Gas Dynamics and Heat and Mass Transfer

Fractional Step Method

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1 Theoretical background

Theorem 1.1 (Helmholtz–Hodge FSM)**.** Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with smooth boundary. Let $\boldsymbol{\omega}\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ be a vector field. Then there exist a smooth function $\varphi\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}$ and a divergence-less smooth vector field $\mathbf{a}\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ such that

$$\boldsymbol{\omega} = \mathbf{a} + \boldsymbol{\nabla}\varphi$$

In addition,

$$\mathbf{a} \cdot \boldsymbol{\nu} = 0 \quad \text{on } \partial\Omega$$

where $\boldsymbol{\nu}$ denotes the outer normal vector to $\partial\Omega$.

Theorem 1.2 (Helmholtz–Hodge)**.** Let $D \subset \mathbb{R}^3$ be a bounded domain. Then every smooth vector field $\mathbf{F}\colon D \to \mathbb{R}^3$ can be decomposed into a sum $\mathbf{F} = \mathbf{F}_1 + \mathbf{F}_2$, where $\mathbf{F}_1$ is an irrotational field and $\mathbf{F}_2$ is a solenoidal field.

Theorem 1.3 (Helmholtz–Hodge)**.** Let $\Omega \subset \mathbb{R}^3$ be a contractible bounded open set with smooth boundary. Let $F\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ be a $\mathcal{C}^\infty(\Omega)$ vector field. Then there exist a function $f \in \mathcal{C}^\infty(\Omega, \mathbb{R})$ and a vector field $H \in \mathcal{C}^\infty(\Omega, \mathbb{R}^3)$ such that

$$F = \boldsymbol{\nabla} f + \boldsymbol{\nabla} \times H$$

Theorem 1.4. Let $\Omega \subset \mathbb{R}^3$ be a contractible bounded open set with smooth boundary. Let $G\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ be a divergence–free $\mathcal{C}^\infty(\Omega)$ vector field, that is to say, $\boldsymbol{\nabla} \cdot G = 0$. Then there exists a $\mathcal{C}^\infty(\Omega)$ vector field $g\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ such that $\boldsymbol{\nabla} \times g = G$.

Notice that the previous theorem says nothing about the uniqueness of the field g.

Assume F is the Schwartz space

Then see Griffith's of Helmholtz's theorem

2 Fractional step method (FSM)

Hereinafter, it is assumed that the studied problems occur in a contractible bounded open set $\Omega \subset \mathbb{R}^3$ with smooth boundary. Besides, these problems last for finite time, that is to say, the time interval is $I = [t_0, t_f] \subset \mathbb{R}$.

2.1 First approach to the FSM

Time integration of the incompressible Navier–Stokes equations

Recall that the Navier–Stokes equations (NS) for an incompressible flow are

$$\begin{cases} \boldsymbol{\nabla} \cdot \mathbf{v} = 0 \\ \rho \dfrac{\partial \mathbf{v}}{\partial t} + (\rho \mathbf{v} \cdot \nabla)\mathbf{v} = -\boldsymbol{\nabla} p + \mu \, \Delta \mathbf{v} \end{cases} \tag{2.1}$$

where $\mathbf{v} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k}$. By defining the operator

$$\mathbf{R}(\mathbf{v}) = \mu \, \Delta \mathbf{v} - (\rho \mathbf{v} \cdot \nabla)\mathbf{v}$$

these equations may be rewritten as

$$\begin{cases} \boldsymbol{\nabla} \cdot \mathbf{v} = 0 \\ \rho \dfrac{\partial \mathbf{v}}{\partial t} = \mathbf{R}(\mathbf{v}) - \boldsymbol{\nabla} p \end{cases} \tag{2.2}$$

