

Droplet Impact Dynamics

*A Seminar Report
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Abstract

Droplet impingement is very common phenomenon in the world around us. This can be seen in the nature as well as in the industries. It is well known that the droplets are formed when there are instabilities such as Rayleigh-Plateau instability, but it is not easy to predict the complex dynamics of droplets. Droplet impact on a solid surface is one such phenomena which intrigues physicists, mathematicians and engineers. For physicists the interest lies in understanding the solution of Navier-stokes equation before and after impact and various intricacies of the boundary conditions on the dry rigid surface, mathematicians study the asymptotic solution of the governing laws of the fluid dynamics and for engineers, droplet impact is of tremendous technological importance as its application lies in silicon chip technology, ink jet printing, internal combustion engines, spray painting and coating, plasma spraying and crop spraying. This report presents with a short review on the droplet impact and a numerical study of droplet impact applying simple contact line and contact angle models.

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Chapter 1

Simulation Methods

1.1 Introduction

In a flow where an interface exists there is a need for interface reconstruction. Hirt (1981) came up with the idea of Volume of Fluid interface (VOF) tracking to approximate the free boundaries in numerical simulations. This method is based on a concept of fractional volume of fluid. This is still widely used due to its flexibility and efficiency compared to other methods. Volume of fluid essentially conserves the mass, where in level set method is better in reconstruction of curved interfaces.

1.2 The Volume of Fluid method

This method starts with defining a quantity called as volume fraction F , for each cell in computational domain. For a binary phase system there is a dark fluid and light fluid. F is the ratio of volume of the dark fluid to the volume of the cell itself. The cells with only light fluid will have $F = 0$ and for only dark fluid $F = 1$. For interfacial cells F will have a value between 0 and 1. The volume of fluid when advected it does not change with respect to the fluid parcel. Hence, it satisfies the following relation,

$$\frac{\partial F}{\partial t} + (\vec{u} \cdot \vec{\nabla})F = 0 \quad (1.1)$$

Now, F can be tracked in time using finite difference technique and use some algorithms to reconstruct the interface. But this methodology goes into problems as the smearing of interface, due to the fact that F is a discontinuous function in spacial and temporal domain. There is need for some other technique to evolve interface in time. Here comes the role

of geometrical reconstruction and tracking of F-field. There are many such algorithms developed to demonstrate this such as SLIC, PLIC, Youngs method, LVIRA, ELVIRA etc.

1.3 Motivation for a new method

A need of new method arises when conventional methods fail. For multiphase flow, we can try to advect a material property say volume fraction of a fluid in the cell in time, which follows the Eq 1.1. If we use finite difference method to solve above equation to advect the volume fraction, the interface does not remain sharp, smears, due to the fact that the volume fraction is a step function but finite differencing tries to smooth it over the time. The conventional numerical methods do not retain the discontinuous property of the function. Hence there is need for methods which conserve the discontinuous material properties in multiphase flows.

1.4 Least Squares of Volume of Fluid Interface Reconstruction Algorithm

The interfaces in Volume of fluid method has no unique way of reconstruction. With a given F-field there are multiple algorithms to represent interface. One such algorithm is Least Squares Volume of Fluid Reconstruction Algorithm proposed by Pilliod and Puckett (2004). It represents interface as a line in 2D and a plane in 3D. Any interface reconstruction algorithm consists two basic steps:-

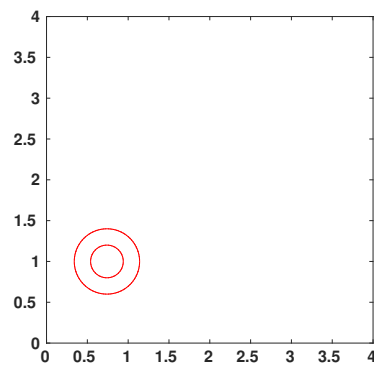
1. Interface Reconstruction
2. Advection of F field

1.5 Interface Reconstruction

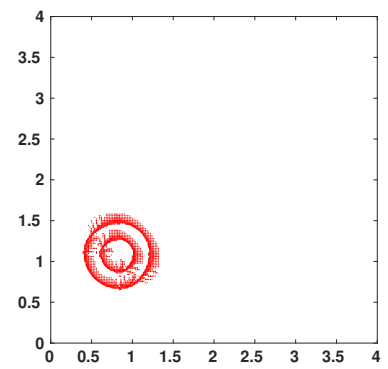
There are many steps involved in interface reconstruction explained in subsections.

