

**Turbulent diapycnal mixing in stratified
shear flows: the influence of Prandtl number
on mixing efficiency and transition at high
Reynolds number
Supplementary Materials**

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1. Verification of DNS Results: Conservation of Energy

The following energy balance equations are reproduced from the main manuscript here by means of verifying the accuracy of the DNS results. Both sides of the following equations have been calculated independently and therefore evaluating the match between RHS and LHS of these equations provides a decent measure to the accuracy of the results. The plots comparing RHS and LHS are presented in figures 1 through 4 only for $Pr = 1, 8, 16$ for conciseness. In fact other simulations resemble these and therefore their corresponding plots are not provided. A shortcoming of this measure entails discrete intervals of the output data during the forward time-stepping code (taken to be about $\Delta t_{\text{save}} = 2$ due to large hard-disk demand), which is imposed by the presence of a time derivative in the left-hand side of all these energy budget equations. As such, huge spikes for example in the plots associated with the three-dimensional kinetic energy balance, σ_{3d} , are very hard to capture temporally, since it needs finer intervals of data output and also explains why the misfit in σ_{3d} is most noticeable. Nevertheless, there is minimal misfit in the relatively smoother regions of σ_{3d} as well as a good agreement (better than approximately 1 part per million) in σ and $\frac{d}{dt}\mathcal{P}$ plots.

$$\frac{d}{dt}\mathcal{K} = -\mathcal{H} + \mathcal{D} \quad (1.1)$$

$$\frac{d}{dt}\mathcal{K}_{3d} = -\mathcal{H}_{3d} + \mathcal{D}_{3d} + \mathcal{S}h + \mathcal{A} \quad (1.2)$$

$$\frac{d}{dt}\mathcal{P} = \mathcal{H} + \mathcal{D}_p \quad (1.3)$$

2. Verification of DNS Results: Resolution

A measure for verifying the accuracy of the DNS results is to compare our grid spacing with the dissipation scales of turbulence, as discussed in the main manuscript. Figure 5a, illustrates the ratio of the biggest resolved spatial scales inside the domain to the Batchelor length scale L_B . Note that, during the flow evolution, L_B has been calculated based on the viscous dissipated energy within $z = \pm 1$ for consistency, although after the KH roll-up and specially during the energetic turbulent phase, energy dissipation extends within $z = \pm 2.5$ (in the cases studied in the main manuscript). Thus our overestimation of L_B suits our goal of designing the mesh spacing conservatively. As the figure shows, the peak of such ratio barely extends beyond 5 and is mostly between 3 and 4.5 during the energetic fully turbulent regime (the flow categorization is introduced in the main paper); thus our numerical experiments had been resolved sufficiently based on the recommended range in literature (between 3 and 6).

We have also illustrated similar variations of the grid size but with respect to the Kolmogorov length scale L_K in figure 5b. As shown in this figure we realized that $\Delta x/L_K$ should not exceed 3.5-4 in the most turbulent times of the flow evolution and therefore the corresponding resolutions for $Pr = 1$ was chosen identical to that of $Pr = 2$.

3. MATLAB Snippet for PDF Sorting

Here we present a MATLAB script for demonstrating the implementation of the PDF sorting algorithm for a simple 1D profile (see Listing 1). This algorithm can be suitably parallelized for actual 3D DNS applications. For further details the reader is referred to the main manuscript.

