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# Effects of the computational domain size on direct numerical simulations of Taylor-Couette turbulence with stationary outer cylinder

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In search for the cheapest but still reliable numerical simulation, a systematic study on the effect of the computational domain ("box") size on direct numerical simulations of Taylor-Couette flow was performed. Four boxes with varying azimuthal and axial extents were used. The radius ratio between the inner cylinder and the outer cylinder was fixed to  $\eta = r_i/r_o = 0.909$ . The outer cylinder was kept stationary, while the inner rotated at a Reynolds number  $Re_i = 10^5$ . Profiles of mean and fluctuation velocities are compared, as well as autocorrelations and velocity spectra. The smallest box is found to accurately reproduce the torque and mean azimuthal velocity profiles of larger boxes, while having smaller values of the fluctuations than the larger boxes. The axial extent of the box directly reflects on the Taylor-rolls and plays a crucial role on the correlations and spectra. The azimuthal extent is found to play a minor role in the simulations, as the boxes are large enough. For all boxes studied, the spectra do not reach a box independent maximum. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4913231>]

Taylor-Couette (TC), the flow between two coaxial and independently rotating cylinders, is commonly used as a basic model and paradigmatic system for shear flows in very diverse topics, for example, probing the stability of astrophysical flows<sup>16</sup> or more direct applications such as bubbly drag reduction.<sup>3,11</sup> TC is very accessible experimentally; as it is a closed system, it has a simple geometry and a high number of symmetries, i.e., azimuthal symmetry in the case of experiments, and in addition axial symmetry in simulations. Experiments of TC have been conducted up to  $Re \sim O(10^6)$ .<sup>9,10,18,19</sup> These large  $Re$  allow for the study of the "ultimate" regime, in which the flow is fully turbulent both in the boundary layers and in the bulk. It is expected that the scaling laws which hold in this regime can be extrapolated to arbitrarily large Reynolds numbers, such as those present in geo- and astro-physics.<sup>12,17</sup>

The flow is sheared by the angular velocity difference between the two cylinders. The driving of the cylinders can be expressed non-dimensionally with two Reynolds numbers:  $Re_i = r_i d \omega_i / \nu$  for the inner cylinder and  $Re_o = r_o d \omega_o / \nu$  for the outer cylinder, where  $r_i$  and  $r_o$  are the inner and outer cylinder radius,  $\omega_i$  and  $\omega_o$  the inner and outer cylinder angular velocity,  $d$  is the gap width,  $d = r_o - r_i$ , and  $\nu$  the kinematic viscosity of the fluid. The shear driving of the flow can then be expressed as a shear Reynolds number  $Re_s = r_i |\omega_i - \omega_o| d / \nu = |Re_i - \eta Re_o|$ , where  $\eta$  is the radius ratio  $\eta = r_i / r_o$ .

Direct numerical simulations (DNS) of TC have received increasing level of sophistication in the last years. The first attempt at high  $Re$  was done using "large" computational boxes by Dong.<sup>6,7</sup> Dong used a periodic aspect ratio of  $\Gamma = 2\pi$ , where  $\Gamma = L/d$ , with  $L$  the axial periodicity length, for  $\eta = 0.5$ , reaching  $Re_s = 8000$ . Ostilla-Mónico *et al.*<sup>23,24</sup> also achieved  $Re_s \approx 8000$  for  $\eta = 0.714$  using large boxes with  $\Gamma = 2\pi$ . A breakthrough was achieved by Brauckmann and Eckhardt,<sup>4,5</sup> who showed that simulation boxes could be heavily reduced in two ways, while still obtaining accurate

data for the torque. For simulation boxes with  $\Gamma = 2\pi$ , three Taylor roll pairs fit in the system. However, only one pair of rolls was sufficient to calculate the torque, so  $\Gamma$  could be reduced to  $\Gamma = 2$  ( $\approx 2\pi/3$ ). Second, simulating the full azimuthal extent of the cylinder is also not necessary to obtain an accurate result for the torque. A cylindrical wedge, with a rotational symmetry can be imposed, and, for  $\eta = 0.714$ , only a *ninth*<sup>4</sup> of the cylinder was necessary. The use of these “small” boxes reduces the computational requirements by a factor  $\sim 30$ , or more, and made later DNS deep inside the ultimate regime by Ostilla-Mónico *et al.*<sup>25,26</sup> possible, who achieved  $Re_s \sim O(10^5)$ . Recently, Shi *et al.*<sup>29</sup> also achieved  $Re_s \sim O(10^5)$  in TC in the quasi-Keplerian regime.

The torque at the inner and outer cylinders is a first order, integral statistic. The finiteness of the computational domain however may play a role for other statistics, both higher order statistics, or one-, two-, and many-point statistics. This is the case, for example, in the channel flow simulations of Lozano-Durán *et al.*,<sup>21</sup> where even if the stream-wise mean velocity profile is well reproduced with small boxes, accurate results for velocity and pressure fluctuations (root mean squared) require larger boxes.