1.5.1 Step I : Obtain F field

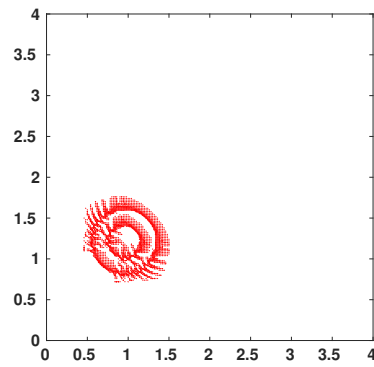
At first a F-field is obtained by knowing the initial free surface and then by calculating the F values in each cell. Then locate a cell having a value of F between 0 and 1.



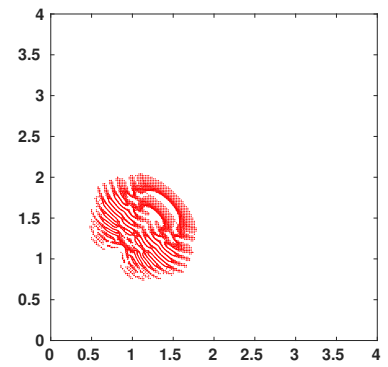
(a) Ini



(b) After advecs



(c) After adve



(d) After ads

Figure 1.1: Advecting volume fraction using finite difference method

1.5.2 Step II : Initial guess of slope

The initial slope of the normal to the interface away from the dark fluid can be obtained using Green-Gauss gradient given by

$$N_x = -\frac{1}{\Delta x}[F_{r+1,c+1} + 2F_{r,c+1} + F_{r-1,c+1} - F_{r+1,c-1} - 2F_{r,c-1} - F_{r-1,c-1}] \quad (1.2)$$

$$N_y = -\frac{1}{\Delta y}[F_{r+1,c+1} + 2F_{r+1,c} + F_{r+1,c-1} - F_{r-1,c+1} - 2F_{r-1,c} - F_{r-1,c-1}] \quad (1.3)$$

1.5.3 Step III : Find Quadrant

Signs of N_x and N_y will determine the quadrant in which the normal points away from the dark fluid present in the cell.

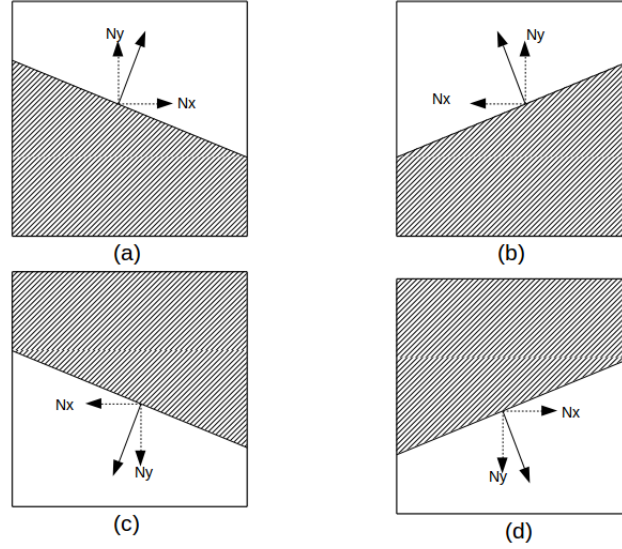


Figure 1.2: (a) First Quadrant (b) Second Quadrant (c) Third Quadrant (d) Fourth Quadrant

1.5.4 Step IV : Calculate angle, θ

The angle, θ is the positive acute angle made by the interface with x-axis if the normal points in first and third quadrant and positive acute angle made by the interface by y-axis if normal points in second and fourth quadrant. θ is defined such that if we rotate the cell such that the normal lies in first quadrant it should make θ with the horizontal axis. So for second and fourth quadrant the θ has to be redefined. Refer to Figure 3.2 for definition of theta. This is required to do since the algorithm is developed in way it works for normal in first quadrant and all other cases has to be modified according to algorithm.

