Derivation of a FV discretization for 1-D transient diffusion equations

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1 Governing equation

Consider a simplified 1-D diffusion equation

$$\frac{du}{dt} = \frac{d}{dx}\left(\frac{du}{dx}\right) \tag{1}$$

with a initial condition

$$u\,|_{t=0} = 0 \tag{2}$$

and Dirichlet boundary condition (BC)

$$u\,|_{x=0} = u_{\mathrm{A}}, u\,|_{x=1} = u_{\mathrm{B}} \tag{3}$$

or Neumann boundary condition (BC)

$$\frac{du}{dx}\,|_{x=0} = q_{\mathrm{A}}, \frac{du}{dx}\,|_{x=1} = q_{\mathrm{B}} \tag{4}$$

2 FV Discretization

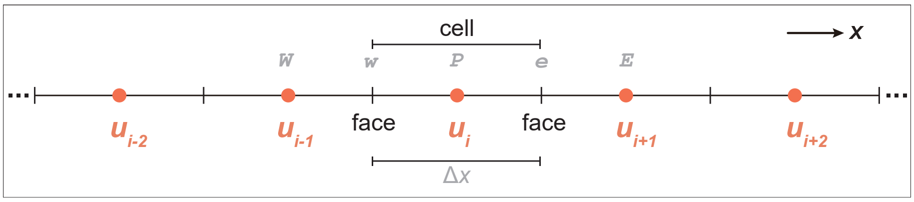

Figure 1: The internal cells of a uniform 1-D cell-centered FV discretization

In a FV discretization, integrating both side of Equ.(2) over a FV cell, we have

$$\int_V \frac{du}{dt} dV = \int_V \frac{d}{dx}\left(\frac{du}{dx}\right) dV \tag{5}$$

where

$$\int_V \frac{du}{dt} dV \approx \Delta V \frac{du}{dt} = \Delta x \Delta y \frac{du}{dt} \tag{6}$$

and

$$\int_{\partial V} \left(\frac{du}{dx}\right) \cdot \mathbf{n} dS \approx \Delta y \left(\frac{du}{dx}\right)_e - \Delta y \left(\frac{du}{dx}\right)_w \tag{7}$$

Substituting Equ.(6) and Equ.(7) into Equ.(5) yields

$$\Delta x \Delta y \frac{du}{dt} = \Delta y \left(\frac{du}{dx}\right)_e - \Delta y \left(\frac{du}{dx}\right)_w \tag{8}$$

Dividing both side of Equ.(8) by $\Delta x \Delta y$, we have

$$\frac{du}{dt} \approx \frac{\left(\frac{du}{dx}\right)_e - \left(\frac{du}{dx}\right)_w}{\Delta x} \tag{9}$$

Approximating $\frac{\partial u}{\partial x}$ by a central difference scheme yields

$$\left(\frac{du}{dx}\right)_e \approx \frac{u_E - u_P}{\Delta x}, \left(\frac{du}{dx}\right)_w \approx \frac{u_P - u_W}{\Delta x} \tag{10}$$

and Equ.(10) becomes

$$\frac{du}{dt} = \frac{\frac{u_E - u_P}{\Delta x} - \frac{u_P - u_W}{\Delta x}}{\Delta x} = \frac{u_E - 2u_P + u_W}{\Delta x^2} \tag{11}$$

or

$$\frac{du}{dt} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \tag{12}$$

Equ.(12) can be rewritten as

$$\frac{du}{dt} = G(t, u) \tag{13}$$

where $\mathbf{G}(t, u)$ is the RHS of Equ.(12)

$$\mathbf{G}(t, u_i) = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \tag{14}$$

which is used by PETSc's **TS** object and implemented in the **TSSetRHSFunction()** for the internal cells.

