1 Forward Equations

For an incompressible fluid, the equations governing the conservation of mass and momentum are

$$\frac{\partial u_j}{\partial x_j} = 0, \tag{1.1}$$

$$\frac{\partial u_i}{\partial t} = -\frac{\partial u_i u_j}{\partial x_j} - \frac{1}{\rho}\frac{\partial p}{\partial x_i} + B_i, \tag{1.2}$$

respectively, where ρ is the constant fluid density, u_i is the i^{th} velocity component, and p is the hydrodynamic pressure. Summation over repeated indices is implied. The viscous flux is

$$B_i \equiv \frac{\mu}{\rho}\frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{1}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right), \tag{1.3}$$

in which μ is the constant viscosity and δ_{ij} is the Kronecker delta. Note that the assumption of constant ρ and μ is not strictly necessary for an incompressible fluid.

1.1 Temporal Discretization

The governing equations are solved using Chorin's fractional-step scheme. The system is discretized in time using the explicit Euler method. In the fractional-step scheme, a "predicted" velocity field u_i^* is computed according to Eq. (1.2) without the pressure derivative, *i.e.*,

$$u_i^* = u_i^t - \Delta t\left(\frac{\partial u_i u_j}{\partial x_j} - B_i\right) + \mathcal{O}(\Delta t). \tag{1.4}$$

A Poisson equation is solved to obtain a pressure field that enforces the divergence-free condition on the velocity field [Eq. (1.1)],

$$\frac{\partial^2 p^*}{\partial x_j^2} = \frac{\rho}{\Delta t}\frac{\partial u_j^*}{\partial x_j}. \tag{1.5}$$

Finally, a "corrected" velocity field is obtained by applying the pressure correction:

$$u_i^{t+1} = u_i^* - \frac{\Delta t}{\rho}\frac{\partial p^*}{\partial x_i} + \mathcal{O}(\Delta t). \tag{1.6}$$

1.2 Spatial Discretization

The system is discretized in space using a fully-staggered grid, in which the velocity components are located at cell faces and the pressure is located at cell centers. A uniform mesh is assumed.

Convective terms are discretized in "divergence form," as they appear in Eq. (1.2), due to several desirable conservation properties on the staggered grid (Morinishi *et al.*, *JCP* 143, 1998). Let us denote the x, y, z components of velocity as $u_1, u_2, u_3 = u, v, w$, respectively. No longer implying summation over repeated indices, we can write the discretized convective terms for the $u_1 = u$ velocity component at a point (i, j, k)

as

$$\begin{aligned}\left(\frac{\partial uu}{\partial x}+\frac{\partial uv}{\partial y}+\frac{\partial uw}{\partial z}\right)_{i,j,k} &= \left(\mathrm{Conv}_{11}+\mathrm{Conv}_{12}+\mathrm{Conv}_{13}\right)_{i,j,k} \\ &= (\mathrm{grad\_x})\left[u^{I,xm}_{i,j,k}u^{I,xm}_{i,j,k}-u^{I,xm}_{i-1,j,k}u^{I,xm}_{i-1,j,k}\right] \\ &+ (\mathrm{grad\_y})\left[u^{I,y}_{i,j+1,k}v^{I,x}_{i,j+1,k}-u^{I,y}_{i,j,k}v^{I,x}_{i,j,k}\right] \\ &+ (\mathrm{grad\_z})\left[u^{I,z}_{i,j,k+1}w^{I,x}_{i,j,k+1}-u^{I}_{i,j,k}w^{I,x}_{i,j,k}\right],\end{aligned} \tag{1.7}$$

where interpolated velocities are defined as

$$\begin{aligned}u^{I,xm}_{i,j,k} &= \frac{1}{2}\left(u_{i+1,j,k}+u_{i,j,k}\right), \\ u^{I,y}_{i,j,k} &= \frac{1}{2}\left(u_{i,j,k}+u_{i,j-1,k}\right), \\ u^{I,z}_{i,j,k} &= \frac{1}{2}\left(u_{i,j,k}+u_{i,j,k-1}\right), \\ v^{I,x}_{i,j,k} &= \frac{1}{2}\left(v_{i,j,k}+v_{i-1,j,k}\right), \\ w^{I,x}_{i,j,k} &= \frac{1}{2}\left(w_{i,j,k}+w_{i-1,j,k}\right),\end{aligned}$$

and (grad_x), etc., contain the denominators of the derivative operators. The order of interpolation and differentiation in the discretized convective terms will be important in the derivation of the discrete-exact adjoint equations.