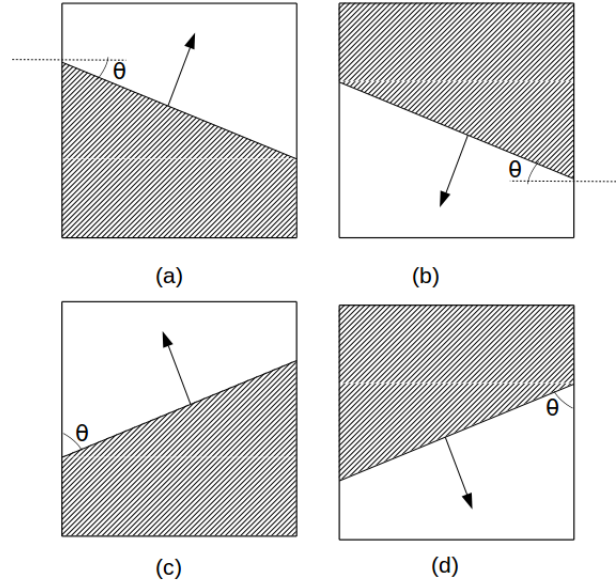


Figure 1.3: Positive acute angle made by the interface with x-axis and y-axis

Equation 3.4 gives the expression for calculating θ

$$\theta = \frac{\pi}{2} - \tan^{-1}\left(\frac{N_x}{N_y}\right) \quad (1.4)$$

Function atan() in GCC

The function `atan()` in GCC returns a value between $-\frac{\pi}{2}$ and $\frac{\pi}{2}$. The slope, $\frac{N_y}{N_x}$ of normal to interface is given as input to `atan[$\frac{N_y}{N_x}$]` return the value of the acute angle made by the x-axis. The returned value is positive when in first and third quadrant and negative when in second and fourth quadrant. To make it positive `fabs` function is used.

$$\beta = \text{atan}\left(\frac{N_y}{N_x}\right) \quad (1.5)$$

$$\alpha = |\beta| \quad (1.6)$$

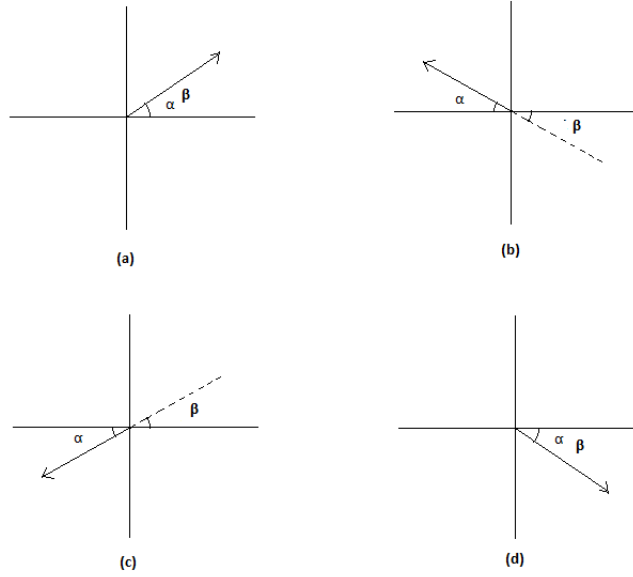


Figure 1.4: Angle value returned by gcc compiler

Hence, the expression for GCC to calculate theta becomes

$$\theta = \frac{\pi}{2} - fabs(atan(\frac{N_x}{N_y})) \quad (1.7)$$

Note: Every step after calculating θ , will have first reorient the normal to the first quadrant.

1.5.5 Step V : Identify shape

If the volume fraction and θ is fixed then the shape of the fluid is independent of the quadrant in which the normal lies in. So there is no need to for reorientation for identifying shape.

