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*Published in:*

Proceedings in applied mathematics and mechanics

*DOI:*

[10.1002/pamm.201900201](https://doi.org/10.1002/pamm.201900201)

*Publication date:*

2019

*Document Version*

Publisher's PDF, also known as Version of record

[Link to publication](#)

*Citation for published version (APA):*

Klünker, A., Schneide, C., Pandey, A., Padberg-Gehle, K., & Schumacher, J. (2019). Lagrangian perspectives on turbulent superstructures in Rayleigh-Bénard convection. *Proceedings in applied mathematics and mechanics*, 19(1), Article 201900201. <https://doi.org/10.1002/pamm.201900201>

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# Lagrangian perspectives on turbulent superstructures in Rayleigh-Bénard convection

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We analyze large-scale patterns in three-dimensional turbulent convection in a horizontally extended square convection cell by means of Lagrangian particle trajectories calculated in direct numerical simulations. Different Lagrangian computational methods, i.e. finite-time Lyapunov exponents, spectral and density-based clustering and transfer operator approaches, are used to detect these large-scale structures, which are denoted as turbulent superstructures of convection.

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## 1 Introduction

We consider turbulent Rayleigh-Bénard convection at a Prandtl number  $Pr = 0.7$  and a Rayleigh number  $Ra = 10^5$  in the three-dimensional domain  $[-8, 8]^2 \times [0, 1]$  as discussed in [1]. In the Eulerian frame of reference, the formation of patterns from the fluid motion is presented e.g. in the time averaged temperature field. In order to consider the Lagrangian perspective, tracer particles are seeded into the simulation domain on a regular mesh with  $N = 512^2$  points at a plane close to the bottom plate, well inside the thermal boundary layer. Each individual tracer particle is advected by the flow. The particle trajectories are analyzed by means of different computational methods with respect to coherent flow behavior as described in the following section 2. By a coherent set we mean a time-dependent region in the physical domain of the flow which is minimally dispersive, a property that is characteristic of a Lagrangian turbulent superstructure. The results of our computations are discussed in section 3.

## 2 Methods

Here we briefly describe the different computational methods that are applied to the tracer trajectories in order to study convection from a Lagrangian point of view.

**Finite-time Lyapunov exponents:** The finite-time Lyapunov exponent (FTLE) measures separation of trajectories over a given time span  $[t_0, t_1]$  and is a heuristic diagnostic for identifying boundaries of coherent sets. It is defined via the maximal eigenvalue of the Cauchy-Green strain tensor obtained from the gradient of the flow map. We approximate this gradient via central differences based on particle positions at times  $t_0$  and  $t_1$ .

**Spectral clustering:** Similar in spirit to [2], we construct a network where the nodes are the Lagrangian trajectories. Two trajectories are linked if their dynamical distance, i.e. the average distance between their particles, is sufficiently small. The network is described by a sparse adjacency matrix  $A$ , with links weighted by the corresponding distance. A normalized cut problem is solved via a generalized graph Laplacian eigenvalue problem [3], where eigenvectors to eigenvalues close to zero indicate almost decoupled subgraphs. These leading eigenvectors are postprocessed by  $k$ -means clustering to extract the coherent sets as groups of trajectories that are closely interconnected.

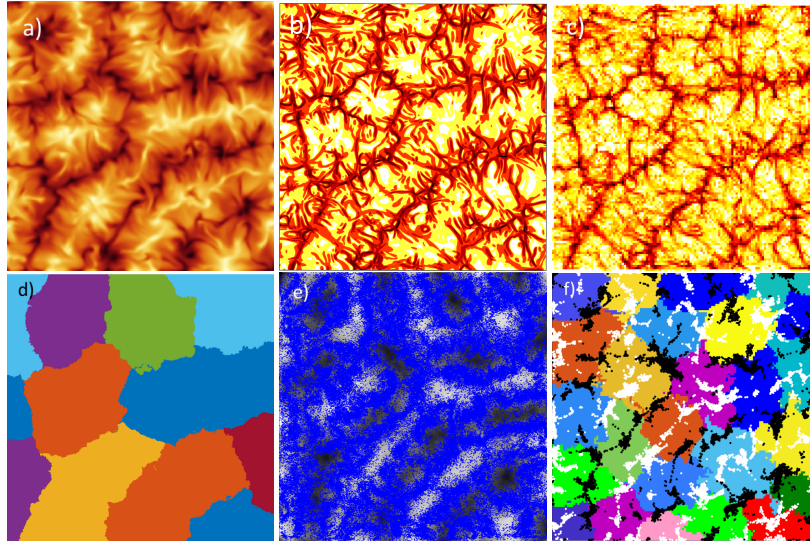
**Density-based clustering:** Using DBSCAN [4], we group trajectories into cluster trajectories and noise, as follows. A trajectory  $X$  that is close to at least  $minPts$  other trajectories (with respect to the dynamical distance) is a core point of a cluster  $C$ . All trajectories in the neighborhood of  $X$  are added to the same cluster  $C$ . They can be core points itself or border points of the cluster  $C$ . This process is repeated for all core points of cluster  $C$ . Trajectories that are not assigned to any cluster are defined as noise.