Time integration of the continuity equation yields

$$\begin{aligned} \int_{t^n}^{t^{n+1}} \boldsymbol{\nabla} \cdot \mathbf{v} \, \mathrm{d}t &= \int_{t^n}^{t^{n+1}} (u_x + v_y + w_z) \, \mathrm{d}t \\ &= \left\{ \beta \left(u_x^{n+1} + v_y^{n+1} + w_z^{n+1} \right) + (1 - \beta) \left(u_x^n + v_y^n + w_z^n \right) \right\} \Delta t \\ &= \left\{ \beta (\boldsymbol{\nabla} \cdot \mathbf{v})^{n+1} + (1 - \beta)(\boldsymbol{\nabla} \cdot \mathbf{v})^n \right\} \Delta t = 0 \end{aligned}$$

where $\beta \in \{0, 0.5, 1\}$ depends upon the selected integration scheme. The implicit scheme ($\beta = 1$) is enough, whence

$$\int_{t^n}^{t^{n+1}} \boldsymbol{\nabla} \cdot \mathbf{v} \, \mathrm{d}t = (\boldsymbol{\nabla} \cdot \mathbf{v})^{n+1} \, \Delta t = 0$$

and, since $\Delta t > 0$, the time–integrated continuity equation is obtained:

$$(\boldsymbol{\nabla} \cdot \mathbf{v})^{n+1} = \boldsymbol{\nabla} \cdot \mathbf{v}^{n+1} = 0 \tag{2.3}$$

Time integration of the momentum equation over $[t^n, t^{n+1}]$ gives

$$\int_{t^n}^{t^{n+1}} \rho \frac{\partial \mathbf{v}}{\partial t} \, \mathrm{d}t = \int_{t^n}^{t^{n+1}} \mathbf{R}(\mathbf{v}) \, \mathrm{d}t - \int_{t^n}^{t^{n+1}} \boldsymbol{\nabla} p \, \mathrm{d}t$$

The evaluation of the first term is exact:

$$\int_{t^n}^{t^{n+1}} \rho \frac{\partial \mathbf{v}}{\partial t} \, \mathrm{d}t = \rho \int_{t^n}^{t^{n+1}} \frac{\partial \mathbf{v}}{\partial t} \, \mathrm{d}t = \rho \, [\mathbf{v}]_{t^n}^{t^{n+1}} = \rho(\mathbf{v}^{n+1} - \mathbf{v}^n)$$

In order to compute the second integral, the two–step Adams–Bashforth method is used as follows:

$$\int_{t^n}^{t^{n+1}} \mathbf{R}(\mathbf{v})\,\mathrm{d}t = \frac{\Delta t}{2}\left\{3\mathbf{R}(\mathbf{v}^n) - \mathbf{R}(\mathbf{v}^{n-1}) + \mathcal{O}(\Delta t^2)\right\}$$

Finally, the third term is evaluated using an implicit integration scheme:

$$\int_{t^n}^{t^{n+1}} \boldsymbol{\nabla} p\,\mathrm{d}t = \left\{\beta(\boldsymbol{\nabla} p)^{n+1} + (1-\beta)(\boldsymbol{\nabla} p)^n + \mathcal{O}(\Delta t)\right\}\Delta t = (\boldsymbol{\nabla} p)^{n+1}\,\Delta t = \boldsymbol{\nabla} p^{n+1}\,\Delta t$$

Therefore, the integrated time–equation is

$$\rho\frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \frac{3}{2}\mathbf{R}(\mathbf{v}^n) - \frac{1}{2}\mathbf{R}(\mathbf{v}^{n-1}) - \boldsymbol{\nabla} p^{n+1} \tag{2.4}$$

Application of the Helmholtz–Hodge theorem

In order to remove $\boldsymbol{\nabla} p^{n+1}$ from (2.4), the equation may be rearranged as

$$\rho\frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} + \boldsymbol{\nabla} p^{n+1} = \rho\frac{\mathbf{v}^{n+1} + \dfrac{\Delta t}{\rho}\boldsymbol{\nabla} p^{n+1} - \mathbf{v}^n}{\Delta t} = \frac{3}{2}\mathbf{R}(\mathbf{v}^n) - \frac{1}{2}\mathbf{R}(\mathbf{v}^{n-1}) \tag{2.5}$$

