Automated Tracking of 3-D Overturn Patches in Direct Numerical Simulation of Stratified Homogeneous Turbulence

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Abstract. Direct numerical simulation is a valuable tool for modeling turbulence, but like "wet lab" simulation, it does not solve the problem of how to interpret the data. Manual analysis, accompanied by visual aids, is a time consuming, error prone process due to the elaborate time-dependent structures appearing in simulations. We describe a technique based on volume tracking, that enables the worker to identify and observe evolving coherent flow structures, eliminating uninteresting background data. Using our techniques we were able to investigate 3-D density overturns in stably stratified homogeneous turbulence, understand entangled physical structures and their dynamical behavior. We describe our technique, which improves on past work by incorporating application-specific knowledge into the identification process. Such knowledge was vital in filtering out spurious information that would have interfered with the experimental method. Representative results are shown which summarize the physical insight gained by the application of the above identification/tracking method.

1   Introduction

Turbulence and turbulent mixing in an ambient stratification, with or without a background shear, are salient small-scale phenomena in the dynamics of geophysical flows. It is through the associated processes that diapycnal mixing and vertical transport of momentum, nutrients and chemicals are effected in naturally stratified fluid bodies, typical examples of which are the thermoclines of the ocean and lakes. In stratified flows, overturns, i.e. regions where heavy fluid

resides over light within the same fluid column, are viewed as an indicator of the ability of the turbulence to overcome the stabilizing effect of the mean stratification and are thus considered active sites of stirring and mixing. Insight gained through the study of the structure and dynamics of overturns often serves as the foundation for parameterization of subgrid scale turbulence and mixing in large scale models. However, ocean measurements of overturns are incomplete because they are restricted to 1-D vertical profiles of density and single-time snapshots of the overturning event. As a result, conflicting interpretations ensue [6,7]. Although laboratory experiments contribute some partial insight into an improved understanding of overturning events, the only way one can obtain the full 3-D detail and temporal evolution of one of these phenomena is through Direct Numerical Simulation (DNS).

The conventional overturning event, often the focus of stratified flow DNS studies, is a single event as described by the roll-up of a vortex sheet overlaid on a vertical density step–referred to as a "stratified shear layer" [14]. However, a turbulent region in the field may consist of a population of overturns dynamically interacting among themselves. Examples are the flow established after the breaking of an internal gravity wave or at the interior of a stratified shear layer at a later time in its evolution. A very accurate approximation to the above two phenomena is stably stratified homogeneous sheared turbulence, the flow we focus on.

Although we have been able to visualize the entire population of 3-D overturns, evaluate the prevalent dynamical balances within the population and calculate their collective contribution to the flow's energy budgets as compared to the rest of the flow [2], we were neither able locally identify a 3-D overturning patch and delineate a zone of influence around it, i.e. a "halo", nor track the patch forward and backward in time. To this end, we devised a technique, and an accompanying library, called MOLD (Managing Overly Large Data Sets) [12], which we present here.

With the aid of MOLD we were able to show that diapycnal mixing within the flow is confined primarily to the halo regions. We were also able to perform a census of the overturn population at a given time and in particular, correlate the age of overturns with a variety of geometric and energetic quantities, which may help scrutinize conflicting theories in this field of research. Monitoring of the evolution of single representative overturns was also possible, increasing our qualitative understanding of these events. Lastly, we were able to compress data sets, by discarding uninteresting data outside the field of interest.

2   Direct Numerical Simulations

We have carried out our computations using DISTUF [5], which performs direct numerical simulations (DNS) of incompressible stably stratified homogeneous sheared and unsheared turbulent flows. The significance of DNS is the elimination of turbulence closure models thus allowing recovery of the fundamental physics directly from simulation results. Complete resolution of all relevant scales

is therefore required. The number of computational grid points needed is proportional to the $Re^{9/4}$, where Re is the integral scale Reynolds number [15].

DISTUF solves the three-dimensional, time-dependent Navier–Stokes, continuity and density equations under the Boussinesq approximation. The numerical solution methodology employs 2nd order finite differences with periodic boundary conditions in all three spatial directions, while allowing the flexibility for shear periodic boundary conditions in the vertical when a background shear is present [5]. The output of DISTUF passes through a post-processing phase (described below) before being written out to disk. The output consists of 4 single precision variables, defined at the locations of a 3-dimensional uniform mesh: density and vector-valued velocity.