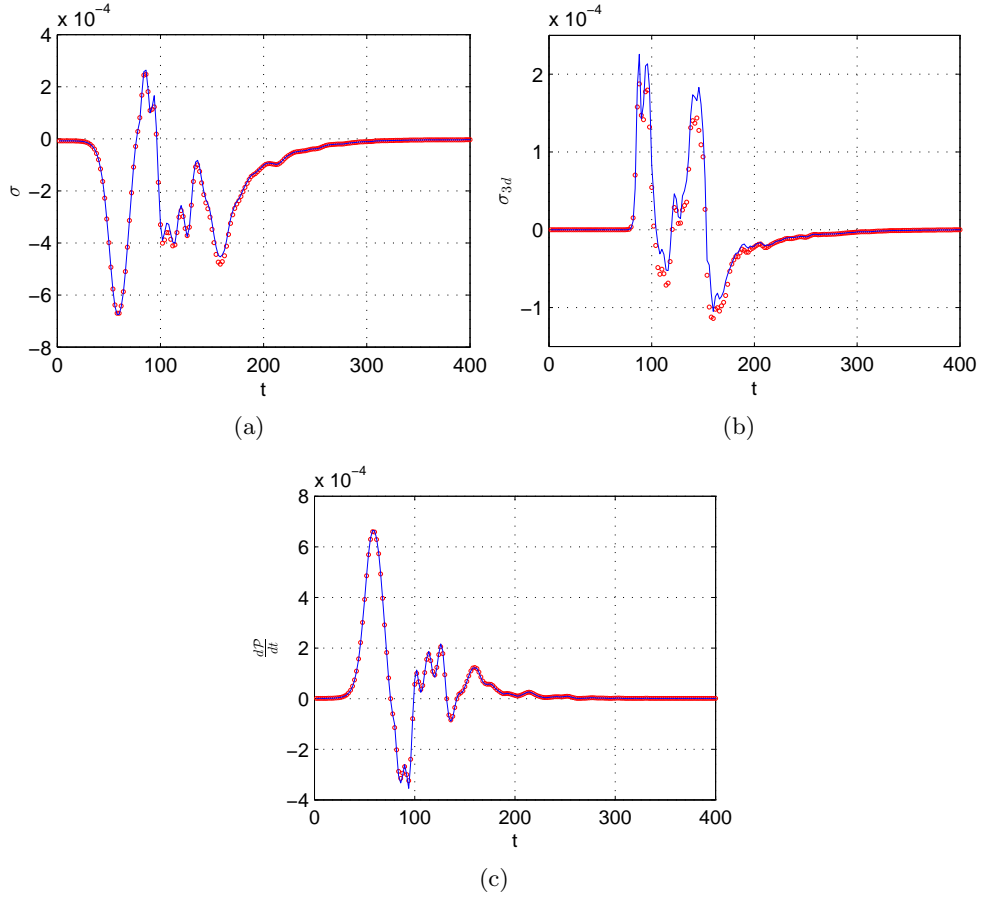
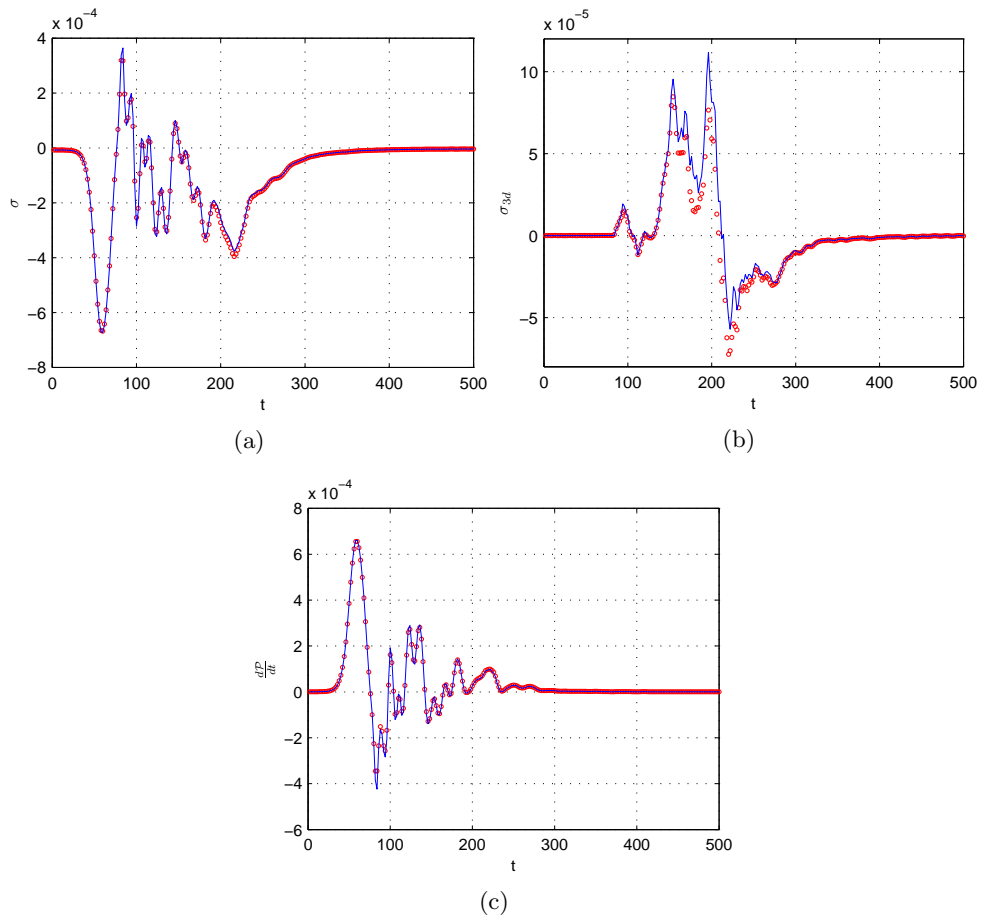
