtained after subtracting the mean temperature profile $\langle T \rangle_{A,t}(z)$. Here, $\langle \cdot \rangle_{A,t}$ is a combined average over the horizontal cross section $A = L^2$ and time t . Using Eq. (6), it is possible to calculate the Nusselt number in an alternative way to Eq. (5), which is given by

$$Nu = 1 + \sqrt{RaPr} \langle H_c(\mathbf{x}, t) \rangle_{V,t}. \quad (8)$$

Computing Nu using this formula, we get $Nu = 4.264 \pm 0.086$, which is in excellent agreement with the former value of Nu computed from near-wall temperature gradient (5). This underlines that the numerical simulations are well-resolved, both in the bulk of the layer and the near-wall regions.

We obtain a sequence of 102 three-dimensional data snapshots of the velocity and temperature fields of RBC flow for times $2001T_f < t < 2103T_f$ with a time interval of $1 T_f$ between successive snapshots. The field data are subsequently interpolated spectrally to a coarser three-dimensional grid with uniform mesh size ℓ in all three space directions (see also Sec. III C). The coarse grid will be used for the data analysis. Note that the original fields are much more finely resolved with a vertically nonuniform spectral element grid, in particular close to the bottom and top walls.

Figure 1 shows two-dimensional slice cuts through the temperature fluctuation field $\theta(\mathbf{x}, t_0)$ in panels (a) and (d), the vertical velocity field $u_z(\mathbf{x}, t_0)$ in panels (b) and (e), and the CHT field $H_c(\mathbf{x}, t_0)$ in panels (c) and (f) at $t_0 = 2052T_f$, which is the snapshot in the middle of the sequence. In the top row of the figure, horizontal cross sections at the midplane at $z = 1/2$ are shown. In the three subsequent rows, we show the corresponding vertical cuts through the volume V at $y = 0$. While the horizontal cuts display the spatial organization of the convection patterns by means of three fields viewed from the top, the vertical cut highlights the thermal plume structures of the convection flow across the layer, which carry the heat from bottom to top.

The horizontal organization into turbulent superstructure patterns, which we observe here in panels (a)–(c) of Fig. 1, remains intact for higher Rayleigh numbers and different Prandtl numbers than discussed here (see, e.g., Refs. [10–12]). With increasing Ra and thus with increasing vigor of the convective turbulence, an ever finer network of linelike thermal plumes forms. These plumes are the structures which protrude vertically from both top and bottom walls, visible in the vertical cross-section plots, such as panel (d) of Fig. 1. As mentioned in Sec. I, the plume network becomes coarser with increasing distance from the wall. This results in prominent plume clusters, which are the superstructures in the bulk of the layer. This process sustains the superstructure pattern, also for higher Rayleigh numbers; in Refs. [13,37], we showed its presence up to $Ra = 10^{11}$.

The characteristic size of cells that form the superstructure pattern depends on the Prandtl number [10]. This dependence

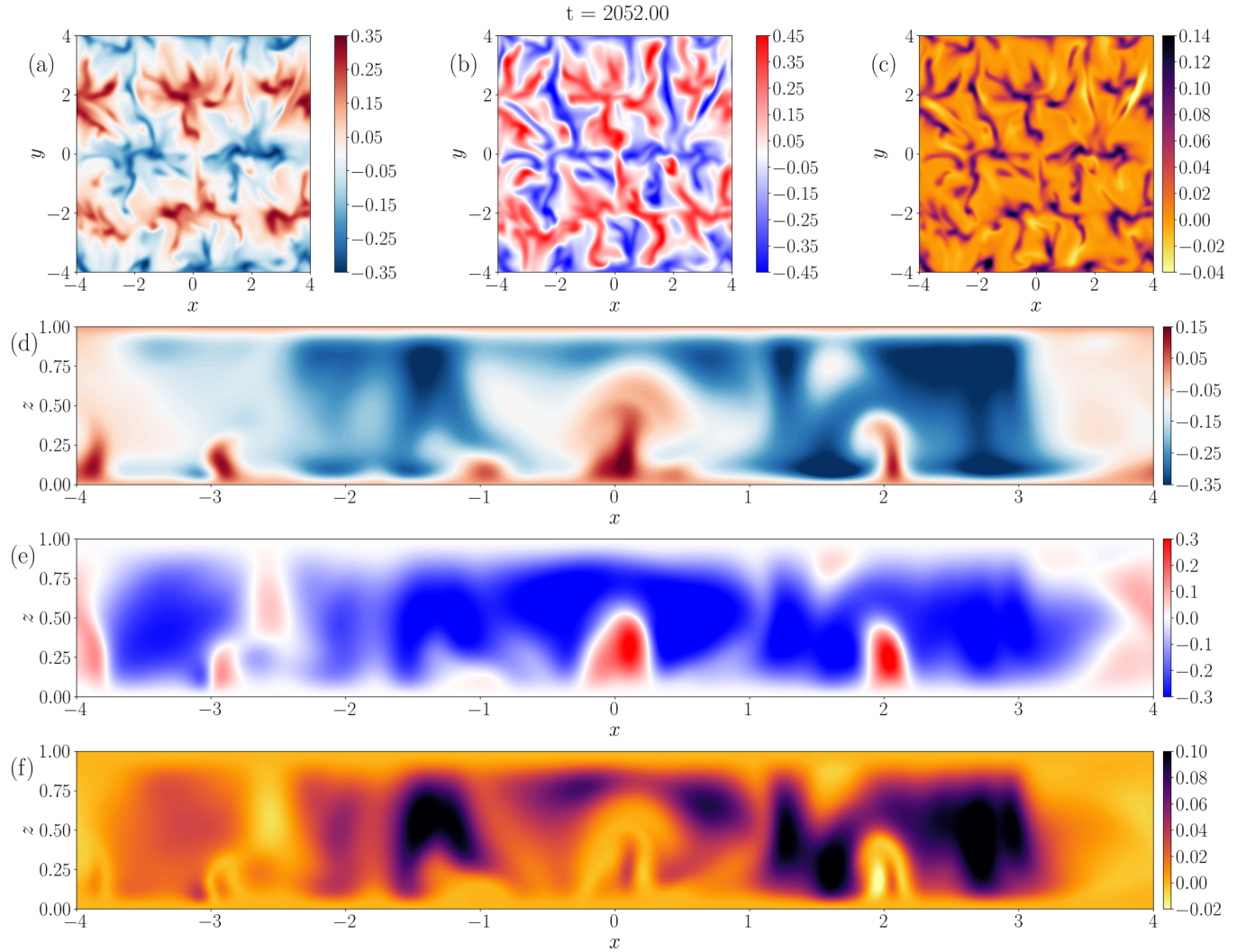


FIG. 1. Snapshots of the temperature fluctuation θ , in panels (a) and (d), the vertical velocity u_z in panels (b) and (e), and convective heat transfer field in panels (c) and (f) for the time instant at $t = 2052 T_f$. The top row displays horizontal cuts at $z = 1/2$, and the three bottom rows vertical cuts at $y = 0$.

is not yet fully understood. However, it is connected to the stem width of the thermal plumes, which are unstable detached fragments of the thermal boundary layer. The boundary layers have a Pr-dependent width that is well documented by scaling theories and simulations [7,9]. In a nutshell, the lower Pr at fixed Ra, the thicker the thermal boundary layer width.

It is seen in Figs. 1(c) and 1(f) that CHT is locally maximal where hot fluid rises and cold fluid sinks to the bottom; in both cases locally $H_c > 0$. Note, that in both cases, heat is carried from the bottom to the top. For the vertical cut at $y = 0$, this is dominantly done by cold fluid falling down as seen by relating panels (d) and (e) with panel (f) of Fig. 1. These fields fluctuate strongly with respect to space and time. We thus smooth the snapshot data by a sliding time average over a time window $[t_k - m, t_k + m]$ of length $\tau = (2m + 1) T_f$ for the upcoming analysis. We will take $m = 2$ and thus a time window of length $5 T_f$. This filtering with respect to time, which will be denoted by $\langle \cdot \rangle_\tau$, highlights the large-scale and gradually evolving convection cells better, which we aim to analyze with the present framework.

Figure 2 provides a three-dimensional view of the fields θ (left) and u_z (right) for the same snapshot as in Fig. 1. Although the structures appear like isosurfaces, they are isovolumes defined by narrow ranges in their corresponding fields. As a result, blue isovolumes in panel (a) denoting negative values of temperature fluctuations are defined by a band of θ corresponding to the interval $[-0.23, -0.22]$. Similarly, the red isovolumes in panel (a) are defined by $\theta \in [0.22, 0.23]$. Correspondingly in panel (b), the low and high values of the vertical velocity u_z are defined by the ranges $[-0.25, -0.24]$ (blue isovolumes) and $[0.24, 0.25]$ (red isovolumes), respectively. We note that the upwelling hot fluid and downwelling cold fluid are equally distributed within the flow domain.

While the short-time fluctuations of the fields are smoothed by the sliding average, mean transport properties of the flow remain unaffected by this procedure. To demonstrate this, we choose a single snapshot at a time t_0 and calculate the mean vertical CHT profile $\langle H_c(t_0) \rangle_A(z)$. This is compared in Fig. 3 with the mean profiles that are obtained from an average that combines the time window-average centered about t_0 and plane average of CHT fields, $\langle H_c \rangle_{A,\tau}(z)$. We see that the

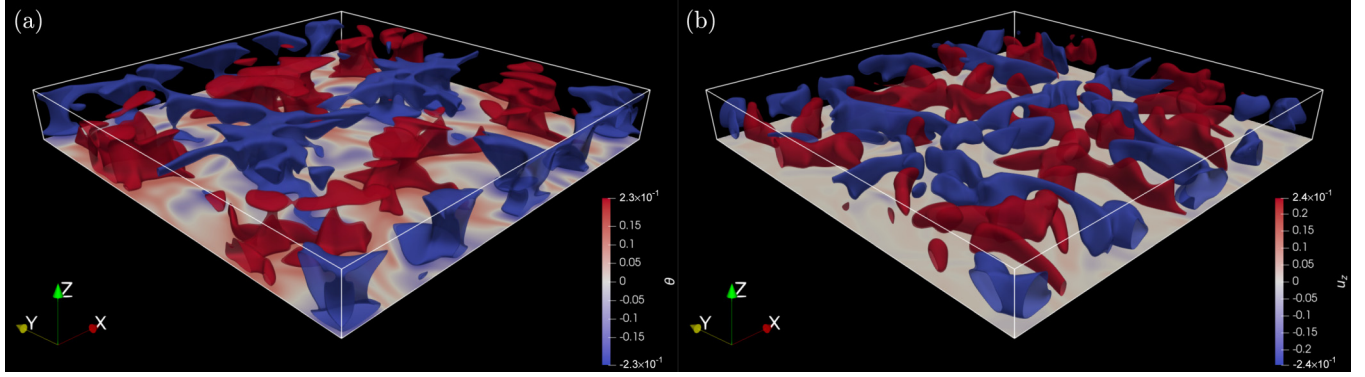


FIG. 2. Three-dimensional structure of (a) θ and (b) u_z at $t = 2052T_f$, corresponding to the snapshots shown in Fig. 1. The faint contours near the bottom walls are at $z = 0.005$. The red regions in panel (a) correspond to $\theta \in [0.22, 0.23]$, and those in panel (b) correspond to $u_z \in [0.24, 0.25]$. The blue regions correspond to $\theta \in [-0.23, -0.22]$ and $u_z \in [-0.25, -0.24]$, respectively.

vertical mean profiles overlap for time windows of different lengths τ , which are indicated in the legend. All CHT profiles are $H_c = 0$ at the walls, which is caused by the no-slip boundary condition at the walls, $z = 0, 1$, which states that $u_x = u_y = u_z = 0$. The averaged CHT profiles become maximal in the center or bulk of the convection layer, as seen in Fig. 3.

