Chapter 3
Piecewise Linear Interpolation Method

3.1 Introduction

In solving problems in computational physics, we often encounter non-linear, mathematical equations which are difficult to solve, or even worse, not amenable to be approaches by analytic methods developed up to now. Then we turn to numerical methods to attack them instead. These methods, when used to compute with high speed computers available at present, often yield some satisfactory solutions. However, there are disadvantages with these methods, such as when they are used to solve the same problems, but may result in different solutions. Sometimes it is hard to determine which method is more accurate. The methods that give solutions consistently converging to those from analytic methods, when such analytic solutions are available, are generally accepted to be applied to problems for which there is no analytic solution in closed form. In this work we investigate a new method developed by Rajamäki and Saarinen (1991).

They explained that the method has the capability to preserve the shape of a propagating distribution and great applicability in many flow problems, such as strong convection, convection-diffusion, and reaction-diffusion problems. Their explanation made us curious to use their method to investigate the transport of cosmic rays across the solar-flare shock. Because this problem is similar those above, the method should be applied to it too if it works with those mentioned by its authors. We find, however, that when the method is applied to determine a solution of a problem having a peak-distribution initial condition, we obtain result that is significantly different from that of an analytic method. Our efforts to implement and test this method constituted a major portion of the work of this thesis. The method is called the Piecewise Linear Interpolation Method or PLIM for short. Before we present details about PLIM, we briefly review linear, first-order, partial differential equations of two independent variables, and the method of characteristics for determining their solutions.

3.2 Linear, First-Order Partial Differential Equations

The following discussion is derived from the literature of Zauderer (1989). Consider a linear, first-order, partial differential equation of two independent variables in the general form

$$a(t,z)\frac{\partial U}{\partial t} + b(t,z)\frac{\partial U}{\partial z} = c(t,z), \tag{3.1}$$

where the unknown variable U is a function of t, z and the coefficients a, b and c are continuously differentiable in some region. We solve eq. (3.1) under the initial condition

$$U(0,z) = f(z), \tag{3.2}$$

where domain is $t \geq 0$ and $0 \leq z \leq L$ and boundary condition at $U(0,0)$ and $U(0,L)$ are supposedly known.

At each point (t,z) where $a(t,z)$ and $b(t,z)$ are defined and not both zero, the left side of eq. (3.1) is a directional derivative of $U(t,z)$ in the direction of $[a,b]$. The equations

$$\begin{aligned} \frac{dt}{ds} &= a(t,z) \\ \frac{dz}{ds} &= b(t,z) \end{aligned} \tag{3.3}$$

determine a family of curves $t = t(s), z = z(s)$ whose tangent vector $[t'(s), z'(s)]$ coincides with the direction of the vector $[a, b]$ at each point where $[a, b]$ is defined and not zero. Therefore, the derivative of $U(t, z)$ along these curves becomes

$$\begin{aligned} \frac{dU}{ds} &= \frac{dU}{ds}(t(s), z(s)) \\ &= \frac{\partial U}{\partial t}\frac{dt}{ds} + \frac{\partial U}{\partial z}\frac{dt}{ds} \\ &= a\frac{\partial U}{\partial t} + b\frac{\partial U}{\partial z}, \end{aligned}$$

consequently yielding

$$\frac{dU}{ds} = c(t, z) \tag{3.4}$$

using the chain rule and eqs. (3.1) and (3.3).

The family of curves $t = t(s)$, $z = z(s)$, and $U = U(s)$, determined by the solution of a system of ordinary differential equations, eqs. (3.3) and (3.4), are called the characteristic curves of the partial differential equation eq. (3.1). Because eq. (3.3) can be solved independently of eq. (3.4), the curves in the (t, z)-plane determined from eq. (3.3) are occasionally also referred to as characteristic base curves. The approach to solve eq. (3.1) by making use of eqs. (3.3) and (3.4) is called the method of characteristics. It is based on a geometric interpretation of the partial differential equation.

The existence and uniqueness theory for ordinary differential equations, assuming certain smoothness conditions on the functions a, b, and c, guarantees that exactly one solution curve $[t(s), z(s), U(s)]$ of eqs. (3.3) and (3.4), i.e., a characteristic curve, passes through a given point (t_0, z_0, U_0) in (t, z, U)-space. As a result, we are not interested in determining a general solution of eq. (3.1), but rather a specific solution $U = U(t, z)$ that passes through or contains a given curve C associated with eq. (3.2). This problem is known as the initial value problem for eq. (3.1).

The method of characteristics for solving the initial value problem for eq. (3.1) proceeds as follows. We assume that the initial curve C associated with eq. (3.2) is given parametrically as

$$\begin{aligned} t &= t(\tau) \\ z &= z(\tau) \\ U &= U(\tau) \end{aligned} \tag{3.5}$$

for a given range of the parameter τ. The curve may be of finite or infinite extent and is required to have a continuous tangent vector at each point. Every value of τ fixes a point on curve C through which a unique characteristic curve passes. The family of characteristic curves determined by the points of curve C may be parameterized as

$$\begin{aligned} t &= t(s,\tau) \\ z &= z(s,\tau) \\ U &= U(s,\tau) \end{aligned} \tag{3.6}$$

with $s = 0$ corresponding to the initial curve C in eq. (3.5). That is, we have

$$\begin{aligned} t(0,\tau) &= t(\tau) \\ z(0,\tau) &= z(\tau) \\ U(0,\tau) &= U(\tau). \end{aligned} \tag{3.7}$$

Eq. (3.6), in general, yields a parametric representation of a surface in (t, z, U)-space that contains the initial curve C. Assuming the equations $t = t(s,\tau)$ and $z = z(s,\tau)$ can be inverted to give s and τ as functions of t and z, which is the case if the Jacobian $z_s t_\tau - t_s z_\tau \neq 0$ on C, these functions can be introduced into the equation $U = U(s,\tau)$. The resulting function $U[s(t,z), \tau(t,z)] = U(t,z)$ satisfies eq. (3.1) in a neighborhood of the curve C in view of eq. (3.4) and the initial condition eq. (3.5), i.e., $U[t(\tau), z(\tau)] = U(\tau)$, and is a unique solution of the given initial value problem. The smoothness requirements placed on the functions

a, b, and c in eq. (3.1) imply that $U(t,z)$ must be continuously differentiable near the curve C.

Now let us consider an equation that will be used in this work and to illustrate the procedures outlined above. If in eq. (3.1) we let $a(t,z) = 1$, $b(t,z) =$ constant b, we obtain

$$\frac{\partial U}{\partial t} + b\frac{\partial U}{\partial z} = c(t,z). \tag{3.8}$$

Eq. (3.8) with an initial condition, eq. (3.2), constitutes initial value problem which will be solved by the method of characteristics in the following. The initial curve C associated with eq. (3.2) is parameterized as

$$\begin{aligned} t &= 0 \\ z &= \tau \\ U &= U(0,\tau) \end{aligned} \tag{3.9}$$

where $t \geq 0$, $0 \leq z \leq L$ and boundary condition of $U(0,0)$ and $U(0,L)$ are given functions. The equations corresponding to Eq. (3.3) are

$$\begin{aligned} \frac{dt}{ds} &= 1 \\ \frac{dz}{ds} &= b, \end{aligned} \tag{3.10}$$

which can be integrated to yield $t = t_0 + s$ and $z = z_0 + bs$. For $s = 0$, a comparison with the first two equations in eq. (3.9), yields $t_0 = 0$ and $z_0 = \tau$, so we obtain the characteristic base curve as

$$\begin{aligned} t &= s \\ z &= \tau + bs. \end{aligned} \tag{3.11}$$

Substituting t and z from eq. (3.11) into eq. (3.4) yields

$$\frac{dU}{ds} = c(s, \tau + bs), \tag{3.12}$$

which can be integrated to obtain

$$U(s,\tau) = U(s=0,\tau) + \int_0^s c(\xi, \tau + b\xi)d\xi. \tag{3.13}$$

Because the Jacobian $z_s t_\tau - t_s z_\tau = -1 \neq 0$, we can find s and τ in terms of t and z (which can be done easily in this case) using eq. (3.11):

$$\begin{aligned} s &= t \\ \tau &= z - bt. \end{aligned} \tag{3.14}$$

Finally, when inserting s and τ from eq. (3.14) into eq. (3.13), we obtain the solution of the initial value problem as

$$U(t,z) = U(0, z - bt) + \int_0^t c(\xi, z - bt + b\xi)d\xi. \tag{3.15}$$

In practice, we usually consider a finite range of z values, so it is necessary to consider a boundary condition for any z-boundary at which the flow is directed inward. When the characteristic enters the domain of interest through a z-boundary, we obtain a formula similar to eq. (3.15). These results are indispensable because they will be used in computations in the next section. Now we have completed the review and are ready to investigate the PLIM method.