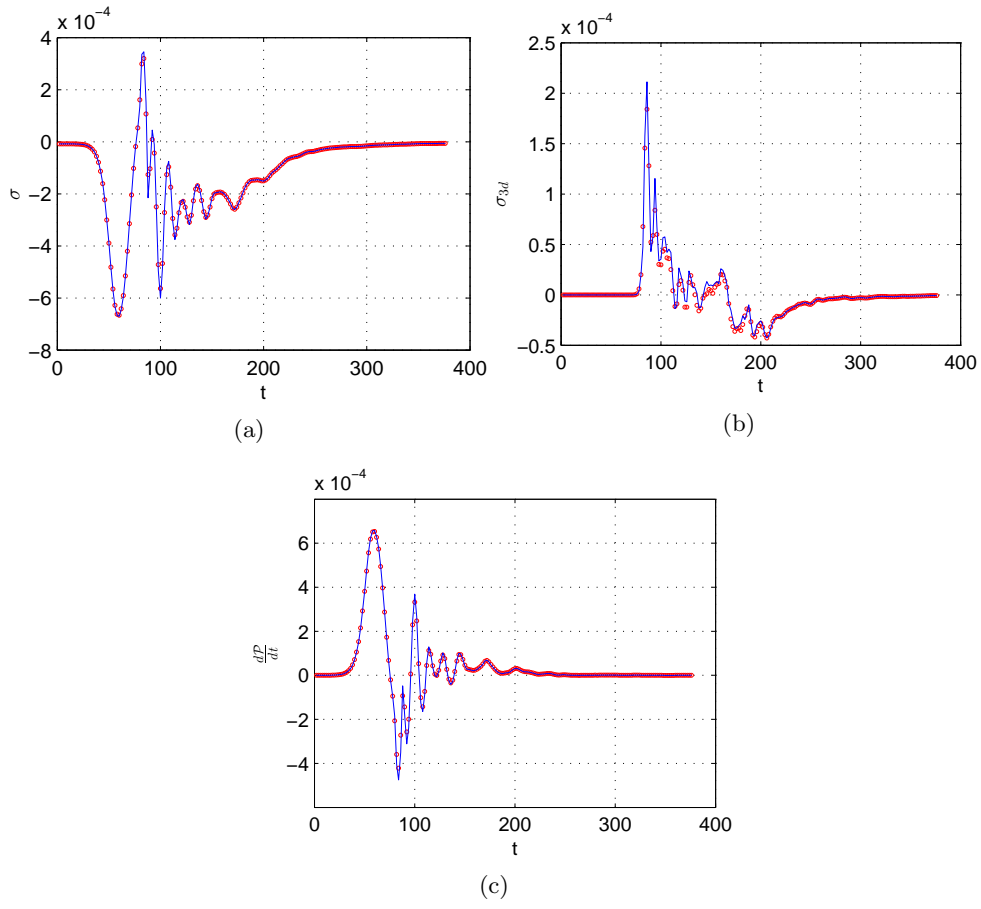
