Contents

1 Overview

Developing the CFD tool was a little more intense than I thought it would be. I developed something similar for my job but I tried to be more general here so that one could insert a geometry and have the tool solve for the flow field. I ended up only implementing geometries that were symmetrical and haven't implemented a 2D CFD approach yet. Looking back, I would also like to try out dual time stepping instead of my iterative solver. It would be interesting to see how the two compare in terms of accuracy and computational time.

Ideally, I would develop a real gas tool and introduce chemical kinetics to simulate chemical reactions and reacting flows. This would involve introducing kinetics and species conservation as well which would be a little more involved. I will need to come back to this eventually.

2 General conservation equations

We will derive the conservation equations for the general 3D case. In the next section, we will look at the 1D case which we used to build the model for the examples above. We conduct our derivations assuming we are looking at a control volume in space that is not moving with the fluid so we have fluid moving in and out of our control volume. Compare this to deriving the equation by following a fluid parcel as it moves through space.

We can start with the general conservation equations, and make simplifications after understanding the general case. Looking at the general case allows us to get comfortable with the equations and the terms and how to translate a physical process into mathematical relations. We will take the infinitesimal volume approach and consider our reference frame to be stationary with respect to the fluid (e.g., control volume is not traveling with a fluid parcel but our reference frame is such that the fluid is passing through the our control volume). First, we look at the conservation of mass.

2.1 Conservation of mass

With the conservation of mass, we have that the change of mass in the control volume is equal to the sum of the mass entering the control volume minus the sum of the mass exiting the control volume as shown in Figure 1.

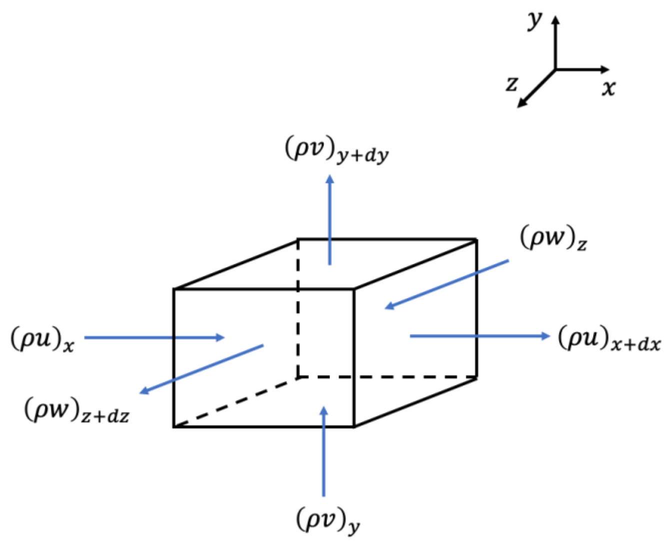

Figure 1: Conservation of mass.

We can write this as a differential equation where we have:

$$change\ of\ mass\ in\ volume\ = mass\ in\ -\ mass\ out$$

Mathematically, this becomes:

$$\frac{\partial(\rho dV)}{\partial t} = [(\rho u)_x - (\rho u)_{x+dx}]dydz +$$

$$[(\rho v)_y - (\rho v)_{y+dy}]dxdz + [(\rho w)_z - (\rho w)_{z+dz}]dxdy$$

Expanding $(\rho u)_{x+dx}$ as a Taylor series gives:

$$(\rho u)_{x+dx} = (\rho u)_x + \frac{\partial(\rho u)_x}{\partial x}dx + \cdots$$

Using only the first two terms on the RHS and plugging into the first equation (using same approach for other components) and simplifying, obtain:

$$\frac{\partial \rho}{\partial t}dxdydz = -\frac{\partial(\rho u)}{\partial x}dxdydz - \frac{\partial(\rho v)}{\partial y}dxdydz - \frac{\partial(\rho w)}{\partial z}dxdydz$$

Simplifying even more:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho u)}{\partial x} - \frac{\partial(\rho v)}{\partial y} - \frac{\partial(\rho w)}{\partial z}$$

Differential form of conservation of mass:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \bar{U})$$

where $\bar{U} = (u, v, w)$

Integral form:

$$\int_V \frac{\partial \rho}{\partial t} dV = -\int_V \nabla \cdot (\rho \bar{U}) dV = \frac{\partial}{\partial t}\int_V \rho dV = -\int_S (\rho \bar{U}) \cdot \hat{n}\, dS$$

where $\hat{n}$ is a unit vector pointing away from the surface element

2.2 Conservation of momentum

Next, we can look at the conservation of momentum. We'll only focus on momentum in the x direction but the results are identical for momentum in the y and z directions. Momentum conservation in the x direction is shown in Figure 2.

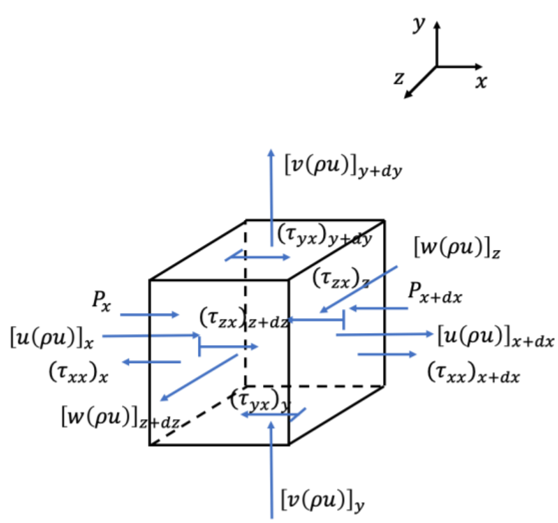

Figure 2: Conservation of momentum.

As explained above, we will focus on momentum in the x direction to simplify the explanation. We have that the change of momentum in the control volume in the x direction is equal to the sum of momentum entering and exiting the control volume in the x direction plus the sum of the body and surface forces. Body forces include pressure and any others (such as gravity but we ignore gravity here). Surface forces are mostly viscous forces (e.g., friction)

We can write this as a differential equation where we have:

$$
\begin{aligned}
&\mathit{change\ of\ momentum\ in\ the\ x\ direction}\\
&\qquad = (\mathit{momentum\ in} - \mathit{momentum\ out})x\\
&\qquad + \mathit{sum\ of\ body\ forces}\ (\mathit{in\ x\ direction})\ \mathit{and\ sum\ of\ viscous\ forces}\ (\mathit{in\ x\ direction})
\end{aligned}
$$

