Multiphase Flows

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Multiphase Flow

- "A multiphase flow is one in which two or more distinct phases coexist."
- Examples:
  - Rain drops falling through atmosphere.
  - Air bubbles rising in water.
  - Water flows with a free surface.
  - Water vapor bubbles forming in boiling water due to phase change.
  - Multiphase flows involving solids: melting of ice, solidification of water
- Multiphase flows have unique features compared to single-phase flows.
  - Surface tension
  - Deformation
  - Breaking and merging of phase interfaces

Qin (2022, p. 225)

Multiphase Flow

- Modeling multiphase flows is challenging due to
  - Material properties (density, viscosity, etc.) are not uniform.
  - The position and movement of the interface are unknown and have to be determined as part of the solution procedure.
- Many numerical methods have been developed for multiphase flows.
  - Marker-and-cell (MAC) method (Harlow and Welch, 1965)
  - Volume-of-fluid (VOF) method (Noh and Woodward, 1976)
  - Smoothed-particle hydrodynamics (SPH) (Gingold and Monaghan, 1977)
  - Level set method (LSM) (Dervieux and Thomasset, 1980)
  - Front tracking method (Unverdi and Tryggvason, 1992)
  - Lattice Boltzmann method (LBM) (Shan and Chen, 1993)
  - Phase-field method (Jacqmin, 1999)

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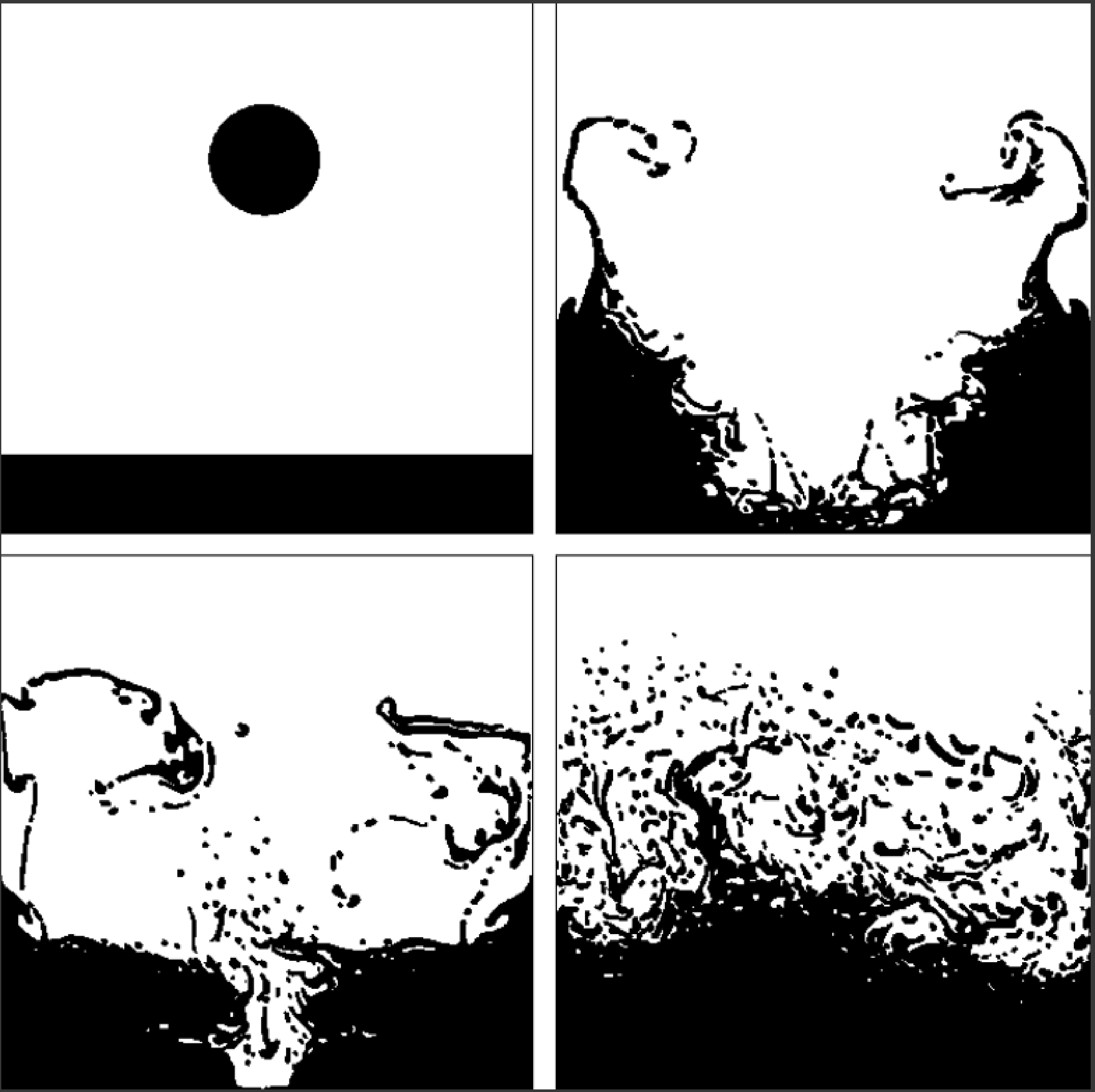
Volume of Fluid (VOF) Method



- The volume of fluid method is a numerical method for tracking and locating the free surface (gas-fluid interface) or fluid-fluid interface.
- However, the Navier-Stokes equations governing the flow must be solved separately.
- The VOF method is based on the marker-and-cell (MAC) method.
- An advantage of the VOF method is that the volume of each phase is well conserved even on a coarse grid.

https://en.wikipedia.org/wiki/Volume_of_fluid_method

VOF: Interface Representation

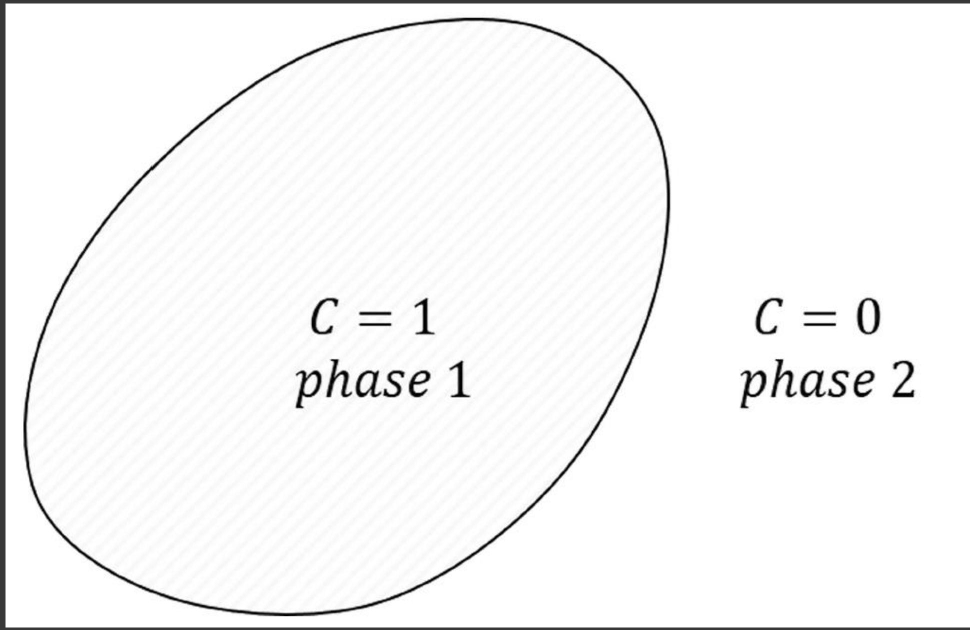
- Consider a fluid flow comprising two immisible phases: liquid and gas.
- Both phases are separated by a sharp interface.
- Assume that there is neither phase change nor chemical reaction in the flow.
- It is crucial to accurately identify and track the interface in such flows.
- This can be done explicitly by tracking massless point particles located along the interface and advecting with the local fluid velocity.
- Alternatively, a marker function can be used to label different phases and represent the interface implicitly.
- The simplest marker function is a step function

$$C(x,y) = \begin{cases} 1 & \text{if phase 1 is present at point } (x,y) \\ 0 & \text{if phase 2 is present at point } (x,y) \end{cases}$$

Qin (2022, p. 226)

VOF: Interface Representation

- The interface is then identified implicitly by the step change of the marker function.
- If the marker function C is discretized by a mesh, some mesh cells may contain both phases (they contain part of the interface).
- The C value at the center of such a cell can be interpreted as the volume average of the marker function in this cell:



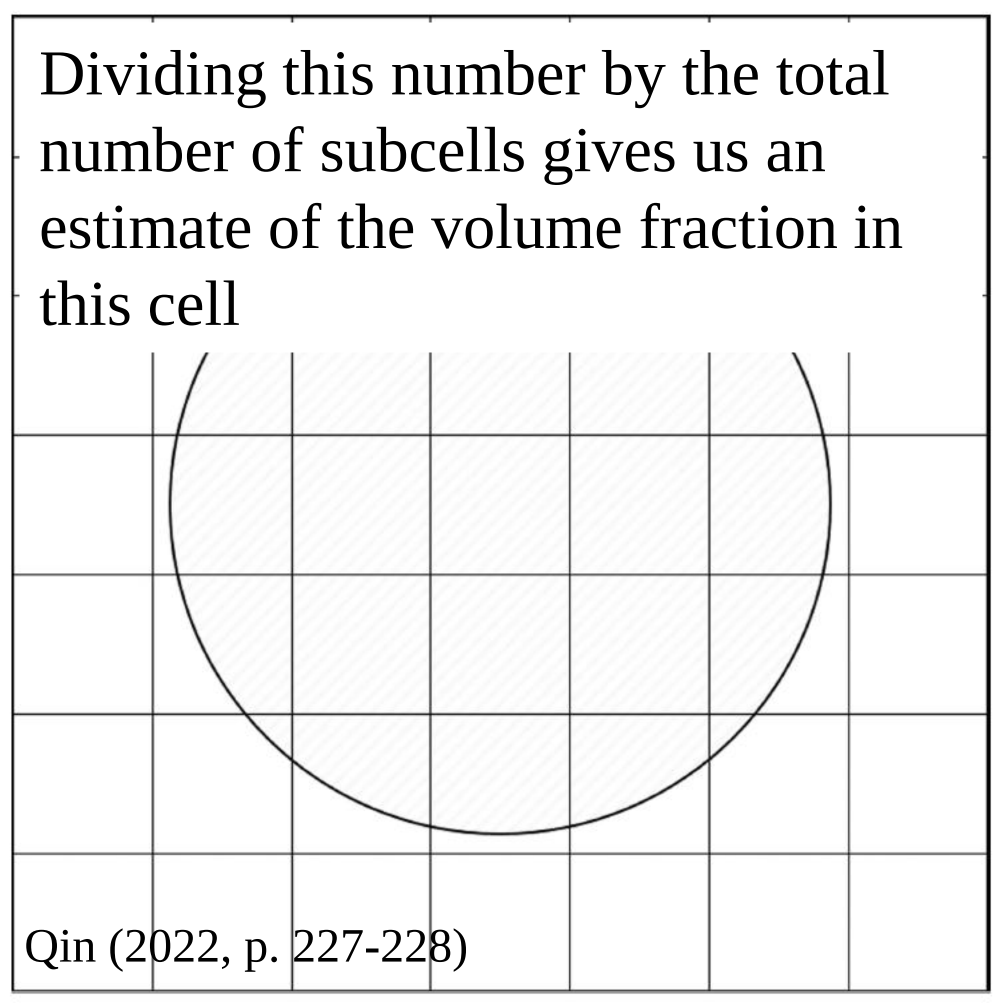
$$C_{i,j} = \frac{1}{V}\int_V C dV = \frac{1 \cdot V_1 + 0 \cdot V_2}{V} = \frac{V_1}{V}$$

where V_1 and V_2 are volume of phase 1 and phase 2 in this cell, respectively, and $V = V_1 + V_2$ is the total volume of this cell.

Qin (2022, p. 226)

VOF: Interface Representation

- It is obvious that $0 < C < 1$ in cells containing interface.
- C then has a physical meaning as the volume fraction of phase 1.
- Suppose we are simulating the motion of an air bubble rising in water.
- "The bubble is initially a circle with known radius and center position, so we know whether a given point is within or without this bubble."
- The volume fraction of the gas phase in each cell can be estimated by splitting each cell into subcells and count the number of subcells whose center is inside the circle.



Qin (2022, p. 227-228)

VOF: Interface Reconstruction

- Given a discretized *C* field as shown in the right figure, how can we reconstruct the interface, i.e., finding the exact location of the interface?
- The piecewise linear interface calcution (PLIC) method (Youngs, 1982) uses a straight line segment to approximate the interface in each cell with $0 < C < 1$.

