Note: what follows is an appendix to the paper *DNS-based predictive control of turbulence: an optimal benchmark for feedback algorithms* which won't appear in the JFM version of this paper. However, it does appear in the version of this article which was included in the following:

BEWLEY T.R. (1999) *Optimal and robust control and estimation of transition, convection, and turbulence.* Stanford University thesis.

Appendix C. Details of numerical method for DNS of controlled turbulent channel flow

The equation governing the flow in the present case (with the forcing in a form slightly generalized from that in the text) is:

$$\mathcal{N}(\mathbf{q}) = \begin{pmatrix} \dfrac{\partial u_j}{\partial x_j} \\ \dfrac{\partial u_i}{\partial t} + \dfrac{\partial u_j u_i}{\partial x_j} - \nu \dfrac{\partial^2 u_i}{\partial x_j^2} + \dfrac{\partial p}{\partial x_i} \end{pmatrix} = \begin{pmatrix} 0 \\ -\delta_{1i}\, P_x(\mathbf{x},t) + f_i(\phi) \end{pmatrix} \qquad \text{in } \Omega$$

with periodic boundary conditions on the velocity on $\Gamma_1^\pm$ and $\Gamma_3^\pm$ (the streamwise and spanwise directions) and a wall-normal control velocity distributed over the walls

$$\mathbf{u} = g_i(\phi) \qquad \text{on } \Gamma_2^\pm,$$

where $\mathbf{n}$ is the unit outward normal to the boundary $\partial\Omega$, and prescribed initial conditions on the velocity

$$\mathbf{u} = \mathbf{u}_0 \qquad \text{at } t = 0.$$

To solve this problem computationally, the continuous flow field must be approximated on a discrete set of points in space. Further, the resulting approximate equation on this finite set of points must be advanced in time using discrete time steps. To minimize the expense of the computation, one desires to use as few spatial points as possible and as large time steps as possible while maintaining accuracy (in both space and time) and stability of the simulation. Since the flow is periodic in the streamwise direction, so that there is no inflow or outflow, it is critical that the numerical errors due to spatial and temporal discretization of the physical problem do not accumulate in a way which causes the simulation to be unstable. Subject this restriction, a scheme with high spatial accuracy is desired. Finally, with a particular spatial discretization, it is found that certain terms of the governing equation have more restrictive time step limitations than do others in the time-advancing algorithm. The most restrictive terms should be taken implicitly to allow for stability at "large" time steps (which, however, must be kept small enough to ensure accuracy of the computation), while other less restrictive terms may be taken explicitly. These issues guide the choice of spatial and temporal discretizations of the current problem, which are discussed in detail below.

C.1. *Spatial discretization*

A grid must be chosen to discretize the flow quantities in space. This grid is chosen to be equispaced and unstaggered in the streamwise (x_1) and spanwise (x_3) directions, allowing Fourier transforms to be used to accurately and efficiently compute all derivatives in these directions. A finite volume approach is used to determine discrete difference expressions for the derivatives in the wall normal direction, which is discretized with a hyperbolic tangent stretching function:

$$x_{2_n} = \frac{\tanh\left(C_s\left(\frac{2\,n}{NY}-1\right)\right)}{\tanh\left(C_s\right)}, \tag{C 1a}$$

with the integer n enumerating the grid in this direction. (A stretching parameter of $C_s = 1.75$ results in a fairly smooth grid, and is used in the present computations.) Note that $n = 0$ corresponds to the lower wall and $n = NY$ corresponds to the upper wall. With this as the base grid, we make the following definitions:

$$x_{2_{n-1/2}} = \frac{1}{2}\left(x_{2_n} + x_{2_{n-1}}\right) \tag{C 1b}$$

$$\Delta x_{2_{n-1/2}} = x_{2_n} - x_{2_{n-1}} \tag{C 1c}$$

$$\Delta x_{2_n} = x_{2_{n+1/2}} - x_{2_{n-1/2}} = \frac{1}{2}\left(\Delta x_{2_{n+1/2}} + \Delta x_{2_{n-1/2}}\right) \tag{C 1d}$$

In this discussion, the subscript n is used to indicate gridpoints at integer x_2 locations, and the subscript $n-1/2$ is used to indicate the gridpoints between these points. The wall-normal component of velocity u_2 is discretized on the n family of gridpoints and the streamwise and spanwise components of velocity u_1 and u_3 and the pressure p are discretized on the $n-1/2$ family of gridpoints. The motivation for staggering the wall-normal component of velocity from the pressure is to couple the pressure at the nodes with n even to the pressure at the nodes with n odd. This is a natural result of a staggered grid, but is not the case in non-staggered configurations. The streamwise and spanwise components of velocity must be discretized at the same x_2 locations as the pressure in order to solve the appropriate discretization of the continuity equation exactly in the fractional step algorithm, as will be shown later in this Appendix.

To interpolate these quantities to the adjacent gridpoints when necessary, the following interpolation formula is used for u_2:

$$\bar{u}_{2_{n-1/2}} = \frac{1}{2}\left(u_{2_n} + u_{2_{n-1}}\right) \qquad \text{(exactly second order)}$$

and the following interpolation formula are used for u_1 and u_3:

$$\bar{u}_{1_n} = \frac{1}{2}\left(u_{1_{n+1/2}} + u_{1_{n-1/2}}\right) \qquad \text{(quasi-second order)}$$

$$\check{u}_{1_n} = \frac{1}{2\,\Delta x_{2_n}}\left(\Delta x_{2_{n+1/2}} u_{1_{n+1/2}} + \Delta x_{2_{n-1/2}} u_{1_{n-1/2}}\right) \qquad \text{(quasi-second order)},$$

$$\check{\check{u}}_{1_n} = \frac{1}{2\,\Delta x_{2_n}}\left(\Delta x_{2_{n-1/2}} u_{1_{n+1/2}} + \Delta x_{2_{n+1/2}} u_{1_{n-1/2}}\right) \qquad \text{(exactly second order)}.$$

Interpolation for p is not required in the staggered grid formulation. As $x_{2_{n-1/2}}$ is midway between x_{2_n} and $x_{2_{n-1}}$, the interpolation formula for $\bar{u}_{2_{n-1/2}}$ is second-order accurate. As x_{2_n} is *not* midway between $x_{2_{n+1/2}}$ and $x_{2_{n-1/2}}$ on the stretched grid, only the interpolation formula for $\check{\check{u}}_{1_n}$ is truly second-order accurate. The formula for $\bar{u}_{1_n}$ and $\check{u}_{1_n}$

are only second-order accurate in the sense that, as NY is increased with the stretching function (C 1a) fixed, $\Delta x_{2_{n+1/2}}/\Delta x_{2_{n-1/2}} \to 1$, and all three forms approach a second order form.

