FINITE POINTSET METHOD (FPM) FOR COMPRESSIBLE FLUID FLOW

ABSTRACT

This paper sums up the upwind ideas in FPM.

1 General remarks

We want to solve the system of conservation equations of gasdynamics

$$\begin{aligned} &\tfrac{\mathrm{d}}{\mathrm{dt}}\rho + \rho \cdot \nabla^T \mathbf{v} \;=\; 0 \\ &\tfrac{\mathrm{d}}{\mathrm{dt}}\left(\rho \mathbf{v}\right) + \left(\rho \mathbf{v}\right) \cdot \nabla^T \mathbf{v} + \nabla p = 0 \\ &\tfrac{\mathrm{d}}{\mathrm{dt}}\left(\rho E\right) + \left(\rho E\right) \cdot \nabla^T \mathbf{v} + \nabla^T \left(p \cdot \mathbf{v}\right) \;=\; 0 \end{aligned} \tag{1.1}$$

where

ρ is the density,

$\mathbf{v} = \begin{pmatrix} u & v & w \end{pmatrix}^T$ is the velocity,

p is the pressure,

$\rho E = \int_0^T c_v \, dT + \frac{\rho}{2} \mathbf{v}^T \mathbf{v}$ is the total energy,

T is the temperature (Kelvin),

c_v is the specific heat capacity.

We have to complete the set of equations by the equation of state

$$p = \rho R T \tag{1.2}$$

with R being the specific gas constant.

The sound speed can be derived by

$$c^2 = kRT \tag{1.3}$$

where

$k = \frac{c_v + R}{c_v}$ is the isentropic exponent.

For the numerical integration, we introduce the so called upwind velocity $\overline{\mathbf{v}}$ and upwind pressure $\overline{p}$, leading to a stabilization of the scheme. Numerically, we solve the modified conservation equations

$$
\begin{aligned}
\tfrac{\mathrm{d}}{\mathrm{dt}}\rho + \rho\cdot\nabla^T\overline{\mathbf{v}} &= 0 \\
\tfrac{\mathrm{d}}{\mathrm{dt}}(\rho\mathbf{v}) + (\rho\mathbf{v})\cdot\nabla^T\overline{\mathbf{v}} + \nabla\overline{p} &= 0 \\
\tfrac{\mathrm{d}}{\mathrm{dt}}(\rho E) + (\rho E)\cdot\nabla^T\overline{\mathbf{v}} + \nabla^T(\overline{p}\cdot\overline{\mathbf{v}}) &= 0
\end{aligned}
$$

The following sections now provide different ways of approaching $\overline{\mathbf{v}}$ and $\overline{p}$.

2 Classical upwind formulation

The classical upwind formulation is given in [1], section 6.2. There, we use the upwind pressure and velocity of the form

$$
\begin{aligned}
\overline{p} &= p - \frac{\rho c}{2}\left(\mathbf{v}^+ - \mathbf{v}^-\right)^T \mathbf{n} \\
\overline{\mathbf{v}} &= \mathbf{v} - \frac{1}{2\rho c}\left(p^+ - p^-\right)\mathbf{n}
\end{aligned}
\tag{2.1}
$$

where $\mathbf{n} = \begin{pmatrix} n_x & n_y & n_z \end{pmatrix}^T = \frac{1}{\|\nabla p\|}\nabla p$ is the upwind direction given by the pressure gradient. Here, we evaluate $\mathbf{v}^+, \mathbf{v}^-$ and p^+, p^- using FPM's approximation tools (east squares approximation) at the upstream location

$$
\begin{aligned}
p^+(\mathbf{x}) &= \tilde{p}(\mathbf{x} + \alpha h\mathbf{n}) \quad & p^-(\mathbf{x}) &= \tilde{p}(\mathbf{x} - \alpha h\mathbf{n}) \\
\mathbf{v}^+(\mathbf{x}) &= \tilde{\mathbf{v}}(\mathbf{x} + \alpha h\mathbf{n}) \quad & \mathbf{v}^-(\mathbf{x}) &= \tilde{\mathbf{v}}(\mathbf{x} - \alpha h\mathbf{n})
\end{aligned}
\tag{2.2}
$$

where α is the upwind parameter that defines the relative distance (compared to smoothing length h) to go upstream in order to evaluate the upwind quantities.

