HISTORICAL REFLECTION ON THE USE OF BOLTZMANN APPROACHES FOR FLUID SYSTEM MODELING

Naser G.[1] and Karney B. W.[2]

[1] Ph.D. Candidate, University of Toronto, Toronto, Canada, gnaser@ecf.utoronto.ca
[2] Professor, University of Toronto, Toronto, Canada, karney@ecf.utoronto.ca

1. ABSTRACT

Ludwig Boltzmann, in the last quarter of the 19th century, discovered how irreversible macroscopic laws could originate from the time-reversible microscopic laws of physics. Although the logic of Boltzmann analysis is indisputable, macroscopic-based methods have traditionally been the prime approaches for solving almost all fluid-related engineering problems, and only recently have the family of Boltzmann techniques become serious contenders for such applications. Using a backdrop of traditional CFD modeling, this paper highlights and summarizes the Boltzmann-based solution techniques.

2. INTRODUCTION

One of the fascinating things about new discoveries is the relationship they bear to previous knowledge. At times true breakthroughs can startlingly revolutionize our view the world. Yet, perhaps even more often, there is a gradual accumulation of small insights or a growing awareness of inconsistencies in existing explanations, that suddenly 'snap' into a new and viable pattern. Such novel ideas, as dramatic as they first appear, are sometimes so completely assimilated that soon one can hardly imaging viewing the world in another way. In considering such changes, perhaps two mistakes are possible: the first is to discount the creative step, and thus to dismiss true inspiration as mere routine; the contrary position is to exaggerate the novelty, and thus downplay the role of progressive development. As in the classic "the glass is half empty/full" challenge, at issue here is another impossible division – in this case, Edison's divide between "inspiration" and "perspiration" in the prescription of a discovery.

Interestingly, though, the description just given need not be limited to scientific discoveries at the fringes of human knowledge. A set of shifting and evolving paradigms is in fact characteristic of all learning and growth, and thus is central to education. As we learn, we gradually distinguish simple and routine events from extraordinary ones, with the great benefit of freeing our concentration to attend to what is most new, challenging and, in many cases, most threatening. As W.H. Vanderburg (1985) argues so well in his excellent *On the Growth of Minds and Culture*, this separation of the routine from the unusual is a key part of the way our minds are linked to a dynamic world.

The connections of these insights and the current task – namely a review of Boltzmann approaches to fluid modelling – are not as obscure as they might first appear. All humans attend most to what is most unexpected and novel, and we often tire or bore quickly of what is most familiar. Thus, when a new approach is discovered, or perhaps rediscovered after having been lost for a while, one would first expect great advances, invigorated exchange, and, almost as likely, slightly over-zealous claims at "how much" is on the verge of being accomplished or discovered. Since our initial progress is always so charged with a special aura of discovery, few things are as heady as initial success;

and yet, knowing as much as we do about the true nature of reality, perhaps few things are as sobering as the conviction that, in the long run, nature will continue to surprise us and confound our well-intended attempts to uncover her secrets. Indeed, a somewhat analogous uncertainty principle appears to lie at the heart of physical reality itself. The inescapable implication is that we must both strive to enlarge our comfort zone, while at the same time maintaining a sense of humility: each new perspective we uncover is of necessity limited and incomplete, and needs a context to give it meaning.

3. SOLUTION APPROACHES TO A FLUID FLOW PROBLEM

Three complimentary viewpoints are often used to solve fluid flow problems, namely microscopic, mesoscopic and macroscopic perspectives. The specific approaches sketched in Fig. 1 (Succi, 2001), each contributes insight lacking in others, but each suffers inherent liabilities. For almost all practical purposes in applied physics, the ability to predict the behavior of the real world strongly depends on the time evolution of macroscopic quantities such as pressure, flow velocity, chemical concentration, temperature, etc. Such terms arise from averages obtained over a huge number of individual trajectories. Since average quantities are most relevant to many "real life" problems of system design and operation, it makes sense to think of mathematical formulations dealing directly with these average quantities (Succi et al, 2002). This is, in fact, the prime task of statistical mechanics. The theory of the lattice Boltzmann equation belongs to the general framework of non-equilibrium statistical mechanics.