The motivation for using interpolation forms which are only second order accurate in the sense described above stems from conservation issues, which are described in the following section. Though the "proper" second-order interpolation formula $\check{\check{u}}_{1_n}$ can be used everywhere, the discretization error of such an interpolation formula results in spurious sources and sinks of energy on a marginally-resolved stretched grid, which can lead to numerical instabilities. Proper use of the above interpolation formulae prevents discretization errors from contributing to the total energy of the flow. Note that a sufficiently smooth grid stretching function is used to minimize the inaccuracies caused by these interpolation formulae for reasonable values of NY.

For the notational convenience of extending difference formulae to the cells adjacent to the walls, we also make the following useful definitions:

$$
\begin{aligned}
&\Delta x_{2_{NY}} = x_{2_{NY}} - x_{2_{NY-1/2}} && \Delta x_{2_0} = x_{2_{1/2}} - x_{2_0}\\
&u_{1_{NY+1/2}} = \bar{u}_{1_{NY}} = g_{1_{NY}}(\phi) && u_{1_{-1/2}} = \bar{u}_{1_0} = g_{1_0}(\phi)\\
&u_{2_{NY+1}} = \bar{u}_{2_{NY+1/2}} = u_{2_{NY}} = g_{2_{NY}}(\phi) && u_{2_{-1}} = \bar{u}_{2_{-1/2}} = u_{2_0} = g_{2_0}(\phi)\\
&u_{3_{NY+1/2}} = \bar{u}_{3_{NY}} = g_{3_{NY}}(\phi) && u_{3_{-1/2}} = \bar{u}_{3_0} = g_{3_0}(\phi).\\
&p_{NY+1/2} = p_{NY} = p_{NY-1/2} && p_{-1/2} = p_0 = p_{1/2}
\end{aligned}
$$

With the spatial discretization of the flow quantities described above, the individual momentum equations are solved at the corresponding velocity points and the continuity equation is solved at the pressure points. The spatial discretization of the derivatives in the governing equation are now made precise:

$$
\begin{pmatrix}
\left.\dfrac{\delta u_j}{\delta x_j}\right|_{n-1/2}\\
\left[\dfrac{\partial u_1}{\partial t} + \dfrac{\delta(u_1 u_j)}{\delta x_j} - \nu\dfrac{\delta^2 u_1}{\delta x_j^2} + \dfrac{\delta p}{\delta x_1}\right]_{n-1/2}\\
\left[\dfrac{\partial u_2}{\partial t} + \dfrac{\delta(u_2 u_j)}{\delta x_j} - \nu\dfrac{\delta^2 u_2}{\delta x_j^2} + \dfrac{\delta p}{\delta x_2}\right]_{n}\\
\left[\dfrac{\partial u_3}{\partial t} + \dfrac{\delta(u_3 u_j)}{\delta x_j} - \nu\dfrac{\delta^2 u_3}{\delta x_j^2} + \dfrac{\delta p}{\delta x_3}\right]_{n-1/2}
\end{pmatrix}
=
\begin{pmatrix}
0\\
-P_x + f_{1_{n-1/2}}(\phi)\\
f_{2_n}(\phi)\\
f_{3_{n-1/2}}(\phi)
\end{pmatrix}
\qquad (C\,2)
$$

All first and second derivatives in the x_1 and x_3 directions are computed in Fourier space according to:

$$
\widehat{\frac{\delta_s q}{\delta x_1}} = i\,k_x\,\hat{q} \qquad \widehat{\frac{\delta_s q}{\delta x_3}} = i\,k_z\,\hat{q} \qquad \widehat{\frac{\delta_s^2 q}{\delta x_1}} = -k_x^2\,\hat{q} \qquad \widehat{\frac{\delta_s^2 q}{\delta x_3}} = -k_z^2\,\hat{q},
$$

where the hat indicates the Fourier transform in the x_1 and x_3 directions with corresponding wavenumbers k_x and k_z, q is an arbitrary flow quantity, and the s subscript is used to emphasize that the derivative is evaluated spectrally. The convective terms involving derivatives in the x_2 direction are computed with quasi-second-order accurate formulae motivated by a finite volume analysis. Written out completely, the convective terms are:

$$\left.\frac{\delta(u_1 u_j)}{\delta x_j}\right|_{n-1/2} = \frac{\delta_s (u_1 u_1)_{n-1/2}}{\delta x_1} + \frac{(\bar{u}_1 u_2)_n - (\bar{u}_1 u_2)_{n-1}}{\Delta x_{2_{n-1/2}}} + \frac{\delta_s (u_1 u_3)_{n-1/2}}{\delta x_3}$$

$$\left.\frac{\delta(u_2 u_j)}{\delta x_j}\right|_{n} = \frac{\delta_s (u_2 \check{u}_1)_n}{\delta x_1} + \frac{(\bar{u}_2 \bar{u}_2)_{n+1/2} - (\bar{u}_2 \bar{u}_2)_{n-1/2}}{\Delta x_{2_n}} + \frac{\delta_s (u_2 \check{u}_3)_n}{\delta x_3}$$

$$\left.\frac{\delta(u_3 u_j)}{\delta x_j}\right|_{n-1/2} = \frac{\delta_s (u_3 u_1)_{n-1/2}}{\delta x_1} + \frac{(\bar{u}_3 u_2)_n - (\bar{u}_3 u_2)_{n-1}}{\Delta x_{2_{n-1/2}}} + \frac{\delta_s (u_3 u_3)_{n-1/2}}{\delta x_3}.$$

