

1 **Single-point structure tensors in turbulent channel flows with smooth and wavy**
2 **walls**

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12 A long-standing problem in turbulence modeling is that the Reynolds stress tensor alone is
13 not necessarily sufficient to characterize the transient and non-equilibrium behaviors of tur-
14 bulence under arbitrary mean deformation or frame rotation. A more complete single-point
15 characterization of the flow can be obtained using the structure Dimensionality, Circulic-
16 ity, and Inhomogeneity tensors. These tensors are one-point correlations of local stream
17 vector gradients and carry non-local information regarding the structure of the flow field.
18 We explore the potential of these tensors to improve understanding of complex turbulent
19 flows using direct numerical simulation of flows in channels with a smooth wall and a
20 two-dimensional sinusoidal wavy wall. To enforce no-slip and no-penetration conditions
21 at wavy-wall boundaries, an immersed boundary method for the stream vector Poisson
22 equation was adopted within the framework of F. S. Stylianou, R. Pecnik, and S. C. Kassinos,
23 *Comput. Fluids*, 106, 54–66 (2015). Results show that the effects of wall waviness
24 on the inclination and aspect ratio of the two-point velocity correlation near the wall are
25 reproduced qualitatively by their corresponding single-point tensor representations. In the
26 outer layer, good quantitative agreement is achieved for both parameters. Additional ob-
27 servations on the structural changes of turbulence due to wall waviness and their relevance
28 to turbulence modeling with surface roughness are discussed. The findings of this investi-
29 gation suggest that single-point structure tensors can be appended to the modeling basis for
30 inhomogeneous flows with geometrically complex boundaries, such as rough-wall flows,
31 to develop improved turbulence models.

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32 I. INTRODUCTION

33 Many turbulent flows in engineering and environmental applications are both at high Reynolds
34 numbers and over rough surfaces. For example, in turbomachines the blade surfaces undergo wear
35 due to pitting, erosion, deposition, etc., which changes their surface roughness. Assessing the
36 ensuing degradation in performance requires accounting explicitly for this wear in simulations.
37 Similarly, accounting for the effects of ice accretion on the leading edges of airfoils is essential to
38 accurate prediction of airfoil performance. The use of ablative materials on re-entry-vehicle nose
39 cones can also result in significant changes to their surface roughness. Computational Fluid Dy-
40 namics (CFD) simulations must therefore account for effects of roughness to estimate accurately
41 design parameters such as heat transfer coefficients. In wall bounded flows, surface roughness
42 can lead to a substantial increase in form drag, associated with a greater intensity of pressure
43 and velocity fluctuations. In each of the preceding examples, the dynamics of the flow is com-
44 plicated further by additional factors such as pressure gradients, unsteadiness, surface curvature,
45 and complex geometries. In spite of rapid increases in computational resources, direct numerical
46 simulations (DNS) of such complex engineering flows remain impractical. At present and for the
47 foreseeable future, the only pragmatic computational approach to simulating such non-equilibrium
48 turbulent boundary layers is to use single-point closures in the vicinity of the wall or throughout
49 the boundary layer.

50 The ability of most single-point closures to model different features of turbulent flows is lim-
51 ited by the fact that the state of the turbulent flow field is expressed only in terms of the Reynolds
52 stresses, as in the case of a second-moment closure approach. This corresponds to a coarse-
53 grained¹ description of the turbulent flow field and limits the features of turbulence that such mod-
54 els can potentially replicate. For instance, Sagaut and Cambon² have shown that in the presence of
55 background rotation, Reynolds stress anisotropy should be decomposed into directional and polar-
56 ization anisotropies, each of which is affected very differently by the pressure-velocity correlations
57 through the action of the Coriolis force. Additionally, this coarse-grained description introduces
58 uncertainty into the modeling problem^{3,4} as all turbulent flows with the same Reynolds stress need
59 not evolve identically under the same strain-rate histories. Kassinos and Reynolds⁵ have shown
60 that using just the Reynolds stresses to characterize the turbulent flow field limits models by es-
61 chewing information regarding dynamically important physics. The Reynolds stresses carry only
62 information on the componentality of turbulence—the relative strengths of different velocity com-

ponents. Kassinos, Reynolds, and Rogers⁶ introduced additional tensors to the modeling basis that add important information to improve turbulence model predictions in homogeneous turbulent flows. These tensors include the Structure Dimensionality tensor, which characterizes the relative uniformity of the turbulence structure in different directions, and the Circularity tensor, which characterizes the large-scale circulation around a particular axis. These tensors are used to describe the structure of the turbulent flow field and their definitions are given in Section II C.

While seminally important in homogeneous flows, the aforementioned effects of coarse-graining are further exacerbated when turbulent flows are inhomogeneous, in regions such as the vicinity of a smooth wall. To explore the ability of these structure tensors to model inhomogeneous flows, it is important to clarify to what extent these tensors represent the same information in homogeneous and inhomogeneous flows. For example, it can be shown⁷ that the Dimensionality tensor represents exactly the characteristics of the two-point velocity correlation in homogeneous turbulence. Specifically, the tensor eigenvalue ratio represents the aspect ratio of the two-point velocity-correlation contour, and the tensor principal-axes inclination represents the contour rotation. This is true under the assumptions of homogeneous turbulence for the scales in the inertial subrange. It is not clear whether such representations still apply near a wall, where turbulence is inhomogeneous and the local Reynolds number is often low.

In this study, we analyze the structure-tensor representation of turbulence above smooth and wavy walls using half-channel DNS simulations. The structural characteristics are compared with the corresponding information represented by the same tensors in the case of homogeneous turbulence. We also analyze whether these tensors capture near-surface changes in the structure of turbulence caused by wall waviness—a simple, two-dimensional surface roughness^{8,9}. Section II summarizes the simulation parameters and provides calculation details of the stream vector and the single-point tensors, which are validated in Section III. In Section IV, we compare characteristics of the actual coherent motions with the tensors and reduce the tensors to principal information that can be used for modeling purposes. An overarching objective of many turbulence modeling efforts is to improve the fidelity of closures by integrating a higher degree of underlying physics within the closure model. To this end, a promising approach is to append to the modeling basis tensors that carry information on features of turbulence physics that are difficult to represent in existing models. In this context, single-point structure tensors appear to be very promising as they are effective measures of non-local characteristics of homogeneous turbulence⁵. In this paper, we show that for complex inhomogeneous turbulence, these tensors contain qualitative information

95 on the structure of the turbulent flow field and we quantify their behavior in the vicinity of a wavy
96 wall.

97 **II. PROBLEM FORMULATION AND METHODOLOGIES**

98 **A. Modeling background**

99 Turbulence theory and the modeling of flows at high Reynolds numbers with complex inhomogeneity are of considerable importance. The atmospheric boundary layer¹⁰ and flows over urban
100 and natural canopies¹¹ are ubiquitous examples of turbulent flows over rough surfaces. Virtually
101 all surfaces of engineering and scientific interest have some roughness and flows over them can be
102 fundamentally different from their smooth-wall counterparts, in terms of their underlying physics
103 and their engineering ramifications. With respect to the former, the innate physics of turbulence
104 close to the wall is affected strongly by roughness. For instance, depending on the roughness
105 height, the surface roughness can either interfere with the dynamics of the buffer-layer viscous
106 production mechanism or interrupt it completely. In terms of flow variables, roughness leads to
107 changes in the mean velocity profiles near the wall, in length scales and in turbulent kinetic energy
108 distributions¹². With respect to the latter, transition to turbulence can be promoted by surface
109 roughness¹³. Surface roughness can lead to changes in both the flow's coherent structures and its
110 behavior far from the wall¹⁴. It can also substantially enhance the Nusselt number in devices such
111 as heat exchangers¹⁵. Moreover, the physics underlying these phenomena can be complicated. For
112 example, the augmentation of heat transfer by roughness is a consequence of an increase in surface
113 area due to roughness, together with increased heat diffusion through roughness-enhanced turbulent
114 motion. Consequently, complex inhomogeneity leads to significant changes in the physics of
115 turbulent flows that may be difficult to describe with existing turbulence models.

117 Established turbulence models like Reynolds stress closures are typically formulated for homogeneous
118 turbulence, while eddy viscosity models are usually developed and calibrated for smooth
119 walled flows. The application of such turbulence closures to rough surface flows typically requires
120 the use of ad hoc techniques. For instance, the equivalent sand grain approach introduces the
121 sand-grain roughness height as a new parameter for the turbulence model, which enables the enhancement
122 of turbulence in the near-wall region, to increase the momentum transport toward the
123 wall and to reproduce the drag increase. However, there is a schism between the physics under-

124 lying these phenomena and the manner in which such approaches reproduce them. For example,
125 equivalent sand-grain roughness models increase the frictional drag even though it arises predom-
126 inantly through pressure forces on roughness elements. Alternatively, various correction terms
127 have been appended to established turbulence models to account for roughness^{16–18}. In addition
128 to being largely empirical, such corrections suffer from a lack of robustness and universality. For
129 instance, the correction by Wilcox¹⁹ profoundly affects the flow over smooth surfaces and causes
130 unrealistically low eddy-viscosity values over regions of high roughness. In the same vein, dif-
131 ferent correction terms have to be formulated to account for the drag increase at the wall due to
132 roughness and the heat transfer augmentation by roughness, with complementary wall functions
133 for each correction etc., resulting in a cumbersome framework that may lack robustness and does
134 not offer consistent fidelity across different flows, or even across all regions of a single turbulent
135 flow. In this light, accounting for the effects of surface roughness in Reynolds-Averaged Navier-
136 Stokes (RANS) simulations has been described as the “Achilles heel of CFD”²⁰.

137 In contrast to conventional closure formulations, elliptic relaxation models have shown some
138 success in predicting turbulence over rough walls^{21–23}. The $v^2 - f$ closure in these studies in-
139 cludes terms that combine the effects of the near-wall velocity-pressure gradient correlation and
140 the anisotropic dissipation rate and, by extension, the near-wall stress anisotropy and the non-local
141 pressure-strain effects. The need for any near wall damping functions is obviated by incorporat-
142 ing near-wall turbulence anisotropy and non-local pressure-strain effects via an elliptic relaxation
143 equation that captures the non-local, wall-blocking effects. This facet is critical in the computa-
144 tion of strongly heterogeneous turbulent flows such as rough wall flows, enabling more accurate
145 prediction of heat transfer, skin friction, and turbulent boundary layer separation. Consequently,
146 the addition of information regarding the turbulence structure may potentially enable better mod-
147 eling of turbulence over complex inhomogeneity. In an analogous scenario, appending turbulence
148 structure tensors to the modeling basis should improve the modeling of non-local physics in sec-
149 ond moment closures. In this investigation, we analyze whether such structure tensors may aid
150 turbulence modeling over complex inhomogeneities. We focus on the nature of information pro-
151 vided by such tensors about turbulence in the vicinity of rough or wavy surfaces, the extent of this
152 information and its distribution over individual tensors.

Wall	Re_τ	k_s^+	k_c/δ	$(L_x, L_z)/\delta$	(n_i, n_j, n_k)	$(\Delta x^+, \Delta z^+)$	$(\Delta y_{\min}^+, \Delta y_{\max}^+)$	Tu_τ/δ	Δt^+
Smooth	1000	0	0	(6, 3)	(512, 256, 512)	(11.7, 5.8)	(0.3, 9.9)	85	0.03
Wavy	1000	75	0.05	(6, 3)	(1024, 226, 512)	(6.0, 6.0)	(0.9, 10.6)	86	0.04

TABLE I. Half-channel DNS simulation summary. Superscript + indicates normalization using friction velocity u_τ and viscous length scale δ_ν . L_x and L_z are domain sizes, δ is the channel half height, k_c is the roughness crest height, T is the total simulation time and Δt is the time step size. $Re_\tau = u_b \delta / \nu$, where u_b is bulk velocity. k_s is the equivalent sand-grain height, which relates the drag of a roughness to that of the sand-grain roughness studied by Nikuradse²⁴.

B. Simulation data

The DNS simulations of this investigation were performed using a well-validated code that solved the governing equations on a staggered grid using second-order, central differences for all terms, second-order accurate Adams-Bashforth semi-implicit time advancement, and Message Passing Interface parallelization. For the wavy-wall case, an immersed boundary method (IBM) based on the volume-of-fluid approach is used to impose no-slip boundary conditions at the surface. The Neumann boundary condition of pressure at the solid-fluid interface is not explicitly imposed. Detailed implementation and validation are provided by Yuan and Piomelli^{25,26}.

The parameters of the DNS simulations are summarized in Table I. Here, x_1 , x_2 , and x_3 (or x , y , and z) are, respectively, the streamwise, wall-normal, and spanwise directions, and u_j (or u , v , and w) are the velocity components in those directions. For both cases, a half channel is simulated to limit computational cost. Such approximation of a full channel as a half channel is widely used in the literature when the focus of the study is not near the channel center line (for example, see Scotti²⁷). No-slip and symmetric boundary conditions ($\partial u / \partial y = 0$, $\partial w / \partial y = 0$, $v = 0$) are applied to the bottom and top boundaries of the simulation domain respectively, and periodic conditions are used in x and z . Following previous publications on rough-walled channel flows using this code^{26,28,29}, a constant pressure gradient is applied to drive the flow. The constant pressure gradient is imposed inside both fluid and solid; in solid, it is balanced by the IBM forcing. Note also that the imposed pressure gradient is the gradient of the space- and time-averaged pressure. The pressure that is solved is the sum of the form-induced pressure (see Eq. 1) and the turbulent fluctuating pressure.

