P.L. Bhatnagar and the BGK Model*

Phoolan Prasad
Department of Mathematics
Indian Institute of Science, Bangalore 560 012
email: prasad@math.iisc.ernet.in, Webpage: http://math.iisc.ernet.in/∼prasad/

Abstract

This lecture briefly describes life and research contributions of P.L. Bhantnagar, the founder Professor and the Head of the Department of Mathematics at IISc, which was established in 1956 as the Department of Applied Mathematics. He was a mathematician, an astrophysicist and fluid dynamicist. The BGK (Bhatnagar, Gross and Krook) model proposed in 1954 became the most important model to solve the integro-differential Boltzmann equation (proposed by Boltzmann in 1872). In BGK model, the nonlinear collision term of the Boltzmann equation is replaced by a simpler term and the model makes the derivation of the transport equations for macroscopic variables much easier. A problem, which is easily solved by the BGK model, is that of relaxation of a state of a fluid to equilibrium. During the last 20 years or so, the BGK model has found an important new application - derivation of numerical schemes, namely kinetic schemes to solve hyperbolic conservation of laws. This is an area of application, which the three authors B, G and K would not have imagined.

1 P.L. Bhatnagar: life and work

I sincerely thank the President, Prof. B.S. Passi and the secretary Dr. (Miss) Shashi Prabha Arya of the Indian Mathematical Society who asked me to give the 19th P.L. Bhatnagar Memorial Lecture. I consider it to be a great honour. P.L. Bhatnagar (PLB) was my teacher. As a topic of this lecture, I chose Bhatnagar himself, not only because Bhatnagar played a very important role in mathematics education and research in India but also because his "BGK Model" has turned out to be one of the most important tools in developing kinetic numerical schemes to solve hyperbolic system of equations - an area of application which none of the three authors : Bhatnagar, Gross and Krook, would have ever imagined.

*19th P.L. Bhatnagar Memorial Award Lecture - 2006, delivered at 72nd Annual Conference of the Indian Mathematical Society at Jabalpur, 27 - 30 December, 2007.

Prof. P. L. Bhatnagar

This lecture will be popular in nature with life and work of PLB and will include only salient features of kinetic numerical schemes developed in the last 20 years. The original paper containing the BGK model was published in 1954 and is one of the most referred research papers from a mathematician from India. An account of personal reminiscences of PLB from a large number mathematicians is available in a special volume: No. 14 of the Mathematics Teachers (India), published in 1978 by the Association of Mathematics Teachers of India. The colourful personality of PLB was described in just one sentence by Tikekar, Prasad and Ravindran (1989) as "There were only a few, who came in contact with PLB and went away unimpressed" in Biographical Memoirs of the Indian National Science Academy, from where I would take some more sentences in this article.

Prabhu Lal was born on August 8, 1912 in Kota in Rajasthan. His parents belonged to a well connected family, which had been advisors to the rulers of the princely state of Kota. His first lessons in arithmatic were from his grandfather, who enjoyed giving him problems to work mentally. Young Prabhu Lal showed promise in his studies from the very beginning since he went to school first in Kota, then the government school at Rampura and Herberter Collage, Kota. He secured first rank in the Intermediate Examination, continued doing outstanding

results securing first rank in the university examinations and supported himself and his family (his elder brother and he were married to two sisters at the same marriage ceremony) with the scholarships he received from matriculation onwards. Some of these and other details of his research are described in [3]. Let me briefly describe some salient features.

Research carrier of PLB started in 1936 as a research student at the university of Allahabad under the supervision of Prof. B.N. Prasad on summability theory but soon he joined Prof. A.C. Banerjee to work in differential equations. Two of his results (with Prof. Banerji, published in Proceeding of National Academy of Sciences, 1938) have been incorporated in the famous book of Kamke: Differential Gleichungen, Vol I. Under the inspiration of Prof. M.N. Saha (Saha, FNA, FRS, was already famous) PLB's, interest slowly shifted to astrophysics and he started working on the spiral nebula and tidal theory of planetary formation. For the best research work in the Faculty of Science, Allahabad University, during 1937-39 he won EG Hill Memorial Prize. He obtained his D.Phil degree for his thesis entitled *On the origin of the solar system.*