0.52	0.16	0	0
1	0.97	0.26	0
1	1	0.78	0
1	1	0.86	0

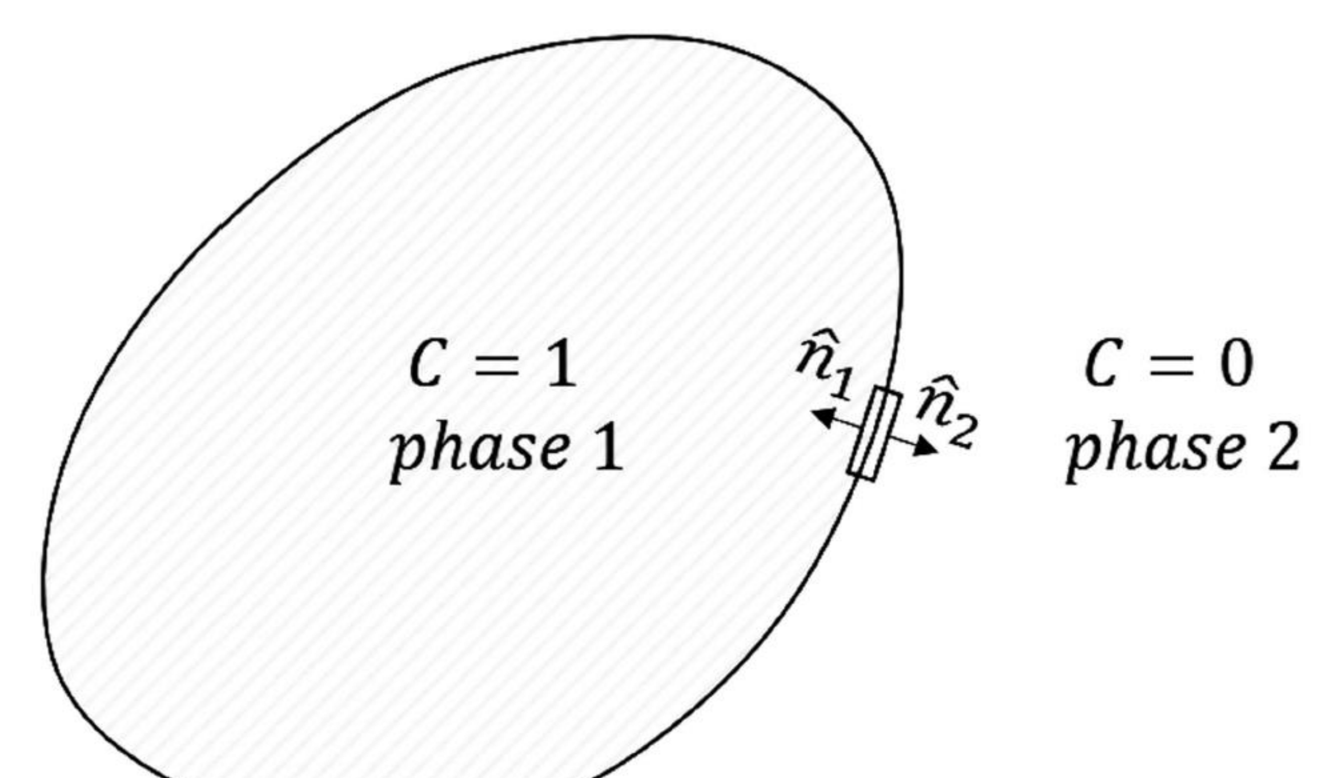
- "In the PLIC method the orientation of the line segment is determined first, and then the exact location of the segment is decided based on the *C* value."

Qin (2022, p. 227)

VOF: Interface Reconstruction

- "If we use a small volume to enclose a segment of the interface as shown in the right figure, the volume integral of the gradient of *C* over this small volume is"

$$\int_V \nabla C dV = \int_S C\hat{\mathbf{n}} dS$$



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- "When the volume is small enough and the interface segment contained in the volume is close to a straight line, we have $\int_V \nabla C dV = \int_S C\hat{\mathbf{n}} dS \approx (1 \cdot \hat{\mathbf{n}}_1 + 0 \cdot \hat{\mathbf{n}}_2)\delta A = \hat{\mathbf{n}}_1 \delta A$

where δA is the area of the interface segment in 3D or the length of the segment in 2D."

VOF: Interface Reconstruction

0.52	0.16	0	0
1	0.97	0.26	0
1	1	0.78	0
1	1	0.86	0

- If we apply this result to control volume (i, j) that contains an interface segment in the right figure, we have

$$\int_V \nabla C dV = (\nabla C)_{i,j}\, \delta V_{i,j} \approx (\hat{\mathbf{n}}_1)_{i,j}\, \delta A_{i,j}$$

- The orientation of the interface segment is then obtained from

$$(\hat{\mathbf{n}}_1)_{i,j} \approx \frac{\delta V_{i,j}}{\delta A_{i,j}} (\nabla C)_{i,j}$$

- This equation tells use the interface orientation can be computed using the gradient of C.
- Since $\hat{\mathbf{n}}_1$ is a unit vector, we then have $(\hat{\mathbf{n}}_1)_{i,j} \approx \dfrac{(\nabla C)_{i,j}}{\left|(\nabla C)_{i,j}\right|}$

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VOF: Interface Reconstruction

- In 2D, the gradient of C is $\nabla C = \frac{\partial C}{\partial x}\hat{\mathbf{i}} + \frac{\partial C}{\partial y}\hat{\mathbf{j}}$
- We can use the second-order central FD to approximate the derivatives.
- More accurate FD approximations are

$$\left(\frac{\partial C}{\partial x}\right)_{i,j} \approx \frac{\left(C_{i+1,j+1} + 2C_{i+1,j} + C_{i+1,j-1}\right) - \left(C_{i-1,j+1} + 2C_{i-1,j} + C_{i-1,j-1}\right)}{8\Delta x}$$

$$\left(\frac{\partial C}{\partial y}\right)_{i,j} \approx \frac{\left(C_{i-1,j+1} + 2C_{i,j+1} + C_{i+1,j+1}\right) - \left(C_{i-1,j-1} + 2C_{i,j-1} + C_{i+1,j-1}\right)}{8\Delta y}$$

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VOF: Interface Reconstruction

- For the cell with $C = 0.26$, the derivatives are approximated as $$\frac{\partial C}{\partial x} = -\frac{0.3875}{\Delta x}, \qquad \frac{\partial C}{\partial y} = -\frac{0.3}{\Delta y}$$
- With $\Delta x = \Delta y$, the unit normal is $\hat{\mathbf{n}} = -0.79\hat{\mathbf{i}} - 0.61\hat{\mathbf{j}}$

0.52	0.16	0	0
1	0.97	0.26	0
1	1	0.78	0
1	1	0.86	0

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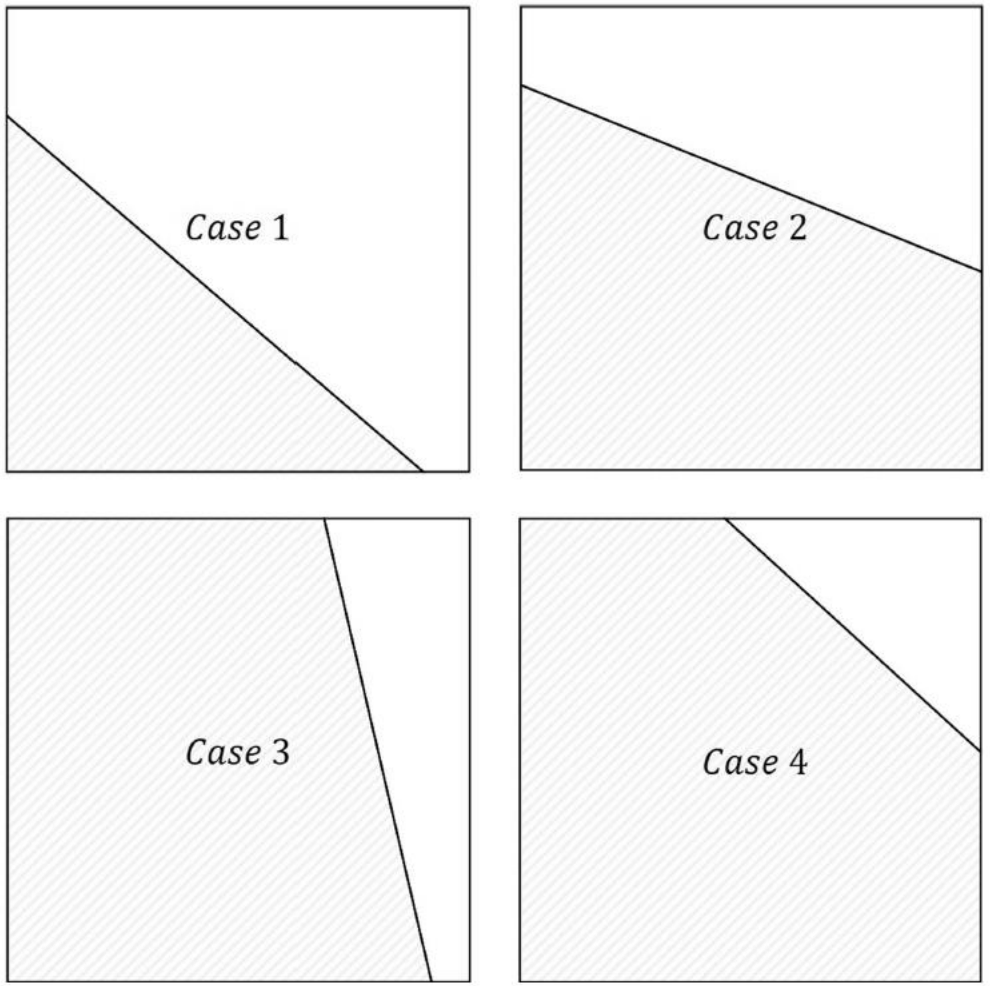
VOF: Interface Reconstruction



- The second step to the interface reconstruction is to determine the exact location of the interface in a cell.
- "If both components of the normal vector of a cell are both negative, the interface approximated by a line segment can only intersect the cell surfaces in 4 possible cases as shown in the right figure."
- "The volume fraction of phase 1 of the cell (the shaded region) is equal to the *C* value of this cell and this value has to be within certain limits for each case."

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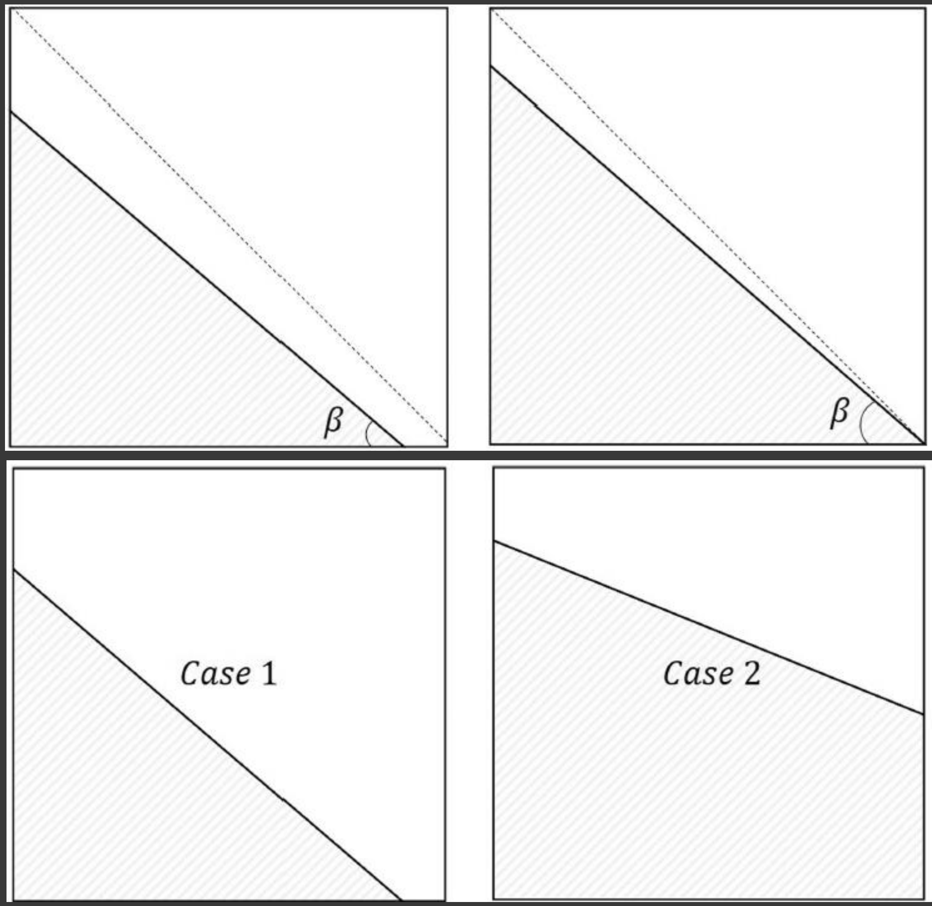
VOF: Interface Reconstruction

- "If the angle β made by the interface with the south interface in case 1 is such that

$$\tan\beta < \frac{\Delta y}{\Delta x}$$

the shaded area cannot exceed a limiting value shown in case 2, otherwise it is no longer case 1 but case 2 configuration."
- "The condition that an interface belongs to case 1 when the above inequality holds is

$$C\Delta x\Delta y \le \tfrac{1}{2}\Delta x\Delta y$$
$$\le \tfrac{1}{2}\Delta x\left(\Delta x\tan\beta\right)$$



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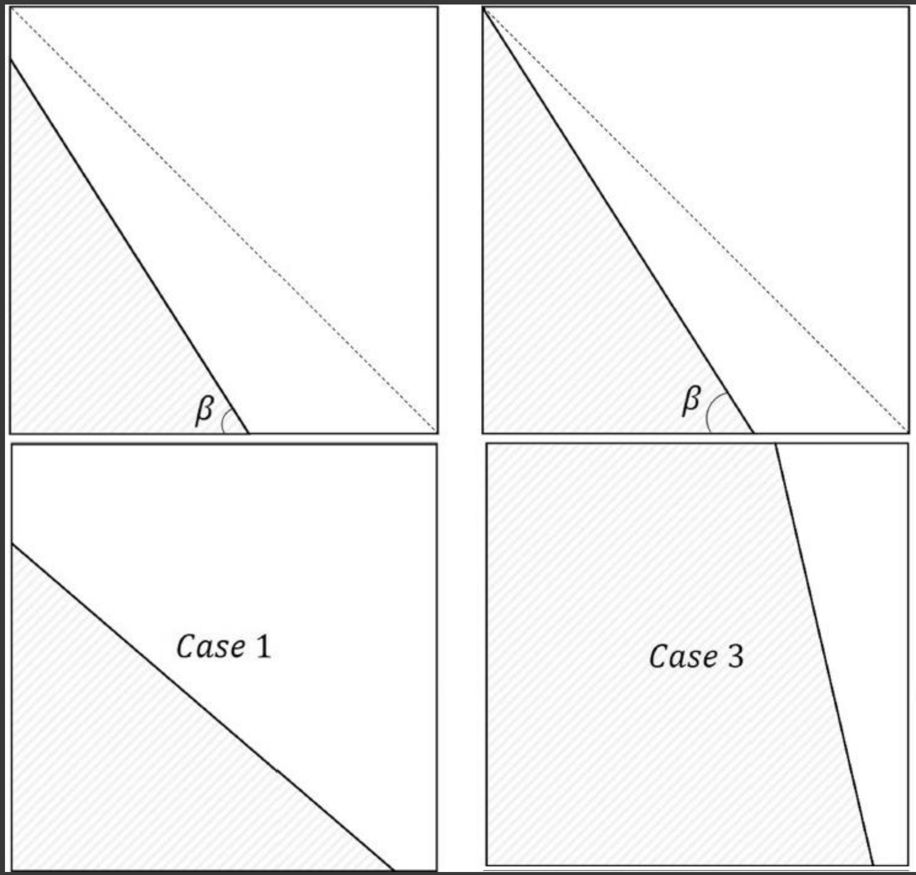
VOF: Interface Reconstruction

- "If $\tan\beta \geq \Delta y/\Delta x$ as shown in the top left panel, the condition for the disposition to be case 1 is" $C\Delta x\Delta y \leq \frac{1}{2}\Delta x\Delta y$

$$\leq \frac{1}{2}\Delta y\left(\frac{\Delta y}{\tan\beta}\right)$$

- "We can find similar conditions for the other three cases following the same idea."