**Transfer operator approach:** A transfer operator  $\mathcal{P}$  describes the evolution of densities under the dynamics. Numerically, a finite rank approximation of this operator is given by a stochastic matrix  $P$  that describes transition probabilities between grid elements that partition the domain over some time span  $[t_0, t_1]$ . To extract minimally dispersive regions (almost-invariant sets [5]), we apply  $k$ -means clustering to the leading eigenvectors of the transition matrix  $P$ . A nonlinear stretching measure similar in spirit to FTLE termed finite-time entropy (FTE) can be computed very efficiently given  $P$  [6].

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**Fig. 1:** a) Time averaged temperature field in the midplane, averaged over  $2.6T_f$ . b) FTLE field computed on time span  $[0, 5.2T_f]$ . c) FTE field computed over same time span as in b). d) Clustering obtained from spectral clustering on  $[0, 10.4T_f]$ , particles plotted at initial positions. e) Midpoints of pseudotrajectories that belong to a dense cluster on  $[0, 80T_f]$ . f) Clustering obtained from the transfer operator method computed on time span  $[52.4T_f, 62.9T_f]$ , cold and hot particles near the midplane are plotted in black and white, respectively.

### 3 Results

Applying the different methods sketched in section 2 to our system, large-scale coherent structures can be detected in the Lagrangian frame of reference (Fig. 1 (b)-(f)), similar to the superstructures obtained in the Eulerian frame of reference (Fig. 1 (a)). The characteristic time scale for these large-scale structures is found to be  $\tau \approx 20T_f$  [1], which is the average turnover time of a Lagrangian particle, where  $T_f$  is the free-fall time unit.

Regions of initial strong separation are identified as FTLE ridges. These are signatures of the boundaries between convection rolls. Due to turbulent dispersion FTLE only gives insightful results on very short time scales  $\ll \tau$  (Fig. 1 (b)). A computation of the FTE field estimated directly from the transition matrix gives very similar results (Fig. 1 (c)).

On time scales comparable to the characteristic time  $\tau$  of the turbulent superstructures, the spectral clustering approach applied to the Lagrangian trajectories turns out to be successful in detecting large-scale structures (Fig. 1 (d)). These structures are found to agree very well with the Eulerian superstructures and appear to be bounded by regions of strong separation as measured by the FTLE field.

For longer time periods beyond  $\tau$  the spectral approach fails, but a density-based clustering applied to pseudo-trajectories (containing sliding window time averaged particle positions) is successful in finding a small coherent set of Lagrangian particles that are trapped for long times in the core of the superstructure circulation rolls and are thus not subject to ongoing turbulent dispersion (Fig. 1 (e)).

Finally, whereas the studies above focus on the emergence of the superstructures, we study turbulent trajectories at later times in the simulation, when the particles are well spread over the 3-dimensional domain. The clusters obtained by a transfer operator approach appear to consist of smaller compartments of a double roll or two neighboring convection rolls (Fig. 1 (f)).

To summarize, through the application of different computational methods on various time spans in Rayleigh-Bénard convection we detect Lagrangian turbulent superstructures that are comparable to those identified in the Eulerian frame of reference. A detailed Lagrangian study of Rayleigh-Bénard convection by means of trajectory clustering is carried out in [1].

**Acknowledgements** This work is supported by the Priority Programme SPP 1881 Turbulent Superstructures of the Deutsche Forschungsgemeinschaft.

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