3.3 The Piecewise Linear Interpolation Method

The Piecewise Linear Interpolation Method (PLIM) was introduced in a recent paper by Rajamäki and Saarinen (1991). However, this paper only presents a rough description of the method, and we have had to figure out many of the details (and correct several errors in the paper) for ourselves. Therefore, the following section summarizes the relevant discussion in the original work, along with some details and corrections that we have worked out. Consider a system of first order partial differential equations,

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial z} = \mathbf{P}, \tag{3.16}$$

where

$$\begin{aligned}
\mathbf{U} &= (U_1, U_2, \ldots, U_n), \quad U_k = U_k(u_1, u_2, \ldots, u_n, t, z) \\
\mathbf{F} &= (F_1, F_2, \ldots, F_n), \quad F_k = F_k(u_1, u_2, \ldots, u_n, t, z) \\
\mathbf{P} &= (P_1, P_2, \ldots, P_n), \quad P_k = P_k(u_1, u_2, \ldots, u_n, t, z),
\end{aligned}$$

and the unknown variables are $u_k = u_k(t, z)$ for $k = 1, 2, \ldots, n$, where n is the number of equations in eq. (3.16). This system of equations is not yet ready for the application of piecewise linear interpolation. Firstly, we need to perform some manipulations as follows:

The $z - t$ space is assumed to be divided into rectangular mesh cells, as shown in Figure 3.1. In these mesh cells the Jacobian matrices

$$\begin{aligned}
\mathbf{W_U} &= \begin{pmatrix} \frac{\partial U_1}{\partial u_1} & \frac{\partial U_1}{\partial u_2} & \cdots & \frac{\partial U_1}{\partial u_n} \\ \frac{\partial U_2}{\partial u_1} & \frac{\partial U_2}{\partial u_2} & \cdots & \frac{\partial U_2}{\partial u_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial U_n}{\partial u_1} & \frac{\partial U_n}{\partial u_2} & \cdots & \frac{\partial U_n}{\partial u_n} \end{pmatrix} \\
\mathbf{W_F} &= \begin{pmatrix} \frac{\partial F_1}{\partial u_1} & \frac{\partial F_1}{\partial u_2} & \cdots & \frac{\partial F_1}{\partial u_n} \\ \frac{\partial F_2}{\partial u_1} & \frac{\partial F_2}{\partial u_2} & \cdots & \frac{\partial F_2}{\partial u_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial F_n}{\partial u_1} & \frac{\partial F_n}{\partial u_2} & \cdots & \frac{\partial F_n}{\partial u_n} \end{pmatrix}
\end{aligned} \tag{3.17}$$

are evaluated by numerical differences. Both $\mathbf{W_U}$ and $\mathbf{W_F}$ are assumed to be constant matrices in each mesh cell. In addition $\mathbf{W_U}$ must be nonsingular, so its inverse $\mathbf{W_U^{-1}}$ must exist.

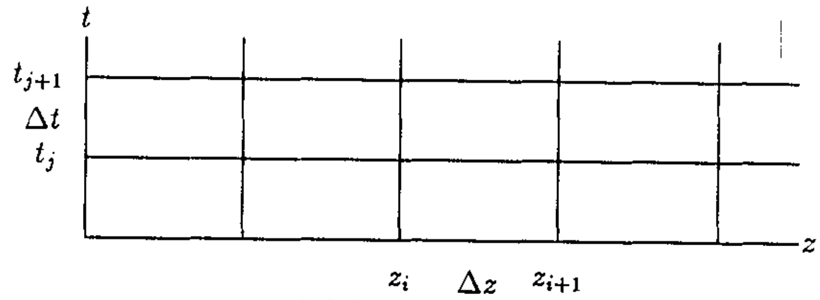

Figure 3.1 Discretization mesh

In the mesh cell, PLIM approximates

$$\begin{aligned}\mathbf{U} &= \mathbf{U_L} + \mathbf{W_U}(\mathbf{u} - \mathbf{u_L}(t,z)) \\ \mathbf{F} &= \mathbf{F_L} + \mathbf{W_F}(\mathbf{u} - \mathbf{u_L}(t,z)),\end{aligned} \tag{3.18}$$

where $\mathbf{u} = (u_1, u_2, \ldots, u_n)$ and the subscript L refers to linear z-t dependent vector functions. We define the cellwise constant velocity matrix as

$$\mathbf{V} = \mathbf{W_F}\mathbf{W_U^{-1}}. \tag{3.19}$$

Multiplying through the first equation of eq. (3.18) by $\mathbf{W_U^{-1}}$, we obtain

$$\mathbf{W_U^{-1}U} = \mathbf{W_U^{-1}U}_L + (\mathbf{u} - \mathbf{u}_L(t,z))$$

and

$$(\mathbf{u} - \mathbf{u}_L(t,z)) = \mathbf{W_U^{-1}}(\mathbf{U} - \mathbf{U}_L). \tag{3.20}$$

Plugging eq. (3.20) into the second equation of eq. (3.18), and using eq. (3.19), we get

$$\mathbf{F} = \mathbf{F}_L + \mathbf{V}(\mathbf{U} - \mathbf{U}_L). \tag{3.21}$$

Thereafter putting this into eq. (3.16) and rearranging yields

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{V}\frac{\partial \mathbf{U}}{\partial z} = \mathbf{P_M}, \tag{3.22}$$

where

$$\mathbf{P_M} = \mathbf{P} - \frac{\partial}{\partial z}(\mathbf{F}_L - \mathbf{V}\mathbf{U}_L).$$

To form equations that are suitable for the application of the piecewise linear interpolation method the matrix $\mathbf{V}$ is diagonalized to yield

$$\mathbf{V} = \mathbf{S}\mathrm{v}\mathbf{S}^{-1}, \tag{3.23}$$

where v is a diagonal matrix which includes eigenvalues of matrix $\mathbf{V}$, i.e., the characteristic velocities of the system of equations. Eq. (3.16) is an initial value problem with respect to time. Thus if the problem is well-posed, all the eigenvalues have to be real. Multiplying eq. (3.22) by $\mathbf{S}^{-1}$ yields

$$\frac{\partial \mathrm{x}}{\partial t} + \mathrm{v}\frac{\partial \mathrm{x}}{\partial z} = \mathrm{p}, \tag{3.24}$$

where $\mathrm{x} = \mathbf{S}^{-1}\mathbf{U}$, $\mathrm{p} = \mathbf{S}^{-1}\mathbf{P}_M$. Hence, n uncoupled, linear equations in the mesh cell have been derived. Now x can be solved by using piecewise linear interpolation. The original vector functions $\mathbf{U}$ and $\mathbf{F}$ are related to x in eq. (3.24) by

$$\begin{aligned} \mathbf{U} &= \mathbf{S}\mathrm{x} \\ \mathbf{F} &= \mathbf{S}\mathrm{v}(\mathrm{x} - \mathbf{S}^{-1}\mathbf{U}_L) + \mathbf{F}_L, \end{aligned} \tag{3.25}$$

where the second equation is obtained by putting eq. (3.23) into eq. (3.21) and using $\mathrm{x} = \mathbf{S}^{-1}\mathbf{U}$.