Structure tensors in channel flow

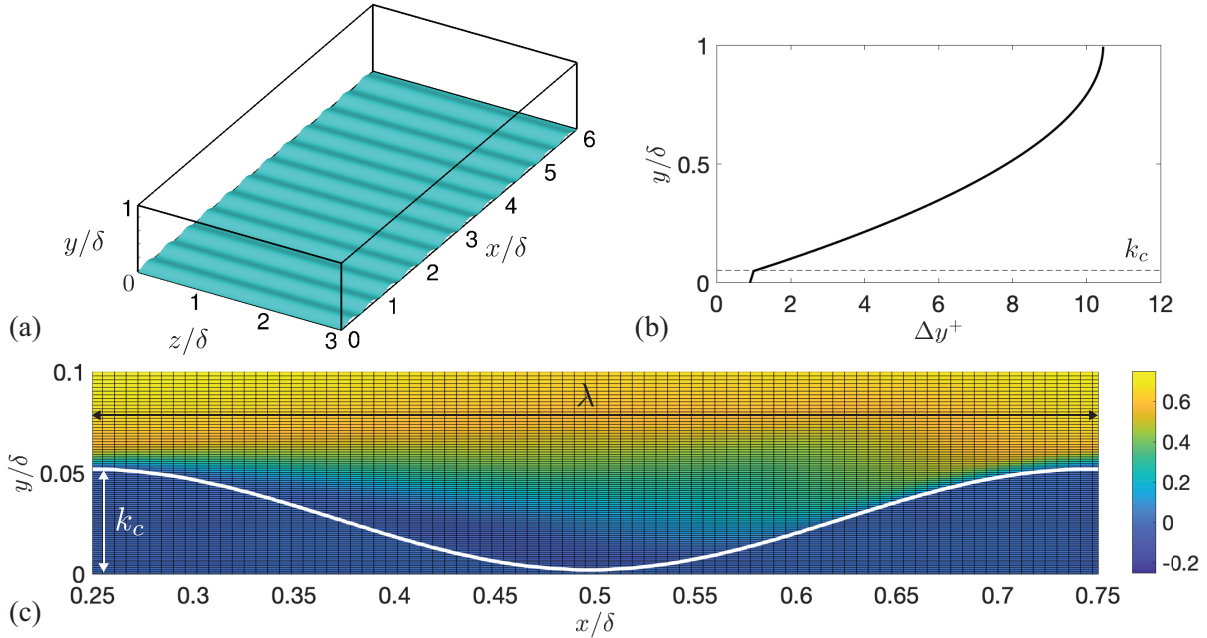


FIG. 1. (a) Simulation domain and the wall geometry of the wavy-wall case. (b) Wall-normal grid sizes in wall units. (c) Contour of time-averaged streamwise velocity overlaid with the mesh to show resolution of local shear layers. λ is the wavelength of the wavy wall.

174 Channel flows with two-dimensional sinusoidal wavy walls have been studied extensively. Ex-
 175 perimental and numerical studies showed that, if the wave height ($2a$, equivalent to k_c herein) to
 176 length (λ) ratio (also called wave slope) is large ($2a/\lambda \geq 0.10$), the flow exhibits a large, unsteady,
 177 recirculation zone downstream of the wave crest^{8,30–32}. This flow can be separated into two zones:
 178 an outer layer, for which the wavy wall is considered as an equivalent roughness, and an inner
 179 region. The latter is characterized by the presence of a region of reverse flow developing down-
 180 stream of the wave crest, forming an intense shear layer above the recirculation region, and a very
 181 thin boundary layer that develops beyond the reattachment point. Away from the wall region, the
 182 logarithmic mean velocity profile, the Reynolds stresses and the two-point velocity correlations
 183 appear not to be affected by the wavy wall^{9,33}. Therefore, such a wall geometry is equivalent
 184 to large-scale two-dimensional roughness. For the waviness simulated here, $2a/\lambda$ is set to 0.10
 185 to generate significant separation regions near the wall and the peak-to-trough height k_c is 0.05δ
 186 (or $k_c^+ = 50$) to yield a flow at the lower limit of the fully rough regime for this surface (the full
 187 rough regime is reached at $k_c^+ = 60$ for $2a/\lambda = 0.10^9$), while maintaining a clear scale separation
 188 between the roughness height and the channel height. The roughness wavelength λ is 0.5δ . Here

189 $y = 0$ is defined as the lowest elevation of the rough surface and the zero-plane location d is defined
 190 as the centroid of the rough-wall drag distribution³⁴ which was at 0.031δ in these simulations.

191 For the wavy-wall case, the simulation domain, wall geometry, grid sizes in y and the spatial
 192 resolution of the local shear layers are shown in Fig. 1. The grid sizes in wall units are smaller
 193 than the DNS study of Maas and Schumann³⁵, who used $\Delta x^+ = \Delta z^+ \approx 10$ and $\Delta y_{\min}^+ = 1.6$
 194 and obtained results that compared well with the experimental measurements of Hudson³⁶. A
 195 domain with $L_x \geq 2\lambda$ and $L_z \geq \lambda$ has been shown sufficient for an accurate evaluation of the
 196 inner-layer statistics³⁷. Keylock et al.³⁸ commented that L_x of more than 3λ is required to ensure
 197 that the x periodic boundary condition does not impact on the inferred dynamics of large-scale
 198 vortical structure. The present L_x value of 12λ is thus considered sufficient. For both simulations,
 199 the maximum Δy^+ and the total simulation time are comparable to DNS of channel flows in the
 200 literature (see, for example, Sillero et al.³⁹).

201 Near the wall, roughness leads to spatial heterogeneity in the flow. Time-averaged perturba-
 202 tions in space are separated from turbulent fluctuations using the double-averaging decomposition
 203 introduced by Raupach and Shaw⁴⁰,

$$\theta(x_i, t) = \langle \bar{\theta} \rangle(y) + \tilde{\theta}(x_i) + \theta'(x_i, t), \quad (1)$$

204 where θ is an instantaneous flow variable, $\langle \theta \rangle$ is the intrinsic spatial average in the (x, z) plane,
 205 $\langle \theta \rangle = 1/A_f \int_{A_f} \theta dA$ (where A_f is the area occupied by fluid at the corresponding y), $\bar{\theta}$ is the aver-
 206 age in both time and z , $\theta' = \theta - \bar{\theta}$ is the instantaneous turbulent fluctuation, and $\tilde{\theta} = \bar{\theta} - \langle \bar{\theta} \rangle$ is the
 207 form-induced fluctuation. The double-averaging technique has been used in the rough-wall tur-
 208 bulence literature to distinguish between turbulent and form-induced fluctuations by, for example,
 209 Coceal, Thomas, and Belcher⁴¹, Pokrajac, McEwan, and Nikora⁴² and Mignot, Barthelemy, and
 210 Hurther⁴³. This decomposition is applied to flow data for both smooth and wavy wall simulations.

211 C. Structure-tensor calculation

212 1. Smooth-wall channel

213 The structure tensors are second-order moments of the three-dimensional instantaneous stream
 214 vector ψ_i which is determined from the Poisson equation

$$-\frac{\partial^2 \psi_i}{\partial x_j \partial x_j} = \omega_i, \quad (2)$$

215 where ω_i is the vorticity vector and ψ_i is related to u_i as $u_i = \varepsilon_{ijk}\psi_{k,j}$, where ε_{ijk} is the Levi-Civita
 216 symbol.

217 Periodic boundary conditions are applied to ψ_i in x and z . Following Stylianou, Pecnik, and
 218 Kassinos⁴⁴, the y boundary conditions of Eq. (2) are imposed as (no summation among Greek
 219 letters)

$$n_\alpha \psi_\alpha + n_\beta \psi_\beta + n_\gamma \psi_\gamma = 0, \quad (3)$$

220

$$-n_\alpha \frac{\partial \psi_\beta}{\partial x_\alpha} - n_\gamma \frac{\partial \psi_\beta}{\partial x_\gamma} = -n_\alpha \frac{\partial \psi_\alpha}{\partial x_\beta} - n_\gamma \frac{\partial \psi_\gamma}{\partial x_\beta} + \varepsilon_{\beta jk} n_j u_k, \quad (4)$$

221 and

$$-n_\alpha \frac{\partial \psi_\gamma}{\partial x_\alpha} - n_\beta \frac{\partial \psi_\gamma}{\partial x_\beta} = -n_\alpha \frac{\partial \psi_\alpha}{\partial x_\gamma} - n_\beta \frac{\partial \psi_\beta}{\partial x_\gamma} + \varepsilon_{\gamma jk} n_j u_k, \quad (5)$$

222 where n_α , n_β and n_γ are the components of the unit normal vector of the surface pointing out of
 223 the fluid domain. Index α corresponds to the maximum absolute component among the three (i.e.
 224 $|n_\alpha| > |n_\beta|, |n_\gamma|$), while the remaining indices, β and γ , are such that a right handed coordinate
 225 system is formed. Each component of ψ_i and ω_i is defined at the cell center. Equation (2) is
 226 recast as a system of linear equations using second-order central differencing (first-order one-sided
 227 differencing at the domain boundaries) and is solved using a successive over-relaxation (SOR)
 228 scheme.

229 The single-point structure tensors include the Reynolds stress (R_{ij}), Dimensionality (D_{ij}), Cir-
 230 cularity (F_{ij}), and Inhomogeneity (C_{ij}) tensors. They are defined by Kassinos, Reynolds, and
 231 Rogers⁶ as

$$R_{ij} = \varepsilon_{ipq} \varepsilon_{jrs} \langle \overline{\psi'_{q,p} \psi'_{s,r}} \rangle, D_{ij} = \langle \overline{\psi'_{k,i} \psi'_{k,j}} \rangle, F_{ij} = \langle \overline{\psi'_{i,k} \psi'_{j,k}} \rangle, C_{ij} = \langle \overline{\psi'_{i,k} \psi'_{k,j}} \rangle \quad (6)$$

232 and so both temporal and spatial averaging of data is carried out to determine these tensor com-
 233 ponents. In this article, we follow the precedent of Kassinos, Reynolds, and Rogers⁶ and classify
 234 these as single-point tensors.

235 Each tensor has a distinct physical meaning. C_{ij} represents the degree of spatial variation of
 236 statistical quantities, as $C_{ij} = \langle \overline{(\psi'_{i,k} \psi'_{k,j})_{,k}} \rangle$, which is zero for the case of homogeneous turbulence.
 237 As such, this tensor characterizes the degree of inhomogeneity of the turbulent flow field. The
 238 Structure Dimensionality tensor D_{ij} represents the relative uniformity of the structure of the tur-
 239 bulent flow field along different coordinate directions. Equivalently, this can be viewed as the
 240 distribution of turbulent kinetic energy along different directions in wavenumber space in a ho-
 241 mogeneous flow. In contrast to the Dimensionality tensor, the Structure Componentality tensor

242 R_{ij} represents the relative strength of fluctuating velocity components along different coordinate
 243 directions. Lastly, $F_{\alpha\alpha}$ represents large-scale circulation around x_α , which can be shown by the
 244 fact that $\Psi'_{\alpha,kk} = -\omega'_\alpha$ and that, if the flow is irrotational around x_α (i.e. $\omega'_\alpha = 0$ everywhere),
 245 $\Psi'_\alpha = \text{constant}$ and consequently $\Psi'_{\alpha,k} = 0$, in which case $F_{\alpha\alpha} = 0$. The connection between F_{ij}
 246 and the vorticity tensor $\langle \overline{\omega'_i \omega'_j} \rangle$ has been pointed out by Stylianou, Pecnik, and Kassinos⁴⁵ near
 247 the wall in a turbulent pipe flow.

248 Instead of using the classical definitions outlined in Eq. (6), we calculate R_{ij} , D_{ij} , and F_{ij} using
 249 an alternative approach given by Stylianou, Pecnik, and Kassinos⁴⁵, as

$$R_{ij} = \varepsilon_{imp} Q_{mjp}, \quad D_{ij} = \varepsilon_{imp} Q_{pmj} + C_{ij}, \quad F_{ij} = \varepsilon_{imp} Q_{jpm} + C_{ji}, \quad (7)$$

250 where $Q_{ijk} = -\langle \overline{u'_j \Psi'_{i,k}} \rangle$ and C_{ij} is calculated according to its definition in Eq. (6). When calculat-
 251 ing these tensors, the use of Eq. (7) results in less numerical error associated with the discretization
 252 of $\Psi_{i,j}$ ⁴⁵. The normalized forms of R_{ij} , D_{ij} , and F_{ij} are obtained by rescaling with their respective
 253 traces, as

$$r_{ij} = R_{ij}/R_{kk}, \quad d_{ij} = D_{ij}/D_{kk}, \quad f_{ij} = F_{ij}/F_{kk}. \quad (8)$$

254 In contrast, C_{ij} is normalized as

$$c_{ij} = C_{ij}/D_{kk}, \quad (9)$$

255 and is not rescaled by C_{kk} because C_{ij} is not positive semi-definite.

256 **2. Immersed boundaries and the stream vector solver**

257 For the wavy-wall case, the Poisson equation (2) for ψ_i is solved over the entire domain, in-
 258 cluding both the fluid and the solid. Two types of ψ_i boundary conditions are imposed: (1) domain
 259 boundary conditions that are the same as in smooth-wall channel flow; and (2) immersed bound-
 260 aries on roughness. For the interface grid cells (the uppermost layer of grid cells of the immersed
 261 wall, either partially or fully solid), the wall boundary conditions (Eqs. (3)–(5)) are imposed with
 262 $\alpha = 2$, $\beta = 3$, and $\gamma = 1$, as the surface normal is predominantly in the y direction.