Soon after he completed his doctoral degree, he was invited to join the St. Stephen's Collage, Delhi, where he spent 16 years first as a lecturer and later as Head of the Department of Mathematics and concurrently as a Reader in Mathematics at Delhi University. These years could be termed as the blossoming years when Bhatnagar was in full bloom. He worked in astrophysics both independently and in collaboration with D.S. Kothari. Pulsation phenomenon had been observed only in "Supergiant Stars". Bhatnagar worked on the theory of anharmonic pulsations of Cepheids and white dwarf stars and found the pulsations lasting for 10^3 years. This work brought important international recognition - reported in Britain as "discovery of a young Indian astrophysicist". This work was quoted in S. Rosseland's book "Pulsation Theory of Variable Stars" published in 1949.

A busy schedule of over 20 hours of teaching per week at St. Stephen did not dampen Bhatnagar's enthusiasm for research. In 1947, he was awarded the D.Sc. degree from the Allahabad University. His interest in stellar structures and interiors led him to study of rarefied gases and ionized media. This was a harbinger of the monumental work he was to do a few years later - what is now known as the BGK Model.

In 1951, Bhatnagar went to Harvard University, Cambridge as a Fullbright scholar for two years. This handsome tall scholar from India was often mistaken in the University corridors for a student. Once he took his place at the lecture rostrum, the students realized that he was indeed a senior faculty. He lectured on mathematical theory of gases based on the mathematically formidable book by S. Chapman and T.G. Cowling. At Harvard, he produced two very important publications (1) a book "Stellar Interiors" jointly with D.H. Menzel and H.K. Sen, published in the International Astrophysical Series and (2) a research paper in Physical Review in 1954 which contained the famous BGK (Bhatnagar, Gross, Krook) model. The Bolzmann equation, governing the evolution of a state of molecules in gases, contains an extremely complicated integral term containing integration with respect to a vector $\mathbf{v}_*$ over R^3 and with respect to $\mathbf{n}$ over a unit hemisphere.

Faced with the reality that the Boltzmann equation was too difficult to handle due to

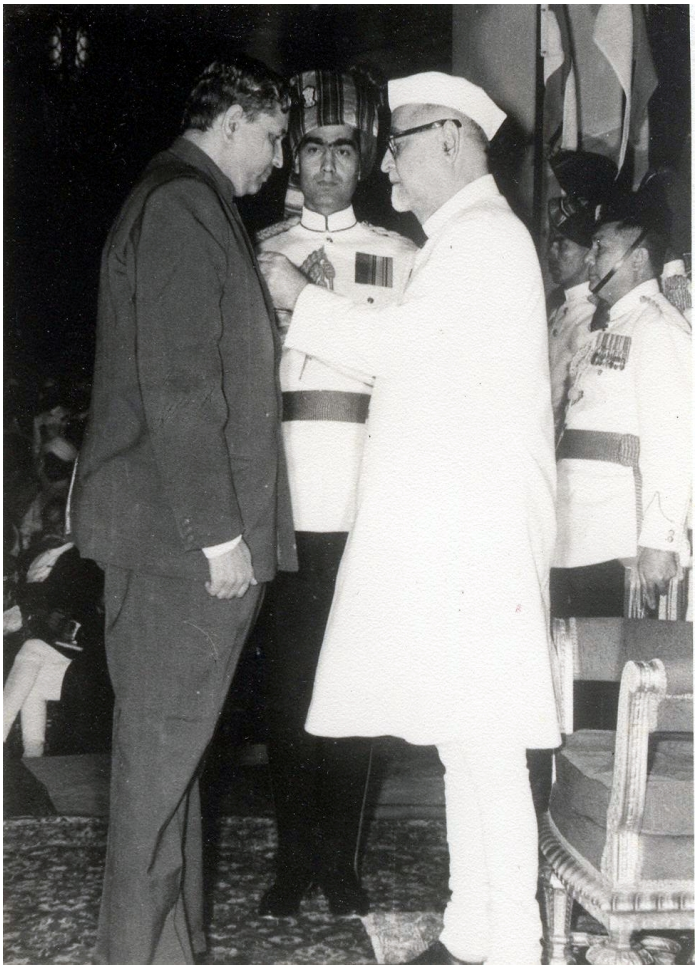
this collision integral term, Bhatnagar, Gross and Krook used their deep understanding of relaxation process of a swarm of molecules towards an equilibrium state to replace this term by a much simpler term free from the integration over a domain in the 5-dimensional half space. This gives a simple, yet a very realistic Boltzmann like equation, which has since been used as alternative to the Boltzmann equation in solving problems in rarefied gas dynamics, plasma physics and the kinetic theory itself.