Nomura and co-workers have previously employed DISTUF in studies of the structure and dynamics of small-scale turbulence in sheared an unsheared flows (see reference no. [3] for a list of previous publications).

In the present work, the simulations performed were at the relatively low microscale Reynolds number range, $20 < Re_\lambda < 30$. The Prandtl number employed was that of air, $Pr = 0.7$. These non-dimensional parameter values stem from computational restrictions [2]. The initial turbulent Froude number of the flow, Fr, was in the range $0.5 < Fr < 2$.. The Froude number represents the relative strength of the inertial forces in the fluid with the respect to the restoring effect of gravity. For a discussion of the physical significance of all other non-dimensional parameters see Diamessis [2].

3   Overturn Phenomena

To identify overturn structures we first apply a technique called Thorpe-sorting [10], which sorts all vertical density profiles in the flow into monotonically stable ones (density decreases with height). The Thorpe displacement, $d(z)$, is the distance a particle in the initial profile is displaced during the sorting. An overturn patch is defined as a contiguous 3-D volume of fluid with $d(z) \neq 0$. For the purpose of conditional sampling and visualization we can then define an *overturn identifier function*, which is a 3-D integer array marking each point in the flow as part of an overturn patch or "non-interesting". A peripheral zone of influence bearing high energetic importance is found to surround all patches [2]. One of our objectives is to quantify the contribution of these peripheral zones, or "*halo*" to the energetics of the overall flow. The thickness of this peripheral zone of influence is dependent on the energetic quantity of interest and generally, this thickness increases with the bounding box height of a feature (i.e. patch). We use an empirical function of patch height to set the halo thickness. Possible improvements to this function based on more physical arguments are discussed in Diamessis [2]. Note also that an unnecessarily thick halo will increase excessively the size of output. Fig. 1a, shows the halo region faithfully following the contour of the exterior surface of a 3-D patch.
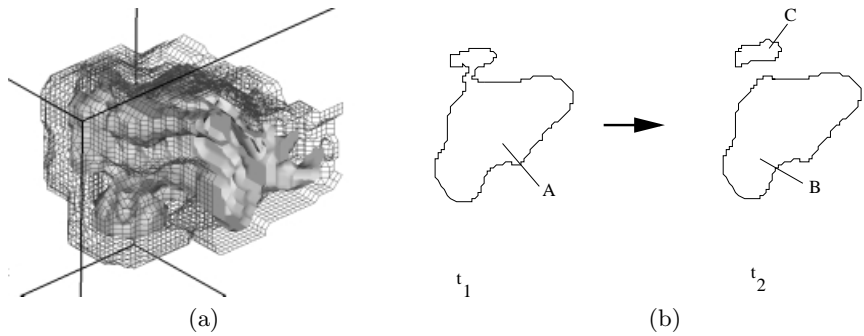
Fig. 1. (a) External surfaces of 3-D overturning patch (opaque) and associated halo region (wireframe contour). (b) An idealized 2-D sketch the pinch-off of a small region of overturned fluid from a large one, attached by a thin strand of fluid. The smaller overturn may eventually re attach to an adjacent larger patch. Time advances in the direction of the arrow.

4   Automated Tracking of Overturn Phenomena

Our primary objective is to follow forward (backward) in time any feature of choice at a given frame along with any offsprings (parents) it may have in subsequent frames. The immediate offspring (parents) of this feature must be governed by the same dynamical process. Only then will the geometrical/energetic information obtained by monitoring the "legacy" of this feature be reliable.

In order to meet our objective, we devised a procedure for tracking the time evolution of the features. The procedure begins by determining the connected components in the overturn objective function mentioned previously [8]. Each connected component identifies a set of points–which we call a "patch"– where the overturn identifier function is true and each point in the patch is connected to at least one other point in the same patch. These properties ensure that all points in a given patch are connected to each other by some path, and that no point has a path to a point in another patch.

Once the patches have been identified, we can track backward toward their genesis–or formation by a merger–and also forward to their eventual extinction. We began with Silver's *volume tracking* technique, which follows the creation, destruction, and evolution of patches [13]. The basic technique is to examine all identified features in the current frame, and to intersect the features against the features of the previous and subsequent frames. Based on the volume fraction of overlap (or no overlap at all) we identify four types of events: merger, splitting, creation, and destruction [13]. Using this information, we can then determine if a patch has broken up into "children" features, has disappeared from the flow, or is an entirely new feature.