Note that the interpolation formulae chosen in the above expressions have been selected deliberately in order to achieve energy conservation, as discussed in the following section. The viscous terms involving derivatives in the x_2 direction are evaluated with a second-order accurate finite difference formula. Written out completely, the viscous terms are:

$$\left.\frac{\delta^2 u_1}{\delta x_j^2}\right|_{n-1/2} = \frac{\delta_s^2 u_{1_{n-1/2}}}{\delta x_1^2} + \left(\frac{u_{1_{n+1/2}} - u_{1_{n-1/2}}}{\Delta x_{2_n}} - \frac{u_{1_{n-1/2}} - u_{1_{n-3/2}}}{\Delta x_{2_{n-1}}}\right) / \Delta x_{2_{n-1/2}} + \frac{\delta_s^2 u_{1_{n-1/2}}}{\delta x_3^2}$$

$$\left.\frac{\delta^2 u_2}{\delta x_j^2}\right|_{n} = \frac{\delta_s^2 u_{2_n}}{\delta x_1^2} + \left(\frac{u_{2_{n+1}} - u_{2_n}}{\Delta x_{2_{n+1/2}}} - \frac{u_{2_n} - u_{2_{n-1}}}{\Delta x_{2_{n-1/2}}}\right) / \Delta x_{2_n} + \frac{\delta_s^2 u_{2_n}}{\delta x_3^2}$$

$$\left.\frac{\delta^2 u_3}{\delta x_j^2}\right|_{n-1/2} = \frac{\delta_s^2 u_{3_{n-1/2}}}{\delta x_1^2} + \left(\frac{u_{3_{n+1/2}} - u_{3_{n-1/2}}}{\Delta x_{2_n}} - \frac{u_{3_{n-1/2}} - u_{3_{n-3/2}}}{\Delta x_{2_{n-1}}}\right) / \Delta x_{2_{n-1/2}} + \frac{\delta_s^2 u_{3_{n-1/2}}}{\delta x_3^2}.$$

The required derivatives of p are given by

$$\left.\frac{\delta p}{\delta x_1}\right|_{n-1/2} = \frac{\delta_s p_{n-1/2}}{\delta x_1}, \qquad \left.\frac{\delta p}{\delta x_2}\right|_{n} = \frac{p_{n+1/2} - p_{n-1/2}}{\Delta x_{2_n}}, \qquad \left.\frac{\delta p}{\delta x_3}\right|_{n-1/2} = \frac{\delta_s p_{n-1/2}}{\delta x_3},$$

$$\left.\frac{\delta^2 p}{\delta x_j^2}\right|_{n-1/2} = \frac{\delta_s^2 p_{n-1/2}}{\delta x_1^2} + \left(\frac{p_{n+1/2} - p_{n-1/2}}{\Delta x_{2_n}} - \frac{p_{n-1/2} - p_{n-3/2}}{\Delta x_{2_{n-1}}}\right) / \Delta x_{2_{n-1/2}} + \frac{\delta_s^2 p_{n-1/2}}{\delta x_3^2}.$$

(The Laplacian of the pressure is required by the Poisson equation to update the pressure in the fractional step algorithm.) Finally, the discretization of the continuity equation is

$$\left.\frac{\delta u_j}{\delta x_j}\right|_{n-1/2} = \frac{\delta_s u_{1_{n-1/2}}}{\delta x_1} + \frac{u_{2_n} - u_{2_{n-1}}}{\Delta x_{2_{n-1/2}}} + \frac{\delta_s u_{3_{n-1/2}}}{\delta x_3}. \qquad \text{(C 3)}$$

C.1.1. *Conservation of mass, momentum, and energy*

An important check on the stability of an incompressible channel flow code is that mass should be conserved to within machine round-off error, and spatial discretization errors should not contribute to the momentum and energy of the flow integrated over the channel volume.

To show that the total mass is conserved, the compressible continuity equation is integrated over the volume under consideration (with the integrals on the right hand side evaluated with a trapezoidal rule in the wall normal direction and spectral rules in the Fourier directions), verifying that numerical errors do not contribute to net sources of mass and thus the discretized system indeed conserves total mass exactly:

$$
\begin{aligned}
\frac{\partial}{\partial t}\int_\Omega \rho\, dV &= -\int_\Omega \frac{\delta\, \rho u_j}{\delta x_j}\, dV \\
&= -\rho \int_x\int_z \sum_{n=1}^{NY} \Delta x_{2_{n-1/2}} \left(\frac{\delta_s u_{1_{n-1/2}}}{\delta x_1} + \frac{u_{2_n} - u_{2_{n-1}}}{\Delta x_{2_{n-1/2}}} + \frac{\delta_s u_{3_{n-1/2}}}{\delta x_3} \right) dx\, dz \\
&= -\rho \int_x\int_z \left(u_{2_{NY}} - u_{2_0}\right)\, dx\, dz \\
&= 0 \implies \text{Mass is conserved.}
\end{aligned}
$$

To show that total momentum is conserved in each direction x_i for cases with $f_i(\phi) = 0$ and $g_i(\phi) = 0$, each component of the momentum equation in (C 2) is integrated over the volume under consideration:

$$
\frac{\partial}{\partial t}\int_\Omega u_i\, dV = -\int_\Omega \left(\frac{\delta\,(u_i u_j)}{\delta x_j} + \frac{\delta p}{\delta x_i} + \delta_{1i}\, P_x - \nu \frac{\delta^2 u_i}{\delta x_j^2} \right) dV
$$