So far, I have copied in this article many points from the article of Tikekar, Prasad and Ravindran and I could present here more from this article, which contains a good description of the life and work of Bhatnagar, which led to many academic and public honours to him after he returned to Delhi University, and there after joined in 1956 the Indian Institute of Science, Bangalore as the founding Professor of the Department of Applied Mathematics. After this, he was invited as vice-chancellor of the Jaipur University, Head of the Mathematics Department of the newly formed Himachal Pradesh University, Member of the Union Public Service Commission and finally as the first Director of the Mehta Research Institute (now renamed as the Harischandra Research Institute). After his wife, Anand Kumari, passed away in 1973, his personal life was far from comfortable. I would suggest the readers of this article to read for details the two references which are available on my web page.

Let me mention here a beautiful book, which PLB wrote in just six months from the reprints of recent articles on the Korteweg-de-Vries equation, which I had carried with me from IISc, Bangalore to the Mehta Research Institute during my stay at MRI in 1975-76. This book is "Nonlinear Waves in One-dimensional Dispersive Systems", published in the series "Oxford Mathematical Monograph" edited by I.G. MacDonald and R. Penrose. The importance of the book was realized by M.J. Lighthill, who had written a foreword for the book before PLB passed away and added in it later "I had written the above words before the deeply regretted and untimely death of Professor Bhatnagar on 5 October 1976, when the world of applied mathematics suddenly lost one of its most respected figures. After the shock of this great loss had subsided, I felt anxious to ensure that Professor Bhatnagar's last book would receive the wide circulation that it richly merits. I am deeply grateful to Dr. Phoolan Prasad for his excellent work as editor. Applied mathematicians owe him a great debt for helping to make this important text generally available". I would like to make a clarification in these words of Lighthill. In the editorial work of this book, three more students of PLB contributed as enthusiastically as me. They are V.G. Tikekar, Renuka Ravindran and Swarnalata Prabhu. The book received good reviews, was immediately translated into Russian and it was used as a text book in USSR. No less than V.E. Zakharov, who has contributed significantly to the development of the theory of solitons, told me "I was surprised to see the first book (a good book) on the subject from a country where no contribution to the theory of solitary wave was made".

PLB received many academic honors, which are described in the reference 3 but let me mention here two public honours. For his service to nation, he was fittingly awarded the Padma Bhushan by the President of India on January 26, 1968. After he passed away on October, 5, 1976 at Allahabad, the most important weekly magazine of India at that time, The Illustrated Weekly of India paid a tribute to his multi-colour personality through a two

page (central pages) article on him by the well known science writer Jagajit Singh.



Padma Bhushan award by the President Zakir Hussain

2 The BGK model and the kinetic scheme

I pass on now to the description of a new application of the BGK model, which picked up vigorously in mid-eighties of the last century. At the time when the biographical memoir of PLB was written for INSA, the application was not yet recognized. This application concerns development of a new numerical method, called *Kinetic or Boltzmann Scheme* to solve a hyperbolic system of conservation laws. Let me first describe the Boltamann equation and BGK model.

There are two ways to describe a fluid motion:

◇ **Kinetic theory**, in which we track the motion of the constituent molecules on a length scale of the order of the mean free path (MFP) of the molecules. In this theory, microscopic

variables: the position $\mathbf{x}$ and velocity $\mathbf{v}$ of each molecules are the quantities which are important.