263 Currently, no local ψ_i reconstruction (similar to, for example, ghost-cell IBM⁴⁶) is performed to
 264 ensure that the fluid-solid interface is sharp, as might be required for a higher numerical accuracy.
 265 The local normal vector of the immersed boundary \vec{n} is obtained from the function $f(x, y, z) = 0$
 266 that describes the plane locally tangent to the solid-fluid interface,

$$\vec{n} = \vec{\nabla} f / |\vec{\nabla} f|. \quad (10)$$

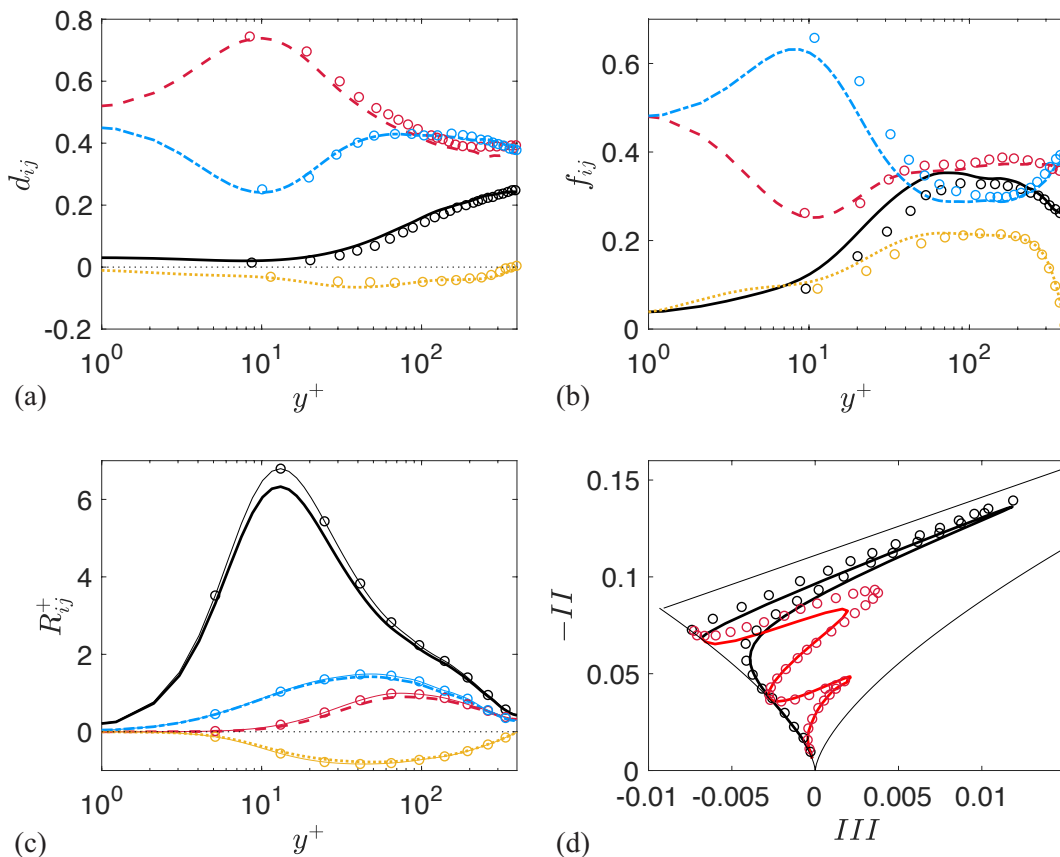


FIG. 2. (a-b) Self-normalized structure tensors obtained from smooth-wall channel flow LES with $Re_\tau = 395$. (c) R_{ij}^+ from Eq. (7) (lines) versus error-free calculation (lines with symbols). Components: 11 (—), 22 (---), 33 (---), 12 (---). (d) Lumley triangle showing anisotropies of d_{ij} (—) and f_{ij} (—). Symbols in (a), (b), (d) are data from Vartdal⁴⁷.

267 Second-order central differencing is used to discretize Eqs. (10) to obtain $\vec{n}(\vec{x})$. It is then used in
 268 Eqs. (3)–(5) on the immersed boundary to enforce these boundary conditions, which are applied
 269 to interface grid cells explicitly at the end of each SOR iteration.

270 III. CODE VALIDATION

271 To validate the stream vector solver without immersed boundaries, ψ_i is calculated from large-
 272 eddy simulation (LES) data of a smooth-wall channel flow with $Re_\tau = 395$. The self-normalized
 273 tensors are compared with results obtained from a similar LES channel-flow simulation by Vart-

274 dal⁴⁷ in Fig. 2(a,b). The two LES simulations share the same domain size of $(2\pi \times 1 \times \pi)\delta$
 275 and similar grid sizes, $(\Delta x, \Delta y_{\min}, \Delta z)^+ \approx (25, 0.6, 9)$. Good agreement is obtained for all compo-
 276 nents, the slight differences attributed to numerical error as Vartdal⁴⁷ calculated structural tensors
 277 through their definitions in Eq. (6) rather than Eq. (7). In Fig. 2(c), the Reynolds stress tensor
 278 obtained from Eq. (7) is compared with that obtained from the calculation of $R_{ij} = \overline{u'_i u'_j}$ which is
 279 free of error from the ψ_i solver. The discrepancy quantifies the numerical error of the tensor calcu-
 280 lation as up to 3% of the local R_{kk} value. A similar error range of 3 – 4% of R_{kk} was also estimated
 281 by Stylianou, Pecnik, and Kassinos⁴⁵ from a pipe flow DNS with $Re_\tau = 180$. For the present DNS
 282 cases with $Re_\tau = 1000$, this error is estimated to be of up to 6% of R_{kk} . The anisotropy invariants
 283 of d_{ij} and f_{ij} tensors are shown within the ‘Lumley triangle’ in Fig. 2(d), from which it can be
 284 seen that the anisotropy invariants computed in this study are very similar to those reported by
 285 Vartdal⁴⁷.

286 It should be noted that the structure tensors obtained from half-channel flow simulations de-
 287 scribed in Sec. IV do not collapse far from the wall with those that would be obtained from full-
 288 channel simulations. This is due to the symmetry boundary condition imposed for the velocity
 289 fields and the boundary conditions for ψ_i imposed by Eqs. (3)-(5) (e.g. $\psi_2 = 0$ at $y = \delta$), which do
 290 not hold for a full channel. Detailed comparison is given in the Appendix. However, the difference
 291 between the structure tensors obtained from a half channel versus a full channel is limited to the
 292 region of $y > \delta/2$, while the effect of the rough wall is later shown to be limited to the near-wall
 293 region. Therefore, a half-channel configuration is considered herein as an efficient and effective
 294 way to demonstrate the rough-wall effect on the structure tensors.

295 To test the implementation of the immersed boundary method in the stream vector solver, a
 296 two-dimensional laminar tilted-channel is used. The channel is tilted in the (x, y) plane at an angle
 297 of 45° from the global coordinates of the Cartesian grid. A uniform grid is used in all directions.
 298 Here, ψ_i is obtained from analytically deduced velocity distributions, instead of velocities from a
 299 simulation with the IBM, to eliminate the error from IBM in the Navier-Stokes solver. In Fig. 3(c),
 300 results for ψ_i using the immersed boundary implementation of the ψ_i solver are compared with
 301 their counterparts obtained for flow in the same channel aligned with these coordinates, without
 302 immersed boundaries. The contour of the only non-zero component ψ_3 is shown in Fig. 3(a)
 303 across the immersed boundary. The velocities, reconstructed from ψ_i using central differencing,
 304 are compared in Fig. 3(d), after transformation to reorient ψ_i and u_i to the coordinates of the
 305 channel. A very good collapse is obtained for all ψ_i and u_i components. Figure 3(b) shows

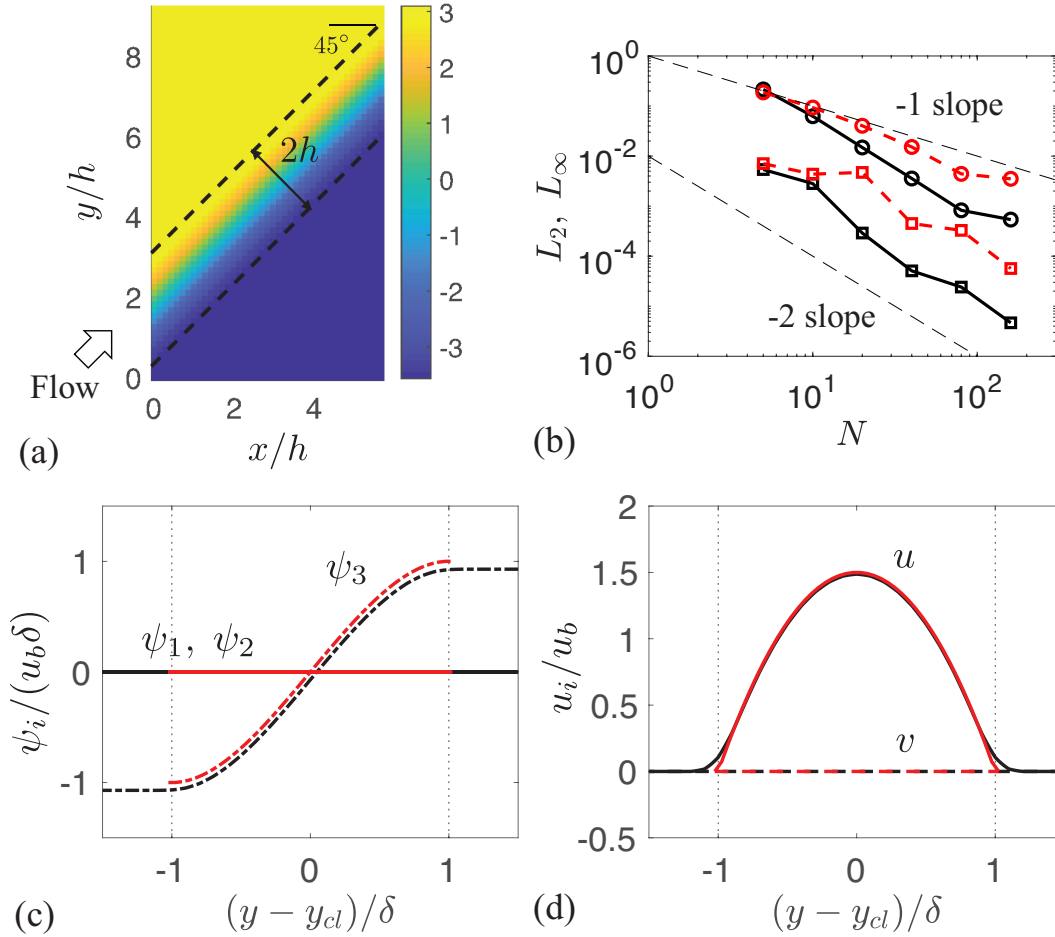


FIG. 3. Validation of the stream vector solver with immersed boundaries using a tilted laminar channel. (a) Distribution of ψ_3 . (b) L_2 -norm (—) and L_∞ -norm (---) errors of reconstructed u (\circ) and v (\square) versus the number of grid points spanning channel height N . Comparison of (c) ψ_i and (d) reconstructed u_i for $N = 10$ between calculations with (black) and without immersed boundaries (red or dark gray). Here y_{cl} is the center-line elevation.

306 the L_2 -norm errors of the reconstructed u and v velocities, which both decrease with increasing
 307 number of grid points across the channel at a second-order rate, while the L_∞ -norm errors decrease
 308 at a rate between first and second orders. The current immersed boundary treatment of the ψ_i
 309 solver is analogous to reconstructing the immersed boundary as a stepwise geometry⁴⁸. Such an
 310 idealization leads to local errors in the vicinity of the immersed boundary, which presumably cause
 311 the L_∞ -norm error to be lower than second order. In this study, these errors are expected to be small
 312 because the wall waviness is well resolved.

313 The tilted channel is a simple test case since the immersed boundary is flat. To perform an error

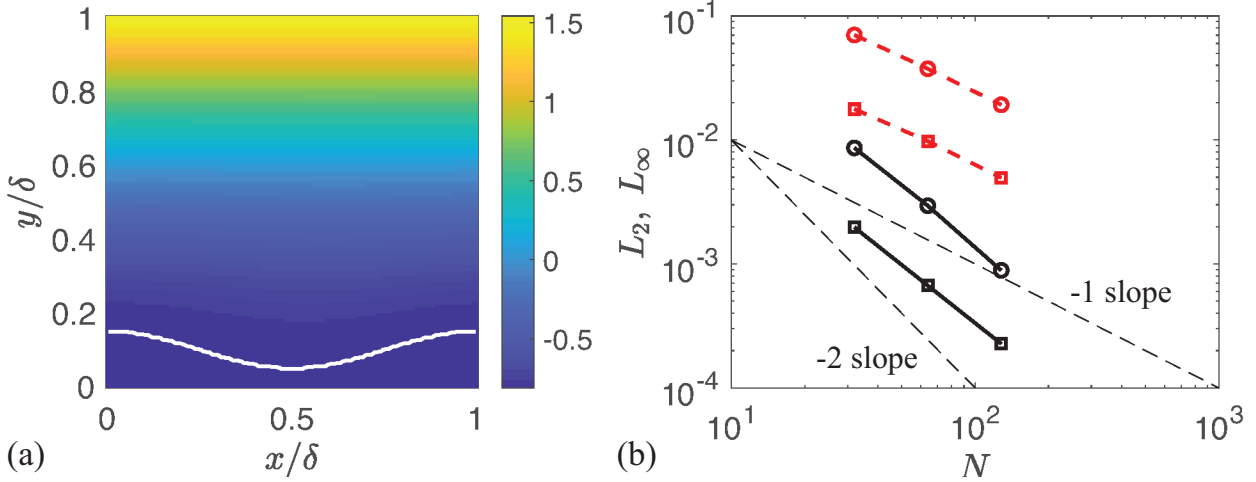


FIG. 4. Validation of the stream vector solver with an immersed boundary using a laminar channel flow with a wavy wall. (a) Distribution of ψ_3^+ . White line: solid-fluid interface. (b) L_2 -norm (—) and L_∞ -norm (---) errors of reconstructed u^+ (\circ) and v^+ (\square) as compared with the actual u^+ and v^+ versus the number of grid points.

