Large eddy simulation of the velocity-intermittency structure for flow over a field of symmetric dunes

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Large eddy simulation of the velocity-intermittency structure for flow over a field of symmetric dunes

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Because of their frequent occurrence and importance in the natural environment, there has been significant interest in refining our understanding of flow over dunes and other bedforms, in particular, their shear layer and flow structure characteristics. However, field-based studies, are reliant on single-, or multi-point measurements, rather than delimiting flow structures from the velocity gradient tensor as is possible in numerical work. Here, we extract pointwise time series from a well-resolved large-eddy simulation to connect these two approaches. The at-a-point analysis technique is termed the velocity-intermittency quadrant method and relates the fluctuating, longitudinal velocity, $u_1(t)$, to its fluctuating pointwise Hölder regularity, $\alpha_1(t)$.

Despite the difference in boundary conditions, our results agree very well with previous experiments, showing the importance, in the region above the dunes, of a quadrant 3 ($u_1 < 0$, $\alpha_1 < 0$) flow configuration. This reflects the formation of hairpin-like structures that form within the shear layer shed from the dune crest. Despite a more active background turbulence level, these large-scale hairpins are a more keenly expressed feature of the flow than the smaller scale features found in a boundary-layer. The quadrant 3 behaviour was less evident when averaging results over four dunes and sixteen transverse locations as this merged together two forms of behaviour. Hence, a clustering technique was used to determine the different groupings in the data, and the quadrant 3 behaviour was prevalent in much of the outer flow when this method was adopted.

Our higher density of sampling beneath the shear layer and close to the bedforms relative to past experimental work reveals a negative correlation between $u_1(t)$ and $\alpha_1(t)$ in this region. This consists of two distinct layers, with quadrant 4 ($u_1 > 0$, $\alpha_1 < 0$) dominant near the wall and quadrant 2 ($u_1 < 0$, $\alpha_1 > 0$) dominant close to the lower part of the separated shear layer. These results are consistent with near-wall entrainment of vorticity into the reattachment region, and entrainment of slow moving and quiescent fluid into a faster, more turbulent shear layer. Thus, our results shed further light on the characteristics of dune-flow in the near-wall region and how that useful information on flow structure can be obtained from single-point, single velocity component measurements.

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1. Introduction

Deformation of an erodible substrate into large-scale bedforms such as dunes, makes understanding turbulence transport in aeolian, fluvial and marine environments complex (Fourrière et al. 2010). While the transport of erodible sand or gravel is a function of instantaneous forces or their time integrated effect (impulse), the development of bedforms affects the spatial distribution of such forces, feeding back into the potential for further erosion to take place (Jackson 1976; Best 2005). Dunes are observed, and are deemed of significance to the dynamics of near-surface boundary layers in various planetary environments (Titus et al. 2015). As a consequence, there have been extensive field studies of flow over such features in aeolian (Lancaster et al. 1996; Wiggs et al. 1996) and fluvial or marine environments (Kostaschuk & Villard 1996; Osborne & Rooker 1999; Kostaschuk 2000; Shugar et al. 2010) as well as many experimental studies (Nelson et al. 1993; Bennett & Best 1995; Venditti & Bennett 2000; Dumas et al. 2005).

While there are also examples of older numerical studies studying the flow structure in these environments (Salvetti et al. 2001; Parsons et al. 2004), it is only recently that high resolution, eddy-resolving numerical studies have been performed (Zedler & Street 2001; Stoesser et al. 2008), and flow structure generation mechanisms have been considered using numerical models (Omidyeganeh & Piomelli 2011, 2013a,b; Chang & Constantinescu 2013). In the context of the two-dimensional dunes that have tended to form the emphasis of previous experimental work (Bennett & Best 1995; Venditti & Bennett 2000; Stoesser et al. 2008; Omidyeganeh & Piomelli 2011; Chang & Constantinescu 2013), recent work has focused on the generation mechanisms behind the large-scale hairpin features generated in such flows, with a variety of mechanisms proposed:

- Stoesser et al. (2008) suggested that these structures are produced close to reattachment of the separated shear layer (SSL) that is generated close to the dune crest;
- Omidyeganeh & Piomelli (2011) focused on the vortex tubes associated with the Kelvin-Helmholtz vortices that are produced in the SSL. They found that the hairpins were a consequence of disturbances to these structures owing to the presence of other structures in the outer part of the dune flow;
- Chang & Constantinescu (2013) examined this looking not only at a fully developed flow with periodic boundary conditions, but also at spatially developing transitional flow where the subdued activity of the smaller scales made identification of the mechanism responsible for the formation of the large-scale coherent structures much clearer. They found that the vortex tube induced by the dune upstream is transported above the SSL of the dune downstream, giving it a greater mean velocity, while retaining more coherence. As the upstream tube passes (and perhaps touches) the tube in the SSL, significant distortion results, leading to the observed hairpin structures that scaled with dune size. Hence, there are some similarities here to the generation of much smaller hairpin structures in the boundary layer (Robinson 1991; Christensen & Adrian 2001; Ganapathisubramani et al. 2003) in terms of velocity gradients inducing lift-off and distortion of initially tranverse-oriented tubes of vorticity. However, the pre-existence of a SSL, and the association with fixed spatial positions (dune crests), rather than a spatially pseudo-random
autogeneration, means that the integrated effect on the velocity structure at a particular location are likely to be very different. In addition to the large-scale hairpins, other types of large scale coherent structures are present in flow over large scale roughness, including “superstreaks” that scale with the size of roughness elements, and koks. These kolk vortices form when the large-scale hairpins interact with the flow field of the dunes downstream (Babakaïff & Hickin 1996; Grigoriadis et al. 2009).

One means of characterising this structure is in terms of the relation between velocity and intermittency and, recently, it has been shown that the outer part of flow over bedforms has a different coupling between the longitudinal velocity component, \( u_1 \), and the intermittency in the dynamics of this signal (Keylock et al. 2013), compared to the structure of boundary-layer flows, jets and wakes. This result has been confirmed by Keylock et al. (2014b) for a dune flow dataset collected under very different experimental conditions (various measuring positions about fixed dunes as opposed to one measuring position and mobile bedforms advected beneath the probe). While the previous experimental studies were able to resolve consistent information on the nature of the velocity-intermittency structure in the outer part of a flow over bedforms, the experimental design for those studies meant that limited information was available beneath the dune crest (the inner flow region). In order to gain an insight into the flow structure in this region, this study uses Large Eddy Simulation (LES) (Sagaut 2002; Geurts 2003; Keylock et al. 2005) to study the flow over sinusoidal bedforms. The simulation provides additional insights into the velocity-intermittency structure of turbulent flow over bedforms, particularly in the near-wall region. In addition, the ability to explain the velocity-intermittency results in terms of the resolved coherent flow structures demonstrates the effectiveness of our quadrant method (Keylock et al. 2012) for capturing flow structure information from single-point, single velocity component data.

The paper is organised as follows: First, we describe the numerical domain and properties of the numerical simulation, as well as validation of the code against previous experimental and numerical studies; Second, we explain the background to, and specific calculation procedure for the velocity-intermittency analysis; The methods section concludes with an explanation of the data clustering/classification technique used to group the 2048 time series analysed into discrete categories; The results section describes vertical profiles of mean velocity and turbulence quantities before examining the correlation between velocity and intermittency at various locations in the flow domain. These correlations are then disaggregated using our quadrant methodology to reveal greater structure to the flow than the correlations imply; The velocity-intermittency structure of the outer and inner regions are then described and linked to the nature of the flow structure at these respective locations.

