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Generalized Boltzmann equation for shallow water flows

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ABSTRACT

This invited review paper introduces the Boltzmann-based approach for the numerical modelling of surface water flows to hydroinformaticians. The paper draws upon earlier work by our group as well as others. This review formulates the generalized Boltzmann equation for 1D and 2D shallow water flows and shows that the statistical moments of these generalized equations provide the classical continuity and momentum equations in shallow waters. The connection between the generalized Boltzmann equation and classical shallow water equations provides a framework for formulating new computational approaches to surface water flows. To illustrate, a first-order explicit scheme based on the generalized Boltzmann equation for 1D shallow waters in frictionless and horizontal channels is formulated. The resulting scheme is applied to the classical dam break problem. Comparison with the analytical solution shows that the Boltzmann-based scheme is highly accurate and free of spurious oscillations, illustrating the potential of the method for surface water problems and other applications.

Key words | Boltzmann equation, unsteady open channel flow, dam break, bore, entropy, numerical model

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INTRODUCTION

Physically based macroscopic modelling of problems in mechanics, hydrodynamics, hydraulics and environmental fluid mechanics often proceeds from applying the fundamental laws of physics to a continuum. In particular, governing equations of mechanics, hydrodynamics, hydraulics and environmental fluid mechanics are often arrived at by applying the principles of mass, momentum and energy to a control volume of size equal to or larger than that required by the continuum hypothesis. These equations are often a system of nonlinear partial differential equations for which exact solutions are not available. Conventional numerical solutions of the governing equations of hydraulic problems are based on techniques such as method of characteristics, finite element and finite difference. Essentially, the role of numerical techniques is to transform the equations of hydraulics into a form suitable for digital computers (Abbot 1991; Abbott & Minns 1998).

Mesoscopic modelling proceeds from the realization that macroscopic (gross) properties of matter and its motion such as density, temperature, pressure, momentum, energy and entropy and the equations governing these gross properties are directly related to the mass and motion of the molecules that constitute the continuum under investigation. In particular, mesocopic theory treats the velocity of particles (atoms or molecules) as a random variable. The statistical moments of the velocity distribution function of particles occupying the control volume of interest provide the density, temperature, pressure, momentum, energy and entropy of this control volume.

An equation describing the evolution of the velocity distribution function of a gas in phase space, defined by the location and momentum of a particle, was introduced in the seminal paper by Boltzmann (1872). The Boltzmann equation is a superset in the sense that its statistical moments provide the classical conservation laws of mass, momentum, energy and entropy (e.g. see Vincenti & Kruger 1965; Jon *et al.* 1996). A generalized Boltzmann-like equations for numerous other

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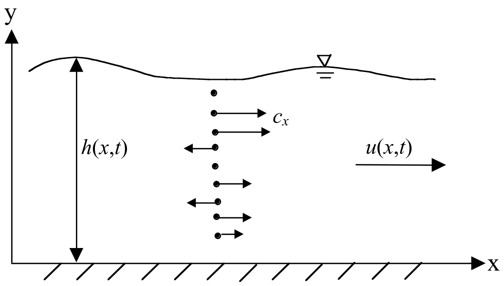

Figure 1 | Sketch of 1D open channel flow.

applications have been formulated and applied. Examples include two-phase flow (Culick 1964), sediment distribution in dense solid-liquid flows (Ni *et al*. 2000), scalar transport (Deng *et al*. 2001), open channel flows (Ghidaoui *et al*. 2001), traffic flow (Helbing 1996; Bellomo & Lo Schiavo 1999) and population dynamics and coagulation processes (Bellomo & Lo Schiavo 1999). This paper derives the generalized Boltzmann equation for 1D and 2D shallow water flows and shows that the moments of these generalized equations provide the classical continuity and momentum in shallow waters. The exploitation of the connection between the generalized Boltzmann equation and the shallow water equations in the formulation of new computational approaches to surface water flows is illustrated for the case of 1D shallow water flows in a frictionless horizontal channel.

HEURISTIC DERIVATION OF THE GENERALIZED BOLTZMANN EQUATION FOR 1D SHALLOW WATER FLOWS

Figure 1 depicts a depth averaged 1D shallow water flow, where x = longitudinal distance (position), y = vertical distance (position), t = time, h = water depth and u = depth-averaged longitudinal velocity. The water depth, $h(x,t)$, is a measure of the vertical length of the stack of the enormous number of water molecules at x and t. The microscopic longitudinal velocity, c_x, of each molecule in the stack is a random variable. The probability density function of c_x for a particle located at x at t is $p(x,t,c_x)$. Therefore, $p(x,t,c_x)dc_x$ is the probability that a water molecule located at x at time t has a microscopic speed in the range $[c_x,c_x+dc_x]$. In addition, $h(x,t)$ $p(x,t,c_x)dc_x$ is the proportion of the water depth at x and t occupied by water molecules whose microscopic speed is in the range $[c_x,c_x+dc_x]$. Moreover, $pc_xh(x,t)p(x,t,c_x)dc_x$ and $pc_x^2h(x,t)p(x,t,c_x)dc_x$ define the contribution of water molecules whose microscopic speed is in the range $[c_x,c_x+dc_x]$ to the mass mass and momentum fluxes at x and t, respectively. The zero and first moments of the probability density function $p(x,t,c_x)$ are