$\diamond$ **Continuum theory**, in which we look at the fluid motion on length scales much larger than the MFP of molecules. At length scales which we encounter in a laboratory, the atmosphere and sea or in stellar models; the individual molecules are no longer important and the state of the fluid is described in terms of some average properties of fluid elements containing billions or much larger number of molecules. These properties are mass density $\rho(\mathbf{x}, t)$, fluid velocity $\mathbf{u}(\mathbf{x}, t)$, fluid stress (or pressure $p(\mathbf{x}, t)$) and other quantities such as internal energy density e of the fluid at a point $\mathbf{x}$ and time t.

Kinetic theory is important also in rarefied gases where the MFP becomes large, for example in outer edge of the atmosphere.

A derivation of the Boltzmann equation

In order to understand physical meaning of each of term, specially the collision integral term, in the Boltzmann equation properly, we need to go through its derivation. For this, we consider a swarm of randomly moving mono-atomic identical molecules. Such a molecule is identified by its position $\mathbf{x} \, \epsilon \, R^3$ and its velocity $\mathbf{v} \, \epsilon \, R^3$. The equations of motion of N particles is

$$\dot{\mathbf{x}}_i = \mathbf{v}_i \tag{1a}$$

$$\dot{\mathbf{v}}_i = \mathbf{X}_i \tag{1b}$$

where $i = 1, 2, ...N$ and $\mathbf{X}_i$ is the force acting on the i th particle divided by the mass of the particle. In a typical situation, a macroscopic volume (say, 1 cm^3) of a gas may contain 10^{20} molecules moving in a very irregular way. For so many molecules (of an order of $N = 10^{20}$), it is not only extremely difficult but also meaningless for any practical purpose to study the $6N$ equations (1). Hence we have to use a different strategy to define a meaningful state of the set of molecules which would give an average behaviour of the set.

Let us first note that $\mathbf{x}_i = (x_i^{(1)}, x_i^{(2)}, x_i^{(3)}), \mathbf{v}_i = (v_i^{(1)}, v_i^{(2)}, v_i^{(3)})$ and then define $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N) \, \epsilon \, R^{3N}, \mathbf{v} = (\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_N) \, \epsilon \, R^{3N}$ and $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, ..., X_N) \, \epsilon \, R^{3N}$. We can now write the $6N$ vector equations (1) into one vector equation

$$\dot{z} = \mathbf{Z}, \quad z \, \epsilon \, R^{6N}, \quad \mathbf{Z} \, \epsilon \, R^{6N} \tag{2}$$

where

$$\mathbf{z} = (\mathbf{x}, \ \mathbf{v}) \text{ and } \mathbf{Z} = (\dot{\mathbf{x}}, \dot{\mathbf{v}}) = (\mathbf{v}, \ \mathbf{X}) \tag{3}$$

The evolution of the state of N particles is described in the *phase space*, a $6N$-dimensional space of $\mathbf{z}$ which consists of a cross product of $3N$ position vectors $\mathbf{x}_i = (x_i^{(1)}, x_i^{(2)}, x_i^{(3)})$ and $3N$ velocity vectors $\mathbf{v}_i = (v_i^{(1)}, v_i^{(2)}, v_i^{(3)})$, $i = 1, 2, ..., \ N$. *Let $P_N(\mathbf{z}, t)$ be the probability density*

of the system of N-particles in the state $\mathbf{z}$ *at any time* t*, so that*

$$\int_{R^{6N}} P_N(\mathbf{z},t)d\mathbf{z} = 1, \quad t \,\epsilon\, R_+ \tag{4}$$

It is possible to show (Cercignani, 1987) that the probability density function satisfies the Liouville equation

$$\frac{\partial P_N}{\partial t} + div_z(P_N\mathbf{Z}) = 0 \tag{5}$$

where the div_z is divergence over the $6N$ dimensional space of $\mathbf{z}$. Note here that $\mathbf{x}_i$ and $\mathbf{v}_i$ are independent. Now we assume that the force $\mathbf{X}_i$ is velocity-independent so that

$$div_{\mathbf{z}}\mathbf{Z} = \sum_{i=1}^{N}\left(\frac{\partial}{\partial \mathbf{x}_i}\,.\,\mathbf{v}_i + \frac{\partial}{\partial \mathbf{v}_i}\,.\,\mathbf{X}_i\right) = 0 \tag{6}$$

where

$$\frac{\partial}{\partial \mathbf{x}_i} = \left(\frac{\partial}{\partial x_i^1}, \frac{\partial}{\partial x_i^2}, \frac{\partial}{\partial x_i^3}\right), \quad \frac{\partial}{\partial \mathbf{v}_i} = \left(\frac{\partial}{\partial v_i^1}\,, \frac{\partial}{\partial v_i^2}\,, \frac{\partial}{\partial v_i^3}\right) \tag{7}$$