The derivatives of the upwind quantities are consequently

$$
\begin{aligned}
\tilde{\nabla}\overline{p} &= \tilde{\nabla}p - \tilde{\nabla}\left(\frac{\rho c}{2}\right)\left(\mathbf{v}^+ - \mathbf{v}^-\right)^T \mathbf{n} - \frac{\rho c}{2}\left(\left(\tilde{\nabla}\left(\mathbf{v}^{+T}\mathbf{n}\right) - \tilde{\nabla}\left(\mathbf{v}^{-T}\mathbf{n}\right)\right)\right) \\
\tilde{\nabla}^T\overline{\mathbf{v}} &= \tilde{\nabla}^T\mathbf{v} - \tilde{\nabla}^T\left(\frac{1}{2\rho c}\right)\left(p^+ - p^-\right)\mathbf{n} - \frac{1}{2\rho c}\left(\tilde{\nabla}^T p^+ - \tilde{\nabla}^T p^-\right)\mathbf{n}
\end{aligned}
\tag{2.3}
$$

3 Simplified, fast upwind formulation

The upwind scheme of section 2 has a major drawback: the evaluation of physical quantities at the locations $\mathbf{x}^+ = \mathbf{x} + \alpha h \mathbf{n}$ and $\mathbf{x}^- = \mathbf{x} - \alpha h \mathbf{n}$. Depending on the upwind direction $\mathbf{n}$, these locations might be outside of the flow domain. The idea of the simplified scheme is to approximate the upwind values by first order Tylor series expansion.

$$\begin{aligned} \overline{p} &= p - \rho c L\left(\mathbf{n}^T \tilde{\nabla}\left(\mathbf{v}^T \mathbf{n}\right)\right) = p - \rho c L\left(n_x^2 u_{\tilde{x}} + n_y^2 v_{\tilde{y}} + n_z^2 w_{\tilde{z}} + \Phi_{mixed}\right) \\ \overline{\mathbf{v}} &= \mathbf{v} - \frac{L}{\rho c}\tilde{\nabla} p \end{aligned} \tag{3.1}$$

where

$L = \alpha h$ is the upwind step size,

$\Phi_{mixed} = n_x n_y v_{\tilde{x}} + n_x n_z w_{\tilde{x}} \quad + \quad n_y n_x u_{\tilde{y}} + n_y n_z w_{\tilde{y}} \quad + \quad n_z n_x u_{\tilde{z}} + n_z n_y v_{\tilde{z}}$ are mixed terms we assume to be of minor importance and therefore neglect them.

The derivatives of the upwind quantities are then

$$\begin{aligned} \tilde{\nabla}\overline{p} &= \tilde{\nabla} p - \tilde{\nabla}\left(\rho c L\right)\left(n_x^2 u_{\tilde{x}} + n_y^2 v_{\tilde{y}} + n_z^2 w_{\tilde{z}}\right) - \left(\rho c L\right)\left(n_x^2 \begin{pmatrix} u_{\tilde{x}\tilde{x}} \\ u_{\tilde{x}\tilde{y}} \\ u_{\tilde{x}\tilde{z}} \end{pmatrix} + n_y^2 \begin{pmatrix} v_{\tilde{y}\tilde{x}} \\ v_{\tilde{y}\tilde{y}} \\ v_{\tilde{y}\tilde{z}} \end{pmatrix} + n_z^2 \begin{pmatrix} w_{\tilde{z}\tilde{x}} \\ w_{\tilde{z}\tilde{y}} \\ w_{\tilde{z}\tilde{z}} \end{pmatrix}\right) \\ \tilde{\nabla}^T \overline{\mathbf{v}} &= \tilde{\nabla}^T \mathbf{v} - \tilde{\nabla}^T\left(\frac{L}{\rho c}\tilde{\nabla} p\right) \end{aligned} \tag{3.2}$$

4 More simplified, fast upwind scheme

In equations (3.1) ff. , the pressure formulation is difficult. However, one could further simplify

$$\begin{aligned} \overline{p} &= p - \rho c L\left(\tilde{\nabla}^T \mathbf{v}\right) \\ \overline{\mathbf{v}} &= \mathbf{v} - \frac{L}{\rho c}\tilde{\nabla} p \end{aligned} \tag{4.1}$$

With this we are on the safe side, the damping in (3.1) would only be smaller by magnitude, never bigger.