The system of equations in eq. (3.24) can be solved separately by the method of characteristics outlined in the preceding section. Each equation is analogous to eq. (3.8), so each component variable x has a solution corresponding to eq. (3.15):

$$x(t,z) = x(0, z - vt) + \int_0^t p(\tau, z - vt + v\tau)\, d\tau \tag{3.26}$$

if the characteristic enters the domain of interest through the boundary at $t = 0$ or

$$x(t,z) = x(t - z/v, 0) + \int_{t-z/v}^{t} p(t - z/v + \tau, v\tau)\, d\tau$$

if the characteristic enters through, say, $z = 0$.

The main problems in finding solutions are related to x at the boundary point where the characteristic enters the mesh cell. If there is no information on the distribution of the variable x in the mesh cell, an accurate numerical solution can be achieved only in the very special case where $v\Delta t/\Delta z$ is an integer for every eigenvalue v. Hence, interpolation is needed to determine x at the incoming boundary point and the scheme *ideally* has the following properties:

1. It is such that any distribution at the boundary of the mesh cell can be reasonably approximated.

2. It preserves the shape of propagating distribution in some sense.

3. Conservation of x in the mesh cell can be satisfied.

4. Overshoots and uncontrolled strong variations can be avoided.

5. The propagation of a front within a mesh cell is described, because fronts are very common in flow problems.

6. It uses values of only one mesh interval, because then no extra schemes are needed for the end points or for the discontinuity points of the z-interval.

The basic idea of PLIM is to form the distribution of x within the mesh cell by representing the unknown variables at each boundary of the mesh cell in terms of a piecewise linear approximation. For convenience in computation we define

$$\begin{aligned} \theta_z &= \frac{z - z_i}{\Delta z} \\ \theta_t &= \frac{t - t_j}{\Delta t}, \end{aligned} \qquad (3.27)$$

and θ without a subscript can stand for either θ_z or θ_t depending on the interpolation, while $x(0,\theta_z)$ or $x(\theta_t,0)$ is denoted by $x(\theta)$.

Define in the interpolation interval

$$x(\theta) = x_L + \Delta x(\theta) \quad \text{for} \quad \theta \in [0,1] \tag{3.28}$$

where x_L refers to linear dependence between the known end points, $x(0)$ and $x(1)$, and $\Delta x(\theta)$ is the deviation from x_L. Defining the zeroth and first central moments for the piecewise linear function $\Delta x(\theta)$, one obtains

$$\begin{aligned} m_0 &= \int_0^1 \Delta x(\theta)\, d\theta \\ m_c &= \int_0^1 \left(\theta - \frac{1}{2}\right) \Delta x(\theta)\, d\theta \end{aligned} \tag{3.29}$$

These moments are useful parameters, since they relate directly to the conservation and shape of $\Delta x(\theta)$.

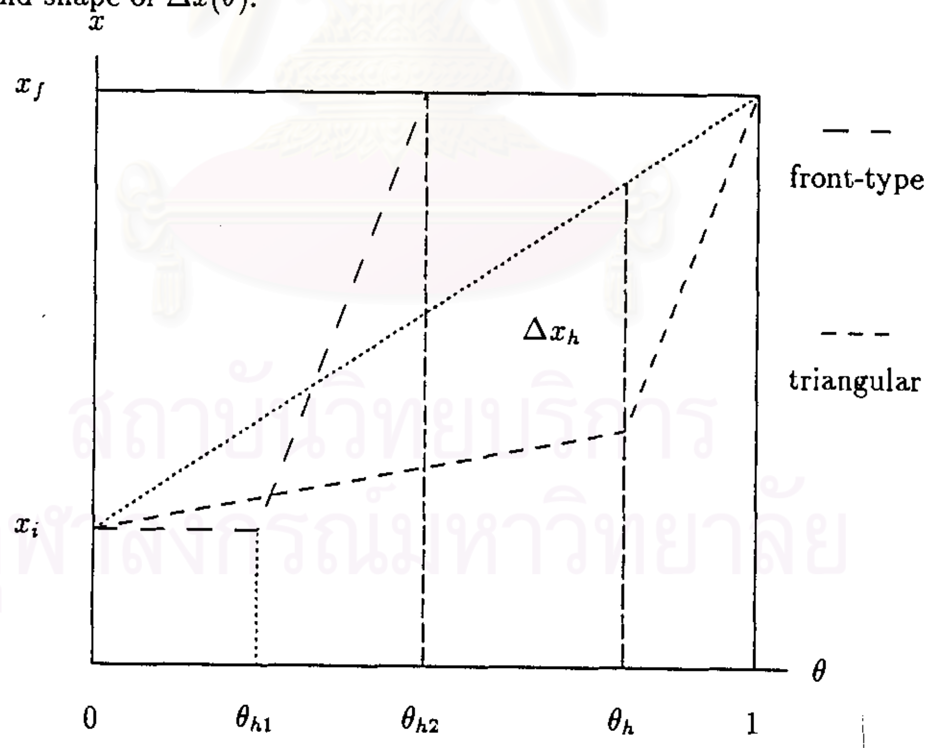

Figure 3.2 Front-type and triangular distributions

Now consider the construction of $\Delta x(\theta)$, as shown in Figure 3.2, between the end points $x(0) = x_i$ and $x(1) = x_f$. The conditions to limit the overshoots, undershoots, and the uncontrolled variations of $x(\theta)$ are

$$\begin{gathered} \min(x_i, x_f) \leq x(\theta) \leq \max(x_i, x_f) \\ \left|\frac{dx(\theta)}{d\theta}\right| \leq \frac{|x_i - x_f|}{\delta}, \end{gathered} \tag{3.30}$$

where δ is a numeric parameter. Rajamäki and Saarinen recommends defining it as

$$\delta = \frac{\delta_1}{|x_i - x_f|} + \delta_2, \tag{3.31}$$

where $\delta_1 = 10^{-7}$ and $\delta_2 = 0.05$ are used in this work.

Under these conditions, two piecewise linear approximating function families can be constructed: the triangular approximations and the front-type approximations as shown in Figure 3.2. Variables Δx_h and θ_h in the triangular approximation or θ_{h1} and θ_{h2} in the front-type approximation can be evaluated using eq. (3.29), and hence $\Delta x(\theta)$ can be evaluated.

The triangular approximation with the joint at position θ_h and height Δx_h results in

$$x(\theta) = \begin{cases} x_i + (x_f - x_i)\theta + \dfrac{\theta}{\theta_h}\Delta x_h, & \text{when } \theta \leq \theta_h \\ x_i + (x_f - x_i)\theta + \dfrac{1-\theta}{1-\theta_h}\Delta x_h, & \text{when } \theta_h \leq \theta, \end{cases} \tag{3.32}$$

and the front-type approximation leads to

$$x(\theta) = \begin{cases} x_i, & \text{when } \theta \leq \theta_{h1} \\ x_i + (x_f - x_i)\dfrac{\theta - \theta_{h1}}{\theta_{h2} - \theta_{h1}}, & \text{when } \theta_{h1} \leq \theta \leq \theta_{h2} \\ x_f, & \text{when } \theta_{h2} \leq \theta. \end{cases} \tag{3.33}$$

The next task is to determine the parameters $\theta_h, \Delta x_h$ or θ_{h1}, θ_{h2} as functions of m_0 and m_c. The conditions defined in eq. (3.30) restrict the acceptable values of these moments. Hence $\Delta x(\theta)$ must be determined using the values

$$|m_0| \le \frac{1}{2}(1-\delta)|x_i - x_f|$$

$$-\left(2|m_0| - \frac{4}{1-\delta}\frac{|m_0|^2}{|x_f - x_i|}\right) \le m_m \le \frac{\left(\frac{|x_f - x_i|}{2} - |m_0|\right)^2}{|x_f - x_i|} - \frac{\delta^2}{4}|x_f - x_i|, \tag{3.34}$$

where $m_m = 6m_c\text{sgn}(x_f - x_i) + \frac{4m_0^2}{|x_f - x_i|} - |m_0|$.