Hence (5) gives the Liouville equation in the form

$$\frac{\partial P_N}{\partial t} + \sum_{i=1}^{N}\mathbf{v}_i\,.\,\frac{\partial P_N}{\partial \mathbf{x}_i} + \sum_{i=1}^{N}\mathbf{X}_i\,.\,\frac{\partial P_N}{\partial \mathbf{v}_i} = 0 \tag{8}$$

The Liouville equation is called *collisionless Boltzmann equation*. When the external force is absent i.e, the force $\mathbf{X}_i$ (on ith particle) $= 0, i = 1\,, 2\,, \ldots\,,\ N$, the equation (8) becomes

$$\frac{\partial}{\partial t}P_N(\mathbf{x}_i, \mathbf{v}_i, t) + \sum_{i=1}^{N}\mathbf{v}_i.\frac{\partial}{\partial \mathbf{x}_i}P_N(\mathbf{x}_i, \mathbf{v}_i, t) = 0 \tag{9}$$

In this Liouville equation, P_N represents the probability density of the state of all N particles in the $6N$ - dimensional space. We now consider the probability density of the state of a single particle, say the 1st particle designated by the subscript 1, which is in the state $(\mathbf{x}_1\,, \mathbf{v}_1)$ at time t. For this, we take N identical particles (and we shall later take $N \to \infty$, which we shall not mention explicitly), which are rigid spheres (we shall take the radius $a \to 0$) with elastic binary collisions. We also assume that the N particles are confined in a region of finite volume. The radius a is the effective radius, i.e. the radius of the sphere with the particle at the centre, such that the spheres about two particles can not penetrate into each other. The one - particle distribution function $P_N^{(1)}$ of the first designated particle is related to P_N by

$$P_N^{(1)}(\mathbf{x}_1, \mathbf{v}_1, t) = \int P_N \prod_{i=2}^{N} d\mathbf{x}_i d\mathbf{v}_i \tag{10}$$

If the particle 1 does not interact with any other particle, it would move in a straight path with a constant velocity (note that we have taken $\mathbf{X}_i = 0$) and it will also satisfy the Liouville

equation $\frac{\partial P_N^{(1)}}{\partial t} + \mathbf{v}_1 . \frac{\partial P_N^{(1)}}{\partial \mathbf{x}_1} = 0$. But when the number N of particles in the region is very large, the particles do collide and further, the rigid sphere assumption means that

$$P_N = 0, \quad (|\mathbf{x}_i - \mathbf{x}_j| < a \ , i \neq j) \tag{11}$$

Taking interactions in to consideration, we find that integration of the Liouville equation (9) over $R^{6(N-1)}$ with respect to $\mathbf{x}_i$ and $\mathbf{v}_i$ $(i = 2 \ , ..., \ N)$ gives not the above mentioned Liouville equation for $P_N^{(1)}(\mathbf{x}_i, \mathbf{v}_i, t)$ but the Liouville equation with an additional interaction term

$$\frac{\partial P_N^{(1)}}{\partial t} + \mathbf{v}_1 . \frac{\partial P_N^{(1)}}{\partial \mathbf{x}_1} = \text{a complicated nonlinear integral term} \tag{12}$$

Derivation of this equation is very involved and runs into many pages [4].