This then becomes (only looking in x direction):

$$
\frac{\partial(\rho u dV)}{\partial t} = \{[u(\rho u)]_x - [u(\rho u)]_{x+dx}\}dydz +
$$

$$
\{[v(\rho u)]_y - [v(\rho u)]_{y+dy}\}dxdz + \{[w(\rho u)]_z - [w(\rho u)]_{z+dz}\}dxdy +
$$

$$
[(\tau_{xx})_{x+dx} - (\tau_{xx})_x]dydz + [(\tau_{yx})_{y+dy} - (\tau_{yx})_y]dxdz +
$$

$$
+[(\tau_{zx})_{z+dz} - (\tau_{zx})_z]dxdy + (P_x - P_{x+dx})dydyz
$$

Expanding terms using Taylor series and simplifying:

$$
\frac{\partial(\rho u)}{\partial t} = -\frac{\partial}{\partial x}[u(\rho u)] -
$$

$$
\frac{\partial}{\partial y}[v(\rho u)] - \frac{\partial}{\partial z}[w(\rho u)] +
$$

$$
\frac{\partial}{\partial x}\tau_{xx} + \frac{\partial}{\partial y}\tau_{yx} + \frac{\partial}{\partial z}\tau_{zx} - \frac{\partial}{\partial x}P
$$

Differential form of conservation of momentum in x direction:

$$
\frac{\partial(\rho u)}{\partial t} = -\frac{\partial}{\partial x}[u(\rho u)] - \frac{\partial}{\partial y}[v(\rho u)] - \frac{\partial}{\partial z}[w(\rho u)] + \frac{\partial}{\partial x}\tau_{xx} + \frac{\partial}{\partial y}\tau_{yx} + \frac{\partial}{\partial z}\tau_{zx} - \frac{\partial}{\partial x}P
$$

$$
\frac{\partial(\rho u)}{\partial t} = -\nabla\cdot(\rho u\overline{U}) + \frac{\partial}{\partial x}\tau_{xx} + \frac{\partial}{\partial y}\tau_{yx} + \frac{\partial}{\partial z}\tau_{zx} - \frac{\partial}{\partial x}P
$$

Similarly for y and z directions:

$$
\frac{\partial(\rho v)}{\partial t} = -\nabla\cdot(\rho v\overline{U}) + \frac{\partial}{\partial x}\tau_{xy} + \frac{\partial}{\partial y}\tau_{yy} + \frac{\partial}{\partial z}\tau_{zy} - \frac{\partial}{\partial y}P
$$

$$
\frac{\partial(\rho w)}{\partial t} = -\nabla\cdot(\rho w\overline{U}) + \frac{\partial}{\partial x}\tau_{xz} + \frac{\partial}{\partial y}\tau_{yz} + \frac{\partial}{\partial z}\tau_{zz} - \frac{\partial}{\partial z}P
$$

We note that momentum has a direction and for each equation above, we should denote a direction. We can simplify the above equations to have:

$$
\frac{\partial(\rho u)}{\partial t} = -\nabla\cdot(\rho u\overline{U}) + \nabla\cdot\sigma_{x} - \frac{\partial}{\partial x}P
$$

$$
\frac{\partial(\rho v)}{\partial t} = -\nabla\cdot(\rho v\overline{U}) + \nabla\cdot\sigma_{y} - \frac{\partial}{\partial y}P
$$

$$
\frac{\partial(\rho w)}{\partial t} = -\nabla\cdot(\rho w\overline{U}) + \nabla\cdot\sigma_{z} - \frac{\partial}{\partial z}P
$$

In the above, $\sigma_x = (\tau_{xx}, \tau_{yx}, \tau_{zx}), \sigma_y = (\tau_{xy}, \tau_{yy}, \tau_{zy}), \sigma_z = (\tau_{xz}, \tau_{yz}, \tau_{zz})$. The above are the differential form of the momentum equation in each direction.

To obtain the integral form, we integrate around our volume (only showing the x direction case first):

$$\int_V \frac{\partial(\rho u)}{\partial t} dV = -\int_V \nabla \cdot (\rho u \bar{U})\, dV + \int_V (\nabla \cdot \sigma_x)\, dV - \int_V \frac{\partial P}{\partial x} dV$$

We can use the divergence theorem on the first two terms on the RHS to obtain:

$$\int_V \frac{\partial(\rho u)}{\partial t} dV = -\int_S (\rho u \bar{U} \cdot \hat{n})\, dS + \int_S (\sigma_x \cdot \hat{n})\, dS - \int_V \frac{\partial P}{\partial x} dV$$

We can do this for the other directions as well and we obtain:

$$x\ direction\colon \int_V \frac{\partial(\rho u)}{\partial t} dV = -\int_S (\rho u \bar{U} \cdot \hat{n})\, dS + \int_S (\sigma_x \cdot \hat{n})\, dS - \int_V \frac{\partial P}{\partial x} dV$$

$$y\ direction\colon \int_V \frac{\partial(\rho v)}{\partial t} dV = -\int_S (\rho v \bar{U} \cdot \hat{n})\, dS + \int_S \left(\sigma_y \cdot \hat{n}\right) dS - \int_V \frac{\partial P}{\partial y} dV$$

$$z\ direction\colon \int_V \frac{\partial(\rho w)}{\partial t} dV = -\int_S (\rho w \bar{U} \cdot \hat{n})\, dS + \int_S (\sigma_z \cdot \hat{n})\, dS - \int_V \frac{\partial P}{\partial z} dV$$

Summing all of these gives:

$$\begin{aligned}\int_V \frac{\partial(\rho u + \rho v + \rho w)}{\partial t} dV \\ &= -\int_S (\rho u \bar{U} \cdot \hat{n} + \rho v \bar{U} \cdot \hat{n} + \rho w \bar{U} \cdot \hat{n})\, dS + \int_S \left(\sigma_x \cdot \hat{n} + \sigma_y \cdot \hat{n} + \sigma_z \cdot \hat{n}\right) dS \\ &\quad - \int_V \left(\frac{\partial P}{\partial x} + \frac{\partial P}{\partial y} + \frac{\partial P}{\partial z}\right) dV\end{aligned}$$

This can be simplified to give our integral form:

$$\int_V \frac{\partial(\rho \bar{U})}{\partial t} dV = -\int_S [\rho \bar{U}(\bar{U} \cdot \hat{n})]\, dS + \int_S (\bar{\sigma}\hat{n})\, dS - \int_V \nabla P\, dV$$

$$\int_V \frac{\partial(\rho \bar{U})}{\partial t} dV = -\int_S [\rho \bar{U}(\bar{U} \cdot \hat{n})]\, dS + \int_S (\bar{\sigma}\hat{n})\, dS - \int_S P\hat{n}\, ds$$

Here, $\bar{\sigma}$ is a matrix representing our viscous forces:

$$\bar{\sigma} = \begin{bmatrix} \tau_{xx} & \tau_{yx} & \tau_{zx} \\ \tau_{xy} & \tau_{yy} & \tau_{zy} \\ \tau_{xz} & \tau_{yz} & \tau_{zz} \end{bmatrix}$$

It's implied but we assume that our velocity vector is a column vector in this analysis. The complete momentum equation should include gravity and other body/surface forces but we neglect these in the derivation as we won't use them in the model.