$$\int_{-\infty}^{\infty} p(x,t,c_x)dc_x = 1 \tag{1}$$

$$\int_{-\infty}^{\infty} c_x p(x,t,c_x)dc_x = u(x,t) \tag{2}$$

Integrating the above moments with respect to water depth give

$$\int_0^{h(x,t)}\int_{-\infty}^{\infty} p(x,t,c_x)dc_x dy = h(x,t) \tag{3}$$

$$\int_0^{h(x,t)}\int_{-\infty}^{\infty} hc_x p(x,t,c_x)dc_x dy = h(x,t)u(x,t) \tag{4}$$

Expressions (3) and (4) provide the connection between the microscopic state of the flow, defined by the probability density function, and the water depth and flow rate per unit width in the channel. Other relations connecting higher moments of $p(x,t,c_x)$ to macroscopic variables, such as the momentum of the flow, are determined later in this paper.

The generalized Boltzmann equation governing the evolution of $h(x,t)p(x,t,c_x)$ in the phase space (x,t,c_x) is obtained by applying the principle of mass balance to the control volume of Figure 2. The volume of this control volume at t is $[\rho hp\Delta c_x\Delta x]_t$ and defines the expected mass at t of the water molecules located between x and $x+\Delta x$ and possessing a microscopic speed in the range $[c_x,c_x+\Delta c_x]$. Similarly, the volume of this control volume at $t+\Delta t$ is $[\rho hp\Delta c_x\Delta x]_{t+\Delta t}$ and defines the expected mass at $t+\Delta t$ of the water molecules located between x and $x+\Delta x$ and possessing a microscopic speed in the range

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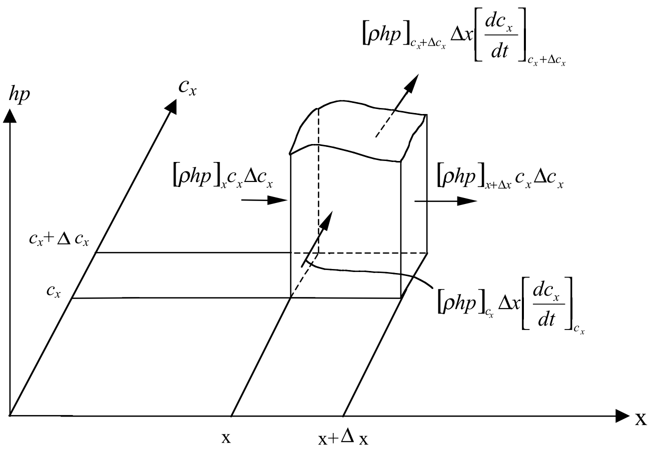

Figure 2 | Control volume in phase space.

$[c_x,c_x+\Delta c_x]$. Therefore, the change in expected mass of the control volume during Δt is

$$[\rho hp\Delta c_x\Delta x]_{t+\Delta t} - [\rho hp\Delta c_x\Delta x]_t = ([(hp]_{t+\Delta t} - [hp]_t))\rho\Delta c_x\Delta x \quad (5)$$

The assumptions that the fluid is incompressible and the control volume is of fixed size are used in (5).

The mass associated with the flux of molecules at x during Δt is equal to the product of c_x, Δt and the area of the control volume at x (i.e. $[c_x\rho hp\Delta c_x]_x$). Therefore, the net mass influx at x during Δt is $[c_x\rho hp\Delta c_x\Delta t]_x$. Similarly, the net mass flux at $x+\Delta x$ during Δt is $[c_x\rho hp\Delta c_x\Delta t]_{x+\Delta x}$. As a result, the net increase of the mass of the control volume due to molecular flux along x is

$$[c_x\rho hp\Delta c_x\Delta t]_{x+\Delta x} - [c_x\rho hp\Delta c_x\Delta t]_x = ([c_x hp]_{x+\Delta x} - [c_x hp]_x)\rho\Delta c_x\Delta t \quad (6)$$

The mass flux at c_x during Δt is equal to the product of molecular acceleration dc_x/dt, Δx and the area of the control volume at c_x (i.e. $[(dc_x/dt)\rho hp\Delta x]_{c_x}$). Therefore, the net mass influx at c_x during Δt *is* $[(dc_x/dt)\rho hp\Delta x\Delta t]_{c_x}$. Similarly, the mass flux at $c_x+\Delta c_x$ during Δt is $[(dc_x/dt)\rho hp\Delta x\Delta t]_{c_x+\Delta c_x}$. As a result, the net increase of the mass of the control volume due to molecular flux along c is

$$\left[\frac{dc_x}{dt}\rho hp\Delta x\Delta t\right]_{c_x+\Delta c_x} - \left[\frac{dc_x}{dt}\rho hp\Delta x\Delta t\right]_{c_x} = \left(\left[\frac{dc_x}{dt}hp\right]_{c_x+\Delta c_x} - \left[\frac{dc_x}{dt}hp\right]_{c_x}\right)\rho\Delta x\Delta t \quad (7)$$