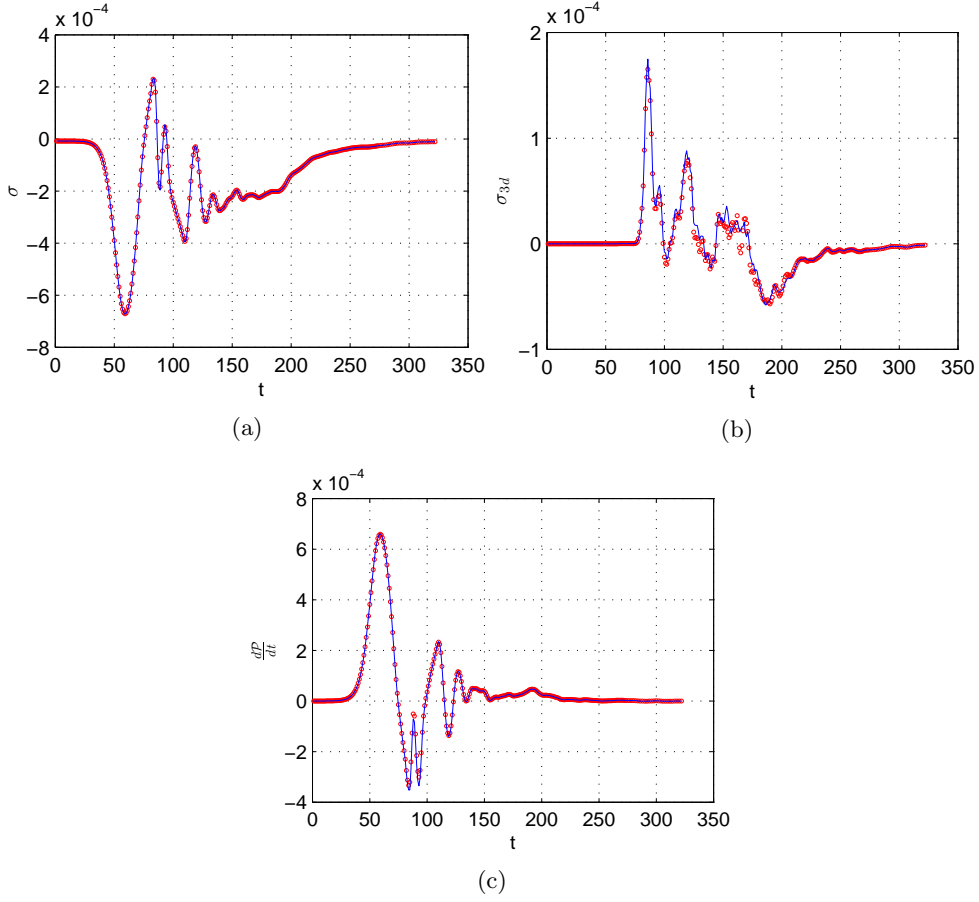
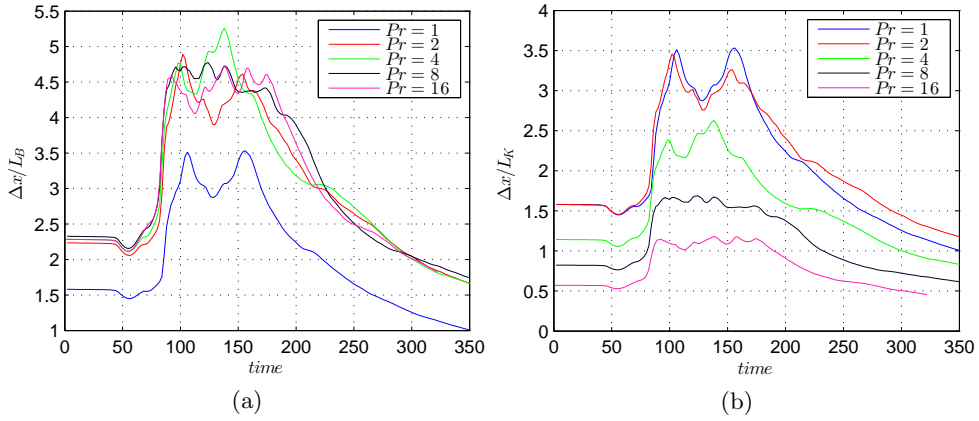