III. ANALYSIS METHOD FOR QUASISTATIONARY FAMILIES OF ALMOST-INVARIANT SETS

As discussed in the introduction, we aim to characterize the three-dimensional fluid motion using the concept of quasistationary families of almost-invariant sets [32]. In our RBC flow setting, a single family is a time-parameterized family of subsets of the cuboidal cell domain. For our turbulent RBC flow, we expect many such families to be present simultaneously, although each individual family may not exist throughout the full time duration we consider from $2001T_f$ to $2103T_f$. The *almost-invariant* aspect of these time-parameterized families

means that for a given family at any given time instant t the instantaneous rate of fluid loss from the family element at time t is very low. The *quasistationary* aspect relates to the families being approximately fixed in the spatial domain through time, and also allows for families to emerge and disappear. These families are the manifestation of the slow dynamics of the large-scale turbulent superstructure patterns; the spatial complement of the families will be responsible for the major fraction of the CHT across the plane layer.

We use the approach of Ref. [32] to construct multiple quasistationary families of almost-invariant sets. This approach rests on a spectral analysis of generators for stochastic drift-diffusion equations, where the drift is given by $\mathbf{u}(t, \mathbf{x})$:

$$d\mathbf{x}_s = \mathbf{u}(t, \mathbf{x}) ds + \epsilon d\mathbf{w}_s, \quad (9)$$

where $\{\mathbf{w}_s\}$ is Brownian motion and $\epsilon > 0$ is small.

A. Almost-invariant sets and generators of steady flows

This section provides background on identifying almost-invariant sets in *steady* flows, i.e., where $\mathbf{u}(t, \mathbf{x}) = \mathbf{u}(\mathbf{x})$; in the

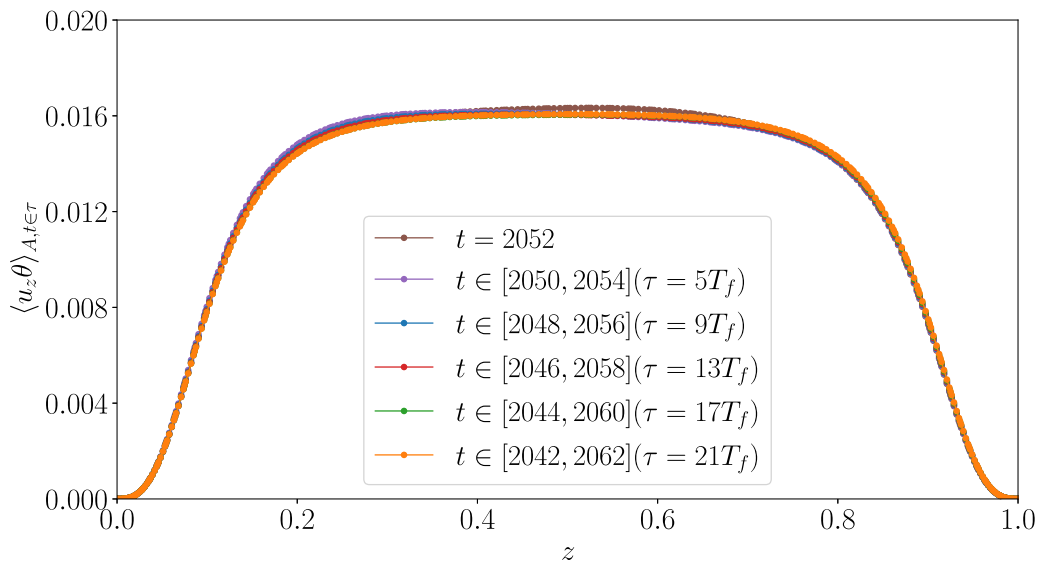


FIG. 3. Mean values of CHT across the horizontal plane at different z levels plotted against these z levels, at $t = 2052T_f$, and averaged over time windows of length 5, 9, 13, 17, and 21 T_f , centered at time $t = 2052T_f$. Similar results are obtained at other times.

next section, we extend these ideas to time-dependent velocity fields. For a steady vector field $\mathbf{u}$, we consider trajectories $\{\mathbf{x}_t\}$ of the stochastic differential equation (SDE) (9). We say that $S \subset M$ is *almost-invariant* if

$$\rho^s(A) := \frac{\text{Prob}(\mathbf{x}_0 \in A, \mathbf{x}_s \in A)}{\text{Prob}(\mathbf{x}_0 \in A)} \approx 1 \quad (10)$$

for short durations s , where Prob is the probability of the event occurring if $\mathbf{x}_0$ is initialized uniformly over M .

Following Ref. [38], one may construct a first-order-in- s formula for $\rho^s(S)$:

$$\rho^s(A) = 1 + \frac{G_A \mathbf{1}_A}{V(A)} s + o(s), \quad (11)$$

where V denotes volume in M and $\mathbf{1}_A$ is the indicator function on A . The operator G_A is defined as

$$G_A f := \lim_{s \rightarrow 0} \int_A \frac{P^s f - f}{s} dV, \quad (12)$$

where P^s is the Perron-Frobenius operator, describing evolution of a density f by the Fokker-Planck equation

$$\frac{\partial f(t, \mathbf{x})}{\partial t} = -\nabla \cdot (\mathbf{u}(\mathbf{x})f(t, \mathbf{x})) + \frac{\epsilon^2}{2} \Delta f(t, \mathbf{x}) \quad (13)$$

for a duration s . From Eq. (12), it is clear that $G_A \mathbf{1}_A \leq 0$ and returning to Eq. (11), we see that almost-invariant sets A should have $G_A \mathbf{1}_A \approx 0$. To obtain multiple almost-invariant sets A , following Ref. [38], one computes several leading real eigenfunctions of the generator G , where

$$Gf := \lim_{s \rightarrow 0} \frac{P^s f - f}{s}. \quad (14)$$

That is, we solve the linear eigenproblem $Gf = \lambda f$ with periodic boundary conditions applied at the vertical “sides” of M and Neumann boundary conditions applied at the floor and ceiling of M .

B. Quasistationary families of almost-invariant sets and the inflated generator

In this and subsequent sections, we assume that $\mathbf{u}$ is time-varying. We define the *spacetime* domain $\mathbb{M} = [0, \tau] \times M$, which should be thought of as a continuum of copies of M across times from 0 to τ . We now define spacetime versions of $\mathbf{u}$, the SDE in Eq. (9), the invariance ratio ρ^s , and the generator G .

Following Ref. [32], we define a time-expanded domain $\mathbb{M} = [0, \tau] \times M$ and construct a stochastic process as so that

- (1) in the time coordinate, introduce diffusion with intensity $a > 0$,
- (2) in the original phase space coordinates, on M at time t , we have the usual SDE on M , namely, diffusion with intensity ϵ and drift given by $\mathbf{u}(t, \cdot)$.

More precisely, we define a spacetime vector field $\mathbf{U}$ by

$$\mathbf{U}(t, \mathbf{x}) = \begin{pmatrix} 0 \\ \mathbf{u}(t, \mathbf{x}) \end{pmatrix}$$

and a spacetime SDE as

$$d\mathbf{X}_s = \mathbf{U}(\mathbf{X}_s) ds + \Sigma d\mathbf{W}_s, \quad (15)$$

where $\mathbf{X} = (t, \mathbf{x}) \in \mathbb{M}$ and

$$\Sigma = \begin{pmatrix} a & 0 \\ 0 & \epsilon \mathbf{I}_3 \end{pmatrix}.$$

The scalar $\epsilon > 0$ continues to represent diffusion in space, and $a > 0$ is the diffusion coefficient along the temporal coordinate. Note that Eq. (15) is an *autonomous* SDE on $\mathbb{M}$.

Similarly to the previous subsection, we will say that the spacetime set $\mathbb{A} \subset \mathbb{M}$ is almost-invariant if Eq. (10),

$$\rho^s(\mathbb{A}) := \frac{\text{Prob}(\mathbf{X}_0 \in \mathbb{A}, \mathbf{X}_s \in \mathbb{A})}{\text{Prob}(\mathbf{X}_0 \in \mathbb{A})} \approx 1, \quad (16)$$

where $\mathbf{X}_0$ is distributed uniformly on $\mathbb{M}$. Let us write the spacetime set $\mathbb{A} = \bigcup_{t \in [0, \tau]} (\{t\} \times A_t)$, where each $A_t \subset M$, $t \in [0, \tau]$, and interpret what almost-invariance in spacetime means. Stochastic trajectory escape from a spacetime set $\mathbb{A}$ can occur in the space coordinates or the time coordinate, and if $\rho^s(\mathbb{A}) \approx 1$, both types of escape should be low.

Low escape in space coordinates means that on most time-slices $\{t\} \times A_t$, one has $\rho^s(A_t) \approx 1$, and therefore at most time instances A_t is almost-invariant in the usual phase space sense.

Low escape in the time coordinate means that the boundary of $\mathbb{A}$ is mostly aligned with the time axis, which means that there is small variation of the boundary of the family A_t with t ; in other words, the family $\{A_t\}_{t \in [0, \tau]}$ is quasistationary.

Note that the sets A_t may be empty during some subintervals of $[0, \tau]$. This flexibility allows for quasistationary families of almost-invariant sets to appear and disappear in time.

Following Ref. [32], one may construct a first-order-in- s formula for $\rho^s(\mathbb{A})$:

$$\rho^s(\mathbb{A}) = 1 + \frac{G_{\mathbb{A}} \mathbf{1}_{\mathbb{A}}}{\mathbb{V}(\mathbb{A})} s + o(s), \quad (17)$$

where $\mathbb{V}$ denotes volume in $\mathbb{M}$. An operator $\mathcal{G}_{\mathbb{A}}$ is defined as

$$\mathcal{G}_{\mathbb{A}} F := \lim_{s \rightarrow 0} \int_{\mathbb{A}} \frac{\mathcal{P}^s F - F}{s} d\mathbb{V}, \quad (18)$$

where $\mathcal{P}^s$ is the Perron-Frobenius operator, describing evolution of a density F by the Fokker-Planck equation

$$\frac{\partial F(\mathbf{X})}{\partial s} = -\nabla \cdot (\mathbf{U}(\mathbf{X})F(\mathbf{X})) + \frac{\Sigma^2}{2} \Delta F(\mathbf{X}) \quad (19)$$

for a duration s . From Eq. (18) it is clear that $\mathcal{G}_{\mathbb{A}} \mathbf{1}_{\mathbb{A}} \leq 0$ and returning to Eq. (17), we see that almost-invariant sets $\mathbb{A}$ should have $\mathcal{G}_{\mathbb{A}} \mathbf{1}_{\mathbb{A}} \approx 0$. To obtain multiple almost-invariant sets A , following Ref. [38] (see also Refs. [39,40]), one computes several leading real eigenfunctions of the generator G , where

$$\mathcal{G}F := \lim_{s \rightarrow 0} \frac{\mathcal{P}^s F - F}{s}. \quad (20)$$

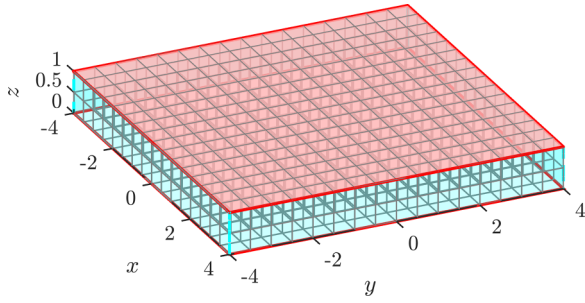


FIG. 4. Sketch of the spatial domain M divided into cubic cells for the construction of the spatial generators G_i on each time slice with side length ℓ . We use periodic boundary conditions on the side walls of the domain (which are highlighted in cyan) and Dirichlet boundary conditions for the temperature field at the top and bottom planes (which are highlighted in red).