$$
= \begin{cases}
-\displaystyle\int_x\int_z \sum_{n=1}^{NY} \Delta x_{2_{n-1/2}} \Bigg[\frac{(\bar u_1 u_2)_n - (\bar u_1 u_2)_{n-1}}{\Delta x_{2_{n-1/2}}} + P_x \\
\qquad - \nu \left(\dfrac{u_{1_{n+1/2}} - u_{1_{n-1/2}}}{\Delta x_{2_n}} - \dfrac{u_{1_{n-1/2}} - u_{1_{n-3/2}}}{\Delta x_{2_{n-1}}} \right) / \Delta x_{2_{n-1/2}} \Bigg] dx\, dz & \text{for } i = 1 \\
-\displaystyle\int_x\int_z \sum_{n=0}^{NY} \Delta x_{2_n} \Bigg[\frac{(\bar u_2 \bar u_2)_{n+1/2} - (\bar u_2 \bar u_2)_{n-1/2}}{\Delta x_{2_n}} + \frac{p_{n+1/2} - p_{n-1/2}}{\Delta x_{2_n}} \\
\qquad - \nu \left(\dfrac{u_{2_{n+1}} - u_{2_n}}{\Delta x_{2_{n+1/2}}} - \dfrac{u_{2_n} - u_{2_{n-1}}}{\Delta x_{2_{n-1/2}}} \right) / \Delta x_{2_n} \Bigg] dx\, dz & \text{for } i = 2 \\
-\displaystyle\int_x\int_z \sum_{n=1}^{NY} \Delta x_{2_{n-1/2}} \Bigg[\frac{(\bar u_3 u_2)_n - (\bar u_3 u_2)_{n-1}}{\Delta x_{2_{n-1/2}}} \\
\qquad - \nu \left(\dfrac{u_{3_{n+1/2}} - u_{3_{n-1/2}}}{\Delta x_{2_n}} - \dfrac{u_{3_{n-1/2}} - u_{3_{n-3/2}}}{\Delta x_{2_{n-1}}} \right) / \Delta x_{2_{n-1/2}} \Bigg] dx\, dz & \text{for } i = 3
\end{cases}
$$

$$
= \begin{cases}
-\displaystyle\int_x\int_z \left[2\,\delta\, P_x - \nu \left(\frac{u_{1_{NY}} - u_{1_{NY-1/2}}}{\Delta x_{2_{NY}}} - \frac{u_{1_{1/2}} - u_{1_0}}{\Delta x_{2_0}} \right) \right] dx\, dz & \text{for } i = 1 \\
-\displaystyle\int_x\int_z \left[p_{NY} - p_0 \right] dx\, dz & \text{for } i = 2 \\
-\displaystyle\int_x\int_z \left[-\nu \left(\frac{u_{3_{NY}} - u_{3_{NY-1/2}}}{\Delta x_{2_{NY}}} - \frac{u_{3_{1/2}} - u_{3_0}}{\Delta x_{2_0}} \right) \right] dx\, dz & \text{for } i = 3.
\end{cases}
$$

In the limit that $\nu \to 0$ with $P_x = 0$, momentum is conserved in the x_1 and x_3 directions. Note that the wall pressure terms may result in small variations in the momentum in the x_2 direction, but non-physical spatial discretization errors do not contribute to this variation. For cases in which $\nu \neq 0$, it is seen that choosing

$$P_x = \frac{1}{V} \int_x \int_z \nu \left(\frac{u_{1_{NY}} - u_{1_{NY-1/2}}}{\Delta x_{2_{NY}}} - \frac{u_{1_{1/2}} - u_{1_0}}{\Delta x_{2_0}} \right) dx\, dz, \tag{C 4}$$

where $V = 2\delta\, L_x\, L_z$ is the volume of the domain under consideration, maintains the x_1 component of momentum (i.e. mass flux) constant by exactly balancing the skin friction integrated over the walls with the force applied by the mean pressure gradient.

The viscous terms of the Navier-Stokes equation result in energy dissipation at the small scales, which, in channel flow, is replenished by the action of the pressure gradient P_x on the flow at the large scale. To show that energy is conserved in cases with $\nu = P_x = f_i(\phi) = g_i(\phi) = 0$, the momentum equation in (C 2) is multiplied by u_i and integrated over the volume under consideration (underbraced sums "telescope" and therefore cancel):

$$\frac{\partial}{\partial t} \int_\Omega \frac{u_i^2}{2}\, dV = - \int_\Omega u_i \left(\frac{\delta\,(u_i u_j)}{\delta x_j} + \frac{\delta p}{\delta x_i} \right) dV$$

$$\begin{aligned}
= -\int_x \int_z \Bigg[& \sum_{n=1}^{NY} \Delta x_{2_{n-1/2}}\, u_{1_{n-1/2}} \left(\frac{\delta_s\,(u_1 u_1)_{n-1/2}}{\delta x_1} + \frac{(\bar{u}_1 u_2)_n - (\bar{u}_1 u_2)_{n-1}}{\Delta x_{2_{n-1/2}}} + \frac{\delta_s\,(u_1 u_3)_{n-1/2}}{\delta x_3} + \frac{\delta_s p_{n-1/2}}{\delta x_1} \right) \\
& + \sum_{n=0}^{NY} \Delta x_{2_n}\, u_{2_n} \left(\frac{\delta_s\,(u_2 \check{u}_1)_n}{\delta x_1} + \frac{(\bar{u}_2 \bar{u}_2)_{n+1/2} - (\bar{u}_2 \bar{u}_2)_{n-1/2}}{\Delta x_{2_n}} + \frac{\delta_s\,(u_2 \check{u}_3)_n}{\delta x_3} + \frac{p_{n+1/2} - p_{n-1/2}}{\Delta x_{2_n}} \right) \\
& + \sum_{n=1}^{NY} \Delta x_{2_{n-1/2}}\, u_{3_{n-1/2}} \left(\frac{\delta_s\,(u_3 u_1)_{n-1/2}}{\delta x_1} + \frac{(\bar{u}_3 u_2)_n - (\bar{u}_3 u_2)_{n-1}}{\Delta x_{2_{n-1/2}}} + \frac{\delta_s\,(u_3 u_3)_{n-1/2}}{\delta x_3} + \frac{\delta_s p_{n-1/2}}{\delta x_3} \right) \Bigg] dx\, dz
\end{aligned}$$