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VOF: Interface Reconstruction

- Let $\alpha \equiv \dfrac{\Delta x}{\Delta y}\tan\beta$. Note that $\tan\beta = \left|\dfrac{\hat{n}_x}{\hat{n}_y}\right|$, so the value of α can be computed after we know the normal vector $\hat{\mathbf{n}}$.
- The conditions $\tan\beta < \Delta y/\Delta x$ and $\tan\beta \geq \Delta y/\Delta x$ can be rewritten as

$$0 < C \leq \alpha/2 \quad \text{if } \alpha < 1$$
$$0 < C \leq 1/2\alpha \quad \text{if } \alpha \geq 1$$

0.52	0.16	0	0
1	0.97	$\boxed{0.26}$	0
1	1	0.78	0
1	1	0.86	0

- For the cell with C = 0.26, we have

$$\alpha = \frac{\Delta x}{\Delta y}\tan\beta = \tan\beta = \left|\frac{-0.79}{-0.61}\right| = 1.29 \rightarrow \alpha \geq 1$$

- So the interface profile belongs to case 1 because

$$0 < (C = 0.26) \leq (1/2\alpha = 0.39)$$

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Conditions for the 4 Interface Configuration Cases

Case	Conditions	
	$\alpha < 1$	$\alpha \geq 1$
1	$0 < C \leq \frac{\alpha}{2}$	$0 < C \leq \frac{1}{2\alpha}$
2	$\frac{\alpha}{2} < C \leq 1 - \frac{\alpha}{2}$	————
3	————	$\frac{1}{2\alpha} < C \leq 1 - \frac{1}{2\alpha}$
4	$1 - \frac{\alpha}{2} < C < 1$	$1 - \frac{1}{2\alpha} < C < 1$

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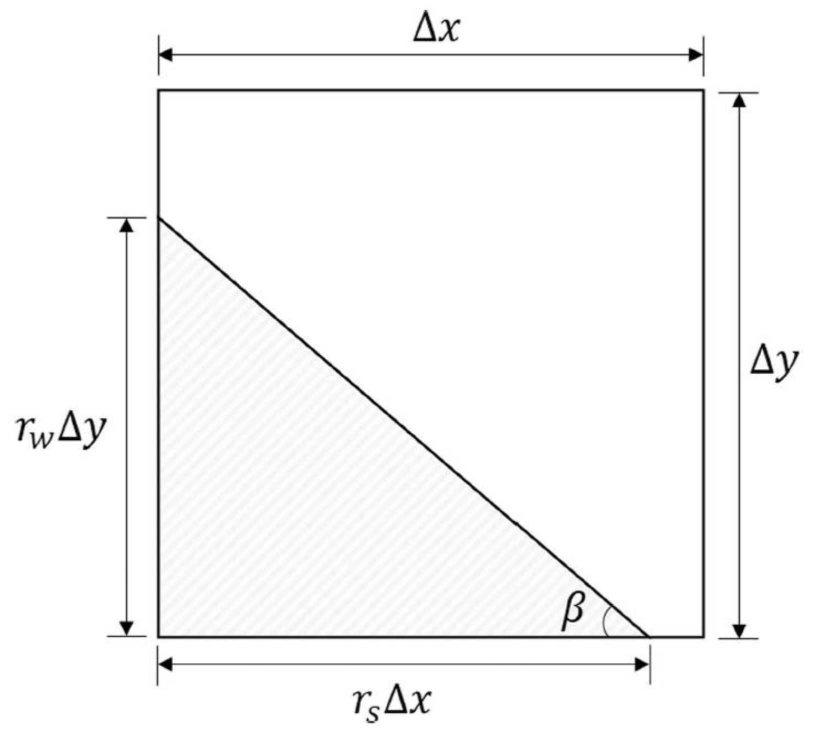
VOF: Interface Reconstruction

- "Once the interface configuration case is determined, the interface reconstruction can be completed by calculating the intercepts the interface make with the cell edges."
- Consider case 1.
- Let r_w and r_s be the fraction of the west and south surfaces of the cell that lie within phase 1, respectively.
- We then have $$\tan\beta = \frac{r_w \Delta y}{r_s \Delta x} \rightarrow \alpha = \frac{\Delta x}{\Delta y}\tan\beta = \frac{r_w}{r_s}$$

$$C\Delta x\Delta y = \frac{1}{2}\left(r_s \Delta x\right)\left(r_w \Delta y\right)$$



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VOF: Interface Reconstruction

- Solving these 2 equations

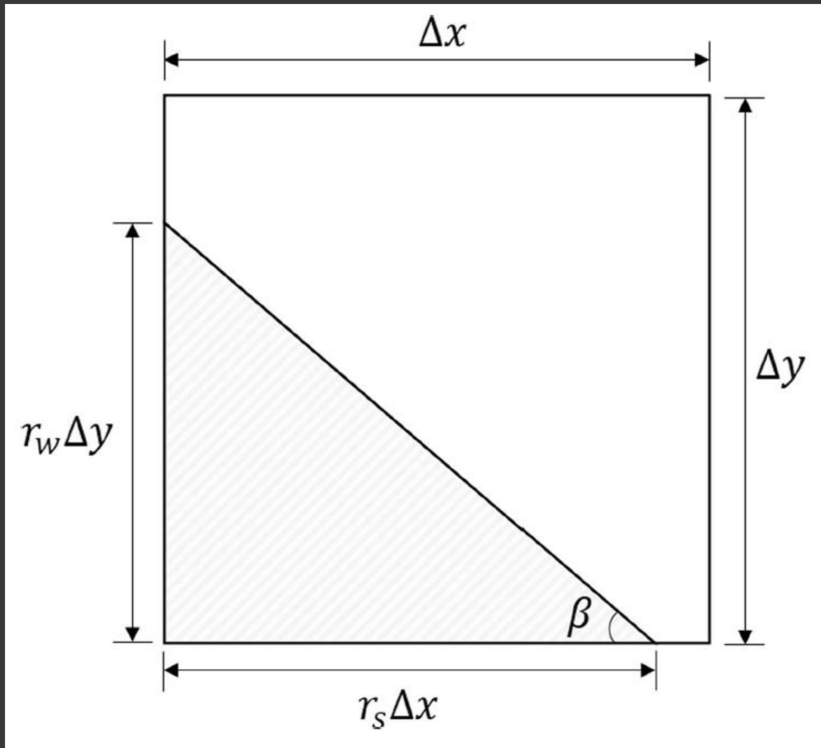
$$\alpha = \frac{r_w}{r_s}, \qquad C\Delta x\Delta y = \frac{1}{2}(r_s\Delta x)(r_w\Delta y)$$

we obtain

$$r_w = \sqrt{2C\alpha}, \qquad r_s = \sqrt{\frac{2C}{\alpha}}$$

- For cell with $C = 0.26$, we have $\alpha = 1.29$.
- So, $r_w = 0.82$ and $r_s = 0.63$.

0.52	0.16	0	0
1	0.97	$\boxed{0.26}$	0
1	1	0.78	0
1	1	0.86	0



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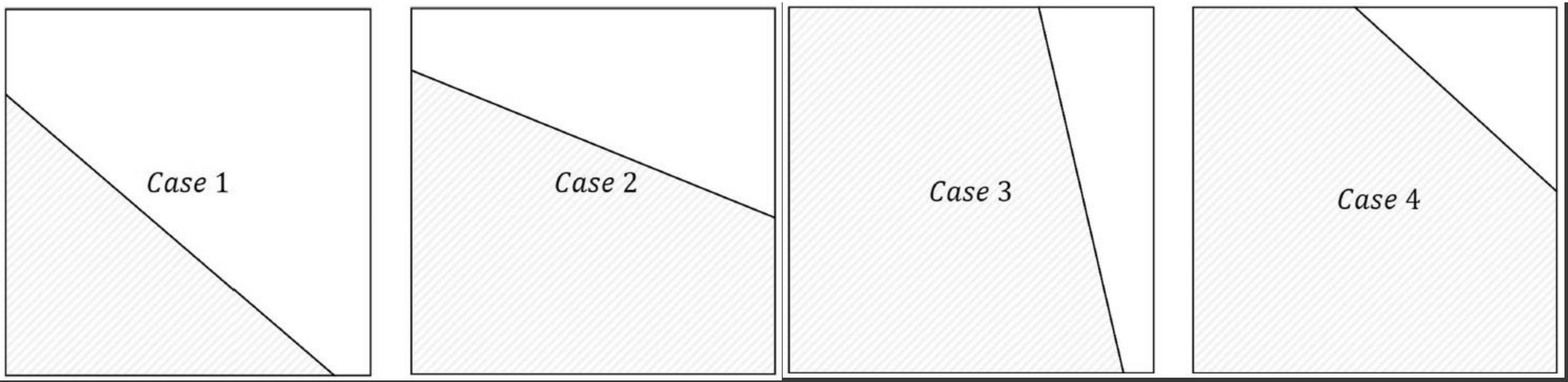
Side Fractions for the 4 Interface Configuration Cases

Case	r_n	r_e	r_w	r_s
1	0	0	$\sqrt{2C\alpha}$	$\sqrt{\frac{2C}{\alpha}}$
2	0	$C - \frac{\alpha}{2}$	$C + \frac{\alpha}{2}$	1
3	$C - \frac{1}{2\alpha}$	0	1	$C + \frac{1}{2\alpha}$
4	$1 - \sqrt{\frac{2(1-C)}{\alpha}}$	$1 - \sqrt{2(1-C)\alpha}$	1	1



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VOF: Interface Advection

- "In the VOF method, the interface is identified by the step change of the marker function C."
- "Therefore, we only need to know how the C field advects with the fluid flow in order to track the interface."
- "Note that C is a label of each fluid particle."
- $C = 1$ for particle in phase 1 (e.g., gas).
- $C = 0$ for particle in phase 2 (e.g., liquid).
- Since we assume that the two phases are immiscible and that there is no phase change, the phase of any fluid particle never change.
- "This implies that the material derivative of C vanishes, i.e.,

$$\frac{DC}{Dt} = \frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C = 0$$

Qin (2022, p. 233)

VOF: Interface Advection

- The advection equation for the marker function can be rewritten as

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(\mathbf{v} C \right) = C \nabla \cdot \mathbf{v}$$

- Integrating the above equation over the (i, j) control volume

$$\int_V \frac{\partial C}{\partial t} dV + \int_V \nabla \cdot \left(\mathbf{v} C \right) dV = \int_V C \nabla \cdot \mathbf{v} dV$$

$$\int_V \frac{\partial C}{\partial t} dV + \int_S C \mathbf{v} \cdot \hat{\mathbf{n}} dS = \int_V C \nabla \cdot \mathbf{v} dV$$

VOF: Interface Advection

- In 2D, the last equation can be approximated as

$$\frac{C_{i,j}^{m+1}-C_{i,j}^{m}}{\Delta t}\Delta x\Delta y+\sum_{k=1}^{4}C_k\mathbf{v}_k\cdot\hat{\mathbf{n}}_k A_k=C_{i,j}^{m}\left(\nabla\cdot\mathbf{v}\right)_{i,j}\Delta x\Delta y$$

where $\hat{\mathbf{n}}_k$ is the unit outward normal vector at the k^{th} surface of the cell,
$\mathbf{v}_k$ is the velocity vector at the k^{th} surface of the cell,
C_k is the C value of the k^{th} surface of the cell,
A_k is the area (length in 2D) of the k^{th} surface of the cell.

- The C flux across the k^{th} surface is defined as

$$F_k=C_k\mathbf{v}_k\cdot\hat{\mathbf{n}}_k$$

- Note that the flux is positive for an outflow.