2 Adjoint Equations

A loss function $\mathcal{L}=g(u^T,v^T,w^T)$ may be defined, where the superscript $(\cdot)^T$ denotes the solution at a final time T. A typical loss function is the mean-squared error (MSE). The adjoint of the velocity field at an intermediate time t is then defined as the gradient of the loss function with respect to the forward solution at time t:

$$\widehat{u}^t \equiv \frac{\partial \mathcal{L}}{\partial u^t}, \quad \widehat{v}^t \equiv \frac{\partial \mathcal{L}}{\partial v^t}, \quad \widehat{w}^t \equiv \frac{\partial \mathcal{L}}{\partial w^t}. \tag{2.1}$$

2.1 Temporal Discretization

The adjoint field is advanced in reverse time over the range $t\in[T-1,0]$. Using dummy indices $(m,n,p)\in(N_x,N_y,N_z)$, the adjoint of the u-component of velocity at a point $(i,j,k)\in(N_x,N_y,N_z)$ is written using the chain rule on $\mathcal{L}$ and substituting Eq. (2.1):

$$\widehat{u}^t_{i,j,k}=\sum_{m,n,p}\left(\widehat{u}^{t+1}_{m,n,p}\frac{\partial u^{t+1}_{m,n,p}}{\partial u^t_{i,j,k}}+\widehat{v}^{t+1}_{m,n,p}\frac{\partial v^{t+1}_{m,n,p}}{\partial u^t_{i,j,k}}+\widehat{w}^{t+1}_{m,n,p}\frac{\partial w^{t+1}_{m,n,p}}{\partial u^t_{i,j,k}}\right). \tag{2.2}$$

We will defer the substitution of $u_{m,n,p}$, etc., until the next sub-section on the discrete-exact adjoint formulation, as the form of the equations depends on the spatial discretization of the forward equations.

Due to the reverse-time nature of the adjoint update, the analog of the Poisson equation [Eq. (1.5)] is solved first to obtain the adjoint pressure,

$$\frac{\partial^2 \widehat{p}}{\partial x_j^2} = \frac{\rho}{\Delta t}\frac{\partial \widehat{u}_j^{t+1}}{\partial x_j}, \tag{2.3}$$

where summation over repeated indices is implied. The "corrected" adjoint field is then obtained by applying the adjoint pressure correction:

$$\widehat{u}_i^* = \widehat{u}_i^{t+1} - \frac{\Delta t}{\rho}\frac{\partial \widehat{p}}{\partial x_i} + \mathcal{O}(\Delta t). \tag{2.4}$$

Finally, the adjoint field at time t is obtained by advancing the convective and viscous terms,

$$\widehat{u}_i^t = \widehat{u}_i^* - \Delta t \left(\mathrm{AdjConv}_i(u_j^t; \widehat{u}_j^*) - \widehat{B}_i\right) + \mathcal{O}(\Delta t), \tag{2.5}$$

where we leave the definition of the adjoint convective operator $\mathrm{AdjConv}_i(u_j^t; \widehat{u}_j^*)$ to the next sub-section. The pressure operator and viscous flux are self-adjoint; therefore, we have written these terms in continuous space. The nonlinear convective terms are not self-adjoint and require consideration of the spatial discretization of the forward equations.