314 analysis near a curved wall, a laminar channel flow with $Re_\tau = 10$ on a wavy wall with $2a/\lambda = 0.1$,
 315 $\lambda/\delta = 1$ (larger λ than that used in the turbulent flow simulations herein) and a x domain size of
 316 1λ is used. Uniform grids are used in both x and y . Simulations are conducted with three spatial
 317 resolutions: $n_i \times n_j = 32^2, 64^2$, and 128^2 . The velocities reconstructed from ψ_i are compared to
 318 the actual velocity obtained from the simulations. Figure 4(a) displays the contour of the only
 319 non-zero component of stream vector, ψ_3 , for the case with a resolution of 128^2 grid points in x
 320 and y . Figure 4(b) shows the order-of-accuracy of reconstructed u and v . The L_∞ -norm errors are
 321 both first-order, while the L_2 -norm errors are almost second order.

322 IV. RESULTS

323 A. The wavy-wall channel

324 To validate the present wavy-wall DNS simulation using the immersed boundary method, we
 325 compare the pressure-drag coefficient with existing studies using experiments or simulations with
 326 body-fitted mesh. The pressure-drag coefficient is determined by integrating the average pressure

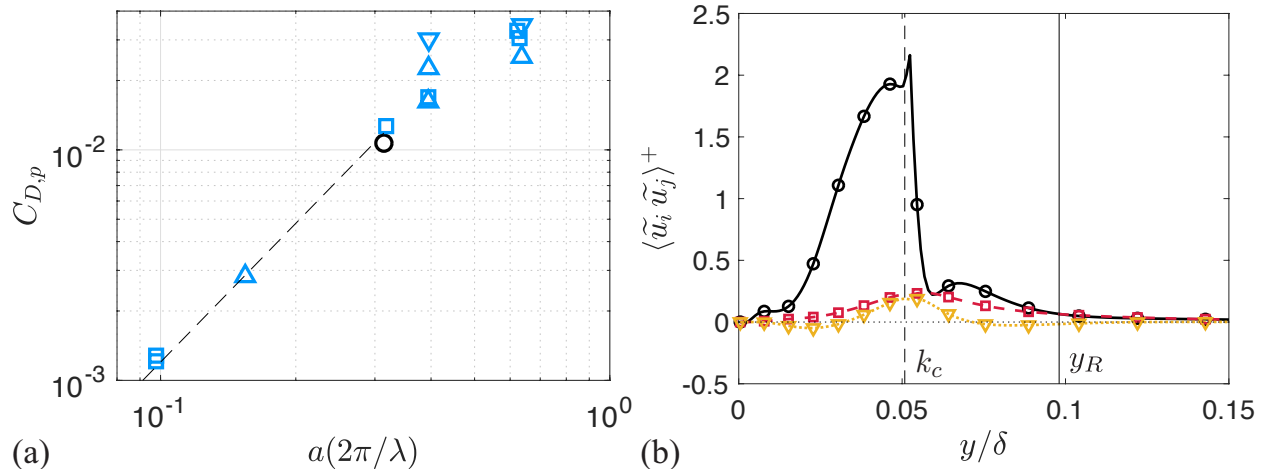


FIG. 5. (a) Wavy-channel pressure drag coefficient comparison with existing studies: \circ present DNS, \square Henn and Sykes³⁷, \triangle Zilker and Hanratty³⁰, ∇ Buckles, Hanratty, and Adrian³¹, --- fitted quadratic relation⁴⁹; (b) dispersive stresses in the wavy-wall case showing the extent of roughness sublayer, y_R . Dispersive stress components: 11 (\circ), 22 (\square), 12 (∇).

327 along the fluid-solid interface (Zilker and Hanratty³⁰) as

$$C_{D,p} = \frac{1}{(1/2)\rho u_b^2 \lambda} \int_0^\lambda \bar{P} \frac{dy}{dx} dx, \quad (11)$$

328 where u_b is the bulk velocity. In Fig. 5, the present value is compared with the values determined
 329 experimentally by Zilker and Hanratty³⁰ with $Re_b \approx 14,000 - 30,000$ and $2a/\lambda = 0.05 - 0.2$ and
 330 by Buckles, Hanratty, and Adrian³¹ with $Re_b \approx 10,700 - 30,000$ and $2a/\lambda = 0.125 - 0.2$. Large-
 331 eddy simulations of Henn and Sykes³⁷ with $Re_b = 57,00 - 10,800$ and $2a/\lambda = 0.03 - 0.2$ are
 332 also compared. These parameters bound the corresponding values of Re_b and wave slope in the
 333 present DNS. As pointed out by Henn and Sykes³⁷, for $a(2\pi/\lambda) \leq 0.31$, $C_{D,p}$ appears insensi-
 334 tive to the Reynolds number variation in this range and the prediction of $C_{D,p} \sim (2\pi a/\lambda)^2$ from
 335 the analytical model for small-amplitude waves⁴⁹ is consistent with these values. The pressure
 336 drag coefficient computed from the present DNS is in very good agreement with reference values,
 337 indicating that modifications of near-wall turbulent structure associated with the mean-flow sep-
 338 aration and reattachment are captured accurately by the immersed boundary method of Yuan and
 339 Piomelli²⁵.

340 The roughness sublayer is defined here as the entire layer within which the streamwise dis-
 341 persive stress is not negligible, i.e. $\langle \tilde{u}^2 \rangle^{1/2} \geq 0.03 \langle \bar{u} \rangle$, which is similar to the definition used by
 342 Pokrajac *et al.*⁵⁰. Figure 5(b) shows the distribution of the dispersive stresses and both the wave

Structure tensors in channel flow

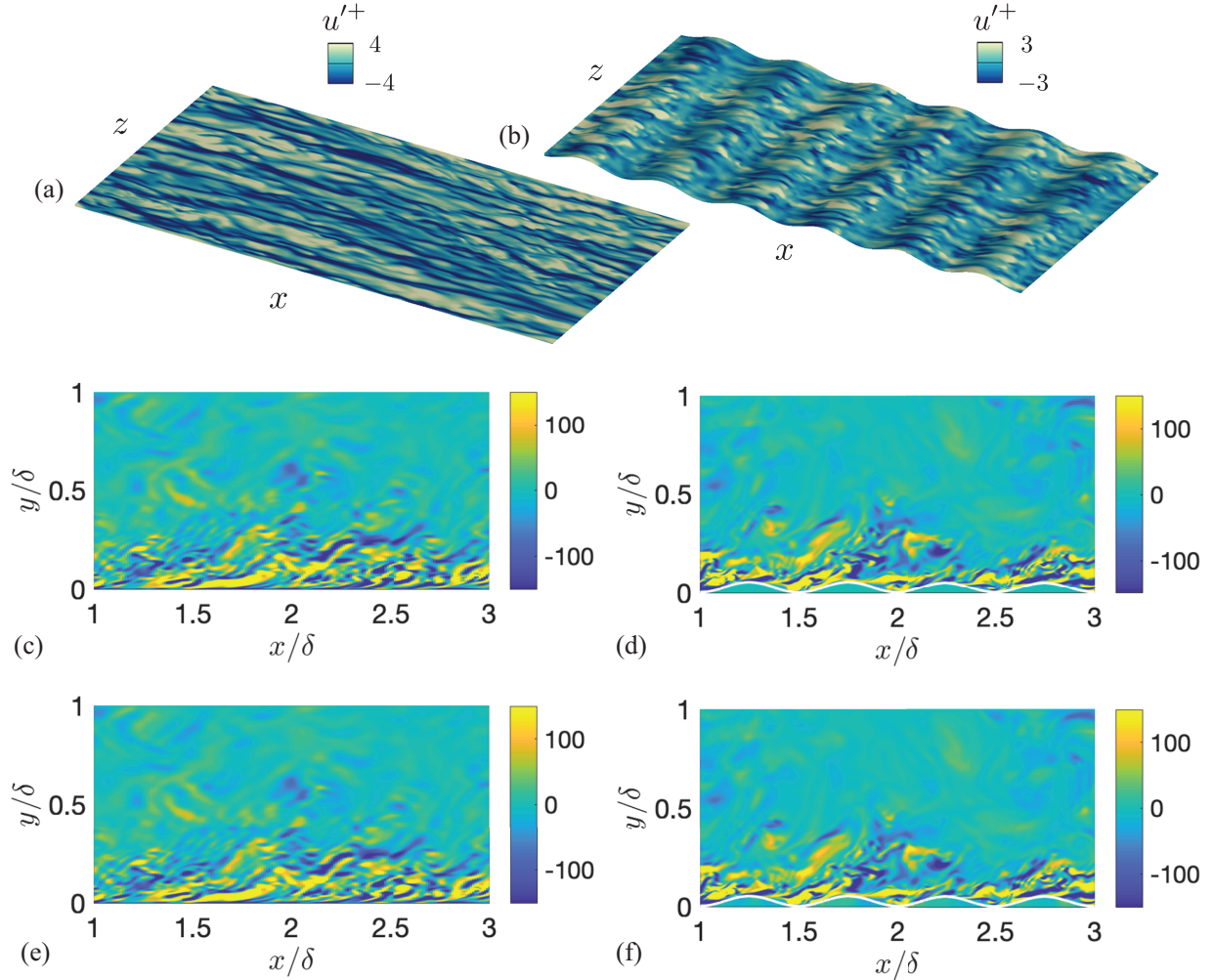


FIG. 6. Instantaneous contours of u'^+ at an elevation of 13 wall units above the wall in 1/4 of the x - z domain (a,b), contours of ω_z^+ of the original DNS velocity (c-d), and ω_z^+ reconstructed from ψ_i (e-d) in the wall-normal plane at $z/\delta = 1.5$, on the smooth wall (a,c,e) and the wavy wall (b,d,f). Solid white lines indicate immersed boundaries. Flow goes from left to right.

343 crest height k_c and the border of the roughness sublayer y_R in the wavy-wall case. The sublayer is
 344 confined mostly to the region $y/\delta \lesssim 0.1$. As will be shown later, this layer contains the majority
 345 of the effects of wall waviness on the structure tensor components.

346 Figure 6(a,b) compares instantaneous values of u'^+ at an elevation of 13 wall units away from
 347 the wall, which corresponds to the buffer layer above the smooth wall, and in the roughness sub-
 348 layer in the wavy-wall case. This elevation was chosen to allow a comparison of the representative
 349 near-wall characteristics in the two flows. Farther away from the wall toward the edge of the rough-
 350 ness sublayer, the velocity contours become increasingly similar in the two cases (not shown). A

351 clear structural change is evident, which is associated with the break-up of low-speed streaks. De
 352 Angelis et al.³² also suggested that the streaks appear to be generated at the reattachment point
 353 and to be extinguished at the next reattachment point with a new cycle starting, based on the ra-
 354 tio of local u' production and dissipation. It will be shown in Section IV B that the single-point
 355 structure tensors capture the shortened streaky motions. Figure 6(c-f) compares the instantaneous
 356 distributions of ω_z^+ in an (x, y) plane obtained using the original DNS velocity data and the vor-
 357 ticity reconstructed from ψ_i , for both cases. It can be seen that the reconstructed fields match the
 358 original fields very well, with or without the immersed fluid-solid boundary.

359 B. Comparison of structure tensors over smooth and wavy walls

360 The structure tensors for flow over smooth and wavy-wall boundaries are compared in Fig. 7
 361 and 8 using logarithmic and linear scales, respectively. The components of the Inhomogeneity
 362 tensor are normalized by wall units, to compare the relative inhomogeneity between different
 363 locations and between cases. For the other tensors, the self-normalized form in Eq. (8) is used to
 364 show differences in their anisotropies.

365 The Inhomogeneity tensor C_{ij} (plotted as its symmetric equivalent $C_{ij} + C_{ji}$) is shown in
 366 Fig. 7(a). The extent of the wall layer within which turbulence has significant inhomogeneity is
 367 important for modeling purposes as, beyond this layer, the state of homogeneous turbulence can be
 368 specified fully by only two structure tensors⁶. Above the smooth wall, the inhomogeneous region
 369 (with non-negligible $C_{ij} + C_{ji}$) extends to $y^+ \approx 30$ whereas, over the wavy wall, the inhomoge-
 370 neous region is confined to the roughness sublayer on account of the roughness-scale form-induced
 371 shear $\partial \tilde{u}_i / \partial x_j$ there. A small peak is visible for the C_{22} component at around k_c . This is perhaps
 372 due to the significant spatial variation of $\partial \tilde{u}_i / \partial y$ associated with the thin attached local mean shear
 373 layers on the peak of the sinusoidal wall and above the mean recirculation regions.

374 In general, waviness increases the near-wall isotropy of r_{ij} , d_{ij} , and f_{ij} , as well as the magni-
 375 tudes of their off-diagonal components. For r_{ij} , this observation is consistent with the findings of
 376 Smalley *et al.*⁵¹, Busse and Sandham⁵² and Flack and Schultz⁵³.