2.3 Conservation of energy

Next, we can look at the conservation of energy. Energy doesn't have a direction but for body forces, our assumptions on the directions influences if the work done on the control volume is positive or negative.

For the conservation of energy, we have that the change of energy in the control volume is equal to the sum of the energy entering and leaving the control volume plus the net rate of energy done on the control volume.

The sum of energy entering and leaving is fairly simple. This is similar to the conservation of mass where we have some energy entering the control volume and some leaving. This can also include heat transfer (e.g., conduction captured in the q" term).

The net rate of energy done on the control volume can be a little trickier. We will focus on the work done from pressure and the shear force. We assume that the pressure at x is acting in the positive x direction.

The pressure at x+dx is acting in the negative x direction. This leads to the work being done by the pressure at x being positive (work done on the control volume). The work from the pressure at x+dx is negative (work done by the control volume). For the viscous stress, we assume that velocity increases in the positive x, y, and z directions. This means we assume that the velocity in the x direction at y+dy is greater than y. This means that the fluid at y+dy is trying to pull the fluid in the control volume in the x direction. The velocity in the x direction at y is less so this fluid is trying to pull the fluid in the -y direction. In this way, the work done by the viscous stress in the x direction at y+dy is positive (see (u*tau)_(yx) in the figure) compared to the viscous stress at y. We again only show forces and flow in the x direction for simplicity but one can expand what we said above to all directions. This is shown in Figure 3.

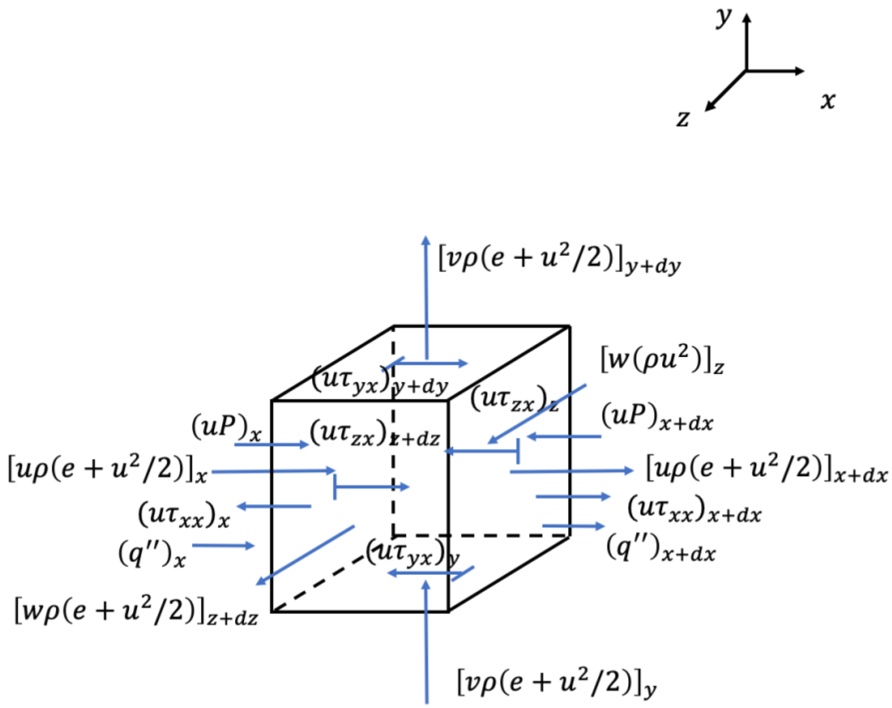

Figure 3: Conservation of energy.

We can write this as a differential equation where we have:

$$\begin{aligned}&\textit{change of energy against time}\\&= (\textit{energy in} - \textit{energy out}) + \textit{sum of work done against control volume}\\&+ \textit{any other heat sources within control volume} \ (\textit{we neglect heat sources but they can occur in nature})\end{aligned}$$

This becomes:

Change of energy = flow of energy in – flow of energy out + rate of energy on volume element

Change of energy:

$$\frac{\partial\left[\rho\left(e+\frac{|\bar{U}|^2}{2}\right)dV\right]}{\partial t}=\frac{\partial\left[\rho\left(e+\frac{|\bar{U}|^2}{2}\right)\right]}{\partial t}dV$$

Flow of energy in – flow of energy out:

$$
\begin{aligned}
&= \left\{\left[u\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]_x - \left[u\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]_{x+dx}\right\}dydz \\
&\quad + \left\{\left[v\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]_y - \left[v\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]_{y+dy}\right\}dxdz \\
&\quad + \left\{\left[w\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]_z - \left[w\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]_{z+dz}\right\}dxdy \\
&\quad = -\frac{\partial}{\partial x}\left[u\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]dxdydz - \frac{\partial}{\partial y}\left[v\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]dxdydz \\
&\quad - \frac{\partial}{\partial z}\left[w\rho\left(e+\frac{u^2}{2}+\frac{v^2}{2}+\frac{w^2}{2}\right)\right]dxdydz = -\nabla\cdot\bar{U}\rho\left(e+\frac{u^2+v^2+w^2}{2}\right)dxdydz
\end{aligned}
$$

Change of energy = flow of energy in – flow of energy out + rate of energy on volume element

Rate of energy by forces:

$$
\begin{aligned}
&\left\{\left[u\tau_{xx}+v\tau_{xy}+w\tau_{xz}-uP\right]_{x+dx} - \left[u\tau_{xx}+v\tau_{xy}+w\tau_{xz}-uP\right]_x\right\}dydz \\
&\quad + \left\{\left[u\tau_{yx}+v\tau_{yy}+w\tau_{yz}-vP\right]_{y+dy} - \left[u\tau_{yx}+v\tau_{yy}+w\tau_{yz}-vP\right]_y\right\}dxdz \\
&\quad + \left\{\left[u\tau_{zx}+v\tau_{zy}+w\tau_{zz}-wP\right]_{z+dz} - \left[u\tau_{zx}+v\tau_{zy}+w\tau_{zz}-wP\right]_z\right\}dxdy \\
&\quad = \frac{\partial}{\partial x}\left[u\tau_{xx}+v\tau_{xy}+w\tau_{xz}-uP\right]dxdydz + \frac{\partial}{\partial y}\left[u\tau_{yx}+v\tau_{yy}+w\tau_{yz}-vP\right]dxdydz \\
&\quad + \frac{\partial}{\partial z}\left[u\tau_{zx}+v\tau_{zy}+w\tau_{zz}-wP\right]dxdydz = \nabla\cdot\bar{\sigma}^T\bar{U}dV - \nabla\cdot\bar{U}P\,dV
\end{aligned}
$$