2.2 Discrete-exact Adjoint

We now return to the definition of the adjoint convective operator. Note that all subsequent derivations assume a uniform mesh. Substituting the forward predictor equations [Eq. (1.4)] and discretized convective terms [Eq. (1.7)] into the expanded expression for $\widehat{u}_{i,j,k}^t$ [Eq. (2.2)] and neglecting the self-adjoint viscous terms, we obtain the adjoint convective operator appearing in the $\widehat{u} = \widehat{u}_1$ equation,

$$\begin{aligned}
&\mathrm{AdjConv}_1\left(u^t, v^t, w^t; \widehat{u}^*, \widehat{v}^*, \widehat{w}^*\right)_{i,j,k} \\
&\quad = \sum_{m,n,p} \widetilde{u}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\mathrm{Conv}^t_{11} + \mathrm{Conv}^t_{12} + \mathrm{Conv}^t_{13}\right]_{m,n,p} \\
&\quad + \sum_{m,n,p} \widetilde{v}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\mathrm{Conv}^t_{21}\right]_{m,n,p} \\
&\quad + \sum_{m,n,p} \widetilde{w}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\mathrm{Conv}^t_{31}\right]_{m,n,p},
\end{aligned} \tag{2.6}$$

where Conv_{21} and Conv_{31} originate from the forward v- and w-equations, respectively.

Expanding terms in Eq. (2.6), we obtain the discrete-exact convective contributions to the $\widehat{u}$-equation at a point (i, j, k). For the Conv_{11} term,

$$\begin{aligned}
&\sum_{m,n,p} \widehat{u}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\mathrm{Conv}^t_{11}\right]_{m,n,p} \\
&\quad = (\mathrm{grad_x}) \sum_{m,n,p} \widehat{u}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[u^{I,xm,t}_{m,n,p} u^{I,xm,t}_{m,n,p} - u^{I,xm,t}_{m-1,n,p} u^{I,xm,t}_{m-1,n,p}\right] \\
&\quad = \frac{1}{4}(\mathrm{grad_x}) \sum_{m,n,p} \widehat{u}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\left(u^t_{m+1,n,p}\right)^2 + 2u^t_{m,n,p}u^t_{m+1,n,p} - 2u^t_{m-1,n,p}u^t_{m,n,p} - \left(u^t_{m-1,n,p}\right)^2\right] \\
&\quad = \frac{1}{2}(\mathrm{grad_x}) \left[\widetilde{u}^*_{i-1,j,k}u^t_{i-1,j,k} + \widehat{u}^*_{i-1,j,k}u^t_{i,j,k} + \widehat{u}^*_{i,j,k}u^t_{i+1,j,k} - \widehat{u}^*_{i,j,k}u^t_{i-1,j,k} - \widehat{u}^*_{i+1,j,k}u^t_{i,j,k} - \widehat{u}^*_{i+1,j,k}u^t_{i+1,j,k}\right] \\
&\quad = (\mathrm{grad_x}) \left[\left(\widehat{u}^*_{i-1,j,k} - \widehat{u}^*_{i,j,k}\right) u^{I,xm,t}_{i-1,j,k} + \left(\widehat{u}^*_{i,j,k} - \widehat{u}^*_{i+1,j,k}\right) u^{I,xm,t}_{i,j,k}\right].
\end{aligned}$$

Several additional terms are present in the discrete-exact adjoint formulation of the convective operator, due to the order of interpolation and differentiation operations, that do not appear in the continuous adjoint formulation.

Similarly, for the Conv_{12} and Conv_{13} terms, respectively,

$$\begin{aligned}
&\sum_{m,n,p} \widehat{u}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\text{Conv}^t_{12}\right]_{m,n,p} \\
&\quad = (\text{grad_y}) \sum_{m,n,p} \widehat{u}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[u^{I,y,t}_{m,n+1,p} v^{I,x,t}_{m,n+1,p} - u^{I,y,t}_{m,n,p} v^{I,x,t}_{m,n,p}\right] \\
&\quad = \frac{1}{2}(\text{grad_y}) \left[\left(\widehat{u}^*_{i,j-1,k} - \widehat{u}^*_{i,j,k}\right) v^{I,x,t}_{i,j,k} + \left(\widehat{u}^*_{i,j,k} - \widehat{u}^*_{i,j+1,k}\right) v^{I,x,t}_{i,j+1,k}\right]
\end{aligned}$$