2. Methods

2.1. Numerical methods and flow domain

The numerical simulations were undertaken using a nondissipative, parallel, finite-volume LES code (Pierce & Moin 2001), which solves the incompressible Navier-Stokes equations on a nonuniform Cartesian mesh. The fractional step algorithm uses a staggered conservative space-time discretization with a semi-implicit iterative method to advance the equations in time. The algorithm is second-order accurate in both space and time. The
numerical method discretely conserves energy (Mahesh et al. 2004) and uses strictly nondissipative (central) discretizations to solve for the momentum and pressure. The subfilter-scale viscosity in the viscous terms is calculated dynamically from the resolved velocity fields (Germano 1992; Pierce & Moin 2001). The flow was driven by imposing the mass flow rate, and the boundary condition at the free-surface was a slip-symmetry condition, where the normal velocity component and the vertical derivatives of the horizontal velocity components were set to zero ($\partial u_1/\partial y = \partial u_3/\partial y = 0$). The dunes were represented with a stair-step approximation, with no slip on each element of the dune surface.

Additional details concerning the numerical method, as well as validation studies are given in Chang et al. (2006, 2007); Chang & Constantinescu (2013, 2015). Grid convergence work was undertaken to underpin the mesh design in those studies. However, it should be emphasized that because of the need to obtain physically meaningful Hölder exponents from the numerical model, which is a more stringent requirement than the appropriate resolution of large scale flow structures, the present study was undertaken on a much finer numerical mesh than these past studies. Indeed, the mesh for the current study was six times finer at 5 wall units (and vertically, 2.5 units in the dune region) than in the simulations reported by Chang & Constantinescu (2013). Hence, the first mesh point is within the viscous sublayer, removing the need for wall functions, and dramatically reducing any dependence on the subgrid model physics. Furthermore, the mesh refinement used in the present study was close to that required by Direct Numerical Simulation (DNS) at the same channel Reynolds number. Hence, because the subgrid scale viscosity from the dynamic Smagorinsky model goes to zero in regions where the resolution approaches that for a well-resolved DNS, this provides another means by which the simulation’s dependence on the representation of subgrid scale physics is reduced.

The numerical domain is shown in Fig. 1 and relevant properties, including the number of computational cells used in each direction, $N_{x,y,z}$, and their size, $\Delta_{x,y,z}$, are given in Table 1. Because the large-scale ‘super-streak’ structures have a streamwise extent greater than that for one dune (Kruse et al. 2003), to capture such structures accurately in a simulation with periodic boundary conditions requires a domain at least three times the length of this structure so that periodic constraints do not impact on the inferred dynamics of the vortices. Hence, the computational domain here, spanning four dune wavelengths, exceeds that in most previous studies. The particular bedforms used in this study were motivated by the work of Günther & von Rohr (2003). Such symmetrical dunes arise in nature when a mobile bed is subject to an oscillating flow, as occurs in tidal environments.
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Table 1. Properties of the flow domain and the mesh for the numerical experiment. The channel height, $h_c$, and inlet depth-averaged, mean velocity, $U$, were both equal to 1 and the mesh sizes $\Delta x, \Delta y, \Delta z$ are non-dimensionalised with respect to $h_c$.

<table>
<thead>
<tr>
<th>Flow variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Re ($\frac{U h}{\nu}$)</td>
<td>6700</td>
</tr>
<tr>
<td>$L_x, L_y, L_z$</td>
<td>4, 1, 5</td>
</tr>
<tr>
<td>$N^L_x, N^L_y, N^L_z$</td>
<td>320, 160, 400</td>
</tr>
<tr>
<td>$\Delta x$</td>
<td>0.0125</td>
</tr>
<tr>
<td>$\Delta y$ (near the dune)</td>
<td>0.00625</td>
</tr>
<tr>
<td>$\Delta z$</td>
<td>0.0125</td>
</tr>
<tr>
<td>Bedform wavelength</td>
<td>$\lambda = h_c$</td>
</tr>
<tr>
<td>Bedform shape</td>
<td>$0.5 h_d \cos 2\pi x / \lambda$</td>
</tr>
<tr>
<td>Dune height, $h_d / h_c$</td>
<td>0.1</td>
</tr>
</tbody>
</table>

The geometry of the bedforms is stated in Table 1. Within the computational domain, time series were extracted from 2048 positions, corresponding to the 32 positions shown in Fig. 2a, replicated over all four bedforms, for sixteen values of the transverse coordinate, $z \lambda \in \{1.0, 1.5, 2.0, 2.3, 2.4, 2.425, 2.45, 2.5, 2.525, 2.55, 2.6, 2.7, 3.0, 3.5, 4.0, 4.5\}$. The time-series were of a 200 $h_c / U$ duration and sampled every $\frac{1}{30} h_c / U$, where $U$ is the temporally and spatially averaged mean flow at the inlet to the domain. The data were obtained after a period of convergence and it was checked that they were stationary from the perspective of the key term needed for our analysis method (the Hölder exponents, $\alpha_1$ described in section 2.3.1). To demonstrate this, we show the time series for $\alpha_1$ for all 32 locations in a given $x - y$ plane for a single dune in Fig. 3. It is clear that the data are
Figure 3. Time series showing the stationarity of the Hölder exponents, $\alpha_1$ for the 32 sampling locations shown in Fig. 2a. From top to bottom we commence with $x/\lambda = \chi.00, y/\lambda = 0.06$, work along increasing $y$ and then move to the next $x/\lambda$ position, finishing at $x/\lambda = \chi.75, y/\lambda = 0.9$. Each series is displaced vertically by an integer value for clarity.

Figure 4. Comparisons of vertical profiles of the $u_1$ velocity component at $x/\lambda = 0.0$ and $x/\lambda = 0.5$ predicted by the LES simulation and measured with two different experimental techniques: Laser Doppler velocimetry (LDV) (Hudson et al. 1996) and particle imaging velocimetry (PIV) (Günther & von Rohr 2003). This figure is taken from Chang, K. and G. Constantinescu (2013), Coherent structures in flow over two-dimensional dunes, Water Resour. Res. 49, 2446-2460, doi:10.1002/wrcr.20239 (copyright American Geophysical Union) and is reproduced with the permission of the AGU.

stationary in their mean, implying a stationary variance to the velocity time series, $u_1$.

2.2. Validation of the LES with experiments and DNS

The LES code has been validated for a wide range of turbulent flows in-
including channel flow over dunes. The reader is referred to Chang & Constantinescu (2013) for a detailed comparison between LES, experiment, and DNS for flow in a channel with dunes at the bottom and a no-slip boundary condition at the top of the domain based on a coarser mesh than adopted here. For example, Fig. 4 compares the vertical velocity profiles obtained at two longitudinal positions (the dune crest, \( x/\lambda = 0.0 \), and the point of minimum elevation, \( x/\lambda = 0.5 \)) for an inflow Reynolds number (flow depth and depth-averaged mean velocity) of 6700, which matched that in the experiments of Günther & von Rohr (2003). Higher order statistical quantities (the root-mean-squared velocity, \( \sigma(u_1) \), and the Reynolds stresses, \(-\langle u_1 u_2 \rangle\)) are compared to a direct numerical simulation (DNS) at a Reynolds number of 6920 by Cherukat et al. (1998) in Fig. 5. It should be noted that this DNS was conducted in a fairly narrow channel and the super streaks over the dunes were not resolved. These super streak features were resolved with the original LES by Chang & Constantinescu (2013) as well as in the current study with a much finer mesh as is clear in Fig. 2.

