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Lagrangian Coherent Structures in Unsteady Flow Fields – Required Resolution of the Field Information

Lagrange'sche kohärente Strukturen in instationären Strömungsfeldern – Benötigte Auflösung der Feldinformation

Anna Slotosch, Maren Gollub, Frieder Kaiser, Bettina Frohnapfel, Jochen Kriegseis
KIT, Institute of Fluid Mechanics (ISTM), Kaiserstr. 10, 76131 Karlsruhe, Germany

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Abstract

Whole-field velocity information – in contrast to single point-data – allows a substantially deeper insight into the investigated flow scenarios, since pattern information is contained beyond only statistical correlations.

As a possible post-processing approach for such field information, the finite-time Lyapunov exponent (FTLE) gains in popularity as it provides essential information, e.g. cause-effect relations of vortex formation and separation. It is calculated based on the Lagrangian flow properties measuring the separation rate of particles to visualize the transport of Lagrangian coherent structures (LCS). Thereby, flow separation, clear vortex boundaries and recirculation zones are identified. Such structures in the flow are often not salient when investigating the Eulerian velocity field or even particle paths. Furthermore, the FTLE takes arbitrary time dependence of dynamical systems into account (see Shadden 2006).

In order to research the influence on different flow characteristics, the spatial resolution of the underlying velocity grid and the mesh of seeded particles are varied through various two and three dimensional flow phenomena. The findings provide valuable insight into the required spatial resolution for the respective flow scenarios. This information in turn serves as mandatory boundary conditions for any experimental effort towards a successful measurement-based FTLE calculation.

Background and Objectives

Most measuring technologies in fluid mechanics (e.g. particle image velocimetry (PIV), laser Doppler anemometry (LDA), hot wire anemometry) deliver Eulerian velocity data that need to be further processed. Lagrangian post-processing in terms of LCS extraction is only feasible for whole-field information, e.g. PIV or CFD data. Such processing provides information about the evolution of the flow and enables clear vortex boundary visualization.

In order to receive the Lagrangian information from unsteady velocity fields, the ordinary differential equation

$$\dot{x}(x_0, t) = v(x(x_0, t), t) \quad (1)$$

has to be solved. Thereby, the Lagrangian particle positions x are connected with the provided Eulerian flow field velocities v. In the Lagrangian description, the coordinate system moves with the particles. Therefore, the calculation is more complex but it is considered beneficial as the results reveal important information on location and dimensions of coherent flow structures, which might uncover cause-effect relations.

Motivated by those advantages over Eulerian post-processing, the calculation of FTLE fields is often used as a basis for LCS extraction. LCS are material manifolds, which act as precise vortex boundaries (Grigoriev 2012). These are represented as material lines in 2D and material surfaces in 3D flows. Haller (2011) defines hyperbolic LCS as locally strongest repelling or attracting material surfaces.

First proposed by Pierrehumbert (1991), the FTLE defines the changing distance of two initially neighboring particles over a particular integration time. An increasing distance between the particles, increases likewise the FTLE-value. Later, Haller and Yuan (2000, 2002) and Shadden *et al.* (2005) provided a profound mathematical description and a new approach to calculate fields, that nowadays are often called classical or flow-map FTLE-fields. A flow-map $\phi_{t_0}^{t}$describes the displacement of a particle from time t_0 to time t. Therefore, the stretching of the infinitesimal small perpetuation with arbitrary direction $\delta\vec{x}_0$ can be calculated using the right Cauchy-Green deformation tensor

$$C = \left(\nabla\phi_{t_0}^{t}\right)^T \nabla\phi_{t_0}^{t}. \tag{2}$$

If the direction of $\delta\vec{x}_0$ is the same as the direction of the eigenvector of C connected to the largest eigenvalue $\lambda_{max}(C)$, the perpetuation is maximized. As such,

$$\sigma_{t_0}^{t} = \frac{1}{t - t_0} ln\sqrt{\lambda_{max}(C)} \tag{3}$$

is called the largest FTLE for forward integration describing how strong the flow is repelled in forward time. Thereby, Shadden *et al.* (2005) defined LCS as ridges of the FTLE-field, which on the one hand precisely define vortex boundaries, but also indicate flow separatrices. More background information and a stepwise mathematical description can be found in Slotosch *et al.* (2014).