Before we continue, it is worth noting that there are two main differences between channels (and pipes) and TC. In TC, a natural constraint on the azimuthal (streamwise) extent of the domain always exists, i.e., the full cylinder, while one could think of channels and pipes extending infinitely. Second, the axial (spanwise) periodicity length in TC fixes the size of the Taylor rolls. The effect of the box-size in the axial direction is not purely numerical. The use of axially periodic conditions in axially “small” computational domains, where only one pair of rolls fits in means that the axial periodicity length sets the wavelength of the Taylor vortices. This wavelength is directly analogous to the wavelength of the Taylor vortices seen in experiments. In large aspect ratio experiments, the physical parameter is the axial length which is given by distance between the end-plates. No preferential wavelength is set for the rolls, but experimental evidence<sup>15,22</sup> suggests that vortex pairs tend to have wavelengths  $\lambda_{TR}$  between  $2 \leq \lambda_{TR} \leq 4$ . These rolls survive up to very large Reynolds numbers, having been observed experimentally up to  $Re_s \sim O(10^6)$  by Huisman *et al.*,<sup>15</sup> and, in the corresponding parameter regimes, all DNS up to now. Taylor rolls have no direct analog in pipes and channel flow between two parallel plates and can still play a large role in the DNS for various physical quantities, even though the torque has been shown to become independent of  $\Gamma$  in the range  $2 \leq \Gamma \leq 4$  at about  $Re_s \sim 3 \cdot 10^4$ .<sup>26</sup>

In this manuscript, we attempt to answer the question: how does the size of the computational domain affect other statistics of TC DNS and in particular higher order moments? To do so, we performed a series of DNS of TC using a second-order finite difference code, with fractional time-stepping detailed in Verzicco and Orlandi.<sup>31</sup> This code has been used for all our previous DNS of TC and has been extensively validated against experiments.<sup>23,25,26</sup>

The radius ratio was fixed to  $\eta = 0.909$  and the inner cylinder was rotated at  $Re_i = 10^5$ , while the outer cylinder was kept stationary, i.e.,  $Re_o = 0$ . This resulted in a total shear driving of  $Re_s = 10^5$ . With the chosen parameters, the simulations are in the fully turbulent (ultimate) regime and still have a strong large-scale axial circulation. A small-gap geometry was chosen, as it has the strongest large-scale rolls.<sup>26</sup> Therefore, we do not expect the effect of  $\eta$  to be significant on the results. By fixing the outer cylinder, we ensure that the flow is fully Rayleigh unstable, i.e.,  $d|\omega r^2|/dr < 0$  everywhere. TC flow in the Rayleigh-stable regime may present other kinds of turbulent structures, Taylor columns instead of Taylor vortices,<sup>30</sup> and this limits the applicability of the present work.

For the parameters mentioned previously, four simulations were conducted with computational boxes of varying sizes. Details of the geometry and resolutions used are available in Table I. The adequacy of the mesh can be further be checked in the spectra shown in later sections. A variable time-step with a maximum Courant-Friedrichs-Lewy (CFL) number of 1.4 was used, which does not reduce the accuracy of the results.<sup>23</sup> Simulations were started from zero-velocity initial conditions on a coarse grid, at low Reynolds numbers. Once these simulations had reached a statistically stationary state, the Reynolds number was increased, and the grid was refined, until the desired Reynolds number and grid refinement was reached. After a sufficiently long time to let transient behaviour die out, simulations were run between 30 large eddy turnover times (defined as  $d/(r_i\omega_i)$ ) in the case of the  $\Gamma 4N10$  run, or up to 70 for the  $\Gamma 2N20$  run. This run-time is smaller than time

TABLE I. Details of the numerical simulations. The first column is the name with which the simulation will be referred to in the chapter. The second column shows  $n_{sym}$ , the order of the rotational symmetry imposed on the system. The third column shows the azimuthal extent of the domain at the mid-gap,  $\tilde{x} = 2\pi(r_i + r_o)/(2dn_{sym})$ . The fourth column gives  $\Gamma$ , the axial periodicity aspect ratio. The fifth column represents the amount of points in the azimuthal, radial, and axial directions used for the simulations. For the uniformly discretized directions, the resolutions used correspond to approximately  $r_o\Delta\theta^+ \approx 9$  and  $\Delta z^+ \approx 3$  in inner cylinder wall units. For the radial direction, points are clustered near the wall using a clipped Chebychev arrangement, with the resolution varying from  $\Delta r^+ \approx 0.3$  near the cylinders to  $\Delta r^+ \approx 4.2$  at the mid-gap. The sixth column shows the non-dimensional torque  $Nu_\omega$ . The last column indicates the line shapes used for Figs. 4–8. The frictional Reynolds number at the inner cylinder  $Re_{\tau,i} = u_{\tau,i}d/(2\nu)$ , is  $Re_{\tau,i} = 1410$  for all cases. The outer cylinder friction number,  $Re_{\tau,o}$ , is  $Re_{\tau,o} = \eta Re_{\tau,i} = 1280$ .

Case	$n_{sym}$	$\tilde{x}$	$\Gamma$	$N_\theta \times N_r \times N_z$	$Nu_\omega$	Line style
$\Gamma 2N20$	20	3.3	2.09	$1024 \times 1024 \times 2048$	$69.5 \pm 0.2$	Solid light blue
$\Gamma 2N10$	10	6.6	2.09	$2048 \times 1024 \times 2048$	$69.4 \pm 0.4$	Solid black
$\Gamma 3N20$	20	3.3	3.00	$1024 \times 1024 \times 3072$	$69.6 \pm 0.2$	Dashed dark green
$\Gamma 4N10$	10	6.6	4.00	$2048 \times 1024 \times 4096$	$69.8 \pm 1.6$	Dash-dot dark red

required to overcome the transient, which is between 100 and 150 time units. For a more detailed analysis of the time-scales in TC flow, we refer the reader to Ostilla-Mónico *et al.*<sup>27</sup>

Throughout this manuscript, the following conventions will be used:  $\langle \phi \rangle_{x_i}$  denotes the average of a quantity  $\phi$  with respect to the independent variable  $x_i$ . The torque  $T$  is non-dimensionalized as a pseudo-Nusselt number<sup>8</sup>  $Nu_\omega = T/T_{pa}$  where  $T_{pa}$  is the torque in the purely azimuthal and laminar state. We also define  $\tilde{r}$ , the normalized radius as  $\tilde{r} = (r - r_i)/d$ , the normalized height as  $\tilde{z} = z/d$ , and the normalized azimuthal distance at the mid-gap as  $\tilde{x} = (r_o + r_i)\theta/(2d)$ .