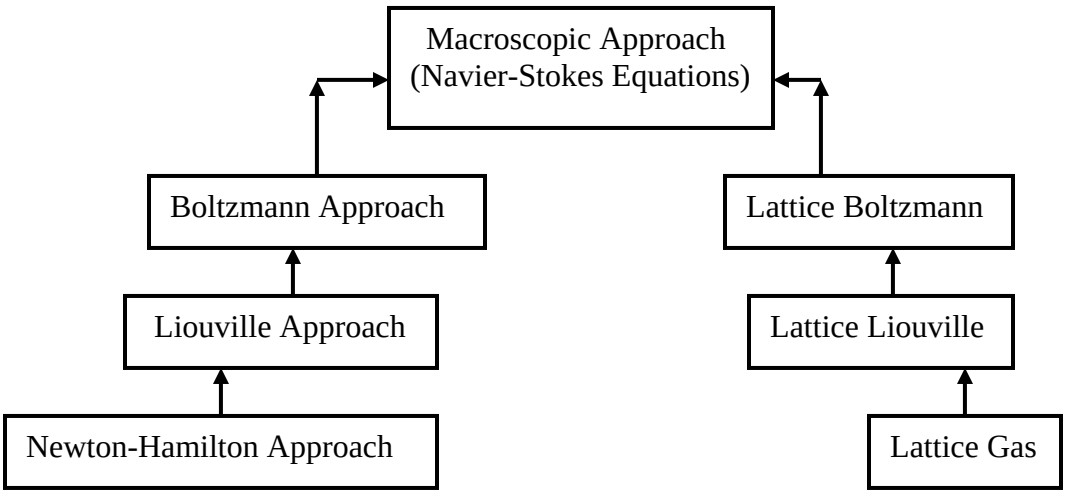

Fig. 1 – Hierarchy of solution approaches (Succi, 2001)

3.1 Newton-Hamilton Approach

The microscopic description of a macroscopic fluid flow system is based on Newtonian mechanics. The mathematical problem generated by Newtonian mechanics is to solve a set of *N* overall nonlinear ordinary differential equations (ODEs):

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = m_i \frac{d\vec{V}_i}{dt} = m_i \vec{a}_i = \vec{F}_i \qquad (1)$$

in which *N* is of the order of Avogadro's number (6×10^{23}). In the above, m_i is the mass of the i^{th} molecule, $\vec{r}_i$ its position vector, $\vec{V}_i = d\vec{r}_i / dt$ its molecule velocity vector, and

$\vec{F}_i$ the force acting upon the i^{th} molecule due to intermolecular interactions (Huang, 1987). In many ways, this component approach is a new technique, contrasting to the apparent unreality of continuum approaches, reminding that macroscopic properties arise from individual components.

To be complete, the ODE, (1), must be solved for all molecules of a substance using appropriate initial and boundary conditions. Yet, the application of Newtonian mechanics to the molecular world creates a huge computational challenge. Since the total number of molecules in a cubic centimeter of any ordinary substance is huge, accounting for the motion of individual molecules by tracing the 6*N* variables of $\vec{r}_i(t)$ and $\vec{V}_i(t)$ is an overwhelming complex scientific and numerical task. Even if it took only one second to store and resolve the conditions for only one molecule of a fluid, it would take 6×10^{23} seconds (around 2×10^{16} years) to determine the conditions for all molecules in a cubic centimeter. Even assuming that such a task was technically possible, the problem of dynamic instabilities would be overwhelming – any small uncertainty in the initial microscopic state would exponentially evolve, thereby shrinking the predictability horizon of the system virtually to zero (Succi et al, 2002). Finally, if all these difficulties are overcome, such a huge amount of information is seldom needed in real world applications.