The mass flux due to molecular acceleration is not commonly encountered in hydraulic modelling and needs further explanation. To this end, recall that the current formulation is focused on molecules residing between x and $x+\Delta x$ and possessing speeds between c_x and $c_x+\Delta c_x$. External forces can cause some of the molecules, which possess speeds outside the range of interest prior to t, to enter this range of interest through acceleration (deceleration) during Δt; thus, the dependence of the flux on the molecular acceleration. Similarly, external forces can cause some of the molecules, which possess speeds inside the range of interest prior to t, to leave this range of interest through acceleration (deceleration) during Δt.

Another physical mechanism that can alter the mass of the control volume in Figure 2 is due to molecular interaction. To explain, molecular interaction such as collisions alters the molecular speeds and their associated probability distribution function. Therefore, molecular interaction can cause some molecules that belong to the range $[x,x+\Delta x]\times[c_x,c_x+\Delta c_x]$ prior to t to exit this range in the time interval $[t,t+\Delta t]$. Alternatively, molecular interaction can cause some molecules that are outside the range $[x,x+\Delta x]\times[c_x,c_x+\Delta c_x]$ prior to t to enter this range in the time interval $[t,t+\Delta t]$. The net source/sink of mass into the range $[x,x+\Delta x]\times[c_x,c_x+\Delta c_x]$ due to molecular interaction is $J\Delta x\Delta t\Delta c_x$. Physically, molecular interaction changes the probability distribution of molecules and results in redistribution of mass, momentum and energy from regions of high concentrations to regions of low concentrations. That is, molecular interaction tends to 'destroy' gradients of mass momentum and energy. In fact, molecular interaction is the origin of macroscopic phenomena such as molecular diffusion and viscous forces. In high Reynolds number flows, the turbulent redistribution of mass, momentum and energy, in the region outside the viscous sub-layer, dominates that of molecular interactions. For the case of depth-averaged shallow water flows, the viscous sub-layer is not resolved since the smallest length scale of interest is equal to the

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water depth. At length scales of the order of the water depth or larger, the contribution of molecular interaction to the redistribution of mass, momentum and energy is negligible. In a manner analogous to macroscopic modelling shallow flows, the loss of momentum to the channel boundary are represented by a wall shear force.

Excluding the effects of molecular interaction, the mass balance principle dictates that the change of mass of the control volume, given by (5), is equal to the net sum of all fluxes, at the control surface, given by (6) and (7). Equating (5) to (6)+(7), dividing through by $\rho\Delta c_x\Delta x\Delta t$, and taking the limit as $(\Delta c_x,\Delta x,\Delta t)$ tends to (0,0,0) gives

$$\frac{\partial f}{\partial t}+c_x\frac{\partial f}{\partial x}+\frac{dc_x}{dt}\frac{\partial f}{\partial c_x}=0 \tag{8}$$

where $f=hp$. Equation (8) is the generalized Boltzmann equation for 1D turbulent shallow water flows. This is a quasi-linear partial differential equation governing the scalar $f=hp$. Mass conservation is the sole fundamental principle that has been invoked to derive (8). Momentum conservation principle can be invoked by relating particle acceleration to external forces through Newton's second law. The result is

$$\frac{\partial f}{\partial t}+c_x\frac{\partial f}{\partial x}+\frac{F_x}{m}\frac{\partial f}{\partial c_x}=0 \tag{9}$$

where $F_x=$ net external forces along x and $m=$ molecular mass. Writing (9) along a particle path gives

$$\frac{df}{dt}=0 \quad \text{if} \quad \frac{dx}{dt}=c \quad \text{and} \quad \frac{dc}{dt}=\frac{F_x}{m} \tag{10}$$

which shows that the distribution function is invariant along the particle path. This is a consequence of neglecting molecular interaction.

The formulation of (8) and (9) involved the principles of mass and momentum principles. Therefore, it is not surprising that the next section shows that the zero and first moments of (9) with respect to c_x provide the well known continuity and momentum equations for shallow waters, respectively.

DERIVATION OF CONTINUITY AND MOMENTUM EQUATIONS FROM MOMENTS OF THE GENERALIZED 1D BOLTZMANN

Continuity equation

The zero moment of (9) with respect to c_x is

$$\int_{-\infty}^{\infty}\frac{\partial f}{\partial t}dc_x+\int_{-\infty}^{\infty}c_x\frac{\partial f}{\partial x}dc_x+\int_{-\infty}^{\infty}\frac{F_x}{m}\frac{\partial f}{\partial c_x}dc_x=0$$

$$\text{or}\ \frac{\partial}{\partial t}\int_{-\infty}^{\infty}f dc_x+\frac{\partial}{\partial x}\int_{-\infty}^{\infty}c_x f dc_x+\frac{F_x}{m}[f]_{-\infty}^{\infty}=0 \tag{11}$$

Invoking (3) and (4), and realizing that the probability of a molecule possessing infinite speed is zero (i.e. $[f]_{-\infty}^{\infty}=0$), (11) becomes

$$\frac{\partial h}{\partial t}+\frac{\partial hu}{\partial x}=0 \tag{12}$$

which is the continuity equation for 1D shallow water flows.