Heat transfer:

$$
(q_x - q_{x+dx})dydz + \left(q_y - q_{y+dy}\right)dxdz + (q_z - q_{z+dz})dydz
$$

$$
= -\frac{\partial q_x}{\partial x}dxdydyz - \frac{\partial q_y}{\partial y}dxdydyz - \frac{\partial q_z}{\partial z}dxdydyz = -\nabla\cdot\bar{q}dV
$$

where $\bar{q} = \left(q_x, q_y, q_z\right)$ and $q_x = -k\frac{\partial T}{\partial x}$ (and similar for other components):

$$
-\nabla\cdot\bar{q}dV = \nabla\cdot(k\nabla T)dV
$$

Differential form of conservation of energy:

$$
\frac{\partial\left[\rho\left(e+\frac{|\bar{U}|^2}{2}\right)\right]}{\partial t} = -\nabla\cdot\left[\bar{U}\rho\left(e+\frac{|\bar{U}|^2}{2}\right)\right] + \nabla\cdot\bar{\sigma}^T\bar{U}dV - \nabla\cdot\bar{U}P\,dV + \nabla\cdot(k\nabla T)
$$

Integral form:

$$
\int_V \frac{\partial\left[\rho\left(e+\frac{|\bar{U}|^2}{2}\right)\right]}{\partial t}dV = \int_V\left\{-\nabla\cdot(\rho e\bar{U}) - \nabla\cdot\left[\bar{U}\rho\left(\frac{|\bar{U}|^2}{2}\right)\right] + \nabla\cdot\bar{\sigma}^T\bar{U}dV - \nabla\cdot\bar{U}P\,dV + \nabla\cdot(k\nabla T)\right\}dV
$$

$$
\int_V \frac{\partial\left[\rho\left(e+\frac{|\bar{U}|^2}{2}\right)\right]}{\partial t}dV = \int_S\left[\left(-\rho e\bar{U} - \bar{U}\rho\left(\frac{|\bar{U}|^2}{2}\right) + \bar{\sigma}^T\bar{U} - \bar{U}P + k\nabla T\right)\cdot\hat{n}\right]dS
$$

I use the differential form for the derivation. We'll see below but I also use the differential form for implementing the 1D conservation equations in the model. The integral form has some advantages (e.g., easier to handle complex geometries, easier to capture discontinuities, more flexibility with numerical techniques) when implementing the equations into a model but we will focus on the differential form for now. I find that the differential form is a little easier to understand and derive.

The integral method will be re-visited when we go 2D (but that has not been implemented yet)

3 1D equations

The examples above are based on a 1D approach that will be explained here. In our general conservation equation derivations, we assumed that the area (dy*dz) when looking in the x direction was constant across the cell. For our 1D model to handle changes in area (symmetrical changes), we need to slightly modify our equations to look at this.

We will follow the same outline as above, first looking at the conservation of mass then momentum then energy. The next section will talk briefly about boundary conditions and the section after that, about how the 1D conservation equations we derive here are solved numerically. We will only look at the differential form in this section

3.1 Conservation of mass

First, we look at the conservation of mass. We see that it is quite similar to the conservation of mass schematic we used in the general section above as shown in Figure 4.

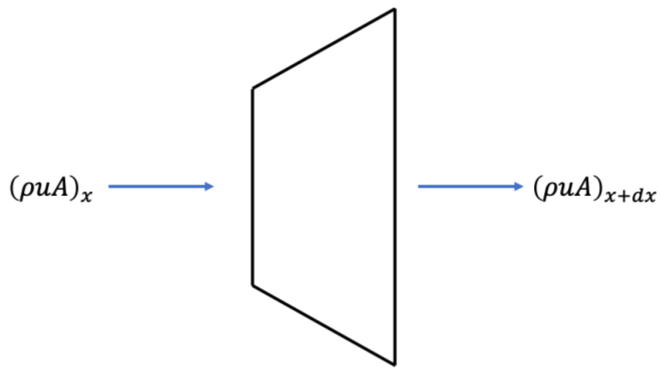

Figure 4: Conservation of mass (1D).

We note that the area is different at the inlet compared to the outlet but we still have:

$$\textit{change of mass in CV} = \textit{mass in} - \textit{mass out}$$

Note that the area is larger at the outlet than the inlet. We could have drawn the schematic with the inlet larger than the outlet and we would get the same result. It will be important to pay attention to this since assumptions on the area change are important in the derivation, particularly in the momentum and energy equations.

Change in mass = mass in – mass out becomes:

$$\frac{\partial(\rho dV)}{\partial t} = (\rho u A)_x - (\rho u A)_{x+dx}$$

$$\frac{\partial(\rho A dx)}{\partial t} = \frac{\partial(\rho A)}{\partial t} dx = -\frac{\partial(\rho u A)}{\partial x} dx$$

$$\frac{\partial(\rho A)}{\partial t} = A\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho u A)}{\partial x}$$

Differential form:

$$\frac{\partial \rho}{\partial t} = -\frac{1}{A}\frac{\partial(\rho u A)}{\partial x}$$

3.2 Conservation of momentum

Next, we look at the conservation of momentum. We note again that it is fairly similar to the general form we had above and it follows the same idea:

$$
\begin{aligned}
&change\ of\ momentum\ in\ the\ x\ direction \\
&\qquad = (momentum\ in\ -\ momentum\ out)x \\
&\qquad + sum\ of\ body\ forces\ (in\ x\ direction)\ and\ sum\ of\ viscous\ forces\ (in\ x\ direction)
\end{aligned}
$$

We do have new body forces due to the change in area compared to the general case above as shown in Figure 5.

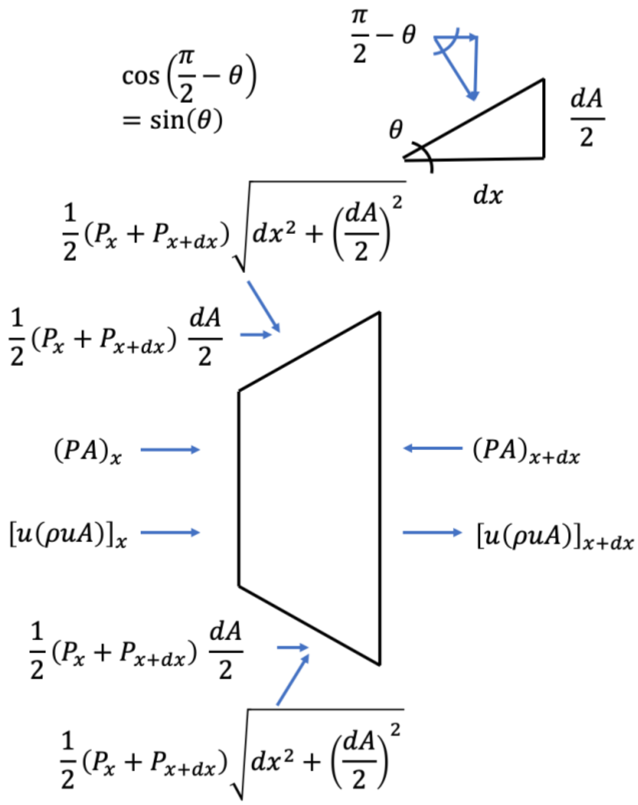

Figure 5: Conservation of momentum (1D).