From Figure 4 if the shape has to be a triangle then,

$$\text{area of fluid, } A = \Delta^2 F$$

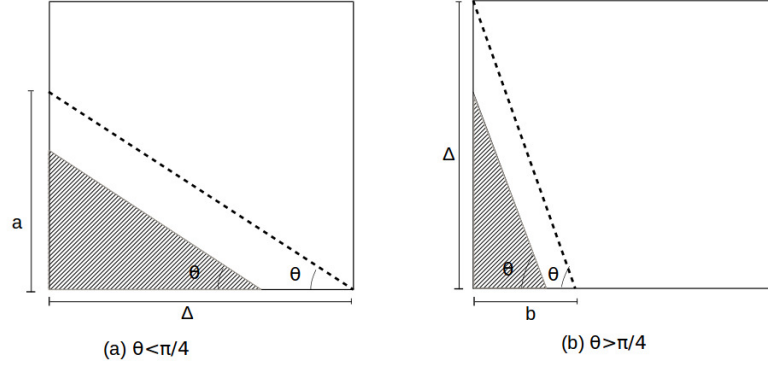


Figure 1.5: Area of the triangle made by dark fluid in the cell

$$a = \Delta \tan \theta \quad \theta < \frac{\pi}{4} \quad (1.8)$$

$$b = \frac{\Delta}{\tan \theta} \quad \theta \geq \frac{\pi}{4} \quad (1.9)$$

$$A \leq \begin{cases} \frac{1}{2} \Delta^2 \tan \theta & \theta < \frac{\pi}{4} \\ \frac{\Delta^2}{2 \tan \theta} & \theta \geq \frac{\pi}{4} \end{cases} \quad (1.10)$$

For trapezium,

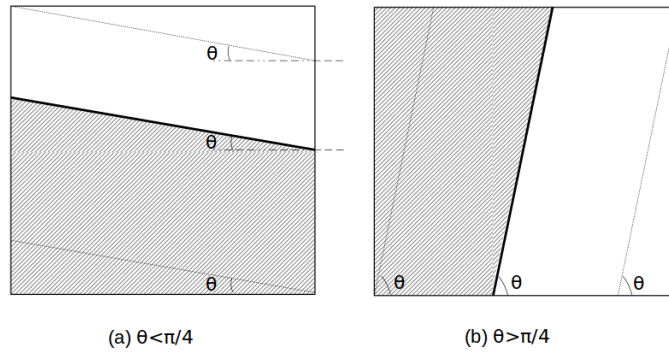


Figure 1.6: Area of a trapezium made by the dark fluid in the cell

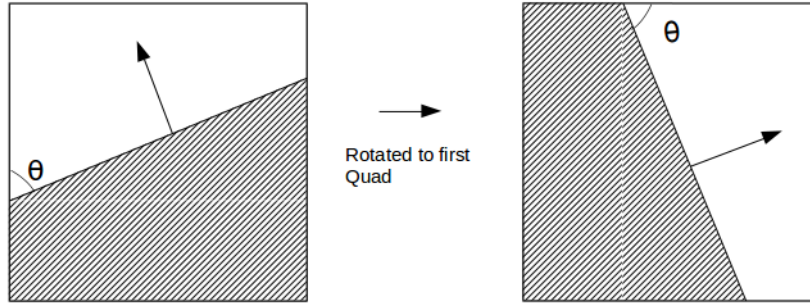


Figure 1.7: When the cell is reoriented to make normal lie in first quadrant

In Figure 3.6, it can be seen that when the cell reoriented to make the normal in first quadrant the θ becomes the angle with the horizontal axis. Hence, the same calculations can be applied to this cell for what is done for first quadrant.

$$A = \begin{cases} (\frac{1}{2}\Delta^2 \tan\theta, (1 - \frac{1}{2}\Delta^2 \tan\theta)) & \theta < \frac{\pi}{4} \\ (\frac{\Delta^2}{2\tan\theta}, (1 - \frac{\Delta^2}{2\tan\theta})) & \theta \geq \frac{\pi}{4} \end{cases} \quad (1.11)$$

For all other cases the shape becomes a compliment of a triangle.

1.5.6 Step VI : Calculate prependicular distance

After reorientation, the prependicular distance will now be always from the LHS corner of the cell.

If shape is a triangle, then

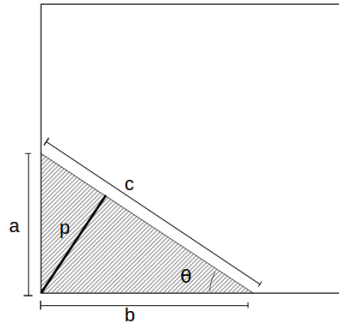


Figure 1.8: Prependicular distance in a triangle

$$c = \frac{b}{\cos\theta}, \quad b = \frac{p}{\sin\theta}, \quad c = \frac{p}{\sin\theta \cos\theta}, \quad \frac{1}{2}pc = F\Delta^2, \quad \frac{p^2}{\sin 2\theta} = F\Delta^2, \quad p = \sqrt{F\Delta^2 \sin 2\theta}$$

