MÉTODO DOS VOLUMES FINITOS APLICADO EM EQUAÇÕES DE CONSERVAÇÃO UNIDIMENSIONAIS

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Sumário

1 Equação da Difusão de Energia

Será aplicado o método dos volumes finitos na equação da difusão como descrito no capítulo 4 de Versteeg e Malalasekera (2007) .

1.1 Volume de Controle

A Fig. 1, ilustra o volume de controle que será adotado para a discretização das equações médias de transporte. O subíndice k representa o elemento discreto de uma tubulação na direção z. As variáveis A_k, S_k e r_k representam, respectimvamente, a área transversal ao escomanto, a superfície lateral e o raio do elemento discreto. O termo $q_{m_{c,p}}$ representa a vazão mássica do componente c na fase p por unidade de volume.

De acordo com a Fig. 1, é possível definir os seguintes termos:

$$dV_k = \pi r_k^2 \Delta z_k \tag{1.1}$$

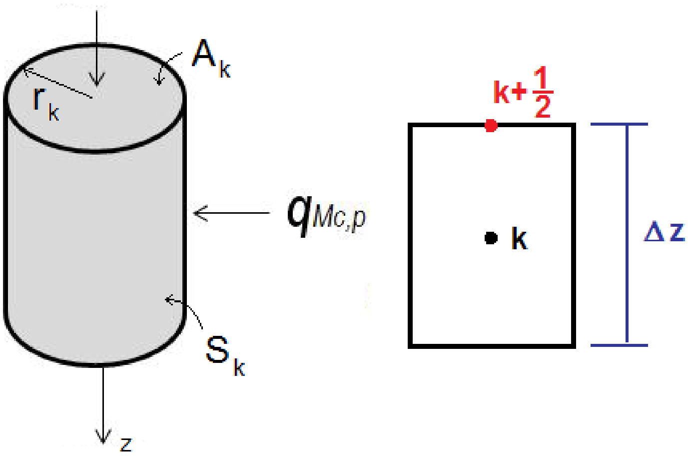

Figura 1: Volume de Controle Unidimensional.

$$A_k = \pi r_k^2 \tag{1.2}$$

$$dS_k = 2\pi r_k \Delta z_k \tag{1.3}$$

1.2 Equação da Difusão

A equação da difusão de energia é dada por:

$$-\nabla \cdot (\kappa \nabla \phi) = S_\phi \tag{1.4}$$

onde κ é a condutividade térmica do fluido, T é a temperatura e S_ϕ é o termo fonte de energia. Integrando no volume de controle:

$$-\iiint\limits_{\text{V.C.}} \nabla \cdot (\kappa \nabla \phi)\, dV = \iiint\limits_{\text{V.C.}} S_\phi dV \tag{1.5}$$

Aplicando o teorema de Gauss:

$$\iiint\limits_{\text{S.C.}} (\kappa \nabla \phi) \cdot \vec{n} dS + \iiint\limits_{\text{V.C.}} S_\phi dV = 0 \tag{1.6}$$

Utilizando o volume de controle unidimensional:

$$-\left[\left(A\kappa \frac{\partial \phi}{\partial x}\right)_{k+\frac{1}{2}} - \left(A\kappa \frac{\partial \phi}{\partial x}\right)_{k-\frac{1}{2}}\right] = (AS_\phi \Delta x)_k \tag{1.7}$$

O termo de derivada será calculado utilizando uma aproximação por diferenças simples, assim:

$$-(A\kappa)_{k+\frac{1}{2}} \frac{\phi_{k+1} - \phi_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} + (A\kappa)_{k-\frac{1}{2}} \frac{\phi_k - \phi_{k-1}}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})} = (AS_\phi \Delta x)_k \tag{1.8}$$

Organizando a equação:

$$
\begin{aligned}
&-(A\kappa)_{k+\frac{1}{2}}\,\frac{\phi_{k+1}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_{k}\right)}+(A\kappa)_{k+\frac{1}{2}}\,\frac{\phi_{k}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_{k}\right)}\\
&\qquad+(A\kappa)_{k-\frac{1}{2}}\,\frac{\phi_{k}}{\frac{1}{2}\left(\Delta x_{k}+\Delta x_{k-1}\right)}-(A\kappa)_{k-\frac{1}{2}}\,\frac{\phi_{k-1}}{\frac{1}{2}\left(\Delta x_{k}+\Delta x_{k-1}\right)}=\left(AS_{\phi}\Delta x\right)_{k}
\end{aligned}
\tag{1.9}
$$

$$
\begin{aligned}
&-2\,(A\kappa)_{k+\frac{1}{2}}\,\frac{\phi_{k+1}}{\left(\Delta x_{k+1}+\Delta x_{k}\right)}+2\,(A\kappa)_{k+\frac{1}{2}}\,\frac{\phi_{k}}{\left(\Delta x_{k+1}+\Delta x_{k}\right)}\\
&\qquad+2\,(A\kappa)_{k-\frac{1}{2}}\,\frac{\phi_{k}}{\left(\Delta x_{k}+\Delta x_{k-1}\right)}-2\,(A\kappa)_{k-\frac{1}{2}}\,\frac{\phi_{k-1}}{\left(\Delta x_{k}+\Delta x_{k-1}\right)}=\left(AS_{\phi}\Delta x\right)_{k}
\end{aligned}
\tag{1.10}
$$

$$
\begin{aligned}
&-\frac{2\,(A\kappa)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_{k}\right)}\phi_{k+1}+\left(\frac{2\,(A\kappa)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_{k}\right)}+\frac{2\,(A\kappa)_{k-\frac{1}{2}}}{\left(\Delta x_{k}+\Delta x_{k-1}\right)}\right)\phi_{k}\\
&\qquad\qquad-\frac{2\,(A\kappa)_{k-\frac{1}{2}}}{\left(\Delta x_{k}+\Delta x_{k-1}\right)}\phi_{k-1}=\left(AS_{\phi}\Delta x\right)_{k}
\end{aligned}
\tag{1.11}
$$

O termo $(A\kappa)_{i\pm\frac{1}{2}}$ será calculado segundo uma interpolação do tipo esquema centrado.

2 Equação Convectiva e Difusiva

Será aplicado o método dos volumes finitos em equações de difusão e convecção como descrito no capítulo 5 de Versteeg e Malalasekera (2007) .

2.1 Equação da Difusão e Convecção

A equação da convecção e difusão é dada por:

$$\nabla \cdot (\rho \vec{v} \phi) = \nabla \cdot (\kappa \nabla \phi) + S_\phi \tag{2.1}$$

onde κ é o coeficiente de difusão, ϕ é a propriedade transportada, $\vec{v}$ é a velocidade do escoamento e S_ϕ é o termo fonte de energia. Integrando no volume de controle:

$$\iiint\limits_{\text{V.C.}} \nabla \cdot (\rho \vec{v} \phi)\, dV = \iiint\limits_{\text{V.C.}} \nabla \cdot (\kappa \nabla \phi)\, dV + \iiint\limits_{\text{V.C.}} S_\phi dV \tag{2.2}$$

Aplicando o teorema de Gauss:

$$\iiint\limits_{\text{S.C.}} (\rho \vec{v} \phi) \cdot \vec{n} dS = \iiint\limits_{\text{S.C.}} (\kappa \nabla \phi) \cdot \vec{n} dS + \iiint\limits_{\text{V.C.}} S_\phi dV \tag{2.3}$$

Utilizando o volume de controle unidimensional:

$$(A\rho \vec{v} \phi)_{k+\frac{1}{2}} - (A\rho \vec{v} \phi)_{k-\frac{1}{2}} = \left(A\kappa \frac{\partial \phi}{\partial x} \right)_{k+\frac{1}{2}} - \left(A\kappa \frac{\partial \phi}{\partial x} \right)_{k-\frac{1}{2}} + (AS_\phi \Delta x)_k \tag{2.4}$$

O termo de derivada será calculado utilizando uma aproximação por diferenças simples, assim:

$$(A\rho\vec{v}\phi)_{k+\frac{1}{2}} - (A\rho\vec{v}\phi)_{k-\frac{1}{2}} = (A\kappa)_{k+\frac{1}{2}} \frac{\phi_{k+1} - \phi_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} - (A\kappa)_{k-\frac{1}{2}} \frac{\phi_k - \phi_{k-1}}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})} + (AS_\phi \Delta x)_k \tag{2.5}$$

Para se calcular a Equação 2.5 deverá se utilizar um metodo adequado de interpolação. Para a escolha do método deverá se analizar o número de Peclet, dado por:

$$P_e = \frac{C_{conv.}}{C_{dif}} = \frac{A\rho u}{\frac{A\kappa}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})}} \tag{2.6}$$

Para baixos números de Peclet o esquema de diferenças centrais é apropriado. Para altos números de Peclet o esquema Upwind é o mais apropriado. Ver Capítulo 5 de (VERSTEEG; MALALASEKERA, 2007) para maiores informações.