377 The normalized Circulicity tensor f_{ij} is plotted in Fig. 7(d). The dominance of the 22 and 33
 378 components of f_{ij} near the smooth wall is due to $\partial u' / \partial y$ and $\partial u' / \partial z$ on account of low- and high-
 379 speed streaks⁴⁵. Furthermore, the rapid increase of the 11 component with increasing distance
 380 from the smooth wall toward a peak at $y^+ \approx 30$ is a consequence of the quasi-streamwise vortices

Structure tensors in channel flow

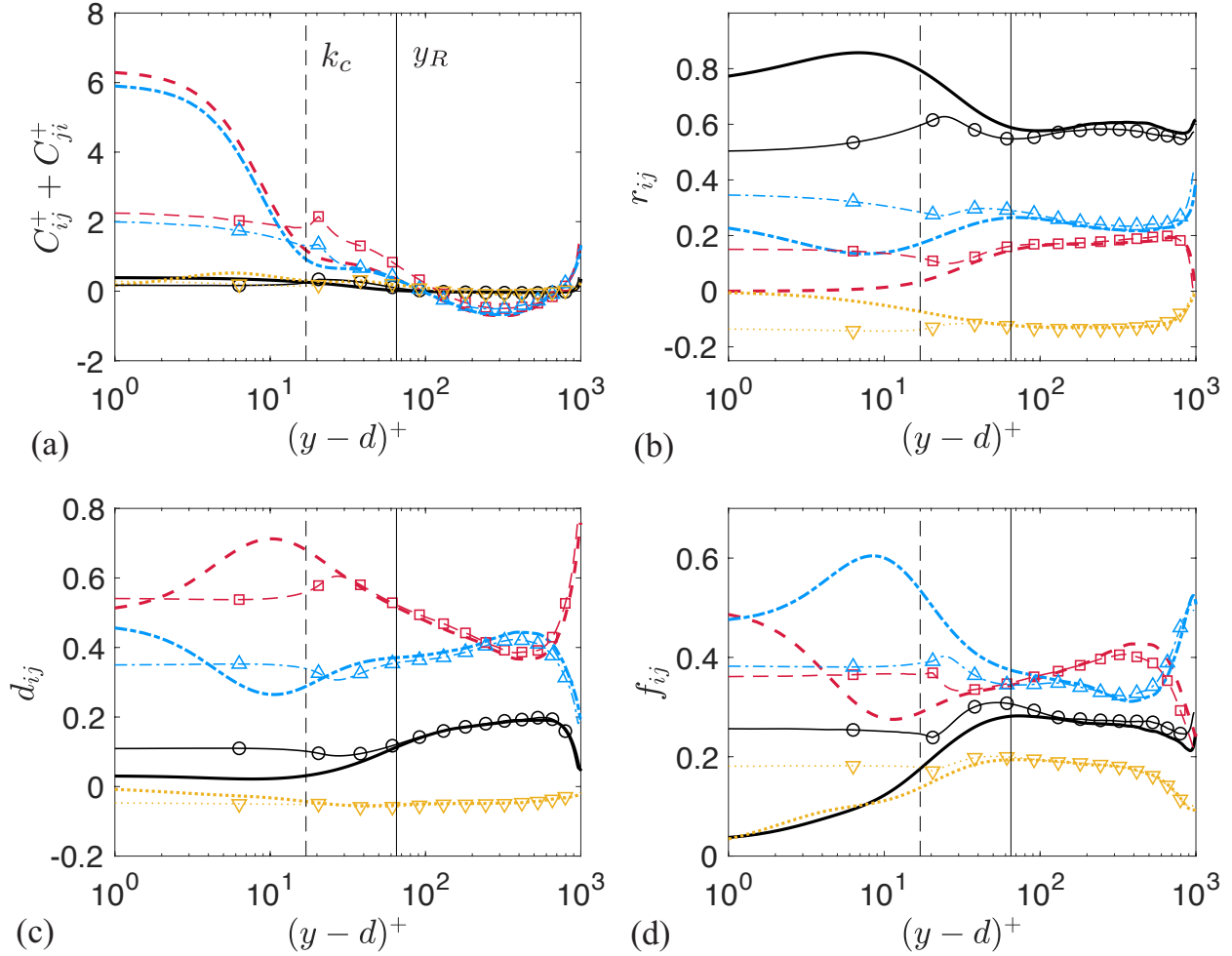


FIG. 7. Inhomogeneity tensor (a) and normalized Reynolds-stress (b), Dimensionality (c) and Circularity tensors (d) along y in logarithmic scale. Smooth-wall components: 11 (—), 22 (---), 33 (- - -), 12 (- · - ·). Lines with symbols show Wavy-wall components: 11 (○), 22 (□), 33 (△), 12 (▽). In the smooth case $(y-d)^+$ reduces to y^+ .

381 in this region. On the wavy wall, all diagonal components remain significant in the vicinity of
 382 the wall, consistent with the presence of roughness-scale three-dimensional vortical structures in
 383 the sublayer of a fully rough flow, such as the head-down and head-up hairpins⁵⁴. Orlandi and
 384 Leonardi⁵⁵ also observed greater isotropy in the vorticity near rough walls than near smooth ones.

385 Lastly, the normalized Dimensionality tensor d_{ij} is plotted in Fig. 7(c). For this structure tensor,
 386 higher values of diagonal components represent shorter coherence in the corresponding direction.
 387 From the figure, it can be seen that, in the roughness sublayer, waviness weakens the streamwise
 388 elongation of structures by enhancing d_{11} , while driving d_{22} and d_{33} closer to equality (similar

Structure tensors in channel flow

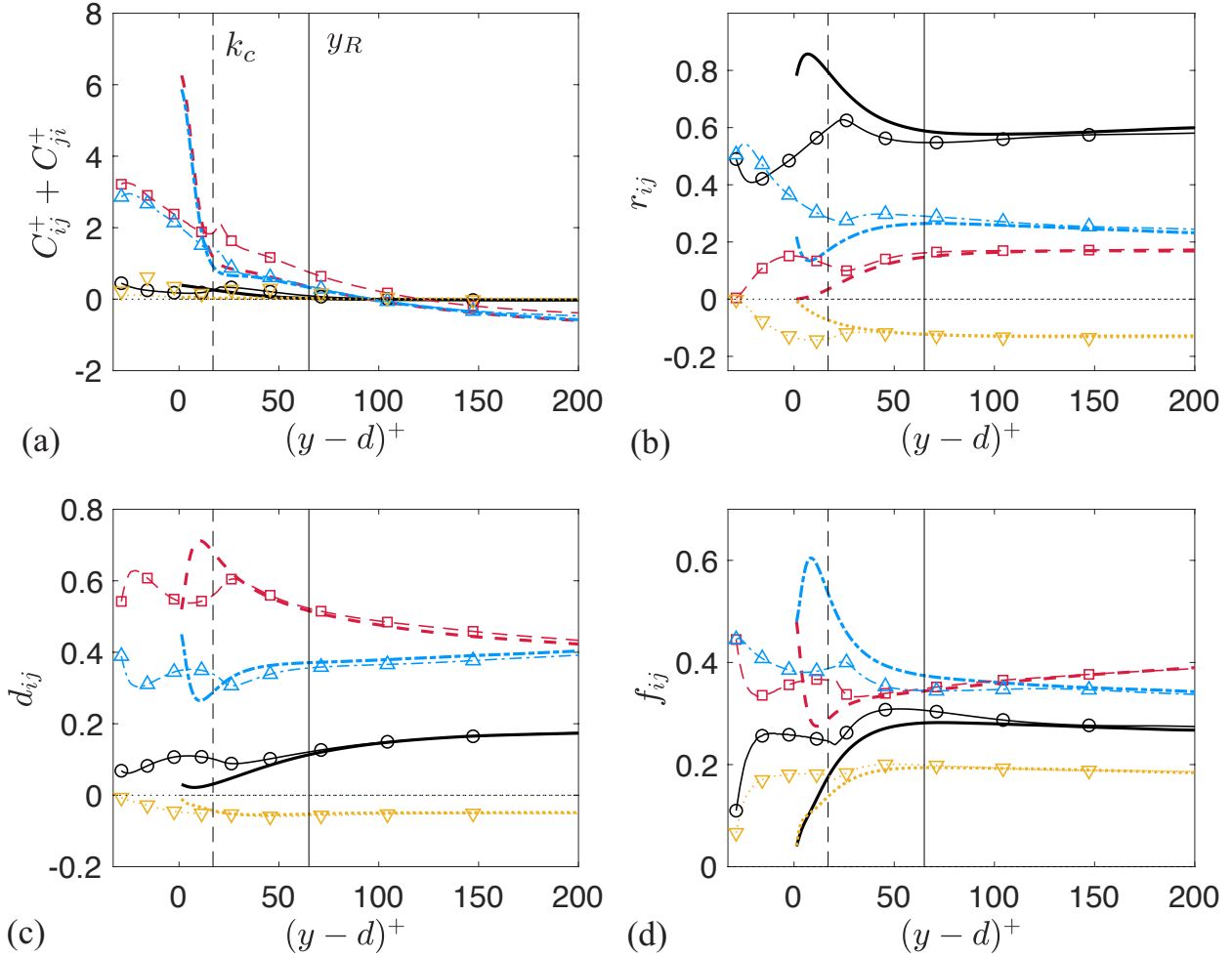


FIG. 8. Inhomogeneity tensor (a) and normalized Reynolds-stress (b), Dimensionality (c) and Circularity tensors (d) along y in linear scale. For legends see Fig. 7.

389 coherence in z and y) as the waviness imposes its scales on the flow. The deductions from this
 390 single-point tensor comparison are consistent with the instantaneous picture of turbulence in Fig. 6.

391 We also note that Townsend’s similarity hypothesis seems to apply not only to turbulence com-
 392 ponentality, but also to Dimensionality and Circularity. Although discernible differences between
 393 the smooth- and wavy-wall flows are observed in the outer layer for f_{ij} in Fig. 7(d), these differ-
 394 ences are no more than 3% of their trace values.

395 To show the spatial variation of various tensors, the (x, y) contours of R_{ij}^+ , D_{ij}^+ and F_{ij}^+ obtained
 396 using statistics of ψ'_i gradients averaged in time and z (instead of time and both x and z as shown
 397 in Fig. 7) are displayed in Fig. 9. The dividing streamline is obtained as the contour line of $\overline{\Psi}_3$
 398 value at the immersed boundary; it quantifies the extend of the separation bubble. The variations

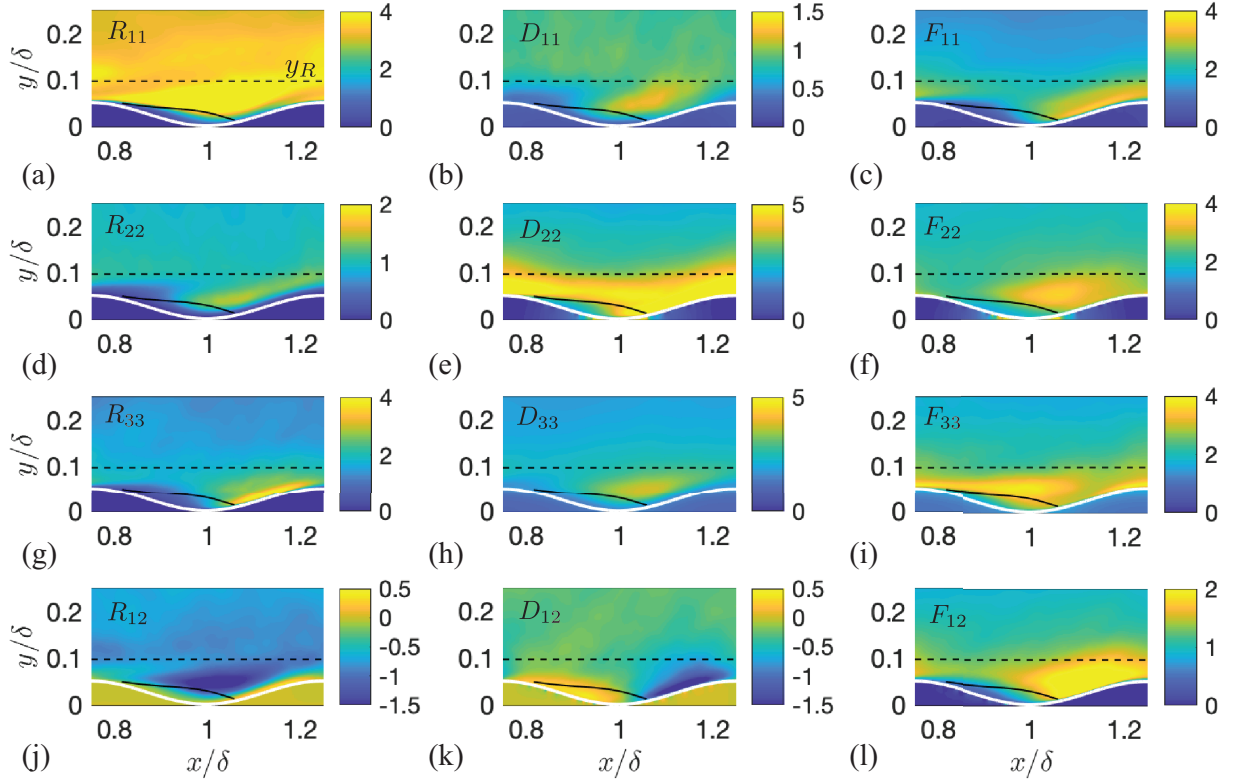


FIG. 9. Contour of 11 (a-c), 22 (d-f), 33 (g-i) and 12 components (j-l) of R_{ij}^+ (a,d,g,j), D_{ij}^+ (b,e,h,k), F_{ij}^+ (c,f,i,l) tensors. White lines indicate solid-fluid interface. Black lines: top of the roughness sublayer (---) and dividing streamline (—).