In practice, we will compute eigenfunctions of the L^2 -adjoint of this operator; see Ref. [32] for details. That is, we solve

$$\begin{aligned} \mathcal{G}^* F^* &= \Lambda F^*, \\ \nabla F(\mathbf{x}) \cdot \mathbf{N}(\mathbf{x}) &= 0, \quad \text{for } \mathbf{x} \in \partial \mathbb{M}, \end{aligned} \quad (21)$$

where

$$\mathcal{G}^* F(t, \mathbf{x}) = \mathbf{U}(t, \mathbf{x}) \cdot \nabla F(t, \mathbf{x}) + \frac{\Sigma^2}{2} \Delta F(t, \mathbf{x}). \quad (22)$$

We have periodic boundary in the x and y coordinates, and apply Neumann boundary conditions on $\partial \mathbb{M} = (\{0, \tau\} \times M) \cup ([0, \tau] \times \partial M)$, where ∂M consists of the floor and ceiling of our three-dimensional physical domain.

The spectrum of $\mathcal{G}^*$ (and of $\mathcal{G}$) consists of eigenvalues $\Lambda_k, k = 1, 2, 3, \dots$ with nonpositive real part, ordered by decreasing real part. The eigenvalue $\Lambda_1 = 0$ has corresponding eigenfunction $F_1^* \equiv 1$. We separate the real eigenvalues into two classes [32,41]. First, so-called *temporal eigenfunctions* with no dependence on $\mathbf{x}$; they have the form $F_k^*(t, \mathbf{x}) = \cos(k\pi t/\tau)$, with corresponding eigenvalues $-(ak\pi/\tau)^2/2$. Second, the remainder of the real eigenfunctions we call *spatial eigenfunctions*; it is these that encode the quasistationary almost-invariant families.

C. Numerical estimation of the inflated generator

We discretize our spacetime domain $\mathbb{M} = [0, \tau] \times M$, where $M = [-4, 4] \times [-4, 4] \times [0, 1] \subset \mathbb{R}^3$, by splitting the time interval $[0, \tau]$ into equidistant time steps $0 = t_0 < t_1 < \dots < t_{K-1} < t_K = \tau$, each separated by $\Delta t = \tau/K$, and subdividing M into N cubes $B_1, \dots, B_N$ of equal side length ℓ . Figure 4 shows an example of what M looks like after it has been split into N cubes.

1. Discretization of spatial generators at each time instant

At time t , we denote the operator corresponding to the right-hand side of Eq. (13) with $\mathbf{u}(\mathbf{x}) = \mathbf{u}(t, \mathbf{x})$ by G^t . To construct an estimate of G^t —called the spatial generator at time t —we use “Ulam’s method for the generator” as introduced in Ref. [38]. This approach is related to an upwind scheme and involves computing integrals representing the rate of flux out of all of the faces of the boxes $\{B_i\}_{i=1}^N$. Let $\mathbf{n}_{ij}$ denote the

unit normal vector to the face $B_i \cap B_j$ pointing out of B_i . We construct an $N \times N$ matrix $\mathbf{G}^t$ as

$$G_{ij}^t = \begin{cases} G_{\text{drift},ij}^t + \frac{\epsilon^2}{2\ell^2}, & i \neq j, \\ -\sum_{j \neq i} G_{ij}^t, & \text{otherwise,} \end{cases} \quad (23)$$

where S denotes surface area and

$$G_{\text{drift},ij}^t = \frac{1}{V(B_j)} \int_{B_i \cap B_j} (\max\{\mathbf{u}(t, \mathbf{x}) \cdot \mathbf{n}_{ij}, 0\}) dS(\mathbf{x}) \quad (24)$$

denotes the deterministic (drift) component of the generator matrix G^t , which corresponds to the first term on the right-hand side of Eq. (13). Note that at most six flux integrals are computed for each three-dimensional box. These integrals are computed numerically using the Julia package `HCubature.jl` [42,43]. All of the default choices for the input arguments are maintained, with the exceptions of the relative and absolute tolerances, which are both set to 10^{-2} for the sake of computational efficiency. We add a small spatial diffusion when the flux integral is nonzero, using

$$\epsilon = \sqrt{0.1\bar{u}\ell}, \quad (25)$$

where $\bar{u}$ is the median RBC velocity magnitude over the entire spacetime domain $\mathbb{M}$ to ensure that the eigenvalue $\Lambda_1 = 0$ is simple. The expression (25) for ϵ is obtained by setting the term $\epsilon^2/2\ell^2$ in Eq. (23) equal to $0.05\bar{u}/\ell$, which corresponds to adding a drift of 5% to the first expression in Eq. (23); see also Ref. [32] for a discussion.

2. Discretization of the inflated generator

To obtain the discretized inflated generator, we note that Eq. (22) can be rewritten as

$$\mathcal{G}F(t, \mathbf{x}) = G_t F(t, \mathbf{x}) + \frac{a^2}{2} \partial_t^2 F(t, \mathbf{x}). \quad (26)$$

To create a discretized spacetime estimate of $\mathcal{G}$, we index first by space, then by time. For the terms G^t in Eq. (26), this means creating a block-diagonal spacetime (st) matrix with generator matrices $\mathbf{G}^t$ on the diagonal:

$$\mathbf{G}_{\text{st}} := \begin{pmatrix} \mathbf{G}^{t_0} & 0 & 0 & 0 & \dots & 0 \\ 0 & \mathbf{G}^{t_1} & 0 & 0 & \dots & 0 \\ 0 & 0 & \mathbf{G}^{t_2} & 0 & \dots & 0 \\ 0 & 0 & 0 & \ddots & & \vdots \\ \vdots & & & \ddots & & \vdots \\ 0 & 0 & \dots & 0 & 0 & \mathbf{G}^{t_K} \end{pmatrix}.$$

To construct the second term on the right-hand side of Eq. (26), we use standard central differencing to estimate the Laplacian in time over the full time interval $[0, \tau]$, and pad with $N \times N$ identity matrices to respect the spacetime indexing:

$$\mathbf{L}_{\text{st}} := \begin{pmatrix} -\mathbf{I}_N & \mathbf{I}_N & 0 & 0 & \dots & 0 \\ \mathbf{I}_N & -2\mathbf{I}_N & \mathbf{I}_N & 0 & \dots & 0 \\ 0 & \mathbf{I}_N & -2\mathbf{I}_N & \mathbf{I}_N & & \vdots \\ 0 & 0 & \mathbf{I}_N & \ddots & \ddots & 0 \\ \vdots & \vdots & & \ddots & -2\mathbf{I}_N & \mathbf{I}_N \\ 0 & 0 & \dots & 0 & \mathbf{I}_N & -\mathbf{I}_N \end{pmatrix} / \Delta t^2.$$

The discretization of $\mathcal{G}$ is then

$$\mathbf{G}_a = \mathbf{G}_{\text{st}} + (a^2/2)\mathbf{L}_{\text{st}}. \quad (27)$$

3. Selecting the temporal diffusion strength

The temporal diffusion matrix in Eq. (27) is scaled by a temporal diffusion strength a . We discuss *a posteriori* and *a priori* heuristics for initial choices of a . Suppose that we seek approximately Q quasistationary families and that the average lifetimes of these families are approximately $(1/\mathcal{T})\tau$. Then, a should be chosen so that the Q th spatial eigenvalue of $\mathbf{G}_a$ is approximately equal to the $\mathcal{T}$ th temporal eigenvalue of $\mathbf{G}_a$. This involves an explicit computation of the eigenvalues of $\mathbf{G}_a$.

In order to create an *a priori* initial estimate of a , we additionally require information about the domain $\mathbb{M}$ in order to estimate the temporal and nontemporal eigenvalues. As discussed earlier, the k th temporal eigenvalue of $\mathbf{G}_a$ is $-(ak\pi/\tau)^2/2$. We now need to compute the eigenvalues of $(\epsilon^2/2)\Delta$ on our spatial domain $M = 8S^1 \times 8S^1 \times [0, 1]$. The eigenfunctions will be combinations of real Fourier modes and of the form

$$\begin{aligned} &\cos(2\pi kx/8)\cos(2\pi ly/8)\cos(\pi mz), \\ &\cos(2\pi kx/8)\sin(2\pi ly/8)\cos(\pi mz), \\ &\sin(2\pi kx/8)\cos(2\pi ly/8)\cos(\pi mz), \\ &\sin(2\pi kx/8)\sin(2\pi ly/8)\cos(\pi mz), \end{aligned}$$

where $k, l, m \in \mathbb{N}$, due to periodicity in the x and y directions and Dirichlet boundary conditions at the domain floor and ceiling. One may verify that the leading eigenvalues of Δ on M are (multiplicities in parenthesis): 0 (1), $-\pi^2/16$ (4), $-\pi^2/8$ (4), $-\pi^2/4$ (4), $-5\pi^2/16$ (8), $-\pi^2/2$ (4), $-9\pi^2/16$ (4), $-5\pi^2/8$ (8), $\dots$. In our experiments, we select $Q = 30$ and $\mathcal{T} = 2$. From the list above, we see that the 30th eigenvalue of $(\epsilon^2/2)\Delta$ is $-5\epsilon^2\pi^2/16$ and the 2nd temporal eigenvalue is $-4a^2\pi^2/2\tau^2$. Following Sec. B 1 [32], there is numerical diffusion introduced by the Ulam-for-the-generator scheme, which means that when determining a heuristic a value, we use an “effective” ϵ defined by

$$\epsilon_{\text{eff}} = \sqrt{1.1\bar{u}\bar{\ell}} \approx 0.1228. \quad (28)$$

Equating these eigenvalues yields

$$a_{\text{init}} = \sqrt{5/32}\epsilon_{\text{eff}}\tau \approx 4.9532. \quad (29)$$

The drift term in Eq. (26) may cause many of the leading $Q = 30$ nontemporal eigenvalues to be complex. Therefore, the estimate for a_{init} in Eq. (29), which assumes all real eigenvalues, may need to be increased in order to match the second temporal eigenvalue with the 30th *real* nontemporal (i.e., spatial) eigenvalue.

We remark that when $Q = \mathcal{T} = 2$ (the simplest case of two quasistationary families with lifetime half of the time extent τ), one may compute the *a priori* heuristic choice for the parameter a as

$$a_{\text{init}} = 2\tau\sqrt{1.1\bar{u}\bar{\ell}}/L_{\text{max}} = 2\epsilon_{\text{eff}}\tau/L_{\text{max}}. \quad (30)$$

L_{max} is the longest side length of the spatial domain M , which in this case will be $\Gamma = 8$. Note that the units of a_{init} in

Eq. (30) are the same as those in Eq. (29) because L_{max} is already part of the numerical coefficient in Eq. (29). The heuristic for a in Eq. (30) was derived in Ref. [32], and has been adjusted by a factor of $2^2 = 4$ here to account for the periodic boundary conditions in the x and y coordinates (see similar periodic/nonperiodic domain discussions in Ref. [41]).