The new parameter m_m introduced to replace m_c is useful because it serves as a pattern-recognizing parameter for different piecewise linear approximations, namely

$$\begin{aligned} m_m &\le 0 \quad \text{for triangular approximation} \\ m_m &> 0 \quad \text{for front-type approximation.} \end{aligned} \tag{3.35}$$

When $m_m \le 0$ (triangular approximation), substituting $\Delta x(\theta)$ from eq. (3.32) into eq. (3.29) and integrating, one obtains

$$\begin{aligned} m_0 &= \frac{\Delta x_h}{2} \\ m_c &= \frac{\Delta x_h}{6}\left(\theta_h - \frac{1}{2}\right) \end{aligned} \tag{3.36}$$

and

$$\begin{aligned} \Delta x_h &= 2m_0 \\ \theta_h &= \frac{3m_c}{m_0} + \frac{1}{2}. \end{aligned} \tag{3.37}$$

When $m_m > 0$ (front-type approximation) we obtain $\Delta x(\theta)$ from eq. (3.28), namely

$$\Delta x(\theta) = x(\theta) - x_L \tag{3.38}$$

where $x_L = x_i + (x_f - x_i)\theta$. Inserting $\Delta x(\theta)$ with $x(\theta)$ from eq. (3.33) into eq. (3.29) and integrating we get for the front-type approximation

$$\begin{aligned} m_0 &= \frac{1}{2}(x_f - x_i)(1 - \theta_{h1} - \theta_{h2}) \\ m_c &= \frac{1}{2}(x_f - x_i)\left[\frac{1}{2}(\theta_{h1} + \theta_{h2}) - \frac{1}{3}(\theta_{h1}^2 + \theta_{h1}\theta_{h2} + \theta_{h2}^2) - \frac{1}{6}\right] \end{aligned} \tag{3.39}$$

which can be solved for θ_{h1}, θ_{h2} in terms of m_0, m_m as

$$\theta_{h1}, \theta_{h2} = \frac{1}{2} - \frac{m_0}{(x_f - x_i)} \pm \left[\left(\frac{1}{2} - \frac{|m_0|}{|x_f - x_i|} \right)^2 - \frac{m_m}{|x_f - x_i|} \right]^{1/2} \qquad (3.40)$$

Eqs. (3.28) – (3.40) show how the piecewise linear distribution of $x(\theta)$ can be represented at all boundaries of the mesh cell. The complete representation for one mesh cell is composed of x_1, x_2, x_3, x_4 at the corner points and $m_{0t1}, m^0_{0z}, m_{0t2}, m_{0z}$ and $m_{ct1}, m^0_{cz}, m_{ct2}, m_{cz}$ at the boundaries as shown in Figure 3.3. All quantities along the lower boundary are known from the initial condition or the results of the previous time step. In the following discussion, we also assume that $v\Delta t < \Delta z$.

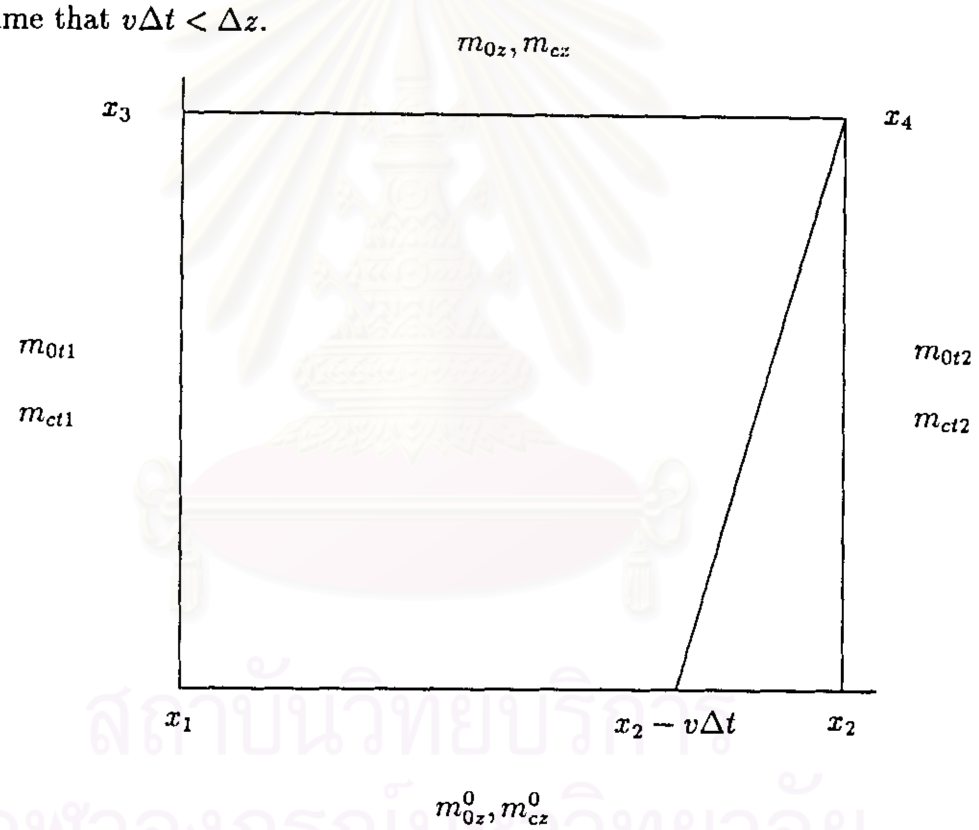

Figure 3.3 Schematic diagram showing all parameters on cell boundaries

Let us recall eq. (3.26), which can be formed in terms of θ_z and θ_t from eq. (3.27) as

$$x(\theta_t, \theta_z) = x(0, \theta_z - k\theta_t) + \Delta t \int_0^{\theta_t} p(\vartheta, \theta_z - k\theta_t + k\vartheta)\, d\vartheta, \qquad (3.41)$$

and when $\theta_z = 1$, we obtain

$$x(\theta_t, 1) = x(0, 1 - k\theta_t) + \Delta t \int_0^{\theta_t} p(\vartheta, 1 - k\theta_t + k\vartheta)\, d\vartheta, \tag{3.42}$$

where $k = v\Delta t/\Delta z$, and in this section we consider only the case $k < 1$. For reducing the computations in testing PLIM with our sample problem, we consider the special of case $p = 0$, so that eq. (3.42) becomes

$$x(\theta_t, 1) = x(0, 1 - k\theta_t), \tag{3.43}$$

which is the value of $x(\theta = 1 - k\theta_t)$ along the x_2-x_4 boundary.