The derivatives of the upwind quantities are now

$$\tilde{\nabla}\overline{p} = \tilde{\nabla}p - \tilde{\nabla}\left(q\left(\tilde{\nabla}^T\mathbf{v}\right)\right) = \tilde{\nabla}p - \tilde{\nabla}^T\left(q\left(\tilde{\nabla}\mathbf{v}\right)\right) - \tilde{\nabla}\times\left(q\left(\tilde{\nabla}\times\mathbf{v}\right)\right) - \begin{pmatrix} q_x v_y - q_y v_x + q_x w_z - q_z w_x \\ q_y u_x - q_x u_y + q_y w_z - q_z w_y \\ q_z u_x - q_x u_z + q_z v_y - q_y v_z \end{pmatrix}$$

$$\tilde{\nabla}^T\overline{\mathbf{v}} = \tilde{\nabla}^T\mathbf{v} - \tilde{\nabla}^T\left(\frac{L}{\rho c}\tilde{\nabla}p\right)$$

where $q = \rho c L$ is simply a shortcut for more compact writing.

With this scheme we are able to prove/show the existence of mathematical damping in the upwind schemes. It is obvious that with the terms $\tilde{\nabla}^T\left(\rho c L\left(\tilde{\nabla}\mathbf{v}\right)\right)$ and $\tilde{\nabla}^T\left(\frac{L}{\rho c}\tilde{\nabla}p\right)$ we have mathematical damping for velocity and pressure, which act as stabilization of the scheme.

5 Quasi-implicit scheme

The fascinating thing comes now. We will show that with a semi-implicit formulation we find the same upwind quantities as in section 4.

From section 1, we have (after slight modifications) the total time derivatives of velocity and pressure by

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{dt}}p + \rho c^2 \cdot \nabla^T\mathbf{v} &= 0 \\ \tfrac{\mathrm{d}}{\mathrm{dt}}\mathbf{v} + \frac{1}{\rho}\nabla p &= 0 \end{aligned}$$

In order to come up with a quasi-implicit scheme, we look slightly into the future, for example we could establish a first order (in time) scheme by

$$\begin{aligned} \frac{\rho^{n+1} - \rho^n}{\Delta t} + \rho\cdot\nabla^T\mathbf{v}^{n+1} &= 0 \\ \frac{\rho\mathbf{v}^{n+1} - \rho\mathbf{v}^n}{\Delta t} + \left(\rho\mathbf{v}\right)\cdot\nabla^T\mathbf{v}^{n+1} + \nabla p^{n+1} &= 0 \\ \frac{\rho E^{n+1} - \rho E^n}{\Delta t} + \left(\rho E\right)\cdot\nabla^T\mathbf{v}^{n+1} + \nabla^T\left(p^{n+1}\cdot\mathbf{v}^{n+1}\right) &= 0 \end{aligned}$$

We might not want to use $\mathbf{v}^{n+1}$ and p^{n+1}, but the values after a certain, intermediate time step size τ, i.e.

$$
\begin{aligned}
&\frac{\rho^{n+1}-\rho^{n}}{\Delta t}+\rho\cdot\nabla^{T}\mathbf{v}_{\tau} \;=\; 0\\
&\frac{\rho\mathbf{v}^{n+1}-\rho\mathbf{v}^{n}}{\Delta t}+(\rho\mathbf{v})\cdot\nabla^{T}\mathbf{v}_{\tau}+\nabla p_{\tau}=0\\
&\frac{\rho E^{n+1}-\rho E^{n}}{\Delta t}+(\rho E)\cdot\nabla^{T}\mathbf{v}_{\tau}+\nabla^{T}\left(p_{\tau}\cdot\mathbf{v}_{\tau}\right) \;=\; 0
\end{aligned}
$$

with $\mathbf{v}_{\tau}=\left(\mathbf{v}^{n}-\frac{\tau}{\rho}\nabla p\right)$ and $p_{\tau}=p^{n}-\tau\rho c^{2}\cdot\nabla^{T}\mathbf{v}$. This gives rise to the general scheme

$$
\begin{aligned}
&\frac{d\rho}{dt}+\rho\cdot\nabla^{T}\mathbf{v}_{\tau} \;=\; 0\\
&\frac{d(\rho\mathbf{v})}{dt}+(\rho\mathbf{v})\cdot\nabla^{T}\mathbf{v}_{\tau}+\nabla p_{\tau}=0\\
&\frac{d(\rho E)}{dt}+(\rho E)\cdot\nabla^{T}\mathbf{v}_{\tau}+\nabla^{T}\left(p_{\tau}\cdot\mathbf{v}_{\tau}\right) \;=\; 0
\end{aligned}
$$

