

# Some notes on Pressure Projection

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## 1 A General Projection Method

Consider the continuity and momentum equations:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}) \quad (1)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} = -\nabla p + \nabla \cdot \mathbf{F} + \mathbf{f} \quad (2)$$

where

$$\mathbf{F} = -(\rho \mathbf{u} \otimes \mathbf{u}) - \boldsymbol{\tau}, \quad (3)$$

$$\mathbf{f} = \rho \mathbf{g}. \quad (4)$$

If we differentiate the continuity equation with respect to time, then we obtain

$$\frac{\partial^2 \rho}{\partial t^2} = -\nabla \cdot \left( \frac{\partial(\rho \mathbf{u})}{\partial t} \right). \quad (5)$$

The momentum equations may be substituted to obtain

$$\nabla^2 p = \frac{\partial^2 \rho}{\partial t^2} + \nabla \cdot \nabla \cdot \mathbf{F} + \nabla \cdot \mathbf{f}, \quad (6)$$

which is a Poisson equation for the pressure. This is exact at this point, and is not tied to any particular numerical algorithm. The only problem is that it is in terms of  $\nabla \cdot \nabla \cdot \mathbf{F}$ , which is somewhat strange (not physically meaningful), and that we don't really have a good way of getting  $\frac{\partial^2 \rho}{\partial t^2}$ .

## 2 Relationship to “Traditional” Projection Methods

### 2.1 Constant Density

Let's consider a forward Euler algorithm for constant density flow. Then the time-discretized form of the momentum equation looks like:

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\nabla p + \nabla \cdot \mathbf{F}^n + \mathbf{f}^n. \quad (7)$$

where the pressure must be such that  $\nabla \cdot \mathbf{u} = 0$  is satisfied. Equation (7) can be written equivalently as

$$\mathbf{u}^* = \mathbf{u}^n - \Delta t (\nabla \cdot \mathbf{F}^n + \mathbf{f}), \quad (8)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla p. \quad (9)$$

This is the traditional fractional step approach. If we take the divergence of (9), we obtain

$$\nabla \cdot \mathbf{u}^{n+1} = \nabla \cdot \mathbf{u}^* - \Delta t \nabla^2 p, \quad (10)$$

which must be identically zero for the continuity constraint to be satisfied. Taking the divergence of (8) and noting that  $\nabla \cdot \mathbf{u}^n = 0$ , we can rewrite the above expression as

$$\nabla \cdot \mathbf{u}^{n+1} = 0 = \Delta t (\nabla \cdot \nabla \cdot \mathbf{F}^n + \nabla \cdot \mathbf{f}^n - \nabla^2 p). \quad (11)$$

In other words, we must solve for the pressure from the Poisson equation

$$\nabla^2 p = \nabla \cdot \nabla \cdot \mathbf{F}^n + \nabla \cdot \mathbf{f}^n. \quad (12)$$

Furthermore, we do not need to use the intermediate velocity at all. In fact, we can use equations (7) and (12) directly to advance the solution in time. I think that this extends to any explicit algorithm (Runge-Kutta, for example).

## 2.2 Variable Density

In the variable density case (and for the forward Euler algorithm), the analog of (8) and (9) becomes

$$(\rho \mathbf{u})^* = (\rho \mathbf{u})^n - \Delta t (\nabla \cdot \mathbf{F}^n + \mathbf{f}^n), \quad (13)$$

$$(\rho \mathbf{u})^{n+1} = (\rho \mathbf{u})^* - \Delta t \nabla p. \quad (14)$$