When persistent high velocity gradients are present in the flow as in the case of strong localized turbulent advection or, in the case of a sheared flow, shear

distortion[1] the tracking algorithm may produce spurious output. If not filtered out, such output may lead to erroneous interpretations of feature physics and the incorrect determination of critically important quantities, such as the *age* of the feature. An example of such a situation may be a small fragment of one patch which pinches off and reconnects to an adjacent patch of totally different dynamical character.

Locally, any small volume of overturned fluid connected by a thin strand of fluid to a larger patch (Fig. 1b) may eventually pinch off due to the straining of the local turbulent flow or the mean shear. Smaller patches may then unexpectedly appear. We found that, if not treated carefully, such small patches can significantly complicate the feature-tracking results by indicating either spurious or dynamically insignificant children (or parents). Such offspring (or parents) can not only complicate but also mislead the tracking process.

We had to modify Silver's algorithm by filtering the tracking output in order to avoid spurious or dynamically insignificant events. The filtering occurs in the case where a feature has multiple children (parents), while tracked forward (backward) in time. In particular, we accept the split (merger) of a feature into (from) two offsprings (parents) only when the offspring have a volume of 0.25 to 2 times (0.25 to 1 times) that of the original feature, when we are tracking in the forward (backward) direction. In the forward direction we wish to avoid two pathologies:

1. *Multiple small features as offspring:* These small features result from the aforementioned pinch-off mechanisms and may either proceed independently to vanish through gravitational collapse or diffusion or eventually attach themselves to other larger features which exhibit totally different dynamics from the main feature under consideration.
2. *Extremely large features as offspring:* These usually result from the rapid attachment of one of the small features mentioned above to an adjacent larger feature. MOLD identifies as the first of all offspring the one most similar geometrically to the original feature. Thus, if a feature has more than one offspring all features, following the first one in the list of descendants, with volume 2 times greater that of the original one are rejected.

With backward tracking, we want to exclude mergers of features which are not of comparable size. For example, a small patch pinches off large patch (A) to rapidly attach itself to another large patch (B). When B is tracked backward in time, A is erroneously treated as a slightly removed parent. Thus, all features of 1/4 the volume of the original one are not tracked backward in time.

An additional complication of intensity increasing with Froude number, Fr of the flow (where the turbulence becomes more energetic and the features more space-filling) is that induced by the formation of a large patch (of height comparable to that of the computational box) which occupies a large fraction–roughly 10 %–of the flow volume. At a time, t_L, subsequent to the initial appearance of

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[1] By shear distortion we mean any geometrical deformation a continuous volume of fluid undergoes due to the local velocity differences associated with the mean shear.

this spatially dominant patch, several smaller offspring of have emerged in the flow due to either the aforementioned pinch-off mechanisms or the gravitational collapse of the patch and its separation into smaller parts. When attempting to compute a patch census at time t_L, one obviously observes several patches of the same age as all patches at this time have their heritage traced back to the same aforementioned dominant patch. To obtain a meaningful census at time t_L we retain only the patch which maps the closest to the original dominant one in terms of geometry. When correlating a given energetic quantity with patch age at time t_L it is found that the value of this quantity for the retained patch dominates its average value computed over all patches of the same age before the filtering process was performed (not shown).

Finally, to maximally free the tracking from any of the above aforementioned spurious effects, we tracked very computational timestep. A more efficient strategy might be to track features adaptively, whereby small features are tracked more frequently than larger ones.

5   Results

We ran DISTUF on an UltraSPARC III uniprocessor. In this paper, we employ a grid resolution of 128^3 and we run for 10.0 dimensionless time units–at 256 time steps per time unit. Such a computation pushes the limit of a workstation, which completes a simulation in about 20 hours. We are interested in ultimately exploring higher, more realistic Reynolds number flows, and are separately exploring a scalable parallel implementation [9]. However, our purpose here is to demonstrate the feasibility of our approach on smaller scale flows. Note that due to the multiple complications introduced by a background shear (§4) we limited our simulations to stratified unsheared flows.