2.2 Método CDS para $\vec{v}$ e ϕ

O método CDS é recomendado para escoamentos com baixo números de Peclet. Utilizando a interpolação por diferenças simples (CDS) para $\vec{v}$ e ϕ:

$$\begin{aligned}(A\rho\vec{v})_{k+\frac{1}{2}} (\phi)_{k+\frac{1}{2}} - (A\rho\vec{v})_{k-\frac{1}{2}} (\phi)_{k-\frac{1}{2}} = \\ (A\kappa)_{k+\frac{1}{2}} \frac{\phi_{k+1} - \phi_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} - (A\kappa)_{k-\frac{1}{2}} \frac{\phi_k - \phi_{k-1}}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})} + (AS_\phi \Delta x)_k\end{aligned} \tag{2.7}$$

$$\begin{aligned}(A\rho\vec{v})_{k+\frac{1}{2}} \frac{\phi_{k+1} + \phi_k}{2} - (A\rho\vec{v})_{k-\frac{1}{2}} \frac{\phi_k + \phi_{k-1}}{2} = \\ (A\kappa)_{k+\frac{1}{2}} \frac{\phi_{k+1} - \phi_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} - (A\kappa)_{k-\frac{1}{2}} \frac{\phi_k - \phi_{k-1}}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})} + (AS_\phi \Delta x)_k\end{aligned} \tag{2.8}$$

Rearranjando os termos da equação:

$$\begin{aligned}\frac{1}{2}(A\rho\vec{v})_{k+\frac{1}{2}} \phi_{k+1} + \frac{1}{2}(A\rho\vec{v})_{k+\frac{1}{2}} \phi_k - \frac{1}{2}(A\rho\vec{v})_{k-\frac{1}{2}} \phi_k - \frac{1}{2}(A\rho\vec{v})_{k-\frac{1}{2}} \phi_{k-1} \\ = (A\kappa)_{k+\frac{1}{2}} \frac{\phi_{k+1}}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} - (A\kappa)_{k+\frac{1}{2}} \frac{\phi_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} \\ - (A\kappa)_{k-\frac{1}{2}} \frac{\phi_k}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})} + (A\kappa)_{k-\frac{1}{2}} \frac{\phi_{k-1}}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})} + (AS_\phi \Delta x)_k\end{aligned} \tag{2.9}$$

$$\left[-\frac{1}{2}\left(A\rho\vec{v}\right)_{k-\frac{1}{2}}-\frac{2\left(A\kappa\right)_{k-\frac{1}{2}}}{\left(\Delta x_k+\Delta x_{k-1}\right)}\right]\phi_{k-1} + \left[\frac{1}{2}\left(A\rho\vec{v}\right)_{k+\frac{1}{2}}-\frac{1}{2}\left(A\rho\vec{v}\right)_{k-\frac{1}{2}}+\frac{2\left(A\kappa\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_k\right)}+\frac{2\left(A\kappa\right)_{k-\frac{1}{2}}}{\left(\Delta x_k+\Delta x_{k-1}\right)}\right]\phi_k + \left[\frac{1}{2}\left(A\rho\vec{v}\right)_{k+\frac{1}{2}}-\frac{2\left(A\kappa\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_k\right)}\right]\phi_{k+1}=\left(AS_\phi\Delta x\right)_k \quad (2.10)$$

Assim:

$$L_k\phi_{k-1}+C_k\phi+R_k\phi_{k+1}=\left(AS_\phi\Delta x\right)_k \quad (2.11)$$

onde:

$$L_k=-\frac{1}{2}\left(A\rho\vec{v}\right)_{k-\frac{1}{2}}-\frac{2\left(A\kappa\right)_{k-\frac{1}{2}}}{\left(\Delta x_k+\Delta x_{k-1}\right)} \quad (2.12)$$

$$R_k=\frac{1}{2}\left(A\rho\vec{v}\right)_{k+\frac{1}{2}}-\frac{2\left(A\kappa\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_k\right)} \quad (2.13)$$

$$C_k=\frac{1}{2}\left(A\rho\vec{v}\right)_{k+\frac{1}{2}}-\frac{1}{2}\left(A\rho\vec{v}\right)_{k-\frac{1}{2}}+\frac{2\left(A\kappa\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_k\right)}+\frac{2\left(A\kappa\right)_{k-\frac{1}{2}}}{\left(\Delta x_k+\Delta x_{k-1}\right)} \quad (2.14)$$

2.3 Método CDS para $\vec{v}$ e UDS para ϕ

O método UDS é recomendado para escoamentos com altos valores do número de Peclet. Utilizando a interpolação pos diferenças centradas para $\vec{v}$ e a interpolação pelo esquema Upwind de primeira ordem UDS para ϕ, o termo $\phi_{k+\frac{1}{2}}$ pode ser expresso como:

$$\phi_{k+\frac{1}{2}}=\phi_k, \quad v_k\geq 0 \quad (2.15)$$

$$\phi_{k+\frac{1}{2}}=\phi_{k+1}, \quad v_k<0 \quad (2.16)$$

Já o termo $\phi_{k-\frac{1}{2}}$ pode ser expresso como:

$$\phi_{k-\frac{1}{2}} = \phi_{k-1}, \quad v_k \geq 0 \tag{2.17}$$

$$\phi_{k-\frac{1}{2}} = \phi_{k}, \quad v_k < 0 \tag{2.18}$$

2.3.1 Velocidades Positivas ($\vec{v_k} \geq 0$)

Para velocidades positivas a Equação 2.5 pode ser escrita como:

$$\begin{aligned}(A\rho\vec{v})_{k+\frac{1}{2}}(\phi)_{k+\frac{1}{2}} - (A\rho\vec{v})_{k-\frac{1}{2}}(\phi)_{k-\frac{1}{2}} = (A\kappa)_{k+\frac{1}{2}}\frac{\phi_{k+1}-\phi_k}{\frac{1}{2}(\Delta x_{k+1}+\Delta x_k)} \\ - (A\kappa)_{k-\frac{1}{2}}\frac{\phi_{k}-\phi_{k-1}}{\frac{1}{2}(\Delta x_{k}+\Delta x_{k-1})} + (AS_\phi\Delta x)_k\end{aligned} \tag{2.19}$$

$$\begin{aligned}(A\rho\vec{v})_{k+\frac{1}{2}}\phi_k - (A\rho\vec{v})_{k-\frac{1}{2}}\phi_{k-1} = (A\kappa)_{k+\frac{1}{2}}\frac{\phi_{k+1}-\phi_k}{\frac{1}{2}(\Delta x_{k+1}+\Delta x_k)} \\ - (A\kappa)_{k-\frac{1}{2}}\frac{\phi_{k}-\phi_{k-1}}{\frac{1}{2}(\Delta x_{k}+\Delta x_{k-1})} + (AS_\phi\Delta x)_k\end{aligned} \tag{2.20}$$

Rearranjando os termos da equação:

$$\begin{aligned}(A\rho\vec{v})_{k+\frac{1}{2}}\phi_k - (A\rho\vec{v})_{k-\frac{1}{2}}\phi_{k-1} = \frac{2(A\kappa)_{k+\frac{1}{2}}}{(\Delta x_{k+1}+\Delta x_k)}\phi_{k+1} - \frac{2(A\kappa)_{k+\frac{1}{2}}}{(\Delta x_{k+1}+\Delta x_k)}\phi_k \\ - \frac{2(A\kappa)_{k-\frac{1}{2}}}{(\Delta x_{k}+\Delta x_{k-1})}\phi_k + \frac{2(A\kappa)_{k-\frac{1}{2}}}{(\Delta x_{k}+\Delta x_{k-1})}\phi_{k-1} + (AS_\phi\Delta x)_k\end{aligned} \tag{2.21}$$

$$\begin{aligned}\left[-(A\rho\vec{v})_{k-\frac{1}{2}} - \frac{2(A\kappa)_{k-\frac{1}{2}}}{(\Delta x_{k}+\Delta x_{k-1})}\right]\phi_{k-1} \\ + \left[(A\rho\vec{v})_{k+\frac{1}{2}} + \frac{2(A\kappa)_{k+\frac{1}{2}}}{(\Delta x_{k+1}+\Delta x_k)} + \frac{2(A\kappa)_{k-\frac{1}{2}}}{(\Delta x_{k}+\Delta x_{k-1})}\right]\phi_k \\ + \left[-\frac{2(A\kappa)_{k+\frac{1}{2}}}{(\Delta x_{k+1}+\Delta x_k)}\right]\phi_{k+1} \\ = (AS_\phi\Delta x)_k\end{aligned} \tag{2.22}$$

Ou seja:

$$L_k \phi_{k-1} + C_k \phi + R_k \phi_{k+1} = (AS_\phi \Delta x)_k \tag{2.23}$$

onde:

$$L_k = -(A\rho\vec{v})_{k-\frac{1}{2}} - \frac{2(A\kappa)_{k-\frac{1}{2}}}{(\Delta x_k + \Delta x_{k-1})} \tag{2.24}$$

$$R_k = -\frac{2(A\kappa)_{k+\frac{1}{2}}}{(\Delta x_{k+1} + \Delta x_k)} \tag{2.25}$$

$$C_k = (A\rho\vec{v})_{k+\frac{1}{2}} + \frac{2(A\kappa)_{k+\frac{1}{2}}}{(\Delta x_{k+1} + \Delta x_k)} + \frac{2(A\kappa)_{k-\frac{1}{2}}}{(\Delta x_k + \Delta x_{k-1})}$$

2.3.2 Velocidades Negativas ($\vec{v_k} < 0$)

Para velocidades negativas a Equação 2.5 pode ser escrita como:

$$\begin{aligned}(A\rho\vec{v})_{k+\frac{1}{2}}(\phi)_{k+\frac{1}{2}} - (A\rho\vec{v})_{k-\frac{1}{2}}(\phi)_{k-\frac{1}{2}} = (A\kappa)_{k+\frac{1}{2}} \frac{\phi_{k+1} - \phi_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} \\ - (A\kappa)_{k-\frac{1}{2}} \frac{\phi_k - \phi_{k-1}}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})} + (AS_\phi \Delta x)_k\end{aligned} \tag{2.26}$$

$$\begin{aligned}(A\rho\vec{v})_{k+\frac{1}{2}}\phi_{k+1} - (A\rho\vec{v})_{k-\frac{1}{2}}\phi_k = (A\kappa)_{k+\frac{1}{2}} \frac{\phi_{k+1} - \phi_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} \\ - (A\kappa)_{k-\frac{1}{2}} \frac{\phi_k - \phi_{k-1}}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})} + (AS_\phi \Delta x)_k\end{aligned} \tag{2.27}$$

Rearranjando os termos da equação:

$$\begin{aligned}(A\rho\vec{v})_{k+\frac{1}{2}}\phi_{k+1} - (A\rho\vec{v})_{k-\frac{1}{2}}\phi_k = \frac{2(A\kappa)_{k+\frac{1}{2}}}{(\Delta x_{k+1} + \Delta x_k)}\phi_{k+1} - \frac{2(A\kappa)_{k+\frac{1}{2}}}{(\Delta x_{k+1} + \Delta x_k)}\phi_k \\ - \frac{2(A\kappa)_{k-\frac{1}{2}}}{(\Delta x_k + \Delta x_{k-1})}\phi_k + \frac{2(A\kappa)_{k-\frac{1}{2}}}{(\Delta x_k + \Delta x_{k-1})}\phi_{k-1} + (AS_\phi \Delta x)_k\end{aligned} \tag{2.28}$$

$$\left[-\frac{2\left(A\kappa\right)_{k-\frac{1}{2}}}{\left(\Delta x_k+\Delta x_{k-1}\right)}\right]\phi_{k-1} \\ +\left[-\left(A\rho\vec{v}\right)_{k-\frac{1}{2}}+\frac{2\left(A\kappa\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_k\right)}+\frac{2\left(A\kappa\right)_{k-\frac{1}{2}}}{\left(\Delta x_k+\Delta x_{k-1}\right)}\right]\phi_k \\ +\left[\left(A\rho\vec{v}\right)_{k+\frac{1}{2}}-\frac{2\left(A\kappa\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_k\right)}\right]\phi_{k+1}=\left(AS_\phi\Delta x\right)_k \quad (2.29)$$

