Pedro André Arroyo Silva

Formulação Variacional e Volumes Finitos 3D para o DDM

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Formulação Variacional

Estudaremos a seguinte Equação Diferencial Parcial

$$
\begin{aligned}
\partial_t u &= \left(\frac{\bar{\sigma}}{1-\kappa\partial_x^2}\right)\partial_x^2 u \\
\partial_x u &= 0 \qquad u \in \partial\Omega,
\end{aligned} \tag{1}
$$

Onde $\kappa = \frac{\ell^4 - h^4}{12\ell^2}$. Lembrando que:

$$
-\int_\Omega \Delta u v dx = \int_\Omega \nabla u \nabla v dx - \int_{\partial\Omega} (\nabla u \cdot n)\, v ds. \tag{2}
$$

Optamos por resolver de maneira implícita a Eq.(1):

$$
\left(1-\kappa\partial_x^2\right)\partial_t u = \bar{\sigma}\partial_x^2 u \tag{3}
$$

$$
\partial_t u - \kappa\partial_x^2\partial_t u = \bar{\sigma}\partial_x^2 u \tag{4}
$$

$$
\int_\Omega v\partial_t u - \kappa\int_\Omega v\partial_x^2\partial_t u = \bar{\sigma}\int_\Omega v\partial_x^2 u, \tag{5}
$$

seja $\partial_t u = \phi$:

$$
\int_\Omega v\phi dx - \kappa\int_\Omega v\partial_x^2\phi dx = \bar{\sigma}\int_\Omega v\partial_x^2 u, \tag{6}
$$

$$
\int_\Omega v\phi dx + \kappa\int_\Omega \frac{dv}{dx}\frac{d\phi}{dx}dx - \kappa\int_{\partial\Omega}\frac{d\phi}{dx}v ds = \bar{\sigma}\int_\Omega \frac{dv}{dx}\frac{du}{dx}dx - \bar{\sigma}\int_{\partial\Omega}\frac{du}{dx}v ds, \tag{7}
$$

$$
\int_\Omega v\phi dx + \kappa\int_\Omega \frac{dv}{dx}\frac{d\phi}{dx} = \bar{\sigma}\int_\Omega \frac{dv}{dx}\frac{du}{dx}dx. \tag{8}
$$

Com isto discretizamos a parte espacial. Nos falta discretizar a parte temporal.

Utilizando Euler implícito, ou seja, $\partial_t u = \dfrac{u^{n+1}-u^n}{\Delta t}$, temos:

$$
\int_\Omega \left(\frac{u^{n+1}-u^n}{\Delta t}\right) v dx + \kappa\int_\Omega \frac{dv}{dx}\frac{d}{dx}\left(\frac{u^{n+1}-u^n}{\Delta t}\right)dx = \bar{\sigma}\int_\Omega \frac{dv}{dx}\frac{d}{dx}u^{n+1}dx, \tag{9}
$$

$$
\int_\Omega u^{n+1} v dx - \Delta t\bar{\sigma}\int_\Omega \frac{dv}{dx}\frac{d}{dx}u^{n+1}dx + \kappa\left[\int_\Omega \frac{dv}{dx}\frac{d}{dx}u^{n+1} - \int_\Omega \frac{dv}{dx}\frac{d}{dx}u^n\right] = \int_\Omega u^n v dx, \tag{10}
$$

$$
\int_\Omega u^{n+1} v dx - \Delta t\bar{\sigma}\int_\Omega \frac{dv}{dx}\frac{d}{dx}u^{n+1}dx + \kappa\int_\Omega \frac{dv}{dx}\frac{d}{dx}u^{n+1}dx = \int_\Omega u^n v dx + \kappa\int_\Omega \frac{dv}{dx}\frac{d}{dx}u^n. \tag{11}
$$

Obtivemos assim, a formulação variacional, Eq.(11), da Eq.(1).

$$
[A]\{u\} = \{F\} \tag{12}
$$

DDM em 2D pelo Método dos Volumes Finitos

Considere a seguinte equação, chamaremos a versão 3D do DDM.

$$\beta C_m \partial_t u = \frac{\nabla \cdot (\sigma \nabla u)}{1 - (\nabla \cdot (\kappa \nabla))} \tag{13}$$

onde

$$\kappa = \begin{pmatrix} \kappa_x & 0 & 0 \\ 0 & \kappa_y & 0 \\ 0 & 0 & \kappa_z \end{pmatrix} \tag{14}$$

os elementos da diagonal são:

$$\kappa_x = \frac{\ell_x^4 - \Delta x^4}{12\ell_x^2}, \quad \kappa_y = \frac{\ell_y^4 - \Delta y^4}{12\ell_y^2}, \quad \kappa_z = \frac{\ell_z^4 - \Delta z^4}{12\ell_z^2} \tag{15}$$

