Jump Conditions

Similarly, we have for the one-dimensional momentum equation and energy equation:

$$
\begin{aligned}
\rho_L v_L^2 + P_L - \rho_L v_L \lambda &= \rho_R v_R^2 + P_R - \rho_R v_R \lambda \\
\rho_L v_L (h_L + v_L^2/2) - \rho_L (\epsilon_L + v_L^2/2)\lambda &= \rho_R v_R (h_R + v_R^2/2) - \rho_R (\epsilon_R + v_R^2/2)\lambda
\end{aligned}
$$

Let us consider the possible cases of discontinuities. The simplest solution is to have $v_L = v_R$ and $P_L = P_R$, in which case $\lambda = v_L = v_R$ is a solution, and ρ_L and ρ_R can take on any combination of values. This is called a *contact discontinuity*. Note that there is no mass flux *across* the discontinuity.

To understand the second type of discontinuity, we go into the frame of the discontinuity so that $\lambda = 0$, which simplifies the calculations. Then we get

$$\begin{aligned}
\rho_L v_L &= \rho_R v_R =: j \\
\rho_L v_L^2 + P_L &= \rho_R v_R^2 + P_R \\
\rho_L v_L (h_L + v_L^2/2) &= \rho_R v_R (h_R + v_R^2/2).
\end{aligned}$$

Now we have a mass flux j across the discontinuity. We can use the first equation to simplify the second one:

$$P_L + j^2/\rho_L = P_R + j^2/\rho_R,$$

or

$$j^2 = \frac{P_R - P_L}{\rho_L^{-1} - \rho_R^{-1}}.$$

Since this is positive, we see that we must either have $\rho_R > \rho_L$ if $P_R > P_L$ or $\rho_L > \rho_R$ if $P_L > P_R$.

Shocks

On the other hand, we have

$$h_L + \frac{1}{2} j^2 \rho_L^{-2} = h_R + \frac{1}{2} j^2 \rho_R^{-2},$$

and hence

$$h_L + \frac{1}{2} j^2 \rho_L^{-2} = h_R + \frac{1}{2} j^2 \rho_R^{-2}.$$

Using our result for j, we can arrive at our final result for the jump conditions at a shock:

$$\begin{aligned}
h_L - h_R + \frac{1}{2} j^2 (\rho_L^{-1} - \rho_R^{-1})(\rho_L^{-1} + \rho_R^{-1}) &= 0 \\
h_L - h_R + \frac{1}{2} (\rho_L^{-1} + \rho_R^{-1})(P_R - P_L) &= 0 \\
\epsilon_L - \epsilon_R + \frac{1}{2} (\rho_L^{-1} - \rho_R^{-1})(P_R + P_L) &= 0
\end{aligned}$$

Results for Perfect Gas

For a perfect gas, we have $P = (\gamma - 1)\rho\epsilon$. Important cases includes $\gamma = 5/3$ and $\gamma = 4/3$ for a non-relativistic and relativistic monoatomic perfact gas. Using the equation of state, we can determine how the compression ratio $\beta = \rho_L/\rho_R$ depends on the pressure jump:

$$\begin{aligned}
[1 + (\gamma - 1)^{-1}] \left(\frac{P_L}{\beta \rho_R} - \frac{P_R}{\rho_R} \right) + \frac{1}{2}(\beta^{-1} + 1)\rho_R^{-1}(P_R - P_L) &= 0 \\
\frac{\gamma}{\gamma - 1} \left(\beta^{-1} P_L - P_R \right) + \frac{1}{2}(\beta^{-1} + 1)(P_R - P_L) &= 0 \\
\frac{\gamma}{\gamma - 1} (P_L - \beta P_R) + \frac{1}{2}(\beta + 1)(P_R - P_L) &= 0
\end{aligned}$$

Now solve for β:

$$\begin{aligned}
\beta &= \frac{\frac{\gamma}{\gamma-1} P_L + \frac{1}{2}(P_R - P_L)}{\frac{\gamma}{\gamma-1} P_R - \frac{1}{2}(P_R - P_L)} = \frac{2\gamma P_L + (\gamma - 1)(P_R - P_L)}{2\gamma P_R - (\gamma - 1)(P_R - P_L)} \\
&= \frac{(\gamma + 1)P_L + (\gamma - 1)P_R}{(\gamma - 1)P_L + (\gamma + 1)P_R}
\end{aligned}$$