Using MOLD we were able to compare the contribution of the patch halo zones to the flow's energy budgets. Diamessis [2] found that the contribution of the patch interior to the diapycnal mixing in the flow was minimal. Visualizations however, did suggest that significant diapycnal mixing occurred in the overturn periphery. MOLD allows us to quantify the diapycnal mixing occurring throughout the halos of all patches in the flow. Fig. 2a indicates that the percentage of total diapycnal mixing occurring within the patches and their halos exceeds the corresponding volume fraction by 10 to 20 %. When the overturns occupy a large fraction (>60 %) the patch halos are where diapycnal mixing is concentrated in the flow.

We were also able to perform a census of all the overturns in the total flow at selected times. Figure 4b shows a patch Reynolds vs. Froude number activity diagram [2,11] for the entire overturn population at selected times of an unsheared $Fr = 1.2$ run. The patches transition from a phase of inertially driven growth to one of gravitational collapse and finally to a viscous-diffusive-buoyant balance of constant patch Rayleigh number [2]. The most important aspect of MOLD, however, is the backward tracking capability, which enabled us to compute the age of each member of the overturn population at a given time of
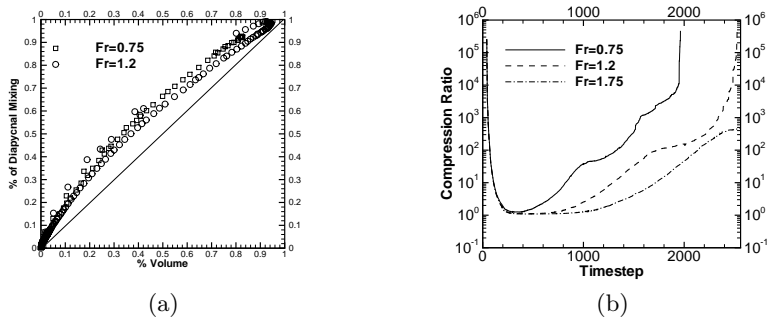
(a)   (b)

Fig. 2. (a) Flow volume fraction occupied by overturn patches and their halos vs. the percentage of the total flow diapycnal mixing occurring within the corresponding regions. Symbols correspond to regularly sampled frames throughout the run evolution. (b) Compression ratio varies over time and is sensitive to the initial turbulent Froude number, Fr. A larger value of Fr is associated with a higher volume-fraction of patches and thus the degrades compression. One non-dimensional timestep is $\Delta t = 1/256$.

interest. We can then correlate age with a variety of geometric and energetic quantities, which allows us to comment on various conflicting theories in the field of ocean microstructure research [7,6]. Figure 3 shows such an example (before and after the age filtering process discussed in §4), a scatter plot of age vs. the length-scale ratio $L_R/\langle L_{T_{3Dmax}}\rangle$ (see Diamessis [2] and [10] for definitions of these length-scales). Time is scaled with the buoyancy frequency N [2,16]. Although the low Re_λ of our DNS doesn't allow us to run the simulations for $Nt > 10^2$, at more advanced times in the flow evolution (Nt> 1.4) one notices a tendency of the length-scale ratio to drop with patch age. This supports Gibson's claim [6] that $L_R/\langle L_{T_{3Dmax}}\rangle$ drops with patch age in contrast to the shear layer findings of Smyth et al. [14]. However, a more detailed investigation of the effect of Re_λ and general flow conditions (i.e. one single event vs. a population of them, overturning instigated at a larger scale vs. the smallest ones etc.) on the above correlation is required before any definitive conclusions are reached.

Although it does not bear full statistical importance, monitoring a few representative individual overturns can give valuable insight into the dynamical evolution of these events. To this end, we identify an overturn of interest at a given time, track it backwards and forwards in time, and plot the time-series of geometrical and energetic quantities. At the meantime an animation of an individual feature along with the associated vortical structures that generate it can also provide an improved understanding of overturn dynamics. Figure 4a shows the activity diagram trajectory of a feature (and its parents) for a $Fr = 1.2$ run. The feature was isolated at a later time of the run. The trajectory is indicative of the aforementioned three phases in patch evolution.