If shape is a trapezium,

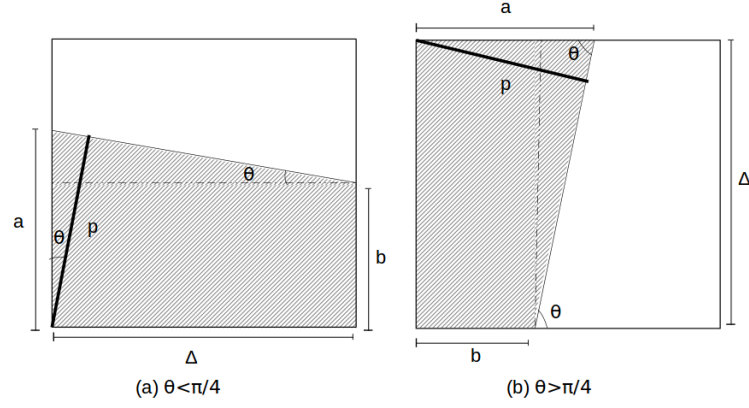


Figure 1.9: Perpendicular distance for a trapezium

$$\begin{aligned} \Delta^2 F &= \frac{(a+b)\Delta}{2}, & a &= \frac{p}{\cos\theta}, & \tan\theta &= \frac{a-b}{\Delta}, & b &= \frac{p}{\cos\theta} - \Delta \tan\theta, \\ \frac{1}{2}\Delta\left(\frac{2p}{\cos\theta} - \Delta \tan\theta\right) &= \Delta^2 F, & p &= \Delta F \cos\theta + \frac{1}{2}\Delta \sin\theta, \end{aligned}$$

For, $\theta < \frac{\pi}{4}$,

$$\begin{aligned} \Delta^2 F &= \frac{(a+b)\Delta}{2}, & a &= \frac{p}{\sin\theta}, & \tan\theta &= \frac{\Delta}{a-b}, & b &= \frac{p}{\sin\theta} - \frac{\Delta}{\tan\theta}, \\ \frac{1}{2}\Delta\left(\frac{2p}{\sin\theta} - \frac{\Delta}{\tan\theta}\right) &= \Delta^2 F, & p &= \Delta F \sin\theta + \frac{1}{2}\Delta \cos\theta \end{aligned}$$

For, $\theta \geq \frac{\pi}{4}$,

For compliment of triangle,

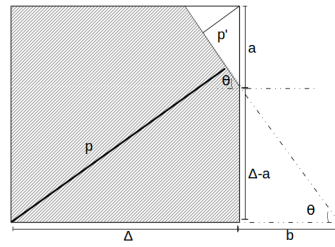


Figure 1.10: Perpendicular distance for compliment of the triangle

$$p' = \sqrt{F\Delta^2 \sin 2\theta}, \quad a = \frac{p'}{\cos\theta}, \quad b = \frac{\Delta - a}{\tan\theta}, \quad p = \Delta(\sin\theta + \cos\theta) - p'$$

1.5.7 Step VII : Extrapolate line

After, reorientation of the line to the first quadrant. A line can be constructed with θ and perpendicular distance using normal form,

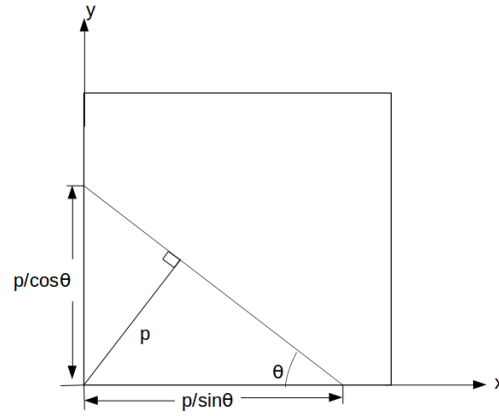


Figure 1.11: Normal form of a line in the cell

$$x \sin \theta + y \cos \theta = p \quad (1.12)$$

Refer to Figure 3.10 for extrapolation,

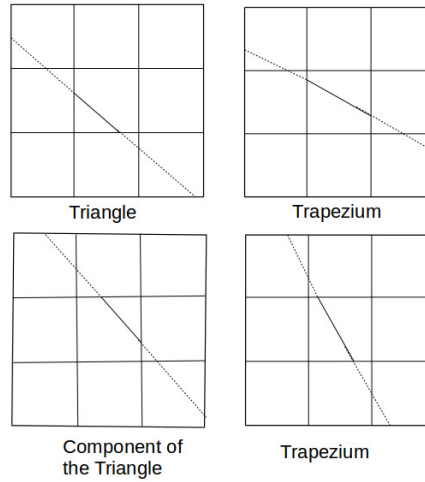


Figure 1.12: Extrapolation of the line in 3 X 3 cell

After extrapolation the new volume fraction calculated under each cell below the line, which then used to calculate the norm.