Taking the divergence of these gives

$$\nabla \cdot (\rho \mathbf{u})^* = - \left( \frac{\partial \rho}{\partial t} \right)^n + \Delta t (\nabla \cdot \nabla \cdot \mathbf{F}^n + \nabla \cdot \mathbf{f}), \quad (15)$$

$$\nabla \cdot (\rho \mathbf{u})^{n+1} = \nabla \cdot (\rho \mathbf{u})^* - \Delta t \nabla^2 p \quad (16)$$

$$= - \left( \frac{\partial \rho}{\partial t} \right)^n + \Delta t (\nabla \cdot \nabla \cdot \mathbf{F}^n + \nabla \cdot \mathbf{f}) - \Delta t \nabla^2 p. \quad (17)$$

Note that for an explicit scheme, we require all terms on the right-hand-side of (1) and (2) at time level  $n$ . This includes the pressure. This implies that the pressure at time level  $n$  is given by the solution to

$$\nabla^2 p^n = \left( \frac{\partial^2 \rho}{\partial t^2} \right)^n + \nabla \cdot \nabla \cdot \mathbf{F}^n + \nabla \cdot \mathbf{f}^n. \quad (18)$$

Table 1: Coefficients for use in equation (19).

$m$	2	3
$\alpha_0$	$\frac{2}{(t^n - t^{n-2})(t^n - t^{n-1})}$	$\frac{6t^n - 2(t^{n-1} + t^{n-2} + t^{n-3})}{(t^n - t^{n-1})(t^n - t^{n-2})(t^n - t^{n-3})}$
$\alpha_1$	$\frac{2}{(t^{n-1} - t^{n-2})(t^{n-1} - t^n)}$	$\frac{4t^n - 2(t^{n-2} + t^{n-3})}{(t^{n-1} - t^n)(t^{n-1} - t^{n-2})(t^{n-1} - t^{n-3})}$
$\alpha_2$	$\frac{2}{(t^{n-2} - t^{n-1})(t^{n-2} - t^n)}$	$\frac{4t^n - 2(t^{n-1} - t^{n-3})}{(t^{n-2} - t^n)(t^{n-2} - t^{n-1})(t^{n-2} - t^{n-3})}$
$\alpha_3$	0	$\frac{4t^n - 2(t^{n-1} - t^{n-2})}{(t^{n-3} - t^n)(t^{n-3} - t^{n-1})(t^{n-3} - t^{n-2})}$

Table 2: Simplified coefficients for equation (19) assuming that  $\Delta t$  is constant.

$m$	2	3
$\alpha_0$	$\frac{1}{\Delta t^2}$	$\frac{2}{\Delta t^2}$
$\alpha_1$	$\frac{-2}{\Delta t^2}$	$\frac{-5}{\Delta t^2}$
$\alpha_2$	$\frac{1}{\Delta t^2}$	$\frac{4}{\Delta t^2}$
$\alpha_3$		$\frac{-1}{\Delta x^2}$

The only problematic term here is  $\left(\frac{\partial^2 \rho}{\partial t^2}\right)^n$ . We could approximate this in various ways. Using Lagrange polynomials, we can derive approximations as

$$\left(\frac{\partial^2 \rho}{\partial t^2}\right)^n = \sum_{i=0}^m \alpha_i \rho^{n-i} \quad (19)$$

where the values of  $\alpha_i$  are given in tables 1 and 2 for variable and fixed  $\Delta t$ , respectively.

While the above discussion used the concept of an intermediate velocity field,  $\mathbf{u}^*$ , this is not required for the derivation of the time-discretized equations. For example, starting with

$$\frac{(\rho \mathbf{u})^{n+1} - (\rho \mathbf{u})^n}{\Delta t} = -\nabla p + \nabla \cdot \mathbf{F}^n + \mathbf{f}^n, \quad (20)$$

and taking its divergence, while requiring that the velocity fields at both time levels satisfy continuity, we obtain

$$\frac{\left(\frac{\partial \rho}{\partial t}\right)^{n+1} - \left(\frac{\partial \rho}{\partial t}\right)^n}{\Delta t} = \nabla^2 p + \nabla \cdot \mathbf{F}^n + \mathbf{f}^n, \quad (21)$$

which is simply a discrete approximation to (18). Thus, there is no requirement to treat anything like  $\mathbf{u}^*$  directly, and the continuous formulation given at the beginning of this document is fully appropriate and consistent.