Ou seja:

$$L_k\phi_{k-1}+C_k\phi+R_k\phi_{k+1}=\left(AS_\phi\Delta x\right)_k \quad (2.30)$$

onde:

$$L_k=-\frac{2\left(A\kappa\right)_{k-\frac{1}{2}}}{\left(\Delta x_k+\Delta x_{k-1}\right)} \quad (2.31)$$

$$R_k=\left(A\rho\vec{v}\right)_{k+\frac{1}{2}}-\frac{2\left(A\kappa\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_k\right)} \quad (2.32)$$

$$C_k=-\left(A\rho\vec{v}\right)_{k-\frac{1}{2}}+\frac{2\left(A\kappa\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1}+\Delta x_k\right)}+\frac{2\left(A\kappa\right)_{k-\frac{1}{2}}}{\left(\Delta x_k+\Delta x_{k-1}\right)} \quad (2.33)$$

3 Acoplamento entre Pressão e Velocidade - Equação de Navier-Stokes

Como descrito no capítulo 6 de Versteeg e Malalasekera (2007) será aplicado o método SIMPLE para o acoplamento pressão velocidade das equações de Navier-Stokes unidimensionais.

3.1 Equação de Navies-Stokes

A equação de Navier-Stokes unidimensional pode ser escrita como:

$$\nabla \cdot (\rho \vec{v}) = S_m \tag{3.1}$$

$$\nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\mu \nabla \vec{v}) + S_u \tag{3.2}$$

A Eq. 3.1 representa a equação da conservação da massa sendo uma equação puramente convectiva. A eq. 3.2 é a conservação da quantidade de movimento sendo uma equação difusiva e convectiva. Observa-se dois fatos que tornam a solução numérica desse conjunto de equações dificil:

1. A Eq. da quantidade de movimento é não linear pois apresenta o produto de velocidades na derivada.

2. As equações estão acopladas entre sí, o que torna inviável a solução delas de forma separada.

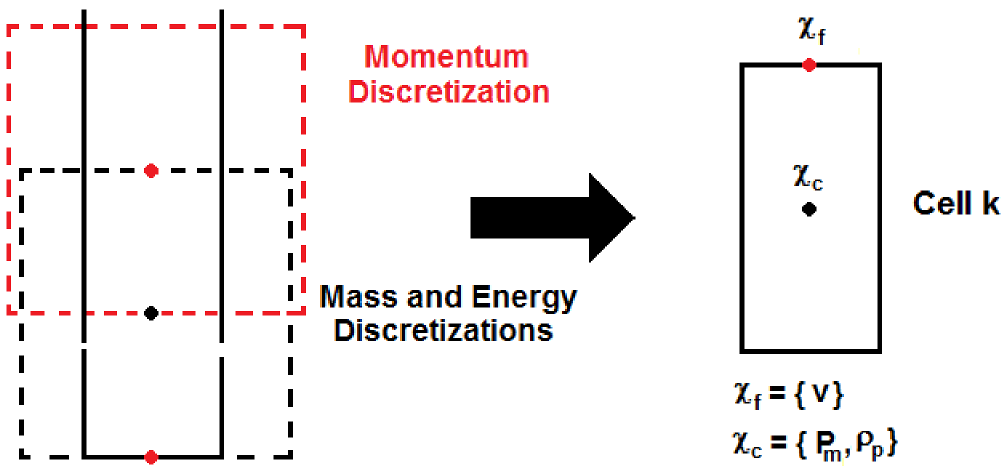

Figura 2: Malha deslocada para solução das equações de Navier-Stokes unidimensionais.

3.2 Malhas Deslocadas (Staggered Grid)

Para facilitar a solução das equações, será adotado o esquema de malhas deslocadas, mostrado na Figura 2. Nesse esquema a pressão é armazenada no centro da célula e a velocidade na face da mesma.

3.3 Equações de Navier-Stokes discretizadas

3.3.1 Conservação da Massa

utilizando o método dos volumes finitos, a equação da conservação da massa pode ser escrita como:

$$\iiint_{\text{V.C.}} \nabla \cdot (\rho \vec{v})\, dV = \iiint_{\text{V.C.}} S_m dV \tag{3.3}$$

Aplicando o teorema de Gauss:

$$\iiint_{\text{S.C.}} (\rho \vec{v}) \cdot \vec{n} dS = \iiint_{\text{V.C.}} S_m dV \tag{3.4}$$

Utilizando o volume de controle unidimensional:

$$(A\rho v)_{k+\frac{1}{2}} - (A\rho v)_{k-\frac{1}{2}} = (A S_m \Delta x)_k \tag{3.5}$$

3.3.2 Conservação da Quantidade de Movimento

A equação da quantidade de movimento pode ser escrita como:

$$\iiint\limits_{\text{V.C.}} \nabla \cdot (\rho \vec{v}\vec{v})\, dV = -\iiint\limits_{\text{V.C.}} \nabla p dV + \iiint\limits_{\text{V.C.}} \nabla \cdot (\mu \nabla \vec{v})\, dV + \iiint\limits_{\text{V.C.}} S_u dV \tag{3.6}$$

Aplicando o teorema de Gauss:

$$\iiint\limits_{\text{S.C.}} (\rho \vec{v}\vec{v}) \cdot \vec{n} dS = -\iiint\limits_{\text{V.C.}} \nabla p dV + \iiint\limits_{\text{S.C.}} (\mu \nabla \vec{v}) \cdot \vec{n} dS + \iiint\limits_{\text{V.C.}} S_u dV \tag{3.7}$$

Utilizando o volume de controle unidimensional:

$$(A\rho vv)_{k+1} - (A\rho vv)_k = -\left(A\Delta x \frac{\partial p}{\partial x}\right)_{k+\frac{1}{2}} + \left(A\mu \frac{\partial v}{\partial x}\right)_{k+1} - \left(A\mu \frac{\partial v}{\partial x}\right)_k + (A\Delta x S_u)_{k+\frac{1}{2}} \tag{3.8}$$

Utilizando diferenças finitas para aproximar os termos das derivadas:

$$\begin{aligned}(A\rho)_{k+1} (vv)_{k+1} - (A\rho)_k (vv)_k = \\ - (A\Delta x)_{k+\frac{1}{2}} \left(\frac{\partial p}{\partial x}\right)_{k+\frac{1}{2}} + (A\mu)_{k+1} \left(\frac{\partial v}{\partial x}\right)_{k+1} - (A\mu)_k \left(\frac{\partial v}{\partial x}\right)_k + (A\Delta x S_u)_{k+\frac{1}{2}}\end{aligned} \tag{3.9}$$

$$\begin{aligned}(A\rho)_{k+1} (vv)_{k+1} - (A\rho)_k (vv)_k = \\ -(A\Delta x)_{k+\frac{1}{2}} \frac{p_{k+1} - p_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} + (A\mu)_{k+1} \frac{v_{k+\frac{3}{2}} - v_{k+\frac{1}{2}}}{\Delta x_{k+1}} - (A\mu)_k \frac{v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}}}{\Delta x_k} + (A\Delta x S_u)_{k+\frac{1}{2}}\end{aligned} \tag{3.10}$$

No lado esquerdo da equação existe um produto de velocidades no centro das células que deverá ser calculado utilizando um algorítimo de interpolação, descrito no Capítulo 2.

3.4 Algorítimo SIMPLE

O algorítimo SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) é um método do tipo previsor-corretor capaz de acoplar as duas equações de Navier-Stokes. Para se utilizar esse metodo é introduzido uma previsão para a velocidade (v^*) para se obter uma previsão para a pressão (p^*). Separando o produto de velocidades e utilizando a Eq. 3.10:

$$\begin{aligned}&(A\rho v)_{k+1}(v^*)_{k+1}-(A\rho v)_k(v^*)_k=\\&-(A\Delta x)_{k+\frac{1}{2}}\frac{p^*_{k+1}-p^*_k}{\frac{1}{2}(\Delta x_{k+1}+\Delta x_k)}+(A\mu)_{k+1}\frac{v^*_{k+\frac{3}{2}}-v^*_{k+\frac{1}{2}}}{\Delta x_{k+1}}-(A\mu)_k\frac{v^*_{k+\frac{1}{2}}-v^*_{k-\frac{1}{2}}}{\Delta x_k}+(A\Delta xS_u)_{k+\frac{1}{2}}\end{aligned} \tag{3.11}$$