D. Extracting individual quasistationary families from eigenvectors of the inflated generator and SEBA

We compute the large-magnitude eigenvalues and the corresponding eigenvectors of the discretized inflated generator $\mathbf{G}_a^*$ with the Arnoldi method using the Julia package `ArnoldiMethod.jl` [44] to obtain the leading real-valued spatial eigenvalues $\Lambda_k^{\text{spat}} < 0$ (with values closer to 0) and their corresponding eigenvectors $\mathbf{F}_k^{\text{spat}}$. To distinguish the real-valued eigenvalues/eigenvectors (spatial and temporal) from their complex-valued counterparts, check that the imaginary part of Λ_k is 0 within a certain tolerance (10^{-12} is sufficient for this study). To distinguish the spatial eigenvalues/eigenvectors from the temporal ones, calculate the variance of the eigenvector $\mathbf{F}_k^*$ on the $K + 1$ blocks of indices $kN + 1, \dots, (k + 1)N$, $k = 0, \dots, K$ (in other words, calculate the variance of the eigenvector data across each point in our spatial domain M for each of the $K + 1$ time steps), then take the average of these variances. If this average spatial variance is close to 0 (again, within a specified tolerance, 10^{-8} was sufficient in this case), then the eigenvector is constant on all points in space for each time step and the eigenvalue/eigenvector pair is therefore temporal. Otherwise, we have a real-valued spatial eigenvalue Λ_k^{spat} and its corresponding eigenvector $\mathbf{F}_k^{\text{spat}}$, the latter of which we use in the SEBA algorithm.

Each of the leading real-valued spatial eigenvectors of the inflated generator $\mathbf{F}_k^{\text{spat}}$ contains signatures of possibly multiple quasistationary families of almost-invariant sets.

To isolate individual families of sets from the span of the leading spatial eigenvectors, as has been done with isolating individual coherent sets within an RBC flow system [25,45], we use the SEBA algorithm [33] to derive a sparse basis for this eigenspace. Each SEBA vector will isolate one quasistationary family of almost-invariant sets.

Let $\mathcal{V} = [\mathbf{F}_1^{\text{spat}} | \mathbf{F}_2^{\text{spat}} | \dots | \mathbf{F}_Q^{\text{spat}}]$ be a matrix whose columns are the leading Q spatial eigenvectors of the inflated generator, let $\mathcal{S}$ be a matrix whose columns form a basis of sparse vectors each of the same length as the spatial eigenvectors $\mathbf{F}_k^{\text{spat}}$, and let $\mu > 0$ be a small sparsity penalty. We seek a sparse array $\mathcal{S}$ whose column space is approximately the same as the column space of $\mathcal{V}$. We achieve this through the following optimization problem:

$$\operatorname{argmin}_{\mathcal{S}, \mathcal{R}} \|\mathcal{V} - \mathcal{S}\mathcal{R}\|_F^2 + \mu\|\mathcal{S}\|_1. \quad (31)$$

We solve Eq. (31) by alternately fixing $\mathcal{R}$ and solving for $\mathcal{S}$ exactly using soft-thresholding, and fixing $\mathcal{S}$ and solving for $\mathcal{R}$ exactly using singular value decomposition (SVD). When the algorithm converges, we are guaranteed a local optimum, which in practice is frequently the global optimum.

The Q columns of $\mathcal{S}$ form our basis of SEBA vectors $\{\mathbf{S}_1, \dots, \mathbf{S}_Q\}$.

ALGORITHM 1. Sparse eigenbasis approximation (SEBA).

Inputs: A matrix $\mathcal{V}$ of size $P \times Q$, whose columns are the Q leading real-valued spatial eigenvectors of $\mathbf{G}_a^*$, $\mathbf{F}_k^{\text{spat}}$, $k = 1, \dots, Q$, each of length P .

Outputs: A $P \times Q$ matrix $\mathcal{S}$, whose columns are the Q SEBA vectors $\mathbf{S}_1, \dots, \mathbf{S}_Q$, which approximately span $\{\mathbf{F}_1^{\text{spat}}, \dots, \mathbf{F}_Q^{\text{spat}}\}$.

1. Define a sparsity parameter $\mu = 0.99/\sqrt{P}$ (the largest possible value) and initialize the rotation matrix $\mathcal{R} = \mathbf{I}_Q$.
2. To avoid degeneracies, apply a tiny random perturbation to any of the eigenvectors $\mathbf{V}_j^{\text{spat}}$ that are constant vectors or close to constant. In practice, this is usually only required for the trivial eigenvector $\mathbf{V}_1^{\text{spat}}$.
3. Apply a soft thresholding to the columns of $\mathcal{S}$:
 $\mathcal{S}_j = C_\mu((\mathcal{V}\mathcal{R}^\top)_j)/\|C_\mu((\mathcal{V}\mathcal{R}^\top)_j)\|$, $j = 1, \dots, Q$, where $C_\mu(z) = \text{sign}(z) \max\{|z| - \mu, 0\}$.
4. Update the orthogonal matrix $\mathcal{R}$: let $USV^\top$ be the singular value decomposition of $\mathcal{S}^\top \mathcal{V}$, and set $\mathcal{R} = UV^\top$.
5. Repeat the previous two steps until the matrix two-norm between the newly calculated matrix $\mathcal{R}$ and the matrix $\mathcal{R}$ calculated from the previous step is below a certain threshold (we used 10^{-12}).
6. Ensure that each column of $\mathcal{S}$ is predominantly nonnegative by setting $\mathcal{S}_j \rightarrow \text{sign}(\sum_{i=1}^P \mathcal{S}_{ij})\mathcal{S}_j$, for $j = 1, \dots, Q$.
7. Scale the columns of $\mathcal{S}$ so that each one has a maximum value of 1: $\mathcal{S}_j \rightarrow \mathcal{S}_j / \max_i \mathcal{S}_{ij}$, for $j = 1, \dots, Q$.
8. Reorder the columns of $\mathcal{S}$ in decreasing order of their minimum value. Those columns with 0 or negative values close to zero are more reliable and appear first in the ordering.

We now summarize the full numerical approach, following Algorithm 1 in Ref. [32], to extracting quasistationary families of almost-invariant sets.

IV. RESULTS

In this section, we provide computational specifics for the inflated generator method applied to our RBC flow system, show relevant results obtained from these methods, and then compare the results from this method with the CHT results shown in Sec. 2 in an attempt to establish a connection between strong convective heat transfer and the lack of quasistationary, almost-invariant flow behavior (or conversely, a connection between low convective heat transfer and quasistationary almost-invariant flow behavior) within this system. We compare these results both qualitatively, through visual comparisons of scalar fields, and quantitatively through computation of the correlation between the maxima of the SEBA vectors produced from the inflated generator method and both instantaneous and time-averaged CHT data.

A. Quasistationary families of almost-invariant sets from the inflated generator

To execute the inflated generator method on the RBC flow system, we follow the steps outlined in Algorithms 1 and 2, starting by discretizing our spatial domain $M = [-4, 4) \times [-4, 4) \times [0, 1]$ into N cubes of equal side length ℓ at each of our $K + 1$ time steps. We take 35 equispaced time steps

ALGORITHM 2. Identify quasistationary families of almost-invariant sets.

Inputs: A state space M , a time-varying velocity field $\mathbf{u}$ on M , a time duration $[t_0, t_0 + \tau]$.

Outputs: Estimates of families of quasistationary almost-invariant sets at discrete time points in $[t_0, t_0 + \tau]$.

1. Discretize the spatial domain M into cubes $B_1, \dots, B_N$, and the time interval $[t_0, t_0 + \tau]$ into time nodes t_k , $k = 0, \dots, K$.
2. Calculate ϵ using Eq. (25) and compute the discrete generator matrices $\mathbf{G}^k$ for $k = 0, \dots, K$ as described in Sec. III C using Eq. (23).
3. Combine the $\mathbf{G}^k$ to form $\mathbf{G}_a$ as described in Sec. III C using Eq. (27), where the temporal strength parameter a is initially selected using Eq. (29).
4. Compute the eigenvalues $0 = \Lambda_1 > \Lambda_2 \geq \dots$ of the sparse matrix $\mathbf{G}_a^*$ whose real parts are closest to 0, along with their corresponding spacetime eigenvectors $\mathbf{F}_1^*, \mathbf{F}_2^*, \dots$. Note that $\mathbf{F}_1^*$ should be a constant vector $\mathbf{1}$.
5. Remove the complex-valued eigenvectors as well as the constant-in-space temporal eigenvectors using the steps outlined at the beginning of this subsection.
6. Isolate Q quasistationary families of almost-invariant sets by applying SEBA to the leading Q spatial eigenvectors (including the trivial constant vector $\mathbf{F}_1^*$) to obtain spacetime SEBA vectors $\mathbf{S}_1, \dots, \mathbf{S}_Q$. Each SEBA vector should support one of these quasistationary families of almost-invariant sets in spacetime.

spaced $\Delta t = 3 T_f$ apart on the time interval $[t_0, t_0 + \tau] = [2001, 2103] T_f$ of length $\tau = 102$. We have tried three different values of ℓ for the inflated generator method in this case, these being 0.25, 0.125, and 0.0625 (which, respectively, gives $N = 4096, 32\,768$, and $262\,144$). In this paper, we focus on the results generated with $\ell = 0.0625$ as this provides the best spatial resolution for M and allows us to identify quasistationary families of almost-invariant sets with greater clarity. We compute the discrete generator matrices $\mathbf{G}^k$ on each of our 35 time steps using Eq. (23). Using Eq. (25), we compute the value for the spatial diffusion parameter $\epsilon \approx 0.0370$, given the box side length $\ell = 0.0625$ and the median velocity $\bar{u}$ over the entire spacetime domain $\mathbb{M}$ taking an approximate value of 0.2195. As we have a large number of flux integrals to compute in this case (at most, $6 \times 262\,144 = 1\,572\,864$ as each cube will have at most six neighboring cubes), we make this process more efficient using standard multithreading in Julia so that multiple flux integrals can be evaluated at once. We then construct the full discretized inflated generator matrix using Eq. (27), which, given $\ell = 0.0625$, will be a relatively large matrix of size $9175\,040 \times 9175\,040$ for our spacetime domain $\mathbb{M} = [2001, 2103] \times M$. Using Eq. (29), we calculate an initial heuristic for the temporal diffusion parameter a , $a_{\text{init}} \approx 4.9532$, given $\tau = 102$ and $L_{\text{max}} = \Gamma = 8$. We then compute the leading eigenvalues/eigenvectors of the discretized inflated generator using the Arnoldi method. To make this process more efficient for a large inflated generator matrix, large matrices such as the inflated generator and the Krylov subspace matrix for the Arnoldi method are defined on a GPU so that matrix multiplications that form part of the

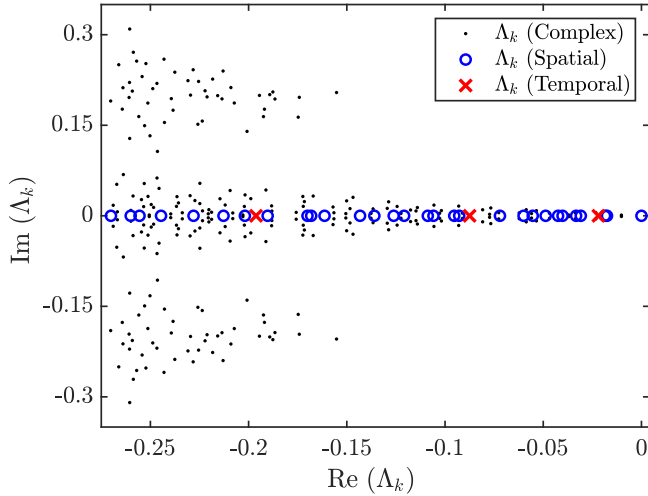


FIG. 5. The spectrum of the inflated generator for the three-dimensional RBC flow with $a = a_{\text{init}} \approx 4.95$, showing the leading 30 real-valued spatial eigenvalues (indicated by blue circles), the first three temporal eigenvalues (indicated by red crosses), and an extensive collection of complex-valued eigenvalues (indicated by black dots).