For a very large number of particles in a given volume ($N \to \infty$ and $a \to 0$ with a suitable relation between N and a, [4]), it is more appropriate to introduce a new *one particle expected mass density function* in phase space (or expected mass per unit volume) $f(\mathbf{x}_1, \mathbf{v}_1, t)$ instead of $P_N^{(1)}$(we now drop the subscript 1 from $\mathbf{x}_1$ and $\mathbf{v}_1$) by

$$f(\mathbf{x}, \mathbf{v}, t) = N \ m \ P_N^{(1)} \tag{13}$$

where m is the mass of one spherical particle of the effective radius a. Then

$$f(\mathbf{x}, \mathbf{v}, t) \, d\,\mathbf{x} \, d\,\mathbf{v} = \begin{cases} \text{expected mass of particles which at time } t \text{ lie in the volume between} \\ (\mathbf{x}, \mathbf{v}) \text{ and } (\mathbf{x} + \mathbf{dx}, \mathbf{v} + \mathbf{dv}) \text{ in the phase space } R^6 \end{cases}$$

The equation (12), when written in terms of f is the celebrated Boltzmann equation

$$\frac{\partial f}{\partial f} + \mathbf{v} . \frac{\partial f}{\partial \mathbf{x}} = Q(f, f) \tag{14}$$

where we note that now $\mathbf{x}$ stands for $\mathbf{x}_1$ and $\mathbf{v}$ for $\mathbf{v}_1$, and the quadratic nonlinear term is given by

$$Q(f, f) = \frac{a^2}{m} \int \{f(\mathbf{v}') f(\mathbf{v}_*') - f(\mathbf{v}) f(\mathbf{v}_*)\} \ |(\mathbf{v} - \mathbf{v}_*) . \mathbf{n}| d\mathbf{n} d\mathbf{v}_* \tag{15}$$

with a simple notation for $f(\mathbf{x}, \mathbf{v}, t)$

$$f(\mathbf{v}) = f(\mathbf{x}, \mathbf{v}, t) \tag{16}$$

and where

$$\mathbf{v}' = \mathbf{v} - \mathbf{n}\{\mathbf{n} . \ (\mathbf{v} - \mathbf{v}_*)\} \tag{17}$$

$$\mathbf{v}_*' = \mathbf{v}_* + \mathbf{n}\{\mathbf{n} . (\mathbf{v} - \mathbf{v}_*)\} \tag{18}$$

and the range of integration with respect to $\mathbf{v}_*$ is over R^3 and that with respect to $\mathbf{n}$ is on the unit hemisphere : $\mid \mathbf{n} \mid = 1 \ , (\mathbf{v} - \mathbf{v}_*) . \mathbf{n} > 0$.

The mass density function $\rho(\mathbf{x}\,t)$, an easily measurable quantity, is given by

$$\rho(\mathbf{x},t) = \int_{R^3} f(\mathbf{x},\mathbf{v},t)d\mathbf{v} \tag{19}$$

Some other important variables in macroscopic continuum model are the fluid velocity $\mathbf{u}(\mathbf{x},t)$, specific total energy e and the specific kinetic energy ε and they are given in terms of f by

$$\begin{bmatrix}\rho\mathbf{u}\\ \rho e\\ \rho\varepsilon\end{bmatrix} = \int_{R^3} f(\mathbf{x},\mathbf{v},t)\begin{bmatrix}\mathbf{v}\\ \frac{1}{2}|\mathbf{v}|^2\\ \frac{1}{2}|\mathbf{v}-\mathbf{u}|^2\end{bmatrix} d\mathbf{v} \tag{20}$$

The macroscopic variables, the gas pressure p, and gas temperature T can be expressed in terms of ρ and e. Further the total energy e is expressed as the sum of the kinetic energy and the specific internal energy ε as $e = \frac{1}{2}|\mathbf{u}|^2 + \varepsilon$. We can also express the stress tensor and heat flux in terms of appropriate moments of f.

At the microscopic level, we just need to solve the Boltzmann equation for a single variable f but at macroscopic level we need solve many equations (such as Navier-Stokes equations) of the fluid motion (which can be derived from the Boltzmann equation - we shall state the results below). The macroscopic model for 5 variables in four independent variables $(\mathbf{x},t)$ is far more simple than the microscopic model for f in seven independent variables. However, there is one application of the Boltzmann or kinetic equation, which picked up in mid-eighties of the last century, and which turns out to be at least as good as the direct use of the macroscopic equations - this application is the derivation of kinetic numerical schemes to solve the macroscopic equations. The schemes are based not on the use of the Boltzmann equation itself but on its approximate form, known as BGK (Bhatnagar - Gross - Krook) model. Before, we describe this application of the BGK model, we mention 4 theorems to highlight a few properties of the solutions of the Boltzmann equation.