$$\begin{aligned}
= -\int_x \int_z \Bigg[& \sum_{n=1}^{NY} \Delta x_{2_{n-1/2}}\, p_{n-1/2} \left(-\frac{\delta_s u_{1_{n-1/2}}}{\delta x_1} - \frac{u_{2_n} - u_{2_{n-1}}}{\Delta x_{2_{n-1/2}}} - \frac{\delta_s u_{3_{n-1/2}}}{\delta x_3} \right) \\
& + \sum_{n=1}^{NY} \Delta x_{2_{n-1/2}} \left(\frac{u_{1_{n-1/2}}^2 + \left(u_{1_n}^2 + u_{1_n}^2\right)/2 + u_{1_{n-1/2}}^2}{2} - p_{n-1/2} \right) \left(\frac{\delta_s u_{1_{n-1/2}}}{\delta x_1} + \frac{\delta_s u_{3_{n-1/2}}}{\delta x_3} \right) dx\, dz \\
& + \sum_{n=1}^{NY} \frac{1}{2} \left(\underbrace{u_{1_{n-1/2}} u_{1_{n+1/2}} u_{2_n} - u_{1_{n-1/2}} u_{1_{n-3/2}} u_{2_{n-1}}} + u_{1_{n-1/2}} u_{1_{n-1/2}} u_{2_n} - u_{1_{n-1/2}} u_{1_{n-1/2}} u_{2_{n-1}} \right) \\
& + \sum_{n=1}^{NY-1} \frac{1}{4} \left(\underbrace{u_{2_n} u_{2_{n+1}} u_{2_{n+1}} - u_{2_n} u_{2_{n-1}} u_{2_n}} + \underbrace{u_{2_n} u_{2_{n+1}} u_{2_n} - u_{2_n} u_{2_{n-1}} u_{2_{n-1}}} + u_{2_n} u_{2_n} u_{2_{n+1}} - u_{2_n} u_{2_n} u_{2_{n-1}} \right) \\
& + \sum_{n=1}^{NY} \frac{1}{2} \left(\underbrace{u_{3_{n-1/2}} u_{3_{n+1/2}} u_{2_n} - u_{3_{n-1/2}} u_{3_{n-3/2}} u_{2_{n-1}}} + u_{3_{n-1/2}} u_{3_{n-1/2}} u_{2_n} - u_{3_{n-1/2}} u_{3_{n-1/2}} u_{2_{n-1}} \right) \Bigg] dx\, dz
\end{aligned}$$

$$= \int_x \int_z \sum_{n=1}^{NY} \Delta x_{2_{n-1/2}} \left(p_{n-1/2} - \frac{u_{1_{n-1/2}}^2 + \dfrac{u_{2_n}^2 + u_{2_{n-1}}^2}{2} + u_{3_{n-1/2}}^2}{2} \right) \left(\frac{\delta_s u_{1_{n-1/2}}}{\delta x_1} + \frac{u_{2_n} - u_{2_{n-1}}}{\Delta x_{2_{n-1/2}}} + \frac{\delta_s u_{3_{n-1/2}}}{\delta x_3} \right) dx\, dz$$

$= 0 \qquad \Longrightarrow$ energy is conserved.

In the above derivation, it was assumed that integration by parts is valid in the spectral directions. Strictly speaking, this is only true if these directions are fully resolved, so that there is no possibility of aliasing. However, no calculation of a turbulent flow is ever "fully resolved". To make them affordable, direct numerical simulations are inevitably conducted with as few modes as possible which still give accurate results. There are two ways of handling the necessary truncation of the Fourier series representation of the flow field under consideration: A) to allow the cascade of energy to higher wavenumbers (due to the nonlinear products) to alias back to lower wavenumbers, hoping that the effect of this aliasing will be minimal, or B) to zero out all higher-order variations resulting from nonlinear products, using the 3/2 dealiasing rule. Method A creates spurious energy sources, as the above derivation does *not* hold when the Fourier series are truncated (due to the fact that integration by parts in the spectral directions is invalid), and thus can lead to an unstable code. Method B constantly drains off the energy of all unresolved modes, and thus energy is not conserved in this case either. However, method B guarantees that no spurious numerical energy *sources* ever appear in the flow due to the Fourier series truncation, and thus can not destabilize the code. Thus, all calculations presented in this report are dealiased in the spectral directions.

Some additional algebra used in the energy conservation proof outlined above now follows (no summation is implied on the subscripts α and β). The step involving the integration by parts in a spectral direction β (neglecting the effects of truncation of the Fourier series) is:

$$\begin{aligned}
\int u_\alpha \frac{\delta_s u_\alpha u_\beta}{\delta x_\beta}\, dx_\beta &= \int \left(u_\alpha^2 \frac{\delta_s u_\beta}{\delta x_\beta} + u_\alpha u_\beta \frac{\delta_s u_\alpha}{\delta x_\beta} \right) dx_\beta \\
&= \int \left(u_\alpha^2 \frac{\delta_s u_\beta}{\delta x_\beta} - u_\alpha \frac{\delta_s u_\alpha u_\beta}{\delta x_\beta} \right) dx_\beta \\
\Rightarrow \int u_\alpha \frac{\delta_s u_\alpha u_\beta}{\delta x_\beta}\, dx_\beta &= \frac{1}{2} \int u_\alpha^2 \frac{\delta_s u_\beta}{\delta x_\beta}\, dx_\beta.
\end{aligned}$$

The x_2 derivatives in the convective terms of the x_2 momentum equation are written:

$$\begin{aligned}
\frac{1}{4} \sum_{n=1}^{NY-1} u_{2_n}^2 \left(u_{2_{n+1}} - u_{2_{n-1}} \right) &= \frac{1}{4} \sum_{n=1}^{NY-1} u_{2_n}^2 \left[\left(u_{2_{n+1}} - u_{2_n} \right) + \left(u_{2_n} - u_{2_{n-1}} \right) \right] \\
&= \frac{1}{2} \sum_{n=1}^{NY} \frac{u_{2_n}^2 + u_{2_{n-1}}^2}{2} \left(u_{2_n} - u_{2_{n-1}} \right).
\end{aligned}$$