The FTLE calculation depends on multiple degrees of freedom, e.g. the resolution of the underlying flow field information that is limited by the capabilities of the applied measuring technique and the available storage size. If the discrete flow field is not fine enough to represent the real flow characteristics any FTLE results are not reliable. Thus, the first question addressed is how many data points, in terms of a velocity grid, are needed along a characteristic length scale in order to capture the structures present at that scale. An answer to this question during the process of experiment design would help choosing the appropriate equipment needed as the measurement capacities limit the resulting data resolution. Equally important is the spatial resolution of the particle mesh.

Equally distributed particles seeded with infinite grid size into the flow would guarantee the identification of all underlying structures resulting in a sharp visualization of the present LCS, while an insufficient number of particles might miss small scale structures. However, computational costs increase with increasing number of particles. Thus, the second question addressed is how dense has the particle mesh to be along a characteristic length scale in order to capture the structures present at that scale. Concerning again the design of an experiment, a third question arises. Is it possible to improve the results provided by a low resolution of the flow data by a high resolution of the particle mesh such that well resolved structures can be extracted despite limited measurement capabilities?

In the following, the influence of velocity grid resolution and particle mesh resolution will be examined based on the two dimensional double gyre flow (see Slotosch *et al.* 2014). This analytical flow field will then also serve as a basis for the development of two strategies, one concerning the velocity grid and one concerning the particle mesh, that allow the determination of the required resolution, respectively. Further, the designed strategies are tested on a more physical two dimensional flow field, namely the Kármán vortex street, and a three dimensional test case comprising a piston vortex.

Results and Discussion

Influence of number of velocity points and number of particle points on the FTLE

In order to study the influence of different resolutions with respect to the number of available velocity data and particles seeded into the flow, two new variables are introduced. For all calculations regarded in this work, the underlying velocity grid is assumed to be equidistant in all spatial directions. If the size of the structure that is to be resolved by FTLE calculations, e.g. a vortex, is known, a certain number of velocity points VP is distributed over a characteristic length L_{char} of the structure. As seen in Figure 1 a) and b), VP is equal to three as three velocity grid points are distributed over the characteristic length represented by the diameter of the vortex. In general, the particle mesh can be different from the velocity grid. Thus an independent number of particle points PP is defined that describes how many particles are seeded along the characteristic length. For the example of the particle mesh used in Figure 1 b) and d), $PP = 5$ as five particles are seeded over L_{char}.

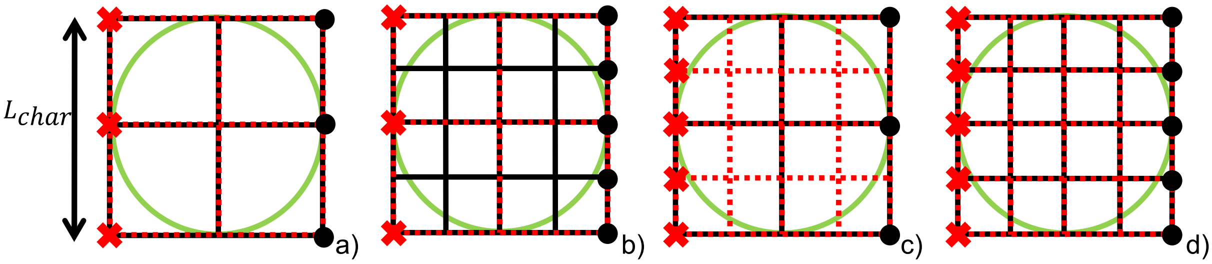

Fig. 1: Possible resolution of the FTLE grid for a vortical structure (green); a) $VP = 3$, $PP = 3$, b) $VP = 3$, $PP = 5$, c) $VP = 5$, $PP = 3$, d) $VP = 5$, $PP = 5$.

The afore-mentioned artificial double gyre comprises two horizontally meandering and counter-rotating vortices, as introduced by Shadden *et al.* (2005) for FTLE studies. This periodically varying analytical flow field is expressed by the stream-function