Normalizations with respect to “wall” variables are denoted with a plus superscript, i.e.,  $\phi^+$ . Wall variables are first averaged azimuthally, axially, and temporally. Then, the frictional velocity at the corresponding cylinder  $u_\tau = \sqrt{\tau_w/\rho}$  is computed, and used as velocity scale, where  $\tau_w$  is the mean friction at the corresponding cylinder and  $\rho$  is the fluid density. As length scale to non-dimensionalize, the viscous length  $\delta_v = \nu/u_\tau$  is used as usual. In these wall variables, we denote the distance to the cylinder(s) with  $r^+$ . For the inner cylinder wall variables, this is defined as  $r^+ = (r - r_i)/\delta_{v,i}$ , while for the outer cylinder wall variables  $r^+ = (r_o - r)/\delta_{v,o}$ .

Table I also shows that  $Nu_\omega$  is the same within the statistical temporal error due to the necessarily limited time averaging for all simulations. This finding, even if expected from previous research, is still remarkable, considering the large-scale flow patterns, i.e., the Taylor rolls, which are still present in the flow. These patterns can be appreciated from Fig. 1. Structures are emitted from the boundary layers. These can be thought of as hairpin vortices or as plumes when speaking in the language common for thermal convection. Plumes tend to attract each other and merge together forming regions with large angular velocity transport, i.e., with a strong correlation between  $u_\theta$  and  $u_r$ .<sup>27</sup> These regions have a very large positive or negative angular velocity transport, which can be orders of magnitude larger than the mean.<sup>25</sup> “Neutral”-transport regions, in the core of the Taylor rolls, lie between them, and in these regions  $u_r$  and  $u_z$  are small. For a more detailed analysis of the dynamics of these regions, see Refs. 25 and 27.

Taylor-rolls are stationary in time. This is displayed by Fig. 2, which shows a pseudocolour plot of the azimuthally and temporally averaged azimuthal velocity  $\langle u_\theta \rangle_{\theta,t}$ . For all panels, a single vortex pair is present, which fills up the whole computational domain. This large-scale structure has little to no effect on the total angular velocity transport. The simulations were ran for more than 30 large eddy turnover times (defined as  $\tilde{t} = d/r_i\omega_i$ ), and this did not significantly modify the position of the roll. Remarkably, for the  $\Gamma 4N10$  case, only one roll pair with wavelength  $\lambda_{TR} = 4$  fills the domain, instead of two “square” rolls with  $\lambda_{TR} = 2$ . This is consistent with the findings that the preferred  $\lambda_{TR}$  increases with  $Re$ , and that large  $Re$  simulations and experiments tend to find rectangular Taylor rolls with  $\lambda_{TR} > 2$ , which however cannot be sustained at lower drivings<sup>26</sup> (cf. the experiments of Huisman *et al.*<sup>15</sup> at  $Re \sim O(10^6)$  who found Taylor rolls with  $\lambda_{TR} > 3$ ).

Long wavelength patterns, present in the axial direction, can also form in the azimuthal direction. Fig. 3 shows a pseudocolour plot of the instantaneous velocity  $u_\theta$  at the mid-gap  $\tilde{r} = 0.5$  for

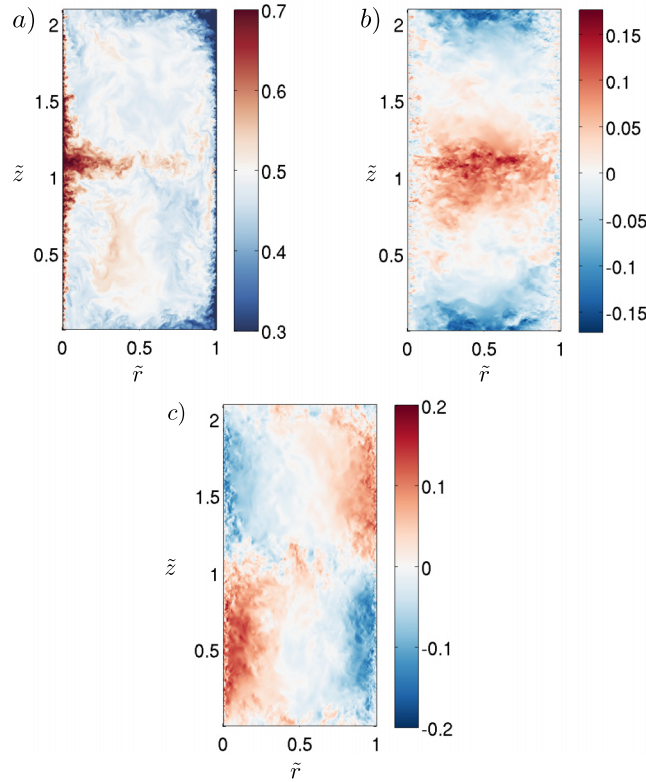


FIG. 1. Pseudocolor of the instantaneous (a) azimuthal, (b) radial, and (c) axial velocities for an azimuthal cut of  $\Gamma 2N20$ . The presence of large scale rolls, which make the flow inhomogeneous, is apparent here.

the  $\Gamma 2N20$  and  $\Gamma 2N10$  cases. The axial signature of the Taylor rolls can be clearly appreciated in the panels. On top of this signature, additional azimuthal patterns can be seen. On both panels of Fig. 3, structures similar to wavy Taylor vortices can be seen, which we will refer to as “wavyness” of the roll. We note that unlike Taylor rolls, long wavelength azimuthal structures are not stationary in time, as they are convected with the mean flow velocity and do not show up on temporal averages.