Arnoldi method can be executed more quickly. We construct the inflated generator matrix using the initial heuristic for a [Eq. (29)].

Figure 5 shows the corresponding eigenspectrum, where the 30 leading real eigenvalues shown as blue circles collectively encode 30 families of quasistationary almost-invariant sets. Real parts closer to zero correspond to stronger quasistationarity and almost-invariance properties. The second temporal eigenvalue roughly matches the 30th nontemporal eigenvalue; however, many of the nontemporal eigenvalues with larger real part than the second temporal eigenvalue are a mix of complex and spatial eigenvalues. In order for the second temporal eigenvalue to match with the 30th spatial eigenvalue (which in this case is the 285th overall), the value of the parameter a would have to be increased to around $a = 9.15$. However, such an increase in a would reduce the amount of temporal variation between time slices of the inflated generator eigenvectors and the SEBA vectors. To emphasize this temporal variation, we reduce a slightly to a value of 4.1 for subsequent experiments with a single value of a .

Since we seek several quasistationary families of almost-invariant sets within this flow system (in this case, roughly 20–30 within the time interval of interest), we take the corresponding eigenvectors $\mathbf{F}_1^{\text{spat}}, \dots, \mathbf{F}_{30}^{\text{spat}}$ of these 30 spatial eigenvalues and we insert these into the SEBA algorithm in order to isolate signatures of the quasistationary families of almost-invariant sets present within the RBC flow system. Since the matrices $\mathcal{V}$, $\mathcal{R}$, and $\mathcal{S}$ will all be large, in similar fashion to what was done with the Arnoldi method, we define all of these matrices on a GPU to make Algorithm 1, in particular steps 3–5 of this Algorithm, more efficient.

After calculating these 30 SEBA vectors $\mathbf{S}_1, \dots, \mathbf{S}_{30}$, we further improve the spatial resolution of these spacetime vectors by interpolating them over a uniform three-dimensional

grid of points within our spatial domain M with mesh size $\ell/2 = 0.03125$.

Figure 6 shows a typical example of a quasistationary family of almost-invariant sets detected for the plane-layer RBC flow system identified through three-dimensional isosurfaces of the SEBA vector $\mathbf{S}_{21}$ taken for example at a level of 0.4 at discrete time steps. As can be seen in Fig. 6, at time $t = 2022T_f$ our spatial domain M is blank, indicating that our family of sets (which will represent a transient plume of fluid comprising an almost-invariant parcel) has not formed yet. However, at $t = 2028T_f$ a red object (representing a member of our family of sets) begins to emerge along the bottom of our fluid layer. This object then begins to grow in size, before reaching the top of our cell at time $t = 2043T_f$ to form our full metastable/almost-invariant flow object. Once fully formed, this transient family of almost-invariant sets retains its shape for roughly 20–25 units of time, until it begins to shrink back down toward the bottom of our cell at around time $t \approx 2061T_f$. By time $t = 2076T_f$, the family of sets has been reduced to a small object sitting at the bottom of the cell, and by time $t = 2082T_f$ the family of sets has vanished completely.

Several quasistationary families of almost-invariant sets are present simultaneously. To illustrate this, Fig. 7 shows four of the many distinct quasistationary families of almost-invariant sets present at time $t = 2052T_f$ (the central point of our time interval), found through four different SEBA vectors ($\mathbf{S}_2$, $\mathbf{S}_{15}$, $\mathbf{S}_{21}$, and $\mathbf{S}_{22}$). In a fifth panel within Fig. 7, we superposition these four vectors to illustrate the four families of sets existing simultaneously at this moment in time. In Fig. 8, we restrict these four SEBA vectors, along with the superposition panel, to the xy midplane with $z = 0.5$. In Fig. 8, two-dimensional restrictions of quasistationary families of almost-invariant sets are identifiable through solid or dark red objects (corresponding to SEBA values of isolevel 0.4 or higher). We again apply a cutoff of 0.4 to both Figs. 7 and 8 so that we can easily visualize the individual quasistationary families of almost-invariant sets.

In order to produce one complete picture of the quasistationary, almost-invariant flow behavior present across our entire spacetime domain $\mathbb{M}$, we calculate the maximum of the 30 SEBA vectors $\mathbf{S}_{\text{max}}$, where

$$(\mathbf{S}_{\text{max}})_i = \max_j \mathbf{S}_{ij}$$

over all $j = 1, \dots, 30$. The full collection of quasistationary, almost-invariant plumes of fluid obtained from $\mathbf{S}_{\text{max}}$ should fill most of our spatial domain M on each time slice, with the remaining filaments of space not covered by these plumes representing regions of faster and less metastable fluid transport. After taking the maximum of the 30 spacetime SEBA vectors $\mathbf{S}_{\text{max}}$ (including the four shown in Figs. 7 and 8), we use $\mathbf{S}_{\text{max}}$ to produce the images shown in Fig. 9. We plot horizontal restrictions of the SEBA maxima at three levels in the xy plane, namely, the “top” (positioned along $z = 1 - \ell = 0.9375$, which is not on the ceiling of the cell but is still within the upper thermal boundary layer for the cooling plate at the top of the cell), the “midplane” ($z = 0.5$, the middlemost horizontal layer), and the “bottom” ($z = \ell = 0.0625$, which is within the lower thermal boundary layer for the heating plate at the bottom of the cell). We also restrict the SEBA maxima

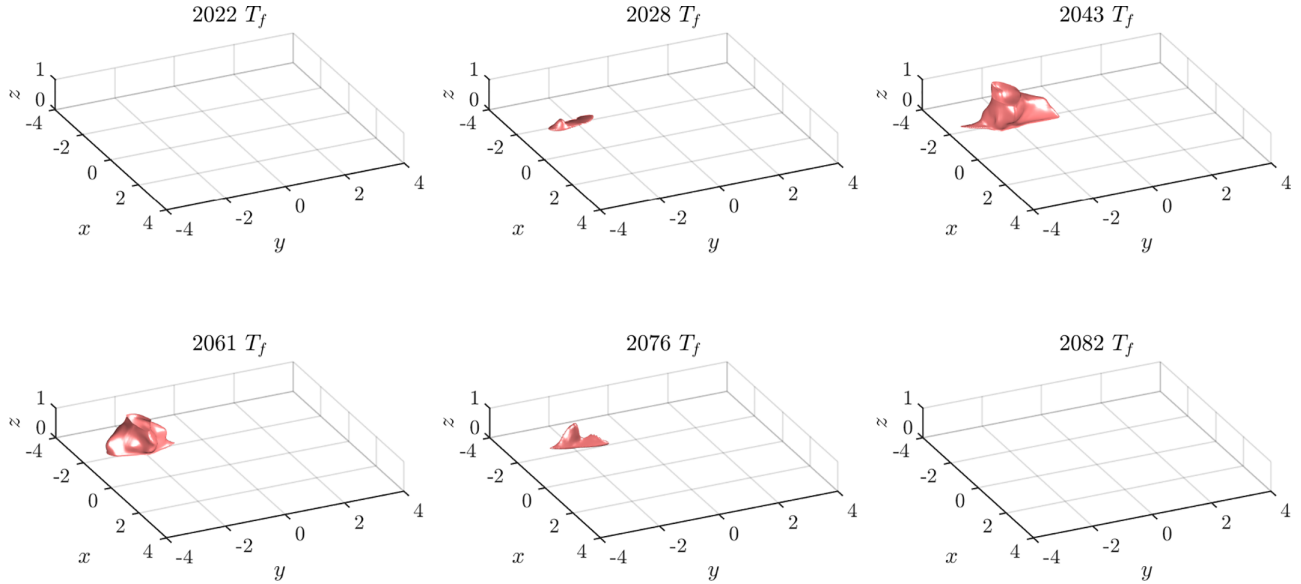


FIG. 6. The evolution of a quasistationary family of almost-invariant sets (a transient plume of fluid forming a metastable parcel) within the RBC flow over six discrete time steps as identified through the SEBA vector $\mathbf{S}_{21}$. A cutoff of 0.4 has been applied to the SEBA vector.

to two vertical midplanes, one in the xz plane (with $y = 0$) and one in the yz plane (with $x = 0$).

In Fig. 9, as was the case in Fig. 8, the regions of our spatial domain colored in red or deep red (corresponding to maximal SEBA values of approximately 0.4 or higher) represent quasistationary, almost-invariant fluid objects present within the RBC flow. Regions colored in light pink represent quasistationary families of almost-invariant sets that are beginning to either emerge or dissipate; while the thin white streaks or filaments correspond to parts of our domain where no almost-invariant behavior is present, and which are more likely to correspond to thin passageways through which parcels of less metastable fluid flow toward the top wall after being heated, or sink toward the bottom wall after being cooled.

In summary, the results of Figs. 6–8 relate to those of Fig. 9 as follows: The first three figures selected particular eigenvectors of the SEBA analysis and displayed their dynamical evolution by means of (1) an isosurface in Fig. 6, (2) different SEBA eigenvector isosurfaces at a fixed time in Fig. 7, and (3) their contours in the horizontal cut at midplane in Fig. 8. All three figures show that individual eigenvectors are localized in space. Figure 9 is a composition obtained from all SEBA eigenvectors when taking the maximum at each point.

B. Qualitative comparisons between SEBA and CHT

We now focus on a connection between the quasistationary families of almost-invariant sets identified from the SEBA

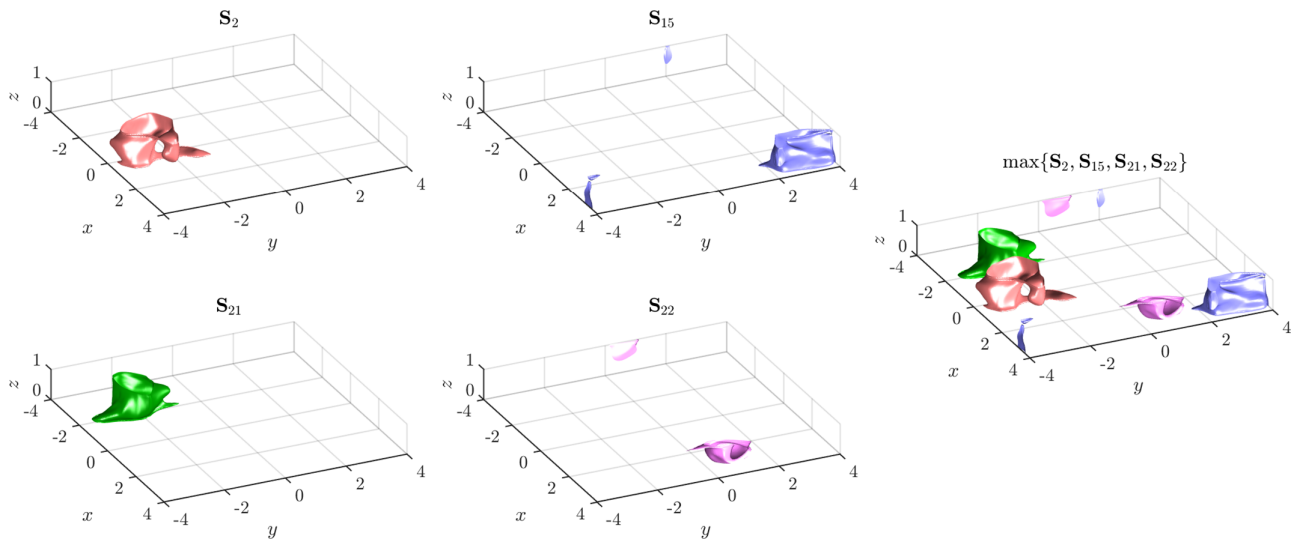


FIG. 7. Three-dimensional isosurfaces for 4 of the 30 SEBA vectors computed for the RBC flow (namely, $\mathbf{S}_2$, $\mathbf{S}_{15}$, $\mathbf{S}_{21}$, and $\mathbf{S}_{22}$) taken at the central time step $2052 T_f$. A cutoff of 0.4 has been applied to each of these SEBA vectors. In a fifth panel (right), we superimpose these four vectors on a single three-dimensional axis to show these four families of sets co-existing within the RBC flow system at time $2052 T_f$.