Momentum equation

The first moment of (9) with respect to c_x is

$$\int_{-\infty}^{\infty}c_x\frac{\partial f}{\partial t}dc_x+\int_{-\infty}^{\infty}c_x^2\frac{\partial f}{\partial x}dc_x+\int_{-\infty}^{\infty}c_x\frac{F_x}{m}\frac{\partial f}{\partial c_x}dc_x=0 \tag{13}$$

Exchanging the order of differentiation and integration in the first two terms in the left hand side of (13), applying integration by parts to the third term on the left hand side of this equation, and invoking (3) and (4), (13) becomes

$$\frac{\partial hu}{\partial t}+\frac{\partial}{\partial x}\int_{-\infty}^{\infty}c_x^2 f dc_x+h\frac{F_x}{m}=0 \tag{14}$$

The second term on the left hand side of (14) can be developed as follows:

$$\int_{-\infty}^{\infty}c_x^2 f dc_x=\int_{-\infty}^{\infty}(u^2+2u(c_x-u)+(c_x-u)^2)f dc_x=hu^2+\int_{-\infty}^{\infty}(c_x-u)^2 f dc_x=hu^2+h\sigma \tag{15}$$

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where σ = standard deviation of p and measures the momentum flux of molecules with respect to a frame of reference moving with macroscopic fluid velocity u. Requiring that the probability density function has a standard deviation equal to $gh/2$ gives

$$\frac{\partial hu}{\partial t}+\frac{\partial(hu^2+gh^2/2)}{\partial x}+h\frac{F_x}{m}=0 \tag{16}$$

which is the classical momentum equation for 1D shallow water flows. Therefore, the zero and first moment of the generalized Boltzmann equation governing the distribution function, where the first three moments of f are h, hu and $hu^2+gh^2/2$, respectively, provide the correct continuity and momentum equation for 1D shallow water flows. That is, equations governing macroscopic dynamics are obtainable from moments of the equation that governs the microscopic dynamics. The generalized Boltzmann equation for 2D shallow water flows and its connection to the classical 2D shallow water equations is developed in the following section.

HEURISTIC DERIVATION OF THE GENERALIZED BOLTZMANN EQUATION FOR 2D SHALLOW WATER FLOWS

In 2D flows, both the microscopic longitudinal and lateral velocities (i.e. c_x and c_z) of each molecule are random variables, where z = longitudinal coordinate. The probability density function associated with c_x and c_z for a molecule located at (x,z) at t is $p(x,z,t,c_x)$. Therefore, $p(x,z,t,c_x)dc_xdc_z$ is the probability that a water molecule located at (x,z) at time t has a microscopic speed in the range $[c_x,c_x+dc_x]\times[c_z,c_z+dc_z]$. In addition, $h(x,z,t)p(x,z,t,c_x)dc_xdc_z$ is the proportion of the water depth at (x,z) and t occupied by water molecules whose microscopic speed is in the range $[c_x,c_x+dc_x]\times[c_z,c_z+dc_z]$. Moreover, $\rho c_xh(x,z,t)p(x,z,t,c_x)dc_x$ and $\rho c_x^2h(x,z,t)p(x,z,t,c_x)dc_x$ define the contribution of water molecules whose microscopic speed is in the range $[c_x,c_x+dc_x]\times[c_z,c_z+dc_z]$ to the longitudinal mass and momentum fluxes at (x,z) and t, respectively. Furthermore, $\rho c_zh(x,z,t)p(x,z,t,c_x)dc_x$ and $\rho c_x^2h(x,z,t)p(x,z,t,c_x)dc_x$ define the contribution of water molecules whose microscopic speed is in the range $[c_x,c_x+dc_x]\times[c_z,c_z+dc_z]$ to the lateral mass and momentum fluxes at (x,z) and t, respectively. Again, letting $f=hp$, the zero and first moments of f are