399 of R_{ij} components shown in Fig. 9(a,d,g,j) match very well with results available in the literature
 400 (for example, see experimental measurements of Hudson et al.⁸). The dominant dynamical phe-
 401 nomena include the following. (i) The detached shear layer corresponding to the \bar{u} inflection point
 402 significantly augments the Reynolds shear stress and u' production. (ii) A thin boundary layer is
 403 generated at the reattachment point, where significant TKE redistribution takes place, mostly from
 404 u' to w' energy. (iii) Flow acceleration on the upslope side leads to increased u' and v' due to pro-
 405 ductions associated with more intense $\partial\bar{u}/\partial x$ and $\partial\bar{v}/\partial x$, respectively. (iv) Below the separated
 406 shear layer, a retarded flow region is formed where the Reynolds stresses are relatively weak and
 407 the TKE is maintained by but diffusion processes, instead of production. Comparing the middle
 408 of the roughness sublayer (e.g. $y \approx d$) in the wavy-wall case and the buffer layer (e.g. $y^+ = 10$) on
 409 the smooth wall, the aforementioned phenomena lead to weaker r_{11} and stronger r_{22} , r_{33} and r_{12}
 410 components on the wavy wall. For the Dimensionality tensor, Fig. 9(b,e,h) show that inside the
 411 detached shear layer the coherent motions are shortened in all directions in an average sense, most

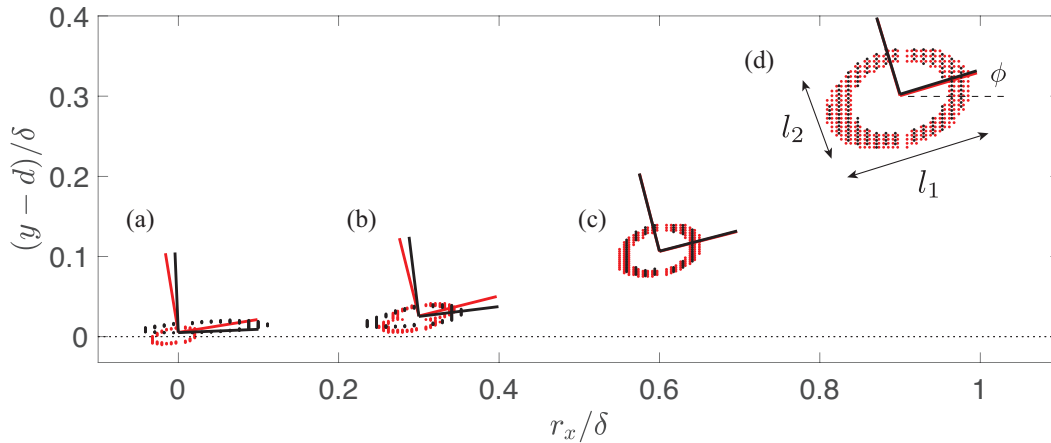


FIG. 10. Contour of the trace of the two-point velocity correlation tensor, $\mathcal{R}_{kk}(r_x, r_y)$ at a contour level between 0.7 and 0.8 centered at $y - d = 5\delta_v$ (a), $25\delta_v$ (b), 0.1δ (c), and 0.3δ (d). Black: smooth case; red (or dark gray): rough case. Short lines indicate axes of the isocontours. Contours are shifted in r_x by 0.3 units for clarity.

412 significantly for the x and z extents. This is probably due to the production of smaller-scale new
 413 turbulence inside the shear layer. The result is a more isotropic D_{ij} tensor near the wall. Fig. 9(f)
 414 shows that F_{33} decreases as the reattachment point is approached, perhaps due to the breakup of
 415 streaky motions (and consequently weaker $\partial u'/\partial y$) as three-dimensional vortical motions are gen-
 416 erated as a result of shear layer roll-up. These vortical motions also lead to augmented F_{22} in the
 417 detached shear layer. In addition, F_{11} appears to increase in the thin boundary layer generated
 418 after reattachment, probably connected to the higher turbulence production resulting in stronger
 419 streamwise vorticity fluctuations. Such damping of F_{33} and augmentation of F_{22} near the reattach-
 420 ment point, as well as the increase of F_{11} in the thin shear layer, lead to an overall more isotropic
 421 Circulicity tensor near the wall as observed in Fig. 7.

422 C. Connection between the Dimensionality tensor and the two-point velocity correlation

423 For homogeneous turbulent flows, Bhattacharya, Kassinos, and Moser⁷ showed that the eigen-
 424 value ratio and principal-axis inclinations of D_{ij} correspond respectively to the aspect ratio and

425 inclination of the isocontour of the trace of two-point velocity correlation tensor

$$\mathcal{R}_{\alpha\beta}(r_i) = \overline{\langle u'_\alpha(x_i, t) u'_\beta(x_i + r_i, t) \rangle} / \overline{\langle u'_\alpha u'_\beta \rangle}, \quad (12)$$

426 where $\vec{r} = r_x \vec{i} + r_y \vec{j}$ is the separation between the two points. For such a connection to be valid, the
427 \vec{r} magnitude must be within the inertial subrange.

428 We now test whether this homogeneous-flow correspondence applies to inhomogeneous tur-
429 bulence at low local Reynolds numbers in the near-wall region, taking care to calculate $\mathcal{R}_{\alpha\beta}(r_i)$
430 only where there is no contribution from within the solid. Values of \mathcal{R}_{kk} ranging from 0.55 to 0.85
431 are used to show the trend and the level of uncertainty in this two-point correlation. Within this
432 \mathcal{R}_{kk} range, all isocontours satisfy $|\vec{r}|^+ > 10$ and so exclude contributions from the dissipative sub-
433 range. In addition, $|\vec{r}|/\mathcal{L} \lesssim 0.25$, where \mathcal{L} is the x extent of the isocontour of $\mathcal{R}_{kk} = 0.3$ at each
434 y -location, which is considered to be a measure of the largest scale of the coherent motion. Thus,
435 the upper cut-off value of $|\vec{r}|$ used here largely (though not completely) excludes the contribution
436 from the integral scales.

437 Figure 10 compares the evolution of the $\mathcal{R}_{kk}(r_x, r_y)$ isocontour along y . The isocontours are
438 identified using \mathcal{R}_{kk} values between 0.7 and 0.8 for demonstration purposes, though using another
439 contour value range does not alter the evolutionary trend. The isocontour axes are identified using
440 principal component analysis. At each y location, the inclination and shape of the isocontour
441 is characterized by: (1) the inclination angle ϕ of the isocontour axis with respect to the (x, y)
442 coordinate; and (2) the aspect ratio (AR), l_1/l_2 , where l_1 is the isocontour length along the principal
443 component and l_2 is the length in the orthogonal direction.

444 In Fig. 11, a comparison is made between the values of ϕ and l_1/l_2 obtained from \mathcal{R}_{kk} iso-
445 contours and their corresponding D_{ij} -tensor representations. Far from the wall, the tensor repre-
446 sentations are very close to the true structural properties (with allowance for scatter in the data)
447 for both smooth- and wavy-wall flows. A good collapse might be expected as the relatively high
448 local Reynolds number results in an inertial subrange of significant extent and the flow is locally
449 homogeneous. Near the wall, waviness leads to a clear increase in the inclination angle and a
450 reduction in the aspect ratio. The tensor representations capture both near-wall changes qualita-
451 tively but not quantitatively according to the relations identified by Bhattacharya, Kassinos, and
452 Moser⁷—possibly because the assumptions of a prominent inertial subrange and homogeneous
453 turbulence do not apply near the wall. The inclusion of information from the Inhomogeneity ten-
454 sor in a structure-tensor-based model of \mathcal{R}_{ij} characteristics might result in better agreement near

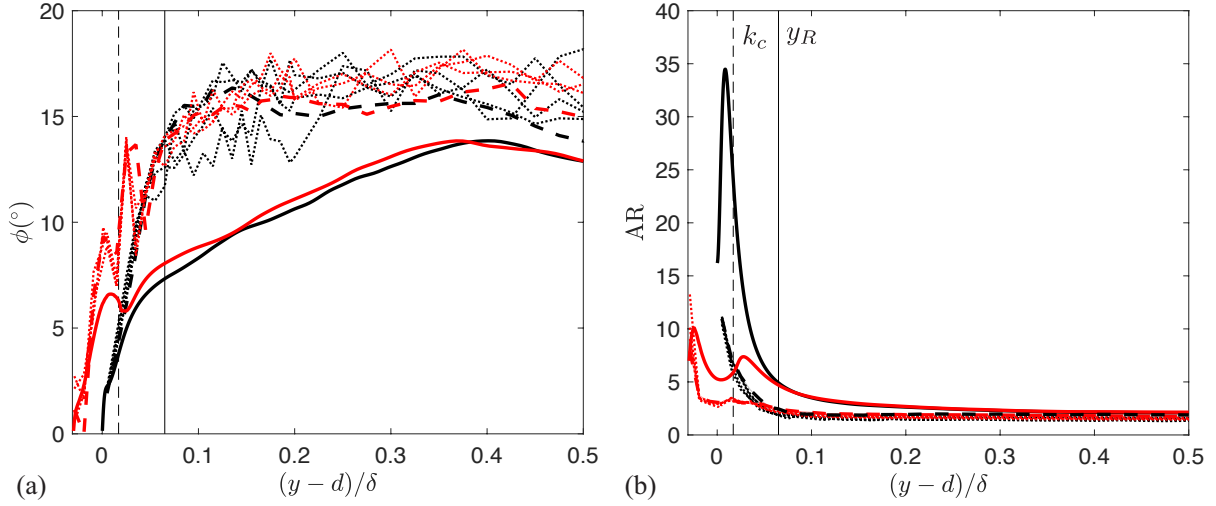


FIG. 11. Properties of the true structure (---) and its tensor prediction (—) in smooth (black) and rough (red or dark gray) cases using \mathcal{R}_{kk} range of 0.55-0.65: (a) inclination angle and (b) aspect ratio (AR) of \mathcal{R}_{kk} isocontour. --- Tensor predictions from \mathcal{R}_{kk} ranges of 0.6-0.7, 0.65-0.75 and 0.75-0.85.

455 the wall—a topic to be explored in future work.

456 D. Principal tensor information

457 For structure-based closures such as that of Kassinos and Reynolds⁵, it is impractical to impose
 458 boundary conditions on each tensor component. Instead, one imposes the minimum amount of
 459 information required to describe the structural change between the wall and the outer layer, both
 460 for smooth and wavy walls. One approach is to decompose a full tensor into: (1) the principal-axis
 461 inclination angle; and (2) a measure of tensor anisotropy which, together with the tensor trace,
 462 describe the principal information of the tensor.

463 In Fig. 12(a), the principal-axis inclination angle is shown for each tensor. For the smooth case,
 464 the inner-layer ($y/\delta < 0.1$) distributions are very similar to the smooth-wall pipe-flow results
 465 obtained by Stylianou, Pecnik, and Kassinos⁴⁵ at $Re_\tau \approx 180$. Waviness results in significantly
 466 higher inclination angles near the wall, comparable to their values at the edge of the roughness
 467 sublayer.

468 The tensor anisotropies may be characterized on a barycentric map⁵⁶, which is designed to
 469 present visually the state of turbulence in an equilateral triangle which weights equally the differ-

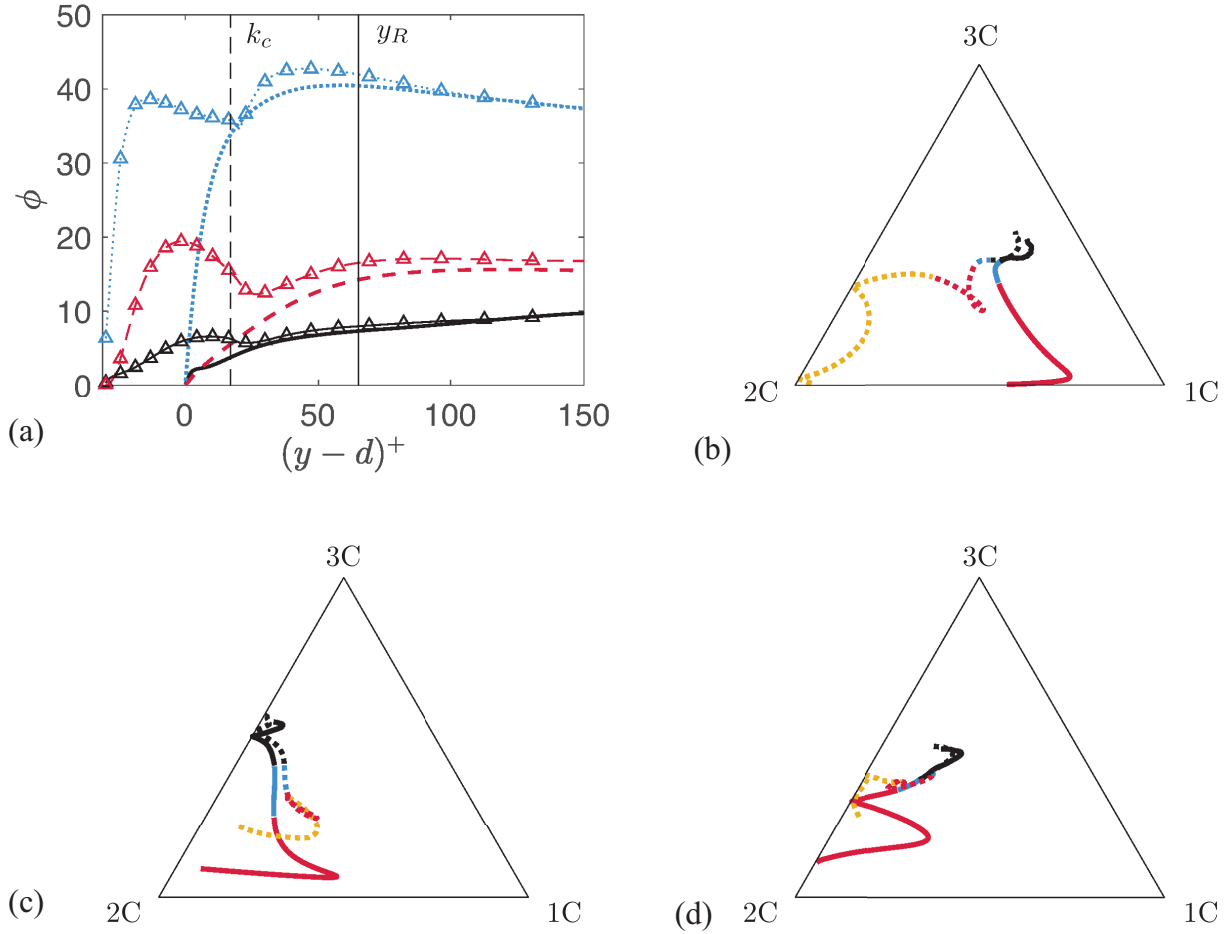


FIG. 12. (a) Inclination angles (in degrees) of principal axes of D_{ij} (—), R_{ij} (---) and F_{ij} (···) tensors for smooth wall (lines) and wavy wall (Δ) cases. Barycentric maps showing the change of anisotropies of R_{ij} (b), D_{ij} (c), and F_{ij} (d) tensors for smooth wall (—) and wavy wall (···) cases. —, ··· : $0.1\delta \leq y \leq 0.6\delta$; —, ··· : overlap region, $50\delta_v \leq y \leq 0.1\delta$ for smooth wall flow and $y_R \leq y \leq 0.1\delta$ for wavy wall flow; — : viscous wall region ($y \leq 50\delta_v$) for smooth wall flow; --- ($d \leq y \leq y_R$) and - - - ($y \leq d$): roughness sublayer for wavy wall flow.