Strong Shocks

For strong shocks with $P_L \gg P_R$, the compression ratio asymptotes to:

$$\beta = \frac{(\gamma+1)P_L + (\gamma-1)P_R}{(\gamma-1)P_L + (\gamma+1)P_R} \to \frac{\gamma+1}{\gamma-1}$$

This means that for a perfect gas the compression ratio is always *finite*, and can only reach $\beta = 4$ for a non-relativistic perfect gas and $\beta = 7$ for a relativistic perfect gas. One interesting case is $\gamma = 1$, which corresponds to *isothermal* conditions. This can be achived if cooling behind the shock is extremely fast, and allows the compression ratio to become arbitrarily large. From the jump condition for th mass flux one can deduce that the velocity jumps from $-v$ ahead of the shock to $-v/\beta$ behind the shock.

Oblique Shocks

The jump conditions can easily be generalised to the case chen the fluid ahead of the shock has a velocity component transverse to the shock. Then the transverse velocity simply remains constant across the shock, $v_{parallel,L} = v_{\|,R}$, while $v_{\perp,L} = \beta^{-1} v_{\perp,R}$. As a result, streamlines undergo "refraction" at an oblique shock.

Some further results on shocks (without proof)

- Entropy increases discontinuously in the direction of the mass flux (i.e. higher in the compressed region)
- The velocity of weak shocks ($P_L \approx P_R$) relative to the upstream medium is given by the speed of sound.
- For strong shocks ($P_L \gg P_R$ or vice versa), the shock velocity can be arbitrarily high.

Example – Advection Equation

Let's begin with a simple example and see how we can solve the *advection equation*

$$\partial_t f + v\partial_x f = 0$$

on a grid. We know how to solve it anlytically:

$$f(t,x) = f(t_0, x - v(t - t_0)).$$

This describes the advection of some field f (e.g. a mass fraction) along the x-direction with velocity v.

Discretisation – Finite-Difference Methods

- Denote the discrete solution with $f_i^n = f(t_n, x_i)$ where x_i and t_n are the values of x and t on the grid.
- Now we *could* approximate

$$(\partial_x f)_i^n \approx \frac{f_{i+1}^n - f_{i-1}^n}{x_{i+1}^n - x_{i-1}^n} \frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x}$$

$$(\partial_t f)_i^n \approx \frac{f_i^{n+1} - f_i^n}{t_{n+1} - t_n} = \frac{f_i^{n+1} - f_i^n}{\Delta t}$$

- Then the discrete form of the equation allows us to obtain f at time t_{n+1}:

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + \frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} = 0$$

- This is called a *finite-difference representation* of the advection equation.

Does this work?

- Let's try to test this algorithm with $v = 1$, $\delta x = 1$, $\delta t = 0.5$, and the following *initial conditions*:

$$f_i^0 = \begin{cases} 1, & \text{i=1...49} \\ 0, & \text{i=50,...100} \end{cases}$$

- We also need *boundary conditions* to calculate the finite-difference representation of $\partial_x f$ at the grid boundaries. For the sake of simplicity, we choose periodic boundary conditions here:

$$f_0^n = f_{100}^n, \qquad f_{101}^n = f_1^n.$$

- When we try this, we get a numerical solution that is completely wrong (see Figure).

Boundary conditions

At the grid boundaries, the finite-difference operators need values for mesh points that are not on the computational grid. In a numerical code, one can either switch to a different finite-difference operator at the boundaries (that is chosen to respect the *mathematical* boundary conditions) or use so called *ghost zones* that are populated with values by copying/reflecting the values of zones inside the computational domain. Common cases include:

- Periodic boundary conditions
- Reflecting (symmetric/antisymmetric) boundary conditions
- Fixed boundary conditions

Periodic boundary conditions are often particularly easy to implement if a programming language offers a command for a cyclic permutation of an array.