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f dc_xdc_z=h(x,z,t) \tag{17}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_xfdc_xdc_zdy=h(x,z,t)u(x,z,t) \tag{18}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_zfdc_xdc_zdy=h(x,z,t)v(x,z,t) \tag{19}$$

where v = velocity along z. The formulation of the generalized Boltzmann equation for 2D shallow water flows which governs the evolution of f in the phase space (x,z,c_x,c_z) and t is analogous to the 1D case. In particular, applying the mass balance principle to a control volume defined in the phase space, invoking Newton's second law to relate molecular acceleration to external forces and neglecting molecular interaction gives

$$\frac{\partial f}{\partial t}+c_x\frac{\partial f}{\partial x}+c_z\frac{\partial f}{\partial z}+\frac{F_x}{m}\frac{\partial f}{\partial c_x}+\frac{F_z}{m}\frac{\partial f}{\partial c_z}=0 \tag{20}$$

where F_z = net external forces along z. Writing (20) along the particle path gives

$$\frac{\partial f}{\partial t}=0 \quad \text{if} \quad \frac{dx}{dt}=c_x\,; \quad \frac{dz}{dt}=c_z\,; \quad \frac{dc_x}{dt}=\frac{F_x}{m} \quad \text{and} \quad \frac{dc_z}{dt}=\frac{F_z}{m} \tag{21}$$

which shows that the distribution function is invariant along the particle path. The next section demonstrates that moments of (20) provide the well known continuity and momentum equations for 2D shallow waters.

DERIVATION OF CONTINUITY AND MOMENTUM EQUATIONS FROM MOMENTS OF THE GENERALIZED 2D BOLTZMANN

Continuity equation

Taking the zero moment of (20) and interchanging the order of differentiation and integration gives

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$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f dc_x dc_z + \frac{\partial}{\partial x}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x f dc_x dc_z + \frac{\partial}{\partial z}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_z f dc_x dc_z + \frac{F_x}{m}\int_{-\infty}^{\infty}[f]_{-\infty}^{\infty} dc_z + \frac{F_z}{m}\int_{-\infty}^{\infty}[f]_{-\infty}^{\infty} dc_x = 0 \quad (22)$$

Invoking (17), (18) and (19), and using the fact that $[f]_{-\infty}^{\infty}=0$, (22) becomes

$$\frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x} + \frac{\partial hv}{\partial z} = 0 \quad (23)$$

which is the continuity equation for 2D shallow water flows.

Momentum equations

Taking the first moment of (20) with respect c_x and c_z, respectively, gives

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x f dc_x dc_z + \frac{\partial}{\partial x}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x{}^2 f dc_z dc_z + \frac{\partial}{\partial z}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x c_z f dc_x dc_z + \frac{F_x}{m}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x \frac{\partial f}{\partial c_x} dc_x dc_z + \frac{F_z}{m}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x \frac{\partial f}{\partial c_z} dc_x dc_z = 0 \quad (24)$$

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_z f dc_x dc_z + \frac{\partial}{\partial x}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x c_z f dc_z dc_z + \frac{\partial}{\partial z}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_z{}^2 f dc_x dc_z + \frac{F_x}{m}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x \frac{\partial f}{\partial c_x} dc_x dc_z + \frac{F_z}{m}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c_x \frac{\partial f}{\partial c_z} dc_x dc_z = 0 \quad (25)$$

Invoking (17), (18) and (19), performing manipulations similar to that in (15) and using the fact that shallow water problems are high Reynolds number (i.e. turbulent interactions dominate molecular interactions) gives

$$\frac{\partial hu}{\partial t} + \frac{\partial (hu^2 + gh^2/2)}{\partial x} + \frac{\partial huv}{\partial z} + h\frac{F_x}{m} = 0 \quad (26)$$

$$\frac{\partial vh}{\partial t} + \frac{\partial huv}{\partial x} + \frac{\partial (v^2 h + gh^2/2)}{\partial z} + h\frac{F_z}{m} = 0 \quad (27)$$

which are the 2D shallow water equations.

Both the current and previous sections formulate a Boltzmann-like equation for 1D and 2D shallow water flows and show that the statistical moments of these generalized equations provide the classical continuity and momentum in shallow waters. The following section illustrates how the generalized Boltzmann equation can be used to formulate novel computational schemes for shallow water flows.

GENERALIZED BOLTZMANN EQUATION AND COMPUTATIONAL HYDRAULICS

Traditionally, computational models for problems in hydraulics, hydrodynamics and environmental fluid mechanics have been based largely on the numerical solution of conservation laws applied to a continuum. More recently, however, numerical schemes based on the Boltzmann equation have been developed and applied to a multitude of problems including shock waves in compressible flows (e.g. Chu 1965; Reitz 1981; Xu *et al*. 1995, 1996), multicomponent and multiphase flows (e.g. Gunstenson *et al*. 1991; Xu 1997*a*; He *et al*. 1998), flows in complex geometries (e.g. Rothman 1988; Chen & Doolen 1998), turbulent flows (e.g. Chen *et al*. 1992; Martinez *et al*. 1994), low Mach number flows (Su *et al*. 1999), heat transfer and reaction diffusion flows (Qian 1993; Xu 1997*b*), open channel flows (Deng 2000; Ghidaoui *et al*. 2001) and mass transport (Deng 2000; Ghidaoui *et al*. 2001). The formulation of a Boltzmann-based numerical solution is motivated by the realization that, since the classical conservation laws are obtained from moments of the Boltzman equation, then the difference form of the classical conservation laws can also be obtained from the difference form of the Boltzmann equation. This approach allows the modeller to take advantage of the mathematical features of the Boltzmann equation. For example, while the advective operator in the Boltzmann equation is quasi-linear, its counterpart in the classical conservation