470 ent limiting states. The one-component (1C) state describes the flow where the tensor-represented
 471 properties (fluctuations, spatial variations, or large scale circulation) exist only in one direction.
 472 The axisymmetric two-component (2C) state describes turbulence where these properties exist
 473 along two directions with equal magnitude, and the isotropic (or three-component 3C) state de-
 474 scribes flow where the properties are of equal strength in all directions.

475 The tensor anisotropies are shown on barycentric maps in Fig. 12(b-d). In Fig. 12(b) it may be

476 seen that on a smooth wall R_{ij} develops from the two-component limit in the buffer layer, where
 477 much of its turbulence kinetic energy (TKE) is in the u' component and associated with the low-
 478 speed streaks, to a state much closer to 3C in and above the overlap region where $y^+ > 50$. In
 479 Fig. 12(c), it can be seen that D_{ij} also transitions from close to the two-component limit at the
 480 wall (due to very long coherence in the x direction with $D_{11} \approx 0$) to an axisymmetric state with
 481 one small eigenvalue far from the wall, with structure elongation predominantly in the x direction
 482 and correspondingly weaker in y and z directions, with $D_{22} \approx D_{33} > D_{11}$. In Fig. 12(d), it can be
 483 seen that very near the wall F_{ij} is near the axisymmetric two-component state because the flow
 484 is dominated by circulation around the y and z axes, as a consequence of low and high velocity
 485 streaks. F_{ij} then changes towards the 3C state with increasing distance from the wall.

486 For flow over the wavy-wall, it is evident that the tensor anisotropy above the roughness sub-
 487 layer follows closely the variation in the smooth case. In the upper part of the roughness sublayer
 488 above the virtual wavy-wall origin ($y > d$), all three structure tensors are at a state close to that in
 489 the overlap region. This is presumably because, inside the roughness sublayer, quasi-streamwise
 490 vortices coexist with smaller-scale eddies generated by mechanisms such as shear-layer roll-up⁵⁷
 491 near local wake regions (see, for examples, Martinuzzi and Tropea⁵⁸ and Talapatra and Katz⁵⁴).
 492 In contrast, a significant departure from the buffer-layer state is observed below the virtual ori-
 493 gin ($y < d$), especially for R_{ij} , which takes the shape of an oblate spheroid other than the prolate
 494 one observed in smooth-wall flow. Busse and Sandham⁵² also observed this behavior in R_{ij} in
 495 the lower part of the sublayer adjacent to a random synthetic wall roughness, and attributed it to
 496 stronger damping of u' motions than v' and w' motions in this layer. Below the virtual wavy-wall
 497 origin, D_{ij} is more isotropic than in their respective buffer-layer states, where a weaker structure
 498 elongation in the x direction yields values of D_{ij} further from the two-component limit. Also,
 499 F_{ij} is further from the 2-component axisymmetric limit in the lower portion of the roughness
 500 sublayer than in the buffer layer, as a result of more significant x -axis circulation caused by three-
 501 dimensional vortices there. From the perspective of turbulence model closure, the upper portion
 502 ($y > d$) of the roughness sublayer of the wavy (fully rough) flow appears to be structurally similar
 503 to the outer layer, in the Componentality, Dimensionality and Circularity of its turbulence.

504 The observation of greater isotropy in turbulence statistics within the roughness sublayer has
 505 important implications for modeling of wavy- and rough-wall flows. For example, in smooth-
 506 wall flows, the sharp near-wall peaks in quantities such as $\langle \overline{u'^2} \rangle$ and TKE require wall functions
 507 in Reynolds-averaged Navier-Stokes closures and render model equations so stiff that smoothing

508 approaches such as elliptic relaxation⁵⁹ are often needed to satisfy boundary conditions. However,
509 in wavy- and rough-wall flows, the degree of turbulence anisotropy is greatly reduced within the
510 roughness sublayer. This observation implies that, although the specification of precise boundary
511 conditions at a virtual origin may not be straightforward, the modeling of a more isotropic tur-
512 bulence may be simpler and may not require such stiff model equations or relaxation techniques
513 to accommodate boundary conditions. This observation is supported by the modeling studies of
514 Brereton and Yuan⁶⁰, who show that the dominant contribution to shear stress in the roughness
515 sublayer in turbulent flows in rough-wall channels comes from the viscous and pressure forces
516 over roughness elements, which can be modeled as an eddy viscosity or an effective local body
517 force. The dominance of this term over the Reynolds and dispersive stresses in the roughness
518 sublayer lessens some of the limitations of Reynolds-stress closures when applied in smooth-wall
519 flows.

520 V. CONCLUSIONS

521 An overarching objective of many turbulence modeling efforts is to improve the fidelity of
522 closures by integrating a higher degree of underlying physics within the closure model. To this
523 end, a promising approach is to append to the modeling basis by adding tensors that carry infor-
524 mation regarding features of turbulence physics that are difficult to represent in existing models.
525 In this context, single-point turbulence structure tensors appear to be very promising as they are
526 effective measures of non-local characteristics of homogeneous turbulence⁵. While the capability
527 of such tensors to improve model fidelity has been verified for homogeneous turbulence, in this
528 work, we show that for complex inhomogeneous turbulence, these tensors also contain qualitative
529 information on the computed turbulence structure, which we quantify throughout the flow over a
530 wavy wall. An immersed-boundary approach for solving the vector Poisson equation is adopted
531 to solve for the stream vector to extract these tensors on an ideal (wavy), two-dimensional rough
532 surface and can potentially be used for establishing databases of single-point structure tensors for
533 structure-based model development for more complex wall-roughness geometries.

534 DNS results show that, in the sublayer adjacent to the rough/wavy surface, turbulence is inho-
535 mogeneous. In this sublayer, the Dimensionality structure tensor describes qualitatively higher-
536 order effects such as the near-wall structure inclination angle on account of waviness, as well as the
537 shortening of streamwise coherence lengths of turbulence motions. Furthermore, the Circularity

Structure tensors in channel flow

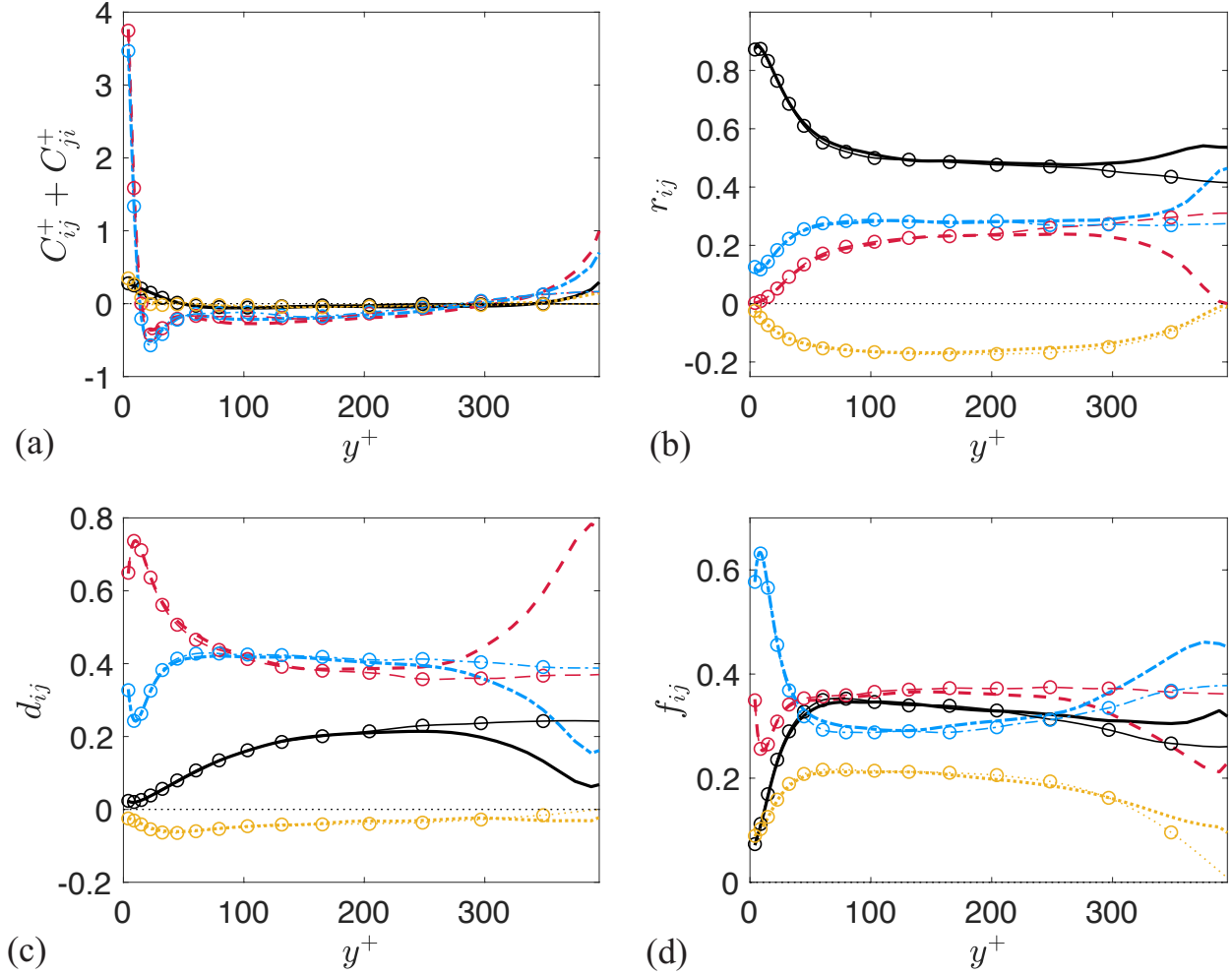


FIG. 13. Comparison of Inhomogeneity tensors (a) and normalized Reynolds-stress (b), Dimensionality (c) and Circularity tensors (d) obtained from a full channel (lines with symbols) and half channel (lines only), both with a smooth wall and $Re_\tau = 395$. Components: 11 (—), 22 (---), 33 (-.-), 12 (....).

538 tensor becomes more isotropic in the sublayer, consistent with the emergence of roughness-scale
 539 eddies. Beyond the roughness sublayer, Townsend's similarity hypothesis appears to apply not
 540 only to the componentality of turbulence, but also to its Dimensionality and Circularity. Even
 541 within the roughness sublayer above the virtual origin, turbulence above a wavy or rough surface
 542 appears to be structurally simpler compared with a smooth-wall flow. This is encouraging from
 543 a modeling standpoint. In general, tensor characteristics such as principal-axis inclination and
 544 anisotropy are shown to be sensitive to both the presence of wall waviness and the distance from
 545 the surface. Thus structure-tensor characteristics may also prove to be useful for imposing wall
 546 boundary conditions for use with structure-based turbulence models.

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551 **Appendix: Structure tensors extracted from a half channel**

552 The half-channel configuration is used in this work as an efficient way to explore the difference
 553 brought by roughness in a channel flow. In this section, we show the discrepancy between the
 554 results obtained from a half channel simulation and a full-channel one. Tensors extracted from the
 555 LES simulations of a full-channel flow with $Re_\tau = 395$ and those from its half-channel counterpart
 556 are compared in Fig. 13. In the region $y/\delta < 0.5$ (or $y^+ < 200$), the two cases collapse perfectly.
 557 In the region $0.5 < y/\delta \leq 1$, differences are increasingly significant as y increases. At $y/\delta = 1$, the
 558 symmetry condition for velocities gives $r_{22} = 0$, causing differences in the other two components
 559 also, since $r_{11} + r_{22} + r_{33} = 1$. The other tensors are also affected due to the identity⁶¹,

$$R_{ij} + D_{ij} + F_{ij} - (C_{ij} + C_{ji}) = \delta_{ij}R_{kk}. \quad (\text{A.1})$$

560 Furthermore, the ψ_i boundary conditions at the top boundary of a half channel do not hold for a
 561 full channel. For example, ψ_2 is set to zero at $y/\delta = 1$ according to Eq. (3) for a half channel, while
 562 for a full channel ψ_2 is free to take any value at the channel center line. Despite these differences,
 563 a half channel is considered effective in studying the roughness effect, which is shown limited to
 564 the near-wall region only.

