Manuscript NPG-2016-72

Title Trajectory encounter number as a diagnostic of mixing potential in fluid flows

Authors Irina I. Rypina and Larry J. Pratt

General comments The study proposes a new diagnostic for evaluation of the mixing potential of fluid flows: the trajectory encounter number. This diagnostic is for a given trajectory defined as the number of other trajectories it approaches to within a pre-defined distance during a specific time interval. The new diagnostic is demonstrated by way of two analytical flows and a data-based flow. The proposed approach is certainly of interest for mixing analyses and, due to its straightforward concept and structure, seems particularly suited for data-based studies. Moreover, the manuscript overall is well written. However, a number of scientific and technical issues arise that must be addressed in a revision in order for the manuscript to become acceptable for publication. Details are below.

Specific comments

1. Line 43: "... property exchange can take place between different water parcels ..." Mention that this exchange happens by diffusion and therefore relies on a concentration difference between two parcels. The relevance of tracer non-uniformity and the fact that mixing potential alone may not suffice is then evident.

2. Lines 49–50: "Our method does not require the initial spacing between trajectories to be small ..." Mustn't the spacing always be sufficiently small to detect the relevant spatial features that determine the mixing properties? In other words, doesn't your method therefore require comparable spacings as other methods in order to properly capture the physics? Your examples in fact employ fairly dense spacings (see also remark below). Please comment.

3. Lines 62–67: encounter number N is determined by the *first* encounter of a given trajectory with other trajectories. This relies on the assumption that in the absence of sources/sinks "most property exchange will occur during the first encounter" and in other cases "... the number of first encounters ... should still be relevant." This is a rather loose argumentation. May the concentration difference between parcel A and B (also in the absence of sources/sinks) not just as well be *larger* – causing *more* property exchange – on e.g. a *second* encounter due to property exchange of parcels and A and B with other parcels in between their first and second encounters? Please provide a stronger physical rationale for this first-encounter ansatz or present it more explicitly as an assumption or hypothesis.

4. Lines 84–86: "... encounter rates ... are locally the largest near a hyperbolic trajectory and along the segments of its associated stable manifolds ..." This exclusive link with stable manifolds is unclear. Don't the high encounter rates result from the rapid dispersion of fluid parcels due to exponential stretching in the homoclinic/heteroclinic tangles delineated by interacting (un)stable manifolds of hyperbolic points? In other words, don't stable and unstable manifolds contribute equally to the high encounter rates in chaotic regions? Hence, it seems more accurate to correlate regions of high N with such tangles instead of only with stable manifolds. Please either better explain the (assumed) role of stable manifolds or link the behaviour with chaotic tangles.

5. Lines 93–94: "... will reveal longer segments of stable manifolds ... illustrated numerically in the next section." It actually more and more seems to reveal the abovementioned homoclinic/heteroclinic tangles instead of the stable manifolds. Consider to this end the Duffing oscillator in Sec. IIa. Here the stable and unstable manifolds of the hyperbolic point form a pair

symmetric about $x = 0$ (as remarked on line 126). Their interaction yields a homoclinic tangle that delineates a figure-8 region about the two islands in Fig. 1. This tangle – and thereby *both* manifolds – coincides with the region of highest encounter rates in Fig. 2. Results on the Bickley jet in Fig. 4 further seem to support this; here correlation actually occurs with the heteroclinic tangles delineated by the interacting (un)stable manifolds of the 3 hyperbolic points instead of only with the stable manifolds. Please comment and, if necessary, modify the discussion.

6. The discussion of Fig. 2 implies that the encounter number indeed adequately captures the dynamics. However, to this end rather smooth distributions (as e.g. in Figs. 2–4) seem necessary, suggesting that the method requires a dense spacing of initial parcel positions in order to work properly. This contradicts the statement "... does not require the initial spacing between trajectories to be small ..." (lines 49-50). Moreover, this suggests that mixing analyses by the encounter number may in fact be far more expensive than standard Poincaré sectioning (typically requiring only a few dozen parcels). Please comment and, if necessary, modify the discussion.

7. The above suggests that Poincaré sectioning outperforms the encounter-number method in periodic flows. Hence, the periodic examples mainly serve to demonstrate the physical validity of the encounter-number method; its true usefulness seems to be for essentially aperiodic flows as e.g. the Gulf stream flow (Sec. IIc). However, the analysis of this flow is rather superficial and open-ended (lines 209–230). It is recommended to deepen this analysis so as to convincingly demonstrate the potential of the method (in particular) for aperiodic flows.

8. Sec. III: it is recommended to demonstrate validity of expressions (1), (2) and (9) for N by comparison with N found via actual parcel trajectories of the corresponding simplified flows.