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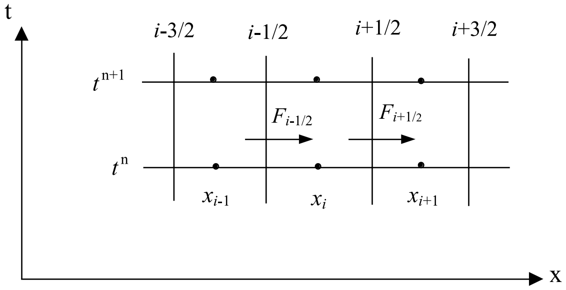

Figure 3 | Sketch of fluxes at cell interface in distance-time space.

laws is nonlinear. In addition, while the Boltzmann equation is a first-order single scalar partial differential equation, the majority of the classical conservation laws (e.g. the shallow water equations and the Navier–Stokes equations) are a system of partial differential equations of at least first order.

The formulation of numerical schemes on the basis of the Boltzmann equation is illustrated for the case of 1D shallow water problems. For clarity and ease of presentation, and without loss of generality, the formulation is carried out for a frictionless horizontal channel. A complete formulation of Boltzmann-based schemes for 1D and 2D shallow water problems with gravitational and frictional forces can be found in Deng (2000) and Ghidaoui *et al*. (2001). Consider the finite volume depicted in Figure 3. Cell i is defined by the range $[x_{i-1/2}, x_{i+1/2}]$. Therefore, $x = x_{i-1/2}$ for all i defines the interface between adjacent cells. Letting $F_x = 0$ and integrating Equations (9) in a numerical cell i from the interface $x_{i-1/2}$ to $x_{i+1/2}$, and time from t^n to t^{n+1} gives

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} (f^{n+1} - f^n) dx + \int_{t^n}^{t^{n+1}} c_x (f_{i-\frac{1}{2}} - f_{i+\frac{1}{2}}) dt = 0 \quad (28)$$

The zero and first moments in c_x of (28) are

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{-\infty}^{\infty} (f^{n+1} - f^n) \begin{bmatrix} 1 \\ c_x \end{bmatrix} dc_x dx + \int_{t^n}^{t^{n+1}} \int_{-\infty}^{\infty} c_x (f_{i-\frac{1}{2}} - f_{i+\frac{1}{2}}) \begin{bmatrix} 1 \\ c_x \end{bmatrix} dc_x dx = 0 \quad (29)$$

Applying (3) and (4) to the first term in the left hand side of (29) and rearranging gives

$$\begin{bmatrix} h \\ hu \end{bmatrix}_i^{n+1} = \begin{bmatrix} h \\ hu \end{bmatrix}_i^n - \frac{1}{\Delta x} \int_{t^n}^{t^{n+1}} \int_{-\infty}^{\infty} c_x (f_{i-\frac{1}{2}} - f_{i+\frac{1}{2}}) \begin{bmatrix} 1 \\ c_x \end{bmatrix} dc_x dt \quad (30)$$

where $\Delta x = x_{i+1/2} - x_{i-1/2}$, and $(h,hu)_i^n =$ average of (h,u) in the cell i at time n. The first term on the right side of (30) is known from the previous time step computations. The explicit integration of the second term on the right hand side of (30) in terms of previously known nodel values requires the evaluation of the distribution function at the cell interface (i.e. $f_{i-1/2}$ for all i). Using Taylor series expansion, the distribution function in either side of $x_{i-1/2}$ is as follows:

$$f(x,t,c_x) = \begin{cases} f_i^n + O(\Delta x, \Delta t) & \text{for } x_{i-3/2} \le x < x_{i-1/2}, \\ t^n \le t \le t^{n+1}, \text{ and } c_x \ge 0 & \\ f_{i+1}^n + O(\Delta x, \Delta t) & \text{for } x_{i-1/2} \le x < x_{i+1/2}, \\ t^n \le t \le t^{n+1}, \text{ and } c_x \le 0 & \end{cases} \quad (31)$$

where $O(\Delta x, \Delta t) =$ order of Δx and Δt. Equation (31) allows a jump in the distribution function across cell interfaces, thus providing the Boltzmann-based scheme with the ability to capture bores and hydraulic jumps.