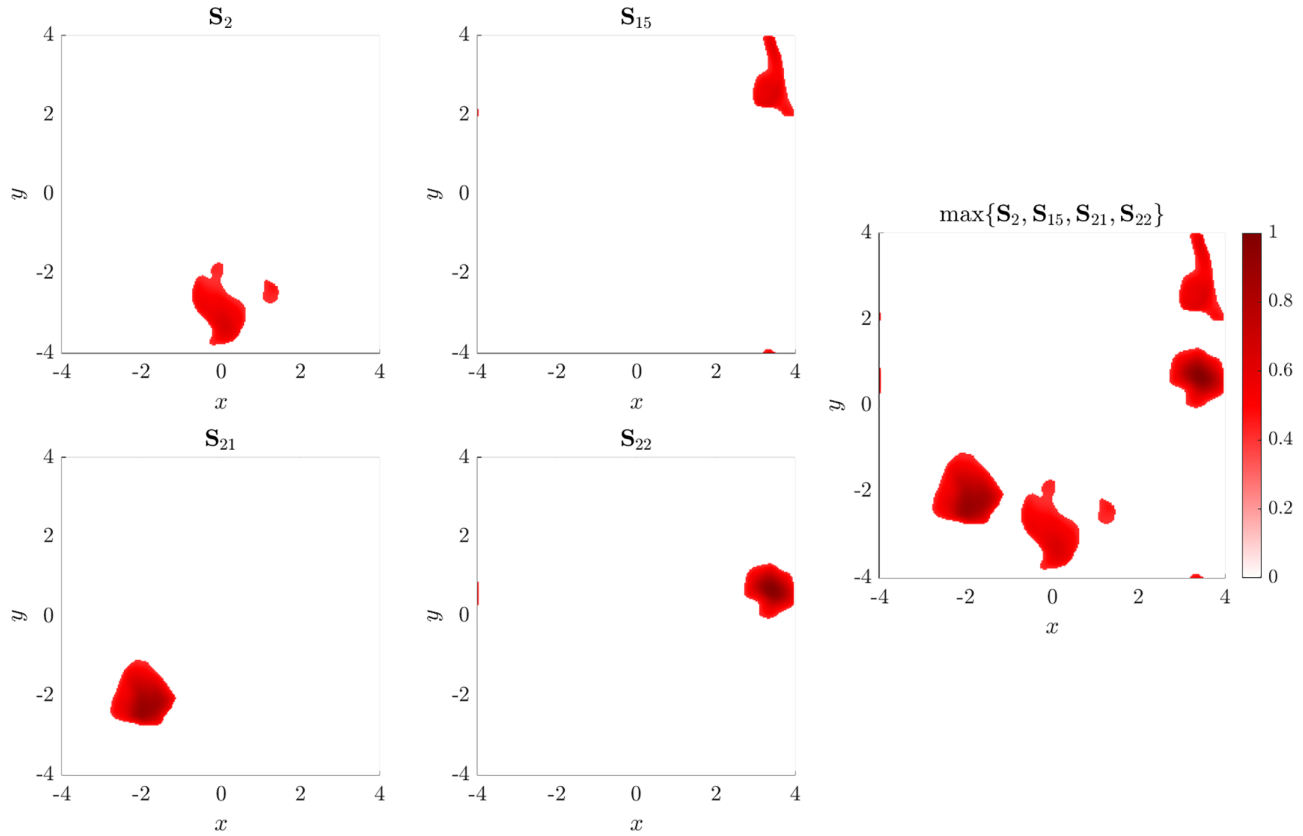


FIG. 8. Snapshots of the same four SEBA vectors shown in Fig. 7 restricted to the horizontal xy midplane (with $z = 0.5$) at the central time step $2052 T_f$. A cutoff of 0.4 has been applied to each of these SEBA vectors. In a fifth panel (right), we take the maximum of these four vectors and restrict this to the xy midplane to demonstrate the coexistence of these four families of sets found through the four SEBA vectors at time $2052 T_f$.

vectors and the values of CHT data for the RBC flow system. We start with a more qualitative approach to doing this by comparing the scalar fields for the SEBA vectors and the CHT data. Figure 10 shows the scalar fields of the maximum of 30 SEBA vectors computed from the inflated generator method with $a = 4.1$ (as discussed in the previous subsection) and the CHT data averaged over $5 T_f$ in the horizontal xy midplane and the vertical xz midplane. The full three-dimensional CHT data are averaged over a window of length $5 T_f$, $[t_k - 2, t_k + 2]$ with $t_k = 2052 T_f$, and is then restricted to the two-dimensional horizontal xy midplane and the vertical xz midplane. We must stress that the SEBA spacetime vectors and CHT data are three dimensional and defined over the entire spatial domain M ; however, for ease of display we restrict the data to these two midplanes for this qualitative analysis. We focus on more quantitative comparisons of the full three-dimensional data in the next two subsections.

Recall that locally enhanced turbulent heat transfer in the RBC layer implies that CHT becomes large and positive; that is the case either if cold fluid is moved from top to bottom ($u_z < 0$ and $\theta < 0$) or hot fluid from bottom to top ($u_z > 0$ and $\theta > 0$). Local maxima of CHT in our manuscript appear to approximately correlate with the interfaces between the almost-invariant sets. These interfaces are the local minima in the SEBA maxima scalar fields, shown in Figs. 9 and 10 [upper row (left) and second row]. The inflated generator

approach thus identifies these enhanced transport regions as the spatial complement to the almost-invariant sets, likely due to the strong transport violating the almost-invariance property. This is seen in Fig. 10 when comparing the first two plots in the top row and the plots in the second and third rows.

For brevity, we restrict the qualitative analysis in this paper to one value of the temporal diffusion parameter $a = 4.1$ for the inflated generator method to produce the SEBA vectors, and one length of time over which we average the CHT data ($5 T_f$). To the naked eye, some connections can be drawn between the SEBA and CHT fields in Fig. 10. For instance, at a region in the neighborhood of the point $(0, 2)$ in the xy midplane, the crucifix-shaped purple object in the CHT field roughly coincides with a web of white filaments centered at the same location in the maximum SEBA field. In the xz midplane, we can also spot some of these similarities, such as a thin white colored stem roughly close to the vertical line $x = -1.5$ in the maximum SEBA field lining up with a purple vertical object (a little thicker than the white stem) in the CHT field. Other examples like these can be deduced from the scalar fields, signifying a potential connection between low SEBA (and therefore less metastable fluid behavior) and high average CHT (corresponding to faster fluid movement as heated fluid rises from the bottom of our cell and cooled fluid sinks from the top). That said, while the regions of high CHT usually take the shape of thicker purple or black

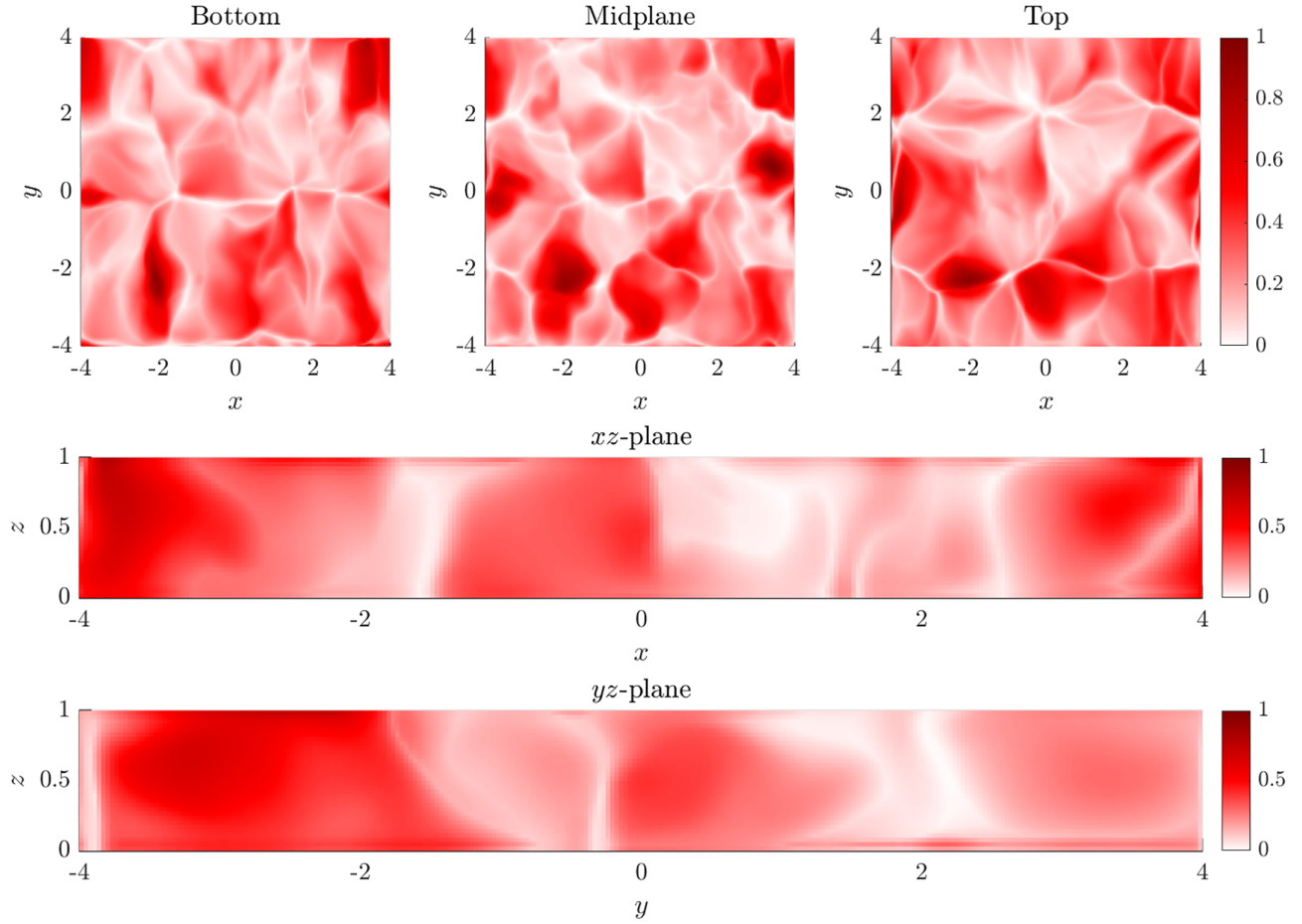


FIG. 9. Snapshots of the maximum of 30 SEBA vectors computed for the RBC flow taken at $2052T_f$ along five two-dimensional restrictions of the spatial domain M . We take horizontal restrictions of the SEBA maxima (shown in the top row) along the xy plane at three vertical levels (from left to right, the “bottom” of the cell ($z = 0.0625$), the “midplane” ($z = 0.5$), and the “top” of the cell ($z = 0.9375$)); and we take vertical restrictions of the SEBA maxima in the xz midplane with $y = 0$ (middle row) and in the yz midplane with $x = 0$ (bottom row).

blobs, the white ridges of minimal SEBA are little more than wafer-thin filaments that separate the quasistationary families of almost-invariant sets.