1.5.8 Step VIII: Calculate Norm

Let the new volume fraction calculated be $\widetilde{F}_{r,c}$. Now the norm which is here the difference of original volume fraction and new volume fraction calculated after the extrapolation are squared and then summed over 3 X 3 stencil. Also, called as L^2 norm,

$$L^2(\widetilde{F}) = \sum_{k,l=-1}^1 (\widetilde{F}_{r+k,c+l} - F_{r+k,c+l})^2 \quad (1.13)$$

1.5.9 Step IX : Minimize Norm

After calculating norm the initial guess of slope and θ is changed with small step size but it should not be confused with rotation of interface or normal. All the steps are repeated to after modifying theta and norm is again calculated. This process repeats when a minima of norm reached. And the final values of θ , shape, and quadrant are assigned to the cell.

1.6 Advection

The equation 3.1 is also solved using geometrical technique by calculating fluxes across the cells and then updating the F-field in each time step. The direct finite differencing will lose the discontinuos property of F-field and cause smearing of interface. The flux is calculated through the wall of the cells in X an Y directions.

For first quadrant all cases are discussed below,

Note:- for all other quadrants the algorithm passes the values as if the normal is in first quadrant and the values returned by it are passed accordingly to the structure. The interface angle with horizontal axis (after rotating the normal to first quadrant) θ is calculated and stored in the structure.

For X-Flux when velocity in x-direction, u is positive then only the right wall of the left cell will affect the flux (See Figure 11)

1.6.1 Flux Calculation

Triangle

For a triangle there are two cases:-

if $\Delta - udt > x_0$, Nothing will leave from the right wall

if $\Delta - udt < x_0$, A triangle leaves.

where x_0 is the x at $y = 0$.

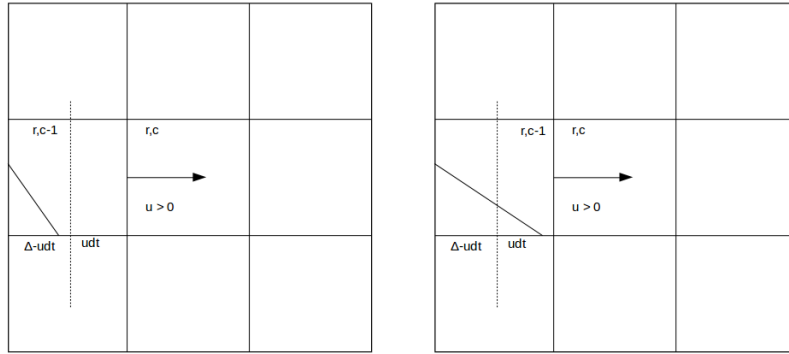


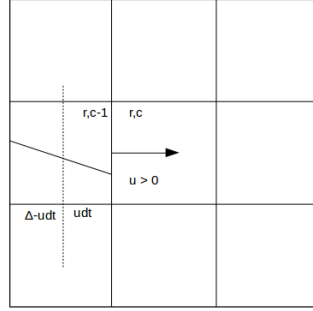
Figure 1.13: Cases for a triangle in flux calculation