We say that the pressure on this face (slanted face due to the change in area) is the average of the inlet and outlet pressures as shown. This force is acting against the face and we can see that the force from the pressure will be perpendicular to that face. From the symmetry, we see that the forces in the y direction from the top and bottom face will cancel. The force in the x direction is new and we have one part from the top face and a second from the bottom face. From the geometry, we know that the x component is F * cos(pi/2-theta) where cos(pi/2-theta) = sin(theta) and sin(theta) = dA/2 / sqrt(dx^2+(dA/2)^2). We note that our dA is assumed positive so we add this pressure force in the x direction. If we assumed dA was negative, we would be subtracting and also have -dA so we would get the same result.

We have:

Change of momentum = flow of momentum in – flow of momentum out + sum of body and surface forces

*neglecting viscous forces

$$\frac{\partial(\rho u dV)}{\partial t} = \{[u(\rho uA)]_x - [u(\rho uA)]_{x+dx}\}$$

$$+[(PA)_x - (PA)_{x+dx}] + 2\frac{1}{2}(P_x + P_{x+dx})\frac{dA}{2}$$

$$\frac{\partial(\rho u dV)}{\partial t} = -\frac{\partial[u(\rho uA)]}{\partial x}dx - \frac{\partial(PA)}{\partial x}dx + PdA + \frac{1}{2}\frac{\partial P}{\partial x}dxdA$$

$$\frac{\partial(\rho u dV)}{\partial t} = \frac{\partial(\rho u A dx)}{\partial t} = -\frac{\partial[u(\rho u A)]}{\partial x}dx - \frac{\partial(PA)}{\partial x}dx + PdA + \frac{1}{2}\frac{\partial P}{\partial x}dxdA$$

We can neglect the last term on the RHS since we have $dxdA$ which we can say is small compared to the other terms but we will keep it for now:

$$\frac{\partial(\rho u A)}{\partial t} = -\frac{\partial[u(\rho u A)]}{\partial x} - \frac{\partial(PA)}{\partial x} + P\frac{dA}{dx} + \frac{1}{2}\frac{\partial P}{\partial x}dA$$

Differential form:

$$\frac{\partial(\rho u)}{\partial t} = -\frac{1}{A}\frac{\partial[u(\rho u A)]}{\partial x} - \frac{1}{A}\frac{\partial(PA)}{\partial x} + P\frac{1}{A}\frac{dA}{dx} + \frac{1}{2}\frac{\partial P}{\partial x}\frac{1}{A}dA$$

$$\frac{\partial(\rho u)}{\partial t} = -\frac{1}{A}\frac{\partial[u(\rho u A)]}{\partial x} - \frac{1}{A}\frac{\partial(PA)}{\partial x} + P\frac{1}{A}\frac{dA}{dx} + \frac{1}{2}\frac{\partial P}{\partial x}dln(A)$$

3.3 Conservation of energy

We look at the conservation of energy next. We again follow the same general procedure as for the general case:

$$\begin{aligned}&\mathit{change\ of\ energy\ against\ time}\\&= (\mathit{energy\ in} - \mathit{energy\ out}) + \mathit{sum\ of\ work\ done\ against\ control\ volume}\\&+ \mathit{any\ other\ heat\ sources\ within\ control\ volume}\ (\mathit{we\ neglect\ heat\ sources\ but\ they\ can\ occur\ in\ nature})\end{aligned}$$

We show our schematic in Figure 6.

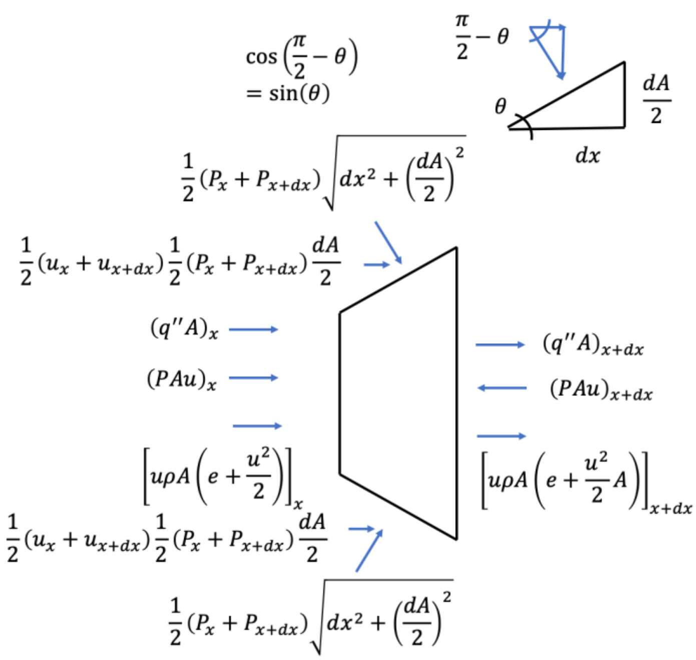

Figure 6: Conservation of energy (1D).

We show in the schematic our new force on the slanted face that we found in the momentum section above for the 1D case. We have to be careful with our new pressure force since no flow is actually going across the boundary so no work is being done. We still want to include the x component of our new pressure force and the average velocity to capture the extra work from our non-symmetrical geometry.

We have:

Change of energy = flow of energy in – flow of energy out + rate of energy on volume element

$$\frac{\partial\left[\rho\left(e+\frac{u^2}{2}\right)dV\right]}{\partial t}$$
$$=\left\{\left[u\rho A\left(e+\frac{u^2}{2}\right)\right]_x-\left[u\rho A\left(e+\frac{u^2}{2}\right)\right]_{x+dx}\right\}$$
$$+[(PAu)_x-(PAu)_{x+dx}]+[(q''A)_x-(q''A)_{x+dx}]$$
$$+\left(u+\frac{du}{2}\right)\left(P+\frac{dP}{2}\right)dA$$

$$\frac{\partial\left[\rho\left(e+\frac{u^2}{2}\right)dV\right]}{\partial t}=\left\{\left[u\rho A\left(e+\frac{u^2}{2}\right)\right]_x-\left[u\rho A\left(e+\frac{u^2}{2}\right)\right]_{x+dx}\right\}$$
$$+[(PAu)_x-(PAu)_{x+dx}]+[(q''A)_x-(q''A)_{x+dx}]+\left(u+\frac{du}{2}\right)\left(P+\frac{dP}{2}\right)dA$$

$$\frac{\partial\left[\rho\left(e+\frac{u^2}{2}\right)Adx\right]}{\partial t}=-\frac{\partial\left[u\rho A\left(e+\frac{u^2}{2}\right)\right]}{\partial x}dx-\frac{\partial(PAu)}{\partial x}dx-\frac{\partial(q''A)}{\partial x}dx+\left(u+\frac{du}{2}\right)\left(P+\frac{dP}{2}\right)dA$$