2.3. Velocity-intermittency analysis

The intermittency of turbulence has long been recognized, resulting in the various forms for the corrections to Kolmogorov’s original (K41) (Kolmogorov 1941) structure function scaling (Kolmogorov 1962; Frisch et al. 1978; She & Leveque 1994), and explicit consideration of multifractal approaches (Mene-
veau & Sreenivasan 1991; Muzy et al. 1991). However, as a consequence of scale-separation arguments (Richardson 1922), the formal links between velocity difference distributions, intermittency, and their possible correlations with the velocity field have received less attention (although note that Kolmogorov permits the values for the coefficients in his revised theory to be a function of the macrostructure of the flow (Kolmogorov 1962) and it is suggested by Frisch et al. (2005) that Kolmogorov recognised this issue in 1941, but ignored it at the time to facilitate the derivation of the $\frac{4}{5}$ law).

In terms of experimental and theoretical investigation into these matters, the relation between the longitudinal velocity difference, over a length, $r$, given by $\Delta u_r = u_x - u_x + r$ and $u_x$ was studied by Praskovsky et al. (1993) who demonstrated the invalidity of the sweeping decorrelation hypothesis. More recently, Hosokawa (2007) showed a dependence between velocity increments and the local velocity sum that was broadly consistent with the conclusion of Praskovsky et al. (1993). Further work on velocity dependence can be seen in studies that move away from considering the velocity increment moments (structure functions) to studying a Fokker-Planck equation for the evolution of the probability density function of the increments (Renner et al. 2001; Keylock et al. 2012). By further conditioning the distribution for $p(\Delta u_r | \Delta u_{2r}, u_x)$, Stresing & Peinke (2010) were able to show the relevance of describing the turbulent energy cascade with a velocity conditioning.

While this conditional distribution function technique is suited to the analysis of long experimental datasets consisting of millions of samples, it is much less appropriate for studying velocity-intermittency properties derived from eddy-resolving numerical studies or shorter duration geophysical field studies. This deficiency of the Fokker-Planck approach was the rationale for the development of a velocity-intermittency analysis framework better suited to the study of shorter duration time series (Keylock et al. 2012). This method is adopted in this paper and explained more thoroughly below. In addition to its links to fundamental questions regarding turbulence cascades and dynamics, this analysis permits an implicit consideration of the role of flow structures in the dynamics from single point time series (from which the velocity gradient tensor cannot be resolved). Hence, identification of the velocity-intermittency structure complements more conventional analysis of turbulent kinetic energy and Reynolds stresses for single-point data by giving information that one can connect to resolved flow structures (Keylock et al. 2014b).

2.3.1. Hölder exponents

Similar to multifractal analyses (Meneveau & Sreenivasan 1991), our velocity-intermittency approach is underpinned by the notion of Hölder exponents. The Hölder exponents for a turbulence velocity time series can be used to identify flow structures from single-point measurements (Keylock 2008) and can be formally related to more classical structure function analysis using the Frisch-Parisi conjecture (Frisch & Parisi 1985):

$$D(\alpha_1) = \min_n (\alpha_1(t)n - \xi_n + 1),$$

where the singularity (multifractal) spectrum, $D(\alpha_1)$, is given by the set of non-empty values for $\alpha_1(t)$, the Hölder exponents for velocity component, $u_1$, and $\xi_n$ is the structure function scaling exponent for the nth moment of the velocity increment distribution. Hence, analysis in terms of the Hölder regularity of the velocity signal provides a di-
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Table 2. Definition of velocity-intermittency quadrants

<table>
<thead>
<tr>
<th>Quadrant</th>
<th>$u_1'$</th>
<th>$\alpha_1'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q1</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>Q2</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>Q3</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Q4</td>
<td>+</td>
<td>-</td>
</tr>
</tbody>
</table>

rect connection to considerations of turbulent intermittency Kolmogorov (1962) and the multifractal structure of turbulent velocity signals (Meneveau & Sreenivasan 1991; Muzy et al. 1991; Arnéodo et al. 1999).

The Hölder exponent is defined through consideration of the differentiability of a signal relative to polynomial approximations about a particular point (Jaffard 1997; Kolwankar & Lévy Véhel 2002). These are given by a Taylor series expansion:

$$p_T(t) = \sum_{i=0}^{m-1} \frac{u_1'(T)}{i!}(t-T)^i$$

where we study a velocity time series, $u_1(t)$, in a neighbourhood, $\delta$, about a position, $T$, and $m$ is the number of times that $u$ is differentiable in $T \pm \delta$. We then state that $u_1(t)$ has a pointwise Hölder exponent, $\alpha_1 \equiv \alpha(u_1) \geq 0$ if a constant $K > 0$ and the polynomial $p_T(t)$ of degree $m$ exist such that

$$|u_1(t) - p_T(t)| \leq K|t-T|^{\alpha} \quad (2.3)$$

The Hölder regularity, $\alpha_1$, of $u_1(t)$ at $T$ is then given by the supremum of $\beta$ that fulfills Eq. 2.3.

We evaluate $\alpha_1$ using a time domain scaling method (Kolwankar & Lévy Véhel 2002; Seuret & Lévy Véhel 2003). This method performed well in a comparative test of various such algorithms (Keylock 2010) and is based on the determination of the oscillations within the vicinity of a particular target position and then a log-log regression of these signal oscillations, $O_{T,\pm \delta}$, within some distance $\delta$ of $T$ against $\delta$, where $O_{T,\pm \delta}$ is given by:

$$O_{T,\pm \delta} = \max [u_1(t \in \{T - \delta, \ldots, T + \delta\})] - \min [u_1(t \in \{T - \delta, \ldots, T + \delta\})]$$

and $\delta$ is distributed logarithmically. In our study $2^1 \leq \delta \leq 2^{10}$ to provide as broad a scaling regime as possible (i.e. spanning integral and inertial scales to incorporate both dune flow turbulent macrostructure (Kruse et al. 2003; Chang & Constantinescu 2013) and cascade effects) while minimizing algorithm end-effect issues (our time series each consist of 6000 values).

2.3.2. Velocity-intermittency quadrants

The approach we use for determining the velocity-intermittency coupling is based on the notion of quadrants, commonly used to characterise boundary-layer flows (Nakagawa & Nezu 1977; Bogard & Tiederman 1986; Keylock et al. 2014a). However, in our formulation, the fluctuating vertical velocity component, $u_3'(t)$ is replaced by the fluctuating pointwise Hölder regularity, $\alpha_1'(t)$ of the fluctuating longitudinal component, $u_1'(t)$ (Keylock et al. 2012). Hence, having obtained $\alpha_1(t)$ from $u_1(t)$, we form quadrants by subtracting the respective mean values, $\alpha_1'(t) \equiv \alpha_1(t) - \langle \alpha_1 \rangle$, $u_1'(t) \equiv u_1(t) - \langle u_1 \rangle$ and then classifying the data based on the sign of the fluctuating terms (Table 2).
To illustrate the method more clearly, we show velocity-intermittency quadrant plots from four selected positions in our numerical domain, combining data from all four dunes, in Fig. 6. We follow the idea in classical quadrant analysis of identifying selected events (ejections and sweeps in the standard analysis) based on a threshold ‘hole size’. Because the units of measurement for our variables differ, we normalise using the respective standard deviations, $\sigma(\ldots)$:

$$\alpha^*_1(t) = \frac{\alpha'_1(t)}{\sigma(\alpha_1)}$$
$$u^*_1(t) = \frac{u'_1(t)}{\sigma(u_1)}$$  \hspace{1cm} (2.5)

We then define our hole size, $H$, as values for the product, $\alpha^*_1(t)u^*_1(t)$, and example thresholds are shown in Fig. 6 for $H \in \{1, 2\}$ as grey, dotted lines. The four locations chosen in Fig. 6 can be seen from Fig. 2 to represent very different local flow environments:

- $(x/\lambda = \chi, 0.00, y/\lambda = 0.90)$ - The outer flow far above the dunes (a);
- $(x/\lambda = \chi, 5.00, y/\lambda = 0.04)$ - Within the shear layer formed by separation at the upstream crest (b);
- $(x/\lambda = \chi, 0.00, y/\lambda = 0.06)$ - Close to the point of separation at the dune crest (c); and,
- $(x/\lambda = \chi, 5.00, y/\lambda = -0.02)$ - Near the bed and in the region of reattachment and recirculation (d).
It is clear from these plots that the velocity-intermittency relations are structured quite differently at the four selected locations. The two locations in the regions directly influenced by shear generated by the dunes, (b) and (c), exhibit a clear negative correlation, with extreme velocity-intermittency states preferentially located in quadrants 2 and 4, respectively. There is a weak positive correlation at position (a), with the general negative skew at this location resulting in a slight preference for extreme states to be located in quadrant 3. The velocity-intermittency plot in the recirculation region is more isotropic (Fig. 6d), without a strong correlation. However, a preference for extreme occurrences to occur in quadrant 4 can be detected.

To quantify this structure, we then count the number of records exceeding a given choice of $H$ in each quadrant, $N_Q(H)$, and plot this as an empirical probability defined as a function of the proportion of the total exceedances at a given $H$:

$$p_Q(H) = \frac{N_Q(H)}{\sum_{Q=1}^{4} N_Q(H)}$$ (2.6)

Hence, the data in Table 3 are extracted from Fig. 6 and are initially expressed as an empirical probability of the full number of points in the data record (such that the values always decrease and tend to 0 as $H$ tends to infinity). The second block of values are those after renormalisation by the total number of points exceeding each threshold, $\sum_{Q=1}^{4} N_Q(H)$ as defined in eq. 2.6. These $p_Q(H)$ values can then be plotted as a function of $H$ for each quadrant. Different examples of these types of plots are shown in Fig. 7 for a range of flows. From this figure, it is clear that turbulent flows in different domains may be readily discriminated from others using this velocity-intermittency analysis. Interpretation of these results was provided previously by Keylock et al. (2012) and Keylock et al. (2013). As an example, it can be seen that quadrant 2 dominates the statistics at large $H$ for the jet data (red line), leading to a large, positive value for the gradient of $p_Q$ and $H$ in this quadrant. This is indicative of regions of low velocity with relatively subdued turbulence driving the extreme statistics, and for the jet experiment, this may be readily interpreted as the entrainment of quiescent fluid from the surrounding fluid into the jet as it expands away from the nozzle. The near-wall boundary layer data (solid green and blue lines) have a positive slope in quadrant 4. This is consistent with the standard ejection-sweep model for flow near the wall (Lu & Willmarth 1973; Bogard & Tiederman 1986) and fast moving sweeps, highly turbulent states dominating the statistics in this region.

Figure 7 also contains information on the velocity-intermittency structure over mobile gravel bedforms, as analyzed by Keylock et al. (2013) using data collected by Singh et al. (2009, 2010). The region analysed was above the shear layer developed at the dune crest and shows a particularly strong quadrant 3 dominance, even relative to boundary-layer flow above 150 wall units (dotted green and blue lines). This reflects the large hairpin-like features that develop in this region as described in previous studies Omidyeganeh & Piomelli (2011); Chang & Constantinescu (2013). Because of their movement upwards from regions of relatively low velocity, these highly turbulent structures are associated with a lower velocity than is typical at this depth, explaining the positive slope in quadrant 3. Recently it has been shown that, despite the very different experimental conditions (fixed, artificial dunes rather than mobile, low-angled gravel bedforms), a well-
known dataset on flow over dunes (Venditti & Bennett 2000) also contains clear evidence of the same velocity-intermittency relation as that seen in Fig. 7 for flow over bedforms Keylock et al. (2014b). This highlights the robustness of our method and the existence of an ‘outer region bedform velocity-intermittency structure’.

In the same way that a given set of lines in Fig. 7 summarises the information in velocity-intermittency quadrant plots such as those in Fig. 6, to examine the velocity-intermittency response at the 2048 locations studied, requires a further distillation of the information contained in plots such as Fig. 7. Following Keylock et al. (2014b), we accomplish this by approximating the behaviour of the $p_Q(H)$ vs $H$ relations by their slopes, $dp_Q/dH$. Hence, the four lines in Fig. 7 are replaced by four gradient values. Subsequent results in this paper express these four values as bar charts.

Using this velocity-intermittency framework, the current study complements previous experimental work by using a well-resolved large-eddy simulation to examine the velocity-intermittency properties of dune flow dynamics, looking in particular at the near-bed region where the previous experimental data undersampled the flow. This was an intrinsic feature of the experiments of Singh et al. (2009, 2010) as the bedforms were free to develop and advect beneath the probe. Hence, the probe had to be positioned so that it sampled the flow above the crest. Therefore, the LES results provide new information on the near-wall velocity-intermittency structure for what is an important, emergent boundary-condition for flows over a mobile bed (Fourrière et al. 2010).

### 2.4. Data classification by K-means clustering

Because we can obtain results from a large number of spatial locations using numerical methods, we employ an automatic data classification technique to see if the natural groupings in the data conform to our understanding of the flow field. That is, averaging results across multiple points can, in the case of a multimodal behaviour, give a result that is not representative of any observed flow state. In such instances, clustering analysis reveals which type of behaviour are present at a particular point. We use the well-known $K$-means clustering method applied to straight line approximations to the proportional occupancy of each quadrant as a function of $H$.  

### Table 3. Calculation of the hole size threshold exceedances for each quadrant for the four locations shown in Fig. 6 (coordinates at the top of each column) and four choices of hole size, $H$. The first set of results are expressed as empirical probabilities of the length of the full data record. The second set of results are given as a function of the number of values exceeding the selected threshold. This is what is defined as $p_Q(H)$ in the text and used for analysis.

<table>
<thead>
<tr>
<th>$H$</th>
<th>(0.0, 0.09)</th>
<th>(0.5, 0.05)</th>
<th>(0.0, 0.06)</th>
<th>(0.5, -0.02)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q1</td>
<td>0.29 0.26 0.25 0.19 0.29 0.21 0.32 0.15 0.32 0.21 0.33 0.22 0.25 0.25 0.27</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q2</td>
<td>0.13 0.12 0.10 0.07 0.16 0.06 0.14 0.04 0.18 0.05 0.17 0.07 0.10 0.10 0.12</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q3</td>
<td>1.0 0.03 0.06 0.05 0.03 0.10 0.03 0.07 0.02 0.12 0.01 0.10 0.03 0.05 0.04 0.07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q4</td>
<td>1.5 0.03 0.03 0.02 0.07 0.01 0.03 0.01 0.08 0.00 0.06 0.01 0.03 0.02 0.04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q1</td>
<td>0.29 0.26 0.25 0.19 0.29 0.21 0.32 0.15 0.32 0.21 0.33 0.22 0.25 0.25 0.27</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q2</td>
<td>0.30 0.28 0.23 0.15 0.37 0.15 0.33 0.09 0.40 0.12 0.39 0.18 0.27 0.25 0.31</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q3</td>
<td>1.0 0.29 0.30 0.25 0.14 0.45 0.12 0.30 0.08 0.48 0.04 0.40 0.15 0.26 0.23 0.36</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q4</td>
<td>1.5 0.26 0.33 0.27 0.12 0.52 0.09 0.40 0.05 0.53 0.02 0.40 0.10 0.28 0.23 0.40</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Figure 7. An analysis of velocity-intermittency for various experiments. The data from flow over mobile bedforms studied by Keylock et al. (2013) are shown as a solid black line, while other lines correspond to data from a turbulent jet experiment (Renner et al. 2001) (red), wake data at 8.5 ms$^{-1}$ (gray dotted) and 24.3 ms$^{-1}$ (gray) (Stresing et al. 2010), and data below 150 wall units (solid lines) and higher into the flow (dotted lines) at 6 ms$^{-1}$ (blue) and 8 ms$^{-1}$ (green) for the upstream boundary layer from the study by Keylock et al. (2012). This figure is modified from: Keylock, C.J., Singh, A., Foufoula-Georgiou, E. 2013. The influence of bedforms on the velocity-intermittency structure of turbulent flow over a gravel bed, Geophysical Research Letters 40, 1-5, doi:10.1002/grl.50337. (copyright American Geophysical Union) and is reproduced with the permission of the AGU.