Consistency

The idea is that the discrete solution will *converge* to the true analytic solution if $\Delta t \to 0$ and $\Delta x \to 0$. In order for that to happen, the discretised equation must be *consistent* with the analytic form, which we can check by using Taylor's theorem:

$$
\begin{aligned}
\frac{f_{i+1}^n - f_{i-1}^n}{x_{i+1}^n - x_{i-1}^n} &= \frac{1}{2\Delta x}\Bigg[f_i + \left(\frac{\partial f}{\partial x}\right)_i \Delta x + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x^2 + \frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i \Delta x^3 + \mathcal{O}(\Delta x \\
&\quad -(f_i - \left(\frac{\partial f}{\partial x}\right)_i \Delta x + \frac{1}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_i \Delta x^2 - \frac{1}{6}\left(\frac{\partial^3 f}{\partial x^3}\right)_i \Delta x^3 + \mathcal{O}(\Delta x^4))\Bigg] \\
&\approx \frac{\partial f}{\partial x} + \frac{1}{6}\frac{\partial^3 f}{\partial x^3}\Delta x^2
\end{aligned}
$$

Playing the same game for the other term, we obtain the so-called *modified equation*:

$$
\frac{\partial f}{\partial t} + C\frac{\partial^2 f}{\partial t^2}\Delta t + v\frac{\partial f}{\partial x} + v\frac{1}{6}\frac{\partial^3 f}{\partial x^3}\Delta x^2 = 0
$$

The Modified Equation

$$\frac{\partial f}{\partial t} + C\frac{\partial^2 f}{\partial t^2}\Delta t + v\frac{\partial f}{\partial x} + v\frac{1}{6}\frac{\partial^3 f}{\partial x^3}\Delta x^2 = 0$$

- **Calculate the coefficient C!**
- You can think of this as the equation that we *actually solve* for $\Delta x \neq 0$ and $\Delta t \neq 0$.
- For $\Delta x \to 0$ and $\Delta t \to 0$, we recover the advection equation as required.
- Hence our finite-difference representation is *consistent*.
- The leading *truncation error* terms in Δt and Δx are of order $\mathcal{O}(\Delta t)$ and $\mathcal{O}(\Delta x^2)$. We therefore say that the scheme is accurate to first-order in time and to second order in space.
- One way to make finite-difference scheme stable is to add a diffusive (or viscous) terms like $\partial^2 f/\partial x^2$ or similar higher-order terms by hand (cp. S. Shelyag's course), and this is also done in SPH. We're going to do it differently now.

Stability

- So our scheme is apparently unstable. . .
- For our finite-difference scheme, there is a rigorous way (von Neumann stability analysis) to determine whether it's stable or unstable. This works only for *linear* PDEs with a linear finite-difference representation **(Why?)**.
- We look at individual Fourier modes of the numerical solution and determine their temporal evolution using the ansatz:

$$f_{i,n} = e^{ikx_i} e^{\omega t_n}.$$

- If $\mathrm{Re}\,\omega > 0$ for any k, there's a blow-up and the scheme is unstable, if $\mathrm{Re}\,\omega \leq 0$ for al k, the scheme is stable.

$$
\begin{aligned}
\frac{f_i^{n+1}-f_i^n}{\Delta t} &= -v\frac{f_{i+1}^n-f_{i-1}^n}{2\Delta x} \\
\frac{e^{\omega\Delta t}-1}{\Delta t}e^{\omega t_n}e^{ikx_i} &= -v\frac{e^{ik\Delta x}-e^{-ik\Delta x}}{2\Delta x}e^{\omega t_n}e^{ikx_i} \\
e^{\omega\Delta t} &= 1-v\left(e^{ik\Delta x}-e^{-ik\Delta x}\right)\frac{\Delta t}{2\Delta x} \\
e^{\omega\Delta t} &= 1-iv\sin k\Delta x\frac{\Delta t}{\Delta x}
\end{aligned}
$$

The amplifcation factor $e^{\omega\Delta}$ has an absolute value of $|e^{\omega\Delta t}|=\sqrt{1+v^2\sin^2 k\Delta x}$, i.e. $|e^{\omega\Delta t}|>1$ for almost all k. Hence the FTCS scheme is unstable.