### 3 Staggered Finite-Volume

Here we assume that the spatial discretization is static (not changing in time). In a finite-volume formulation, equations (1) and (2) are written as

$$\int_{V_s} \frac{\partial \rho}{\partial t} dV = - \int_{S_s} \rho \mathbf{u} \cdot \mathbf{n} \cdot \mathbf{n} dS, \quad (22)$$

$$\int_{V_x} \frac{\partial \rho u}{\partial t} dV = \int_{S_x} \mathbf{F} \cdot \mathbf{n}_x \cdot \mathbf{n} dS - \int_{V_x} \frac{\partial p}{\partial x} dV, \quad (23)$$

$$= \int_{S_x} (\mathbf{F} \cdot \mathbf{n}_x - p \mathbf{n}_x) \cdot \mathbf{n} dS, \quad (24)$$

$$\int_{V_y} \frac{\partial \rho v}{\partial t} dV = \int_{S_y} \mathbf{F} \cdot \mathbf{n}_y \cdot \mathbf{n} dS - \int_{V_y} \frac{\partial p}{\partial y} dV, \quad (25)$$

$$= \int_{S_y} (\mathbf{F} \cdot \mathbf{n}_y - p \mathbf{n}_y) \cdot \mathbf{n} dS, \quad (26)$$

$$\int_{V_z} \frac{\partial \rho w}{\partial t} dV = \int_{S_z} \mathbf{F} \cdot \mathbf{n}_z \cdot \mathbf{n} dS - \int_{V_z} \frac{\partial p}{\partial z} dV, \quad (27)$$

$$= \int_{S_z} (\mathbf{F} \cdot \mathbf{n}_z - p \mathbf{n}_z) \cdot \mathbf{n} dS \quad (28)$$

Here the s, x, y, and z subscripts indicate the scalar, x-staggered, y-staggered and z-staggered control volumes, respectively. Taking the time-derivative of (22) we obtain

$$\int_{V_s} \frac{\partial^2 \rho}{\partial t^2} dV = - \int_{S_s} \frac{\partial \rho \mathbf{u}}{\partial t} \cdot \mathbf{n} dS \quad (29)$$

$$= - \int_{V_s} \nabla \cdot \frac{\partial \rho \mathbf{u}}{\partial t} dV. \quad (30)$$

Note that we cannot directly substitute (23), (25) and (27) since they apply on different volumes than (29) does. Thus, the discrete form of (29) is given as

$$[{}^{s_v} I {}^{s_v}] \left( \frac{\partial^2 \rho}{\partial t^2} \right) = - [{}^{s_v} I {}^{s_x}] [{}^{s_z} R {}^{x_v}] \left( \frac{\partial \rho u}{\partial t} \right) - [{}^{s_v} I {}^{s_y}] [{}^{s_z} R {}^{y_v}] \left( \frac{\partial \rho v}{\partial t} \right) - [{}^{s_v} I {}^{s_z}] [{}^{s_z} R {}^{z_v}] \left( \frac{\partial \rho w}{\partial t} \right) \quad (31)$$

#### 3.1 Spatial Discretization

We define  $G$ ,  $R$ , and  $I$  as gradient, interpolant, and integral operators, respectively. For a general operator,  $\mathcal{Q}$ ,  $[{}^a \mathcal{Q}^b]$  indicates that the operator consumes a field located at  $b$  and produces a field located at  $a$ . For example,