3.2 Liouville Approach

While the Newton-Hamilton approach deals with molecular positions and velocities (Succi et al, 2002), the Liouville approach considers the so-called distribution functions $f_N\left(\vec{r}_1,\vec{V}_1,\cdots,\vec{r}_N,\vec{V}_N,t\right)$ which describe the probability of having molecule 1 at position $\vec{r}_1$ with velocity $\vec{V}_1$, and so on up to molecule *N* at position $\vec{r}_N$ with velocity $\vec{V}_N$ at time *t*. Trajectories are replaced here by the notion of phase-space fluids obeying a 6*N*-dimensional continuity equation, known as the Liouville equation (Succi et al, 2002):

$$\frac{\partial f_N}{\partial t}+\sum_{i=1}^{N}\vec{V}_i\cdot\frac{\partial f_N}{\partial \vec{r}_i}+\vec{a}_i\cdot\frac{\partial f_N}{\partial v_i}=0 \qquad (3)$$

where $\vec{a}_i=\vec{F}_i/m_i$ is the acceleration of the i^{th} molecule of mass m_i under the action of force $\vec{F}_i$. Unfortunately, however, as is obvious the Liouville equation not only does not remove the difficulties in Newtonian approach arise from the huge amount of information being handled but also, since f_N is a continuum 6*N*-dimensional field, the amount of computational information required for the Liouville approach grows exponentially. Nonetheless, the Liouville equation represents a very valuable step, not because it is mathematically solvable, but because it sets the stage for an elegant and powerful procedure that consistently eliminates irrelevant information (Succi et al, 2002). In fact, f_N can be integrated over single-particle coordinates in order to define a low-order reduced distribution function of:

$$f_M = f_{12\cdots M<N}=\int f_{12\cdots N}\,dz_{M+1}\cdots dz_N \qquad (4)$$

where $dz_k=dx_k dV_k$ and $k=M+1,\cdots N$. As Succi et al (2002) argued, the result is the following set of *M*-equations:

$$\frac{\partial f_M}{\partial t} + \sum_{i=1}^{N} \vec{V}_i \cdot \frac{\partial f_M}{\partial \vec{r}_i} + \vec{a}_i \cdot \frac{\partial f_M}{\partial \vec{V}_i} = C_M \qquad (5)$$

in which C_M represents the effects of intermolecular interactions. In the presence of a *b*-body potential, C_M involves only *b* upper-lying distributions $f_{M+1}, \cdots, f_{M+b}$. Fortunately, most interesting macroscopic observables, such as density, pressure, temperature, and energy, often depend only on one or two body distributions, so effort can be channeled into the lower levels (M = 1 and 2).

3.3 Boltzmann Approach

As quoted in Succi et al (2002), Boltzmann constructed a model in 1872 that he thought could describe the time development of a gas, whether in equilibrium or not. The Boltzmann model implied the so-called *H*-theorem, describing a quantity equal to entropy in equilibrium that must always increase with time. He showed how irreversible macroscopic laws such as 2nd law of thermodynamics could originate in time reversible laws of microscopic physics. Most macroscopic phenomena are irreversible and look quite different when run backward in time. Boltzmann argued that this irreversible behavior arises from more fundamental microscopic laws governing the behavior of the constituents of the systems obeying the irreversible laws. At first, it seemed that Boltzmann had successfully proved the 2nd law; but, then, it turned out that since molecular collisions were assumed reversible, his derivation could be run in reverse, which would then imply the opposite of the 2nd law! Later it was realized that Boltzmann's original model implicitly assumed that molecules are uncorrelated before each collision, but not afterwards, thereby introducing a fundamental asymmetry in time (Wolfram, 2002). In responding to objections concerning reversibility, Boltzmann realized (around 1876) that in a gas there are many more states that seem random than seem orderly. This realization led him to argue that entropy must be proportional to the logarithm of the number of possible states of a system, and to formulate ideas about ergodicity (Wolfram, 2002). The Boltzmann equation is expressed as (Xu et al, 1995):

$$\frac{\partial f}{\partial t} + \vec{V} \cdot \vec{\nabla} f + \vec{a} \cdot \frac{\partial f}{\partial \vec{V}} = J(f) \qquad (6)$$

where f is the non-equilibrium probability density of finding a particle with mass m at position $\vec{r}$ and at time t with velocity $\vec{V}$ and acceleration $\vec{a} = \vec{F}/m$ in which $\vec{F}$ is the net external forces acting on the particle. The left-hand side represents free motion in the phase space $(\vec{r}, \vec{V})$ and the right-hand side denotes the effects of binary collisions of particles arising from molecular interactions. The Boltzmann equation relies on the famous molecular chaos assumption:

$$f_{12}\left(\vec{r}_1, \vec{V}_1, \vec{r}_2, \vec{V}_2\right) = f_1\left(\vec{r}_1, \vec{V}_1\right) \times f_2\left(\vec{r}_2, \vec{V}_2\right) \qquad (7)$$

which considers no correlation between molecules entering a binary collision. It is precisely this arbitrary assumption that breaks time reversal symmetry; it is clear that after a collision takes place, molecules must be correlated due to the mass, momentum, and energy conservations. The essence of the molecular chaos assumption is that these post collisional correlations decay exponentially fast in time so that the probability of the two particles' colliding with each other again in a correlated state after any finite time

lapse is virtually zero (Succi et al, 2002). Breaking time-reversal symmetry allows a process to be irreversible. This is, in fact, Boltzmann's most profound contribution to statistical mechanics after his discovery of a quantitative measure of irreversibility, the celebrated *H*-theorem (Boltzmann, 1872 cited in Brush 2003):

$$H(t) = \int f\left(\vec{r},\vec{V},t\right) \times \ln\left[f\left(\vec{r},\vec{V},t\right)\right] d\vec{V} \cdot d\vec{r} \qquad (8)$$

In fact, the Boltzmann *H*-function provides a quantitative measure of irreversibility and can be directly related to the concept of entropy (i.e., entropy $S = -K_B H$).

Boltzmann showed that the H-function never increases but must always decrease or remain constant regardless of the details of the collision operator. Moreover, *H* must approach a value and remain constant thereafter. In that case, the corresponding final value of *f* is the Maxwellian distribution (Brush, 2003). Indeed, the *H*-theorem takes the role of a conceptual bridge between microscopic and macroscopic behavior of a system. Unfortunately, however, Boltzmann derived his theory without demonstrating under what conditions it has solutions (Succi et al, 2002). While leaving mathematical rigor behind, the *H* theorem is nonetheless a monumental contribution to modern science, since it showed for the first time the way to a grand unification of two fundamental and hitherto disconnected domains of science: mechanics and thermodynamics.

Modern developments reveal the practical importance of Boltzmann equation. With a shift in focus from actual particles (real atoms or molecules) to quasi particles, the Boltzmann equation became applicable well beyond the original framework (i.e., rarefied gas dynamics; Kadanoff and Baym, 1962). Today Boltzmann approaches are used in a vast variety of fields in statistical mechanics including engineering and applied physics such as neutron and radiation transport, electron transport in semiconductors, hadronic plasmas, fluid flow problems, groundwater flow, and many others.

The adequacy of Boltzmann description was quite controversial at the time and to a certain degree at least this remains so. Zermelo and Loschmidt claimed that Boltzmann description was not adequate (Goldstein, 2001). As cited in Goldstein (2001), Loschmidt argued that since the classical equations of motion are time reversible, it is possible to obtain a solution to these equations that violate the macroscopic laws by time reversing solutions that obey them. Zermelo also pointed out reasons for the existence of such anti-thermodynamic solutions showing that anti-thermodynamic behavior is just as consistent with the macroscopic laws as thermodynamic behavior.

3.4 Macroscopic or Continuum Approach

Macroscopic quantities such as fluid density (ρ), momentum (*M*), energy (*E*), and other parameters are obtained using integration of the kinetic molecular distribution function *f* over velocity space:

$$\rho(\vec{r},t) = m\int f(\vec{r},\vec{V},t)\, d\vec{V} \qquad (9\text{-a})$$

$$M(\vec{r},t) = \rho(\vec{r},t)\vec{U}(\vec{r},t) = m\int f(\vec{r},\vec{V},t)\vec{V}(\vec{r},t)\, d\vec{V} \qquad (9\text{-b})$$

$$\rho(\vec{r},t)E(\vec{r},t) = m\int f(\vec{r},\vec{V},t) \times \frac{v^2}{2}\, d\vec{V} \qquad (9\text{-c})$$