Finally, the terms involving $\check{u}_\alpha$ are written:

$$\begin{aligned}
\sum_{n=1}^{NY-1} \Delta x_{2_n}\, u_{2_n} \frac{\delta_s \left(u_2 \check{u}_\alpha \right)_n}{\delta x_\alpha} &= \frac{1}{2} \sum_{n=1}^{NY-1} \left(\Delta x_{2_{n+1/2}}\, u_{2_n} \frac{\delta_s u_{2_n} u_{\alpha_{n+1/2}}}{\delta x_\alpha} + \Delta x_{2_{n-1/2}}\, u_{2_n} \frac{\delta_s u_{2_n} u_{\alpha_{n-1/2}}}{\delta x_\alpha} \right) \\
&= \frac{1}{4} \sum_{n=1}^{NY-1} \left(\Delta x_{2_{n+1/2}}\, u_{2_n}^2 \frac{\delta_s u_{\alpha_{n+1/2}}}{\delta x_\alpha} + \Delta x_{2_{n-1/2}}\, u_{2_n}^2 \frac{\delta_s u_{\alpha_{n-1/2}}}{\delta x_\alpha} \right) \\
&= \frac{1}{2} \sum_{n=1}^{NY-1} \Delta x_{2_{n-1/2}} \frac{u_{2_n}^2 + u_{2_{n-1}}^2}{2} \frac{\delta_s u_{\alpha_{n-1/2}}}{\delta x_\alpha}.
\end{aligned}$$

C.2. *Temporal discretization of flow problem*

The temporal discretization used in the present work is identical to that used by Akselvoll & Moin (1995), and therefore will be written here with minimal explanation. The reader is referred to Akselvoll & Moin (1995) for a clear description of the details of the derivation of this temporal discretization.

Let the operator A_i represent the terms treated explicitly (third order Runge-Kutta) and B_i represent the terms treated implicitly in the Navier Stokes equation (C 2):

$$\begin{aligned}\frac{u_i^k - u_i^{k-1}}{\Delta t} &= \beta_k \left(B_i(u_j^k) + B_i(u_j^{k-1}) \right) + \gamma_k A_i(u_j^{k-1}) + \zeta_k A_i(u_j^{k-2}) \\ &\quad + 2\beta_k \left(-\frac{\delta p^k}{\delta x_i} - \delta_{1i} P_x + f_i(\phi^{k-1}) \right) \\ \frac{\delta u_i^k}{\delta x_i} &= 0,\end{aligned}$$

where the explicit and implicit operators are given, as in Akselvoll & Moin (1995), by:

$$\begin{aligned}A_1(u_j) &= \frac{\delta}{\delta x_1}\left[\nu \frac{\delta u_1}{\delta x_1}\right] + \frac{\delta}{\delta x_3}\left[\nu \frac{\delta u_1}{\delta x_3}\right] - \frac{\delta u_1 u_1}{\delta x_1} - \frac{\delta u_3 u_1}{\delta x_3} \\ A_2(u_j) &= \frac{\delta}{\delta x_1}\left[\nu \frac{\delta u_2}{\delta x_1}\right] + \frac{\delta}{\delta x_3}\left[\nu \frac{\delta u_2}{\delta x_3}\right] - \frac{\delta u_1 u_2}{\delta x_1} - \frac{\delta u_3 u_2}{\delta x_3} \\ A_3(u_j) &= \frac{\delta}{\delta x_1}\left[\nu \frac{\delta u_3}{\delta x_1}\right] + \frac{\delta}{\delta x_3}\left[\nu \frac{\delta u_3}{\delta x_3}\right] - \frac{\delta u_1 u_3}{\delta x_1} - \frac{\delta u_3 u_3}{\delta x_3} \\ B_1(u_j) &= \frac{\delta}{\delta x_2}\left[\nu \frac{\delta u_1}{\delta x_2}\right] - \frac{\delta u_2 u_1}{\delta x_2} \\ B_2(u_j) &= \frac{\delta}{\delta x_2}\left[\nu \frac{\delta u_2}{\delta x_2}\right] - \frac{\delta u_2 u_2}{\delta x_2} \\ B_3(u_j) &= \frac{\delta}{\delta x_2}\left[\nu \frac{\delta u_3}{\delta x_2}\right] - \frac{\delta u_2 u_3}{\delta x_2}.\end{aligned}$$

The Runge-Kutta coefficients used in the present computations are:

$$\begin{aligned}\beta_1 &= \frac{4}{15}, & \beta_2 &= \frac{1}{15}, & \beta_3 &= \frac{1}{6}, \\ \gamma_1 &= \frac{8}{15}, & \gamma_2 &= \frac{5}{12}, & \gamma_3 &= \frac{3}{4}, \\ \zeta_1 &= 0, & \zeta_2 &= -\frac{17}{60}, & \zeta_3 &= -\frac{5}{12}.\end{aligned}$$

An important key to the success of the present approach is that wall-normal derivatives may be linearized (without loss of overall accuracy of the method) according to

$$\overline{B}_2(u_j^k) = \frac{\delta}{\delta x_2}\left[\nu \frac{\delta u_2^k}{\delta x_2}\right] - 2\frac{\delta u_2^{k-1} u_2^k}{\delta x_2} + \frac{\delta u_2^{k-1} u_2^{k-1}}{\delta x_2}. \tag{C 5}$$

The fractional step method for the flow problem may now be written out (in order of computation in the actual code) as follows. The right hand sides, containing all terms computed explicitly, are first computed:

$$R_1 = u_1^{k-1} + \beta_k \Delta t \left(\frac{\delta}{\delta x_2} \left[\nu \frac{\delta u_1^{k-1}}{\delta x_2} \right] - \frac{\delta u_2^{k-1} u_1^{k-1}}{\delta x_2} \right)$$

$$+ \gamma_k \Delta t A_1(u_j^{k-1}) + \zeta_k \Delta t A_1(u_j^{k-2}) + 2\beta_k \Delta t \left(-\frac{\delta p^{k-1}}{\delta x_1} - P_x + f_1(\phi^{k-1}) \right)$$

$$R_2 = u_2^{k-1} + \beta_k \Delta t \left(\frac{\delta}{\delta x_2} \left[\nu \frac{\delta u_2^{k-1}}{\delta x_2} \right] \right)$$

$$+ \gamma_k \Delta t A_2(u_j^{k-1}) + \zeta_k \Delta t A_2(u_j^{k-2}) + 2\beta_k \Delta t \left(-\frac{\delta p^{k-1}}{\delta x_2} + f_2(\phi^{k-1}) \right)$$

$$R_3 = u_3^{k-1} + \beta_k \Delta t \left(\frac{\delta}{\delta x_2} \left[\nu \frac{\delta u_3^{k-1}}{\delta x_2} \right] - \frac{\delta u_2^{k-1} u_3^{k-1}}{\delta x_2} \right)$$

$$+ \gamma_k \Delta t A_3(u_j^{k-1}) + \zeta_k \Delta t A_3(u_j^{k-2}) + 2\beta_k \Delta t \left(-\frac{\delta p^{k-1}}{\delta x_3} + f_3(\phi^{k-1}) \right).$$