Now the unknown value x_4 in Figure 3.3 can be obtained by eq. (3.43) with $\theta_t = 1$, i.e.,

$$x_4 = x(1, 1) = x(0, 1 - k), \tag{3.44}$$

and because we already have in hand the distribution of $x(0, \theta_z)$ as derived above. Then $x(0, 1 - k)$ can be evaluated using eq. (3.32) or (3.33). The next task is to evaluate the moments m_{0t2} and m_{ct2} as follows

1. When the distribution between x_1 and x_2 is a triangular approximation:

   - For $1 - k \leq \theta_h$, we obtain a triangular distribution on the x_2-x_4 boundary:

$$x(\theta) = \begin{cases} x_2 + (x_4 - x_2)\theta + \dfrac{\theta}{\theta_v}\Delta x_v, & \text{when } \theta \leq \theta_v \\ x_2 + (x_4 - x_2)\theta + \dfrac{1 - \theta}{1 - \theta_v}\Delta x_v, & \text{when } \theta_v \leq \theta, \end{cases} \tag{3.45}$$

   where

$$\begin{aligned} \theta_v &= \frac{1 - \theta_h}{k} \\ \Delta x_v &= \frac{\Delta x_h}{k\theta_h}(k + \theta_h - 1). \end{aligned} \tag{3.46}$$

Comparing with eq. (3.36) we obtain immediately

$$\begin{aligned} m_{0t2} &= \frac{\Delta x_v}{2} &&= \frac{\Delta x_h}{2k\theta_h}(k+\theta_h-1) \\ m_{ct2} &= \frac{\Delta x_v}{6}\left(\theta_v-\frac{1}{2}\right) &&= \frac{\Delta x_h}{6k\theta_h}(k+\theta_h-1)\left(\frac{1-\theta_h}{k}-\frac{1}{2}\right). \end{aligned} \tag{3.47}$$

- For $1-k \geq 0$, the distribution on the x_2-x_4 boundary is a linear function, thus $\Delta x(\theta) = x(\theta) - x_L \equiv 0$, yielding

$$m_{0t2} = m_{ct2} = 0. \tag{3.48}$$

2. When the distribution between x_1 and x_2 is a front-type approximation:

- For $1-k \leq \theta_{h1}$, then the distribution on the x_2-x_4 boundary is front-type:

$$x(\theta) = \begin{cases} x_2, & \text{when } \theta \leq \theta_{v1} \\ x_2 + (x_4 - x_2)\dfrac{\theta-\theta_{v1}}{\theta_{v2}-\theta_{v1}}, & \text{when } \theta_{v1} \leq \theta \leq \theta_{v2} \\ x_4, & \text{when } \theta_{v2} \leq \theta, \end{cases} \tag{3.49}$$

where

$$\begin{aligned} \theta_{v1} &= \frac{1-\theta_{h2}}{k} \\ \theta_{v2} &= \frac{1-\theta_{h1}}{k}, \end{aligned} \tag{3.50}$$

and we obtain using eq. (3.39)

$$\begin{aligned} m_{0t2} &= \frac{x_4-x_2}{2}(1-\theta_{v1}-\theta_{v2}) \\ &= \frac{x_4-x_2}{2}\left(1-\frac{2}{k}+\frac{\theta_{h1}+\theta_{h2}}{k}\right) \\ m_{ct2} &= \frac{1}{2}(x_4-x_2)\left\{\frac{1}{2}(\theta_{v1}+\theta_{v2})\right. \\ &\quad \left.-\frac{1}{3}(\theta_{v1}^2+\theta_{v1}\theta_{v2}+\theta_{v2}^2)-\frac{1}{6}\right\} \\ &= \frac{1}{2}(x_4-x_2)\left\{1-\frac{1}{k}+(\theta_{h1}+\theta_{h2})\left(\frac{1}{k}-\frac{1}{2}\right)\right. \\ &\quad \left.-\frac{1}{3k}(\theta_{h1}^2+\theta_{h1}\theta_{h2}+\theta_{h2}^2)-\frac{k}{6}\right\}. \end{aligned} \tag{3.51}$$

- For $\theta_{h1} \leq 1-k \leq \theta_{h2}$, we obtain a triangular distribution on the x_2-x_4 boundary similar to eq. (3.45) but with

$$\begin{aligned} \theta_v &= \frac{1-\theta_{h2}}{k} \\ \Delta x_v &= \frac{1}{2}(x_2 - x_4)\frac{1-\theta_{h2}}{k}. \end{aligned} \tag{3.52}$$

Then we get

$$\begin{aligned} m_{0t2} &= \frac{\Delta x_v}{2} \\ &= (x_4 - x_2)\frac{(\theta_{h2}-1)}{2k} \\ m_{ct2} &= \frac{\Delta x_v}{6}\left(\theta_v - \frac{1}{2}\right) \\ &= \frac{x_4 - x_2}{6k}(\theta_{h2}-1)\left(\frac{1-\theta_{h2}}{k} - \frac{1}{2}\right). \end{aligned} \tag{3.53}$$

- For $\theta_{h2} \leq 1-k$, the distribution at x_2-x_4 boundary is a linear (constant) function, so $\Delta x(\theta) = x(\theta) - x_L = 0$, yielding

$$m_{0t2} = m_{ct2} = 0. \tag{3.54}$$

The values of x_3 , m_{0t1} , and m_{ct1} are calculated in a similar fashion.

Two moment values, m_{0z}, m_{cz}, must still be evaluated. Before doing that we define

$$\begin{aligned} I_0 &= \int_0^1 x(\theta)\, d\theta \\ I_c &= \int_0^1 \left(\theta - \frac{1}{2}\right) x(\theta)\, d\theta. \end{aligned} \tag{3.55}$$

Consequently, we obtain the relations between them and moments defined in eq. (3.29) as

$$\begin{aligned} I_0 &= m_0 + \frac{x_f + x_i}{2} \\ I_c &= m_c + \frac{x_f - x_i}{12}. \end{aligned} \tag{3.56}$$

Figure 3.4 illustrates I_0's and I_c's at each boundary.

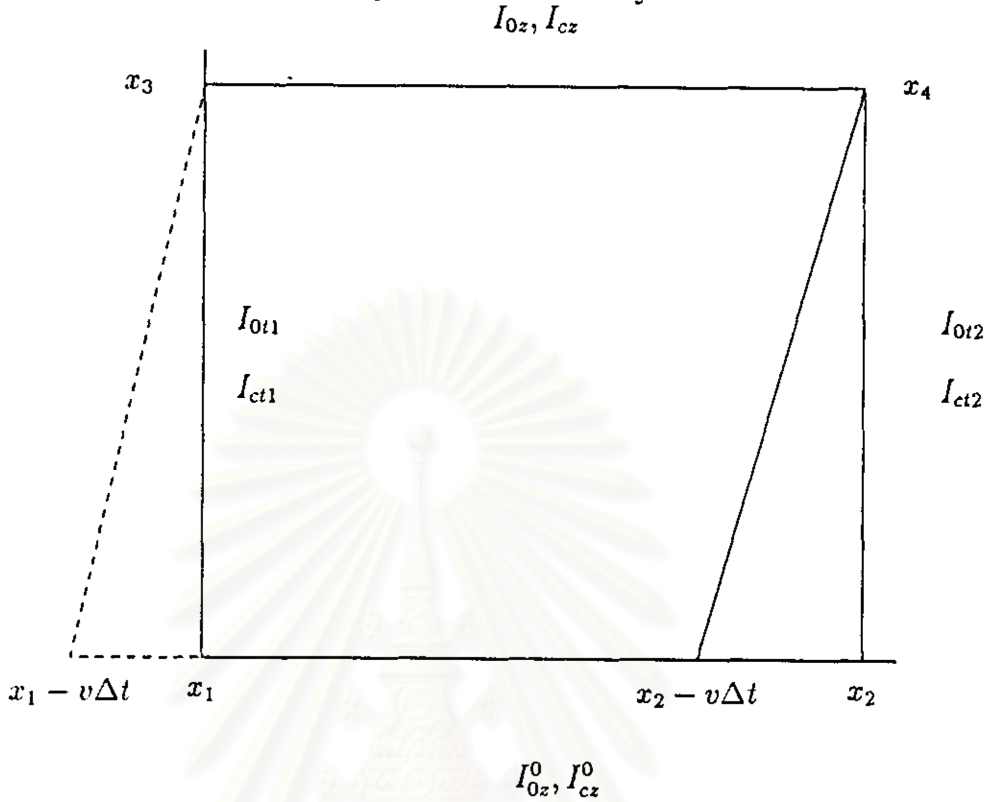

Figure 3.4 Schematic diagram showing I_0 and I_c on a boundary

Physically, if x is interpreted as a flux of particles, its integral with proper limits respective to distance is the number of particles, which should be conserved at any time, i.e., at $\theta_t = 0$ and at a later time $\theta_t = 1$ these integrals should be equal:

$$\int_{-k}^{1-k} x(0,\theta_z)\, d\theta_z = \int_0^1 x(1,\theta_z)\, d\theta_z, \tag{3.57}$$

and with some modifications we obtain another relation

$$\int_{-k}^{1-k} \left(\theta_z + k - \frac{1}{2}\right) x(0,\theta_z)\, d\theta_z = \int_0^1 \left(\theta_z - \frac{1}{2}\right) x(1,\theta_z)\, d\theta_z. \tag{3.58}$$