in which m is the molecular mass and $\vec{U}$ is the macroscopic velocity vector at a position $\vec{r}$ and at time t. The traditional model of fluid flows used in applied physics and engineering is based on a set of partial differential equations (PDEs) known as the Navier-Stokes equations (NSEs). These equations were originally derived in the 1840s on the basis of conservation laws and first-order approximations. Interestingly, though, they can also be derived from molecular dynamics if one assumes sufficient randomness in microscopic molecular processes. Assuming small deviations from local thermodynamic equilibrium and using (9-a, b, and c) for a small control volume of flow, the Navier-Stokes equations (continuity and momentum) of flow dynamics for a fluid with kinematic viscosity of υ at the macroscopic level are obtained as:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{U}) = 0 \qquad \text{(10-a)}$$

$$\frac{\partial \vec{U}}{\partial t} + (\vec{U} \cdot \vec{\nabla})\vec{U} = -\frac{1}{\rho}\vec{\nabla} P + \upsilon \nabla^2 \vec{U} + \vec{B}_f \qquad \text{(10-b)}$$

in which B_f represents the body forces per unit mass (typically gravity). The left side of (10-b) represents the flow acceleration and the right side is the total effective force acting on the control surfaces per unit mass of control volume. At a mathematical level, analysis of NSEs has not yet fully established the formal uniqueness and existence of solutions. Indeed, there is even some evidence that singularities might almost inevitably form, which would imply a breakdown of the equations, and perhaps a need to account for underlying molecular processes (Wolfram, 2002).

The main challenge with NSEs is that although explicit solutions are sometimes available for flows with very low Reynolds numbers and simple geometries, even in the regime of flow where regular arrays of eddies are produced, analytical methods have never yielded complete explicit solutions. In this regime, and more generally in almost all high Reynolds-number flows, however, numerical approximations are realistically the only possible approach. Indeed, it has become increasingly common to see numerical results given far into the turbulent regime, leading sometimes to the assumption that turbulence has somehow been derived from the NSEs (Wolfram, 2002). But just what such numerical results actually have to do with detailed solutions to the NSEs is not clear. One the other hand, it turns out to be be almost impossible to distinguish whatever genuine instability and apparent randomness may be implied by the NSEs from artifacts that are introduced through the discretization procedure used to numerically solve the equations. Turbulent flows at higher Reynolds numbers involve eddies with a wide range of sizes that thus require prohibitively large amounts of information to be numerically captured. In practice, therefore, semi-empirical models of turbulence tend to be used - often "eddy viscosities" or other closure approaches that have no direct relation to the NSEs.

A number of researchers (Ghidaoui et al, 2001, Chen et al, 1998, Gunstension et al, 1991, Abbott and Minns, 1998, Frisch et al, 1986, Su et al, 1999) have argued that there are considerable advantages to mesoscopic Boltzmann approach over the traditional macroscopic approaches. These include the following attributes:

1. The advective operator in the macroscopic approach (10-b) is nonlinear; whereas the corresponding term in Boltzmann approach (6) is linear, permitting superposition;

2. Since the probability distribution function of particles is scalar, the Boltzmann approach can be simply extended for a multidimensional fluid flow problem;
3. The Boltzmann approach can be easily implemented for fluid flow problems with complex boundary conditions;
4. The fact that the (6) is a linear ODE and probability distribution function of particles/molecules is scalar make the analysis of the turbulent open channel flow problems much easier, since a direct numerical simulation and large eddies is possible;
5. The solution of an incompressible fluid flow problem is much easier and do not involve the difficult solution of the Poisson equation since it is simply the limit of (6) as the Mach number approaches zero;
6. The physics of any waves and or diffusion processes are handled simultaneously with the flow equations, and there is no need for operator splitting; and finally,
7. No characteristics decomposition is required to solve the equations.

Yet the novelty and "strangeness" of the Boltzmann approach compared to traditional CFD modelling is a barrier to some, and wide adoption will depend on demonstrating not only its equivalence, but its computational and physical superiority in a range of applications. In this context, it is worthwhile introducing one more promising Boltzmann variant, the so-called lattice Boltzmann method.