We will now quantify the effect of these patterns and thus of the computational box size on the flow. We start with one-point statistics, in particular with the mean azimuthal velocity. The left panel of Fig. 4 shows the azimuthally, temporally, and axially averaged azimuthal velocity  $\langle u_\theta \rangle_z$  at

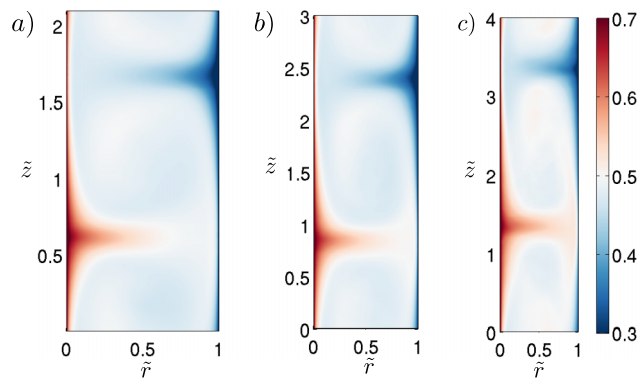


FIG. 2. Azimuthally and time-averaged azimuthal velocity  $\bar{u}_\theta$  for the cases (a)  $\Gamma 2N20$ , (b)  $\Gamma 3N20$ , and (c)  $\Gamma 4N10$ . As  $\Gamma$  increases, the Taylor roll pair also grows, filling the entire box. In these panels (and also in Figs. 1 and 3), there is a slight preference for blue (low velocity) regions in the plots, because the mean azimuthal velocity in the bulk is slightly below 0.5 due to the inherent asymmetry between both cylinders.

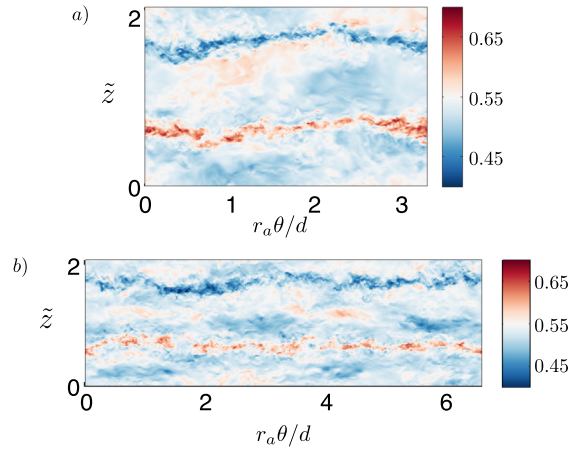


FIG. 3. Instantaneous azimuthal velocity  $u_\theta$  at the mid-gap  $\tilde{r}_a$  for the cases (a)  $\Gamma 2N20$  and (b)  $\Gamma 2N10$ , as a function of the azimuthal variable  $\theta$ . Increasing  $n_{sym}$  allows larger wavelength structures to fit in the simulation. These structures do not seem to form from visual inspection.

the inner cylinder in inner cylinder wall units, while the right panel of Fig. 4 shows the so-called diagnostic function  $\Xi^+ = du^+/d(\log r^+)$ , which is the local slope of a lin-log plot of the profile.

Only little variation between all cases can be seen between these panels. In the right panel, a slight decrease of the intercept of the logarithmic profile is observed for the  $\Gamma 3N20$  and  $\Gamma 4N10$  simulations. This is caused by the remnant axial dependence of  $u_\theta$ , which increases with increasing  $\Gamma$ . On the other hand, there are no appreciable differences in the boundary layers between the  $\Gamma 2N20$  and  $\Gamma 2N10$  simulations indicating that the azimuthal extent of the box is enough to capture the mean profiles in the boundary layer.

Fig. 5 shows the velocity fluctuation profiles at the inner cylinder. The root mean square (rms) of a field  $\phi$  is computed as  $\phi' = \langle \langle \phi^2 \rangle_{\theta,t} - \langle \phi \rangle_{\theta,t}^2 \rangle_z$ . Note that the order of the axial average and subtraction operations is crucial due to the remnant and significant axial dependence in the mean velocity fields (cf. Fig. 2). Axially averaging before subtracting results in rms values which are considerably higher, but originate simply from the Taylor rolls and have nothing to do with the underlying statistics.

While the box-size can be seen to play a small effect on the  $u_\theta^+$  profile, it is critical for other averages else. In general, increased box sizes lead to increased fluctuations, in line with what is seen in channels.<sup>21</sup> The effect of increasing the azimuthal size of the domain on the fluctuations can be appreciated by comparing the  $\Gamma 2N10$  and the  $\Gamma 2N20$  cases. There is a clear increase in the