Differential form:

$$\frac{\partial\left[\rho\left(e+\frac{u^2}{2}\right)\right]}{\partial t}=-\frac{1}{A}\frac{\partial\left[u\rho A\left(e+\frac{u^2}{2}\right)\right]}{\partial x}-\frac{1}{A}\frac{\partial(PAu)}{\partial x}-\frac{1}{A}\frac{\partial(q''A)}{\partial x}+\frac{1}{A}\left(u+\frac{du}{2}\right)\left(P+\frac{dP}{2}\right)\frac{dA}{dx}$$

We now have our differential form conservation equations for the 1D case with a changing area (symmetric change). In the next section, we will talk about the boundary conditions and then in the section after that, talk about how we implement the equations and solve them numerically.

4 Boundary conditions

Handling boundary conditions is easier for the 1D case compared to 2D or even 3D. The full list of boundary conditions to handle is:

- Inlet conditions
- Outlet conditions
- Wall conditions (flow and thermal/temperature)
    - Flow: no slip (velocity equal to 0) or no flow through boundary (V*n=0 where V is velocity vector, n is unit vector perpendicular to surface)
    - Thermal/temperature: Constant temperature at wall or heat flux (this could vary)

We will only consider the inlet and outlet conditions. When we go to 2D, we will have to consider the wall boundary conditions. We simplify our approach to the inlet conditions and only allow specifying pressure and temperature (and velocity if the flow is sonic or supersonic). Specifying pressure and temperature is similar to having a constant air supply at some conditions (e.g., ambient temperature at elevated pressure).

Similarly, at the outlet, we only specify pressure (if the flow is subsonic at the outlet).

The following schematic (Figure 7) illustrates what we specify according to the Mach number at the inlet or outlet:

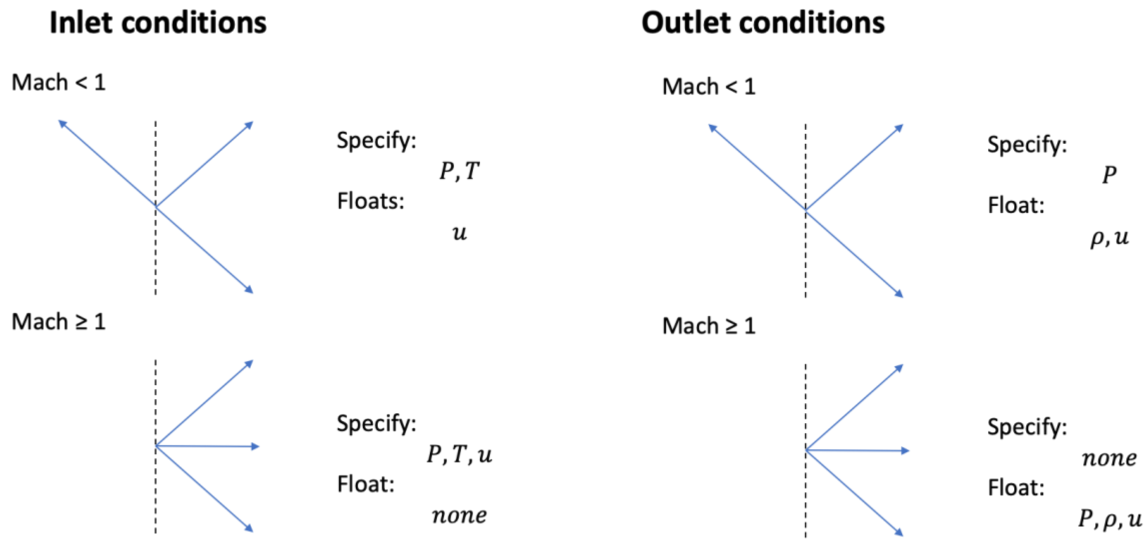

Figure 7: Flow boundary conditions (inlet and outlet).

The mathematical reason is a little complex but in the above schematic, we show the characteristic lines for the different mach number conditions at the inlet and the outlet. Essentially, how to specify inlet and outlet boundary conditions simplifies down to the number of characteristic lines entering the control volume. So for example, with a subsonic flow at the inlet, we have two characteristic lines entering the control volume so we specify the pressure and temperature. We could also specify, say density and velocity. We don't do this because physically, it is easier to understand us having a constant pressure and temperature supply and allowing the velocity to float to match whatever flow is being pulled from our source.

At the outlet with a subsonic flow, we specify pressure only. This makes sense where we have a valve and can control the outlet pressure (e.g., open to ambient conditions).

For the supersonic case, we first need to either specify if the inlet is supersonic or subsonic. In the diverging example above, we specified a sonic inlet for one example to give us the result we want. When the model sees the user specifies a sonic flow at the inlet, the model calculates the sonic velocity based on the inlet temperature and pins the inlet velocity to be sonic. In this case, all inlet conditions are specified.

At the outlet, the model determines based on the velocity and the temperature, if the flow is subsonic or not. If the flow is subsonic, the model uses the pressure boundary condition specified. If the flow becomes supersonic, the model determines that the flow is supersonic and lets all variables at the outlet boundary float.

5 Solver information

In this section, I will describe how the solver works. It is a semi-implicit method where the at each time step, the model iterates until some convergence criteria is met. There are weights in the solver that can be modified to make the solution more or less implicit. With a more implicit solution, the error will be smaller but with the increasing number of iterations, the model will take longer to run.

I'll first modify the equations a bit to make them easier to implement then I will talk about how the solution is found, mainly using the conservation of mass equation as an example.

First, I will start with our 1D equations and simplify them a bit before implementing them. This will save some computation time and make any debugging easier once the code is written.