At vertical boundaries we know from eq. (3.43) that $x(\theta_t, \theta_z = 1) = x(0, \theta_z =$

$1 - k\theta_t)$, so

$$
\begin{aligned}
I_{0t2} &= \int_0^1 x(\theta_t, 1)\, d\theta_t &&= \frac{1}{k}\int_{1-k}^{1} x(0,\theta_z)\, d\theta_z \\
I_{ct2} &= \int_0^1 \left(\theta_t - \frac{1}{2}\right) x(\theta_t, 1)\, d\theta_t &&= \frac{1}{k}\int_{1-k}^{1} \left(\frac{1-\theta_z}{k} - \frac{1}{2}\right) x(0,\theta_z)\, d\theta_z
\end{aligned}
\tag{3.59}
$$

and $x(\theta_t, \theta_z = 0) = x(0, \theta_z = -k\theta_t)$, so

$$
\begin{aligned}
I_{0t1} &= \int_0^1 x(\theta_t, 0)\, d\theta_t &&= \frac{1}{k}\int_{-k}^{0} x(0,\theta_z)\, d\theta_z \\
I_{ct1} &= \int_0^1 \left(\theta_t - \frac{1}{2}\right) x(\theta_t, 0)\, d\theta_t &&= \frac{1}{k}\int_{-k}^{0} \left(-\frac{\theta_z}{k} - \frac{1}{2}\right) x(0,\theta_z)\, d\theta_z.
\end{aligned}
\tag{3.60}
$$

From eq. (3.57) we obtain

$$
\begin{aligned}
I_{0z} &= \int_{-k}^{1-k} x(0,\theta_z)\, d\theta_z \\
&= \int_{-k}^{0} x(0,\theta_z)\, d\theta_z + \int_{0}^{1} x(0,\theta_z)\, d\theta_z + \int_{1}^{1-k} x(0,\theta_z)\, d\theta_z \\
&= kI_{0t1} + I_{0z}^0 - kI_{0t2}.
\end{aligned}
$$

Using eq. (3.59) and (3.60), we obtain

$$
I_{0z} = I_{0z}^0 + k(I_{0t1} - I_{0t2}) \tag{3.61}
$$

and eq. (3.58) yields

$$
\begin{aligned}
I_{cz} &= \int_{-k}^{1-k} \left(\theta_z + k - \frac{1}{2}\right) x(0,\theta_z)\, d\theta_z \\
&= k\int_{-k}^{1-k} x(0,\theta_z)\, d\theta_z + \int_{-k}^{0} \left(\theta_z - \frac{1}{2}\right) x(0,\theta_z)\, d\theta_z \\
&\quad + \int_{0}^{1} \left(\theta_z - \frac{1}{2}\right) x(0,\theta_z)\, d\theta_z + \int_{1}^{1-k} \left(\theta_z - \frac{1}{2}\right) x(0,\theta_z)\, d\theta_z.
\end{aligned}
$$

Using eq. (3.59) and (3.60), and after much laborious work, we finally get

$$
I_{cz} = I_{cz}^0 + k^2(I_{ct2} - I_{ct1}) + \frac{k}{2}(I_{0z} + I_{0z}^0 - I_{0t2} - I_{0t1}). \tag{3.62}
$$

Next, we want eq. (3.61) and (3.62) in terms of moments using eq. (3.56) with proper substitutions for m_0, m_c, x_i and x_f, obtaining

$$\begin{aligned} m_{0z} &= m_{0z}^0 + k(m_{0t1} - m_{0t2}) + \frac{1}{2}(x_1 + x_2 - x_3 - x_4) \\ &\quad + \frac{k}{2}(x_1 - x_2 + x_3 - x_4) \\ m_{cz} &= m_{cz}^0 + k^2(m_{ct2} - m_{ct1}) + \frac{k}{2}(m_{0z} + m_{0z}^0 - m_{0t2} - m_{0t1}) \\ &\quad + \frac{1}{12}(k^2 - 1)(x_1 - x_2 - x_3 + x_4). \end{aligned} \tag{3.63}$$

In case where PLIM conditions are violated i.e. $I_{0z} < \Delta z.\min(x_3, x_4)$ or $I_{0z} > \Delta z.\max(x_3, x_4)$, we will adjust x_3 in that I_{0z} must conserve. New x_3' is computed from

$$x_3' = \frac{I_{0z} - \delta' x_4/2}{\Delta z - \delta'/2}$$

where δ' is given. Thereafter we recompute m_{0z} and m_{cz} from x_3' and the others with old value.

Now we have determined the procedure for evaluating the unknown variables of a mesh cell. In the next section we apply the method to two sample problems.

3.4 Numerical Results

The PLIM has been tested with two simple problems. The first has distribution at incoming boundary of two-step function, and the second has distribution of rising exponentially and at a certain point dropping suddenly to zero. The results of computation by PLIM were compared with the analytic solution. We find that the results for the first problem agrees precisely, but those for the second differs significantly such that the conservation of shape breakdowns. The two problems have the same equation,

$$\frac{\partial x}{\partial t} + v\frac{\partial x}{\partial z} = 0 \tag{3.64}$$

Problem 1: Eq. (3.64) with initial and boundary condition as follows:

$$\begin{aligned} x(0,z) &= \begin{cases} 1, & \text{when } z \leq z_0 \\ 0, & \text{when } z \geq z_0 \end{cases} \\ x(t,0) &= 1, \text{ for } t \geq 0 \end{aligned} \tag{3.65}$$

Before we solve problem 1, eq. (3.65) must be approximated reasonably to be used by PLIM. We know that $M\Delta z \leq z_0 \leq (M+1)\Delta z$ for a positive integer M. For $z < M\Delta z$ we set $x(0,z) \equiv 1$, and for $z > (M+1)\Delta z$ we set $x(0,z) \equiv 0$, but for $M\Delta z \leq z_0 \leq (M+1)\Delta z$ we approximate $x(0,z)$ so that eq. (3.30) is not violated, having a finite slope. Then eq. (3.65) is approximated by

$$\begin{aligned} x(0,z) &= \begin{cases} 1, & \text{when } z \leq z_0 - \beta \\ \frac{1}{2\beta}(z_0 + \beta - z), & \text{when } z_0 - \beta < z \leq z_0 + \beta \\ 0, & \text{when } z > z_0 + \beta \end{cases} \\ x(t,0) &= 1, \text{ fort} \geq 0 \end{aligned} \tag{3.66}$$

for a given $\beta \geq 0$.

An analytic solution of eq. (3.64) with the initial and boundary condition eq. (3.66) is obtained by using eq. (3.15):

$$x(t,z) = x(0, z - vt) \tag{3.67}$$

where the integral term in eq. (3.15) is zero here. When replacing z in eq. (3.66) with $z - vt$ we obtain the analytic solution from eq. (3.67)

$$x(t,z) = \begin{cases} 1, & \text{when } z \leq vt + z_0 - \beta \\ \frac{1}{2\beta}[z_0 + \beta - (z - vt)], & \text{when } vt + z_0 - \beta < z \leq vt + z_0 + \beta \\ 0, & \text{when } z > vt + z_0 + \beta \end{cases} \tag{3.68}$$

Now the PLIM solution of eq. (3.64) with the initial and boundary condition eq. (3.66) is obtained by using the procedure detailed in the preceding section. Below are the results of PLIM with the analytic solution, eq. (3.68), shown for comparison.