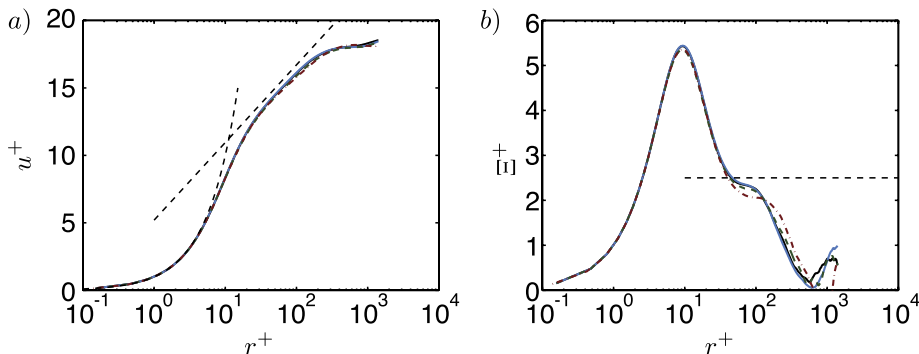


FIG. 4. (a): Axially, azimuthally, and time-averaged azimuthal velocity in inner cylinder wall units. The dashed lines indicate  $u^+ = r^+$  and  $u^+ = 2.5 \log r^+ + 5.2$ . (b): Diagnostic function  $\Xi^+ = du^+/d(\log r^+)$ . Dashed line indicates  $\Xi^+ = 2.5$ . Very little to no dependence on the box-size can be seen near the boundary layers, while differences can be appreciated from  $r^+ > 500$ , i.e., in the bulk. In the bulk,  $u_\theta$ , has a strong axial dependence, and this is probably causing the discrepancies. For both panels, symbols are as in Table I.



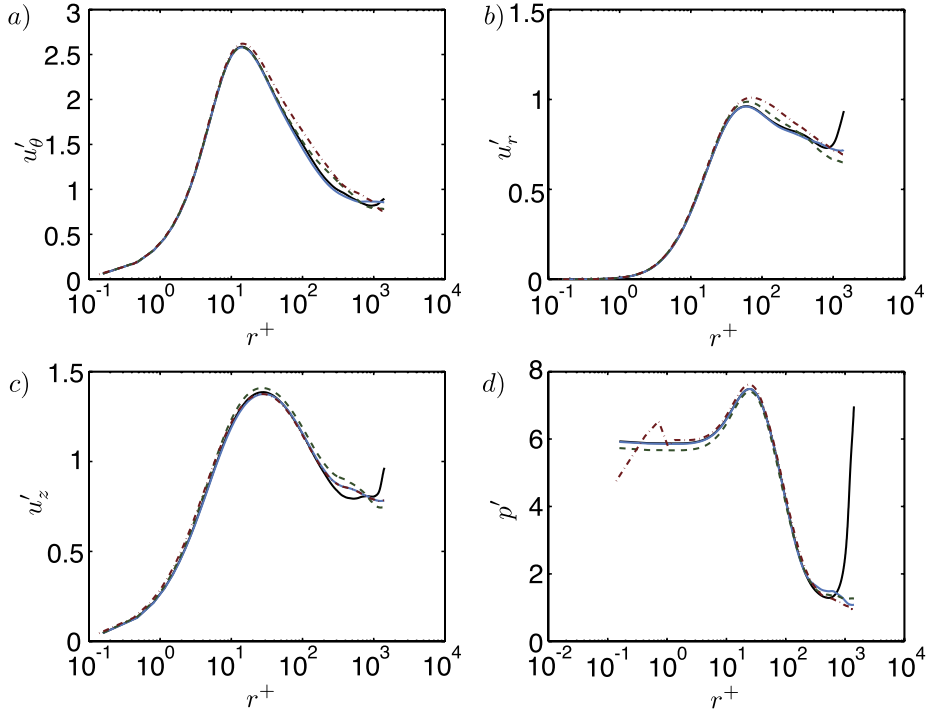


FIG. 5. Velocity and pressure fluctuations near the inner cylinder in inner cylinder wall units for all simulations. Symbols are as in Table I.

$u_r^+$  and  $u_z^+$  fluctuations in the bulk. This is a direct reflection of the increased mobility of the rolls. The axial extent of the domain can also be seen to affect the velocity fluctuation profiles. A larger axial domain, i.e., increasing  $\Gamma$ , again leads to larger fluctuations in the boundary layer due to the increased mobility of the plumes and the increased axial dependence of the velocity.

Finally, the pressure fluctuations become *smaller* for larger domains. This is probably due to the pressure playing a damping role on the velocity fluctuations in the smaller domains. Again, this is in line with what is seen in channels.<sup>21</sup> The geometric (computational) constraint on the flow inside the boundary layers is enforced through these pressure fluctuations. The sharp increase of velocity fluctuations in the bulk seen for the  $\Gamma 2N10$  case also results in a sharp increase of pressure fluctuations in the bulk.

Fig. 6 shows the two-point autocorrelation function for all velocity fields in both axial and azimuthal direction. Two main effects of the box size can be seen on the flow. The azimuthal extent of the box plays a negligible role in the decorrelation in all panels. If one compares the  $\Gamma 2N10$  case to the  $\Gamma 2N20$  cases, both show a region of anti-correlation at around  $\tilde{r}\theta \approx 1.6$ . This suggests that  $n_{\text{sym}} = 20$  is large enough to capture the largest structures in the azimuthal extent, with wavelength equal to the small-box size  $\tilde{r}\theta \approx 3.3$ . This can be confirmed by visual inspection of Fig. 3, where the right panel seems to consist of two copies of the left panel. We also note that the azimuthal decorrelation lengths are an order of magnitude smaller than those seen in plane Couette flow,<sup>2</sup> which have allowed TC simulations to reach higher  $Re_\tau$  with heavily reduced computational costs. Current state-of-the-art plane Couette simulations “only” reach  $Re_\tau = 550$  while requiring  $2.2 \times 10^9$  points.<sup>1</sup>

On the other hand, the axial extent plays an important role in *both* axial and azimuthal correlations. As expected, the axial autocorrelations are dominated by the effect of Taylor rolls. This is especially true in the case of the radial velocity autocorrelation  $R_{rr}$ . The axial velocity autocorrelation  $R_{zz}$  remains relatively unaffected, as axial velocities in the mid-gap are very small (cf. Fig. 3). Additionally, increasing  $\Gamma$  allows for a faster drop of  $R_{\theta\theta}$  in the azimuthal direction but not for faster drops in  $R_{rr}$  and  $R_{zz}$ . This is due to the larger cores of the Taylor rolls, which result in more mixing.