and

$$\begin{aligned}
&\sum_{m,n,p} \widehat{u}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\text{Conv}^t_{13}\right]_{m,n,p} \\
&\quad = (\text{grad_z}) \sum_{m,n,p} \widehat{u}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[u^{I,z,t}_{m,n,p+1} w^{I,x,t}_{m,n,p+1} - u^{I,z,t}_{m,n,p} w^{I,x,t}_{m,n,p}\right] \\
&\quad = \frac{1}{2}(\text{grad_z}) \left[\left(\widehat{u}^*_{i,j,k-1} - \widehat{u}^*_{i,j,k}\right) w^{I,x,t}_{i,j,k} + \left(\widehat{u}^*_{i,j,k} - \widehat{u}^*_{i,j,k+1}\right) w^{I,x,t}_{i,j,k+1}\right].
\end{aligned}$$

From the contributions of the v- and w- equations to the $\widehat{u}$-equation [the last two terms in Eq. (2.6)], two new terms appear. In the v-equation, the term Conv_{21} is written

$$\left.\frac{\partial vu}{\partial x}\right|_{i,j,k} = \left[\text{Conv}_{21}\right]_{i,j,k} = (\text{grad\_x}) \left[v^{I,x}_{i+1,j,k} u^{I,y}_{i+1,j,k} - v^{I,x}_{i,j,k} u^{I,y}_{i,j,k}\right], \tag{2.7}$$

making use of the interpolation operators

$$\begin{aligned}
u^{I,y}_{i,j,k} &= \frac{1}{2}\left(u_{i,j,k} + u_{i,j-1,k}\right), \\
v^{I,x}_{i,j,k} &= \frac{1}{2}\left(v_{i,j,k} + v_{i-1,j,k}\right).
\end{aligned}$$

Note that the derivative in Eq. (2.7) is evaluated at y-faces, as is required for terms in the v-equation.

Upon substituting the expression for Conv_{21} [Eq. (2.7)] into the $\widehat{v}$-contribution to the $\widehat{u}$-equation [in Eq. (2.6)], we obtain

$$\begin{aligned}
&\sum_{m,n,p} \widehat{v}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\text{Conv}^t_{21}\right]_{m,n,p} \\
&\quad = (\text{grad_x}) \sum_{m,n,p} \widehat{v}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[v^{I,x,t}_{m+1,n,p} u^{I,y,t}_{m+1,n,p} - v^{I,x,t}_{m,n,p} u^{I,y,t}_{m,n,p}\right] \\
&\quad = \frac{1}{2}(\text{grad_x}) \left[\left(\widehat{v}^*_{i-1,j,k} - \widehat{v}^*_{i,j,k}\right) v^{I,x,t}_{i,j,k} + \left(\widehat{v}^*_{i-1,j+1,k} - \widehat{v}^*_{i,j+1,k}\right) v^{I,x,t}_{i,j+1,k}\right].
\end{aligned}$$

Now, note that this derivative is evaluated at x-faces, as is required for terms in the $\widehat{u}$-equation! Similarly, for the contribution of Conv_{31} to the $\widehat{u}$-equation, we obtain

$$\begin{aligned}
&\sum_{m,n,p} \widehat{w}^*_{m,n,p} \frac{\partial}{\partial u^t_{i,j,k}} \left[\text{Conv}^t_{31}\right]_{m,n,p} \\
&\quad = \frac{1}{2}(\text{grad_x}) \left[\left(\widehat{w}^*_{i-1,j,k} - \widehat{w}^*_{i,j,k}\right) w^{I,x,t}_{i,j,k} + \left(\widehat{w}^*_{i-1,j,k+1} - \widehat{w}^*_{i,j,k+1}\right) w^{I,x,t}_{i,j,k+1}\right].
\end{aligned}$$

As before, note that this derivative is evaluated at x-faces.

The discrete-exact convective terms appearing in the $\widehat{v}$- and $\widehat{w}$-equations can be derived by repeating the steps above for these equations. These terms are implemented in the `adjoint.py` module of *PyFlow* but are omitted here for brevity.