$$\psi(x, y, t) = 0.1 \sin\big(\pi f(x, t)\big) \sin(\pi y), \tag{4}$$

which is evaluated over the domain $[0,2] \times [0,1]$ with

$$f(x, t) = 0.25 \sin(0.2\pi t)\, x^2 + (1 - 0.5\ \sin(0.2\pi t))\, x. \tag{5}$$

For more details on double gyre flow please refer to Shadden *et al.* (2005). The characteristic length scale of the double gyre is chosen to be equal to the size of the domain in y-direction as each of the two vortices compromises half of the evaluated domain. In the following, only the results of forward integration are considered as both, repelling and attracting LCS, look alike in such an oscillatory flow. Three example results for the FTLE calculation with an integration time of 1.5 perturbation periods are shown in Figure 2. The picture in the middle shows an FTLE field calculated based on the finest considered resolution, such that $PP = VP = 1001$. Note that this resolution is defined as reference for the subsequent parameter studies, initially justified on the grounds of qualitative visual inspection. The red/yellow color denotes high FTLE values, which reveals a sharp and continuous LCS. As such, repulsion of particles normal to the LCS and a corresponding folding or stretching parallel to the LCS takes place, which is caused by the incompressibility of the fluid. Furthermore, no cross flux should occur due to the separating character of LCS being material lines (see Shadden *et al.* 2005).

Since PP and VP span a two dimensional parameter space, a subsequent systematic variation of either degree of freedom is performed. For instance, either VP stays constant and PP changes or vice versa. As expected, small variations of either parameter lead to no or negligible changes in the resulting FTLE field, which confirms the unnecessary high resolution of the reference case. Nonetheless, as the resolution becomes coarser clear differences can be seen. A coarse resolution of the particle mesh as shown on the left in Figure 2 results in a smearing of the FTLE value. No clear continuous ridge can be detected anymore, although the positions of high FTLE value do not differ from the finest resolution. In contrast, a coarsening of the velocity grid (compare Figure 2 (right)) still yields a highly resolved sharp LCS but its shape and location are changed. These observations are also made if a coarser basis resolution is chosen.

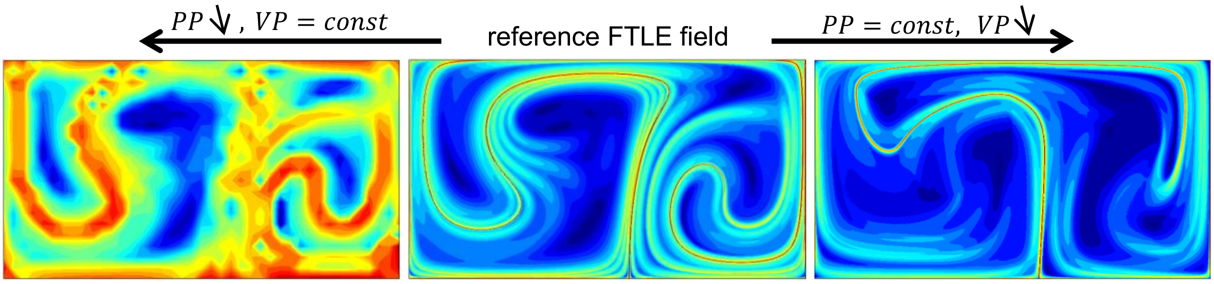

Fig. 2: FTLE field calculated for the double gyre flow with varying number of particle mesh points and velocity grid points.

Consequently, the following three important conclusions can be drawn from this simple illustrative comparison:

1. The resolution of the particle mesh determines the sharpness of the FTLE result.
2. The resolution of the velocity grid determines the shape of the FTLE ridges.
3. A highly resolved particle mesh cannot compensate for a poorly resolved velocity grid.

Relative Error

As seen before, the resolution of available velocity data has an important impact on the position of an LCS in the flow field. This is, because the FTLE can only capture the characteristics transported by the measured data. Consequently, if a defined structure with length scale L_{char} is to be found by experimental measurements, it is important to choose an appropriate resolution.

The solution of an FTLE calculation provides as many FTLE values as particles were seeded into the flow. As such, the number of FTLE values is independent of VP and a pointwise comparison of the FTLE results of varying velocity grid resolutions is possible. A relative discrepancy or error ε for a given FTLE field in comparison to the reference FTLE field can then be calculated for every particle i, expressed by the ratio of absolute difference to the sum of the FTLE values

$$\varepsilon(i) = \frac{|\sigma_i| - |\sigma_{i,ref}|}{\sigma_i + \sigma_{i,ref}}, \text{ with } i \in N. \quad (6)$$

To determine a global error estimate, the median $\hat{\varepsilon}$ of all obtained errors $\varepsilon(i)$ is taken as the characteristic measure for comparison. A distribution of $\hat{\varepsilon}$ for variations of VP obtained for different resolutions of PP can be seen in Figure 3. Given that, for instance, an error of 3% is (arbitrarily) defined as the acceptance threshold, then $VP \geq 10$ would yield the desired resolution with good LCS positioning for the double gyre flow.

