# 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 $\rho$ is the constant fluid density, $u_i$ is the $i^{\text{th}}$ 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 $\mu$ is the constant viscosity and $\delta_{ij}$ is the Kronecker delta. Note that the assumption of constant $\rho$ and $\mu$ 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,

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

where $\mathrm{Conv}_{21}$ and $\mathrm{Conv}_{31}$ 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 $\mathrm{Conv}_{11}$ term,

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

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 $\mathrm{Conv}_{12}$ and $\mathrm{Conv}_{13}$ terms, respectively,

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

and

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

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 $\mathrm{Conv}_{21}$ is written

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

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 $\mathrm{Conv}_{21}$ [Eq. (2.7)] into the $\widehat{v}$-contribution to the $\widehat{u}$-equation [in Eq. (2.6)], we obtain

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

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 $\mathrm{Conv}_{31}$ to the $\widehat{u}$-equation, we obtain

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

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

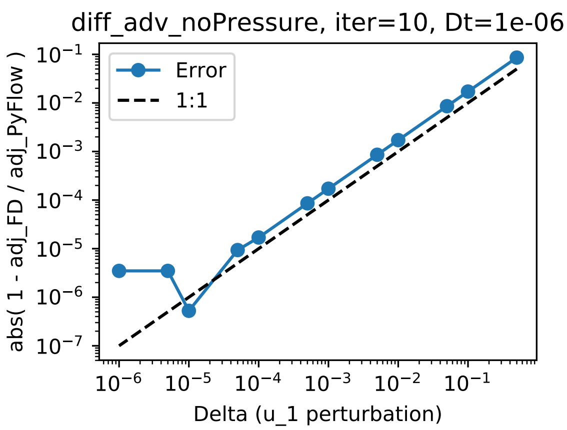
$$\widehat{u}_0^* = \frac{\partial \mathcal{L}}{\partial u_0} = \frac{\mathcal{L}^* - \mathcal{L}}{\Delta u} + \mathcal{O}(\Delta u)$$

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

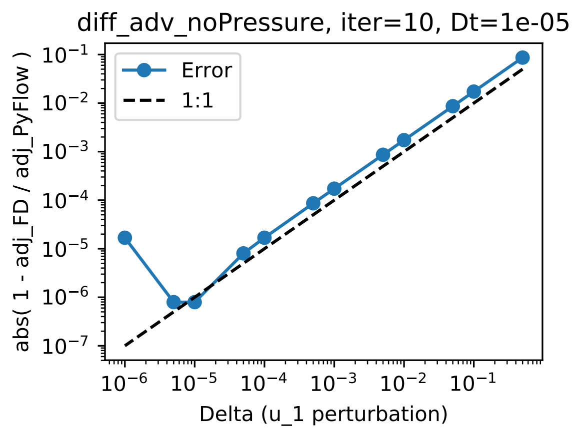
$$\epsilon_{\text{rel}} = \text{abs}\left(1 - \frac{\widehat{u}_0^*}{\widehat{u}_0}\right)$$

## 3.2 Notes

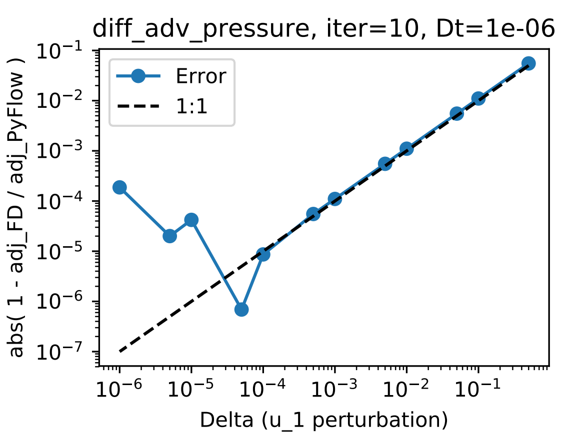
- The magnitude of the adjoint $\widehat{u}_0$ is $\mathcal{O}(10^{-5})$, so truncation-error saturation can be expected for $\epsilon_{\text{rel}} \lesssim 10^{-10}$.
- The continuous versions of the self-adjoint viscous diffusion and pressure terms are implemented, and these terms converge as expected.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



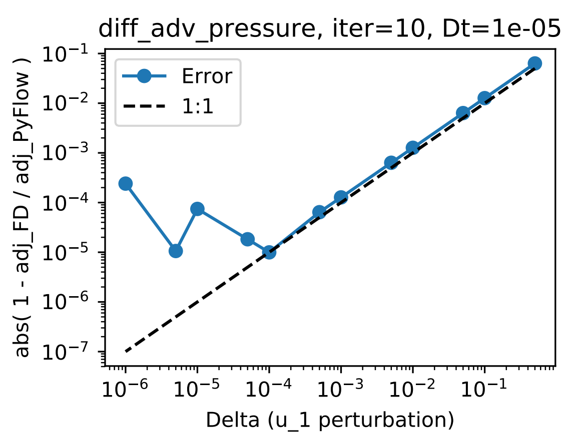

(a) Viscous and convective terms, $n_{\text{iter}} = 10$, $\Delta t = 10^{-6}$ s




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




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




(d) Navier-Stokes equations, $n_{\text{iter}} = 10$, $\Delta t = 10^{-5}$ 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 ($n_{\text{iter}} \cdot \Delta t$) is increased by a factor of 10 in the right column.