Figure 1: Comparing independent numerical evaluations of the left-hand side (circles) and right-hand side (blue curve) of (a) total kinetic energy balance equation as reproduced in (1.1), (b) kinetic energy of three-dimensional perturbations (1.2) and (c) potential energy balance (1.3); at $Pr = 1$, $Re = 6000$, $Ri_0 = 0.12$.

Figure 2: Similar to figure 1 but for $Pr = 2$.

Figure 3: Similar to figure 1 but for $Pr = 8$.

Figure 4: Similar to figure 1 but for $Pr = 16$.Figure 5: The time variations of (a) $\Delta x / L_B$ and (b) $\Delta x / L_K$ where Δx represents an approximation for the fixed grid spacing and L_K and L_B denote the Kolmogorov and Batchelor length scales respectively; highlighting the sufficiency of the resolution employed in all the DNS studies reported in the main manuscript.

Listing 1: A MATLAB snippet demonstrating the implementation of parallel PDF sorting algorithm as explained in the main manuscript

```

% Purpose: A 1D prototype for parallel sorting algorithm used for
%          adiabatic restratification of the evolving density
%          field based on probability density function (PDF) and
%          Chebyshev transformation.
%          More details can be found in [1,2].
%
%
% Written by :      Hesam Salehipour
%                  h.salehipour@utoronto.ca
%                  September 8th , 2013
%
%
% NOTE: If you found this short script useful *please cite*:
%
% [1] Tseng, Y. & Ferziger, J. H. 2001 "Mixing and available
%      potential energy in stratified flows", Physics of Fluids
%      13, 1281.
% [2] Salehipour, H., Peltier, W. R. & Mashayek, A. 2015 "Turbulent
%      diapycnal mixing in stratified shear flows: the influence of
%      Prandtl number on mixing efficiency and transition at high
%      Reynolds number", J. Fluid Mech.

```

```

clear all; clc; close all;
nz= 5e3;
z=linspace(-15,15,nz);
rho=1-tanh(z);
%rho = 2*sin(z);    % choose your profile!

% Sort using pdf approach
np = 250;
nbins = 3*np-1;      %nbins = 3*(np+1)-2;

rmax=max(rho);
rmin=min(rho);
dr=rmax-rmin;

% Step 1: Build the reference monotonically decreasing profile using
%          Chebyshev transformation.
theta=zeros(1,np+1);
rhob =zeros(1,np+1);
for i=1:np+1

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    theta(i)=pi*(i-1)/np;
    rhob(i)=rmin+dr/2*(1+cos(theta(i)));
end
theta = theta/2;
rhobmax = rhob(2) + (rhob(1)-rhob(2))*cos(theta);
rhobmin = rhob(np)-(rhob(np)-rhob(np+1))*cos(theta(np+1:-1:1));
%rhobmid = 0.5*(rhob(1:np)+rhob(2:np+1));
rhobmid = rhob(1:np);

% Step 2: Calculate the PDF for the grid points of each node.
rho_base=zeros(1,nbins);
rpdf = zeros(1,nbins);
dzi = z(2)-z(1);
rho_base(np+1:2*np-2) = rhobmid(2:np-1);

for i=1:np
    rho_base(i) = (rhobmax(i)+rhobmax(i+1))/2;
    rho_base(i+2*np-2) = (rhobmin(i)+rhobmin(i+1))/2;
    for j=1:nz
        if (rho(j)>rhobmax(i+1) && rho(j)<=rhobmax(i))
            rpdf(i) = rpdf(i) + dzi;
        elseif (rho(j)>rhobmin(i+1) && rho(j)<=rhobmin(i))
            rpdf(i+2*np-2) = rpdf(i+2*np-2) + dzi;
        end
    end
end
for i=2:np-1
    for j=1:nz
        if (rho(j)>rhob(i+1) && rho(j)<=rhob(i))
            rpdf(i+np-1) = rpdf(i+np-1) + dzi;
        end
    end
end
end

% NOTE: In parallel: do a global sum of "rpdf"

% Step 3: Build the reference height associated with the sorted profile.
zb=zeros(1,nbins);
for i=2:nbins
    zb(i)=zb(i-1)+rpdf(i-1);
end

plot(rho_base,zb,'bo-')
hold on;
plot(rho,z+15,'r')

```