This connection is not perfect, as there are a few visual inconsistencies between the two fields. This is particularly true in the opposite case, where we seek connections between high SEBA (quasistationary families of almost-invariant sets) and low CHT (reduced transfer of heat from reduced fluid movement as large metastable objects form). As we can see in Fig. 10, while there are some overlaps between the red regions of the SEBA fields and the deep orange or yellow regions of the CHT fields, the shapes of the red objects in the SEBA field do not completely line up with orange or yellow objects in the CHT field. These observations suggest a qualitative connection (albeit weak) does exist between SEBA and CHT when the movement of fluid is more rapid and convective heat transfer is stronger, but not within regions of the domain where fluid movement is more quasistationary and metastable (or at least, not to as great an extent).

In the xy midplane, we note that the $|\theta|$ field, much like the CHT (H_c) field, does share common features with the SEBA field, particularly between the thin white streaks of the SEBA field and the yellow regions of high $|\theta|$, reinforcing that there is some connection between regions of less metastable fluid

advection and increased temperature fluctuation (in absolute value, disregarding whether this is a net positive or negative fluctuation). However, when we focus on the vertical xz mid-plane, it is much more difficult to develop some connection between SEBA and the $|\theta|$ field, in contrast to CHT.

Thus, it appears that it is difficult to detect transient almost-invariant regions in this turbulent flow using physical properties of the fluid directly, and one requires the more specialized inflated generator method, which targets precisely the emergence and dissipation of almost-invariant objects.

C. Correlation between SEBA and CHT

We quantitatively compare the SEBA field and other fields such as CHT by computing correlations. Let $\text{SEBA}_{t,i}$ and $\text{CHT}_{t,i}$, respectively, denote the values of the SEBA and CHT fields at time t and pixel i . Pearson’s correlation coefficient at time t is computed with

$$\text{Corr}_t(\text{SEBA}, \text{CHT}) := \frac{\sum_{i=1}^N (\text{SEBA}_{t,i} - \overline{\text{SEBA}_t})(\text{CHT}_{t,i} - \overline{\text{CHT}_t})}{\sqrt{\sum_{i=1}^N (\text{SEBA}_{t,i} - \overline{\text{SEBA}_t})^2} \sqrt{\sum_{i=1}^N (\text{CHT}_{t,i} - \overline{\text{CHT}_t})^2}}, \quad (32)$$

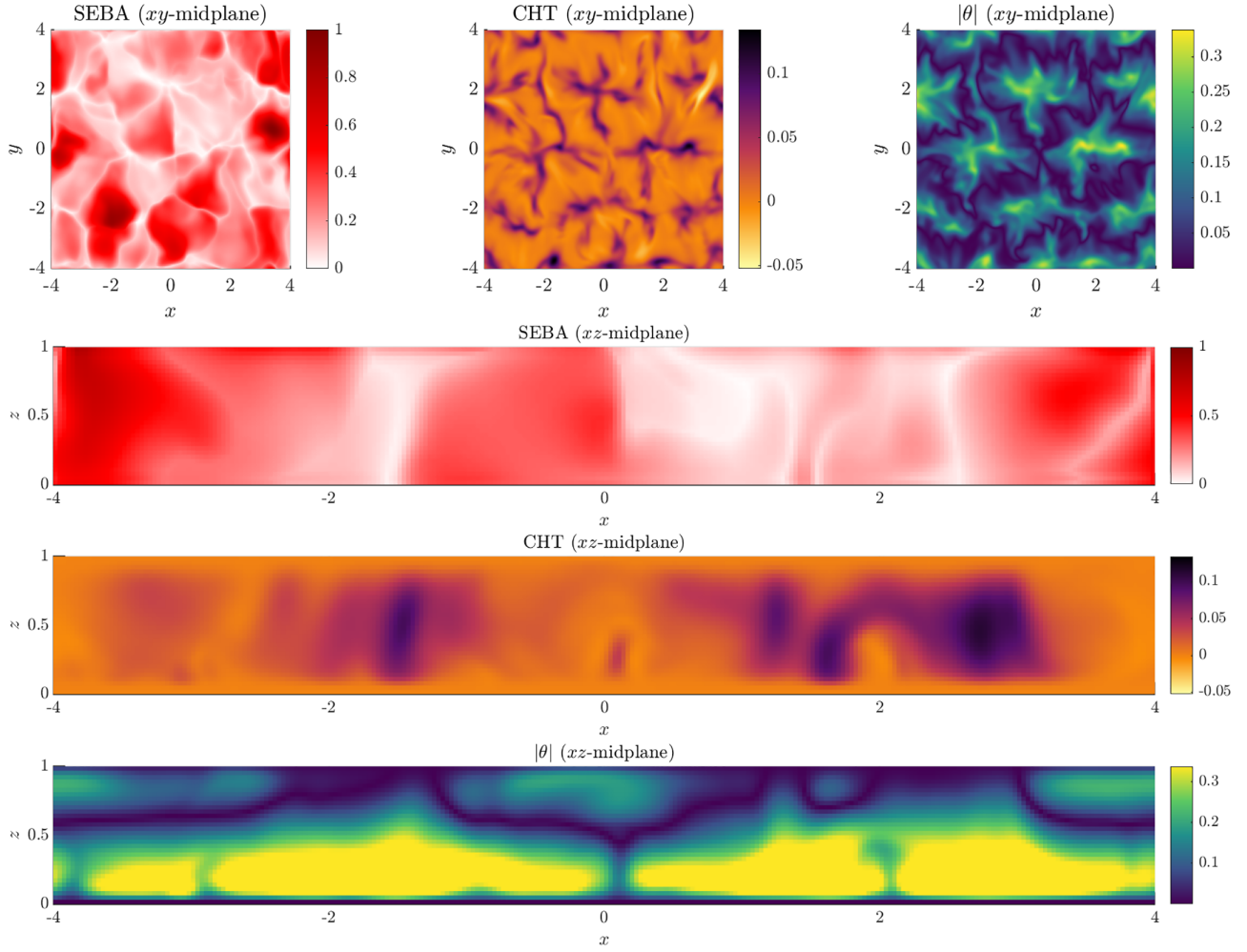


FIG. 10. The maximum of 30 SEBA vectors [first row (left) and second row], CHT averaged over $5 T_f$ [first row (middle) and third row] and $|\theta|$ also averaged over $5 T_f$ [first row (right) and fourth row] for the RBC flow taken at time $2052 T_f$. We restrict these three-dimensional quantities to the horizontal xy midplane (with $z = 0.5$) in the first row, and to the vertical xz midplane (with $y = 0$) in all subsequent rows.

where

$$\overline{\text{SEBA}}_t = \frac{1}{N} \sum_{i=1}^N \text{SEBA}_{t,i} \quad \text{and} \quad \overline{\text{CHT}}_t = \frac{1}{N} \sum_{i=1}^N \text{CHT}_{t,i}.$$

In Fig. 11, we plot the correlation between the full three-dimensional SEBA data and CHT data against time at every $3 T_f$ (as this is the temporal resolution of the SEBA spacetime vectors). We also plot the correlation between SEBA and CHT restricted to the xy midplane. In this instance, we focus on

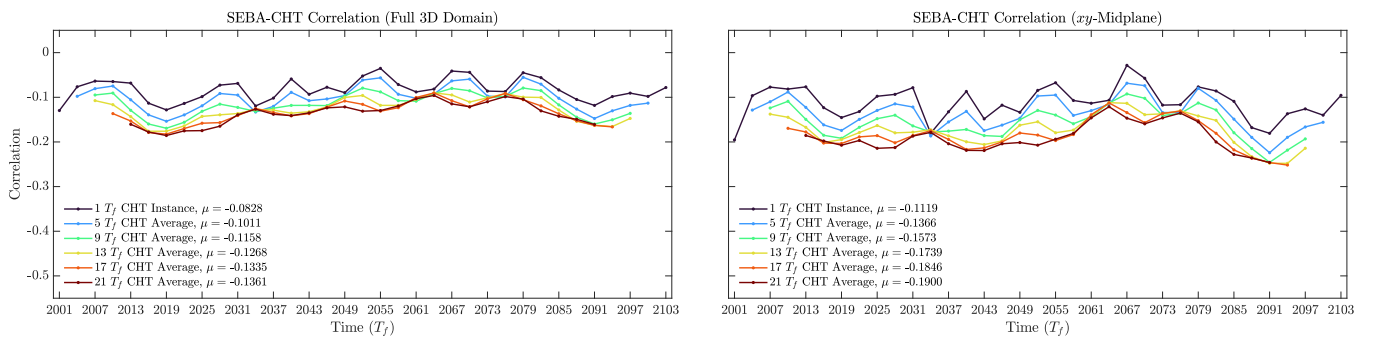


FIG. 11. Plots of correlation values between SEBA and CHT against time. In the left-hand panel, we take SEBA and CHT data over the entire three-dimensional spatial domain M and in the right-hand panel we restrict the data to the xy midplane. The SEBA vectors have been computed from the inflated generator method with a set to 4.1. Each color represents the length of time over which the CHT data are averaged, and the correlation values are plotted at the midpoints t_k of the time intervals $[t_k - m, t_k + m]$ over which we compute the averages for the CHT data. Included in the plot's legend are the means of the correlation values μ taken over time for each curve.

SEBA data computed from the inflated generator with $a = 4.1$, while the CHT data are taken at instantaneous moments in time, and are also averaged over subintervals of time of length 5, 9, 13, 17, and 21. The subintervals in question take the form $[t_k - m, t_k + m]$, where t_k is the central time point of the interval and $m = 2p$, $p = 1, \dots, 5$. The correlation values computed between SEBA and average CHT are plotted at these central time points t_k .

From the left-hand graph in Fig. 11, we observe a (weak) negative correlation between SEBA and CHT. This correlation is considerably weaker when we calculate it using single-time instances of CHT; however, as the length of the time window over which we compute CHT averages increases, the correlation between SEBA and CHT becomes more negative and therefore improves. This implies that the removal of noise/diffusion from the CHT data by averaging the data helps improve the correlation between CHT and SEBA. One could argue that it is possible to improve the correlation values even further by taking CHT averages over longer time windows than those already considered (e.g., in the region of 60–90 T_f). However, the observed “bunching” of the curves as the time window length increases suggests that we are approaching some limit for the improvement of these correlation values, where increasing the window of time over which we average the CHT data will only be effective at improving the correlation up to a point.