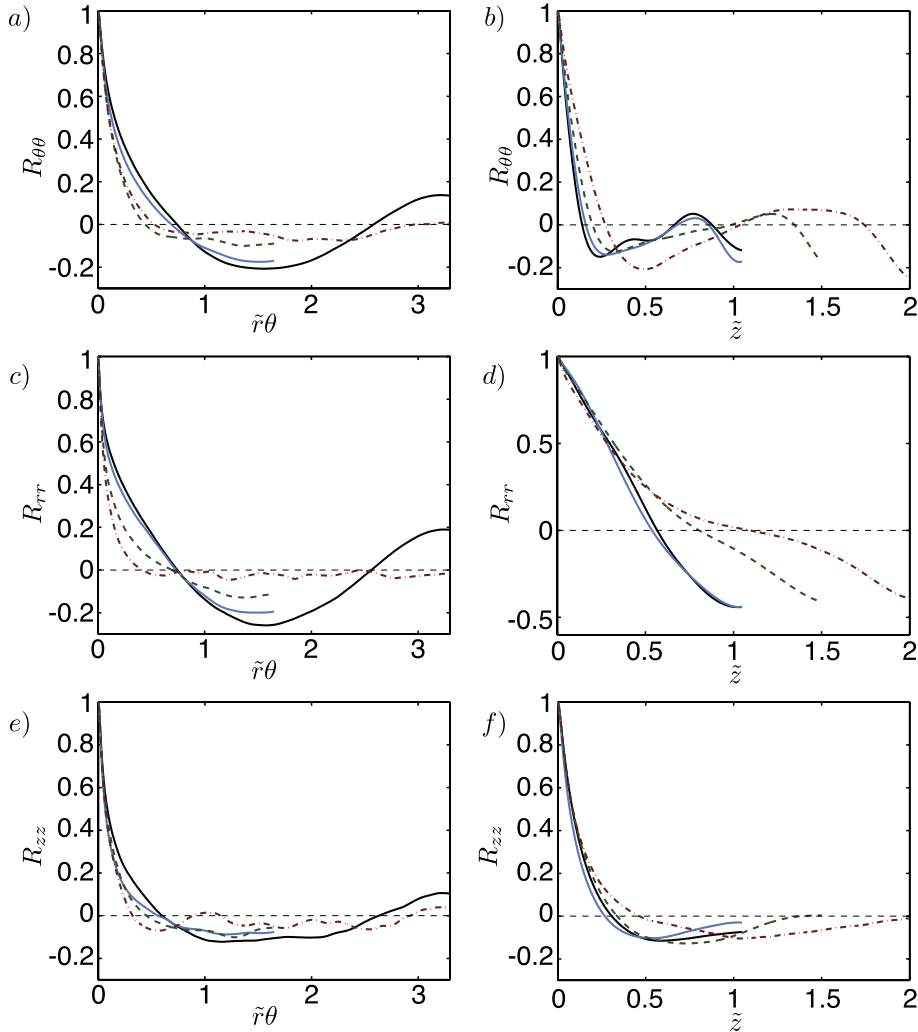


FIG. 6. Two-point autocorrelation functions at the mid-gap ( $\tilde{r} = 0.5$ ) for all simulations. Left panels: autocorrelations in the azimuthal direction ( $\theta$ ), right panels: autocorrelations in the axial directions. The three rows are for each velocity component. Top row: azimuthal, middle row: radial and bottom row: axial. Symbols are as in Table I.

In these regions, the radial and axial velocities are small, so  $R_{rr}$  and  $R_{zz}$  are dominated by the strongly correlated regions seen in Fig. 1.

We now turn to the velocity spectra. Fig. 7 shows the premultiplied velocity spectra in the inner cylinder boundary layer ( $r^+ \approx 12$ ), while Fig. 8 shows the spectra at the mid-gap ( $\tilde{r} = 0.5$ ). In both figures, the size of the computational box can be seen to play a negligible role for the spectra at the small scales, while, as seen in Ref. 27, the large scales contain a very significant amount of energy both deep inside the boundary layer and in the bulk.

Inside the boundary layer, there are two main energy containing scales- that of the plumes at high  $k$ , and that of the Taylor rolls, at low  $k$ . In the mid-gap, the plumes have merged with each other, and the main energy content can be found only in the large scales. It is apparent from both figures that the maximum of the spectra is not converged to their very large box-size value. The box is not large enough to contain all large scales which are energetic. Even then, good collapse for the small scales can be seen. The largest scales contain energy from all three velocity components, and not only for the azimuthal and spanwise components, which is the case in channels<sup>13</sup> and plane Couette.<sup>1</sup> All mid-gap spectra neither display clearly the inertial range Kolmogorov scaling with  $-5/3$  scaling nor the  $-1$  scaling for the  $E_{\theta\theta}$  in the  $\theta$ -direction predicted by Perry and Chong.<sup>28</sup> This is consistent with the experimental findings of Lewis and Swinney<sup>20</sup> and those of Huisman *et al.*<sup>14</sup>