A first-order approximation to the integrals in (30) is obtained from (31) as follows:

$$\int_{t^n}^{t^{n+1}} \int_{-\infty}^{\infty} c_x f_{i-\frac{1}{2}} \begin{bmatrix} 1 \\ c_x \end{bmatrix} dc_x dt = \int_{t^n}^{t^{n+1}} \int_{0}^{\infty} c_x f_i^n \begin{bmatrix} 1 \\ c_x \end{bmatrix} dc_x dt + \int_{t^n}^{t^{n+1}} \int_{-\infty}^{0} c_x f_{i+1}^n \begin{bmatrix} 1 \\ c_x \end{bmatrix} dc_x dt \quad (32)$$

Physically, the first term on the right hand side of (32) represents the contribution to the mass and momentum fluxes at the cell interface by molecules moving along the positive x direction. Similarly, the second term on the right hand side of (32) represents the contribution to the mass and momentum fluxes at the cell interface by molecules moving along the negative x direction. Therefore, while flux splitting schemes derived directly from the shallow water equations are based on wave motion, flux splitting schemes derived from the Boltzmann equation are based on particle motion. In particular, flux splitting schemes

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derived from the shallow water equations require characteristic decomposition of the advective matrix so as to delineate negative and positive waves. On the other hand, flux splitting derived from the Boltzmann equation at the cell interface is the algebraic sum of the flux associated with molecules possessing positive speeds and of the flux associated with molecules possessing negative speeds (see Equation (32)), thus avoiding characteristic decomposition of the advective matrix. Note, however, that the explicit integration (32) requires the specification of the shape of the distribution function. Ghidaoui *et al.* (2001) showed that the local equilibrium distribution function in 1D shallow water flows is Gaussian and has the following form:

$$f(x,c_x,t)=h\left(\frac{1}{\sqrt{\pi gh}}e^{-\frac{(c_x-u)^2}{gh}}\right) \tag{33}$$

It is trivial to check that insertion of (33) in (9) and taking the zero and first moment of the resulting equation leads to the shallow water equations. Therefore, (33) is used to evaluate the right hand side of (32) and the result is

$$\Delta t\begin{bmatrix}\dfrac{hu}{2}\operatorname{erfc}(-\boldsymbol{F})+\dfrac{h\sqrt{gh}}{2\pi}e^{-\boldsymbol{F}^2}\\ \dfrac{hu^2+gh^2/2}{2}\operatorname{erfc}(-\boldsymbol{F})+\dfrac{uh\sqrt{gh}}{2\pi}e^{-\boldsymbol{F}^2}\end{bmatrix}_{i-1}^{n}+\Delta t\begin{bmatrix}\dfrac{hu}{2}\operatorname{erfc}(\boldsymbol{F})-\dfrac{h\sqrt{gh}}{2\pi}e^{-\boldsymbol{F}^2}\\ \dfrac{hu^2+gh^2/2}{2}\operatorname{erfc}(\boldsymbol{F})-\dfrac{uh\sqrt{gh}}{2\pi}e^{-\boldsymbol{F}^2}\end{bmatrix}_{i}^{n} \tag{34}$$

where $\boldsymbol{F}=u/\sqrt{gh}$ = local Froude number; and erfc = complementary error function. Expression (34) provides the Boltzmann-based mass and momentum fluxes at cell interface $i-1/2$ in terms of the known values of (y,u) at nodes $(i-1, n)$ and (i,n) for all i. Therefore, inserting (34) in place of the integral terms in the right hand side of (30) gives the first-order explicit Boltzmann-based scheme for 1D shallow waters in a frictionless and horizontal channels. It must be emphasized that the final expression of the scheme does not contain the distribution function f (i.e. it involves h and u only). That is, the generalized Boltzmann equation is only used to formulate the flux given by (34). In fact, modellers can simply insert (34) in place of the integral terms on the right hand side of (30) and code the resulting scheme without any knowledge of Boltzmann theory!

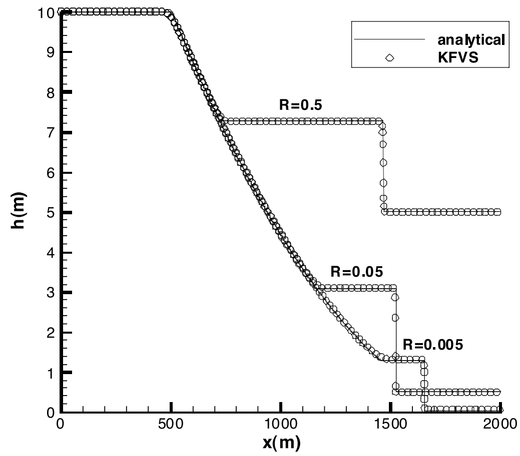

Figure 4 | Water depth profile for 1D dam break problem with different R values (Δx=1.0m, Cr=0.6, t=50s, S_f=0.0, S_0=0.0).

The accuracy and efficiency of the Boltzmann scheme in modelling discontinuous and smooth surfaces is illustrated using the classical dam break problem. In particular, consider an infinitely wide, horizontal and frictionless channel of length of 2000 m with a dam situated at its mid-length. Let R denote the ratio of the initial water depth downstream of the dam to the initial water depth upstream of the dam. The current simulation is performed at R values of 0.5, 0.05 and 0.005. In addition, the influence of Courant number on the accuracy of the scheme is examined by comparing solutions obtained with Courant numbers of 0.1, 0.6 and 0.9. The results of the test cases are shown in Figures 4 and 5. It is clear from these figures that the numerical results are very close to the analytical solution for all depth ratios and all Courant numbers. The difference between the computed and the exact solution, as measured by the L_1^n norm, is in all cases lower than 0.6%. Figure 5 shows that the shock resolution is quite insensitive to the Courant number and the shock front is spread over about $3\Delta x$. This is very little smearing considering that Nyquist's theorem states that a grid of size Δx cannot resolve a structure smaller than $2\Delta x$.