Start with equations in differential form:

$$\frac{\partial \rho}{\partial t} = -\frac{1}{A}\frac{\partial(\rho u A)}{\partial x}$$

$$\frac{\partial(\rho u)}{\partial t} = -\frac{1}{A}\frac{\partial(\rho u^2 A)}{\partial x} - \frac{\partial P}{\partial x}$$

$$\frac{\partial\left[\rho\left(e+\frac{u^2}{2}\right)\right]}{\partial t} = -\frac{1}{A}\frac{\partial\left[u\rho\left(e+\frac{u^2}{2}\right)A\right]}{\partial x} - \frac{1}{A}\frac{\partial(uPA)}{\partial x} - \frac{1}{A}\frac{\partial(q''A)}{\partial x} + uP\frac{1}{A}\frac{dA}{dx}$$

This can be further simplified (saves some computational steps later) if we multiply the conservation of mass by u and subtract it from the conservation of momentum:

$$\frac{\partial(\rho u)}{\partial t} - u\frac{\partial \rho}{\partial t} = -\frac{1}{A}\frac{\partial(\rho u^2 A)}{\partial x} + \frac{1}{A}u\frac{\partial(\rho u A)}{\partial x} - \frac{\partial P}{\partial x}$$

$$\rho\frac{\partial u}{\partial t} = -\rho u\frac{\partial u}{\partial x} - \frac{\partial P}{\partial x}$$

$$\frac{\partial \rho}{\partial t} = -\frac{1}{A}\frac{\partial(\rho u A)}{\partial x}$$

$$\rho\frac{\partial u}{\partial t} = -\rho u\frac{\partial u}{\partial x} - \frac{\partial P}{\partial x}$$

$$\frac{\partial\left[\rho\left(e+\frac{u^2}{2}\right)\right]}{\partial t} = -\frac{1}{A}\frac{\partial\left[u\rho\left(e+\frac{u^2}{2}\right)A\right]}{\partial x} - \frac{1}{A}\frac{\partial(uPA)}{\partial x} - \frac{1}{A}\frac{\partial(q''A)}{\partial x}$$

The conservation of energy equation can be simplified by multiplying the conservation of momentum equation by u and subtracting from the conservation of energy equation:

$$\frac{\partial(\rho e)}{\partial t} + u\rho\frac{\partial u}{\partial t} + \frac{u^2}{2}\frac{\partial \rho}{\partial t} - u\rho\frac{\partial u}{\partial t}$$
$$= -\frac{1}{A}\frac{\partial(u\rho e A)}{\partial x} - \rho u^2\frac{\partial u}{\partial x} - \frac{1}{A}\frac{u^2}{2}\frac{\partial(u\rho A)}{\partial x} + \rho u^2\frac{\partial u}{\partial x} - \frac{1}{A}\frac{\partial(uPA)}{\partial x} + u\frac{\partial P}{\partial x} - \frac{1}{A}\frac{\partial(q''A)}{\partial x} + uP\frac{1}{A}\frac{dA}{dx}$$

$$\frac{\partial(\rho e)}{\partial t} + \frac{u^2}{2}\frac{\partial \rho}{\partial t} = -\frac{1}{A}\frac{\partial(u\rho e A)}{\partial x} - \frac{1}{A}\frac{u^2}{2}\frac{\partial(u\rho A)}{\partial x} - uP\frac{d(lnA)}{dx} - P\frac{\partial u}{\partial x} - \frac{1}{A}\frac{\partial(q''A)}{\partial x}$$

$$\frac{\partial \rho}{\partial t} = -\frac{1}{A}\frac{\partial(\rho u A)}{\partial x}$$

$$\rho\frac{\partial u}{\partial t} = -\rho u\frac{\partial u}{\partial x} - \frac{\partial P}{\partial x}$$

$$\frac{\partial(\rho e)}{\partial t} + \frac{u^2}{2}\frac{\partial \rho}{\partial t} = -\frac{1}{A}\frac{\partial(u\rho e A)}{\partial x} - \frac{1}{A}\frac{u^2}{2}\frac{\partial(u\rho A)}{\partial x} - P\frac{\partial u}{\partial x} - uP\frac{d(lnA)}{dx} - \frac{1}{A}\frac{\partial(q''A)}{\partial x}$$

Re-arranging conservation of energy to get:

$$\rho\frac{\partial e}{\partial t} + e\frac{\partial \rho}{\partial t} + \frac{u^2}{2}\frac{\partial \rho}{\partial t} = -\frac{1}{A}e\frac{\partial(\rho u A)}{\partial x} - u\rho\frac{\partial e}{\partial x} - \frac{1}{A}\frac{u^2}{2}\frac{\partial(\rho u A)}{\partial x} - P\frac{\partial u}{\partial x} - uP\frac{d(lnA)}{dx} - \frac{1}{A}\frac{\partial(q''A)}{dx}$$

Multiply conservation of mass by e and multiply conservation of mass by $\frac{u^2}{2}$ and subtract from conservation of energy to get:

$$\rho\frac{\partial e}{\partial t} + e\frac{\partial \rho}{\partial t} - e\frac{\partial \rho}{\partial t} + \frac{u^2}{2}\frac{\partial \rho}{\partial t} - \frac{u^2}{2}\frac{\partial \rho}{\partial t}$$
$$= -\frac{1}{A}e\frac{\partial(\rho u A)}{\partial x} + \frac{1}{A}e\frac{\partial(\rho u A)}{\partial x} - u\rho\frac{\partial e}{\partial x} - \frac{1}{A}\frac{u^2}{2}\frac{\partial(\rho u A)}{\partial x} + \frac{1}{A}\frac{u^2}{2}\frac{\partial(\rho u A)}{\partial x} - P\frac{\partial u}{\partial x} - uP\frac{d(lnA)}{dx}$$
$$-\frac{1}{A}\frac{\partial(q''A)}{dx}$$

$$\frac{\partial \rho}{\partial t} = -\frac{1}{A}\frac{\partial(\rho u A)}{\partial x}$$

$$\rho\frac{\partial u}{\partial t} = -\rho u\frac{\partial u}{\partial x} - \frac{\partial P}{\partial x}$$

$$\rho\frac{\partial e}{\partial t} = -u\rho\frac{\partial e}{\partial x} - P\frac{\partial u}{\partial x} - uP\frac{d(lnA)}{dx} - \frac{1}{A}\frac{\partial(q''A)}{dx}$$

In the first iteration, we only consider gasses that obey the ideal gas law ($P = \rho RT$), expand the heat flux, q'', and assume that fluid properties are, at least, constant across the time step so we ultimately obtain:

$$c_v\rho\frac{\partial T}{\partial t} = -c_v u\rho\frac{\partial T}{\partial x} - P\frac{\partial u}{\partial x} + k\frac{\partial^2 T}{\partial x^2} - uP\frac{d(lnA)}{dx} + k\frac{\partial T}{\partial x}\frac{d(lnA)}{dx}$$

Our final set of equations are shown below. These are the equations we will implement in the code to solver for density, temperature, and velocity at each time step. Pressure is found using our equation of state (ideal gas law).

$$\frac{\partial\rho}{\partial t} = -\frac{1}{A}\frac{\partial(\rho uA)}{\partial x}$$

$$\rho\frac{\partial u}{\partial t} = -\rho u\frac{\partial u}{\partial x} - \frac{\partial P}{\partial x}$$

$$c_v\rho\frac{\partial T}{\partial t} = -c_v u\rho\frac{\partial T}{\partial x} - P\frac{\partial u}{\partial x} + k\frac{\partial^2 T}{\partial x^2} - uP\frac{d(lnA)}{dx} + k\frac{\partial T}{\partial x}\frac{d(lnA)}{dx}$$