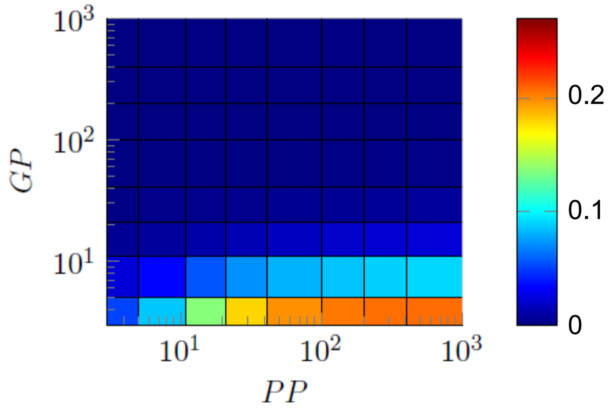

Fig. 3: Relative error distribution for the double gyre flow with varying VP and PP.

As further seen in Figure 3, the relative error increases with increasing PP. This is caused by two reasons. First, the numerical noise floor in the small FTLE values increases. Second, as an increasing PP sharpens the LCS, the spatial gradients of the FTLE become steeper. As such, the deviation in FTLE value of two particles increases faster with a higher resolution. These observations show, that if the LCS of two velocity fields are slightly shifted to each other, due to for example a small shift in camera position between two measurements, the method of relative error might lead to large discrepancies although the velocity resolution is sufficient. Hence, good confidence in the reproducibility of the data that is to be compared is mandatory for a successful application of the method.

Sum criterion

After the underlying velocity field is constructed, the resolution of the particle mesh PP has to be chosen in order to sharply capture the LCS. Because the number of seeded particles determines the number of resultant FTLE values, two different resolutions cannot be immediately compared. Therefore, the FTLE field is summed up to a total FTLE value. Regarding the development of this sum in Figure 4 a), two major observations are made. First, with changing VP and constant PP (blue arrow), the sum converges quickly towards a constant, as the FTLE calculation converges towards the highest resolution. In the second case, where VP is constant and PP changes (red arrow), the sum rises not only because the number of summed values rises with increasing PP but also the FTLE value itself increases with increasing PP. It is important to note, that the slope of the sum converges towards a straight line with inclination $2{:}1$ in loglog scale (compare Figure 4 b), which directly correlates with the particle refinement rate in two dimensional space.

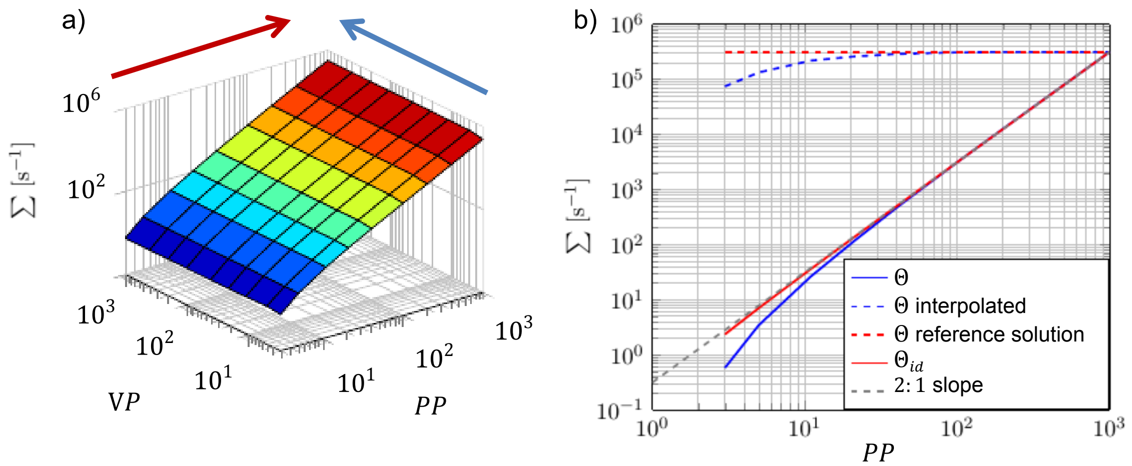

Fig. 4: Sum of FTLE values for a) span of parameter space and b) varying PP at $VP = 1001$.