3 Adjoint Verification

3.1 Methodology

1. Advance NS equations n_{iter} time steps of size Δt to obtain solution u_n and objective function $\mathcal{L}$

$$\begin{aligned}\mathcal{L} &= g(u_n, v_n, w_n) \\ &= \text{mean}\left[(u_n - u_{\text{target}})^2\right]\end{aligned}$$

2. Advance *PyFlow* adjoint n_{iter} steps in reverse to obtain $\widehat{u}_0$
3. Perturb the initial velocity field $u_0^* = u_0 + \Delta u$, then advance n_{iter} steps, size Δt, to obtain u_n^* and $\mathcal{L}^*$
4. Approximate the perturbation-based adjoint using finite differences:

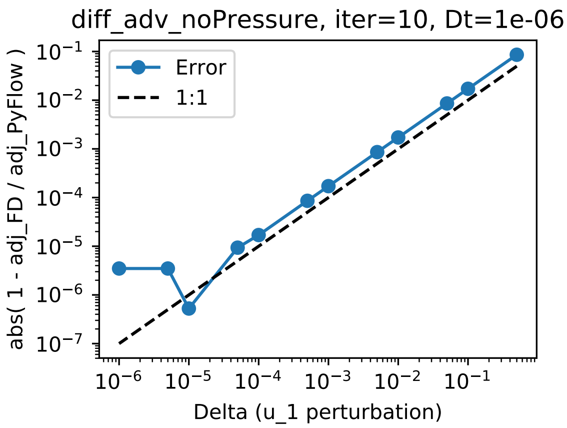
$$\widehat{u}_0^* = \frac{\partial \mathcal{L}}{\partial u_0} = \frac{\mathcal{L}^* - \mathcal{L}}{\Delta u} + \mathcal{O}(\Delta u)$$

5. Compute the convergence of the perturbation-based adjoint to the *PyFlow* adjoint as the relative error:

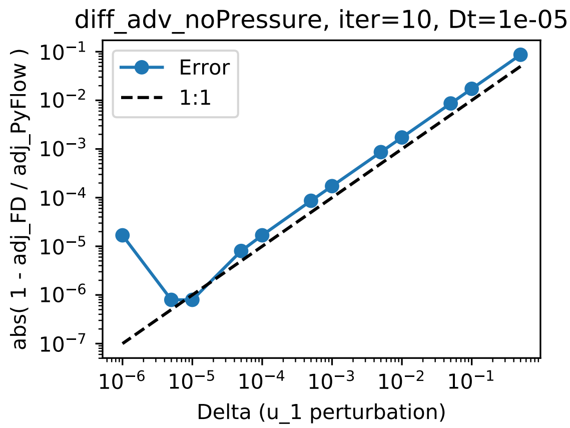
$$\epsilon_{\text{rel}} = \text{abs}\left(1 - \frac{\widehat{u}_0^*}{\widehat{u}_0}\right)$$

3.2 Notes

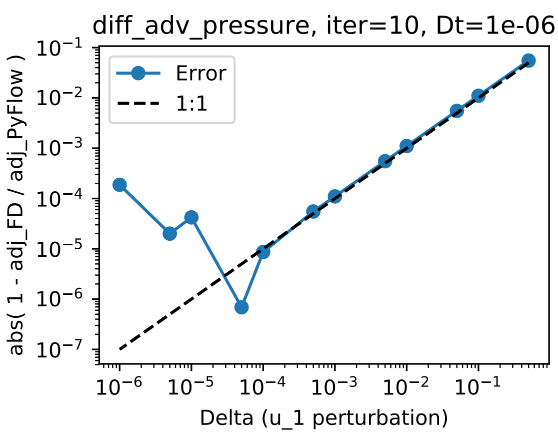
- The magnitude of the adjoint $\widehat{u}_0$ is $\mathcal{O}(10^{-5})$, so truncation-error saturation can be expected for $\epsilon_{\text{rel}} \lesssim 10^{-10}$.
- The continuous versions of the self-adjoint viscous diffusion and pressure terms are implemented, and these terms converge as expected. The range of convergence is insensitive to both n_{iter} and Δt.
- The adjoint converges as expected when the discrete-exact convective terms are implemented. Again, the range of convergence is insensitive to both n_{iter} and Δt.
- The pressure correction reduces the error marginally within the asymptotic range of convergence.