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VOF: Interface Advection

- We can then rewrite

$$\frac{C_{i,j}^{m+1} - C_{i,j}^{m}}{\Delta t}\Delta x \Delta y + \sum_{k=1}^{4} C_k \mathbf{v}_k \cdot \hat{\mathbf{n}}_k A_k = C_{i,j}^{m} \left(\nabla \cdot \mathbf{v}\right)_{i,j} \Delta x \Delta y$$

as

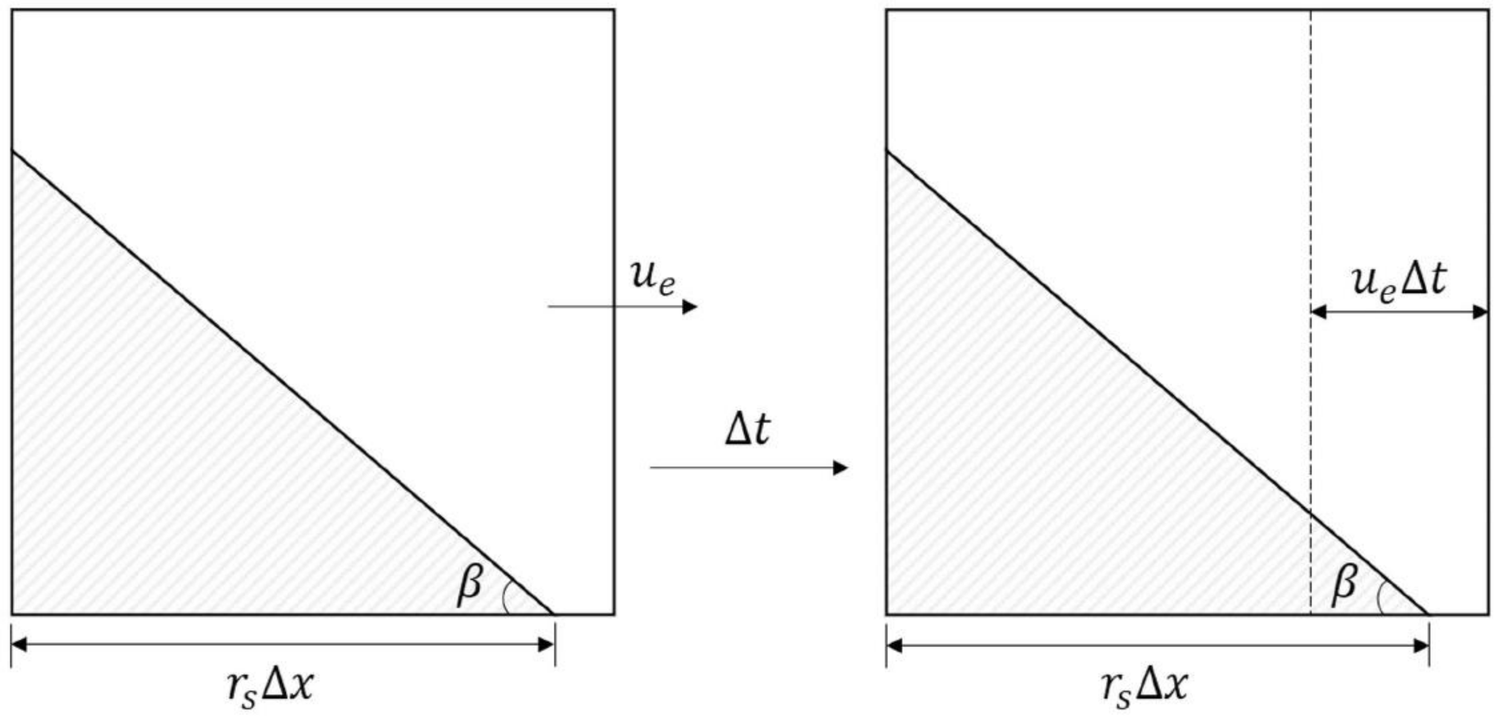
$$\frac{C_{i,j}^{m+1} - C_{i,j}^{m}}{\Delta t} = -\frac{F_e + F_w}{\Delta x} - \frac{F_n + F_s}{\Delta y} + C_{i,j}^{m} \left(\nabla \cdot \mathbf{v}\right)_{i,j}$$

- If this numerical scheme is applied to advect the C field, numerical diffusion will gradually smear the C field (more cells with $0 < C < 1$) causing the interface to grow thicker over time.
- The advection equation tells us that both fluid phases (represented by the C field) simply advect with the local fluid velocity.

Qin (2022, p. 236)

VOF: Interface Advection

- "We may directly calculate the amount of each phase getting into or out of a control volume."
- Suppose that a cell has a case 1 interface configuration and the fluid velocity at its east surface is $u_e > 0$.
- In Δt time period, the fluid right to the dash line in the right panel will leave this cell and enter its east neighboring cell.
- "This cell then loses some volume of phase 1 to its east neighboring cell."



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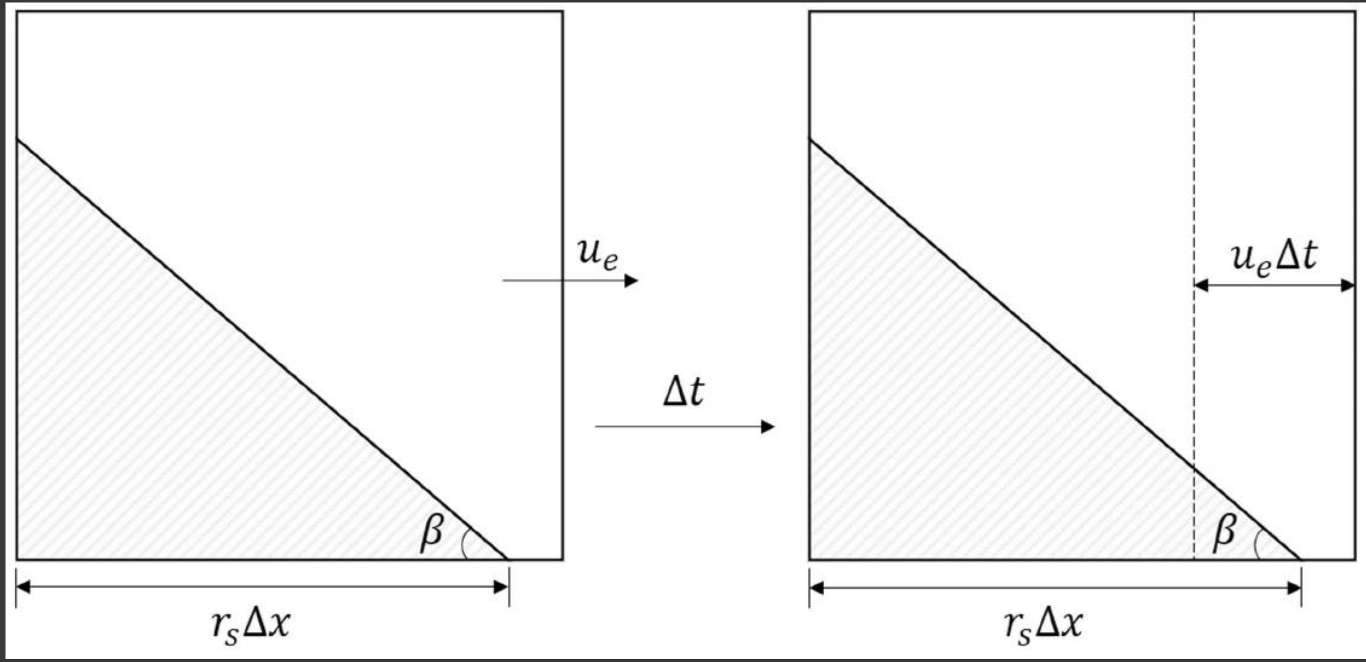
VOF: Interface Advection

- "The amount of this volume change is

$$V_e = \begin{cases} 0 & \text{if } u_e \Delta t < (1 - r_s)\Delta x \\ 0.5 \tan\beta \left[u_e \Delta t - (1 - r_s)\Delta x \right]^2 & \text{if } (1 - r_s)\Delta x \le u_e \Delta t < \Delta x \end{cases}$$

- We require $u_e \Delta t < \Delta x$, otherwise we will run out of fluid in this cell after Δt.
- This leads to the CFL condition

$$\max\left[\frac{\max(|u|)\Delta t}{\Delta x}, \frac{\max(|v|)\Delta t}{\Delta y} \right] < 1$$



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VOF: Interface Advection

- "The C flux leaving the (i, j) cell through its east surface is"

$$F_e(i,j) = u_e C_e = u_e\left(\frac{V_e}{u_e \Delta t \Delta y}\right) = \frac{V_e}{\Delta t \Delta y}$$

- "The east neighborint cell, the $(i + 1, j)$ cell, gains the same amount of flux via its west surface:"

$$F_w(i+1,j) = -F_e(i,j)$$

- The negative sign is added to the flux because it is an inflow of the $(i + 1, j)$ cell.
- The information about the flux is always provided by the upstream or "donor" cell.

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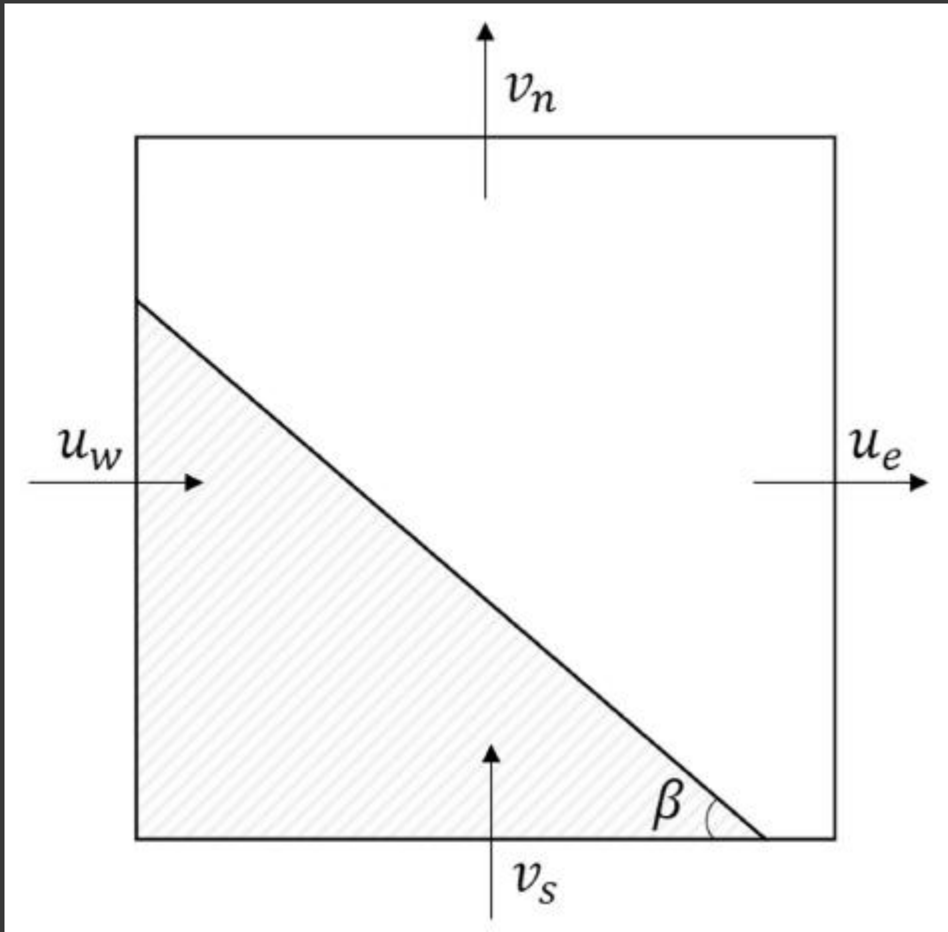
VOF: Interface Advection

- Consider a cell shown in the right figure.
- This cell is a donor in terms of fluxes across its north and east surfaces while an acceptor for the fluxes across its west and south surfaces.
- Donors and acceptors always appear in pairs.



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Volume Transfer through East and West Surfaces

Case	V_w (if $u_w < 0$)	V_e (if $u_e > 0$)
1	if $\lvert u_w\rvert \Delta t < r_s \Delta x$ $\lvert u_w\rvert \Delta t\,(r_w \Delta y - 0.5\lvert u_w\rvert \Delta t \tan\beta)$ else $C\Delta x \Delta y$	if $u_e \Delta t < (1 - r_s)\Delta x$ 0 else $0.5 \tan\beta\,[u_e \Delta t - (1 - r_s)\Delta x]^2$
2	$\lvert u_w\rvert \Delta t\,(r_w \Delta y - 0.5\lvert u_w\rvert \Delta t \tan\beta)$	$u_e \Delta t\,(r_e \Delta y + 0.5 u_e \Delta t \tan\beta)$
3	if $\lvert u_w\rvert \Delta t < r_n \Delta x$ $\lvert u_w\rvert \Delta t \Delta y$ elseif $\lvert u_w\rvert \Delta t < r_s \Delta x$ $\lvert u_w\rvert \Delta t \Delta y - 0.5 \tan\beta\,(\lvert u_w\rvert \Delta t - r_n \Delta x)^2$ else $C\Delta x \Delta y$	if $u_e \Delta t < (1 - r_s)\Delta x$ 0 elseif $u_e \Delta t < (1 - r_n)\Delta x$ $0.5 \tan\beta\,[u_e \Delta t - (1 - r_s)\Delta x]^2$ else $u_e \Delta t \Delta y - (1 - C)\Delta x \Delta y$
4	if $\lvert u_w\rvert \Delta t < r_n \Delta x$ $\lvert u_w\rvert \Delta t \Delta y$ else $\lvert u_w\rvert \Delta t \Delta y - 0.5 \tan\beta\,(\lvert u_w\rvert \Delta t - r_n \Delta x)^2$	if $u_e \Delta t < (1 - r_n)\Delta x$ $u_e \Delta t\,(r_e \Delta y + 0.5 u_e \Delta t \tan\beta)$ else $u_e \Delta t \Delta y - (1 - C)\Delta x \Delta y$

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Volume Transfer through North and South Surfaces

Case	V_s (if $v_s < 0$)	V_n (if $v_n > 0$)
1	if $\|v_s\|\Delta t < r_w \Delta y$	if $v_n \Delta t < (1 - r_w)\Delta y$
	$\|v_s\|\Delta t\,(r_s \Delta x - 0.5\|v_s\|\Delta t \tan\beta)$	0
	else	else
	$C\Delta x \Delta y$	$0.5 \tan\beta\,[v_n \Delta t - (1 - r_w)\Delta y]^2$
2	if $\|v_s\|\Delta t < r_e \Delta y$	if $v_n \Delta t < (1 - r_w)\Delta y$
	$\|v_s\|\Delta t \Delta x$	0
	elseif $\|v_s\|\Delta t < r_w \Delta y$	elseif $v_n \Delta t < (1 - r_e)\Delta y$
	$\|v_s\|\Delta t \Delta x - 0.5 \tan\beta\,(\|v_s\|\Delta t - r_e \Delta y)^2$	$0.5 \tan\beta\,[v_n \Delta t - (1 - r_w)\Delta y]^2$
	else	else
	$C\Delta x \Delta y$	$v_n \Delta t \Delta x - (1 - C)\Delta x \Delta y$
3	$\|v_s\|\Delta t\,(r_s \Delta x - 0.5\|v_s\|\Delta t \tan\beta)$	$v_n \Delta t\,(r_n \Delta x + 0.5 v_n \Delta t \tan\beta)$
4	if $\|v_s\|\Delta t < r_e \Delta y$	if $v_n \Delta t < (1 - r_e)\Delta y$
	$\|v_s\|\Delta t \Delta x$	$v_n \Delta t\,(r_n \Delta x + 0.5 v_n \Delta t \tan\beta)$
	else	else
	$\|v_s\|\Delta t \Delta x - 0.5 \tan\beta\,(\|v_s\|\Delta t - r_e \Delta y)^2$	$v_n \Delta t \Delta x - (1 - C)\Delta x \Delta y$

Qin (2022, p. 239)