Uma definição importante utilizada no método SIMPLE são os termos de correção, dados por:

$$p=p^*+p' \tag{3.12}$$

$$v=v^*+v' \tag{3.13}$$

onde p' é a correção da pressão e v' da velocidade. Subtraindo a Equação 3.11 da 3.10:

$$\begin{aligned}&(A\rho v)_{k+1}(v)_{k+1}-(A\rho v)_k(v)_k-\left((A\rho v)_{k+1}(v^*)_{k+1}-(A\rho v)_k(v^*)_k\right)=\\&-(A\Delta x)_{k+\frac{1}{2}}\frac{p_{k+1}-p_k}{\frac{1}{2}(\Delta x_{k+1}+\Delta x_k)}+(A\mu)_{k+1}\frac{v_{k+\frac{3}{2}}-v_{k+\frac{1}{2}}}{\Delta x_{k+1}}-(A\mu)_k\frac{v_{k+\frac{1}{2}}-v_{k-\frac{1}{2}}}{\Delta x_k}+(A\Delta xS_u)_{k+\frac{1}{2}}\\&-\left(-(A\Delta x)_{k+\frac{1}{2}}\frac{p^*_{k+1}-p^*_k}{\frac{1}{2}(\Delta x_{k+1}+\Delta x_k)}+(A\mu)_{k+1}\frac{v^*_{k+\frac{3}{2}}-v^*_{k+\frac{1}{2}}}{\Delta x_{k+1}}-(A\mu)_k\frac{v^*_{k+\frac{1}{2}}-v^*_{k-\frac{1}{2}}}{\Delta x_k}+(A\Delta xS_u)_{k+\frac{1}{2}}\right)\end{aligned} \tag{3.14}$$

$$
\begin{aligned}
&(A\rho v)_{k+1}\left[v_{k+1}-v_{k+1}^{*}\right]-(A\rho v)_{k}\left[v_{k}-v_{k}^{*}\right]= \\
&-\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_{k}\right)}\left(p_{k+1}-p_{k}\right)+\frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\left(v_{k+\frac{3}{2}}-v_{k+\frac{1}{2}}\right)-\frac{(A\mu)_{k}}{\Delta x_{k}}\left(v_{k+\frac{1}{2}}-v_{k-\frac{1}{2}}\right)+\left(A\Delta xS_u\right)_{k+\frac{1}{2}} \\
&+\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_{k}\right)}\left(p_{k+1}^{*}-p_{k}^{*}\right)-\frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\left(v_{k+\frac{3}{2}}^{*}-v_{k+\frac{1}{2}}^{*}\right)+\frac{(A\mu)_{k}}{\Delta x_{k}}\left(v_{k+\frac{1}{2}}^{*}-v_{k-\frac{1}{2}}^{*}\right)-\left(A\Delta xS_u\right)_{k+\frac{1}{2}}
\end{aligned}
\tag{3.15}
$$

$$
\begin{aligned}
&(A\rho v)_{k+1}\left[v_{k+1}-v_{k+1}^{*}\right]-(A\rho v)_{k}\left[v_{k}-v_{k}^{*}\right]= \\
&\qquad -\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_{k}\right)}\left[\left(p_{k+1}-p_{k+1}^{*}\right)-\left(p_{k}-p_{k}^{*}\right)\right] \\
&\qquad +\frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\left[\left(v_{k+\frac{3}{2}}-v_{k+\frac{3}{2}}^{*}\right)-\left(v_{k+\frac{1}{2}}-v_{k+\frac{1}{2}}^{*}\right)\right] \\
&\qquad -\frac{(A\mu)_{k}}{\Delta x_{k}}\left[\left(v_{k+\frac{1}{2}}-v_{k+\frac{1}{2}}^{*}\right)-\left(v_{k-\frac{1}{2}}-v_{k-\frac{1}{2}}^{*}\right)\right]
\end{aligned}
\tag{3.16}
$$

O método SIMPLE utiliza a seguinte aproximação para se definir a equação corretora:

$$
\begin{aligned}
&-(A\rho v)_{k}\left[v_{k}-v_{k}^{*}\right]= \\
&\qquad +\frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\left[\left(v_{k+\frac{3}{2}}-v_{k+\frac{3}{2}}^{*}\right)-\left(v_{k+\frac{1}{2}}-v_{k+\frac{1}{2}}^{*}\right)\right] \\
&\qquad -\frac{(A\mu)_{k}}{\Delta x_{k}}\left[\left(v_{k+\frac{1}{2}}-v_{k+\frac{1}{2}}^{*}\right)-\left(v_{k-\frac{1}{2}}-v_{k-\frac{1}{2}}^{*}\right)\right]
\end{aligned}
\tag{3.17}
$$

Observa-se que apesar desses termos serem deprezados na equação corretora, essa equação continua respeitando a conservação da massa, como descrito por Versteeg e Malalasekera (2007) . Dessa forma:

$$
(A\rho v)_{k+1}\left[v_{k+1}-v_{k+1}^{*}\right]=-\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_{k}\right)}\left[\left(p_{k+1}-p_{k+1}^{*}\right)-\left(p_{k}-p_{k}^{*}\right)\right] \tag{3.18}
$$

$$
v_{k+1}^{\prime}=-\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_{k}\right)(A\rho v)_{k+1}}\left[\left(p_{k+1}-p_{k+1}^{*}\right)-\left(p_{k}-p_{k}^{*}\right)\right] \tag{3.19}
$$

ou em termos do bloco k:

$$v'_k = -\frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_k + \Delta x_{k-1}\right)(A\rho v)_k}\left[p'_k - p'_{k-1}\right] \tag{3.20}$$

Assim a velocidade real do fluido pode ser escrita como:

$$v_k = v^*_k - \frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_k + \Delta x_{k-1}\right)(A\rho v)_k}\left[p'_k - p'_{k-1}\right] \tag{3.21}$$

A equação da massa discretizada ao redor do ponto k foi escrita como (Equação 3.5):

$$(A\rho v)_{k+\frac{1}{2}} - (A\rho v)_{k-\frac{1}{2}} = (AS_m\Delta x)_k \tag{3.22}$$

É possível perceber que a velocidade real dada pelo método simple (Equação 3.21) é dada no centro da célula, enquanto a velocidade na equação da massa é na face da célula. Dessa forma é necessário se utilizar um método de interpolação para v_k.

3.5 Conservação da Massa utilizando o método UDS

Utilizando o método upwind de primeira ordem para discretizar a velocidade:

3.5.1 Velocidades Positivas ($v_{k+\frac{1}{2}} \geq 0$)

Dessa forma:

$$v_{k+1} = v_{k+\frac{1}{2}} \tag{3.23}$$

$$v_k = v_{k-\frac{1}{2}} \tag{3.24}$$

Substituindo a Equação 3.21 na conservação da massa:

$$(A\rho)_{k+\frac{1}{2}}(v)_{k+\frac{1}{2}} - (A\rho)_{k-\frac{1}{2}}(v)_{k-\frac{1}{2}} = (AS_m\Delta x)_k \tag{3.25}$$

$$(A\rho)_{k+\frac{1}{2}}\left(v^*_{k+1}-\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_k\right)(A\rho v)_{k+1}}\left[p'_{k+1}-p'_k\right]\right)$$
$$-(A\rho)_{k-\frac{1}{2}}\left(v^*_{k}-\frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k}+\Delta x_{k-1}\right)(A\rho v)_{k}}\left[p'_{k}-p'_{k-1}\right]\right)=(AS_m\Delta x)_k \quad (3.26)$$

$$-(A\rho)_{k+\frac{1}{2}}\left(\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_k\right)(A\rho v)_{k+1}}\left[p'_{k+1}-p'_k\right]\right)$$
$$+(A\rho)_{k-\frac{1}{2}}\left(\frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k}+\Delta x_{k-1}\right)(A\rho v)_{k}}\left[p'_{k}-p'_{k-1}\right]\right)=$$
$$(AS_m\Delta x)_k-(A\rho)_{k+\frac{1}{2}}\,v^*_{k+1}+(A\rho)_{k-\frac{1}{2}}\,v^*_k \quad (3.27)$$

$$-(A\rho)_{k+\frac{1}{2}}\left(\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_k\right)(A\rho v)_{k+1}}\right)p'_{k+1}+(A\rho)_{k+\frac{1}{2}}\left(\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_k\right)(A\rho v)_{k+1}}\right)p'_k$$
$$+(A\rho)_{k-\frac{1}{2}}\left(\frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k}+\Delta x_{k-1}\right)(A\rho v)_{k}}\right)p'_k-(A\rho)_{k-\frac{1}{2}}\left(\frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k}+\Delta x_{k-1}\right)(A\rho v)_{k}}\right)p'_{k-1}=$$
$$(AS_m\Delta x)_k-(A\rho)_{k+\frac{1}{2}}\,v^*_{k+1}+(A\rho)_{k-\frac{1}{2}}\,v^*_k \quad (3.28)$$

$$(A\rho)_{k-\frac{1}{2}}\left(\frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k}+\Delta x_{k-1}\right)(A\rho v)_{k}}\right)p'_{k-1}$$
$$-(A\rho)_{k-\frac{1}{2}}\left(\frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k}+\Delta x_{k-1}\right)(A\rho v)_{k}}\right)p'_k-(A\rho)_{k+\frac{1}{2}}\left(\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_k\right)(A\rho v)_{k+1}}\right)p'_k$$
$$+(A\rho)_{k+\frac{1}{2}}\left(\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}\left(\Delta x_{k+1}+\Delta x_k\right)(A\rho v)_{k+1}}\right)p'_{k+1}=$$
$$-(AS_m\Delta x)_k+(A\rho)_{k+\frac{1}{2}}\,v^*_{k+1}-(A\rho)_{k-\frac{1}{2}}\,v^*_k \quad (3.29)$$

Utilizando uma notação simplificada:

$$a_l p'_{k-1}+a_c p'_k+a_r p'_{k+1}=-(AS_m\Delta x)_k+(A\rho)_{k+\frac{1}{2}}\,v^*_{k+1}-(A\rho)_{k-\frac{1}{2}}\,v^*_k \quad (3.30)$$

onde:

$$a_l = (A\rho)_{k-\frac{1}{2}} \left(\frac{(A\Delta x)_{k-\frac{1}{2}}}{\frac{1}{2}(\Delta x_k + \Delta x_{k-1})(A\rho v)_k} \right) \tag{3.31}$$

$$a_r = (A\rho)_{k+\frac{1}{2}} \left(\frac{(A\Delta x)_{k+\frac{1}{2}}}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_{k})(A\rho v)_{k+1}} \right) \tag{3.32}$$

$$a_c = -a_l - a_r \tag{3.33}$$

A Equação 3.30 é a expressão para a correção da pressão em cada célula do domínio. Com os valores de correção de pressão é possível corrigir a velocidade do escoamento com a Equação 3.21. A Figura 3 mostra um fluxograma com as etapas de cálculo do método SIMPLE.