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[2] Turbulent patches in the field are believed by some researchers [6] to have ages in the range $0 < Nt < 1000$.
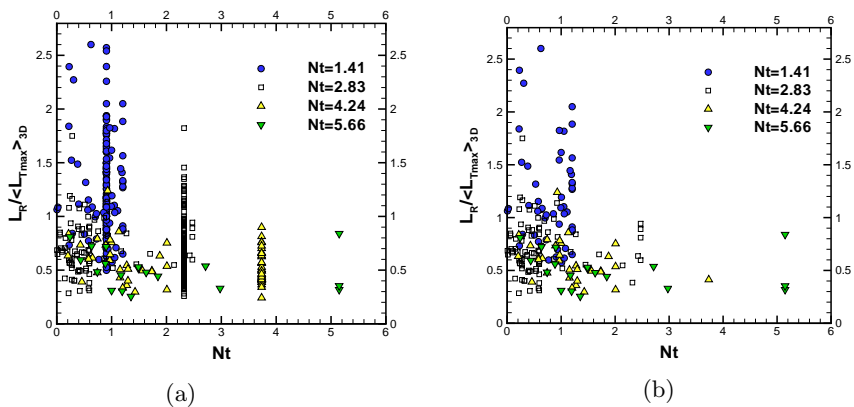
Fig. 3. Scatter plots of the lengthscale ratio $L_R/\langle L_{T_{3Dmax}}\rangle$ vs. age in buoyancy units. Patch population sampled at select times during a $Fr = 1.2$ run. (a) Before filtering process discussed in §4. (b) After filtering process.
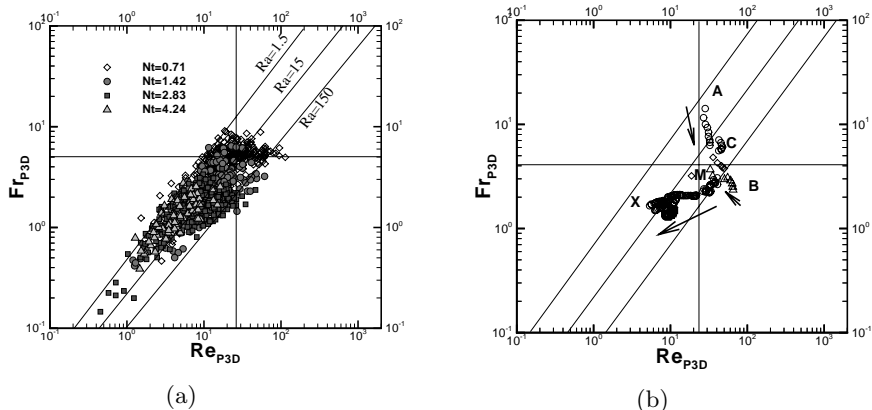

Fig. 4. Activity diagrams for $Fr = 1.2$ run. Shown are lines of critical patch Froude and Reynolds numbers. Diagonal lines are lines of constant patch Rayleigh number. (a) Overturn population at select times. (b) Trajectory of a representative individual patch identified at time $Nt \approx 5$ and tracked backward and forward. A,B and C represent locations of generation of first parent patches, M is location of mergers and X is location of termination of patch lifetime. Arrows indicate advancement in time.

6   Discussion and Conclusions

We have demonstrated automated tracking techniques that enabled us to meet our objectives of increasing the knowledge about overturn phenomena, which are only partially understood. We have implemented our techniques through the

MOLD library [12]. MOLD is also able to compress datasets, by eliminating background data which can safely be ignored. We realized a factor of 2.8 in compression, but compression increases to about 22 when halos are eliminated. We can use this capability to support animation, which requires an increased sampling frequency in time. We note, however, that when following a single feature, we can reduce data access time significantly, since MOLD will access only the data demanded.

With increasing computational power it is vital that data sets contain the minimal amount of data needed to enable scientific discovery. Users are beginning to accept that they can no longer archive large datasets, but rather, must maintain large data sets on-line (see for example Data Cutter[1]). The methodology offered by MOLD supports this technological climate, and offers the possibility to provide *adaptive storage and retrieval* of large scientific data sets.

We are currently applying MOLD to the study of Taylor-Green vortex instability. In this case, there is no halo, and the structures are compact. We expect MOLD to realize qualitative reductions in disk storage requirements. This work will be carried out on a parallel version of DISTUF, called KDISTUF [9], which has been written with the KeLP system [4].

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