To solve these equations, we first approximate the differential equations using the finite difference method. We will then discuss how the equations are solved to find a solution at each time step.

$$\frac{\partial\rho}{\partial t} = -\frac{1}{A}\frac{\partial(\rho uA)}{\partial x}$$

$$\rho\frac{\partial u}{\partial t} = -\rho u\frac{\partial u}{\partial x} - \frac{\partial P}{\partial x}$$

$$c_v\rho\frac{\partial T}{\partial t} = -c_v u\rho\frac{\partial T}{\partial x} - P\frac{\partial u}{\partial x} + k\frac{\partial^2 T}{\partial x^2} - uP\frac{d(lnA)}{dx} + k\frac{\partial T}{\partial x}\frac{d(lnA)}{dx}$$

Now need to discretize, we begin by looking at point i and considering the points before and after, $i-1$ and $i+1$, respectively. For the velocity, we get:

$$u_{i-1} = u_i - \frac{du_i}{dx}dx + \frac{d^2u_i}{dx^2}\frac{(dx)^2}{2} - \cdots + (-1)^n\frac{d^nu_i}{dx^n}\frac{(dx)^n}{n!}$$

$$u_{i+1} = u_i + \frac{du_i}{dx}dx + \frac{d^2u_i}{dx^2}\frac{(dx)^2}{2} + \cdots + \frac{d^nu_i}{dx^n}\frac{(dx)^n}{n!}$$

Subtracting the first form the second we get:

$$u_{i+1} - u_{i-1} = 2\frac{du_i}{dx}dx + 2\frac{d^3u_i}{dx^3}\frac{(dx)^3}{3!} + 2\frac{d^5u_i}{dx^5}\frac{(dx)^5}{5!} + \cdots$$

$$u_{i+1} - u_{i-1} = 2\frac{du_i}{dx}dx + 2\frac{d^3u_i}{dx^3}\frac{(dx)^3}{3!} + 2\frac{d^5u_i}{dx^5}\frac{(dx)^5}{5!} + \cdots$$

This can be put into this form:

$$\frac{du_i}{dx} = \frac{u_{i+1} - u_{i-1}}{2dx} - 2\frac{d^3u_i}{dx^3}\frac{(dx)^2}{3!} - 2\frac{d^5u_i}{dx^5}\frac{(dx)^4}{5!} - \cdots$$

So we obtain:

$$\frac{du_i}{dx} = \frac{u_{i+1} - u_{i-1}}{2dx} + O(dx)^2$$

If we add the two original equations, we obtain:

$$u_{i-1} + u_{i+1} = 2u_i + 2\frac{d^2u_i}{dx^2}\frac{(dx)^2}{2} + 2\frac{d^4u_i}{dx^4}\frac{(dx)^4}{4!} + \cdots$$

Similarly to the previous exercise, we obtain:

$$\frac{d^2u_i}{dx^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(dx)^2} - 2\frac{d^4u_i}{dx^4}\frac{(dx)^2}{4!} - 2\frac{d^6u_i}{dx^6}\frac{(dx)^4}{6!} - \cdots = \frac{u_{i+1} - 2u_i + u_{i-1}}{(dx)^2} - O(dx)^2$$

The final equations we have:

$$\frac{\partial\rho}{\partial t} = -u\frac{\partial\rho}{\partial x} - \rho\frac{\partial u}{\partial x} - \rho u\frac{d(lnA)}{dx}$$

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - \frac{1}{\rho}\frac{\partial P}{\partial x}$$

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} - \frac{P}{c_v\rho}\frac{\partial u}{\partial x} - \frac{1}{c_v\rho}\left(uP - k\frac{\partial T}{\partial x}\right)\frac{d(lnA)}{dx} + \frac{1}{c_v\rho}k\frac{\partial^2 T}{\partial x^2}$$

We can then put into numerical form using our derivative approximations:

$$\frac{\rho_i^{n+1} - \rho_i^n}{\Delta t} = -u_i^n\frac{\rho_{i+1}^n - \rho_{i-1}^n}{2\Delta x} - \rho_i^n\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} - u_i^n\rho_i^n\frac{\ln(A_{i+1}) - \ln(A_{i-1})}{2\Delta x}$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -u_i^n\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} - \frac{1}{\rho_i^n}\frac{P_{i+1}^n - P_{i-1}^n}{2\Delta x}$$

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = -u_i^n\frac{T_{i+1}^n - T_{i-1}^n}{2\Delta x} - \frac{P_i^n}{c_v\rho_i^n}\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}$$
$$-\frac{1}{c_v\rho_i^n}\left(u_i^nP_i^n - k\frac{T_{i+1}^n - T_{i-1}^n}{2\Delta x}\right)\frac{\ln(A_{i+1}) - \ln(A_{i-1})}{2\Delta x} + \frac{1}{c_v\rho_i^n}k\frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(dx)^2}$$

To find a solution, we first find the time derivative based on the current step. We then find an approximation for the next time using the time derivatives we found at the current step. We then want to find the time derivative again at our approximated next step. We then use weights (X for time derivative found using current step, Y for time derivative found at approximated next step) to find a weighted time derivative. We then keep iterating on our approximated next step until we converge. We use a convergence error term to determine when the solution converges or not.

To make the solution more stable, we want to first guess (approximate) the values at $n+1$, and then correct by iterating until we find a mostly implicit solution. We call this a semi-implicit iterative procedure. We only demonstrate the process using the momentum equation

First we find u_i^{n+1} by solving the equation below for u_i^{n+1}

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -u_i^n\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} - \frac{1}{\rho_i^n}\frac{P_{i+1}^n - P_{i-1}^n}{2\Delta x}$$

We now have an approximation for u_i at $n+1$ and introduce the weights X, Y and iterate. We use the weighted average (using the weights) to adjust our approximation of u_i at $n+1$ by solving the following equation for u_i^{n+1}:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{Xu_i^n + Yu_i^{n+1}}{(X+Y)^2}\frac{(Xu_{i+1}^n + Yu_{i+1}^{n+1}) - (Xu_{i-1}^n + Yu_{i-1}^{n+1})}{2\Delta x}$$
$$-\frac{1}{X\rho_i^n + Y\rho_i^{n+1}}\frac{(XP_{i+1}^n + YP_{i+1}^{n+1}) - (XP_{i-1}^n + YP_{i-1}^{n+1})}{2\Delta x}$$

We then iterate using the new approximation until $(u_i^{n+1})_N - (u_i^{n+1})_{N-1} < \epsilon$ where N is the number of iterations.

The solution should approximate an implicit solution if $Y \gg X$. The same procedure is used for the other two conservation equations. The four variables (u, P, ρ, T) are coupled with each other (with the ideal gas law being used as the fourth relationship) which can slow the solution down but with sufficient weights, the solution should remain stable.