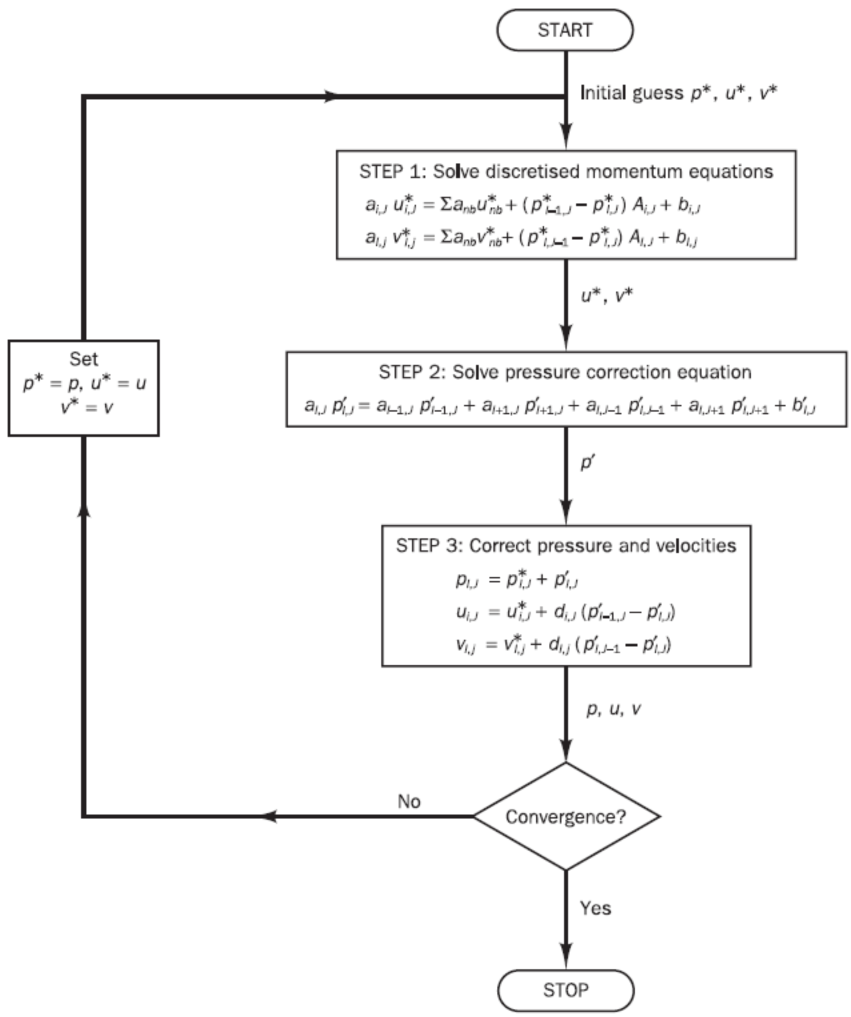

Figura 3: Fluxograma do método SIMPLE.

3.6

3.7 Quantidade de Movimento utilizando interpolação UDS

A equação da conservação da quantidade de movimento (Equação 3.10) foi definida como:

$$(A\rho v)_{k+1}\, v^*_{k+1} - (A\rho v)_k\, v^*_k =$$
$$-(A\Delta x)_{k+\frac{1}{2}}\, \frac{p^*_{k+1} - p^*_k}{\frac{1}{2}\left(\Delta x_{k+1} + \Delta x_k\right)} + (A\mu)_{k+1}\, \frac{v^*_{k+\frac{3}{2}} - v^*_{k+\frac{1}{2}}}{\Delta x_{k+1}} - (A\mu)_k\, \frac{v^*_{k+\frac{1}{2}} - v^*_{k-\frac{1}{2}}}{\Delta x_k} + (A\Delta x S_u)_{k+\frac{1}{2}} \tag{3.34}$$

O método UDS é recomendado para escoamentos com altos valores do número de Peclet. Utilizando a interpolação pos diferenças centradas para $\vec{v}$ e a interpolação pelo esquema Upwind de primeira ordem UDS para ϕ, o termo $\phi_{k+\frac{1}{2}}$ pode ser expresso como:

$$\phi_{k+\frac{1}{2}} = \phi_k, \quad v_k \geq 0 \tag{3.35}$$

$$\phi_{k+\frac{1}{2}} = \phi_{k+1}, \quad v_k < 0 \tag{3.36}$$

Já o termo $\phi_{k-\frac{1}{2}}$ pode ser expresso como:

$$\phi_{k-\frac{1}{2}} = \phi_{k-1}, \quad v_k \geq 0 \tag{3.37}$$

$$\phi_{k-\frac{1}{2}} = \phi_k, \quad v_k < 0 \tag{3.38}$$

3.7.1 Velocidades Positivas ($\vec{v_k} \geq 0$)

$$\begin{aligned}&(A\rho v)_{k+1}\, v^*_{k+\frac{1}{2}} - (A\rho v)_k\, v^*_{k-\frac{1}{2}} = \\ &- A_{k+\frac{1}{2}} \left(p^*_{k+1} - p^*_k\right) + (A\mu)_{k+1} \frac{v^*_{k+\frac{3}{2}} - v^*_{k+\frac{1}{2}}}{\Delta x_{k+1}} - (A\mu)_k \frac{v^*_{k+\frac{1}{2}} - v^*_{k-\frac{1}{2}}}{\Delta x_k} + (A\Delta x S_u)_{k+\frac{1}{2}}\end{aligned} \tag{3.39}$$

Rearranjando:

$$\begin{aligned}&\left[-(A\rho v)_k - \frac{(A\mu)_k}{\Delta x_k}\right] v^*_{k-\frac{1}{2}} \\ &\quad + \left[(A\rho v)_{k+1} + \frac{(A\mu)_k}{\Delta x_k} + \frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\right] v^*_{k+\frac{1}{2}} \\ &\quad \left[-\frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\right] v^*_{k+\frac{3}{2}} \\ &= \\ &- A_{k+\frac{1}{2}} \left(p^*_{k+1} - p^*_k\right)\end{aligned} \tag{3.40}$$

Que pode ser simplificada como:

$$a_{vl} v^*_{k-\frac{1}{2}} + a_{vc} v^*_{k+\frac{1}{2}} + a_{vr} v^*_{k+\frac{3}{2}} = -A_{k+\frac{1}{2}} \left(p^*_{k+1} - p^*_k\right) \tag{3.41}$$

onde

$$a_{vl} = -(A\rho v)_k - \frac{(A\mu)_k}{\Delta x_k} \tag{3.42}$$

$$a_{vc} = (A\rho v)_{k+1} + \frac{(A\mu)_k}{\Delta x_k} + \frac{(A\mu)_{k+1}}{\Delta x_{k+1}} \tag{3.43}$$

$$a_{vr} = -\frac{(A\mu)_{k+1}}{\Delta x_{k+1}} \tag{3.44}$$

3.7.2 Velocidades Negativas ($\vec{v_k} < 0$)

$$
\begin{aligned}
&(A\rho v)_{k+1}\, v^*_{k+\frac{3}{2}} - (A\rho v)_k\, v^*_{k+\frac{1}{2}} = \\
&- A_{k+\frac{1}{2}} \left(p^*_{k+1} - p^*_k\right) + (A\mu)_{k+1} \frac{v^*_{k+\frac{3}{2}} - v^*_{k+\frac{1}{2}}}{\Delta x_{k+1}} - (A\mu)_k \frac{v^*_{k+\frac{1}{2}} - v^*_{k-\frac{1}{2}}}{\Delta x_k} + (A\Delta x S_u)_{k+\frac{1}{2}}
\end{aligned}
\tag{3.45}
$$

Rearranjando:

$$
\begin{aligned}
&\left[-\frac{(A\mu)_k}{\Delta x_k}\right] v^*_{k-\frac{1}{2}} \\
&+ \left[- (A\rho v)_k + \frac{(A\mu)_k}{\Delta x_k} + \frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\right] v^*_{k+\frac{1}{2}} \\
&\left[(A\rho v)_{k+1} - \frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\right] v^*_{k+\frac{3}{2}} \\
&= \\
&- A_{k+\frac{1}{2}} \left(p^*_{k+1} - p^*_k\right)
\end{aligned}
\tag{3.46}
$$

Que pode ser simplificada como:

$$
a_{vl} v^*_{k-\frac{1}{2}} + a_{vc} v^*_{k+\frac{1}{2}} + a_{vr} v^*_{k+\frac{3}{2}} = -A_{k+\frac{1}{2}} \left(p^*_{k+1} - p^*_k\right) \tag{3.47}
$$

onde

$$
a_{vl} = -\frac{(A\mu)_k}{\Delta x_k} \tag{3.48}
$$

$$
a_{vc} = (A\rho v)_k + \frac{(A\mu)_k}{\Delta x_k} + \frac{(A\mu)_{k+1}}{\Delta x_{k+1}} \tag{3.49}
$$

$$
a_{vr} = (A\rho v)_{k+1} - \frac{(A\mu)_{k+1}}{\Delta x_{k+1}} \tag{3.50}
$$

3.7.3 Condição de Contorno a Esquerda

3.7.3.1 Pressão constante

A velocidade pode ser calculada utilizando a equação da continuidade:

$$v_k = v_{k+\frac{1}{2}} \frac{A_{k+\frac{1}{2}}}{A_k} \tag{3.51}$$

A fronteira possui velocidade, utilizando Bernouli, a pressão estática pode ser calculada por:

$$\begin{aligned} p_k &= p_{BC} - \frac{1}{2}\left(\rho v^2\right)_k & (3.52) \\ &= p_{BC} - \frac{1}{2}\rho_k \left(\frac{A_{k+\frac{1}{2}}}{A_k} v_{k+\frac{1}{2}}\right)^2 & (3.53) \end{aligned}$$

Velocidades positivas

$$a_{vl} v^*_{k-\frac{1}{2}} + a_{vc} v^*_{k+\frac{1}{2}} + a_{vr} v^*_{k+\frac{3}{2}} = -A_{k+\frac{1}{2}} \left(p^*_{k+1} - p_{BC}\right) \tag{3.54}$$

onde:

$$a_{vl} = 0 \tag{3.55}$$

$$\begin{aligned} a_{vc} = &\left[\left(-\left(A\rho v\right)_k - \frac{(A\mu)_k}{\Delta x_k}\right) \frac{A_{k+\frac{1}{2}}}{A_k}\right] + \left[\frac{1}{2}\left(\rho A v\right)_k \left(\frac{A_{k+\frac{1}{2}}}{A_k}\right)^2\right] \\ &+ \left(A\rho v\right)_{k+1} + \frac{(A\mu)_k}{\Delta x_k} + \frac{(A\mu)_{k+1}}{\Delta x_{k+1}} \end{aligned} \tag{3.56}$$

$$a_{vr} = -\frac{(A\mu)_{k+1}}{\Delta x_{k+1}} \tag{3.57}$$

3.7.4 Condição de contorno a direita

A velocidade pode ser calculada utilizando a equação da continuidade:

$$(\rho A v)_{k+1} = (\rho A v)_{k+\frac{1}{2}} \tag{3.58}$$

A fronteira possui velocidade, utilizando Bernouli, a pressão estática pode ser calculada por:

$$p_{k+1} \quad = \quad p_{BC} \tag{3.59}$$

Velocidades positivas

$$a_{vl} v^*_{k-\frac{1}{2}} + a_{vc} v^*_{k+\frac{1}{2}} + a_{vr} v^*_{k+\frac{3}{2}} = -A_{k+\frac{1}{2}} \left(p_{BC} - p^*_k\right) \tag{3.60}$$

onde

$$a_{vl} = -\left(A \rho v\right)_k - \frac{(A\mu)_k}{\Delta x_k} \tag{3.61}$$

$$a_{vc} = \left(A \rho v\right)_{k+\frac{1}{2}} + \frac{(A\mu)_k}{\Delta x_k} \tag{3.62}$$

$$a_{vr} = 0 \tag{3.63}$$

4 Algorítimo COUPLE - Equação de Navier-Stokes com formulação full-implicit

No Capítulo 3 foi utilizado o método SIMPLE para o acoplamento entre a pressão e velocidade nas equações de Navier-Stoker. Nesse capítulo será utilizada uma formulação totalmente implícita, capaz de resolver essas equações utilizando o método de Newton-Rapson.