If we base the implicit time shift τ on the sound speed and the smoothing length with the proportionality factor α, then we have $\tau=\alpha\frac{h}{c}$ and obtain

$$
\begin{aligned}
p_{\tau}&=p-\alpha h\rho c\cdot\nabla^{T}\mathbf{v}=p-L\rho c\cdot\nabla^{T}\mathbf{v}\\
\mathbf{v}_{\tau}&=\left(\mathbf{v}-\frac{\alpha h}{\rho c}\nabla p\right)=\left(\mathbf{v}-\frac{L}{\rho c}\nabla p\right)
\end{aligned}
$$

Please compare with section 4. We see that p_{τ} and $\overline{p}$ are similar, as well as $\mathbf{v}_{\tau}$ and $\overline{\mathbf{v}}$ are similar.

6 Generalization

There are two principle upwind methods:

6.1 Method 1 (original method)

$$
\begin{aligned}
\overline{p}_{orig}&=p-\frac{\rho c}{2}\left(\mathbf{v}^{+}-\mathbf{v}^{-}\right)^{T}\mathbf{n}\quad\text{with } \mathbf{v}^{+}(\mathbf{x})=\tilde{\mathbf{v}}(\mathbf{x}+\alpha h\mathbf{n})\;\text{ and }\;\mathbf{v}^{-}(\mathbf{x})=\tilde{\mathbf{v}}(\mathbf{x}-\alpha h\mathbf{n})\\
\overline{\mathbf{v}}_{orig}&=\mathbf{v}-\frac{1}{2\rho c}\left(p^{+}-p^{-}\right)\mathbf{n}\quad\text{with } p^{+}(\mathbf{x})=\tilde{p}(\mathbf{x}+\alpha h\mathbf{n})\;\text{ and }\;p^{-}(\mathbf{x})=\tilde{p}(\mathbf{x}-\alpha h\mathbf{n})
\end{aligned}
\qquad (6.1)
$$

With

αh the upwind step length

$\mathbf{n} = \frac{1}{\|\nabla p\|}\nabla p$ the upwind direction

6.2 Method 2 (simplified)

$$\begin{aligned} \overline{p}_{simp} &= p - \rho c L\left(\tilde{\nabla}^T \mathbf{v}\right) \\ \overline{\mathbf{v}}_{simp} &= \mathbf{v} - \frac{L}{\rho c}\tilde{\nabla} p \end{aligned} \tag{6.2}$$

With

$L = \begin{cases} \text{either } \beta \cdot \Delta t \cdot c \\ \text{or} \quad \gamma \cdot h \end{cases}$ the upwind step length (needed in the Tylor series expansion)

6.3 Combined method

We can bring both methods together into one

$$\begin{aligned} \overline{p}_{general} &= p - \frac{\rho c}{2}\left(\mathbf{v}^{+} - \mathbf{v}^{-}\right)^T \mathbf{n} - \rho c L\left(\tilde{\nabla}^T \mathbf{v}\right) \\ \overline{\mathbf{v}}_{general} &= \mathbf{v} - \frac{1}{2\rho c}\left(p^{+} - p^{-}\right)\mathbf{n} - \frac{L}{\rho c}\tilde{\nabla} p \end{aligned} \tag{6.3}$$

How are the upwind lengths chosen?

FPM1 (original)

$\alpha = 0.2$

$L = 0$

FPM1 (simplified – implemented in VPS)

$\alpha = 0$

$\beta = 0$

$\gamma = 0.2$

FPM3

$$\alpha = 0$$

$$\beta = \begin{cases} 0.5 & if \quad \nabla^T \mathbf{v} > 0 \ \ \text{(rarefaction)} \\ 0 & \text{elsewise} \end{cases}$$

$$\gamma = \begin{cases} 0.0 & if \quad \nabla^T \mathbf{v} > 0 \ \ \text{(rarefaction)} \\ 0.2 & \text{elsewise} \end{cases}$$

7 Conclusions

- The upwind formulation induces proper mathematical damping terms.

- The quasi-implicit formulation is similar to the upwind formulation $\Leftrightarrow$ the upwind formulation is similar to the quasi-implicit formulation. Both formulations can be combined into a generalized upwind function.

8 Literature

[1] Jörg Kuhnert, „General Smoothed Particle Hydrodynamics", dissertation, University of Kaiserslautern, 1999