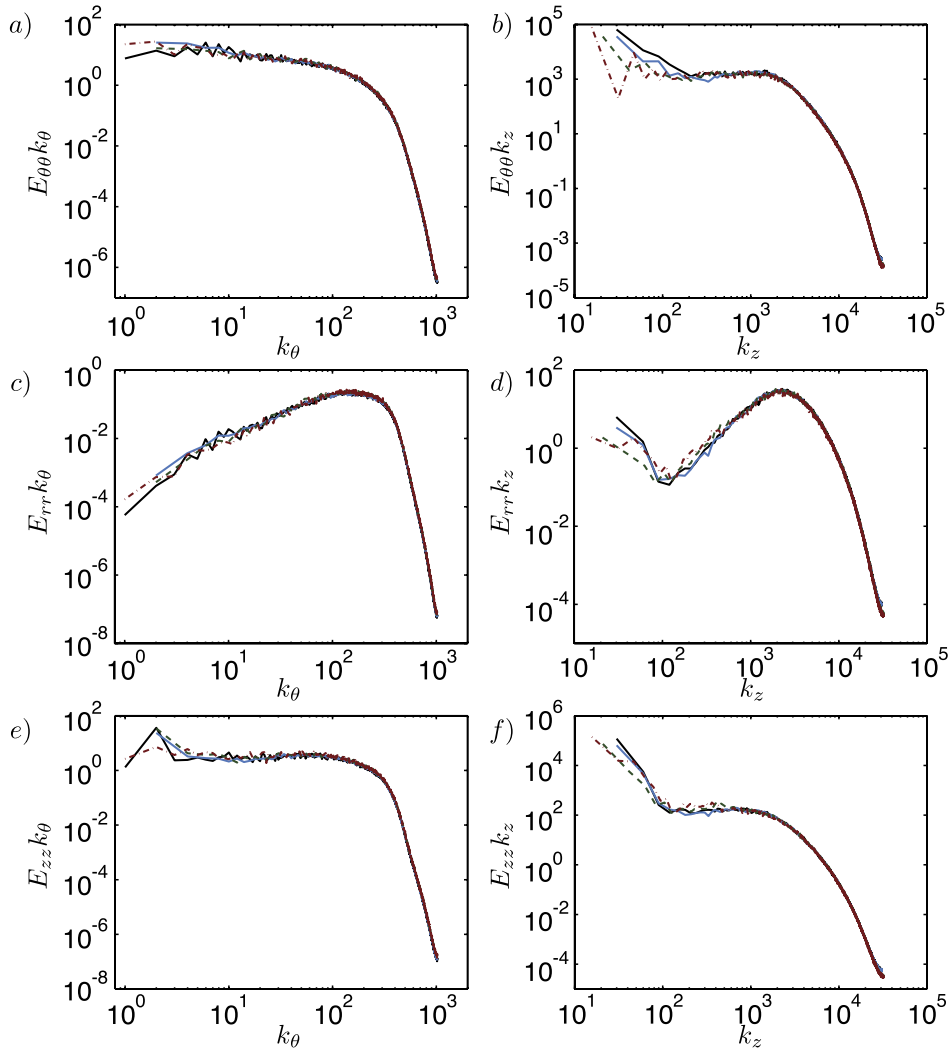


FIG. 7. Premultiplied azimuthal (left column) and axial (right column) spectra for the azimuthal (top), radial (middle) and axial (bottom) velocities at  $r_i^+ \approx 12$ . Symbols are as in Table I.

Saw-tooth patterns indicating preferred even or odd modes can be seen for the axial spectra for all cases. Increasing  $\Gamma$  shifts the maxima in  $k_z$  accordingly, to accommodate for the different size of the Taylor-roll. We note that inside the boundary layer, simulations with larger  $\Gamma$  have a smaller energy peak at the Taylor-roll wavelength  $k_z$ . This means that the Taylor-roll has a larger effect on the plume generation and its aspect ratio is smaller. Using a small domain may artificially strengthen the roll and lead to an increased correlation inside the boundary layer. Further increases in  $\Gamma$  will accommodate for more rolls. This was seen to produce a very sharp dropoff in the spectra for  $k_z < k_{TR}$  by Dong.<sup>6</sup> The effect of end-plates has also been omitted, and this will require attention in the future.

Remarkably, sawtooth behaviour at low frequencies is also present in the azimuthal direction if the azimuthal extent of the domain is increased. A preference for even modes over odd modes is indicated, and this again suggests the fundamental wavelength of the system is  $\tilde{r}\theta \approx 3.3$ , i.e., half the domain. This is further evident that the statistics for the  $\Gamma 2N10$  case can be accurately reproduced with the  $\Gamma 2N20$  case.

However, the spectra are not saturated, i.e., a clear maximum is not seen. This means that all the energy containing scales are not captured, and thus extending the azimuthal extent of the simulation seems to be a necessity to fully capture these scales, which do not affect the flow significantly, as