That is, for the equations in this subsection, $\gamma \equiv \frac{dp_Q}{dH}$, for each quadrant at each sampling location. The $K$-means approach defines clusters by minimizing the within cluster sum-of-squares difference. Hence, with $i = 1, \ldots, k$ clusters and $j = 1, \ldots, \eta$ data vectors ($k < \eta$), one seeks to minimize

$$\arg\min_{S} = \sum_{i=1}^{k} \sum_{\gamma_j} S_i ||\gamma_j - \mu_i||^2$$

From an initial guess of the $k$ means, $\mu_1^{(0)}, \ldots, \mu_k^{(0)}$, the standard algorithm alternates between assignment and update steps:

$$S_i^{(t)} = \{\gamma_j : ||\gamma_j - \mu_i^{(t)}||^2 \leq ||\gamma_j - \mu_\ell^{(t)}||^2 \forall \ 1 \leq \ell \leq k\}$$

Following the assignment of $\gamma_j$ to just one $S_i$, the cluster means are updated:

$$\mu_i^{(t+1)} = \frac{1}{|S_i^{(t)}|} \sum_{\gamma_j \in S_i^{(t)}} \gamma_j$$

The optimal number of clusters, $K \in k$, is obtained from consideration of two criteria after convergence ($t = \infty$), where $\delta_{i,j} = ||\gamma_j - \mu_i^{(\infty)}||^2$:

- For a given $j = J$, we define $(D_1)_J = \min\{\delta_{1,j}^{(\infty)}, \ldots, \delta_{k,j}^{(\infty)}\}$, $(D_k)_J = \max\{\delta_{1,j}^{(\infty)}, \ldots, \delta_{k,j}^{(\infty)}\}$. Hence, $(D_1/D_2)_J$ is a measure cluster distinctiveness for vector $j$. The average ratio over all $\eta$ vectors is then a summarial measure of the effectiveness of ease of classification into
clusters:

\[ \langle D_1 / D_2 \rangle = \frac{1}{\eta} \sum_{j=1}^{\eta} (D_1 / D_2)_j \]  

The effectiveness of the variance partitioning over all clusters is given by the mean distance of the members of a cluster to the cluster centroid, \( \mu_i \), then averaged over all \( k \) clusters:

\[ \delta_{av} = \frac{1}{k} \sum_{i=1}^{k} \frac{1}{|S_i(\infty)|} \sum_{\eta_i \in S_i(t)} \delta_{i,j} \]  

In the analysis below, we use these two methods to discern the optimal number of clusters in our data, which we then interpret physically in terms of quadrant-dominance.

3. Results

3.1. Elementary flow properties

Vertical profiles for the time-averaged longitudinal velocity component, \( \langle u_1 \rangle \), the standard deviation of \( u_1 \), \( \sigma(u_1) \), and the primary Reynolds stress component, \(-\langle u_1 u_2 \rangle\) are shown in Fig. 8 as a function of longitudinal coordinate, \( x \). The results shown are also averaged over the 16 choices for \( z \) and the four dunes, as indicated by the “av” subscript. The position notation, \( x = \chi, 75 \), for example, means that rather than identifying a specific dune (e.g. \( x = 1.75 \)) results have been averaged or compiled over all four dunes, \( \chi \in \{1, 2, 3, 4\} \).

These data show the expected pattern of an increasing mean velocity above the dune crest, and a decrease in the standard deviation and Reynolds stress both above and beyond \( y = h_d \), highlighting the shear layer development at this height. It is interesting to note that peak values for \( \sigma(u_1)_{av} \) are similar at \( x = \chi, 25 \) and \( x = \chi, 50 \), and only decay by about 10% by \( x = \chi, 75 \). In contrast, average Reynolds stresses nearly double from \( x = \chi, 25 \) to \( x = \chi, 50 \), and then return to approximately the \( x = \chi, 25 \) values by \( x = \chi, 75 \).

In the \( \sigma(u_1) \) results, in particular, but also with the Reynolds stresses, there is a clear ‘bulge’ to the profile at \( y/\lambda \sim 0.5 \), which constrains with the rapid decay from the wall seen in a boundary-layer. It can be seen in the total vorticity plane in Fig. 2b that coherent structures with significant vorticity are penetrating to at least this height in the domain. These are associated with the upstream vortex tube overlying the SSL (Chang & Constantinescu 2013), increasing the longitudinal turbulence effects in this region and highlighting the complexity of the bedform flow environment.

The variability in the results shown in Fig. 8 for each of the four dunes was calculated on a point-by-point basis and peaked at the height of the shear layer, where the difference between maximum and minimum values was of the order of 10%. It should be noted that because of the strong vertical gradients of the flow variables in this region, slight differences in the vertical location of the shear layer can have a dramatic impact on the calculated difference statistics. Because of this, and because there was no systematic trend in these statistics, in addition to the temporal stationarity shown in Fig. 3, the results were deemed also to be spatially stationary.

3.2. Average relations between \( u_1 \) and \( \alpha_1 \)

The general structure of the correlation between \( u_1 \) and \( \alpha_1 \) as a function of position is shown in Fig. 9. One observes a peak negative correlation just above the crest \( (x/\lambda = \)
Figure 8. Vertical profiles of $\langle u_1 \rangle$ (top row), $\sigma(u_1)$ (middle row) and $-\langle u_1'u_2' \rangle$ (bottom row) averaged over sixteen choices for $z$ and the four dunes. The values in each column are a function of longitudinal position, $x$.

Figure 9. The median correlation, $R(u_1, \alpha_1)$, between $u_1$ and $\alpha_1$, determined over all dunes, $\chi \in \{1, 2, 3, 4\}$, on the centreline of the domain ($z = 2.5/\lambda$). The lower panel focuses on the near-wall region.

$\chi_{0.00}, y/\lambda = 0.06$, and this zone moves downwards and expands past the crest, appearing to reach a maximum vertical extent at $x/\lambda = chi_{0.50}$ where it extends from $-0.03 < y/\lambda < 0.03$. Positive correlations are more prevalent higher into the flow ($y/\lambda > 0.7$), except for $x/\lambda \in \{\chi_{0.00}, 0.25\}, y/\lambda = 0.2$ where a positive correlation is also found. These results are indicative of general Q2 or Q4 dominance in the lower flow, with Q1 or Q3 dominant in the outer flow.
Figure 10. Bar charts of the slopes extracted from quadrant plots similar to Fig. 7 for the 32 positions sampled within the dune region. Results are averaged over the four dunes, and over seven central locations in the transverse direction: \( z = \frac{2}{425}, 2, 45, 2, 5, 2, 525, 2, 55, 2, 6, 2, 7 \). Quadrants are in ascending order from bottom to top in each subplot. Black shading indicates the pattern of Q2 dominance described in the text and corresponding to the centroid of cluster \( K_5 \), grey indicates a pattern of Q4-dominated flow similar to the centroid of cluster \( K_1 \), green indicates the pattern of positive \( Q_2 \) and negative \( Q_1 \) slopes similar to cluster \( K_2 \), while red shading shows some evidence of Q3 dominance corresponding to \( K_4 \). Blue shading shows quadrant patterns that do not qualitatively match any of the identified cluster centroids.