Theorem 1: The states of the thermodynamics equilibrium (i.e, states, in which $\frac{\partial f}{\partial t} = 0$ and $\frac{\partial f}{\partial \mathbf{x}} = 0$, which imply $Q(f,f) = 0$) are characterized by the Maxwellian distributions

$$M(\mathbf{v}-\mathbf{u}) = A\ exp\{-\frac{|\ \mathbf{v}-\mathbf{u}\ |^2}{\beta}\} \tag{21}$$

where $A\ \epsilon\ R_+$, $\mathbf{u}\ \epsilon\ R^3$, $\beta\ \epsilon\ R_+$ are arbitrary parameters.

Note 1: When $f(\mathbf{x},\mathbf{v},\ t)\ = M(\mathbf{v}-\mathbf{u})$ given by (21), then the parameter $\mathbf{u}$ in it is indeed the macroscopic velocity defined by (20) and A and β are given in terms of $\rho(\mathbf{x},t)$ and appropriately defined temperature $T(\mathbf{x},t)$ (from (19) and (20)) as

$$A = \{2\pi RT(\mathbf{x},t)\}^{-3/2}\rho(\mathbf{x},t)\ ,\quad \beta = 2RT(\mathbf{x},t) \tag{22}$$

and R is the Boltzmann constant of the gas.

Note 2: The argument $(\mathbf{x},t)$ in $\mathbf{u}$, ρ and T appear for the state on macro scale in local

thermodynamic equilibrium at $(\mathbf{x}, t)$. On microscale $\frac{\partial M}{\partial t} = 0$ and $\frac{\partial M}{\partial x} = 0$. The fluid in motion is in local thermodynamic equilibrium at $(\mathbf{x}\ , t)$.

Definition: For any distribution function $f(\mathbf{x}, \mathbf{v}, t)$, we define

$$H(f) = \int_{R^3} f\ log\ f\ d\ \mathbf{v} \tag{23}$$

When f is a Maxwellian $M(\mathbf{v}-\mathbf{u})$, the function H is closely related to the thermodynamic entropy. To see deep meaning to this statement, for any f, we define for a region $D\ \epsilon\ R^3$, filled with a gas, a function $\mathcal{H}$

$$\mathcal{H} = \int_D H(f) d\ \mathbf{x} \tag{24}$$

and state a theorem

Theorem 2 : Boltzmann's H-theorem. When f evolves according to the Boltzmann equation, then for a nonporus and nonconducting wall ∂D , we have

$$\frac{d\ \mathcal{H}}{d\ t} \leq 0 \tag{25}$$

and $\mathcal{H}$ is constant when f is Maxwellian $M(\mathbf{v} - \mathbf{u})$.

Note: The Boltzmann equation describes the evolution ("relaxation") towards a state of minimum $\mathcal{H}$. The final state is a steady state and thus a Maxwellian having the maximum entropy.

For a mathematical description of a gas in motion at a macroscopic level it is assumed that the gas is in local equilibrium in microscopic level at any $(\mathbf{x}, t)$.

Given any microscopic state f, (20) gives a macroscopic state $(\rho, \mathbf{u}, e$ or $p)$ of fluid in motion. But when f is locally Maxwellian at $(\mathbf{x}, t)$ given by (21) and (22), then we get a very important type of motion stated in the following theorem

Theorem 3: For $f =$ Maxwellian M, the macroscopic variables mass: density ρ, fluid velocity $\mathbf{u}$ and the gas pressure p; satisfy the Euler equations of motion

$$\rho_t + < \nabla, \rho\mathbf{u} >= 0 \tag{26}$$

$$(\rho u_i)_t + < \nabla, \rho\mathbf{u}u_i > + \nabla p = 0,\ i = 1, 2, 3 \tag{27}$$

$$(\rho e)_t + < \nabla, (\rho e + p)\mathbf{u} >= 0 \tag{28}$$

where we note that the total energy e is expressible in terms of $|\mathbf{u}|^2$ and the kinetic energy ε (see the equations in (20) and the note below it).