Now by defining the vector field

$$\mathbf{v}^p = \mathbf{v}^{n+1} + \frac{\Delta t}{\rho}\boldsymbol{\nabla} p^{n+1} \tag{2.6}$$

equation (2.5) becomes

$$\rho\frac{\mathbf{v}^p - \mathbf{v}^n}{\Delta t} = \frac{3}{2}\mathbf{R}(\mathbf{v}^n) - \frac{1}{2}\mathbf{R}(\mathbf{v}^{n-1}) \tag{2.7}$$

Equation (2.6) states that the vector field $\mathbf{v}^p\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ can be expressed as the sum of the divergence–free vector field $\mathbf{v}^{n+1}$ and the gradient $\boldsymbol{\nabla}\left(\frac{\Delta t}{\rho} p^{n+1}\right)$. By the Helmholtz–Hodge theorem, the decomposition of $\mathbf{v}^p$ is unique. Applying the divergence operator on both sides of (2.6) and using equation (2.3) yields

$$\boldsymbol{\nabla}\cdot\mathbf{v}^p = \frac{\Delta t}{\rho}\boldsymbol{\nabla}\cdot\boldsymbol{\nabla} p^{n+1}$$

whence a Poisson equation for the pressure is found:

$$\Delta p^{n+1} = \frac{\rho}{\Delta t}\boldsymbol{\nabla}\cdot\mathbf{v}^p$$

Whenever the pressure on the boundary of Ω is given by a known function $P\colon \partial\Omega \to \mathbb{R}$, the following Cauchy problem can be posed:

$$\begin{cases} \Delta p^{n+1} = \dfrac{\rho}{\Delta t}\boldsymbol{\nabla}\cdot\mathbf{v}^p & \text{in } \Omega \\ p^{n+1} = P & \text{on } \partial\Omega \end{cases} \tag{2.8}$$

Existence and uniqueness of the problem

Finally, the velocity at time t^{n+1} is given by

$$\mathbf{v}^{n+1} = \mathbf{v}^p - \frac{\Delta t}{\rho}\boldsymbol{\nabla} p^{n+1} \tag{2.9}$$

Algorithm 1 Fractional Step Method – First approach

1. Evaluation of $\mathbf{R}(\mathbf{v}^n)$
2. Evaluation of $\mathbf{v}^p$:
$$\mathbf{v}^p = \mathbf{v}^n + \frac{\Delta t}{\rho}\left[\frac{3}{2}\mathbf{R}(\mathbf{v}^n) - \frac{1}{2}\mathbf{R}(\mathbf{v}^{n-1})\right]$$
3. Solve the problem
$$\begin{cases} \Delta p^{n+1} = \dfrac{\rho}{\Delta t}\boldsymbol{\nabla}\cdot\mathbf{v}^p & \text{in } \Omega \\ p^{n+1} = P & \text{on } \partial\Omega \end{cases}$$
4. Compute $\mathbf{v}^{n+1}$:
$$\mathbf{v}^{n+1} = \mathbf{v}^p - \frac{\Delta t}{\rho}\boldsymbol{\nabla} p^{n+1}$$

Algorithm

2.2 The checkerboard problem

Notice that (2.9) is a vector equation, hence expanding it by components gives:

$$\begin{cases} u^{n+1} = u^p - \dfrac{\Delta t}{\rho} p_x^{n+1} \\ v^{n+1} = v^p - \dfrac{\Delta t}{\rho} p_y^{n+1} \\ w^{n+1} = w^p - \dfrac{\Delta t}{\rho} p_z^{n+1} \end{cases} \tag{2.10}$$

Consider the discretization of the x–component of (2.10):

$$u_P^{n+1} = u_P^p - \frac{\Delta t}{\rho}\left(\frac{p_E^{n+1} - p_W^{n+1}}{2\,\Delta x}\right) \tag{2.11}$$

Notice that the discrete approximation of $\boldsymbol{\nabla} p^{n+1}$ is independent of p_P^{n+1}.