VOF: Interface Advection

- "After we obtain the fluxes across all four surfaces of a cell, we can evaluate the overall change in its C value as"

$$\frac{C_{i,j}^{m+1}-C_{i,j}^{m}}{\Delta t}=-\frac{F_e+F_w}{\Delta x}-\frac{F_n+F_s}{\Delta y}+C_{i,j}^{m}\left(\nabla\cdot\mathbf{v}\right)_{i,j}$$

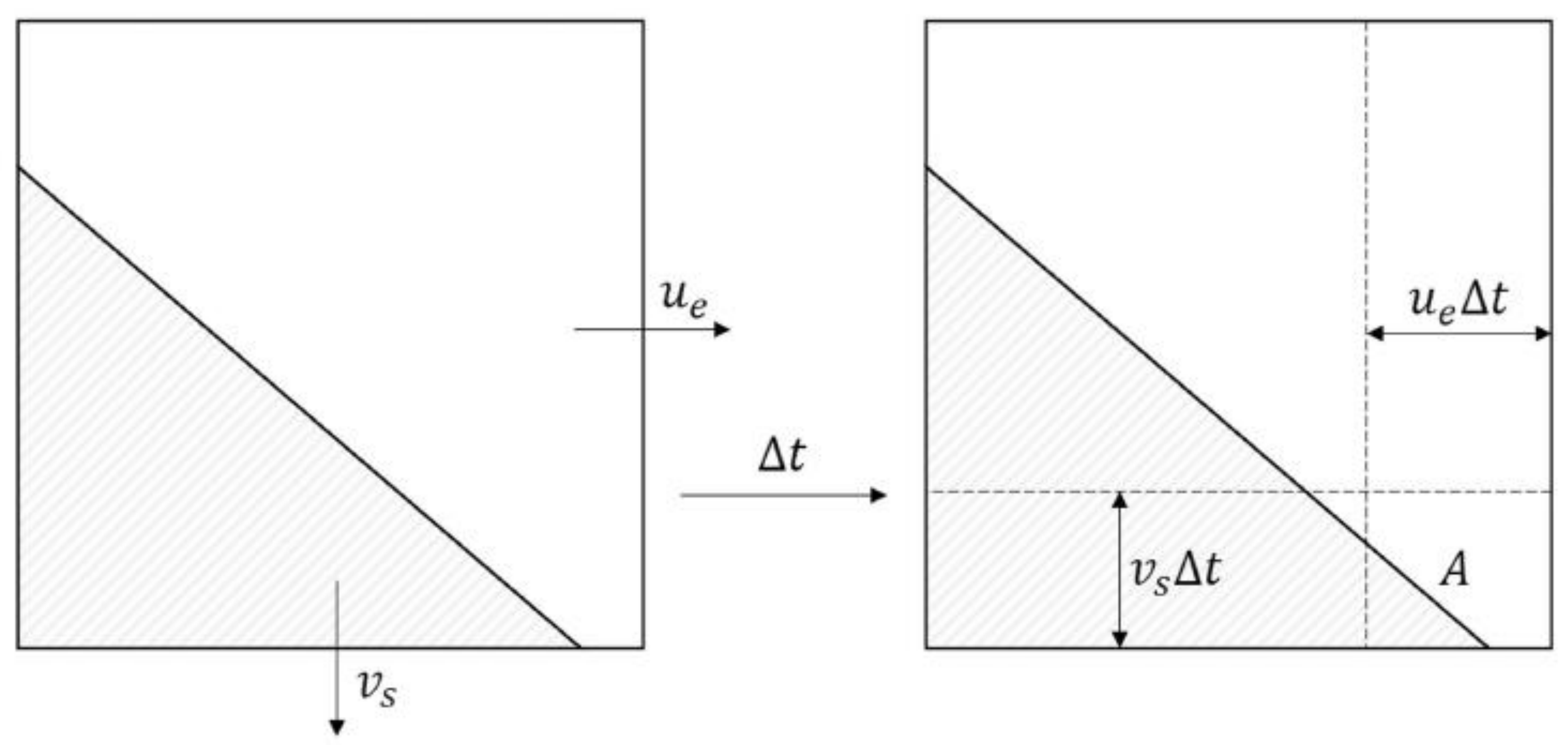
$$=-\frac{F_e+F_w}{\Delta x}-\frac{F_n+F_s}{\Delta y}+C_{i,j}^{m}\left(\frac{u_e-u_w}{\Delta x}+\frac{v_n-v_s}{\Delta y}\right)$$

- There are still some issues that must be addressed.
- The first issue is that we may double-count some fluxes.
- This issue is illustrated in the example in the next slide.

Qin (2022, p. 238)

VOF: Interface Advection

"If fluid flows out of a cell through its east and south surfaces, we will count the fluid right to the vertical dashed line as F_e and that below the horizontal dashed line as F_s. Not that the fluid in the corner area (marked by letter A) is counted twice."



Qin (2022, p. 238)

VOF: Interface Advection

- The second issue is how to obtain second-order accuracy in time.
- A solution to the second issue is to use a fractional time step method and alternate explicit and implicit schems in those fractional steps.
- To solve the first issue, we can advect the *C* field horizontally in one fractional step and vertically in another fractional step.
- These result in the procedure for advancing the *C* field described in the next slide.

Qin (2022, p. 239)

VOF: Interface Advection

- "First, evaluate F_e and F_w according to the C field at the m^{th} time step and advect C horizontally:"

$$\frac{C_{i,j}^{*} - C_{i,j}^{m}}{\Delta t} = -\frac{F_e + F_w}{\Delta x} + C_{i,j}^{*}\left(\frac{u_e - u_w}{\Delta x}\right)$$

- "Then reconstruct the interface and evaluate F_n and F_s based on the C^* field and then advance C to the new time step:"

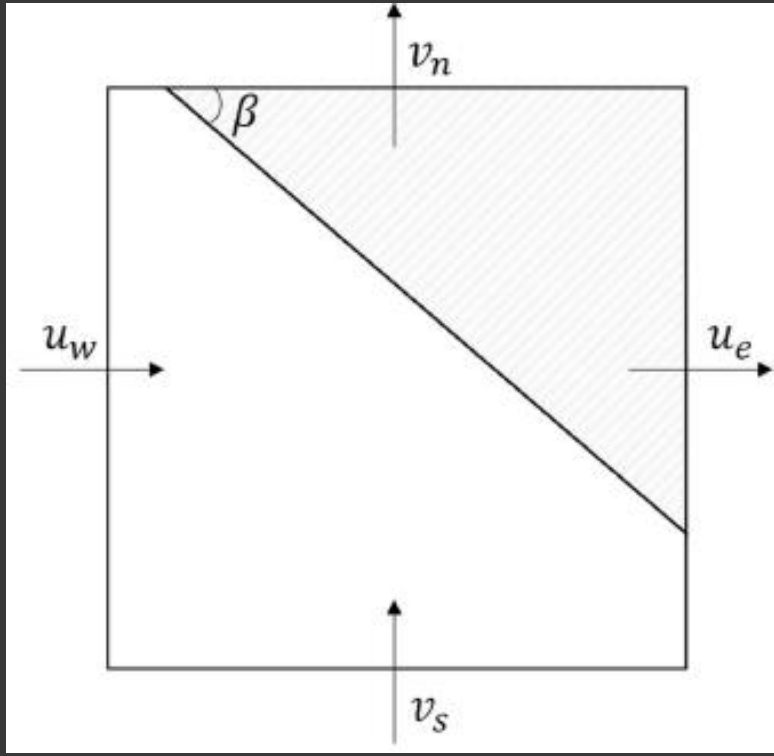
$$\frac{C_{i,j}^{m+1} - C_{i,j}^{*}}{\Delta t} = -\frac{F_n^{*} + F_s^{*}}{\Delta y} + C_{i,j}^{*}\left(\frac{v_n - v_s}{\Delta y}\right)$$

- Note that the advection direction is alternated at each fractional time step.
- An implicit scheme is used in the first fractional step while an explicit scheme is used in the second fractional step.

Qin (2022, p. 240)

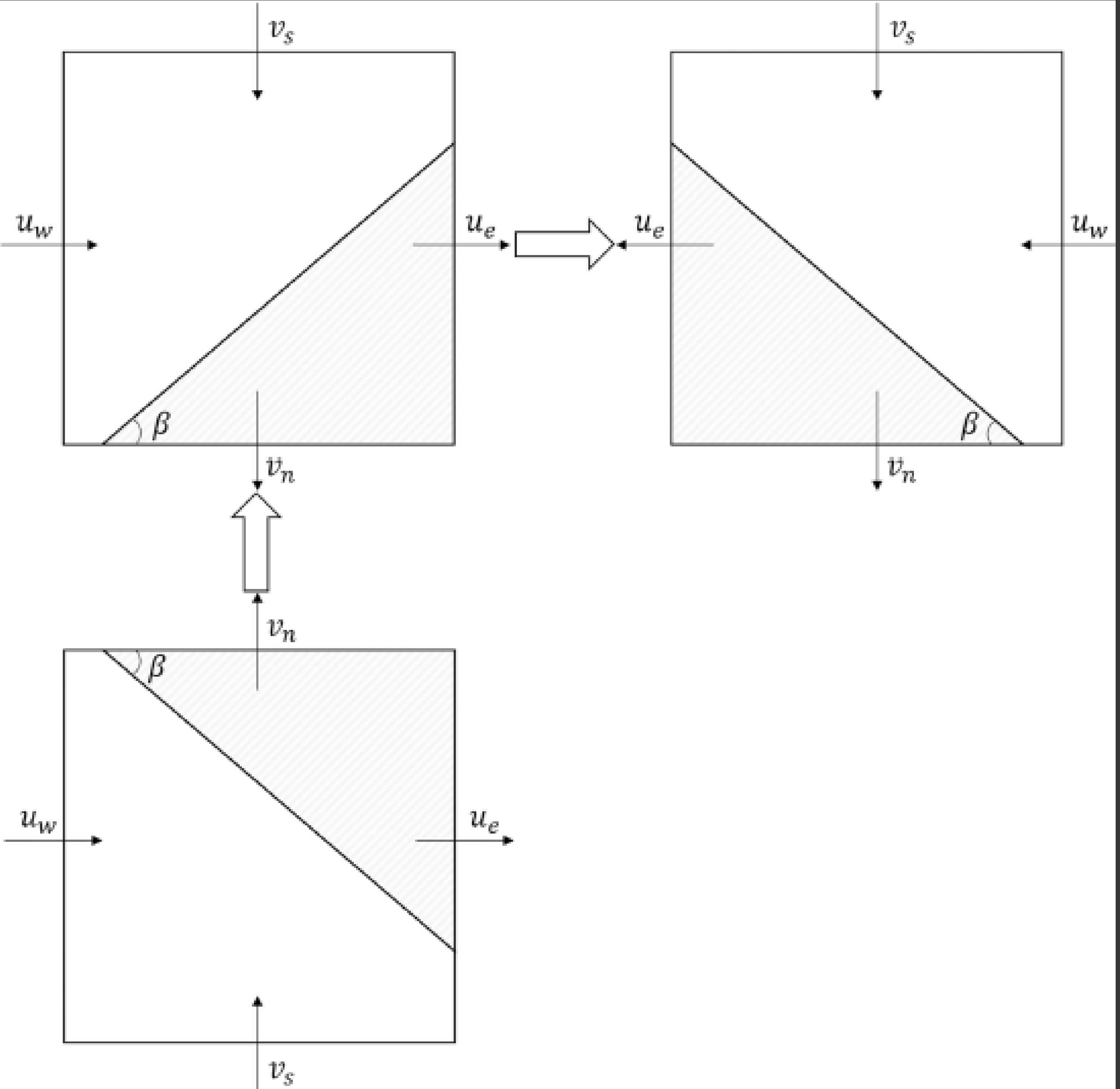
VOF: Interface Advection

- "The last subtletly involed in the interface reconstruction and advection procedure is that all formulas given in last 4 tables are for the situation when both components of the interface normal vectors are negative, and special care is needed if the interface is oriented differently."
- If the interface segment in a cell is as shown in the right figure, both components of the normal vectors are positive.
- "We can first flip it vertically and then horizontally to turn it into the 'standard' configuration."



Qin (2022, p. 240)

VOF: Interface Advection



- "All the formulas can still be used but we need to use -u_w to replace u_e in the formulas."
- "Similar changes have to be made for the other surface velocities."
- "Once the result is obtained, we have to flip backwards to the original cell and assigned the result to it properly."

Qin (2022, p. 240-241)

VOF: Interface Advection

- "For example, suppose u_e for the real-world cell is positive, and we want to find F_e for this cell."
- "We will calculate F_w of the 'standard' cell by substituting u_w in the F_w formula with the $-u_e$ value of the real-world cell."
- "After we find this flux, we will interpret it as the flux leaving the real cell via its east surface, i.e., as F_e."

Qin (2022, p. 240)

Example: Interface Transport by Uniform Velocity

- "The C field corresponding to a gas bubble immersed in a liquid is shown in the right figure."
- "The radius of the bubble is 0.3 and it is initially centered at (0.5, 0.5)."
- "The fluid velocity is uniform: $u = v = 1$."
- "The mesh size is $\Delta x = \Delta y = 0.25$."
- "The gas phase will regarded as phase 1."
- The CFL condition can be rewritten as

$$\Delta t < \min\left[\frac{\Delta x}{\max\left(|u|\right)}, \frac{\Delta y}{\max\left(|v|\right)}\right] = 0.25$$

- Here, we use $\Delta t = 0.125$.