Note that the pressure is accounted for explicitly in the above expressions. With the right hand sides computed, the implicit (tridiagonal) problem for the x_2 component of a (non-divergence-free) intermediate field $\hat{\mathbf{u}}$ may be solved based on the linearized treatment of the implicit wall-normal derivatives:

$$\left\{ 1 - \beta_k \Delta t \frac{\delta}{\delta x_2} \left[\nu \frac{\delta \cdot}{\delta x_2} \right] + 2\beta_k \Delta t \frac{\delta u_2^{k-1} \cdot}{\delta x_2} \right\} \hat{u}_2 = R_2.$$

With $\hat{u}_2$ computed, the implicit problems for the x_1 and x_3 components of $\hat{\mathbf{u}}$ may be solved:

$$\left\{ 1 - \beta_k \Delta t \frac{\delta}{\delta x_2} \left[\nu \frac{\delta \cdot}{\delta x_2} \right] + \beta_k \Delta t \frac{\delta \hat{u}_2 \cdot}{\delta x_2} \right\} \hat{u}_1 = R_1$$

$$\left\{ 1 - \beta_k \Delta t \frac{\delta}{\delta x_2} \left[\nu \frac{\delta \cdot}{\delta x_2} \right] + \beta_k \Delta t \frac{\delta \hat{u}_2 \cdot}{\delta x_2} \right\} \hat{u}_3 = R_3.$$

Finally, a Poisson equation for the pressure update $\varphi = p^k - p^{k-1}$ is computed based on the divergence of this intermediate field:

$$\frac{\delta \varphi}{\delta x_i \delta x_i} = \frac{1}{2\beta_k \Delta t} \frac{\delta \hat{u}_i}{\delta x_i}.$$

The pressure update term φ is then used both to project the intermediate velocity field $\hat{\mathbf{u}}$ onto a divergence free field $\mathbf{u}^k$

$$u_i^k = \hat{u}_i - 2\beta_k \Delta t \frac{\delta \varphi}{\delta x_i},$$

and, of course, to update the pressure p^k itself

$$p^k = p^{k-1} + \varphi.$$

C.3. *Temporal Discretization of Adjoint Problem*

The temporal discretization for the adjoint problem follows closely that of the flow problem developed in the previous section. The equation governing the adjoint is

$$\mathcal{N}'(\mathbf{q})^* \, \mathbf{q}^* = \begin{pmatrix} -\dfrac{\partial u_j^*}{\partial x_j} \\ -\dfrac{\partial u_i^*}{\partial t} - u_j\Big(\dfrac{\partial u_i^*}{\partial x_j} + \dfrac{\partial u_j^*}{\partial x_i}\Big) - \nu \dfrac{\partial^2 u_i^*}{\partial x_j^2} - \dfrac{\partial p^*}{\partial x_i} \end{pmatrix} = \begin{pmatrix} 0 \\ f_i^* \end{pmatrix} \qquad \text{in } \Omega$$

with boundary conditions, initial conditions, and interior forcing terms f_i^* which vary from case to case, as outlined in the main text. In order to simplify the notation for the remainder of this appendix, in which superscripts indicate the Runge-Kutta substep, the tilde notation ($\tilde{}$) will be adopted for the adjoint field rather than the asterisk notation (*).

Let the operator A_i represent the terms treated explicitly (third order Runge-Kutta) and B_i represent the terms treated implicitly in the adjoint equation (above):

$$\begin{aligned} \frac{\tilde{u}_i^k - \tilde{u}_i^{k-1}}{-\Delta t} &= \beta_k \left(B_i(\tilde{u}_j^k) + B_i(\tilde{u}_j^{k-1}) \right) + \gamma_k A_i(\tilde{u}_j^{k-1}) + \zeta_k A_i(\tilde{u}_j^{k-2}) \\ &\quad + 2\beta_k \left(\frac{\delta \tilde{p}^k}{\delta x_i} + \tilde{f}_i \right) \\ \frac{\delta \tilde{u}_i^k}{\delta x_i} &= 0 \end{aligned}$$

where the explicit and implicit operators are given by :

$$\begin{aligned} A_1(\tilde{u}_j) &= \frac{\delta}{\delta x_1}\left[\nu \frac{\delta \tilde{u}_1}{\delta x_1}\right] + \frac{\delta}{\delta x_3}\left[\nu \frac{\delta \tilde{u}_1}{\delta x_3}\right] + 2u_1 \frac{\delta \tilde{u}_1}{\delta x_1} + u_2 \frac{\delta \tilde{u}_2}{\delta x_1} + u_3\Big(\frac{\delta \tilde{u}_1}{\delta x_3} + \frac{\delta \tilde{u}_3}{\delta x_1}\Big) \\ A_2(\tilde{u}_j) &= \frac{\delta}{\delta x_1}\left[\nu \frac{\delta \tilde{u}_2}{\delta x_1}\right] + \frac{\delta}{\delta x_3}\left[\nu \frac{\delta \tilde{u}_2}{\delta x_3}\right] + u_1 \frac{\delta \tilde{u}_2}{\delta x_1} - 2u_2\Big(\frac{\delta \tilde{u}_1}{\delta x_1} + \frac{\delta \tilde{u}_3}{\delta x_3}\Big) + u_3 \frac{\delta \tilde{u}_2}{\delta x_3} \\ A_3(\tilde{u}_j) &= \frac{\delta}{\delta x_1}\left[\nu \frac{\delta \tilde{u}_3}{\delta x_1}\right] + \frac{\delta}{\delta x_3}\left[\nu \frac{\delta \tilde{u}_3}{\delta x_3}\right] + u_1\Big(\frac{\delta \tilde{u}_3}{\delta x_1} + \frac{\delta \tilde{u}_1}{\delta x_3}\Big) + u_2 \frac{\delta \tilde{u}_2}{\delta x_3} + 2u_3 \frac{\delta \tilde{u}_3}{\delta x_3} \end{aligned}$$