This observation yields the conclusion that the FTLE value has to converge towards a constant with increasing PP. It has been shown by Shadden *et al.* (2005), that this assumption is valid if the Euclidean norm of the Jacobian is restricted with a constant k such that

$$\left\| \frac{\mathrm{d}\phi_{t_0}^{t}}{\mathrm{d}x} \right\| \leq e^{k|t-t_0|} \tag{7}$$

holds for all t. For this condition to be true, the underlying velocity field needs to be Lipschitz continuous (Verhulst 1996). If this condition is fulfilled, the sum of all FTLE values Θ can be expressed by

$$\Theta = \sum_{i=1..N} \sigma_i = \bar{\sigma} N, \tag{8}$$

where N is the number of particles and $\bar{\sigma}$ the average FTLE value. For the double gyre flow, the sum of an ideal FTLE distribution is then expressed by

$$\Theta_{id} = \bar{\sigma} N = \bar{\sigma}\,(2\,PP^2 - PP). \tag{9}$$

Knowing the mean FTLE value of the finest resolution, the actual sum can now be compared with the theoretical sum. If, for instance, a discrepancy of 3% is allowed, than $PP \geq 52$ holds for all tested VP. This theoretical estimate is confirmed by the qualitative observations. However, in practice it seems most convenient to start with a coarse PP and do a step wise refinement until the mean value does not change 'significantly' anymore.

Combination of the criteria

Both, the relative error and the sum criterion are tested for all kinds of possible combinations of VP and PP. Subsequently, a map is created that is composed of the maximum error for all possible combinations. Based on a tolerated deviation of 3 % for both criteria, the resultant error map for the forward integration of the double gyre flow can be divided into four regions, as seen in the top left of Figure 5. All results lying in the lower left corner are neither valid in terms of the sum criterion, nor the relative error, while the results in the upper right corner are denoted as valid by both criteria. As such, the combinations of PP and VP in the top right corner lead to sharp and well positioned LCS. In the other two regions only one out of the two criteria is considered as a valid data set in comparison to the reference resolution, because either the results are blurry or not well positioned. Consequently, the most efficient and meaningful result is the valid combination with smallest necessary resolution in VP and PP as this is the combination with least experimental and computational effort. As the FTLE results for backward and forward integration are simply mirrored, the results of the presented criteria remain the same for backward integration (see Figure 5, bottom left).

Kármán vortex street

The Kármán vortex street is chosen as a test flow to vary the independency of the chosen characteristic length scale and to test the applicability of the criteria in an open domain, which means that the particles can leave the region of interest. The flow field is obtained from numerical simulations at $Re = 150$. Applying the presented criteria with a characteristic length equal to the cylinders diameter yields the error maps shown in the middle column of Figure 5. It can be seen, that the slopes of the relative error criterion (black line) differ slightly between forward and backward integration due to the different FTLE results, since attracting and repelling patterns differ in shape (cp. Gollub 2015). Nonetheless, the error maps result in similar predicted optimal resolutions for both integration directions. If a different characteristic length scale is chosen, the same qualitative error maps are obtained although the quantitative values for PP and VP change. Because the resultant resolution suggestions lead to the same total number of velocity data points and particles in the whole domain, it can be concluded that the criteria are independent of the chosen characteristic length scale. Moreover, these findings also show, that the criteria are not limited to closed fluid domains as long as the flow is Lipschitz continuous and Equation (7) is fulfilled.

Piston vortex
As three dimensional test case, a numerically calculated piston vortex that travels through an open fluid domain is chosen. Here, the FTLE results of forward and backward integration differ significantly from each other (see Kaiser 2014). This example also shows significant differences in the resultant error maps (cp. Figure 5, right column). First, it should be noted that the sum criterion approaches a $3:1$ slope with increasing PP resolution, which matches the refinement rate in three dimensional space. Note that in this case the error maps indicate s tolerance level for the sum criterion of 5%. This decision is made because little refinement in three dimensional space leads to much higher computational effort and it was found, that for $PP \geq 60$ and constant VP, the change in $\bar{\sigma}$ was below 3%. Additionally, qualitative comparison supports this decision. Nonetheless, a crossing of the two criteria boundaries is only found for forward integration. Thus, for backward integration no clear combination of PP and VP that results in accurate results with clear least computational effort can be found at this stage. Instead, the examiner has to choose an appropriate set within the valid domain that matches with the available experimental and computational resources.