This weak correlation observed between SEBA and CHT is likely due to the fact that we are computing these correlation values over the entire three-dimensional spatial domain M , and the correlation between these quantities is weaker within some parts of the domain compared to others, such as the thermal boundary layers along the top and bottom of the cell. To that end, we also compute the correlation between SEBA and CHT after restricting these datasets to the xy midplane, with the graphs for these correlation values shown in the right-hand panel of Fig. 11. Similar to the left panel in Fig. 11, the time window over which we compute CHT averages changes, but the temporal diffusion parameter a remains fixed at 4.1. We do not observe a great difference between the correlation values for the three-dimensional data and the xy -midplane data when CHT is defined on a single time step. However, as the length of the time window over which we compute the CHT averages increases, we see an improvement in these correlation values compared to those generated using the full three-dimensional data. These correlation values are still relatively weak as they roughly range between -0.25 and -0.1 (when CHT has been averaged).

A likely reason for this lack of a stronger correlation is to do with the observation of a weaker qualitative connection between high SEBA and low-to-medium CHT values in the xy midplane, as observed in Fig. 10. For a stronger negative correlation between these two quantities (i.e., corresponding to a correlation value close to -1), quasistationary families of almost-invariant sets (identified through high values of SEBA) would have to align near perfectly with regions of M corresponding to low to no convective heat transfer. At the same time, the correlation values are not zero because we do observe some qualitative connections between low SEBA and high CHT. The volume covered by these relatively thin filaments is much smaller compared to the volume covered

by the metastable plumes of fluid identified through quasistationary families of almost-invariant sets and low CHT; hence, this correlation between SEBA and CHT exists over a lower volume of M and contributes to the correlation values being closer to 0 in Fig. 11.

D. Correlation between SEBA and other quantities

To further test the possible connections between SEBA and the characteristics of our RBC flow system, we extend this analysis further by calculating the correlation between SEBA and several other key quantities for the RBC flow. To this end, we take correlations between SEBA and the following fields:

- Temperature fluctuation θ , and its absolute value $|\theta|$;
- Vertical velocity u_z , and its absolute value $|u_z|$;
- Convective heat transfer H_c , and its absolute value $|H_c|$;
- Magnitude of horizontal velocity $\|(u_x, u_y, 0)^T\|$;
- Magnitude of horizontal gradient of temperature fluctuation $\|(\partial\theta/\partial x, \partial\theta/\partial y, 0)^T\|$.

We average these quantities over subintervals of time of length $5 T_f$ centered at t_k , $[t_k - 2, t_k + 2]$, as we did previously with the CHT data. Figure 12 displays these correlation values across time for both the full three-dimensional spatial domain M and the restriction to the xy midplane. The mean correlation values across time are included in the legend of Fig. 12. We observe particularly weak correlation between SEBA and the quantities θ , $|\theta|$, u_z , $\|(u_x, u_y, 0)^T\|$, and $\|(\partial\theta/\partial x, \partial\theta/\partial y, 0)^T\|$ across the full three-dimensional domain. The correlation between SEBA and $|u_z|$ is somewhat less than between SEBA and H_c and $|H_c|$; therefore, we can be confident that our analysis focuses on CHT. Restricting our calculations to the xy midplane greatly improves the correlation between SEBA and $|\theta|$, with the mean correlation changing from -0.0247 across the full spatial domain M to -0.1720 across the xy midplane. Restricted to the midplane, the correlation with $|\theta|$ exceeds the correlations with CHT. A reason for this observation might be that the strongest plume clusters, which have clear $|\theta|$ signatures, will be observed in the xy midplane, while smaller-scale structures formed at the floor and ceiling may become washed out by turbulent mixing by the time they reach the xy midplane. This was also observed in Ref. [13].

Finally, to benchmark against a featureless scalar field, we computed the correlations between SEBA and a constant scalar field, and between CHT and a constant scalar field. The magnitudes of these correlations across all time windows shown in Fig. 11 were at least an order of magnitude smaller (not shown) than the values shown in Figs. 11 and 12.

E. Impact of the temporal diffusion parameter a

To identify what sort of impact (if any) the temporal diffusion parameter a used to construct the inflated generator has on the correlation results presented in the previous subsection, we rerun the inflated generator method for a smaller value of a and two larger values of a than the original value of 4.1 and perform similar correlation analysis using the SEBA vectors generated. As a convenient way of doing this, we rerun the inflated generator method for $a/2 = 2.05$, $2a = 8.2$, and $4a = 16.4$. The results are shown in Fig. 13, where we calculate the mean correlation values between SEBA and CHT across the

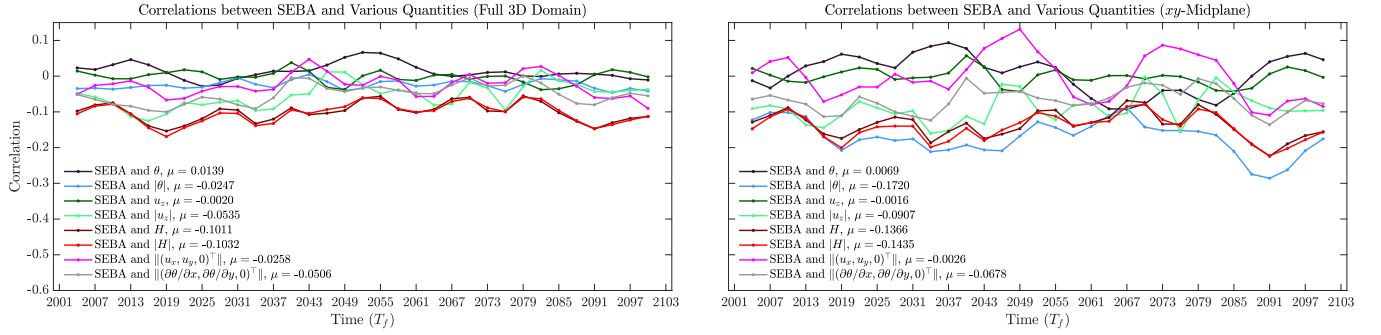


FIG. 12. Plots of correlation values between SEBA and various other quantities against time: temperature fluctuation θ , vertical velocity u_z , and convective heat transfer H_c ; along with the absolute values of these quantities $|\theta|$, $|u_z|$, $|H_c|$; horizontal speed $\|(u_x, u_y, 0)^\top\|$, and the norm of the horizontal gradient of θ , $\|(\partial\theta/\partial x, \partial\theta/\partial y, 0)^\top\|$. In the left-hand panel, we compute these correlations over the entire three-dimensional spatial domain M and in the right-hand panel we restrict these calculations to the xy midplane. The SEBA vectors have been computed from the inflated generator method with a set to 4.1. Each color represents one of the quantities of interest. The data for each of the quantities are averaged over a duration of $5 T_f$, and the correlation values are plotted at the midpoints t_k of the time intervals $[t_k - 2, t_k + 2]$ over which we compute the averages for these quantities. Included in the plot's legend are the means of the correlation values μ taken over time for each curve.

full time interval $[2001, 2103] T_f$ and plot these against the lengths of the time windows over which we compute the CHT averages. Analogously with Fig. 11, the left-hand plot shows correlation values computed for three-dimensional SEBA and CHT data, while the right-hand plot shows these values for SEBA and CHT data restricted to the xy midplane.

Between our two smaller values of a (2.05 and 4.1), we see roughly no impact on the correlation between SEBA and single-time instances of CHT; though as the time window taken to compute the CHT averages increases in length, the mean correlation values improve for the larger $a = 4.1$ and plateau a little more quickly when $a = 2.05$. When $a = 8.2$, we find better mean correlation values when using single-time instances of CHT data, and the correlation values continue to improve as we average CHT over a larger time window. However, when we increase a to 16.4, we do not observe any further improvements to our correlation results. Instead, while the mean correlation values for $a = 16.4$ are better than those for $a = 2.05$ and 4.1, these means are slightly worse (in the sense that they have value closer to 0, when we wish them to tend more toward -1) than those recorded for $a = 8.2$. Hence, increasing the value of the temporal diffusion parameter a for

the inflated generator does improve the correlation between SEBA and CHT but only up to a point, after which the correlation values either plateau or start to recede toward 0.

V. CONCLUSION

The main objective of our study was the application of a recent method to detect and analyze quasistationary families of almost-invariant sets of convective heat transfer in a plane-layer Rayleigh-Bénard convection flow. In this flow, heat that is supplied at the bottom of the layer is carried to the top, amplified by turbulent motion of the fluid layer. The method that we used to extract these families of sets is based on the so-called generator of the Perron-Frobenius or transfer operator that is inflated from space to spacetime to capture the transient dynamics of the almost-invariant sets in time. The scalar field that was mainly analyzed in our study is the convective heat transfer field $H_c(x, t)$, which is the product of the vertical velocity component, u_z , and the temperature fluctuation, $\theta(x, t)$. The quasistationary families of almost-invariant sets are obtained as eigenvectors of the discretized version of the inflated generator and a subsequent SEBA.

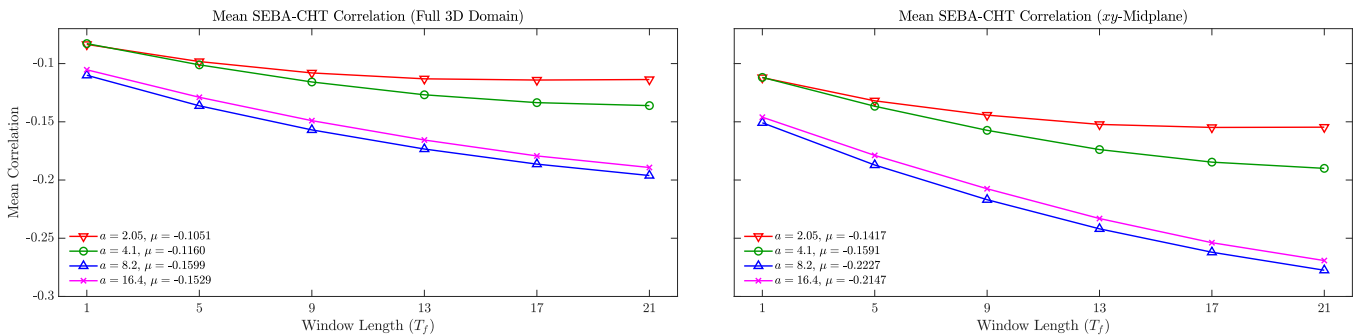


FIG. 13. Plots of the mean correlation values (over the full time interval $[2001, 2103] T_f$) between SEBA and CHT data over the entire three-dimensional spatial domain M (left) and restricted to the xy midplane (right) against the lengths of the time windows used to calculate the average CHT data. The colors (and symbols) in these plots represent the a values used when executing the inflated generator method. Included in the plot's legend are the means of the mean correlation values μ taken over the window lengths for each curve.

In our three-dimensional data analysis, we demonstrated qualitative and quantitative correlations between the patterns of convective heat transfer and the computed SEBA vectors and thus the capability of this analytical approach to extract the formation and dissipation of transient almost-invariant sets in the complex dynamics of a turbulent convection flow. This implies that the mathematical framework applied here can describe the gradual transient dynamics of the large-scale patterns in the plane-layer convection flow, the turbulent superstructures, and reveal its central role for the turbulent heat transfer.

Possible extensions of this work for the future could be as follows. If the convection dynamics proceeds in a more complex setting, e.g., in a thin shell that is subject to rotation, then the transport patterns will become latitude-dependent and meridional transport might be suppressed. The transport barriers that would form in such a flow configuration should be identifiable by the present framework. Finally, an application of the framework to higher Rayleigh and different Prandtl

numbers would be interesting to explore the robustness of the algorithm in processing increasing data sizes.

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DATA AVAILABILITY

Code and data used in this work are available at [46], and on Zenodo [47].

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