3 Discretization on the left boundary

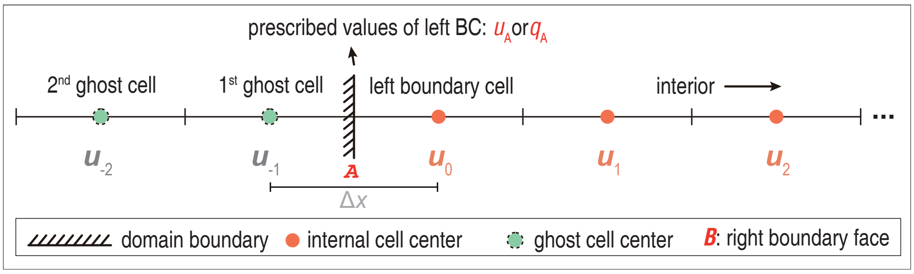

Figure 2: The left side of the uniform 1-D cell-centered FV discretization with ghost cells outside the boundary

3.1 Dirichlet BC

For a given Dirichlet BC u_A at left domain boundary A, linear interpolation relates u_A, u_0 and u_{-1}

$$u_{\mathrm{A}} = \frac{u_0 + u_{-1}}{2} \Rightarrow u_{-1} = 2u_{\mathrm{A}} - u_0 \tag{15}$$

Therefore Equ.(10) becomes

$$\left(\frac{du}{dx}\right)_w = \left(\frac{du}{dx}\right)_{\mathrm{A}} \approx \left(\frac{u_i - u_{i-1}}{\Delta x}\right)_{\mathrm{A}} = \frac{u_0 - u_{-1}}{\Delta x} = \frac{u_0 - (2u_{\mathrm{A}} - u_0)}{\Delta x} = \frac{2u_0 - 2u_{\mathrm{A}}}{\Delta x} \tag{16}$$

and

$$\left(\frac{du}{dx}\right)_e \approx \left(\frac{u_i - u_{i-1}}{\Delta x}\right)_e = \frac{u_1 - u_0}{\Delta x} \tag{17}$$

The RHS of Equ.(12) becomes:

$$\mathbf{G}(u_{\mathrm{A}}, t) = \left(\frac{du}{dx}\right)_{\mathrm{w}}^{e} = \left(\frac{du}{dx}\right)_{\mathrm{A}}^{e} \approx \frac{u_1 - 2u_0 + u_{-1}}{\Delta x^2} = \frac{u_1 - 2u_0 + (2u_{\mathrm{A}-u_0})}{\Delta x^2} = \frac{u_1 - 3u_0 + 2u_{\mathrm{A}}}{\Delta x^2} \tag{18}$$

3.2 Neumann BC

For a given Neumann BC q_A at left domain boundary A, an approximation of q_A relates u_A, u_0 and u_{-1}

$$q_{\mathrm{A}} = \left(\frac{du}{dx}\right)_{\mathrm{A}} \approx \frac{u_0 - u_{-1}}{\Delta x} \Rightarrow u_{-1} = u_0 - q_{\mathrm{A}}\Delta x \tag{19}$$

The RHS of Equ.(12) becomes:

$$\mathbf{G}(u_{\mathrm{B}}, t) = \left(\frac{du}{dx}\right)_{\mathrm{w}}^{e} = \left(\frac{du}{dx}\right)_{\mathrm{A}}^{e} \approx \frac{u_1 - 2u_0 + u_{-1}}{\Delta x^2} = \frac{u_1 - 2u_0 + (u_0 - q_{\mathrm{A}}\Delta x)}{\Delta x^2} = \frac{u_1 - u_0 - q_{\mathrm{A}}\Delta x}{\Delta x^2} \tag{20}$$

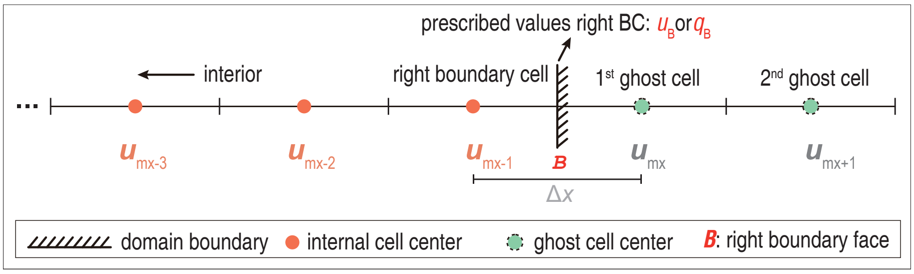

Figure 3: The right side of the uniform 1-D cell-centered FV discretization with ghost cells outside the boundary