Finite-difference stencils

The form of the finite-difference operator that represent the discretised equation is sometimes visualised in graphical form as a “stencil”:

- FTCS (forward time, centered space):
- Leapfrog:
- Backward Euler (1st order implicit):

Domains of Dependence

To assess the stability behaviour of a numerical scheme, it is sometimes useful to consider the numerical *domain of dependence*, i.e. the set of mesh points that influence (directly or indirectly) the numerical solution at a given mesh point:

Characteristics and Upwinding

Understanding how information (in physical terms: waves) travels in a fluid helps to

- explain why certain discretisation schemes are unstable
- and (conversely) to construct schemes that reproduce the behaviour of the physical system described by the equations.

Let us consider how the solution of the advection equation varies along a curve $x(t)$:

$$\begin{aligned}\frac{\mathrm{d}u}{\mathrm{d}t} &= \frac{\partial u}{\partial t} + \frac{\mathrm{d}x}{\mathrm{d}t}\frac{\partial u}{\partial x} \\ &= -v\frac{\partial u}{\partial x} + \dot{x}\frac{\partial u}{\partial x} = (\dot{x} - v)\,\frac{\partial u}{\partial x}\end{aligned}$$

Regardless of the value of $\partial u/\partial x$, $\mathrm{d}u/\mathrm{d}t$ is zero along the curve if $\dot{x} = v$. In other words, u is constant along curves with $\dot{x} = v$. These curves (straight lines in this cases) are called *characteristics* of the advection equation.

Upwinding – Numerical and Physical Domain of Dependence

- The solution of the advection equation (or, generally, a system of linear partial differential equations) can be found by tracing the characteristics back in time.
- If the numerical domain of dependence of a finite-difference scheme doesn't include the characteristics, then it is bound to be unstable.
- It may still be unstable if regions outide the physical domain of dependence are "weighted" too much in the finite-difference operator.
- A way to construct stable scheme is to use *upwind* differences, i.e. one-sided differences aligned with the physical domain of dependence (though upwinding alone is not always sufficient to achieve stability).

Determing Characteristic Speeds – Euler equations

The Euler equations are a non-linear system of equations. Let us focus on the one-dimensional case. We can formally write the 1D Euler equations as a vector equation:

$$\frac{\partial}{\partial t}\left(\begin{array}{c}\rho \\ \rho u \\ \rho(\epsilon+u^2/2)\end{array}\right)+\frac{\partial}{\partial x}\left(\begin{array}{c}\rho v \\ \rho u^2+P \\ \rho(\epsilon+u^2/2)u+Pu\end{array}\right)=0$$

or

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{F}(\mathbf{U})}{\partial x}=0.$$

This is called a *flux-conservative* equation, $\mathbf{U}$ is the *state vector* and $\mathbf{F}$ is the flux function. It can be cast into *quasi-linear* form:

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{F}}{\partial \mathbf{U}}\cdot\frac{\partial \mathbf{U}}{\partial x}=\frac{\partial \mathbf{U}}{\partial t}+\mathbf{J}\cdot\frac{\partial \mathbf{U}}{\partial x}=0.$$

Here, the *flux Jacobian* $\mathbf{J}=\partial\mathbf{U}/\partial x$ is a matrix containing the derivatives of all components of $\mathbf{F}$ with respect to all components of $\mathbf{U}$.

Determing Characteristic Speeds – Quasilinear System of Equations

If we have a quasi-linear system

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{J} \cdot \frac{\mathbf{U}}{\partial x} = 0,$$

where we assume that $\mathbf{J}$ does not depend on x and t, then we can compute $\mathrm{d}\mathbf{U}/\mathrm{d}t$ along a curve $x(t)$ with $\lambda = \dot{x}(t)$ in a similar way as we did for the advection equation:

$$\begin{aligned} \frac{\mathrm{d}\mathbf{U}}{\mathrm{d}t} &= \lambda \frac{\partial U}{\partial x} - \mathbf{J} \cdot \frac{\mathbf{U}}{\partial x} \\ \frac{\mathrm{d}\mathbf{U}}{\mathrm{d}t} &= \frac{\partial}{\partial x} \left(\lambda \mathbf{U} - \mathbf{J} \cdot \mathbf{U} \right) \end{aligned}$$