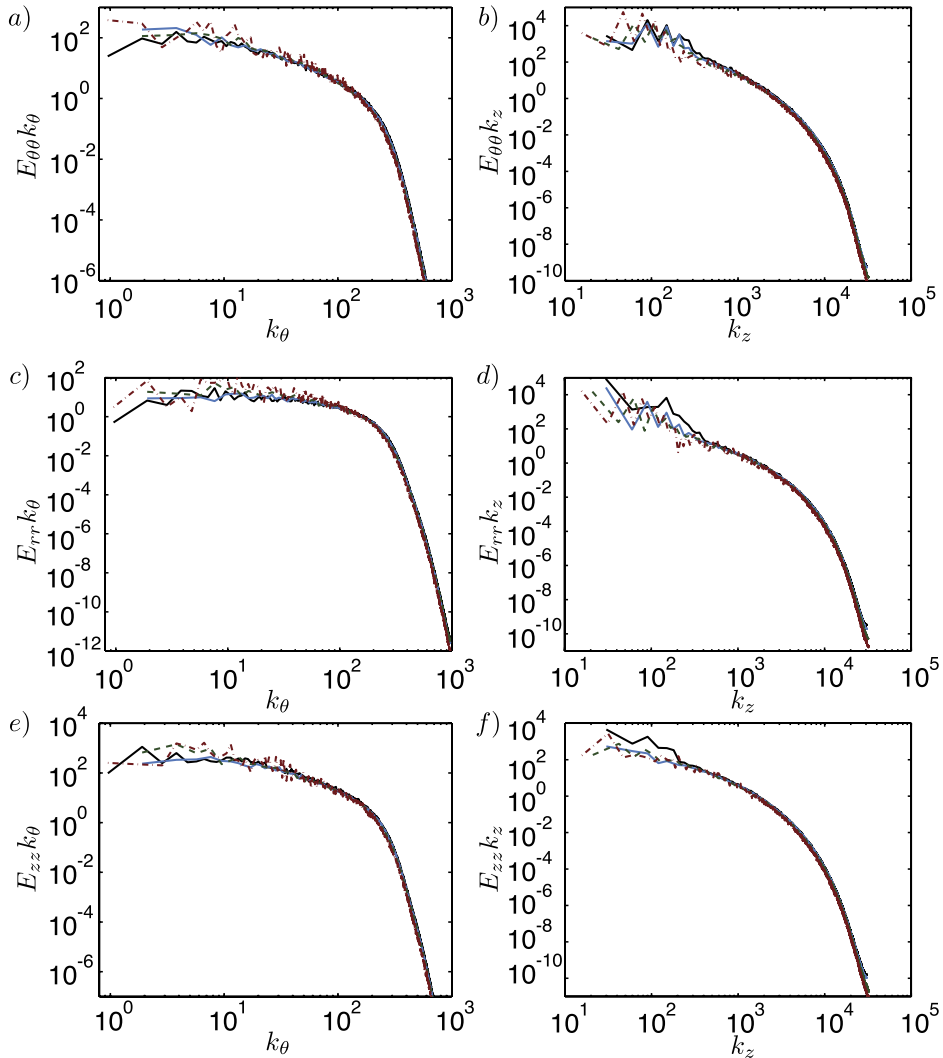


FIG. 8. Premultiplied azimuthal (left column) and axial (right column) spectra for the azimuthal (top), radial (middle), and axial (bottom) velocities at the mid-gap  $\tilde{r} = 0.5$ . Symbols are as in Table I. No significant effect of the box size is seen for the small wavelength (large  $k$ ) scales, while for the large scales, the azimuthal size of the domain appears to play a role in the axial structure of the rolls. The “wavy” modulations seen in Fig. 3 are clearly reflected in the spectra.

$n_{\text{sym}} = 20$  boxes are able to reproduce the main features. It could also be the case that the spectra will not saturate even if  $n_{\text{sym}} = 1$ , and thus all large scales would be energy containing due to the natural finiteness of the azimuthal extent. This point seems to require further study.

In summary, a systematic study of the effect of the computational box size on TC DNS was performed. From previous studies,<sup>4</sup> it was already known that small boxes can obtain accurate results for the non-dimensional torque. Furthermore, similar to what was found by Lozano-Durán *et al.*<sup>21</sup> for DNS of channel flow, small boxes also have accurate mean azimuthal (streamwise) velocity profiles in the boundary layers. Larger boxes are needed in order to obtain box-independent results for fluctuation values, two-point autocorrelations, and low-wavelength spectra. The artificial truncation of the spectra by using a reduced box does not bring about significant changes in its structure at low wavelengths— even if the most energetic scales are not accounted for. Azimuthally small boxes show a reduced level of fluctuations, even if the fundamental wavelengths are already captured.

In the axial direction, things are different. The size of the underlying Taylor roll dominates the autocorrelations, especially for the radial velocity. As we mentioned previously, the effect of the

computational box-size in the axial direction is not purely numerical; the wavelength of the Taylor vortex is a physical parameter. In experimental and natural realizations of TC, the wavelength of the Taylor rolls is determined by the axial constraints, i.e., end plates or periodicity. It appears from recent work<sup>22,26</sup> that for larger  $\Gamma$  domains, which can accommodate more than a pair of rolls, the preferred wavelength of Taylor rolls increases with increasing  $Re$ . This effect cannot be captured in small box simulations but can lead to bifurcations at high Reynolds numbers.<sup>15</sup> Future work should consider simulating large  $\Gamma \sim O(10)$  to check the window of coexistence of different states at high  $Re$ , and how these affect the flow.

In the near future, a study of larger TC boxes seems mandatory, as to determine the minimal box size for accurate statistics of the velocity and pressure fluctuations and higher order moments. It can be the case that the axial extent is too small and thus non-physical, and that the azimuthal extent is not to capture all wavelengths. It is also unclear where the increased level of fluctuations of the  $\Gamma_{2N10}$  case comes from. These increased fluctuations may provide a way for the system to overcome the energy barrier, and to switch between vortical states, i.e., from two vortex pairs with  $\lambda_{TR} = 2$  to one vortex pair with  $\lambda_{TR} = 4$ . Another reason for doubting their physicality comes from the correlations, as the  $\Gamma = 2$  cases show unusually large decorrelation lengths in the azimuthal direction, and this might cause the formation of said patterns.

We also point out that the size of this minimal box is larger than that required for channels. The largest box in this manuscript, for which it is not clear yet whether its statistics are box-independent, has relative dimensions of 8 half-gap lengths in the axial (spanwise) direction and  $4.2\pi$  in the azimuthal (streamwise) direction, while accurate statistics were obtained for a box of size  $\pi$  half-gaps in the spanwise direction and  $2\pi$  half-gaps in the streamwise direction in Lozano-Durán *et al.*<sup>21</sup>

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