565 **REFERENCES**

- 566 ¹J. O’Neil and C. Meneveau, “Spatial correlations in turbulence: Predictions from the multifractal
 567 formalism and comparison with experiments,” *Phys. Fluids A* **5**, 158–172 (1993).
- 568 ²P. Sagaut and C. Cambon, *Homogeneous turbulence dynamics*, Vol. 10 (Cambridge University
 569 Press, 2008).
- 570 ³A. A. Mishra, G. Iaccarino, and K. Duraisamy, “Sensitivity of flow evolution on turbulence
 571 structure,” *Phys. Rev. Fluids* **1**, 052402–1–11 (2016).

- 572 ⁴A. A. Mishra, K. Duraisamy, and G. Iaccarino, “Estimating uncertainty in homogeneous turbu-
573 lence evolution due to coarse-graining,” *Phys. Fluids* **31**, 025106–1—14 (2019).
- 574 ⁵S. C. Kassinos and W. C. Reynolds, “A structure-based model for the rapid distortion of ho-
575 mogeneous turbulence,” Report TF-61 (Thermosciences Division, Department of Mechanical
576 Engineering, Stanford University, 1994).
- 577 ⁶S. C. Kassinos, W. C. Reynolds, and M. M. Rogers, “One-point turbulence structure tensors,”
578 *J. Fluid Mech.* **428**, 213–248 (2001).
- 579 ⁷A. Bhattacharya, S. C. Kassinos, and R. D. Moser, “Representing anisotropy of two-point
580 second-order turbulence velocity correlations using structure tensors,” *Phys. Fluids* **20**, 101502–
581 1—13 (2008).
- 582 ⁸J. D. Hudson, L. Dykhno, and T. J. Hanratty, “Turbulence production in flow over a wavy wall,”
583 *Exp. Fluids* **20**, 257–265 (1996).
- 584 ⁹S. Nakagawa and T. J. Hanratty, “Particle image velocimetry measurements of flow over a wavy
585 wall,” *Phys. Fluids* **13**, 3504–3507 (2001).
- 586 ¹⁰E. Bou-Zeid, C. Meneveau, and M. B. Parlange, “Large-eddy simulation of neutral atmospheric
587 boundary layer flow over heterogeneous surfaces: Blending height and effective surface rough-
588 ness,” *Water Resour. Res.* **40**, W02505 (2004).
- 589 ¹¹J. Finnigan, “Turbulence in plant canopies,” *Annu. Rev. Fluid Mech.* **32**, 519–571 (2000).
- 590 ¹²J. Jiménez, “Turbulent flows over rough walls,” *Annu. Rev. Fluid Mech.* **36**, 173–196 (2004).
- 591 ¹³H. Schlichting and K. Gersten, *Boundary-layer theory* (Springer, 2016).
- 592 ¹⁴R. J. Adrian, C. D. Meinhart, and C. D. Tomkins, “Vortex organization in the outer region of
593 the turbulent boundary layer,” *J. Fluid Mech.* **422**, 1–54 (2000).
- 594 ¹⁵E. K. Kalinin and G. A. Dreitser, “Heat transfer enhancement in heat exchangers,” *Advances in*
595 *Heat Transfer* **31** (1998).
- 596 ¹⁶D. C. Wilcox, “Reassessment of the scale-determining equation for advanced turbulence mod-
597 els,” *AIAA J.* **26**, 1299–1310 (1988).
- 598 ¹⁷A. Hellsten and S. Laine, “Extension of the $k - \omega$ shear-stress transport turbulence model for
599 rough-wall flows,” *AIAA J.* **36**, 1728–1729 (1998).
- 600 ¹⁸T. Knopp, B. Einfeld, and J. B. Calvo, “A new extension for $k - \omega$ turbulence models to account
601 for wall roughness,” *Int. J. Heat Fluid Flow* **30**, 54–65 (2009).
- 602 ¹⁹D. C. Wilcox, “Formulation of the $k - \omega$ turbulence model revisited,” *AIAA J.* **46** (2008).

- 603 ²⁰V. C. Patel, “Perspective: flow at high Reynolds number and over rough surfaces—Achilles heel
604 of CFD,” *Journal of Fluids Engineering* **120**, 434—444 (1998).
- 605 ²¹J. George, A. De Simone, G. Iaccarino, and J. Jimenez, “Modeling roughness effects in turbu-
606 lent boundary layers by elliptic relaxation,” in *Proc. Summer Program, Center for Turbulence*
607 *Research* (2010) pp. 119–128.
- 608 ²²L. Wei, X. Ge, J. George, and P. Durbin, “Modeling transition on smooth and rough blades,” in
609 *ASME 2016 Fluids Engineering Division Summer Meeting collocated with the ASME 2016 Heat*
610 *Transfer Summer Conference and the ASME 2016 14th International Conference on Nanochan-*
611 *nels, Microchannels, and Minichannels* (American Society of Mechanical Engineers Digital
612 Collection, 2016).
- 613 ²³L. Wei, X. Ge, J. George, and P. Durbin, “Modeling of laminar-turbulent transition in boundary
614 layers and rough turbine blades,” *Journal of Turbomachinery* **139**, 111009 (2017).
- 615 ²⁴J. Nikuradse, “Laws of flow in rough pipes,” NACA Technical Memorandum 1292 (1933).
- 616 ²⁵J. Yuan and U. Piomelli, “Numerical simulations of sink-flow boundary layers over rough sur-
617 faces,” *Phys. Fluids* **26**, 015113–1—015113–28 (2014).
- 618 ²⁶J. Yuan and U. Piomelli, “Roughness effects on the Reynolds stress budgets in near-wall turbu-
619 lence,” *J. Fluid Mech.* **760**, R1 (2014).
- 620 ²⁷A. Scotti, “Direct numerical simulation of turbulent channel flows with boundary roughened
621 with virtual sandpaper,” *Phys. Fluids* **18**, 031701–1—4 (2006).
- 622 ²⁸J. Yuan and U. Piomelli, “Estimation and prediction of the roughness function on realistic sur-
623 faces,” *J. Turbul.* **15**, 350–365 (2014).
- 624 ²⁹J. Yuan, G. J. Brereton, G. Iaccarino, A. A. Mishra, and M. Vartdal, “Single-point structure
625 tensors in rough-wall turbulent channel flow,” in *Proceedings of the 2018 Summer Program*
626 (2018).
- 627 ³⁰D. P. Zilker and T. J. Hanratty, “Influence of the amplitude of a solid wavy wall on a turbulent
628 flow. part 2. separated flows,” *J. Fluid Mech.* **90**, 257–271 (1979).
- 629 ³¹J. Buckles, T. J. Hanratty, and R. J. Adrian, “Turbulent flow over large-amplitude wavy sur-
630 faces,” *J. Fluid Mech.* **140**, 27–44 (1984).
- 631 ³²V. De Angelis, P. Lombardi, and S. Banerjee, “Direct numerical simulation of turbulent flow
632 over a wavy wall,” *Phys. Fluids* **9**, 2429–2442 (1997).
- 633 ³³E. Napoli, V. Armenio, and M. De Marchis, “The effect of the slope of irregularly distributed
634 roughness elements on turbulent wall-bounded flows,” *J. Fluid Mech.* **613**, 385–394 (2008).

- 635 ³⁴P. S. Jackson, “On the displacement height in the logarithmic velocity profile,” *J. Fluid Mech.*
636 **111**, 15–25 (1981).
- 637 ³⁵C. Maas and U. Schumann, “Direct numerical simulation of separated turbulent flow over a wavy
638 boundary,” in *Flow Simulation with High-Performance Computers II* (Vieweg+ Teubner Verlag,
639 1996) pp. 227–241.
- 640 ³⁶J. D. Hudson, *The effect of a wavy boundary on turbulent flow*, Ph.D. thesis, University of Illinois
641 (1993).
- 642 ³⁷D. S. Henn and R. I. Sykes, “Large-eddy simulation of flow over wavy surfaces.” *J. Fluid Mech.*
643 **383**, 75–112 (1999).
- 644 ³⁸C. J. Keylock, K. S. Chang, and G. S. Constantinescu, “Large eddy simulatiojn of the velocity-
645 intermittency structure for flow over a field of symmetric dunes,” *J. Fluid Mech.* **805**, 656–685
646 (2016).
- 647 ³⁹J. Sillero, J. Jimenez, and R. D. Moser, “Two-point statistics for turbulent boundary layers and
648 channels at Reynolds numbers up to $\delta^+ \approx 2000$,” *Phys. Fluids* **26** (2014).
- 649 ⁴⁰M. R. Raupach and R. H. Shaw, “Averaging procedures for flow within vegetation canopies,”
650 *Bound.-Lay. Meteorol.* **22**, 79–90 (1982).
- 651 ⁴¹O. Coceal, T. G. Thomas, and S. E. Belcher, “Spatial variability of flow statistics within regular
652 building arrays,” *Bound.-Lay. Meteorol.* **125**, 537–552 (2007).
- 653 ⁴²D. Pokrajac, I. McEwan, and V. Nikora, “Spatially averaged turbulent stress and its partition-
654 ing,” *Exp. Fluids* **45**, 73–83 (2008).
- 655 ⁴³E. Mignot, E. Barthelemy, and D. Hurther, “Double-averaging analysis and local flow char-
656 acterization of near-bed turbulence in gravel-bed channel flows,” *J. Fluid Mech.* **618**, 279–303
657 (2009).
- 658 ⁴⁴F. S. Stylianou, R. Pecnik, and S. C. Kassinis, “A general framework for computing the turbu-
659 lence structure tensors,” *Comput. Fluids* **106**, 54–66 (2015).
- 660 ⁴⁵F. S. Stylianou, R. Pecnik, and S. C. Kassinis, “Analyzing a turbulent pipe flow via the one-
661 point structure tensors: Vorticity crawlers and streak shadows,” *Comput. Fluids* **140**, 450–477
662 (2016).
- 663 ⁴⁶R. Mittal and G. Iaccarino, “Immersed boundary methods,” *Annu. Rev. Fluid Mech.* **37**, 239–261
664 (2005).
- 665 ⁴⁷M. Vartdal, “Computing turbulence structure tensors in plane channel flow,” *Comput. Fluids*
666 **136**, 207–211 (2016).

- 667 ⁴⁸E. A. Fadlun, R. Verzicco, P. Orlandi, and J. Mohd-Yusof, “Combined immersed-boundary
668 finite-difference methods for three-dimensional complex flow simulations,” *J. Comput. Phys.*
669 **161**, 35–60 (2000).
- 670 ⁴⁹N. Wood and P. Mason, “The pressure force induced by neutral, turbulent flow over hills.” *Q. J.*
671 *Roy. Meteor. Soc.* **119**, 1233–1267 (1993).
- 672 ⁵⁰D. Pokrajac, L. J. Campbell, V. Nikora, and I. Manes, C. adn McEwan, “Quadrant analysis of
673 persistent spatial velocity perturbations over square-bar roughness,” *Exp. Fluids* **42**, 413–423
674 (2007).
- 675 ⁵¹R. J. Smalley, S. Leonardi, R. A. Antonia, L. Djenidi, and P. Orlandi, “Reynolds stress
676 anisotropy of turbulent rough wall layers,” *Exp. Fluids* **33**, 31–37 (2002).
- 677 ⁵²A. Busse and N. D. Sandham, “Parametric forcing approach to rough-wall turbulent channel
678 flow,” *Journal of Fluid Mechanics* **712**, 169–202 (2012).
- 679 ⁵³K. A. Flack and M. P. Schultz, “Roughness effects on wall-bounded turbulent flows,” *Phys.*
680 *Fluids* **26**, 101305 (2014).
- 681 ⁵⁴S. Talapatra and J. Katz, “Coherent structures in the inner part of a rough-wall channel flow
682 resolved using holographic PIV,” *J. Fluid Mech.* **711**, 161–170 (2012).
- 683 ⁵⁵P. Orlandi and S. Leonardi, “Direct numerical simulation of three-dimensional turbulent rough
684 channels: parameterization and flow physics,” *J. Fluid Mech.* **606**, 399–415 (2008).
- 685 ⁵⁶S. Banerjee, R. Krahl, F. Durst, and C. Zenger, “Presentation of anisotropy properties of turbu-
686 lence, invariants versus eigenvalue approaches,” *J. Turbul.* **8**, N32 (2007).
- 687 ⁵⁷R. L. Simpson, “Turbulent boundary-layer separation,” *Annu. Rev. Fluid Mech.* **21**, 205–34
688 (1989).
- 689 ⁵⁸R. Martinuzzi and C. Tropea, “The flow around surface-mounted, prismatic obstacles placed in
690 a fully developed channel flow,” *ASME J. Fluids Eng.* **115**, 85–92 (1993).
- 691 ⁵⁹P. A. Durbin, “A Reynolds stress model for near-wall turbulence,” *J. Fluid Mech.* **249**, 465–498
692 (1993).
- 693 ⁶⁰G. J. Brereton and J. Yuan, “Wall-roughness eddy viscosity for Reynolds-Averaged closures,”
694 *Int. J. Heat Fluid Fl.* **73**, 74–81 (2018).
- 695 ⁶¹S. C. Kassinos, C. A. Langer, S. L. Haire, and W. C. Reynolds, “Structure-based turbulence
696 modeling for wall-bounded flows,” *Int. J. Heat Fluid Flow* **21**, 599–605 (2000).