4.1 Mátodo de Newton-Rapson

A formulação implícita do problema será realizada utilizando-se o método de Newton-Raphson, descrito por:

$$R_k^\nu + \sum_j^{NoBlocks} \frac{\partial R_k^\nu}{\partial x_j} \left(x_j^{(\nu+1)} - x_j^{(\nu)} \right) = 0 \tag{4.1}$$

ou em notação matricial:

$$J^\nu \delta x^{\nu+1} = -R^\nu \tag{4.2}$$

onde J é a matriz Jacobiano do problema, R é o vetor de resíduos e δx é a variação da solução do problema.

Os resíduos para a equação da conservação da massa, Equação 3.5, são dados por:

$$R_k^m = (A\rho v)_{k+\frac{1}{2}} - (A\rho v)_{k-\frac{1}{2}} - (AS_m\Delta x)_k \tag{4.3}$$

Os resíduos para a equação da quantidade de movimento, Equação 3.10, desprezando termos fonte, são dados por:

$$R_k^p = (A\rho)_{k+1}(vv)_{k+1} - (A\rho)_k (vv)_k$$
$$+ (A\Delta x)_{k+\frac{1}{2}} \frac{p_{k+1} - p_k}{\frac{1}{2}(\Delta x_{k+1} + \Delta x_k)} - (A\mu)_{k+1} \frac{v_{k+\frac{3}{2}} - v_{k+\frac{1}{2}}}{\Delta x_{k+1}} + (A\mu)_k \frac{v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}}}{\Delta x_k} \quad (4.4)$$

4.2 Derivadas Parciais

4.2.1 Derivada da Massa em relação a pressão

$$\frac{\partial R_k^m}{\partial p_{k-1}} = \frac{\partial R_k^m}{\partial p_k} = \frac{\partial R_k^m}{\partial p_{k+1}} = 0 \quad (4.5)$$

4.2.2 Derivada da Massa em relação a velocidade

$$\frac{\partial R_k^m}{\partial v_{k+\frac{1}{2}}} = \frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[(A\rho v)_{k+\frac{1}{2}} - (A\rho v)_{k-\frac{1}{2}} - (AS_m\Delta x)_k\right] \quad (4.6)$$

$$\frac{\partial R_k^m}{\partial v_{k+\frac{1}{2}}} = (A\rho)_{k+\frac{1}{2}} \quad (4.7)$$

$$\frac{\partial R_k^m}{\partial v_{k-\frac{1}{2}}} = \frac{\partial}{\partial v_{k-\frac{1}{2}}}\left[(A\rho v)_{k+\frac{1}{2}} - (A\rho v)_{k-\frac{1}{2}} - (AS_m\Delta x)_k\right] \quad (4.8)$$

$$\frac{\partial R_k^m}{\partial v_{k-\frac{1}{2}}} = -(A\rho)_{k-\frac{1}{2}} \quad (4.9)$$

4.2.3 Derivada da Quantidade de Movimento em relação a pressão

4.2.3.1 Derivada em relação ao bloco a esquerda

$$\frac{\partial R_k^p}{\partial p_{k-1}} = \frac{\partial}{\partial p_{k-1}} \left[(A\rho)_{k+1} (vv)_{k+1} - (A\rho)_k (vv)_k \right]$$
$$+ \frac{\partial}{\partial p_{k-1}} \left[(A\Delta x)_{k+\frac{1}{2}} \frac{p_{k+1} - p_k}{\frac{1}{2} (\Delta x_{k+1} + \Delta x_k)} - (A\mu)_{k+1} \frac{v_{k+\frac{3}{2}} - v_{k+\frac{1}{2}}}{\Delta x_{k+1}} + (A\mu)_k \frac{v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}}}{\Delta x_k} \right] \tag{4.10}$$

$$\frac{\partial R_k^p}{\partial p_{k-1}} = 0 \tag{4.11}$$

4.2.3.2 Derivada em relação ao bloco ao centro

$$\frac{\partial R_k^p}{\partial p_k} = \frac{\partial}{\partial p_k} \left[(A\rho)_{k+1} (vv)_{k+1} - (A\rho)_k (vv)_k \right]$$
$$+ \frac{\partial}{\partial p_k} \left[(A\Delta x)_{k+\frac{1}{2}} \frac{p_{k+1} - p_k}{\frac{1}{2} (\Delta x_{k+1} + \Delta x_k)} - (A\mu)_{k+1} \frac{v_{k+\frac{3}{2}} - v_{k+\frac{1}{2}}}{\Delta x_{k+1}} + (A\mu)_k \frac{v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}}}{\Delta x_k} \right] \tag{4.12}$$

$$\frac{\partial R_k^m}{\partial p_k} = \frac{\partial}{\partial p_k} \left[\frac{2 (A\Delta x)_{k+\frac{1}{2}}}{(\Delta x_{k+1} + \Delta x_k)} (p_{k+1} - p_k) \right] \tag{4.13}$$

$$\frac{\partial R_k^p}{\partial p_k} = -\frac{2 (A\Delta x)_{k+\frac{1}{2}}}{(\Delta x_{k+1} + \Delta x_k)} \tag{4.14}$$

4.2.3.3 Derivada em relação ao bloco a direita

$$\frac{\partial R_k^p}{\partial p_{k+1}} = \frac{\partial}{\partial p_{k+1}} \left[(A\rho)_{k+1} (vv)_{k+1} - (A\rho)_k (vv)_k \right]$$
$$+ \frac{\partial}{\partial p_{k+1}} \left[(A\Delta x)_{k+\frac{1}{2}} \frac{p_{k+1} - p_k}{\frac{1}{2} (\Delta x_{k+1} + \Delta x_k)} - (A\mu)_{k+1} \frac{v_{k+\frac{3}{2}} - v_{k+\frac{1}{2}}}{\Delta x_{k+1}} + (A\mu)_k \frac{v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}}}{\Delta x_k} \right] \tag{4.15}$$

$$\frac{\partial R_k^p}{\partial p_{k+1}} = \frac{\partial}{\partial p_{k+1}} \left[\frac{2\left(A\Delta x\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1} + \Delta x_k\right)} \left(p_{k+1} - p_k\right) \right] \tag{4.16}$$

$$\frac{\partial R_k^p}{\partial p_{k+1}} = \frac{2\left(A\Delta x\right)_{k+\frac{1}{2}}}{\left(\Delta x_{k+1} + \Delta x_k\right)} \tag{4.17}$$

4.2.4 Derivada da Quantidade de Movimento em relação a velocidade

4.2.4.1 Derivada em relação ao bloco a esquerda

$$\begin{aligned}\frac{\partial R_k^p}{\partial v_{k-\frac{1}{2}}} &= \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\left(A\rho\right)_{k+1} \left(vv\right)_{k+1} - \left(A\rho\right)_k \left(vv\right)_k \right] \\ &+ \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\left(A\Delta x\right)_{k+\frac{1}{2}} \frac{p_{k+1} - p_k}{\frac{1}{2}\left(\Delta x_{k+1} + \Delta x_k\right)} - \left(A\mu\right)_{k+1} \frac{v_{k+\frac{3}{2}} - v_{k+\frac{1}{2}}}{\Delta x_{k+1}} + \left(A\mu\right)_k \frac{v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}}}{\Delta x_k} \right]\end{aligned} \tag{4.18}$$

$$\frac{\partial R_k^p}{\partial v_{k-\frac{1}{2}}} = \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\left(A\rho\right)_{k+1} \left(vv\right)_{k+1} - \left(A\rho\right)_k \left(vv\right)_k \right] + \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\left(A\mu\right)_k \frac{v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}}}{\Delta x_k} \right] \tag{4.19}$$

$$\frac{\partial R_k^p}{\partial v_{k-\frac{1}{2}}} = \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\left(A\rho\right)_{k+1} \left(vv\right)_{k+1} \right] - \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\left(A\rho\right)_k \left(vv\right)_k \right] + \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\frac{\left(A\mu\right)_k}{\Delta x_k} \left(v_{k+\frac{1}{2}} - v_{k-\frac{1}{2}} \right) \right] \tag{4.20}$$

$$\frac{\partial R_k^p}{\partial v_{k-\frac{1}{2}}} = \left(A\rho\right)_{k+1} \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\left(vv\right)_{k+1} \right] - \left(A\rho\right)_k \frac{\partial}{\partial v_{k-\frac{1}{2}}} \left[\left(vv\right)_k \right] - \frac{\left(A\mu\right)_k}{\Delta x_k} \tag{4.21}$$

$$\frac{\partial R_k^p}{\partial v_{k-\frac{1}{2}}} = \left(A\rho\right)_{k+1} \frac{\partial \left(vv\right)_{k+1}}{\partial v_{k-\frac{1}{2}}} - \left(A\rho\right)_k \frac{\partial \left(vv\right)_k}{\partial v_{k-\frac{1}{2}}} - \frac{\left(A\mu\right)_k}{\Delta x_k} \tag{4.22}$$