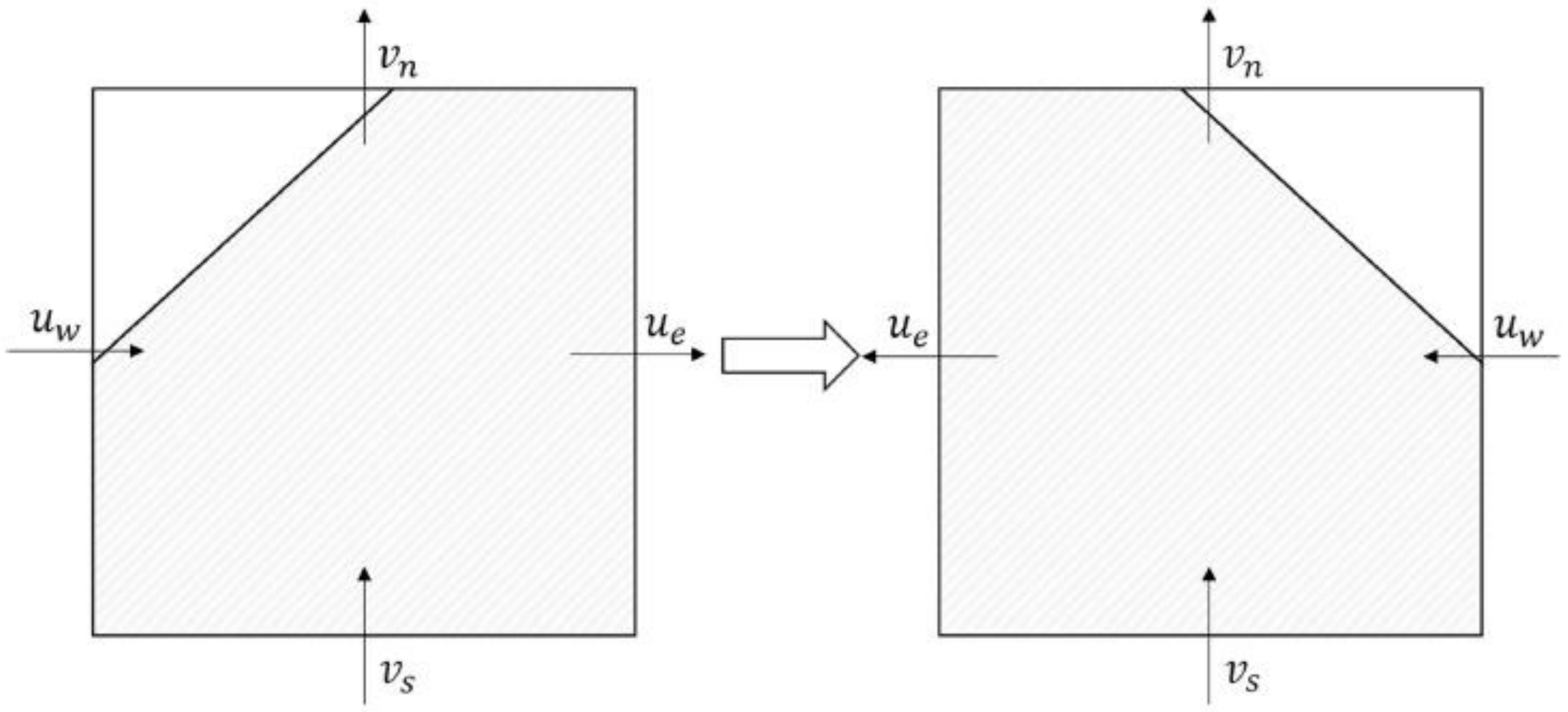
0	0.092	0.092	0
0.092	0.948	0.948	0.092
0.092	0.948	0.948	0.092
0	0.092	0.092	0

Qin (2022, p. 241)

Example: Interface Transport by Uniform Velocity

- Consider the (2, 3) cell marked by the blue square .
- Let's reconstruct the interface for this cell.
- The normal vector for this cell is $\hat{n}_x = 0.7, \hat{n}_y = -0.7$
- Since $\hat{n}_x > 0$, we will flip this cell horizontally to turn it into the standard configuration.

0	0.092	0.092	0
0.092	$\boxed{0.948}$	0.948	0.092
0.092	0.948	0.948	0.092
0	0.092	0.092	0



This cell has $\alpha = 1$. According to the tables in Slides 17 and 20, the interface arrangement is in case 4 and $r_n = r_e = 0.6778$.

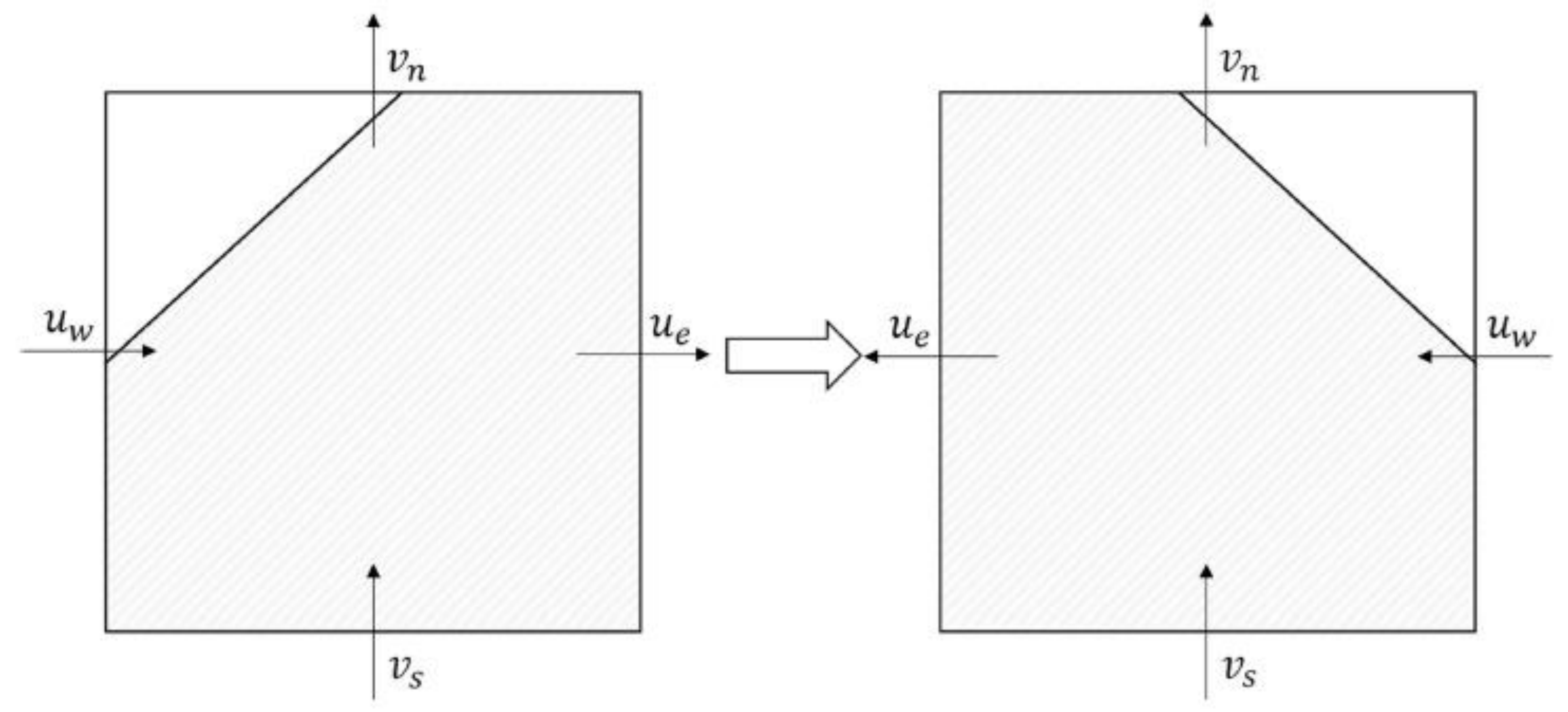
Qin (2022, p. 242)

Example: Interface Transport by Uniform Velocity

- Let's calculate the horizontal fluxes across the surfaces of this cell.
- Using $-u_e = -1$ in place of u_w in equations of the table on Slide 29, we find the gas volume moved out of this cell across its west surface is

$$V_w = |u_w| \Delta t \Delta y = 0.0313$$

- Therefore, $F_w = V_w / \Delta t \Delta y = 1$ for this flipped cell, which is F_e of the original cell. At this point, we should update the F_w value of its east neighboring cell to -1.



Qin (2022, p. 242)

Example: Interface Transport by Uniform Velocity

- Similarly, F_w of the current (2, 3) cell should be updated when we calculate F_e of its west neighboring (1, 3) cell.
- We find that $F_w(2, 3) = -F_e(1, 3) = -0.1846$.
- Using the equation

$$\frac{C^*_{i,j} - C^m_{i,j}}{\Delta t} = -\frac{F_e + F_w}{\Delta x} + C^*_{i,j}\left(\frac{u_e - u_w}{\Delta x}\right)$$

we can find the intermediate C^* value of the current cell as

$$C^*_{2,3} = \frac{C^0_{2,3} - \Delta t \dfrac{F^0_e(2,3) + F^0_w(2,3)}{\Delta x}}{\left[1 - \Delta t\left(\dfrac{u_e - u_w}{\Delta x}\right)\right]} = \frac{0.948 - 0.125 * \dfrac{1 - 0.1846}{0.25}}{1 - 0} = 0.5404$$

0	0.092	0.092	0
0.092	$\boxed{0.948}$	0.948	0.092
0.092	0.948	0.948	0.092
0	0.092	0.092	0

- The superscript 0 indicates the values based on the initial C distribution.

Qin (2022, p. 242-243)

Example: Interface Transport by Uniform Velocity

- Similarly, we can calculate the C^* field (right figure), according to which we can construct the interface again.
- We then compute the vertical fluxes based on the reconstructed interface as $F_n^* = 0.3907$ and its F_s^* is updated when we calculate F_n^* of its south neighboring (2, 2) cell: $F_s^*(2,3) = -F_n^*(2,2) = -0.6901$

0	0.0087	0.1672	0.0087
0	0.5404	1	0.5404
0	0.5404	1	0.5404
0	0.0087	0.1672	0.0087

- We can now calculate the C value of the (2, 3) cell at the next time step as

$$C_{2,3}^1 = C_{2,3}^* - \Delta t \frac{F_n^*(2,3) + F_s^*(2,3)}{\Delta y} + C_{2,3}^* \Delta t \left(\frac{v_n - v_s}{\Delta y} \right)$$

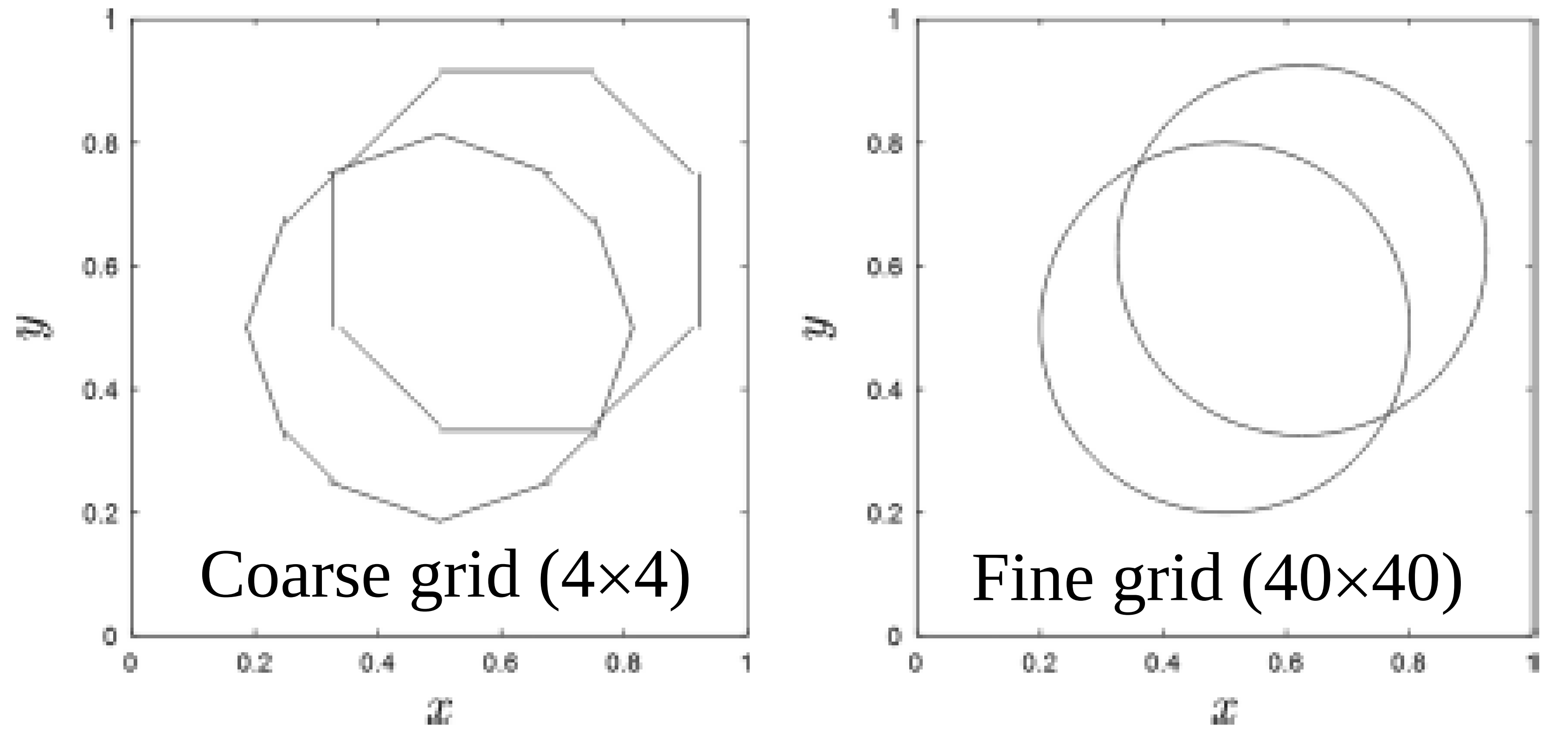
$$= 0.5404 - 0.125 * \frac{0.3907 - 0.6901}{0.25} + 0 = 0.6901$$

Qin (2022, p. 243)

Example: Interface Transport by Uniform Velocity

- The whole C field at $t = 0.125$ is shown one the right.
- "In the next time step, one should advect the C field vertically and then horizontally."
- Initial and final interfaces are shown below (left panel).

0	0.204	0.667	0.204
0	0.69	1	0.69
0	0.204	0.667	0.204
0	0	0	0



The interface is transported to the northeast as expected. The right panel shows the result on a fine grid.