As outlined above, in order to summarise the quadrant-based results effectively, we found the linear slopes, \( \frac{dp_Q}{dH} \), of the occupancy-\( H \) plots (Fig. 7) for each quadrant. Results averaged over all positions are shown in Fig. 10 and highlight which specific quadrants explain the correlations observed in Fig. 9. Spatial differences in the vertical and horizontal directions are clear. The trend for stronger negative correlations towards the bed seen in Fig. 9 is actually made up of two distinct regions:

- Flow near the bed (\( y/\lambda \lesssim 0.02 \), coloured in grey) dominated by strong positive slopes for Q4, with negative values for the other quadrants; and,
- The \( 0.02 < y/\lambda < 0.06 \) region (black colour) dominated by positive slopes for Q2 with negative slopes for the other terms.

Immediately adjacent to the dune, there are also locations (green colour) where both Q2 and Q4 have positive slopes that are reduced in magnitude, but are still sufficient to yield negative correlations in Fig. 9.

The previous study of the velocity-intermittency structure for dune flow was based on the experimental work of Venditti & Bennett (2000). In that experiment, the shape of the bedforms differed from that used here (sinusoidal here, asymmetric in Venditti & Bennett (2000)) and there were also relatively few samples collected below the dune crest. The second lowest row of samples were 50% of the bedform height above the crest (\( y/h_d = 1.5 \)). This corresponded well to the mean elevation in the experimental data of Singh et al. (2009), permitting Keylock et al. (2014b) to compare velocity-intermittency characteristics to those in Keylock et al. (2013), which showed an excellent agreement, and a clear Q3 dominance at this height. This led to the suggestion of a dune flow class for the flow above the shear layer that forms at the dune crest as one with a Q3-dominant
Velocity-intermittency for flow over symmetric dunes

Figure 11. Selection of the number of clusters. The mean ratio between the minimum distance to a cluster centroid, $D_1$, and the second smallest distance to a cluster centroid, $D_2$, as a function of the number of clusters, is shown in panel (a). Panel (b) shows the average distance to a cluster centroid averaged over all clusters.

velocity-intermittency structure (see the black line in Fig. 7). The asymmetry of the dunes in the Venditti & Bennett (2000) dataset meant that there was $15h_d$ between crests, and $2h_d$ from the point of minimum elevation to the next crest, compared to $10h_d$ and $5h_d$, respectively, here. The region of Q3 dominance was most clearly expressed $9h_d$ or more from the crest for the asymmetric case. In the current case, this most closely corresponds to $x = \chi_{0.0}$, but Fig. 2 shows qualitatively, and Chang & Constantinescu (2013) described more thoroughly how vortices from the upstream dune are deflected above the separated shear layer from the current dune, as noted above. Hence, it is to be anticipated that as a consequence of this deflection, the region of maximum Q3 dominance at $x = \chi_{0.0}$ will be displaced upwards from the dune crest. Indeed, this was found to be the case, with the data from $x/\lambda \in \{\chi_{0.0}, \chi_{2.5}\}, y/\lambda = 0.2$ with the clearest Q3 dominance (red shading in Fig. 10). That this is the region affected by vortex generation from the crest of the previous dune may be inferred from the right-hand edge of the background frame in Fig. 2a and the investigation by Chang & Constantinescu (2013). Hence, the region exhibiting positive values for Q3 is in the upper half of the shear layer, where crest-generation processes are not affected by recirculation and near-wall phenomena. This region extends into the flow directly above the crest of the dune that is positioned immediately downstream. The Q3 dominance in these regions occurs both because the advection of large-scale structures is less than the mean flow (as forward momentum has been transferred into angular momentum), and because the hairpin-like structures that form in this region (Fig. 2a,b) are moving upward through the flow from regions of lower mean velocity. Because large magnitude velocity fluctuations (hence, intermittency) are associated with their passage, there is a $u'_1 < 0, \alpha'_1 < 0$ (or Q3) dominance at large $H$.

3.3. Summary of location-specific velocity-intermittency behaviour

In order to go beyond the average results at each position shown in Fig. 10 a statistical classifier of the velocity-intermittency structure at all positions was employed (rather than undertaking an averaging operation). Consequently, a $K$-means clustering algorithm, was used to automatically classify types of observed velocity-intermittency behaviour as described above.

The quadrant slope results, $dp_Q/dH$, for the velocity-intermittency structure at 2048 positions (32 locations in a given $x-y$ plane, 16 transverse positions, and 4 dunes) were analysed. The primary criterion used to determine the optimal number of clusters is given...
by Eq. 2.10 and, as shown in Fig. 11a, either three or five clusters were optimal. Supple-
menting this analysis with Eq. 2.11, as shown in Fig. 11b, \( K = 5 \) was deemed optimal
and these natural groupings in the data are shown in Fig. 12. The shading used here
respects that used in Fig. 10 for highlighting particular velocity-intermittency relations,
and \( n_K \) is the number of vectors assigned to a given cluster (from 2048). The sampling
bias towards the bed, clearly affects any interpretation of these values with respect to
the global prominence of particular flow states, but the most commonly observed cluster,
\( K_5 \), is that with strong \( Q_2 \) dominance, followed by a weaker \( Q_2 \) dominance in \( K_2 \). Al-
together, there were 1049 cases (51.2% of 2048) where \( \frac{dp}{dH} Q \) for \( Q_2 \) was greater than
+0.05 and 65% of the time, these cases occurred at \( y = 0.06 \), which accounted for 50% of
the sampled positions.

Although only two of the thirty two locations in Fig. 10 showed a dominant \( Q_3 \) state
(and slopes for \( \frac{dp}{dH} Q \) in \( Q_2 \) were still positive there), cluster \( K_4 \), with a clear \( Q_3 \)
dominant state, is the third most numerous cluster, occurring 19.6% of the time. In fact,
there were 382 cases (18.7% of 2048) where \( \frac{dp}{dH} Q \) for \( Q_3 \) was greater than +0.05 and
54% of the time, these cases occurred at \( y \in \{0.1, 0.2\} \), which equates to a quarter of
the sampled locations overall and a dominance in the primary region above the shear-
layer generated at the crest, which is compatible with our past results (Keylock et al. 2013, 2014b). The single most important positions for \( K_4 \) occurrence
were \( x/\lambda = \chi_{00}, y/\lambda = 0.2 \) (11% of total occurrences), \( x/\lambda = \chi_{25}, y/\lambda = 0.2 \) (9%), and
then \( x/\lambda = \chi_{50}, y/\lambda = 0.1 \) and \( x/\lambda = \chi_{75}, y/\lambda = 0.1 \) (both 8%). This reduction of
\( y \) with \( x \) for locations with dominant \( Q_3 \) extremes, shows that the sites at
\( x/\lambda \in \{\chi_{00, \chi_{25}}\} \) are capturing the dynamics above the SSL generated from
the previous dune, while \( x/\lambda \in \{\chi_{50, \chi_{75}}\} \) reflect the conditions above the SSL generated from the current dune's crest. More generally, and indicating that this \( K_4 \), \( Q_3 \)-dominant flow state is a characteristic of the outer part of flow over dunes,
88% of occurrences were at \( y/\lambda \geq 0.1 \), which equated to half the sampled locations, but
86% of the flow depth.