$$\begin{aligned} B_1(\tilde{u}_j) &= \frac{\delta}{\delta x_2}\left[\nu \frac{\delta \tilde{u}_1}{\delta x_2}\right] + u_2 \frac{\delta \tilde{u}_1}{\delta x_2} \\ B_2(\tilde{u}_j) &= \frac{\delta}{\delta x_2}\left[\nu \frac{\delta \tilde{u}_2}{\delta x_2}\right] + u_1 \frac{\delta \tilde{u}_1}{\delta x_2} + u_3 \frac{\delta \tilde{u}_3}{\delta x_2} \\ B_3(\tilde{u}_j) &= \frac{\delta}{\delta x_2}\left[\nu \frac{\delta \tilde{u}_3}{\delta x_2}\right] + u_2 \frac{\delta \tilde{u}_3}{\delta x_2} \end{aligned}$$

The fractional step method for adjoint problem may now be written out (in order of computation in the actual code) as follows. The right hand sides, containing all terms computed explicitly, are first computed:

$$\begin{aligned}\tilde{R}_1 &= \tilde{u}_1^{k-1} - \beta_k \Delta t \left(\frac{\delta}{\delta x_2} \left[\nu \frac{\delta \tilde{u}_1^{k-1}}{\delta x_2} \right] + u_2^{k-1} \frac{\delta \tilde{u}_1^{k-1}}{\delta x_2} \right) \\ &\quad - \gamma_k \Delta t A_1(\tilde{u}_j^{k-1}) - \zeta_k \Delta t A_1(\tilde{u}_j^{k-2}) - 2\beta_k \Delta t \left(\frac{\delta \tilde{p}^{k-1}}{\delta x_1} + \tilde{f}_1 \right) \\ \tilde{R}_2 &= \tilde{u}_2^{k-1} - \beta_k \Delta t \left(\frac{\delta}{\delta x_2} \left[\nu \frac{\delta \tilde{u}_2^{k-1}}{\delta x_2} \right] + u_1^{k-1} \frac{\delta \tilde{u}_1^{k-1}}{\delta x_2} + u_3^{k-1} \frac{\delta \tilde{u}_3^{k-1}}{\delta x_2} \right) \\ &\quad - \gamma_k \Delta t A_2(\tilde{u}_j^{k-1}) - \zeta_k \Delta t A_2(\tilde{u}_j^{k-2}) - 2\beta_k \Delta t \left(\frac{\delta \tilde{p}^{k-1}}{\delta x_2} + \tilde{f}_2 \right) \\ \tilde{R}_3 &= \tilde{u}_3^{k-1} - \beta_k \Delta t \left(\frac{\delta}{\delta x_2} \left[\nu \frac{\delta \tilde{u}_3^{k-1}}{\delta x_2} \right] + u_2^{k-1} \frac{\delta \tilde{u}_3^{k-1}}{\delta x_2} \right) \\ &\quad - \gamma_k \Delta t A_3(\tilde{u}_j^{k-1}) - \zeta_k \Delta t A_3(\tilde{u}_j^{k-2}) - 2\beta_k \Delta t \left(\frac{\delta \tilde{p}^{k-1}}{\delta x_3} + \tilde{f}_3 \right).\end{aligned}$$

With the right hand sides computed, the implicit (tridiagonal) problems for a (non-divergence-free) intermediate field $\hat{\mathbf{u}}$ may be solved:

$$\left\{ 1 + \beta_k \Delta t \frac{\delta}{\delta x_2} \left[\nu \frac{\delta \cdot}{\delta x_2} \right] + \beta_k \Delta t \, u_2^k \frac{\delta \cdot}{\delta x_2} \right\} \hat{u}_1 = \tilde{R}_1$$

$$\left\{ 1 + \beta_k \Delta t \frac{\delta}{\delta x_2} \left[\nu \frac{\delta \cdot}{\delta x_2} \right] + \beta_k \Delta t \, u_2^k \frac{\delta \cdot}{\delta x_2} \right\} \hat{u}_3 = \tilde{R}_3$$

$$\left\{ 1 + \beta_k \Delta t \frac{\delta}{\delta x_2} \left[\nu \frac{\delta \cdot}{\delta x_2} \right] \right\} \hat{u}_2 = \tilde{R}_2 - \beta_k \Delta t \left(u_1 \frac{\delta \hat{u}_1^k}{\delta x_2} + u_3 \frac{\delta \hat{u}_3^k}{\delta x_2} \right).$$

Finally, a Poisson equation for the adjoint pressure update $\tilde{\varphi} = \tilde{p}^k - \tilde{p}^{k-1}$ is computed based on the divergence of this intermediate field:

$$\frac{\delta \tilde{\varphi}}{\delta x_i \delta x_i} = \frac{1}{2\beta_k \Delta t} \frac{\delta \hat{u}_i}{\delta x_i}.$$

The adjoint pressure update term $(\tilde{p}^k - \tilde{p}^{k-1})$ is then used both to project the intermediate velocity field $\hat{\mathbf{u}}$ onto a divergence free field $\tilde{\mathbf{u}}^k$

$$\tilde{u}_i^k = \hat{u}_i - 2\beta_k \Delta t \frac{\delta \tilde{\varphi}}{\delta x_i},$$

and, of course, to update the adjoint pressure $\tilde{p}^k$ itself

$$\tilde{p}^k = \tilde{p}^{k-1} + \tilde{\varphi}.$$