Qin (2022, p. 243)

Flow Field Calculation

- "Since the interface advects with the fluid flow, we need to solve for the flow field to complete the multiphase flow calculation."
- This can be accomplished using the projection method to solve the continuity equation and the momentum equations on a staggered grid with pressure, density, viscosity, marker function stored at the cell center and velocities stored at the cell surfaces.
- "Due to the presence of two phases, flow field variables may experience a sudden jump across the phase interface."
- "To capture such sharp changes, one may solve the Navier-Stokes equations in each phase separately which requires boundary conditions to be applied at the interface for each phase."

Qin (2022, p. 244, 247)

Flow Field Calculation

- "An alternative is to treat all phases as one single fluid with varying physical properties."
- "For the cells that contain both phases, an overall density will be assigned to this fictitious fluid:"

$$\rho = \frac{m}{V} = \frac{m_1 + m_2}{V} = \frac{\rho_1 V_1 + \rho_2 V_2}{V} = \rho_1 C + \rho_2 \left(1 - C\right)$$

- For the viscosity, a harmonic mean of the viscosities of the two phases usually gives more accurate results than an arithmetic mean with the following reasoning.

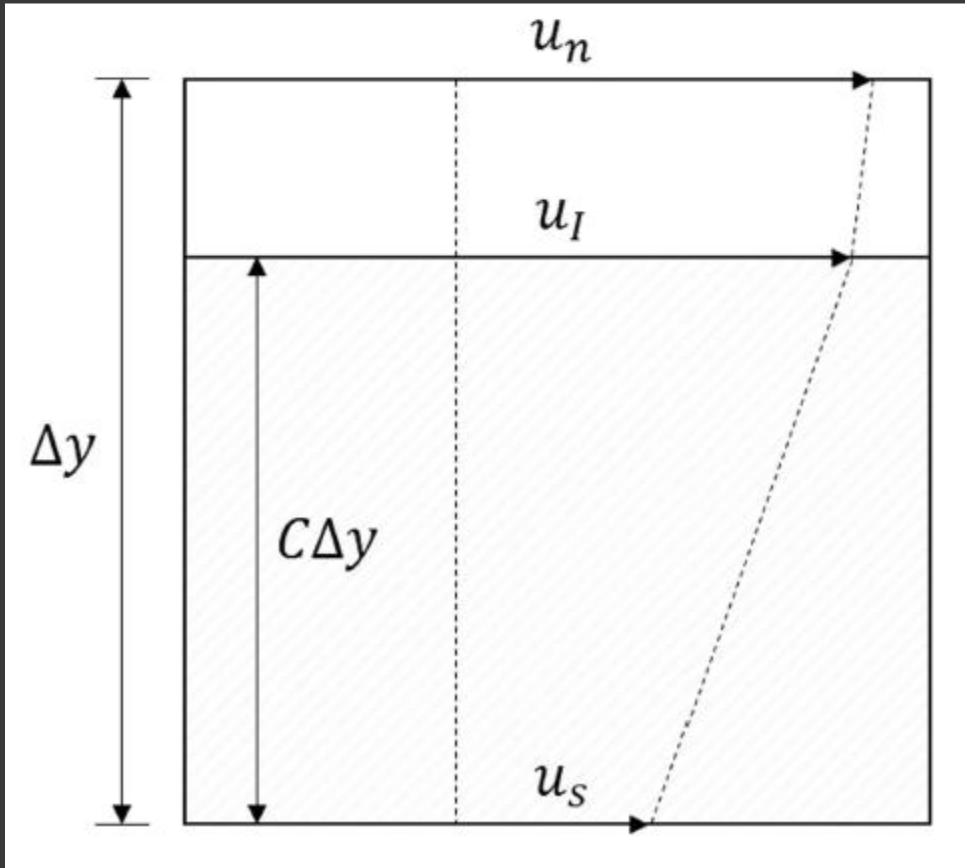
Qin (2022, p. 247)

Flow Field Calculation

- Consider a control volume containing a horizontal phase interface.
- The height of phase 1 is $C\Delta y$ where C is the volume fraction of phase 1.
- "The shear stress acting on this control volume should be

$$\tau_{yx} = \mu \frac{\partial u}{\partial y} \approx \mu \frac{u_n - u_s}{\Delta y}$$

where μ is the effective fluid viscosity of this control volume.



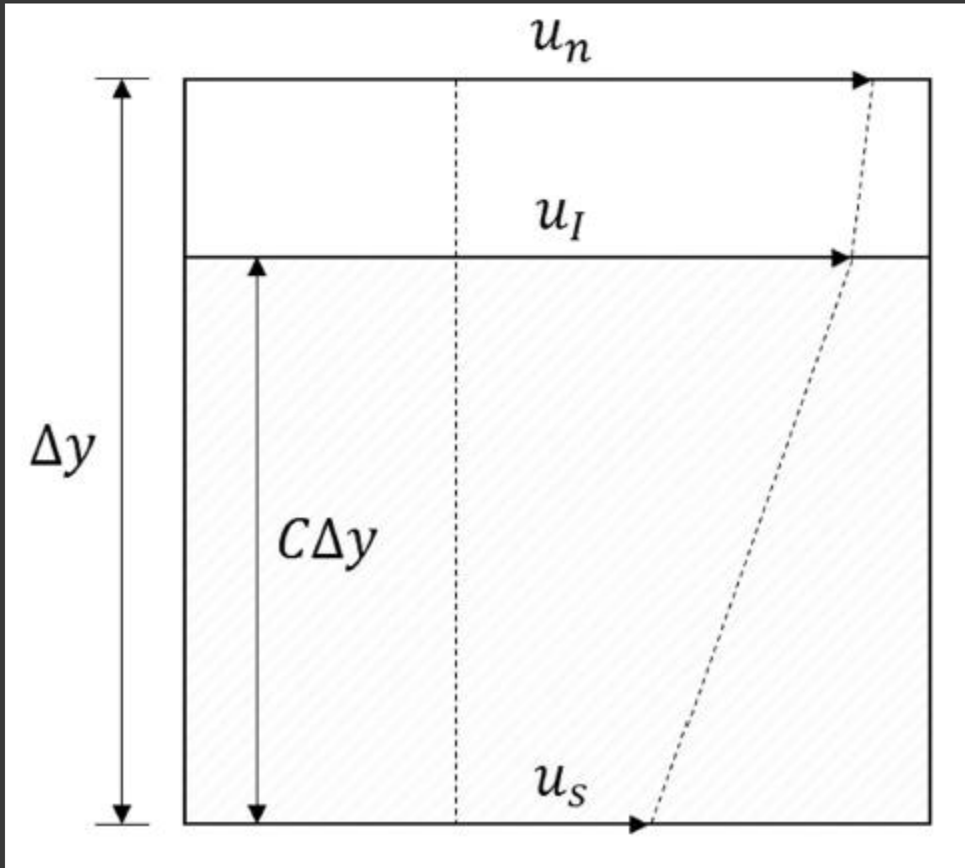
Flow Field Calculation

- "The shear stress can also be evaluated using the velocity profile of phase 2 in this cell alone:"

$$\tau_{yx} = \mu_2 \left(\frac{\partial u}{\partial y} \right)_2 \approx \mu_2 \frac{u_n - u_I}{(1-C)\Delta y}$$

- "Similarly, we may calculate the shear stress using the velocity profile of phase 1 as

$$\tau_{yx} = \mu_1 \left(\frac{\partial u}{\partial y} \right)_1 \approx \mu_1 \frac{u_I - u_s}{C\Delta y}$$



Flow Field Calculation

- Equating these expressions yields

$$\frac{u_n - u_I}{\frac{1-C}{\mu_2}\Delta y} = \frac{u_I - u_s}{\frac{C}{\mu_1}\Delta y} = \frac{u_n - u_s}{\frac{1}{\mu}\Delta y} \quad \rightarrow \quad u_I = \frac{\frac{C}{\mu_1}u_n + \frac{1-C}{\mu_2}u_s}{\frac{1-C}{\mu_2} + \frac{C}{\mu_1}}$$

- Substituting the value of u_I into one of the expressions yields

$$\frac{u_n - u_s}{\left(\frac{1-C}{\mu_2} + \frac{C}{\mu_1}\right)\Delta y} = \frac{u_n - u_s}{\frac{1}{\mu}\Delta y}$$

- This leads to the expression for the effective viscosity as $\mu = \dfrac{1}{\frac{1-C}{\mu_2} + \frac{C}{\mu_1}}$

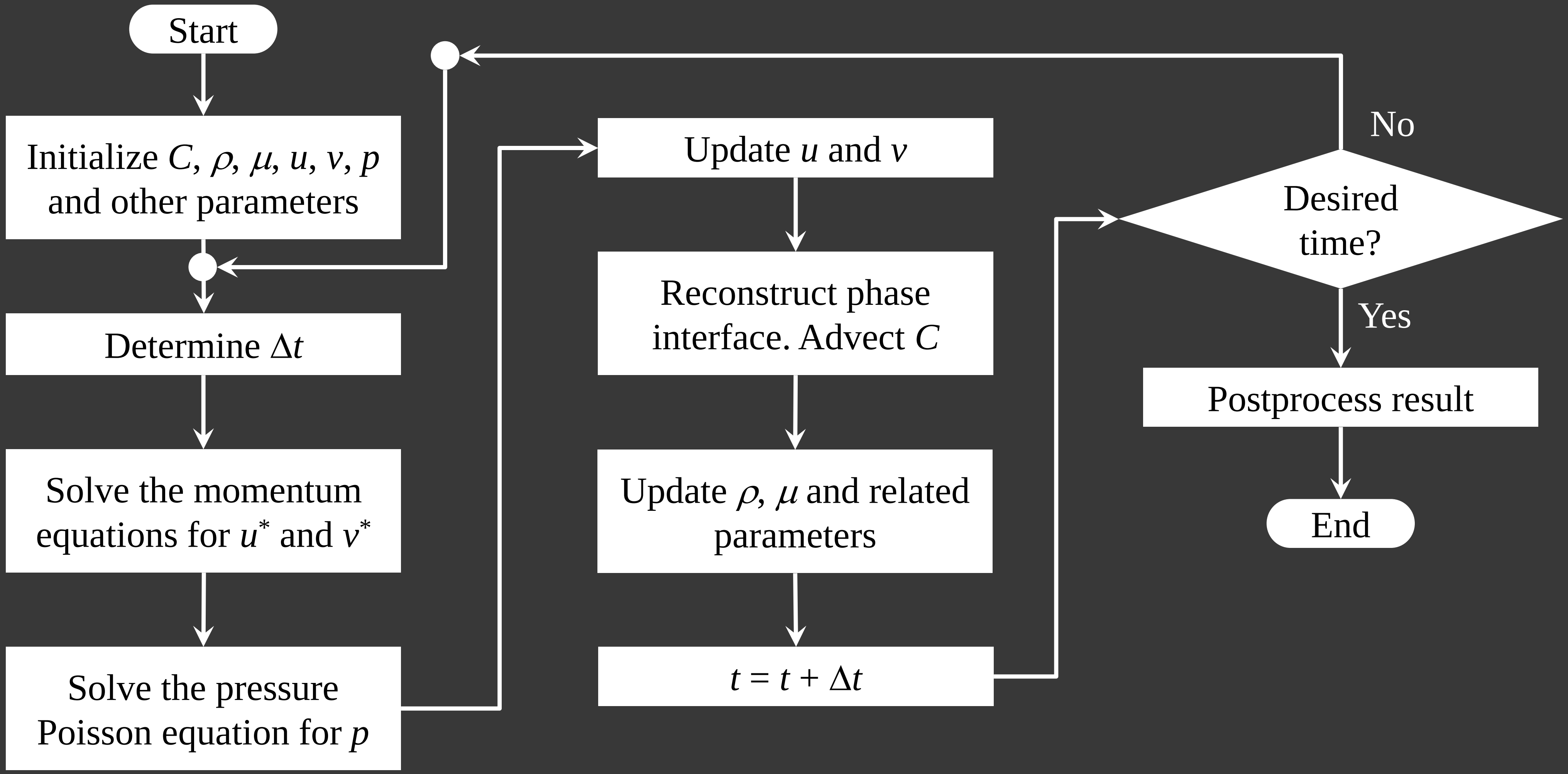
Qin (2022, p. 248)

Flow Field Calculation

- "After the effective density and viscosity have been determined, we can use the projection method to solve for the flow field."

Qin (2022, p. 249)

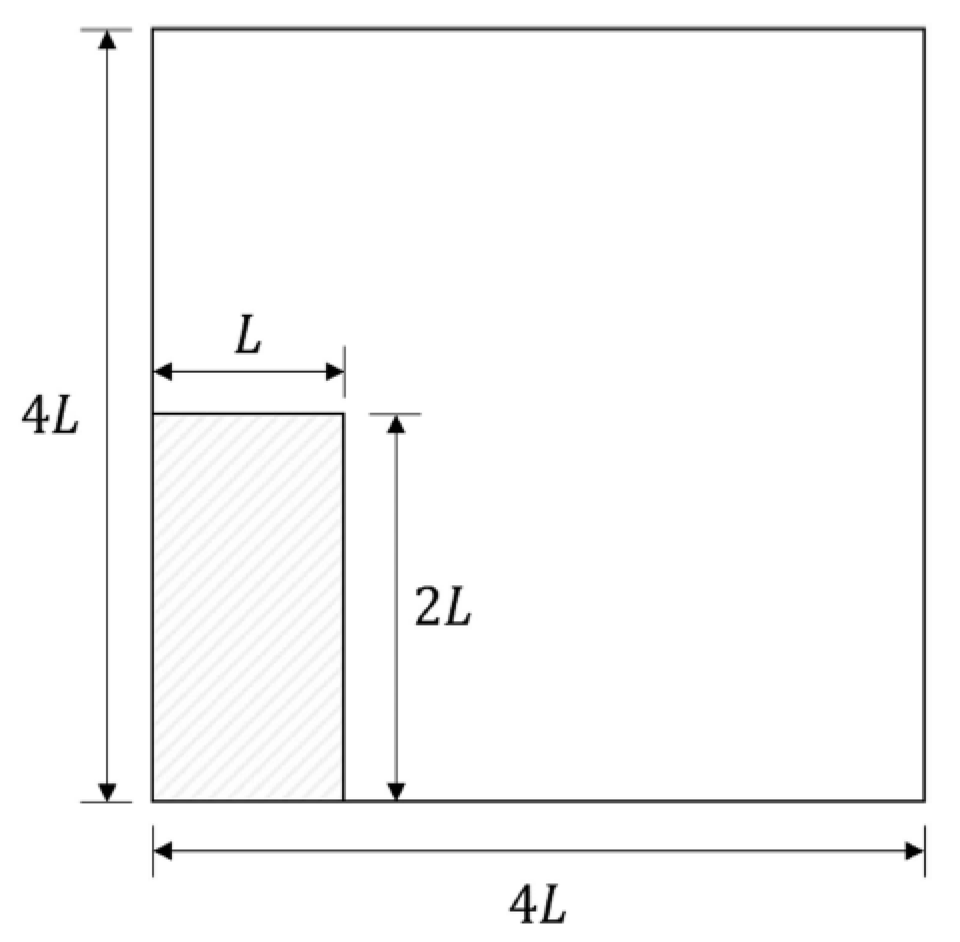
Flowchart of VOF+Projection Method



Qin (2022, p. 251)