Figure 12. The five cluster centroids extracted using the \( K \)-means algorithm displayed in a
similar form to the results in Fig. 10, with the shading for each cluster respecting that used in
that figure (cluster \( K_3 \) does not feature there). The data plotted in the bar graphs are tabulated
in the bottom right.
Velocity-intermittency for flow over symmetric dunes

Figure 13. The percentage of times (from 64 occurrences; four dunes and sixteen lateral positions) that particular $K$-means clusters are expressed at each longitudinal and vertical position considered. Shading indicates which cluster is dominant (grey, green, white, red and black for $K_1$ to $K_5$ dominance, respectively), with locations where no cluster dominates shown in blue.

Figure 14. The centroid of the cluster exhibiting Q3 dominance ($K_4$), together with results from data collected by Singh et al. (2009) and analysed by Keylock et al. (2013) (labeled Singh et al.) and the longitudinally averaged results for four vertical heights ($y/h_d \in \{0.75, 1.5, 2.25, 3.0\}$) from data collected by Venditti & Bennett (2000) and analysed by Keylock et al. (2014b).

Subsequent analysis in Fig. 13 shows the histogram of occurrences of different cluster membership at the 32 locations in the $x - y$ plane, with shading indicating the cluster dominating at a particular position, and blue used when none of the five identified clusters appears to dominate the histogram. Given that averaging the response over different cluster types leads to a mean quadrant response that blends together different quadrant dominant states, Fig. 13 is a more representative map of velocity-intermittency structure than Fig. 10.
3.4. Outer flow velocity-intermittency structure and associated flow structures

Figure 13 shows that clusters $K_3$ (Q1 dominance) and $K_4$ (Q3 dominance) are of greatest importance for most of the flow depth ($y/\lambda > 0.1$). However, with the exception of $x = 0.00, y/\lambda = 0.20$, one cluster does not dominate the results as clearly as in the near-wall locations. This is why the simple averaging over all sites in Fig. 10 departs from Fig. 13 to a greater extent in the outer flow. In addition to the observation that cluster $K_4$ (with its Q3 dominance) occurs more frequently in the outer region, what is seen in Fig. 13 is that $K_4$ occurs more often than any other cluster for all $x/\lambda$ at $y/\lambda = 0.2$, and $x/\lambda \in \{\chi, 0.5, \chi, 0.75\}$ for $y/\lambda = 0.1$. Because $y/\lambda = 0.2$ corresponds to $y/h_d = 1.5$, these results correspond directly to regions of Q3 dominance in the previous experimental work (Keylock et al. 2013, 2014b) and Fig. 14 compares the numerical results from this study with those experiments. Results are shown for the data of Venditti & Bennett (2000) at various choices for $y/h_d$, including $y/h_d = 1.5$, and those of Singh et al. (2009), which were obtained with a mobile bed at an average dimensionless flow depth of $y/h_d = 1.5$. It is clear that the Q3 velocity-intermittency signal is consistent for two physical experiments with asymmetric bedforms but very different experimental procedures (Venditti & Bennett 2000; Singh et al. 2009), and our numerical experiment for symmetric bedforms. Hence, the flow structures located in this region (Fig. 2) induce a quadrant structure that is extreme in its Q3 dominance relative to other flow types studied (Fig. 7). However, it is most similar to the outer part of a boundary-layer, where it is well-known that the flow dynamics are affected by hairpin vortex packets generated near the wall and advected higher into the flow (Christensen & Adrian 2001; Hurther et al. 2007). As is clear from Fig. 8, the point of maximum shear is below this region of Q3 dominance. However, the positive gradient of $\langle u_1 \rangle$ above this height induces a lift on the flow structures associated with the upper part of the shear layer. This results in the production of the hairpins discussed by Omidyeganeh & Piomelli (2011) and clearly associated with locations of high total vorticity in Fig. 2b. Lift-up of the hairpins leads to regions of intense vorticity in $0.07 < y/\lambda < 0.5$ moving slower than the surrounding ambient and a Q3 velocity-intermittency structure. Such vortical structures can be observed at various points in Fig. 2b and at $x/\lambda = 3.9, y/\lambda = 0.2$ in Fig. 2a. That these structures have a hairpin shape and are, consequently, discontinuous in $z$ explains why the mean results in Fig. 10 contrast with those in Fig. 13. While positive slopes for Q3 are observed in this region in Fig. 10, there is a stronger Q2 presence in the mean. That this is a mixing of states is seen by the clustering showing that $K_5$ with its Q2 dominance is also important at $y/\lambda \in \{0.1, 0.2\}$. Note that $dp_Q/dH$ for Q2 in $K_5$ and Q3 in $K_4$ are 0.18 and 0.11, respectively (from the table in Fig. 12). This difference is approximately respected in the Q2 and Q3 bars in the blue plots in Fig. 10 at $x/\lambda \in \{\chi, 0.5, \chi, 0.75\}$ and $x/\lambda \in \{\chi, 0.5, \chi, 7.5\}$, However, the Q3 bars are rather longer than $0.11/\pi$ the length of those for Q2, explaining the $K_4$ dominance in Fig. 13, and suggesting that the hairpins are wider close to their point of maximum curvature than their typical separation, which is supported qualitatively from the Q-surfaces shown in Fig. 2b. That the quadrant 3 dominance seen in our numerical results and the previous experimental data and shown in Fig. 14 is stronger than that in the outer
part of the boundary-layer (Fig. 7) indicates that where they arise, these
hairpin structures are a stronger feature of the flow field than boundary-layer
hairpins even though the background turbulence intensities in the region of
the separated shear layer are higher than those seen in near the wall.

The ‘bulge’ in $\sigma(u_1)$ at $y/\lambda \sim 0.5$ seen in Fig. 8 identifies the presence of
the overlying shear layer from the upstream dune (Chang & Constantinescu
2013). From Fig. 12 it is clear that we see a $K_3$ dominance at $y/\lambda = 0.5$, indicating the importance of $Q_1$ in this region. Reference to Fig. 7 shows
that $Q_1$ dominance is associated with our previous study of wake dynamics
(Keylock et al. 2012), which makes sense in this context: While the SSL from
the current dune is subject to active shearing and hairpin formation and
lift-off, with our geometry, the overlying features were generated at least 10
dune heights earlier, and while straining is still active, vortex production has
dropped. Hence, we see the ‘bulge’ in $\sigma(u_1)$, but not in $-\langle u_1' u_2' \rangle$.

3.5. Near-bed velocity-intermittency structure and associated flow structures

An important advantage of the numerical simulations compared to the pre-
vious experimental studies is the opportunity to sample flow characteristics
close to the bed in the lee of the dune crest more easily than in the previous
experimental studies of dune velocity-intermittency structure. In this region
(the bottom plots in the first three columns of Fig. 10 and Fig. 13), the level
of agreement between the analyses is very clear as highlighted by the identi-
cal shading at the same locations. Quadrant 4 dominance ($K_1$, grey) occurs in
the sites closest to the bed in the lee, with $K_2$ (green) dominant immediately
above these locations. The weakly positive values for both $Q_2$ and $Q_4$ in $K_2$
suggests this is a transitional case, separating the near-wall flow where $Q_4$ is
the most important quadrant, and the overlying $Q_2$ dominance in $K_5$ (black).
This interpretation is supported by the fact that the second most common
configuration in the $K_2$-dominant regions shaded in green at $x \geq \chi.50$ is the
$K_5$ grouping, and that the $K_2$ grouping is the second most common where $K_5$
is dominant (black locations in Fig. 13). The exceptions to this are the $K_2$
dominant locations closest to the dune crest at $(x/\lambda = \chi.00, y/\lambda = 0.06)$ and $(x/\lambda = \chi.25, y/\lambda = 0.04)$, where $K_1$ is the second most common cluster and $K_5$
is third. Figure 12 shows that $K_1$ is dominated by $Q_4$ behaviour, and this is
the dominant cluster closest to the bed at $x/\lambda \in \{\chi.25, \chi.50\}$.