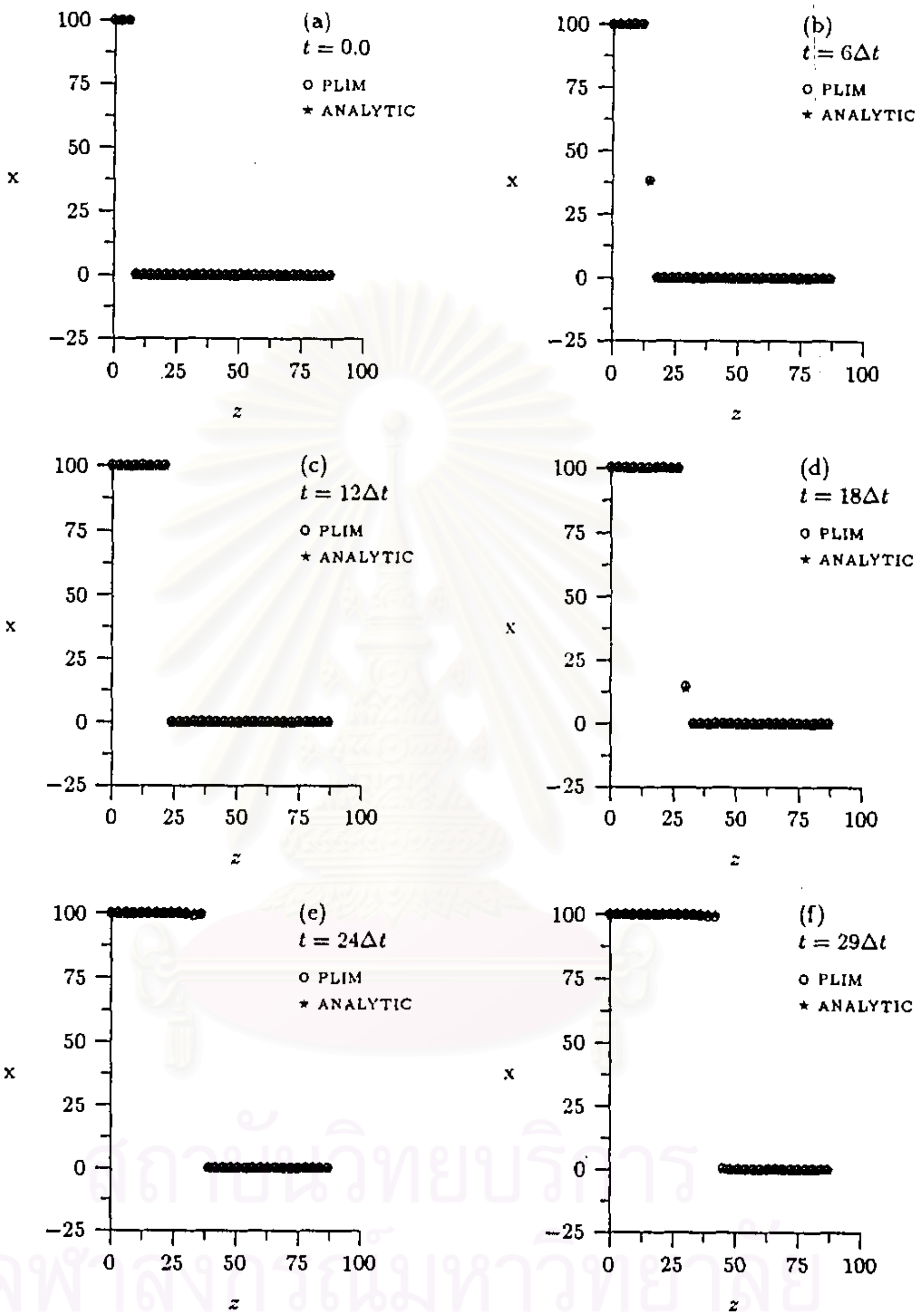

Figure 3.5 Analytic and PLIM solutions of problem 1

Problem 2: Eq. (3.64) with initial and boundary conditions as follows:

$$
\begin{aligned}
x(0,z) &= \begin{cases} e^{-(z_0-z)/\lambda}, & \text{when } z \leq z_0 \\ 0, & \text{when} z \geq z_0 \end{cases} \\
x(t,0) &= e^{-(z_0+vt)/\lambda}, \text{ for } t \geq 0.
\end{aligned}
\tag{3.69}
$$

In the same way as the preceding problem, we approximate eq. (3.69) reasonably to be used by PLIM. We know that $M\Delta z \leq z_0 \leq (M+1)\Delta z$ for a positive integer M. For $t = 0$, we keep $x(0, z) \equiv 0$ for $z > (M+1)\Delta z$. For $z < M\Delta z$ we consider

$$x(0, z) = e^{-(z_0 - z)/\lambda}, \tag{3.70}$$

and compute the integral

$$I_{i0} = \Delta z \int_0^1 x(0, z_i + \theta\Delta z) d\theta.$$

We obtain

$$I_{i0} = \lambda x(0, z_i)(e^{\Delta z/\lambda} - 1), \tag{3.71}$$

and next we compute the integral

$$I_{ic} = \Delta z \int_0^1 \left(\theta - \frac{1}{2}\right) x(0, z_i + \theta\Delta z) d\theta$$

to obtain

$$I_{ic} = x(0, z_i)e^{\Delta z/\lambda} - \frac{\lambda}{\Delta z} I_{i0} - \frac{I_{i0}}{2}, \tag{3.72}$$

where $z_i = i\Delta z$, and $i = 0, 1, 2, \ldots, M-1$. We then can compute the moments m_{i0} and m_{ic} from the relation

$$\begin{aligned} m_{i0} &= I_{i0} - \frac{1}{2}[x(0, z_i + \Delta z) + x(0, z_i)] \\ m_{ic} &= I_{ic} - \frac{1}{12}[x(0, z_i + \Delta z) - x(0, z_i)] \end{aligned} \tag{3.73}$$

where $x(0, z_i)$ and $x(0, z_i + \Delta z)$ are computed from eq. (3.70). We can also compute pattern-recognizing moments m_{im} from m_{i0} and m_{ic} above and find that they are negative, so we use the triangular approximation to approximate eq. (3.69) for $z < M\Delta z$. From eq. (3.73), we can compute the triangular approximation variables:

$$\begin{aligned} \Delta x_{ih} &= 2m_{i0} \\ \theta_{ih} &= \frac{3m_{ic}}{m_{i0}} + \frac{1}{2} \end{aligned} \tag{3.74}$$

Then we obtain the approximate initial condition function $X(0,z)$ for $z < M\Delta z$ as

$$X(0,z) = x(0,z_i)+[x(0,z_i+\Delta z)-x(0,z_i)]\theta_i+\begin{cases} \dfrac{\theta_i}{\theta_{ih}}\Delta x_{ih}, & \text{when } 0 \le \theta_i \le \theta_{ih} \\ \dfrac{1-\theta_i}{1-\theta_{ih}}\Delta x_{ih}, & \text{when } \theta_{ih} < \theta_i \le 1 \end{cases} \tag{3.75}$$

where $\theta_i = (z - z_i)/\Delta z$. Now for $M\Delta z \le z \le (M+1)\Delta z$ the front-type approximation should be more reasonable than the triangular approximation and we approximate $x(0,z)$ as $X(0,z)$ given by

$$X(0,z) = \begin{cases} x(0,z_M), & \text{when } z_M \le z \le z_0 - \beta \\ \dfrac{x(0,z_M)}{2\beta}(z_0+\beta-z), & \text{when } z_0-\beta < z \le z_0+\beta \\ 0, & \text{when } z > z_0+\beta. \end{cases} \tag{3.76}$$