Superscripts indicate the precise type of operator. For example,  $[{}^{x_s} G {}^{s_v}]$  is a discrete gradient operator that operates on a scalar cell center field ( $s_v$ ) and produces a field at an x staggered surface field ( $x_s$ ), while  $[{}^{y_v} I {}^{y_v}]$  is

a volume integral operator on the  $y$ -staggered volume. Using this notation, we may write (23) and (26) as

$$[x_v I^{x_v}] \frac{\partial \rho u}{\partial t} = [x_v I^{x_x}] (F_{xx}) + [x_v I^{x_y}] (F_{yx}) + [x_v I^{x_z}] (F_{zx}) - [x_v I^{x_v}] [x_v R^{s_x}] [s_x G^{s_v}] (p), \quad (32)$$

$$= [x_v I^{x_x}] (F_{xx}) + [x_v I^{x_y}] (F_{yx}) + [x_v I^{x_z}] (F_{zx}) - [x_v I^{x_v}] [x_v R^{s_v}] (p), \quad (33)$$

$$[y_v I^{y_v}] \frac{\partial \rho v}{\partial t} = [y_v I^{y_x}] (F_{xy}) + [y_v I^{y_y}] (F_{yy}) + [y_v I^{y_z}] (F_{zy}) - [y_v I^{y_v}] [y_v R^{s_y}] [s_y G^{s_v}] (p), \quad (34)$$

$$= [y_v I^{y_x}] (F_{xy}) + [y_v I^{y_y}] (F_{yy}) + [y_v I^{y_z}] (F_{zy}) - [y_v I^{y_v}] [y_v R^{s_v}] (p), \quad (35)$$

$$[z_v I^{z_v}] \frac{\partial \rho w}{\partial t} = [z_v I^{z_x}] (F_{xz}) + [z_v I^{z_y}] (F_{yz}) + [z_v I^{z_z}] (F_{zz}) - [z_v I^{z_v}] [z_v R^{s_z}] [s_z G^{s_v}] (p), \quad (36)$$

$$= [z_v I^{z_x}] (F_{xz}) + [z_v I^{z_y}] (F_{yz}) + [z_v I^{z_z}] (F_{zz}) - [z_v I^{z_v}] [z_v R^{s_v}] (p). \quad (37)$$

Here we assume that  $p$  is located at scalar cell centers.

### 3.1.1 Discretization of $\mathbf{F}$

**The shear stress.** The shear stress,  $\tau$ , must be formed at momentum cell surfaces. In general we have

$$\tau_{ij} = -\mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \delta_{ij} \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k}.$$

If we are transporting  $\rho \mathbf{u}$ , then we must interpolate  $\rho$  to the momentum CV centers to obtain the velocity components,

$$(u^{x_v}) = \frac{(\rho u)}{[x_v R^{s_v}]} (\rho), \quad (38)$$

$$(v^{y_v}) = \frac{(\rho v)}{[y_v R^{s_v}]}, \quad (39)$$

$$(w^{z_v}) = \frac{(\rho w)}{[z_v R^{s_v}]}. \quad (40)$$

At this point, if we use one ghost cell for  $\rho$ ,  $\rho \mathbf{u}$ , and  $\mathbf{u}$ , then there is no valid ghost information remaining in  $(u^{x_v})$ ,  $(v^{y_v})$  and  $(w^{z_v})$ , and a ghost update (with associated BC updates) must be performed. I don't see a way around this.

Assuming that we have a velocity available at staggered cell centroids, the velocity gradients are formed at cell faces to form the stress components as

$$\begin{aligned} \tau_{xx} &= -2 [x_v R^{s_v}] (\mu) [x_v G^{x_v}] (u) \\ &\quad - \frac{2}{3} [x_v R^{s_v}] (\mu) ([x_v G^{x_v}] (u) + [x_v R^{y_v}] [y_v G^{y_v}] (v) + [x_v R^{z_v}] [z_v G^{z_v}] (w)), \\ \tau_{yx} &= -[x_v R^{s_v}] (\mu) ([x_v R^{y_v}] [y_v G^{y_v}] (v) + [x_v G^{x_v}] (u)), \\ \tau_{zx} &= -[x_v R^{s_v}] (\mu) ([x_v R^{z_v}] [z_v G^{z_v}] (w) + [x_v G^{x_v}] (u)). \end{aligned}$$