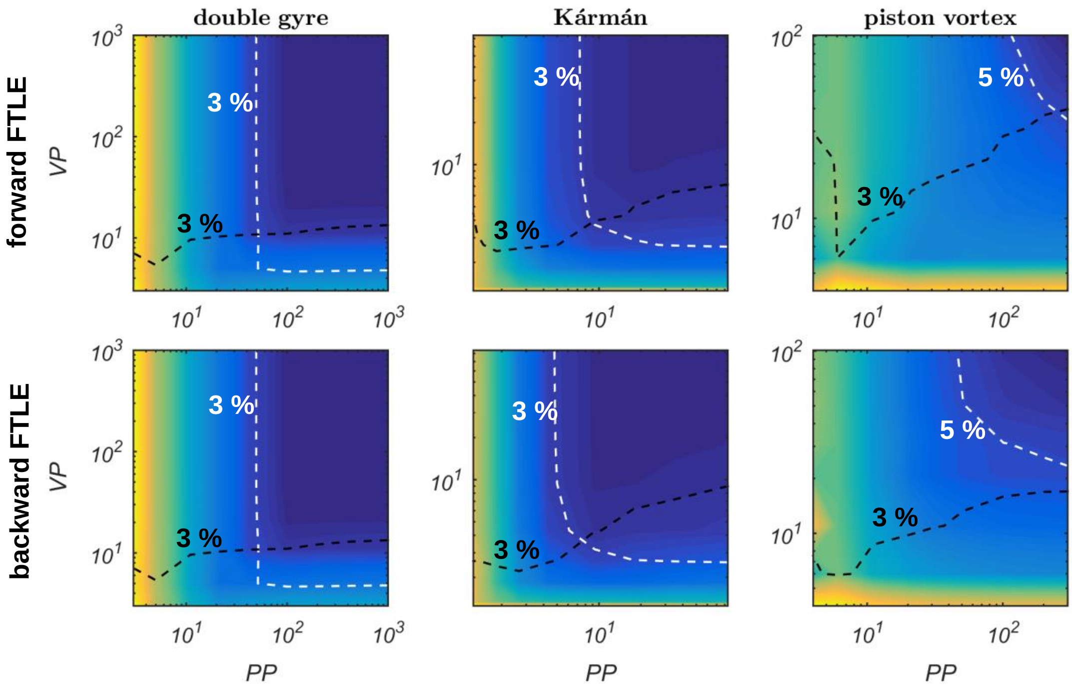

Fig. 5: Error maps for presented test cases based on the sum criterion (white) and the relative error criterion (black).

Conclusions and Future Work

Comparing the quantitative results with qualitative observations and an allowed deviation of 3%, both tested criteria show good agreement in all three test cases. It is important, that for the sum criterion to be applicable, the separation rate of particles, thus the corresponding maximum possible FTLE value has to be limited. In a closed domain such as the double gyre flow this condition is automatically satisfied, while in open flow domains the chosen extrapolation methods dominate the estimated separation rate in case a particle leaves the domain. As such, the methods used have to be Lipschitz continuous. If this condition is satisfied, the sum criterion can be used to determine the number of particles necessary for an FTLE calculation that leads to well resolved LCS. The observations further propose that there is no need to compare with a reference FTLE field of fine resolution, as the inclination of FTLE sum depends directly on the number of particles in the domain. As such, it is sufficient to evaluate the deviation of the FTLE sum with respect to the expected slope. In other words, a compari-

son of the mean FTLE value in terms of a particle mesh independence study can be carried out.
The relative error criterion determines whether the resultant LCS is in the correct position. Unfortunately, it might fail, if some particles are positioned right on an FTLE ridge that moves minimal with the next refinement level. In such cases, the relative error will locally rise significantly. Taking the median as global measurement, this disadvantage is compensated to a certain degree. Note, however, that particularly for high PP the sum of small ridge displacement might cumulate to a large deviation if the median is affected.

The resolutions for both, velocity grid and particle mesh, based on a characteristic length were found to be different for the three test cases. As such, it is not possible to make a general statement on velocity data points or particles needed through the characteristic scale of the flow field. One reason might be the additional dependence of all the results on time stepping and integration time that adds an additional (temporal) degree of freedom to the characteristic length scale needed to fully describe the unsteady flow scenarios. Despite this drawback, it is possible to find the solution necessary to obtain sharp and well positioned LCS based on FTLE calculation for all tested cases.

In future it is therefore intended to further refine the relative error criterion based on a neighbor search to compensate the disadvantages. Additionally, both criteria have to be tested on their dependence of time scaling, which also leads to the need of a third criterion determining the necessary temporal resolution of the FTLE calculation.

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