Next we consider the boundary condition

$$x(t,0) = e^{-(z_0+vt)/\lambda}. \tag{3.77}$$

Computing the integral

$$I_{j0} = \Delta t \int_0^1 x(t_j+\theta\Delta t, 0)d\theta,$$

we obtain

$$I_{j0} = -\frac{\lambda}{v}x(t_j,0)(e^{-v\Delta t/\lambda}-1), \tag{3.78}$$

and then computing the integral

$$I_{jc} = \Delta t \int_0^1 \left(\theta - \frac{1}{2}\right) x(t_j+\theta\Delta t,0)d\theta,$$

we obtain

$$I_{jc} = -\frac{\lambda}{v}x(t_j,0)e^{-v\Delta t/\lambda} + \frac{\lambda}{v\Delta t}I_{j0} - \frac{I_{j0}}{2}, \tag{3.79}$$

where $t_j = j\Delta t$, and $j = 0, 1, 2, \ldots$ indicates the grid point along the t axis. We now can compute moments m_{j0} and m_{jc} from

$$\begin{aligned} m_{j0} &= I_{j0} - \frac{1}{2}[x(t_j + \Delta t, 0) + x(t_j, 0)] \\ m_{jc} &= I_{jc} - \frac{1}{12}[x(t_j + \Delta t, 0) - x(t_j, 0)] \end{aligned} \tag{3.80}$$

We can then compute pattern-recognizing moments m_{jm} from m_{j0} and m_{jc} above and find that they are all negative, so we use the triangular approximation to approximate eq. (3.77). From eq. (3.80) we can compute the triangular approximation variables:

$$\begin{aligned} \Delta x_{jh} &= 2m_{j0} \\ \theta_{jh} &= \frac{3m_{jc}}{m_{j0}} + \frac{1}{2}. \end{aligned} \tag{3.81}$$

Then we obtain $X(t, 0)$ as an approximation to $x(t, 0)$:

$$X(t,0) = x(t_j,0) + [x(t_j+\Delta t,0) - x(t_j,0)]\theta_j + \begin{cases} \dfrac{\theta_j}{\theta_{jh}}\Delta x_{jh}, & \text{when } 0 \le \theta_j \le \theta_{jh} \\ \dfrac{1-\theta_j}{1-\theta_{jh}}\Delta x_{jh}, & \text{when } \theta_{jh} < \theta_j \le 1. \end{cases} \tag{3.82}$$

where $\theta_j = (t - t_j)/\Delta t$. Now we have completed the approximation of eq. (3.69), yielding of eqs. (3.75), (3.76), and (3.82).

An analytic solution of eq. (3.64) with the initial and boundary condition eqs. (3.75), (3.76), and (3.82) is obtained by using eq. (3.15) as in the first problem. When replacing z in eqs. (3.75) and (3.76) with $z - vt$, we obtain the analytic solution. If $z - vt < M\Delta z$ we get eq. (3.75) with $\theta_i = (z - vt - z_i)/\Delta z$ as the analytic solution. If $z - vt \ge M\Delta z$ we get from eq. (3.76):

$$X(t,z) = \begin{cases} x(0, z_M), & \text{when } z_M \le z - vt \le z_0 - \beta \\ \dfrac{x(0,z_M)}{2\beta}[z_0 + \beta - (z - vt)], & \text{when } z_0 - \beta < z - vt \le z_0 + \beta \\ 0, & \text{when } z - vt > z_0 + \beta. \end{cases} \tag{3.83}$$

Now the PLIM solution of eq. (3.64) with the initial and boundary conditions of eq. (3.75), (3.76), and (3.82) is obtained by using the procedure detailed in the preceding section. Below are the results of PLIM with the analytic solution above shown for comparison:

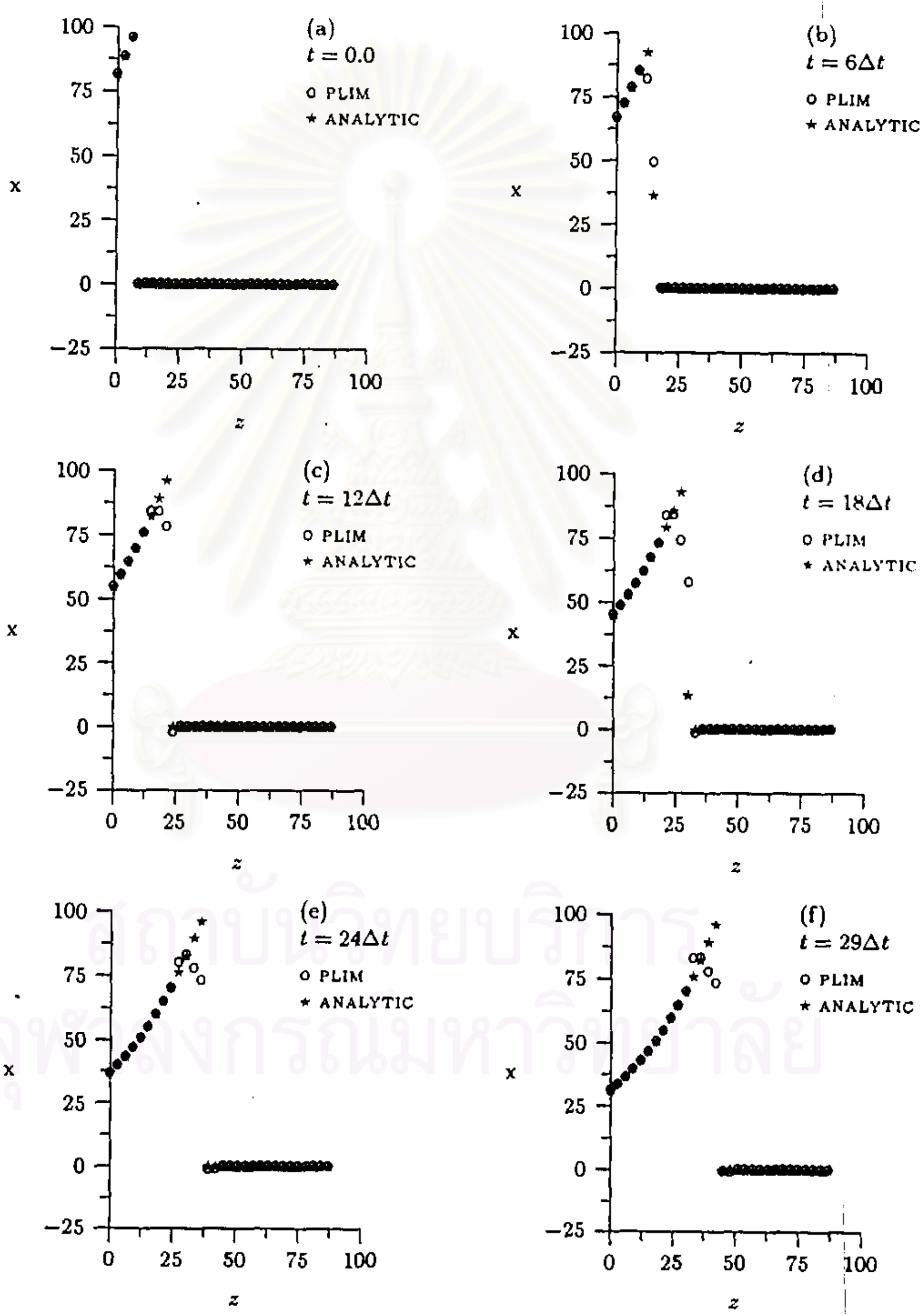

Figure 3.6 Analytic and PLIM solutions of problem 2

We use $v = 0.123$, $\Delta t = 0.10$, $\Delta z = 0.03$, $\beta = 0.005$ in both problems.

3.5 Conclusion

From figure 3.5 we find that a step function conserves its shape when it is moving. The PLIM solution agrees well with analytic one. In figure 3.6 we find that the shape of a peak function deteriorates gradually while it is moving. In addition, the solution near the peak computed by PLIM does not agree with those computed by analytic method. These shows that PLIM can not be applied to peak function while it works very well with step function. So it cannot be used to investigate the transport of cosmic rays across the solar-flare shock.