3.5 Lattice Boltzmann Method

Lattice Boltzmann method (LBM) is a mesoscopic particle based approach to simulate fluid flows. It is becoming a serious alternative to traditional methods for computational fluid dynamics (Chen et al, 1998). LBM is especially well suited to simulate flows around complex geometries, and they are straightforwardly implemented on parallel machines. Historically, LBM developed from lattice gases, although it can also be derived directly from (6) (He and Luo, 1997). In lattice gases, particles "live in" or are assumed to occupy the nodes of a discrete lattice. Using a LBM, the simulation involves in a two-step procedure usually called propagation and collision phases (Rivet and Boom, 2001). Within the propagation phase, the particles jump from one lattice node to the next, according to their discrete velocity, after which the particles collide and obtain new velocities through a collision phase. The collision operator differs between many LBMs. In the BGK method, the particle distribution after propagation is gradually relaxed towards the equilibrium distribution.

4. CONCLUSION

The adequacy of Boltzmann theory has been debated and controversial since it was developed. This article briefly reviews several solution approaches applicable to fluid flow problems and highlights the advantages and disadvantages of mesoscopic and macroscopic approaches. In a more detailed discussion on the importance of the Boltzmann theory, Schrodinger (cited in Goldstein, 2001) reviewed these developments and provided that excellently conclude this review: "the spontaneous transition from order to disorder is the quintessence of Boltzmann theory...This theory really grants an understanding and does not…reason away the dissymmetry of things by means of a prior sense of direction of time…No one who has once understood Boltzmann theory will ever have recourse to such expedients…No perception in physics has ever seemed more important to me than that of Boltzmann-despite Plank and Einstein".

5. ACKNOLEGEMENT

The authors would like here to thank Prof. Mohamed Ghidaoui who read an earlier version of this paper and provided a number of constructive suggestions.

6. REFERENCES

Abbott, M. B. and Minns, A. W., (1998), *Computational Hydraulics*, Bookfield, Vt; Andershot, England: Ashgate, 556P.

Brush S. G., (2003), *The Kinetic Theory of Gases: An Anthology of Classic Papers with Historical Commentary*, Imperial College Press, UK.

Chen, S., Doolen and G. D., (1998), Lattice Boltzmann Method for Fluid Flows, *Annual Review in Fluid Mechanics*, No. 30, 329-364.

Ghidaoui, M. S., Deng, J. Q., Gray, W. G., and Xu, K., (2001), A Boltzmann Based Model for Open Channel Flows, *International Journal of Numerical Methods Fluids*, No. 35, 449-494.

Goldstein S., (2001), Boltzmann Approach to Statistical Mechanics, *arXiv:cond-mat/0105242 V. 1*.

Gunstension, A. K., Rothman, D. H., Zaleski, S., and Zanetti, G., (1991), Lattice Boltzmann Model for Immiscible Fluids, *Physics Review A*, **43**(8), 4320-4327.

Frisch, U., Hasslacher, B., and Pomeau, Y., (1986), Lattice Gas for Navier-Stokes Equations, *Physical Review Letters*, **56**(14), 1505-1508.

He, X. and Luo, L., (1997), Theory of the lattice Boltzmann method: from the Boltzmann equation to the lattice Boltzmann equation, *Phys. Rev. E* 56, 6811.

Huang, K., (1987), *Statistical Mechanics*, 2nd Edition, Wiley, New York, 512P.

Kadanoff, L. and Baym, G., (1962), *Quantum Statistical Mechanics*, Frontiers in Physics Series, Benjamin, New York.

Rivet, J. P. and Boom, J. P., (2001), *Lattice Gas Hydrodynamics*, Cambridge Nonlinear Science Series No. 11, Cambridge: Cambridge University Press.

Su, M., Xu, K., and Ghidaoui, M. S., (1999), Low Speed Flow Simulation by the Gas Kinetic Scheme, *Journal of Computational Physics*, **150**, 17-39.

Succi, S., Karlin, I. V., and Chen, H, (2002), Colloquium: Role of the H Theorem in Lattice Boltzmann Hydrodynamic Simulations, *Rev. Mod. Phys.*, **74**(4), 1203-1220.

Succi, S., (2001), *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond*, Oxford: Clarendon Press; New York: Oxford University Press, 288P.

Wolfram, S., (2002), *A New Kind of Science*, Champaign, IL, 1197P.

Xu, K., Martinelli L., and Jameson, A., (1995), A Gas Kinetic Finite Volume Methods: Flux Vector Splitting and Artificial Diffusion, *Journal of Computational Physics*, **120**, 48-65.