4 Discretization on the right boundary

4.1 Dirichlet BC

For a given Dirichlet BC u_B at the left domain boundary B, linear interpolation relates u_B, u_{mx} and u_{mx-1}

$$u_{\mathrm{B}} = \frac{u_{mx} + u_{mx-1}}{2} \Rightarrow u_{mx} = 2u_{\mathrm{B}} - u_{mx-1} \tag{21}$$

Therefore Equ.(10) becomes

$$\left(\frac{du}{dx}\right)_e = \left(\frac{du}{dx}\right)_{\mathrm{B}} \approx \left(\frac{u_i - u_{i-1}}{\Delta x}\right)_{\mathrm{B}} = \frac{u_{mx} - u_{mx-1}}{\Delta x} = \frac{(2u_{\mathrm{B}} - u_{mx-1}) - u_{mx-1}}{\Delta x} = \frac{2u_{\mathrm{B}} - 2u_{mx-1}}{\Delta x} \tag{22}$$

and

$$\left(\frac{du}{dx}\right)_w \approx \left(\frac{u_i - u_{i-1}}{\Delta x}\right)_w = \frac{u_{mx-1} - u_{mx-2}}{\Delta x} \tag{23}$$

The RHS of Equ.(12) becomes:

$$\begin{aligned}\mathbf{G}(u_{\mathrm{B}}, t) = \left(\frac{du}{dx}\right)_{\mathrm{w}}^{e} = \left(\frac{du}{dx}\right)_{\mathrm{B}}^{e} &\approx \frac{u_{mx} - 2u_{mx-1} + u_{mx-2}}{\Delta x^2} = \frac{(2u_{\mathrm{B}} - u_{mx-1}) - 2u_{mx-1} + u_{mx-2}}{\Delta x^2} \\ &= \frac{u_{mx-2} - 3u_{mx-1} + 2u_{\mathrm{B}}}{\Delta x^2}\end{aligned} \tag{24}$$

4.2 Neumann BC

For a given Neumann BC q_B at the right domain boundary B, an approximation of q_B relates q_B, u_{mx}, $u_{mx-1}$and u_{mx-2}

$$q_{\mathrm{B}} = \left(\frac{du}{dx}\right)_{\mathrm{B}} \approx \frac{u_{mx} - u_{mx-1}}{\Delta x} \Rightarrow u_{mx} = u_{mx-1} + q_{\mathrm{B}}\Delta x \tag{25}$$

The RHS of Equ.(12) becomes:

$$\begin{aligned}\mathbf{G}(u_{\mathrm{B}}, t) = \left(\frac{du}{dx}\right)_{\mathrm{w}}^{e} = \left(\frac{du}{dx}\right)_{\mathrm{B}}^{e} &\approx \frac{u_{mx} - 2u_{mx-1} + u_{mx-2}}{\Delta x^2} \\ &= \frac{(u_{mx-1} + q_{\mathrm{B}}\Delta x) - 2u_{mx-1} + u_{mx-2}}{\Delta x^2} \\ &= -\frac{u_{mx-1} - u_{mx-2} - q_{\mathrm{B}}\Delta x}{\Delta x^2}\end{aligned} \tag{26}$$

Table 1: Summary of RHS function for 1-D FV discretization

	$\mathbf{G}(t, u_i)$	
	Dirichlet BC	Neumann BC
internal	$\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$	
Left	$\frac{u_1 - 3u_0 + 2u_{\mathrm{A}}}{\Delta x^2}$	$\frac{u_1 - u_0 - q_{\mathrm{A}}\Delta x}{\Delta x^2}$
Right	$\frac{u_{mx-2} - 3u_{mx-1} + 2u_{\mathrm{B}}}{\Delta x^2}$	$-\frac{u_{mx-1} - u_{mx-2} - q_{\mathrm{B}}\Delta x}{\Delta x^2}$