Referee report on "Particle Clustering and Subclustering as a Proxy for Mixing in Geophysical Flows" by Rishiraj Chakraborty et al.

General comments

The study of Lagrangian coherent behaviour by means of clustering approaches is a research topic of current interest. In this manuscript, the authors apply a graph-based method to identify regions of dense mixing in a specific example of a two-dimensional flow (shallow water equations on the *f*-plane). The work builds on the trajectory-network approach introduced by Padberg-Gehle and Schneide (2017), where a network is built with Lagrangian trajectories serving as nodes. Two nodes are linked when the underlying trajectories have come ε-close at least once in the time span under consideration, which is coded in a binary adjacency matrix. While in Padberg-Gehle and Schneide (2017) ε is chosen in dependence of the initial grid size and the particle density in order to ensure a connected but sparse network, the authors of the manuscript under review concentrate on local, dense mixing regions. For this they consider the cut-off radius ε to be smaller than the mesh size of the grid where particles are initialized. The resulting network is then typically disconnected. The largest connected components, which the authors call clusters, are then further studied using two community detection approaches, namely the *Quick* algorithm introduced by Liu and Wong (2008) to find maximal quasi-cliques (i.e. dense subgraphs) and the classical spectral method by Shi and Malik (2000) for the solution of a normalized cut problem. The methods are tested on one specific example system.

While the manuscript is well written, contains some original ideas and altogether adds to the current research in the cluster-based study of Lagrangian coherence, there are some issues that have to be worked on in my view before the manuscript can meet the high standards for publication in NPG. Major issues include the question of the robustness of the methods, the lack of a critical comparison with other (network-based) mixing indicators, as well as the question of the relevance of the detected regions.

Specific comments

1) The detection of dense sub-clusters by means of the *Quick* algorithm is stressed several times throughout the manuscript as giving more robust results compared to spectral clustering. This however is not convincingly demonstrated in the paper. In particular, it would be interesting to see how the detected dense subclusters depend on the cut-off radius ε in the network construction and on the two quasi-clique parameters. While the cumulative clusters already differ significantly for two different values of ε (40% and 20% mesh size, Fig. 6/7), I assume that the dense sub-clusters as shown in Figs. 8--11 would vary considerably depending on the three parameters in the method. If a very small ε is chosen, then I also expect that the results would differ when the initial grid points are shifted. Also, how do the dense subclusters look like when ε is chosen larger than the mesh size? The results of corresponding numerical studies (also for instantaneous clusters) should be presented in the paper.

2) Adding to 1): When comparing Fig. 6 and 7 (p13) can any conclusions about the “perfect” thresholding distance ε be made?

3) The relation to other graph properties (e.g. as addressed on p20, l4) is not explored at all. For instance, can the detected structures also be related to a large node degree and/or a large local clustering coefficient? The manuscript would greatly benefit from a corresponding numerical comparison.

4) On p22 (l13) the authors write that “The striking similarities… indicate that dense interaction and thereby mixing is a characteristic of coherent structures.” The dense subclusters appear to be located at the boundary of coherent vortices, but do not make up the entire boundary, which however may

be specific to the choice of parameters and initial conditions. The overall relevance of the detected small structures for transport and mixing remains unclear to me as mixing here seems to be very localized. Also, depending on the choice of parameters, the detected regions and their interpretations may differ significantly (see also point (1) above).

5) On p22 (l1) the authors write: “This helped us validate our method for finding dense subclusters.” This statement refers to a comparison of cumulative clusters plus subclustering and instantaneous clusters. If both approaches find the same regions here then it would be interesting for the reader which way is less expensive and which way is more robust.

6) The clustering approach proposed in the manuscript has also some relation to the concept of the trajectory encounter volume as introduced by Rypina, Pratt (NPG, 2017). The authors should refer to this work as well.

7) Section 2.3.1: The description of the Quick algorithm by Liu and Wong (2008) is very technical. As the details are not referred to later in the text, the authors should focus on the main idea of the algorithm and delegate the details to an appendix.

8) In Figure 5, I assume that with the given parameters, the clique of size 4 could be extended by including the node right next to this subgraph (?).

9) Fig. 2/3: In general, an adjacency matrix only has only 1s on the diagonal in the case of self-loops, which is not the case in this construction.

10) Figs. 2--4 can be merged into one.

11) In the introduction many different methods for studying Lagrangian coherence are discussed, but corresponding references are missing.

12) p12 (l18): A reference to Shi & Malik (2000) for the normalized cut problem is missing.

13) p13 Fig. 6: A “transition from time 52 to 53 in Fig. 6” is mentioned in the text, but there is no time frame 53 in Fig. 6. In the caption it says: “Cumulative clusters … tracked at later times”. However, this would show the particles coloured according to first time step but plotted at later times. From the idea of cluster merging etc. I assume the clustering is performed individually for each of the plotted times.

14) In view of including further numerical studies, the authors should consider condensing the presentation of some the current results that are demonstrated in very much detail in Figs. 6-16.

Technical comments (typos, etc.)

- p11 l18 & 23: missing {
- p.3 l. 4: Hadjighasem et al …. “However, these principles only apply in the early stages…” should rather be something like: “only apply in finite time intervals…”
- p.9 l. 1: “We find sub-clusters with a minimum size of…” rather say “We search for sub-clusters with a minimum size of … throughout our analysis of the double jet flow…”.
- p17 l3 should rather be “Fig. 14 shows the temporal evolution of the spectral sub-clusters of cluster 1 found at time 50.”
- p21 l5 “…identify regions where the density of mixing is relatively higher than other portions of the cumulative clusters.” What is the "density of mixing"?
- p21 l6 “… involve the most mixing.” Rather say “strongest mixing.”