Dam Break Problem

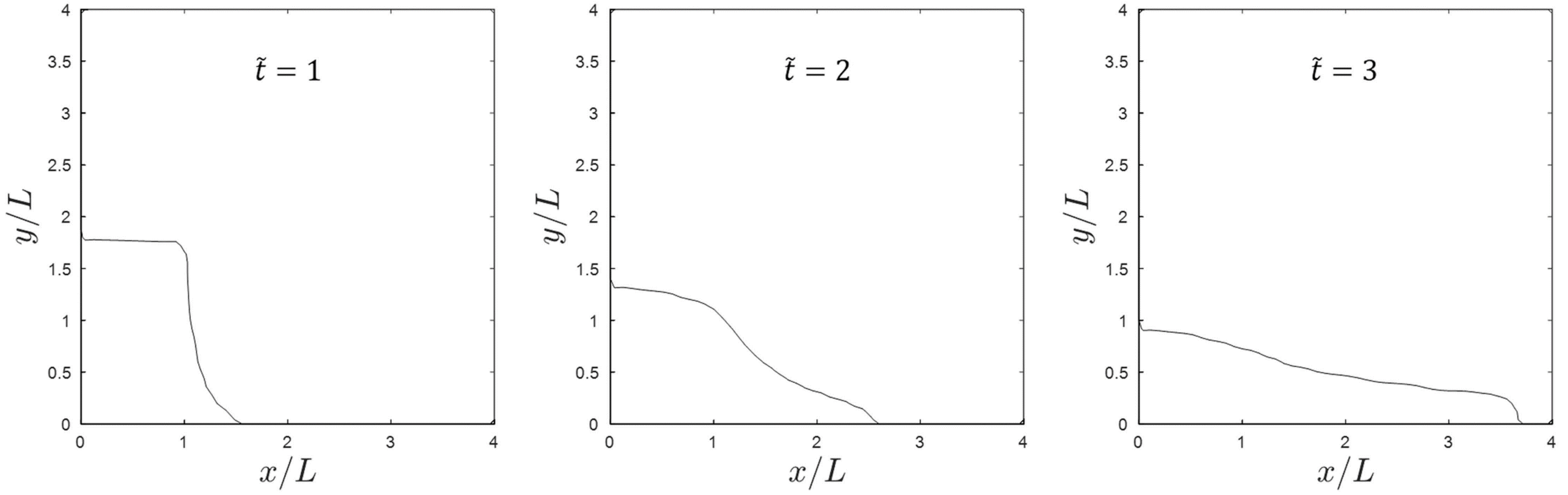
- The dam break problem is a multiphase-flow problem with water confined in a compartment formed by the vertical wall of a tank and a partition plate simulating a dam.
- In this simulation, the density and viscosity of water and air at 25°C are used.
- A slip condition is applied at the tank walls.
- For example, the boundary conditions at the lower wall are $\partial u/\partial y = 0,\ v = 0$
- Here L is used as the length scale, $\sqrt{gL}$ is used as the velocity scale, nondimensional time $\tilde{t} = t\sqrt{2g/L}$



Qin (2022, p. 250, 252)

Dam Break Problem

- The boundary condition for C at the tank walls can be $C = 1$ or $\nabla C \cdot \hat{\mathbf{n}} = 0$ where $\hat{\mathbf{n}}$ is the normal vector of the wall.



Qin (2022, p. 253)

Level-Set Method: Interface Representation

- "In the level-set method, the interface is described by a set of points where a continuous marker function takes a particular value."
- "For example, a circular interface centered at the origin with radius R can be represented by the set of points (x, y) at which the marker function"

$$\phi(x,y)=\sqrt{x^2+y^2}-R=0$$

- "The level-set function is no unique."
- The same circular interface can also be represented by the zero level of the function

$$\psi(x,y)=x^2+y^2-R^2$$

- Function $\phi(x, y)$ is a signed distance function whose value is the least distance between a point (x, y) and the interface represented by the function.

Qin (2022, p. 259)

Level-Set Method: Interface Representation

- The sign of function $\phi(x, y)$ also tells us that the point (x, y) is outside of the interface when the sign is positive. Otherwise, it is inside the interface.
- "This feature allows us to compute many quantities very easily."
- "For instance, if the interface is maintained at a constant temperature T_I and we want to estimate the temperature gradient magnitude at point (x, y) close to the interface, we may simply use

$$\left|\nabla T(x,y)\right| \approx \left|\frac{T(x,y)-T_I}{\phi(x,y)}\right|$$

- The signed distance function ϕ is a solution of the eikonal equation $\left|\nabla\phi\right|=1$ whose zero level will be used from now on to represent an interface.

Qin (2022, p. 261)

Level-Set Method: Interface Advection

- "Since the interface is now associated to one level of a continuous level-set function ϕ, and it advects with the local flow velocity $\mathbf{v}$, it is natural to solve an unsteady convection equation of ϕ to track the interface:

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0$$

- In the VOF method, the volume fraction function C is a discrete function.
- In contrast, the level-set function ϕ is continuous.

Qin (2022, p. 261)

Level-Set Method: Example

- "An interface is initially a circle of radius 0.2π and centered at $(0.5\pi, 0.75)$ in a domain which span from 0 to π in both x- and y-directions."
- The velocity field is

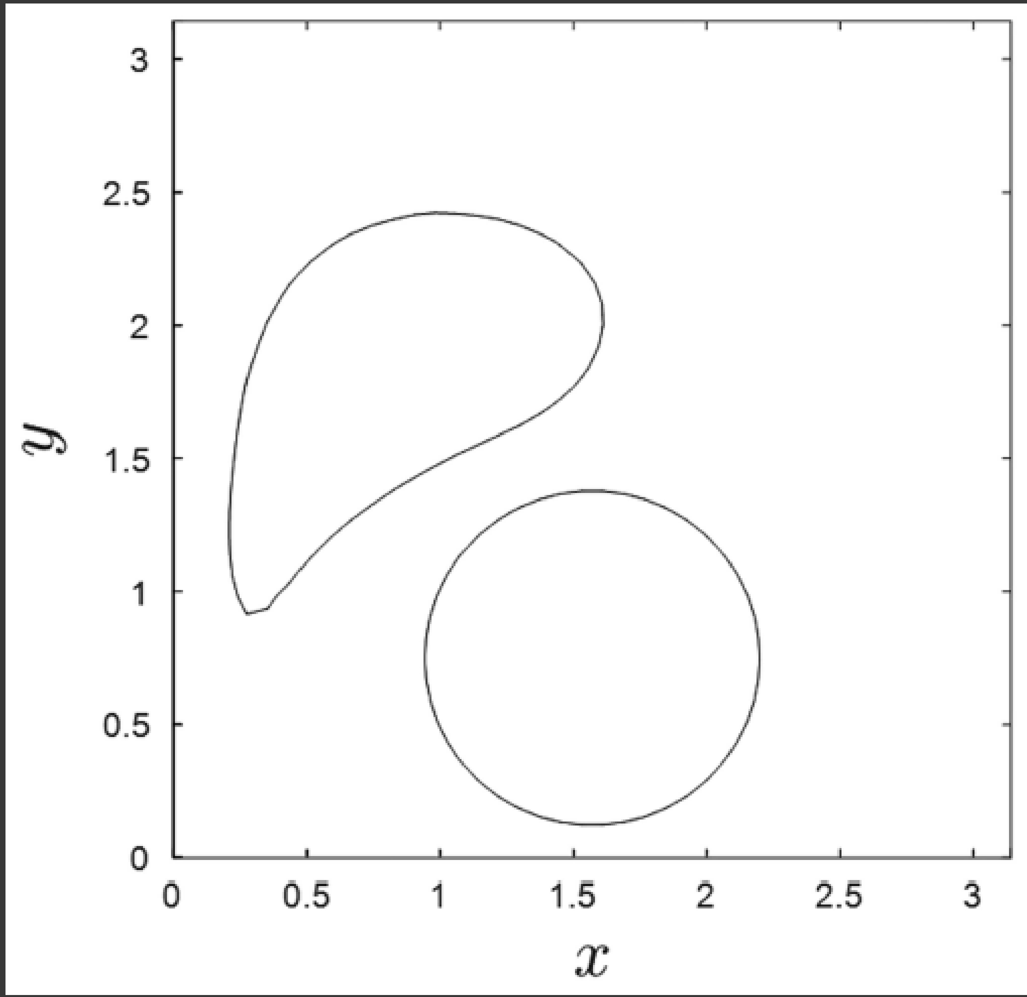
$$u = -\sin x \cos y, \qquad v = \cos x \sin y$$

  which satisfies the incompressibility condition $\nabla \cdot \mathbf{v} = 0$.
- A 40×40 mesh is used with $\Delta t = 0.0025$ are used to calculate the evolution of the interface until $t = 2.5$ s using the second-order ENO scheme for the convection term and the second-order Runge-Kutta method for numerical time integration.

Qin (2022, p. 261)

Level-Set Method: Example

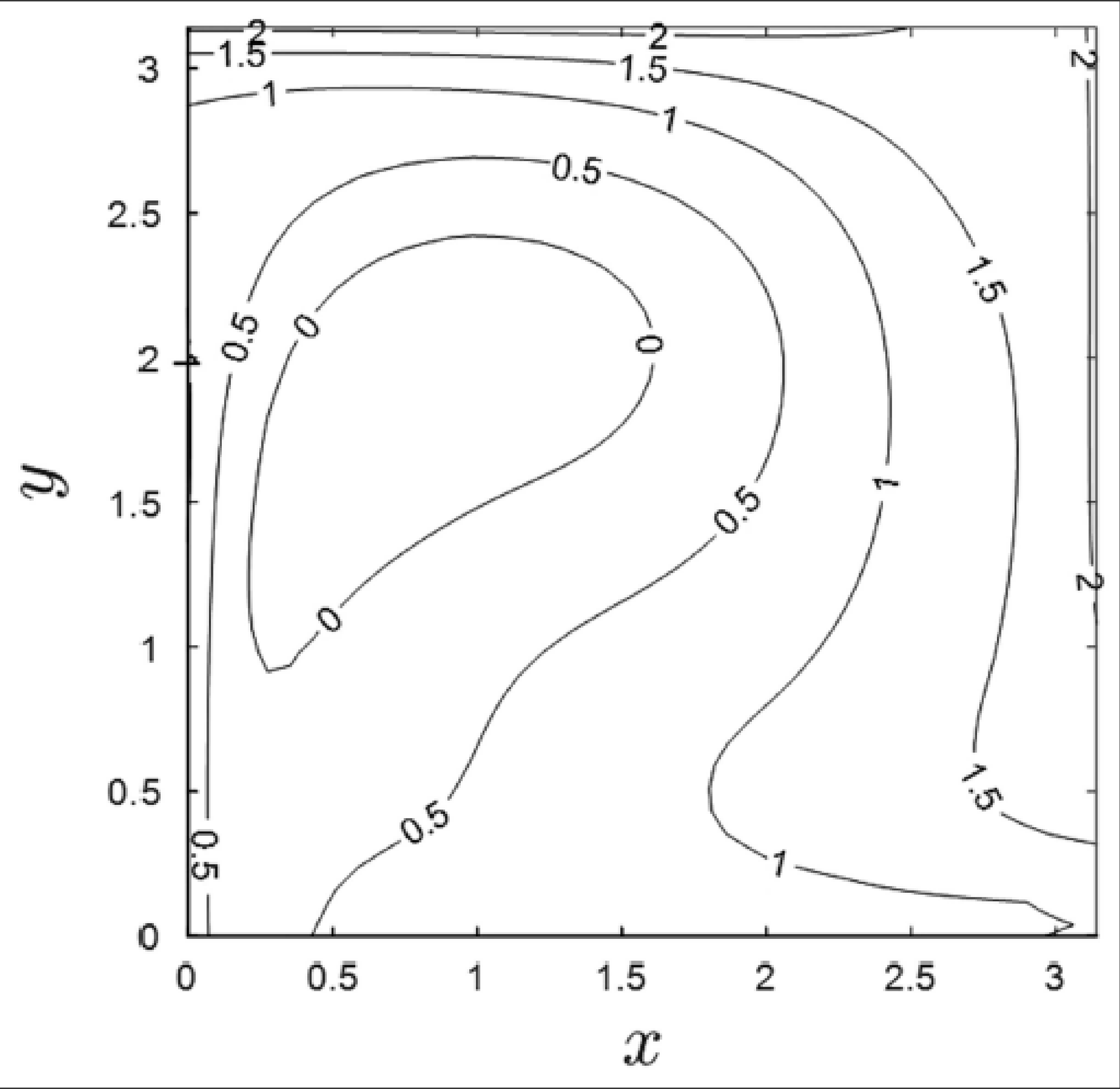
- The initial and final interfaces as shown in the right figure.
- Since the fluid is incompressible, the volume enclosed by the surface should be constant.
- However, the volume enclosed by the final interface is lower by the initial volume by about 0.85%.
- The varying-volume problem is due to numerical diffusion.
- So, higher-order schemes are needed.



Qin (2022, p. 263)

Level-Set Method: Example

- Another issue is that the values of ϕ no longer corresponds to signed distances.
- For example, points on the contour line $\phi = 0.5$ have different distances from the interface.
- This problem occurs because the velocity is not uniform.



Qin (2022, p. 263)

Reinitialization of Level-Set Function

- A

References

- G. Qin, 2022, Computational Fluid Dynamics For Mechanical Engineering, CRC Press.