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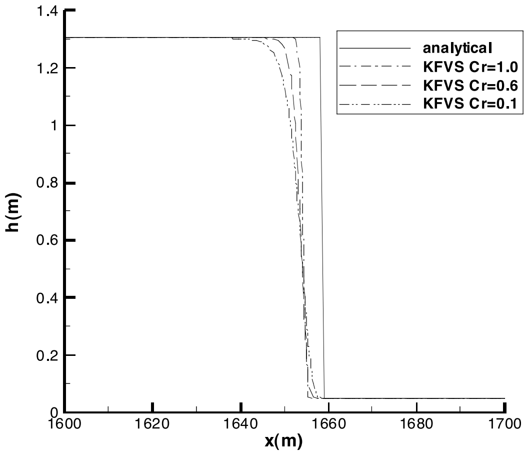

Figure 5 | Effect of *Cr* on shock resolution (Δx=1.0*m*, *t*=50*s*, S_f=0.0, S_0=0.0, *R*=0.005).

Introspection

The generalized Boltzmann equation presented in this paper describes particle motion that is consistent with mass and momentum equations for shallow waters. Admittedly, the motion of particles as described by the generalized Boltzmann equation does not represent the true motion of water particles in surface flows; instead, it represents the motion of a set of abstract (fictitious) particles whose macroscopic dynamics is consistent with the shallow water equations. In fact, the subject of this paper could have been introduced as follows. Take a fictitious set of particles whose velocity distribution function is represented by

$$f(x,c_x,c_z,t)=h\left(\frac{1}{\pi gh}e^{-\frac{(c_x-u)^2+(c_z-v)^2}{gh}}\right) \quad (35)$$

such that

$$\frac{\partial f}{\partial t}+c_x\frac{\partial f}{\partial x}+c_z\frac{\partial f}{\partial z}+\frac{F_x}{m}\frac{\partial f}{\partial c_x}+\frac{F_z}{m}\frac{\partial f}{\partial c_z}=0 \quad (36)$$

The zero and first moments of (35) and (36) are the shallow water equations. This connection between the motion of the fictitious fluid as described by (35) and (36) and the shallow water equations provides a framework for formulating schemes on the basis of (35) and (36).

CONCLUSIONS

Generalized Boltzmann equations for 1D and 2D shallow water flows are derived. It is shown that the zero and first moments of the 1D and 2D generalized Boltzmann equations provide the classical continuity and momentum equations for 1D and 2D shallow water flows, respectively. This connection between the generalized Boltzmann equation and the classical shallow water equations is used to formulate a first-order explicit finite volume Boltzmann-based model for 1D unsteady open channel flows. The splitting of the mass and momentum fluxes into their positive and negative components is determined on the basis of particle motion. Therefore, the current scheme avoids the mathematically tedious and computationally costly operation associated with the characteristic decomposition of the advective matrix.

The resulting scheme is applied to the classical dam break problem. Comparisons with analytical solutions confirm the high accuracy as well as the robustness of the Boltzmann-based scheme. All the computational results are free of spurious oscillations and unphysical shocks (i.e. expansion shocks). The stability requirement of the scheme requires that the Courant number is less or equal to 1.0. The scalar character of the generalized Boltzmann distribution function means that the current scheme is easily extended to multidimensional flows in irregular geometries.

In general, the formulation and application of generalized Boltzmann equations provides a novel way of thinking about and modelling problems in applied sciences. In addition, this approach has been successful in explaining macroscopic phenomena such as mass diffusion and viscous dissipation in terms of molecular motion. That is, the Boltzmann approach provides the explicit link between a macroscopic and mesoscopic view of nature. Last, as illustrated in this paper, the connection between the generalized Boltzmann equation and continuum mechanics provides a novel route to formulating numerical schemes in applied sciences.

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NOTATION

c_x,c_z particle velocity in x and z directions, respectively
C_r Courant number
erfc complementary error function
f nonequilibrium particle distribution function
$\boldsymbol{F}$ Froude number
F_x.F_z external forces in x and z directions, respectively
g acceleration due to gravity
h water depth
i,j integer denoting spatial cell location
J interaction function
m particle mass
n integer denoting time nodal location
p probability density function
R the ratio of the initial depth in either side of the dam
$\boldsymbol{S}_0$ slope vector of the channel
$\boldsymbol{S}_f$ friction slope vector of the channel
t,t^n time, time at $n\Delta t$
u,v macroscopic velocities of the fluid in x and z directions, respectively
Δt time step
(x,z) space coordinates
ρ density of the fluid

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