JCS: need to carefully go through the ghost information. I think that interpolating the density will result in not enough information to form velocity gradients. Also, we need to look at the result of interpolating the velocity

### gradients around...

The stress for the  $y$ - and  $z$ -momentum equations is obtained analogously. Note that in forming the stress tensor we chose to take gradients of the velocities at their natural locations. This requires a special gradient operator. There are alternatives such as  $[G^{y_v x_s}] (v^{y_v}) \approx [G^{x_v x_s}] [R^{y_v x_v}] (v^{y_v})$ .

**The advecting velocities.** We can obtain the advecting velocities by interpolating the staggered-cell velocities obtained from equations (41)-(43). However, we may also obtain them for each momentum cell by interpolating the momentum and density to the cell surface. For example, for the  $x$ -momentum equation we have

$$(u^{x_x}) = \frac{[^{x_x} R^{x_v}] ((\rho u) (\rho u))}{[^{x_x} R^{s_v}] (\rho)}, \quad (41)$$

$$(v^{x_y}) = \frac{[^{x_y} R^{y_v}] ((\rho v) (\rho v))}{[^{x_y} R^{s_v}] (\rho)}, \quad (42)$$

$$(w^{x_z}) = \frac{[^{x_z} R^{z_v}] ((\rho w) (\rho w))}{[^{x_z} R^{s_v}] (\rho)}. \quad (43)$$

This choice is more convenient since it does not require any explicit updates of ghost information to form the convective contribution to  $\mathbf{F}$ .

### 3.1.2 The Discrete Poisson Equation

**NOTE: I still need to rework this section a little bit.**

Here are a few possible discretization approaches for equation (6) and the  $\nabla p$  term in the momentum equations:

1.  $\nabla p$  is calculated at scalar faces so that  $\frac{\partial p}{\partial x}$  is given discretely as  $[^{s_x} G^{s_v}] (p)$ . Then the term in the momentum equation is  $[^{x_v} I^{x_v}] [^{x_v} R^{s_x}] [^{s_x} G^{s_v}] (p)$ . Substituting (32), (34) and (36) into (31), we find

$$\begin{aligned} [^{s_v} I^{s_v}] \left( \frac{\partial^2 \rho}{\partial t^2} \right) = & - [^{s_v} I^{s_x}] [^{s_x} R^{x_v}] [^{x_v} I^{x_x}] (F_{xx}) - [^{s_v} I^{s_x}] [^{s_x} R^{x_v}] [^{x_v} I^{x_y}] (F_{yx}) - [^{s_v} I^{s_x}] [^{s_x} R^{x_v}] [^{x_v} I^{x_z}] (F_{zx}) \\ & + [^{s_v} I^{s_x}] [^{s_x} R^{x_v}] [^{x_v} I^{x_v}] [^{x_v} R^{s_x}] [^{s_x} G^{s_v}] (p), \\ & - [^{s_v} I^{s_y}] [^{s_y} R^{y_v}] [^{y_v} I^{y_x}] (F_{xy}) - [^{s_v} I^{s_y}] [^{s_y} R^{y_v}] [^{y_v} I^{y_y}] (F_{yy}) - [^{s_v} I^{s_y}] [^{s_y} R^{y_v}] [^{y_v} I^{y_z}] (F_{zy}) \\ & + [^{s_v} I^{s_y}] [^{s_y} R^{y_v}] [^{y_v} I^{y_v}] [^{y_v} R^{s_y}] [^{s_y} G^{s_v}] (p) \\ & - [^{s_v} I^{s_z}] [^{s_z} R^{z_v}] [^{z_v} I^{z_x}] (F_{xz}) - [^{s_v} I^{s_z}] [^{s_z} R^{z_v}] [^{z_v} I^{z_y}] (F_{yz}) - [^{s_v} I^{s_z}] [^{s_z} R^{z_v}] [^{z_v} I^{z_z}] (F_{zz}) \\ & + [^{s_v} I^{s_z}] [^{s_z} R^{z_v}] [^{z_v} I^{z_v}] [^{z_v} R^{s_z}] [^{s_z} G^{s_v}] (p). \end{aligned} \quad (44)$$