If λ is an *eigenvalue* and $\mathbf{U}$ is an eigenvector of $\mathbf{J}$, then we again have $\mathrm{d}\mathbf{U}/\mathrm{d}t = 0$. If we diagonalise using $\mathbf{J} = \mathbf{P}^{-1}\mathbf{D}\mathbf{P}$ (with a diagonal matrix $\mathbf{D} = \mathrm{diag}(\lambda_1, \lambda_2, \ldots)$) and introducing the vector of *characteristic variables* $\mathbf{c} = \mathbf{P} \cdot \mathbf{U}$, we find

$$\frac{\partial \mathbf{c}}{\partial t} + D \cdot \frac{\partial \mathbf{c}}{\partial x} = 0,$$

Flux Jacobian for the Euler Equations

The non-linear case where $\mathbf{J}$ depends on $\mathbf{U}$ and hence on x and t is more complicated, but the result still holds: The solution can be decoupled into waves propagating with speeds corresponding to the eigenvalue of the flux Jacobian. If we use an ideal gas equation of state$\rho\epsilon = P/\gamma - 1$, we obtain the following flux Jacobian:

$$\mathbf{J} = \begin{pmatrix} 0 & 1 & 0 \\ \frac{1}{2}(\gamma-3)u^2 & (3-\gamma)u & (\gamma-1) \\ -u\gamma\epsilon - \frac{1}{2}(2-\gamma)u^3 & \gamma\epsilon + (\frac{3}{2}-\gamma)u^2 & \gamma u \end{pmatrix}$$

- The eigenvalues are $u+c$, $u-c$, u, and where $c = \sqrt{\gamma P/\rho}$ is the sound speed. **Try to verify this with Mathematica.**
- The three families of characteristics (plus, minus, zero) correspond to left-going sound waves right-going sound waves and an "entropy" wave that is just advected with the fluid.
- If we want to use upwind differences for the Euler equations, we'd have to decompose into characteristic variables first becaue the characteristics can go into different directions.

Riemann Invariants – Non-Linear Case

In the non-linear case, one can still determine *Riemann invariants* that are conserved along characteristics. We start from the quasi-linear form

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{J} \cdot \frac{\partial \mathbf{U}}{\partial x} = 0.$$

Now we look for function $R_i(\mathbf{U})$ that is conserved along the characteristic with speed λ_i.

$$\frac{\mathrm{d}R_i}{\mathrm{d}t} = \frac{\partial R}{\partial \mathbf{U}} \cdot \frac{\mathrm{d}U}{\mathrm{d}t} = \frac{\partial R_i}{\partial \mathbf{U}} \cdot \left(\lambda_i \frac{\partial \mathbf{U}}{\partial x} - \mathbf{J} \cdot \frac{\partial \mathbf{U}}{\partial x}\right) = \frac{\partial R_i}{\partial \mathbf{U}} \cdot (\lambda_i - \mathbf{J}) \cdot \frac{\partial \mathbf{U}}{\partial x}$$

If $\partial R_i/\partial \mathbf{U}$ is a *left eigenvector* of $\mathbf{J}$, then R_i is invariant along the trajectory. (You may verify that this is true for the characteristic variables in the linear case).

Primitive Form of the Equations

The characteristics may equally be obtained from the *primitve form of the equations*,

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ u\\ P\end{pmatrix}+\begin{pmatrix}u & \rho & 0\\ 0 & u & \frac{1}{\rho}\\ 0 & \rho c^2 & u\end{pmatrix}\cdot\frac{\partial}{\partial x}\begin{pmatrix}\rho\\ u\\ P\end{pmatrix}=0,$$

which also happens to be quasilinear. The coefficient matrix has left eigenvectors $(-c^2, 0, 1)$, $(0, 1, 1/(c\rho))$, and $(0, 1, -1/(c\rho))$. Thus the Riemann invariants for the zero, minus and plus characteristics are:

$$s\ (\text{entropy}), u+\int\frac{\mathrm{d}P}{c\rho}, u-\int\frac{\mathrm{d}P}{c\rho}$$

For isentropic flow, we can integrate these:

$$s\ (\text{entropy}), u+\frac{2c}{\gamma-1}, u-\frac{2c}{\gamma-1}$$