Figure 7 shows that positive $Q_4$ dominance near the wall is entirely ex-
pected based on the velocity-intermittency structure of boundary-layer flow
below 150 wall units. However, the values for $dp_{Q=4}/dH$ are much greater than
have been found for a boundary-layer flow, particularly at $x/\lambda = \chi.00, y = 0.02$
and $x/\lambda = \chi.25, y/\lambda \in \{-0.02, -0.04\}$, suggesting that a different mechanism
than the sweep events that arise as part of the near-wall bursting cycle is
responsible. Instead, the mechanism is a consequence of the impingement of
the lower part of the SSL on the wall, and the concomitant occurrence of rel-
avely rapid ($u_1' > 0$), and highly turbulent ($u_1' < 0$) vortical structures into
this region (Castro & Haque 1987; Furuichi et al. 2004). Three such vortical
structures can be seen impinging on the wall in Fig. 2a as indicated by patches of positive $\omega_z$ at $x/\lambda \in \{3.35, 3.45, 3.55\}$. Transport of such vorticity back
toward the dune crest explains why $K_1$ is the second most frequented cluster
at $(x/\lambda = \chi.00, y/\lambda = 0.06)$ and $(x/\lambda = \chi.25, y/\lambda = 0.04)$. 
The generation of coherent structures by shearing over the dune crest is very clear from the Q-criterion results in Fig. 2b. Furthermore, Fig. 2a also shows the development of a shear layer at the dune crest and the generation of vortical structures in the wake that effectively increase the depth of this feature from a narrow band of vorticity at $x/\lambda = 3.0$ to something that extends from $0 \leq y/\lambda < 0.1$ at $x/\lambda = 3.6$. This corresponds very well to the region of $K_5$ dominance in Fig. 10 and 13. Note that positive values for Q2 (the defining feature of $K_5$) are associated with the behaviour of a jet in Fig. 7 (and are also important for the structure of near-wall boundary-layer flow). This is because the entrainment of quiescent fluid with little turbulence ($u'_1 < 0, \alpha'_1 > 0$) into the jet at the turbulent-non turbulent interface dominates the extreme statistics at large $H$. The Q2 dominance immediately below the SSL may also be explained in terms of a similar entrainment mechanism: the recirculation region on the underside of the shear layer has a weakly negative $\langle u'_1 \rangle$ and a lower turbulence level than the sheared region. Hence, as the shear layer entrains such fluid, these 'patches' dominate the large $H$ statistics.

4. Conclusion

Our Large Eddy Simulation (LES) of the velocity-intermittency structure of flow over symmetrical bedforms has revealed important commonalities with our previous experimental studies despite the differences in Reynolds numbers and the precise geometry of the bedforms. For the region immediately above that of active shearing from the dune crest, we find the $u'_1 < 0, \alpha'_1 < 0$ quadrant 3 (Q3) cases dominate extreme flow events and there was excellent agreement with our experimental studies of this problem in different reference frames (see Fig. 14). Previous investigations such as that by Omidyeganeh & Piomelli (2011) found hairpin vortex formation in the dune field was related to the presence of other structures in the outer dune flow, and Chang & Constantinescu (2013) highlighted the importance of the upstream shear layer as an outer flow characteristic that affected large-scale hairpin development. That the quadrant 3 dominant cluster $K_4$ occurs preferentially in the outer flow in both laboratory and numerical studies for dune flows, as well as in the near-wall region of a boundary-layer, indicates that this is a signature of these hairpin structures and they can be clearly seen at this height in Fig. 2. Averaging the results at different transversal positions blended together two states: that of Q3 dominance reflected in $K_4$ and the generally underlying Q2 dominant state ($K_5$ as shown in Fig. 13. This highlights the utility of a data clustering and classification methodology, rather than simple arithmetic averaging.

As we have previously noted, the degree of Q3 dominance seen in the outer flow over a dune is unusual relative to jets, boundary-layers and wakes (Fig. 7). Hence, it is an important signature of this type of flow environment. That this signature relates so closely to the large scale flow structures in this region, shows that our velocity-intermittency quadrant technique reveals information on flow structure from single-point measurements of the $u_1$ velocity component. It is also important to highlight that this technique works successfully with relatively short time-series, as first shown by Keylock et al. (2012). This may be contrasted with methods based on conditioning velocity increments at some separation $r$ on those at $2r$ and the velocity state, which require millions
of points to converge (Stresing & Peinke 2010). Hence, not only is the method of use in numerical studies, where time-series will typically be over fewer integral scales than well-resolved laboratory wind tunnel measurements, but it will be of use in field studies that attempt to understand the dynamics of large-scale systems (Parsons et al. 2005). Thus, this method can be applied to help fluvial scientists and engineers gain an enhanced understanding of the processes affecting mixing dynamics and sediment transport.

An important advantage of our numerical study compared to the experimental investigations of velocity-intermittency structure is that we have been able to study the near-wall flow field in much greater detail than was possible in those studies. The negative correlation between $u$ and $\alpha$ near the wall actually consists of two distinct regions: a near-wall region where reattachment of part of the separated shear layer injects vorticity at the bed into the recirculation region (Castro & Haque 1987), leading to a dominant quadrant 4 state where $u > 0$ and $\alpha < 0$ (as seen at the wall in the lee of the dune in Fig. 2a), and a region higher into the flow domain, on the underside of the shear layer, where the shear layer dynamics are influenced by the entrainment of relatively slow and quiescent fluid, leading to a dominant quadrant 2 state where $u < 0$ and $\alpha > 0$. There is a resemblance between this mechanism and that observed in a turbulent jet flow (Keylock et al. 2012), and both have the strong quadrant 2 response (Fig. 7).

While the velocity-intermittency quadrant technique has been shown to be a useful way to characterise the flow field from single-point measurements, the implications of the success of this method for developing improved closure schemes for environmental flows forced in a complex fashion should also be noted (Keylock 2015). Kolmogorov noted the potential importance of flow macrostructure on turbulence structure (Kolmogorov 1962) (see his equations 3 and 4). Such couplings across scales are clearer in shear flows than they are in homogeneous isotropic turbulence (Keylock et al. 2016a), and suggest corrections to standard modelling methods for such flows. For example, while classical test filtering in the sense of Germano (1992) (see Meneveau (2012) for a recent review) permits the Smagorinsky coefficient in the subfilter-scales of a LES to vary dynamically, velocity-intermittency coupling implies refined perspectives on the relation between production and dissipation (Vassilicos 2015; Keylock et al. 2016b), and an alternative approach to closure development. One such model can be derived by expanding about a base Kolmogorov $-\frac{5}{3}$ spectrum to obtain additional components that correspond to fluctuations in dissipation (Horiuti et al. 2016) that may be a consequence of macroscale coupling. An alternative, and more empirical, but more direct velocity-intermittency framework would be to use the Hölder exponent as a means to scale velocity fluctuations and develop fractal-based closures (Scotti & Meneveau 1999; Basu et al. 2004) into a multifractal formulation where the velocity field guides the value of the selected Hölder exponent. This is a topic of ongoing research.

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