For the second case where a part of triangle leaves which is also a triangle, the area of the part which leaves is given by,

$$Flux = \frac{1}{2}(x_0 - del + udt)^2 \tan \theta$$

Trapezium

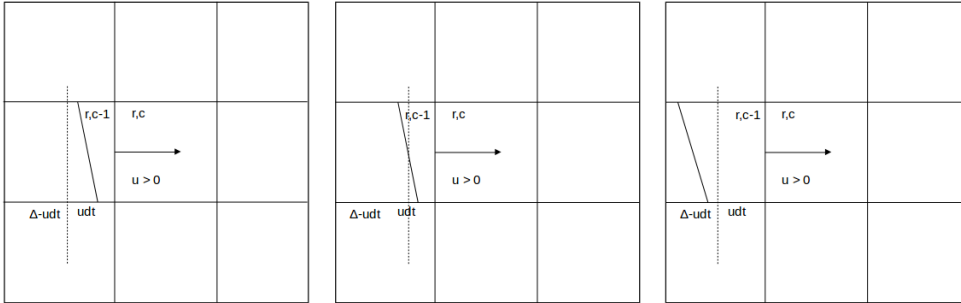
Two types of trapezium can be in the first quadrant, $\theta < \frac{\pi}{4}$, and $\theta > \frac{\pi}{4}$, (See Figure 12 and 13)

Figure 1.14: Flux calculation for trapezium for $\theta < \frac{\pi}{4}$

For $\theta < \frac{\pi}{4}$,

$$Flux = \frac{1}{2}(y_0 - ((\Delta - udt) * \tan\theta) + y_{del}) * udt$$

For $\theta > \frac{\pi}{4}$,

Figure 1.15: (a) $\Delta - udt < x_{del}$, (b) $\Delta - udt \geq x_{del}$ and $\Delta - udt < x_0$, (c) $\Delta - udt \geq x_0$

For $\Delta - udt < x_{del}$, a trapezium leaves the cell and the Flux is given by,

$$Flux = \frac{\Delta}{2}(x_{del} - (2(\Delta - udt)) + x_0)$$

For $\Delta - udt \geq x_{del}$ and $\Delta - udt < x_0$, a triangle leaves the cell and the flux is given by,

$$Flux = \frac{1}{2 \tan \theta} (y_0 - (\Delta - udt) \tan \theta)^2$$

For $\Delta - udt \geq x_0$, nothing leaves from the cell

Compliment of a triangle

For compliment of a triangle two cases arise, (See Figure 15)

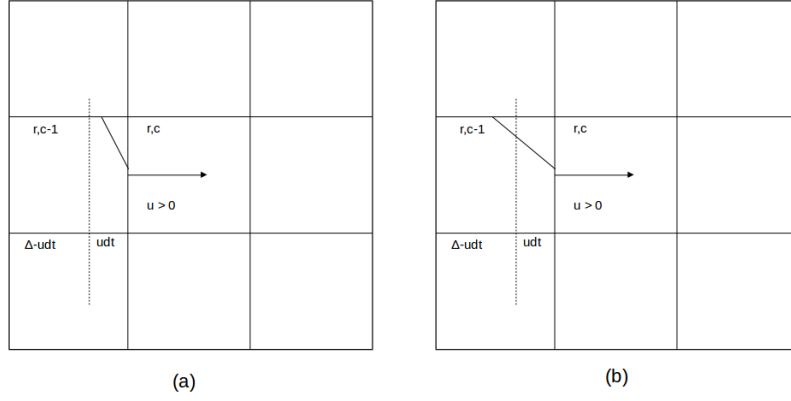


Figure 1.16: (a) $\Delta - udt < x_{del}$, (b) $\Delta - udt \geq x_{del}$

if $\Delta - udt < x_{del}$, A 5-Sided figure leaves, and Flux is given by,

$$Flux = \Delta(x_{del} - \Delta + udt) + \frac{1}{2}((\Delta + y_{del})(\Delta - x_{del})), \text{ (sum of rectangle and trapezium)}$$

or, if $\Delta - udt \geq x_{del}$, A trapezium leaves, and Flux is given by,

$$Flux = \frac{udt}{2}(y_{del} + y_0 - (\Delta - udt) \tan \theta)$$

1.6.2 Rectangle

For rectangle (See Figure 17)

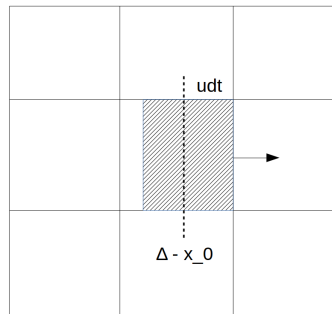


Figure 1.17: Flux calculation for rectangle

if $\Delta - udt \leq x_0$, A Nothing leaves

$$Flux = 0$$

or, if $\Delta - udt \geq x_0$, A rectangle leaves, and Flux is given by,
 $Flux = \Delta(udt)$

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