4.2.4.2 Derivada em relação ao bloco central

$$\frac{\partial R_k^p}{\partial v_{k+\frac{1}{2}}} = \frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[(A\rho)_{k+1}(vv)_{k+1} - (A\rho)_k (vv)_k\right] + \frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[(A\Delta x)_{k+\frac{1}{2}} \frac{p_{k+1}-p_k}{\frac{1}{2}(\Delta x_{k+1}+\Delta x_k)} - (A\mu)_{k+1}\frac{v_{k+\frac{3}{2}}-v_{k+\frac{1}{2}}}{\Delta x_{k+1}} + (A\mu)_k \frac{v_{k+\frac{1}{2}}-v_{k-\frac{1}{2}}}{\Delta x_k}\right] \tag{4.23}$$

$$\frac{\partial R_k^p}{\partial v_{k+\frac{1}{2}}} = \frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[(A\rho)_{k+1}(vv)_{k+1} - (A\rho)_k (vv)_k\right] + \frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[-\frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\left(v_{k+\frac{3}{2}}-v_{k+\frac{1}{2}}\right) + \frac{(A\mu)_k}{\Delta x_k}\left(v_{k+\frac{1}{2}}-v_{k-\frac{1}{2}}\right)\right] \tag{4.24}$$

$$\frac{\partial R_k^p}{\partial v_{k+\frac{1}{2}}} = (A\rho)_{k+1}\frac{\partial (vv)_{k+1}}{\partial v_{k+\frac{1}{2}}} - (A\rho)_k \frac{\partial (vv)_k}{\partial v_{k+\frac{1}{2}}} + \frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[\frac{(A\mu)_{k+1}}{\Delta x_{k+1}}\left(v_{k+\frac{1}{2}}\right) + \frac{(A\mu)_k}{\Delta x_k}\left(v_{k+\frac{1}{2}}\right)\right] \tag{4.25}$$

$$\frac{\partial R_k^p}{\partial v_{k+\frac{1}{2}}} = (A\rho)_{k+1}\frac{\partial (vv)_{k+1}}{\partial v_{k+\frac{1}{2}}} - (A\rho)_k \frac{\partial (vv)_k}{\partial v_{k+\frac{1}{2}}} + \frac{(A\mu)_{k+1}}{\Delta x_{k+1}} + \frac{(A\mu)_k}{\Delta x_k} \tag{4.26}$$

4.2.4.3 Derivada em relação ao bloco a direita

$$\frac{\partial R_k^p}{\partial v_{k+\frac{3}{2}}} = \frac{\partial}{\partial v_{k+\frac{3}{2}}}\left[(A\rho)_{k+1}(vv)_{k+1} - (A\rho)_k (vv)_k\right] + \frac{\partial}{\partial v_{k+\frac{3}{2}}}\left[(A\Delta x)_{k+\frac{1}{2}} \frac{p_{k+1}-p_k}{\frac{1}{2}(\Delta x_{k+1}+\Delta x_k)} - (A\mu)_{k+1}\frac{v_{k+\frac{3}{2}}-v_{k+\frac{1}{2}}}{\Delta x_{k+1}} + (A\mu)_k \frac{v_{k+\frac{1}{2}}-v_{k-\frac{1}{2}}}{\Delta x_k}\right] \tag{4.27}$$

$$\frac{\partial R_k^p}{\partial v_{k+\frac{3}{2}}} = (A\rho)_{k+1}\frac{\partial (vv)_{k+1}}{\partial v_{k+\frac{3}{2}}} - (A\rho)_k \frac{\partial (vv)_k}{\partial v_{k+\frac{3}{2}}} - \frac{(A\mu)_{k+1}}{\Delta x_{k+1}} \tag{4.28}$$

As derivadas da velocidade devem ser calculadas de acordo com o método de interpolação escolhido.

4.3 Interpolação CDS

Utilizando o método CDS, as derivadas parciais das velocidades são calculadas por:

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k-\frac{1}{2}}}=\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k-\frac{1}{2}}}=0 \tag{4.29}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k-\frac{1}{2}}}=\frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k-\frac{1}{2}}}=2v_{k}\frac{\partial}{\partial v_{k-\frac{1}{2}}}\left[\frac{v_{k+\frac{1}{2}}+v_{k-\frac{1}{2}}}{2}\right]=v_{k} \tag{4.30}$$

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+\frac{1}{2}}}=\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k+\frac{1}{2}}}=2v_{k+1}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[\frac{v_{k+\frac{3}{2}}+v_{k+\frac{1}{2}}}{2}\right]=v_{k+1} \tag{4.31}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k+\frac{1}{2}}}=\frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k+\frac{1}{2}}}=2v_{k}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[\frac{v_{k+\frac{1}{2}}+v_{k-\frac{1}{2}}}{2}\right]=v_{k} \tag{4.32}$$

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+\frac{1}{2}}}=\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k+\frac{1}{2}}}=2v_{k+1}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[\frac{v_{k+\frac{3}{2}}+v_{k+\frac{1}{2}}}{2}\right]=v_{k+1} \tag{4.33}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k+\frac{1}{2}}}=\frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k+\frac{1}{2}}}=2v_{k}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[\frac{v_{k+\frac{1}{2}}+v_{k-\frac{1}{2}}}{2}\right]=v_{k} \tag{4.34}$$

4.4 Interpolação UDS

Utilizando o método UDS, as derivadas parciais das velocidades são calculadas por:

4.4.0.4 $v_{k+\frac{1}{2}}\geq 0$:

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k-\frac{1}{2}}}=\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k-\frac{1}{2}}}=0 \tag{4.35}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k-\frac{1}{2}}}=\frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k-\frac{1}{2}}}=2v_{k}\frac{\partial}{\partial v_{k-\frac{1}{2}}}\left[v_{k-\frac{1}{2}}\right]=2v_{k} \tag{4.36}$$

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k+\frac{1}{2}}} = 2v_{k+1}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[v_{k+\frac{1}{2}}\right] = 2v_{k+1} \tag{4.37}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k+\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k+\frac{1}{2}}} = 2v_{k}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[v_{k-\frac{1}{2}}\right] = 0 \tag{4.38}$$

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k+\frac{1}{2}}} = 2v_{k+1}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[v_{k+\frac{1}{2}}\right] = 2v_{k+1} \tag{4.39}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k+\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k+\frac{1}{2}}} = 2v_{k}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[v_{k-\frac{1}{2}}\right] = 0 \tag{4.40}$$

4.4.0.5 $v_{k+\frac{1}{2}} \geq 0$:

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k-\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k-\frac{1}{2}}} = 0 \tag{4.41}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k-\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k-\frac{1}{2}}} = 2v_{k}\frac{\partial}{\partial v_{k-\frac{1}{2}}}\left[v_{k+\frac{1}{2}}\right] = 0 \tag{4.42}$$

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k+\frac{1}{2}}} = 2v_{k+1}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[v_{k+\frac{3}{2}}\right] = 0 \tag{4.43}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k+\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k+\frac{1}{2}}} = 2v_{k}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[v_{k+\frac{1}{2}}\right] = 2v_{k} \tag{4.44}$$

$$\frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k+1}}{\partial v_{k+1}}\frac{\partial v_{k+1}}{\partial v_{k+\frac{1}{2}}} = 2v_{k+1}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[v_{k+\frac{3}{2}}\right] = 0 \tag{4.45}$$

$$\frac{\partial\left(vv\right)_{k}}{\partial v_{k+\frac{1}{2}}} = \frac{\partial\left(vv\right)_{k}}{\partial v_{k}}\frac{\partial v_{k}}{\partial v_{k+\frac{1}{2}}} = 2v_{k}\frac{\partial}{\partial v_{k+\frac{1}{2}}}\left[v_{k+\frac{1}{2}}\right] = 2v_{k} \tag{4.46}$$

4.5 Construção da Matriz Jacobiana

Existem duas formas práticas de se montar a matriz jacobiano, a primeira é se agrupar as equações por tipo para formar o resíduo, e a segunda é se agrupar as equações a partir das células.

4.5.1 Jacobiano com equações agrupadas:

Agrupando as equações do mesmo tipo no Jacobiano:

$$\begin{bmatrix} \frac{\partial R_1^m}{\partial p_1} & \frac{\partial R_1^m}{\partial p_2} & \frac{\partial R_1^m}{\partial p_3} & \cdots & \frac{\partial R_1^m}{\partial p_n} & \frac{\partial R_1^m}{\partial v_1} & \frac{\partial R_1^m}{\partial v_2} & \frac{\partial R_1^m}{\partial v_3} & \cdots & \frac{\partial R_1^m}{\partial v_n} \\ \frac{\partial R_2^m}{\partial p_1} & \frac{\partial R_2^m}{\partial p_2} & \frac{\partial R_2^m}{\partial p_3} & \cdots & \frac{\partial R_2^m}{\partial p_n} & \frac{\partial R_2^m}{\partial v_1} & \frac{\partial R_2^m}{\partial v_2} & \frac{\partial R_2^m}{\partial v_3} & \cdots & \frac{\partial R_2^m}{\partial v_n} \\ \frac{\partial R_3^m}{\partial p_1} & \frac{\partial R_3^m}{\partial p_2} & \frac{\partial R_3^m}{\partial p_3} & \cdots & \frac{\partial R_3^m}{\partial p_n} & \frac{\partial R_3^m}{\partial v_1} & \frac{\partial R_3^m}{\partial v_2} & \frac{\partial R_3^m}{\partial v_3} & \cdots & \frac{\partial R_3^m}{\partial v_n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial R_n^m}{\partial p_1} & \frac{\partial R_n^m}{\partial p_2} & \frac{\partial R_n^m}{\partial p_3} & \cdots & \frac{\partial R_n^m}{\partial p_n} & \frac{\partial R_n^m}{\partial v_1} & \frac{\partial R_n^m}{\partial v_2} & \frac{\partial R_n^m}{\partial v_3} & \cdots & \frac{\partial R_n^m}{\partial v_n} \\ \frac{\partial R_1^p}{\partial p_1} & \frac{\partial R_1^p}{\partial p_2} & \frac{\partial R_1^p}{\partial p_3} & \cdots & \frac{\partial R_1^p}{\partial p_n} & \frac{\partial R_1^p}{\partial v_1} & \frac{\partial R_1^p}{\partial v_2} & \frac{\partial R_1^p}{\partial v_3} & \cdots & \frac{\partial R_1^p}{\partial v_n} \\ \frac{\partial R_2^p}{\partial p_1} & \frac{\partial R_2^p}{\partial p_2} & \frac{\partial R_2^p}{\partial p_3} & \cdots & \frac{\partial R_2^p}{\partial p_n} & \frac{\partial R_2^p}{\partial v_1} & \frac{\partial R_2^p}{\partial v_2} & \frac{\partial R_2^p}{\partial v_3} & \cdots & \frac{\partial R_2^p}{\partial v_n} \\ \frac{\partial R_3^p}{\partial p_1} & \frac{\partial R_3^p}{\partial p_2} & \frac{\partial R_3^p}{\partial p_3} & \cdots & \frac{\partial R_3^p}{\partial p_n} & \frac{\partial R_3^p}{\partial v_1} & \frac{\partial R_3^p}{\partial v_2} & \frac{\partial R_3^p}{\partial v_3} & \cdots & \frac{\partial R_3^p}{\partial v_n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial R_n^p}{\partial p_1} & \frac{\partial R_n^p}{\partial p_2} & \frac{\partial R_n^p}{\partial p_3} & \cdots & \frac{\partial R_n^p}{\partial p_n} & \frac{\partial R_n^p}{\partial v_1} & \frac{\partial R_n^p}{\partial v_2} & \frac{\partial R_n^p}{\partial v_3} & \cdots & \frac{\partial R_n^p}{\partial v_n} \end{bmatrix} \begin{bmatrix} \delta p_1 \\ \delta p_2 \\ \delta p_3 \\ \vdots \\ \delta p_n \\ \delta v_1 \\ \delta v_2 \\ \delta v_3 \\ \vdots \\ \delta v_n \end{bmatrix} = - \begin{bmatrix} \delta R_1^m \\ \delta R_2^m \\ \delta R_3^m \\ \vdots \\ \delta R_n^m \\ \delta R_1^p \\ \delta R_2^p \\ \delta R_3^p \\ \vdots \\ \delta R_n^p \end{bmatrix} \tag{4.47}$$