Combining the terms on  $p$  and rearranging,

$$\begin{aligned} \left[ \begin{array}{c} [s_v I^{s_x}] [s_z R^{x_v}] [x_v I^{x_v}] [x_v R^{s_x}] [s_x G^{s_v}] + \\ [s_v I^{s_y}] [s_z R^{y_v}] [y_v I^{y_v}] [y_v R^{s_y}] [s_y G^{s_v}] + \\ [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_v}] [z_v R^{s_z}] [s_z G^{s_v}] \end{array} \right] (p) &= [s_v I^{s_v}] \left( \frac{\partial^2 \rho}{\partial t^2} \right) \\ &+ [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_x}] (F_{xx}) + [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_y}] (F_{yx}) + [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_z}] (F_{zx}) \\ &+ [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_x}] (F_{xy}) + [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_y}] (F_{yy}) + [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_z}] (F_{zy}) \\ &+ [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_x}] (F_{xz}) + [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_y}] (F_{yz}) + [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_z}] (F_{zz}) \end{aligned}$$

Note that in the case where we have a uniform mesh,  $[x_v R^{s_x}]$ ,  $[s_x R^{x_v}]$  and their corresponding  $y$  and  $z$  operators are all identity operators. For stretched meshes, however, these are not identity operators and will affect ghost cell availability.

2.  $\nabla p$  is calculated at momentum volumes so that  $\frac{\partial p}{\partial x}$  is given discretely as  $[x_v G^{s_v}] (p)$ . The pressure term in the momentum equations is thus  $[x_v I^{x_v}] [x_v G^{s_v}] (p)$ . Substituting (32), (34) and (36) into (31), we find

$$\begin{aligned} [s_v I^{s_v}] \left( \frac{\partial^2 \rho}{\partial t^2} \right) &= - [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_x}] (F_{xx}) - [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_y}] (F_{yx}) - [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_z}] (F_{zx}) \\ &+ [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_v}] [x_v G^{s_v}] (p) \\ &- [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_x}] (F_{xy}) - [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_y}] (F_{yy}) - [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_z}] (F_{zy}) \\ &+ [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_v}] [y_v G^{s_v}] (p) \\ &- [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_x}] (F_{xz}) - [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_y}] (F_{yz}) - [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_z}] (F_{zz}) \\ &+ [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_v}] [z_v G^{s_v}] (p). \end{aligned} \quad (46)$$

Note that this is very similar to (44) but the pressure gradient is calculated differently, eliminating the requirement for an extra interpolant.

$$\begin{aligned} \left[ \begin{array}{c} [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_v}] [x_v G^{s_v}] + \\ [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_v}] [y_v G^{s_v}] + \\ [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_v}] [z_v G^{s_v}] \end{array} \right] (p) &= [s_v I^{s_v}] \left( \frac{\partial^2 \rho}{\partial t^2} \right) \\ &+ [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_x}] (F_{xx}) + [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_y}] (F_{yx}) + [s_v I^{s_x}] [s_x R^{x_v}] [x_v I^{x_z}] (F_{zx}) \\ &+ [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_x}] (F_{xy}) + [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_y}] (F_{yy}) + [s_v I^{s_y}] [s_y R^{y_v}] [y_v I^{y_z}] (F_{zy}) \\ &+ [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_x}] (F_{xz}) + [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_y}] (F_{yz}) + [s_v I^{s_z}] [s_z R^{z_v}] [z_v I^{z_z}] (F_{zz}) \end{aligned}$$

As previously, in the case of a uniform mesh,  $[s_x R^{x_v}]$  and the corresponding  $y$  and  $z$  direction operators are identity operators.