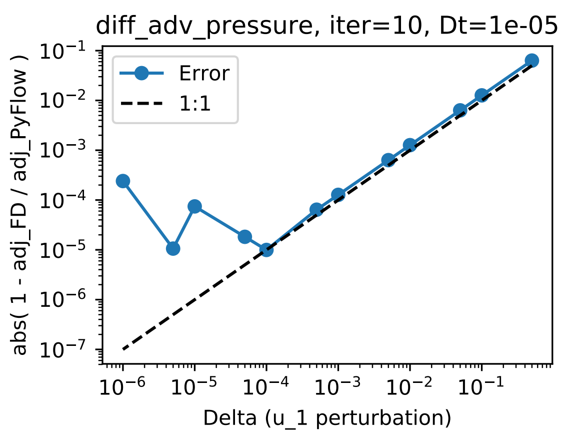
(a) Viscous and convective terms, $n_{\mathrm{iter}} = 10$, $\Delta t = 10^{-6}\,\mathrm{s}$



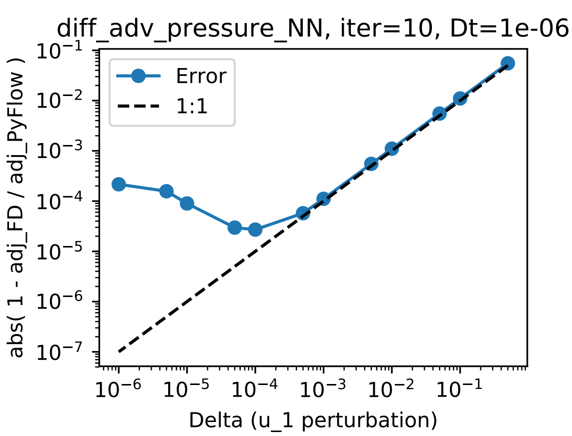
(b) Viscous and convective terms, $n_{\mathrm{iter}} = 10$, $\Delta t = 10^{-5}\,\mathrm{s}$



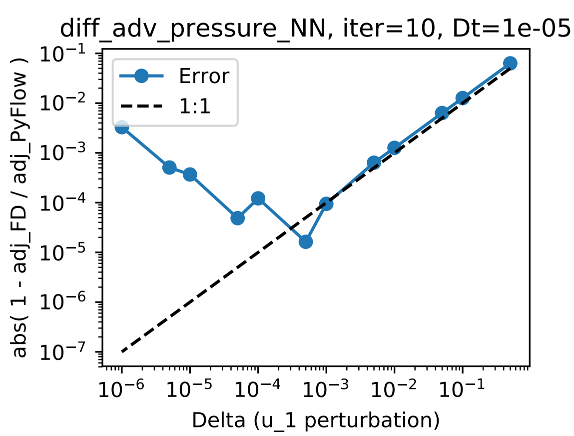
(c) Navier-Stokes equations, $n_{\mathrm{iter}} = 10$, $\Delta t = 10^{-6}\,\mathrm{s}$



(d) Navier-Stokes equations, $n_{\mathrm{iter}} = 10$, $\Delta t = 10^{-5}\,\mathrm{s}$



(e) Navier-Stokes with ML model, $n_{\mathrm{iter}} = 10$, $\Delta t = 10^{-6}\,\mathrm{s}$



(f) Navier-Stokes with ML model, $n_{\mathrm{iter}} = 10$, $\Delta t = 10^{-5}\,\mathrm{s}$

Figure 1: Convergence of the adjoint solution. The pressure solver is omitted in the top row and included in the bottom row. The total solution time ($n_{\mathrm{iter}} \cdot \Delta t$) is increased by a factor of 10 in the right column.