Substituindo as derivadas calculadas:

$$\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & \frac{\partial R_1^m}{\partial v_1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & \frac{\partial R_2^m}{\partial v_1} & \frac{\partial R_2^m}{\partial v_2} & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \frac{\partial R_3^m}{\partial v_2} & \frac{\partial R_3^m}{\partial v_3} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & \frac{\partial R_n^m}{\partial v_n} \\ \frac{\partial R_1^p}{\partial p_1} & \frac{\partial R_1^p}{\partial p_2} & 0 & \cdots & 0 & \frac{\partial R_1^p}{\partial v_1} & \frac{\partial R_1^p}{\partial v_2} & 0 & \cdots & 0 \\ 0 & \frac{\partial R_2^p}{\partial p_2} & \frac{\partial R_2^p}{\partial p_3} & \cdots & 0 & \frac{\partial R_2^p}{\partial v_1} & \frac{\partial R_2^p}{\partial v_2} & \frac{\partial R_2^p}{\partial v_3} & \cdots & 0 \\ 0 & 0 & \frac{\partial R_3^p}{\partial p_3} & \cdots & 0 & 0 & \frac{\partial R_3^p}{\partial v_2} & \frac{\partial R_3^p}{\partial v_3} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{\partial R_n^p}{\partial p_n} & 0 & 0 & 0 & \cdots & \frac{\partial R_n^p}{\partial v_n} \end{bmatrix} \begin{bmatrix} \delta p_1 \\ \delta p_2 \\ \delta p_3 \\ \vdots \\ \delta p_n \\ \delta v_1 \\ \delta v_2 \\ \delta v_3 \\ \vdots \\ \delta v_n \end{bmatrix} = - \begin{bmatrix} \delta R_1^m \\ \delta R_2^m \\ \delta R_3^m \\ \vdots \\ \delta R_n^m \\ \delta R_1^p \\ \delta R_2^p \\ \delta R_3^p \\ \vdots \\ \delta R_n^p \end{bmatrix} \tag{4.48}$$

4.5.2 Jacobiano com células agrupadas:

Agrupando as derivadas com relação as células no Jacobiano:

$$\begin{bmatrix} \frac{\partial R_1^p}{\partial p_1} & \frac{\partial R_1^p}{\partial v_1} & \frac{\partial R_1^p}{\partial p_2} & \frac{\partial R_1^p}{\partial v_2} & \frac{\partial R_1^p}{\partial p_3} & \frac{\partial R_1^p}{\partial v_3} & \cdots & \frac{\partial R_1^p}{\partial p_n} & \frac{\partial R_1^p}{\partial v_n} \\ \frac{\partial R_1^m}{\partial p_1} & \frac{\partial R_1^m}{\partial v_1} & \frac{\partial R_1^m}{\partial p_2} & \frac{\partial R_1^m}{\partial v_2} & \frac{\partial R_1^m}{\partial p_3} & \frac{\partial R_1^m}{\partial v_3} & \cdots & \frac{\partial R_1^m}{\partial p_n} & \frac{\partial R_1^m}{\partial v_n} \\ \frac{\partial R_2^p}{\partial p_1} & \frac{\partial R_2^p}{\partial v_1} & \frac{\partial R_2^p}{\partial p_2} & \frac{\partial R_2^p}{\partial v_2} & \frac{\partial R_2^p}{\partial p_3} & \frac{\partial R_2^p}{\partial v_3} & \cdots & \frac{\partial R_2^p}{\partial p_n} & \frac{\partial R_2^p}{\partial v_n} \\ \frac{\partial R_2^m}{\partial p_1} & \frac{\partial R_2^m}{\partial v_1} & \frac{\partial R_2^m}{\partial p_2} & \frac{\partial R_2^m}{\partial v_2} & \frac{\partial R_2^m}{\partial p_3} & \frac{\partial R_2^m}{\partial v_3} & \cdots & \frac{\partial R_2^m}{\partial p_n} & \frac{\partial R_2^m}{\partial v_n} \\ \frac{\partial R_3^p}{\partial p_1} & \frac{\partial R_3^p}{\partial v_1} & \frac{\partial R_3^p}{\partial p_2} & \frac{\partial R_3^p}{\partial v_2} & \frac{\partial R_3^p}{\partial p_3} & \frac{\partial R_3^p}{\partial v_3} & \cdots & \frac{\partial R_3^p}{\partial p_n} & \frac{\partial R_3^p}{\partial v_n} \\ \frac{\partial R_3^m}{\partial p_1} & \frac{\partial R_3^m}{\partial v_1} & \frac{\partial R_3^m}{\partial p_2} & \frac{\partial R_3^m}{\partial v_2} & \frac{\partial R_3^m}{\partial p_3} & \frac{\partial R_3^m}{\partial v_3} & \cdots & \frac{\partial R_3^m}{\partial p_n} & \frac{\partial R_3^m}{\partial v_n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial R_n^p}{\partial p_1} & \frac{\partial R_n^p}{\partial v_1} & \frac{\partial R_n^p}{\partial p_2} & \frac{\partial R_n^p}{\partial v_2} & \frac{\partial R_n^p}{\partial p_3} & \frac{\partial R_n^p}{\partial v_3} & \cdots & \frac{\partial R_n^p}{\partial p_n} & \frac{\partial R_n^p}{\partial v_n} \\ \frac{\partial R_n^m}{\partial p_1} & \frac{\partial R_n^m}{\partial v_1} & \frac{\partial R_n^m}{\partial p_2} & \frac{\partial R_n^m}{\partial v_2} & \frac{\partial R_n^m}{\partial p_3} & \frac{\partial R_n^m}{\partial v_3} & \cdots & \frac{\partial R_n^m}{\partial p_n} & \frac{\partial R_n^m}{\partial v_n} \end{bmatrix} \begin{bmatrix} \delta p_1 \\ \delta v_1 \\ \delta p_2 \\ \delta v_2 \\ \delta p_3 \\ \delta v_3 \\ \vdots \\ \delta p_n \\ \delta v_n \end{bmatrix} = - \begin{bmatrix} \delta R_1^p \\ \delta R_1^m \\ \delta R_2^p \\ \delta R_2^m \\ \delta R_3^p \\ \delta R_3^m \\ \vdots \\ \delta R_n^p \\ \delta R_n^m \end{bmatrix} \tag{4.49}$$

Substituindo as derivadas:

$$\begin{bmatrix} \frac{\partial R_1^p}{\partial p_1} & \frac{\partial R_1^p}{\partial v_1} & \frac{\partial R_1^p}{\partial p_2} & \frac{\partial R_1^p}{\partial v_2} & 0 & 0 & \cdots & 0 & 0 \\ 0 & \frac{\partial R_1^m}{\partial v_1} & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \frac{\partial R_2^p}{\partial v_1} & \frac{\partial R_2^p}{\partial p_2} & \frac{\partial R_2^p}{\partial v_2} & \frac{\partial R_2^p}{\partial p_3} & \frac{\partial R_2^p}{\partial v_3} & \cdots & 0 & 0 \\ 0 & \frac{\partial R_2^m}{\partial v_1} & 0 & \frac{\partial R_2^m}{\partial v_2} & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial R_3^p}{\partial v_2} & \frac{\partial R_3^p}{\partial p_3} & \frac{\partial R_3^p}{\partial v_3} & \cdots & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial R_3^m}{\partial v_2} & 0 & \frac{\partial R_3^m}{\partial v_3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \frac{\partial R_n^p}{\partial p_n} & \frac{\partial R_n^p}{\partial v_n} \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & \frac{\partial R_n^m}{\partial v_n} \end{bmatrix} \begin{bmatrix} \delta p_1 \\ \delta v_1 \\ \delta p_2 \\ \delta v_2 \\ \delta p_3 \\ \delta v_3 \\ \vdots \\ \delta p_n \\ \delta v_n \end{bmatrix} = - \begin{bmatrix} \delta R_1^p \\ \delta R_1^m \\ \delta R_2^p \\ \delta R_2^m \\ \delta R_3^p \\ \delta R_3^m \\ \vdots \\ \delta R_n^p \\ \delta R_n^m \end{bmatrix} \tag{4.50}$$

Observa-se que o Jacobiano com células agrupadas resulta em uma matriz com maior peso na diagonal, o que facilita os métodos numéricos. Dessa forma esse Jacobiano será implementado.

Referências

VERSTEEG, H. K.; MALALASEKERA, W. *An Introduction to Computational Fluid Dynamics*. [S.l.]: Pearson Education, 2007.