$\ell_x = 100\mu m$, $\ell_y = 25\mu m$ e $\ell_z =?$. A condutividade é dada por

$$\sigma = \begin{pmatrix} \sigma_x & 0 & 0 \\ 0 & \sigma_y & 0 \\ 0 & 0 & \sigma_z \end{pmatrix} \tag{16}$$

podendo escolher as condutividade, por exemplo $\sigma_x = 0.0008mS/cm$, $\sigma_y = 0.0001mS/cm$, $\sigma_z =?$, as quais dependerão do modelo celular que está sendo utilizado.
Da Equação (13) temos:

$$[1 - (\nabla \cdot (\kappa \nabla))]\, u = \nabla \cdot (\sigma \nabla u) \tag{17}$$

$$[1 - (\nabla \cdot (\kappa \nabla))] \left(\frac{u_{i,j,k}^{n+1} - u_{i,j,k}^{n}}{\Delta t} \right) = \nabla \cdot \left(\sigma \nabla u_{i,j,k}^{n+1} \right) \tag{18}$$

$$\left(\frac{u_{i,j,k}^{n+1} - u_{i,j,k}^{n}}{\Delta t} \right) - \frac{\nabla \cdot \left(\kappa \nabla u_{i,j,k}^{n+1} \right)}{\Delta t} - \frac{\nabla \cdot \left(\kappa \nabla u_{i,j,k}^{n} \right)}{\Delta t} = \nabla \cdot \left(\sigma \nabla u_{i,j,k}^{n+1} \right) \tag{19}$$

Depois das devidas discretizações

Tomando $\alpha = \frac{\beta C_m}{\Delta t}$, multiplicando ambos lados da equação por $\Delta x \Delta y \Delta z$, e considerando que σ_x, σ_y e σ_z são constantes temos:

$$
\begin{aligned}
&\left(\alpha \Delta x \Delta y \Delta z + \frac{2\sigma_x}{\Delta x}\Delta y \Delta z + \frac{2\sigma_y}{\Delta y}\Delta x \Delta z + \frac{2\sigma_z}{\Delta z}\Delta x \Delta y + 2\frac{\kappa_x \Delta y \Delta z}{\Delta t \Delta x} + 2\frac{\kappa_y \Delta x \Delta z}{\Delta t \Delta y} + 2\frac{\kappa_z \Delta x \Delta y}{\Delta t \Delta z}\right) u^*_{i,j,k} \\
&- \left(\frac{\sigma_x \Delta y \Delta z}{\Delta x} + \frac{\kappa_x \Delta y \Delta z}{\Delta t \Delta x}\right) u^*_{i+1,j,k} - \left(\frac{\sigma_x \Delta y \Delta z}{\Delta x} + \frac{\kappa_x \Delta y \Delta z}{\Delta t \Delta x}\right) u^*_{i-1,j,k} \\
&- \left(\frac{\sigma_y \Delta x \Delta z}{\Delta y} + \frac{\kappa_y \Delta x \Delta z}{\Delta t \Delta y}\right) u^*_{i,j+1,k} - \left(\frac{\sigma_y \Delta x \Delta z}{\Delta y} + \frac{\kappa_y \Delta x \Delta z}{\Delta t \Delta y}\right) u^*_{i,j-1,k} \\
&- \left(\frac{\sigma_z \Delta x \Delta y}{\Delta z} + \frac{\kappa_z \Delta x \Delta y}{\Delta t \Delta z}\right) u^*_{i,j,k+1} - \left(\frac{\sigma_z \Delta x \Delta y}{\Delta z} + \frac{\kappa_z \Delta x \Delta y}{\Delta t \Delta z}\right) u^*_{i,j,k-1} \\
&= \\
&\left(\alpha \Delta x \Delta y \Delta z + \frac{2\kappa_x \Delta y \Delta z}{\Delta t \Delta x} + \frac{2\kappa_y \Delta x \Delta z}{\Delta t \Delta y} + \frac{2\kappa_y \Delta x \Delta y}{\Delta t \Delta z}\right) u^n_{i,j,k} \\
&- \left(\frac{\kappa_x \Delta y \Delta z}{\Delta t \Delta x}\right) u^n_{i+1,j,k} - \left(\frac{\kappa_x \Delta y \Delta z}{\Delta t \Delta x}\right) u^n_{i-1,j,k} \\
&- \left(\frac{\kappa_y \Delta x \Delta z}{\Delta t \Delta y}\right) u^n_{i,j+1,k} - \left(\frac{\kappa_y \Delta x \Delta z}{\Delta t \Delta y}\right) u^n_{i,j-1,k} \\
&- \left(\frac{\kappa_y \Delta x \Delta y}{\Delta t \Delta z}\right) u^n_{i,j,k+1} - \left(\frac{\kappa_y \Delta x \Delta y}{\Delta t \Delta z}\right) u^n_{i,j,k-1}
\end{aligned}
\tag{20}
$$