9. Lines 310–311: "... vector flux of the scalar of interest. This linkage is made explicit by ..." This same concept of a net scalar flux (and corresponding trajectories) is in fact also adopted in studies on convective heat transfer and chemically-reacting flows [1, 2, 3, 4, 5]. Please mention this for a stronger connection with similar research and literature.

10. Line 324: "Although this lack of uniqueness may seem troublesome ..." This ambiguity is in fact resolved in [5] by attaching physical validity to such an additional vector instead of treating it as an arbitrary field (see also remark below).

11. Lines 347–348: "... it is most convenient to make use of the flexibility in the definition of the tracer flux ..." This suggests that the method produces arbitrary results and its physical meaning therefore is questionable. However, this approach can in fact be provided with a sound physical basis using the approach following [5]. Key to this is that, given linear transport equations, a scalar field c governed by a transport equation of the form (10) admits expression as the difference between two other physically-meaningful scalar fields c_A and c_B, each governed by

$$\frac{\partial c_A}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{F}_A = S_A, \qquad \frac{\partial c_B}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{F}_B = S_B, \tag{1}$$

with $\boldsymbol{F}_{A,B}$ and $S_{A,B}$ the corresponding fluxes and source terms, respectively. In [5], $S_A = S_B = 0$ and $\boldsymbol{F}_A$ and $\boldsymbol{F}_B$ are diffusive flux and advective-diffusive flux, respectively, of the same initial condition $c_A(\boldsymbol{x}, 0) = c_B(\boldsymbol{x}, 0) = g(\boldsymbol{x})$. In the current manuscript, also $S_A = S_B = 0$ yet $\boldsymbol{F}_A$ and $\boldsymbol{F}_A$ now both are the advective flux (i.e. $\boldsymbol{F}_{A,B} = \boldsymbol{u}c_{A,B}$) of the *different* initial conditions $c_A(\boldsymbol{x}, 0) = c_0$ and $c_B(\boldsymbol{x}, 0) = C_0(\boldsymbol{x})$. Hence, both problems, though physically different, allow for treatment by the same concept. Transport of difference $c' = c_B - c_A$ is governed by

$$\frac{\partial c'}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{F}' = S', \quad \boldsymbol{F}' = \boldsymbol{F}_B - \boldsymbol{F}_A, \quad S' = S_B - S_A, \tag{2}$$

with here $S' = 0$ and $\boldsymbol{F}' = \boldsymbol{u}c' = \boldsymbol{u}(c_B - c_A)$ the flux of c' (i.e. the anomaly and its flux in line 348). Thus anomaly c' in fact concerns the scalar transport relative to a physical reference state c_A instead of some arbitrary state. Here the reference state happens to remain uniform in time due to the advective transport of a uniform initial condition, i.e. $c_A(\boldsymbol{x}, t) = c_A(\boldsymbol{x}, 0) = c_0$, yet the approach holds equally for any non-uniform (evolving) state c_A (enabling its employment also for more complicated problems).[1] Moreover, note that $\boldsymbol{u}$ needn't be divergence-free. It is recommended to modify the discussion in Sec. IV according to the above in order to eliminate the (incorrect) impression of a conceptual flaw in the method.

Minor technical issues and corrections

1. Figs. 2–4: specify the spacing of the initial parcel positions.
2. Line 153: pronounces → pronounced
3. Line 231: the title of Sec. III is rather long and confusing. Please consider a more compact title.
4. Line 266: reference moving → reference frame moving

[1] A. Bejan, Convection Heat Transfer, Wiley, New York (1995).

[2] V.A.F. Costa, Bejan's heatlines and masslines for convection visualization and analysis, Appl. Mech. Rev. 59 (2006), 127.

[3] S. Mahmud, R. A. Fraser, Visualizing energy flows through energy streamlines and pathlines, Int. J. Heat Mass Transfer 50 (2007), 3990.

[4] A. Mukhopadhyay, X. Qin, S. K. Aggarwal, I. K. Puri, On extension of "heatline" and "massline" concepts to reacting flows through use of conserved scalars, ASME J. Heat Transfer 124 (2002), 791.

[5] M. F. M. Speetjens, A generalised Lagrangian formalism for thermal analysis of laminar convective heat transfer, Int. J. Therm. Sci. 61 (2012), 79.

[1] Reference state c_A in [5] e.g. corresponds with the non-uniform and unsteady temperature field due to diffusive heat transfer only; $c' = c_B - c_A$ is the contribution to the total advective-diffusive temperature field c_B due to the flow $\boldsymbol{u}$ (i.e. $c' \neq 0$ only if $\boldsymbol{u} \neq \boldsymbol{0}$) and thus captures the thermal transport that is effectively induced by the fluid motion.