3. If we treat the pressure term in the momentum equations as a surface integral as in (33), (35) and (37), then we have variants of (45) and (47).

**Boundary conditions on the pressure Poisson system.** There is a subtle issue regarding  $(F)$ . If it is formed from fields with a single ghost cell, it will require a ghost update prior to its use in forming the Poisson equation.

However, it is not clear what boundary conditions should be used for this term. Therefore, we choose to apply conditions on the pressure (or its gradient) instead. James: perhaps the BC paper can shed some light on this.

### 3.2 Time Integration

Assume we transport a set of scalars  $\eta_i$  in one of two forms:

$$\begin{aligned}\frac{\partial \rho \eta_i}{\partial t} &= -\nabla \cdot (\rho \eta_i) - \nabla \cdot \mathbf{j}_{\eta_i} + s_{\eta_i}, \\ \frac{\partial \eta_i}{\partial t} &= -\frac{\mathbf{u}}{\rho} \cdot \nabla \eta - \frac{1}{\rho} \nabla \cdot \mathbf{j}_{\eta_i} + \frac{1}{\rho} s_{\eta_i}.\end{aligned}$$

At time level  $n$ , we assume that  $\rho^n$ ,  $(\rho \mathbf{u})^n$ , and the scalars  $(\rho \eta_i)^n$  (or  $\eta_i^n$ ) are known. Additionally, we have a state relationship  $\rho = \mathcal{G}(\eta_i)$ . Given this, an explicit time-integration scheme may look like:

1. Calculate  $\mathbf{F}$  as discussed in §3.1.1.
2. Estimate  $\frac{\partial^2 \rho}{\partial t^2}$ . Could do this by setting

$$\left(\frac{\partial^2 \rho}{\partial t^2}\right)^n \approx \frac{-\nabla \cdot (\rho \mathbf{u}) - \left(\frac{\partial \rho}{\partial t}\right)^n}{\Delta t},$$

which would require storage of  $\frac{\partial \rho}{\partial t}$ , and implies

$$\left(\frac{\partial \rho}{\partial t}\right)^{n+1} \approx -\nabla \cdot (\rho \mathbf{u})^n.$$

Alternatively, we could use backward-difference expansions on  $\rho$ .

3. Calculate  $p$  from one of the Poisson equations described in §3.1.2.
4. Calculate the full RHS of the momentum equations as  $\frac{\partial \rho \mathbf{u}}{\partial t} = \mathbf{F} - \nabla p$ .
5. Calculate the RHS of the equations for  $\eta_i$ .
6. Find  $\rho^{n+1}$ ,  $(\rho \mathbf{u})^{n+1}$ ,  $(\rho \eta_i)^{n+1}$  (or  $\eta_i^{n+1}$ ).
  - (a) If we are transporting  $\eta_i$  then find  $\eta_i^{n+1}$  and calculate  $\rho^{n+1} = \mathcal{G}(\eta_i^{n+1})$ ?
  - (b) If we are transporting  $(\rho \eta_i)$  find  $(\rho \eta_i)^{n+1}$  and then find  $\rho^{n+1}$  and  $\eta_i^{n+1}$  by solving the nonlinear system

$$\begin{aligned}\rho &= \mathcal{G}(\eta_i) \\ \rho \eta_i &= \rho \cdot \eta_i\end{aligned}$$

for  $\rho^{n+1}$  and  $\eta_i^{n+1}$ .



(c) Check to see if

$$\sum_{i=1}^{n_\eta} \frac{\partial \eta_i}{\partial t} \frac{\partial \rho}{\partial \eta_i} \stackrel{?}{=} -\nabla \cdot (\rho \mathbf{u}).$$

7. Set  $n + 1 \rightarrow n$  and return to step 1.