When $f =$ Maxwellian, each fluid element has relaxed locally to equilibrium with a constant velocity $\mathbf{u}$. In this case, the dissipative processes like viscosity and heat conduction cease to

exist. However, when f deviates from the Maxwellian distribution, it is possible to derive the macroscopic equations, in which additional viscous and heat conduction terms appear. These are also well known equations in fluid mechanics and I do not write them here.

The BGK Model This model describes the evolution of $f(\mathbf{x}, \mathbf{v}, t)$ through the equation

$$\frac{\partial f}{\partial t} + \mathbf{v}.\frac{\partial f}{\partial \mathbf{x}} = \frac{M(\mathbf{v}) - f}{\nu} \equiv J(f) \tag{29}$$

where $M(\mathbf{v})$ is the local Maxwellian given by (21) and (22) and ν is a small positive number. We have written here simply $\mathbf{v}$ for $\mathbf{v} - \mathbf{u}$.

The BGK collision term $J(f)$ is so chosen that the conditions (31) and (32) below are satisfied. We first note that the Boltzmann collision term $Q(f, f)$ satisfies an important relation

$$\int_{R^3} Q(f, f) \begin{bmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{bmatrix} d\mathbf{v} = \mathbf{0}, \text{ for} f \geq 0 \tag{30}$$

which forms the basis of the theories mentioned earlier and many other results related to solutions of the Boltzmann equation. Hence solutions of any model equation, approximating the Boltzmann equation must satisfy (30) i.e.,

$$\int_{R^3} J(f) \begin{bmatrix} 1 \\ \mathbf{v} \\ |\mathbf{v}|^2 \end{bmatrix} d\mathbf{v} = \mathbf{0}, \text{ for} f \geq 0 \tag{31}$$

and

$$\int_{R^3} (\log\, f)\; J(f)\; d\mathbf{v} \leq 0 \tag{32}$$

with equality if and only if f is Maxwellian. The simple BGK model contains the most basic features of the Boltzmann collision integral and has been extensively used in various applications since it was proposed in 1954.

The kinetic numerical scheme of Euler equations (23) - (25) is derived using the BGK model (26). The development of numerical schemes based on kinetic theory for compressible flow started in 1960s (see Xu (1998)for details). Sanders and Prendergast were one of the first to propose in 1974 a Kinetic Scheme, known as Beam scheme. The Kinetic Flux Vector Scheme is originally due to Pullin (1980), which was presented in a different way by Deshpande (1986). It looks mysterious that a discretization of the equation (14) for the motion of N molecules (say, $N = 10^{20}$) could be used efficiently to solve numerically equations valid on a macroscale. It is this unusual relatively recent approach and the mystery associated with it that prompted me to include a discussion (though very briefly) on it in a write up on BGK model. We shall see here that we need not trace each molecule individually. We describe the method in 2 steps.

Step 1 : Note that, given a local macrostate i.e. $\rho, \mathbf{u}, p$ (or T) at $(\mathbf{x}, t_n)$, we can use (21) to construct the Maxwellian

$$M(\mathbf{x}, \mathbf{v} - \mathbf{u}, t_n) = f_n(\mathbf{x}, \mathbf{v}), \quad \text{say} \tag{33}$$

at time $t_n = n\triangle t$, where $\triangle t$ is the time step used in numerical integration.

Step 2 : Then we set up an initial value problem to solve the BGK model equations (29) for $t > t_n$ with initial data at $t = t_n$

$$f(\mathbf{x}, \mathbf{v}, t = t_n) = f_n(\mathbf{x}, \mathbf{v}) \tag{34}$$

This step is hard. When ν is very small so that the relaxation to equilibrium takes place at a microscale, at each $(\mathbf{x}, t)$ at a macroscale in space and time, the fluid is in equilibrium. We approximate this evolution process of fluid motion on a macrostep $\triangle t = t_{n+1} - t_n$ in time, in two substeps by splitting the kinetic equation

$$f_t + < \mathbf{v}, \nabla_{\mathbf{x}} > f = J(f) \tag{35}$$

into a collisionless evolution transport equation

Step 2a

$$f_t + < \mathbf{v}, \nabla_{\mathbf{x}} > f = 0 \tag{36}$$

during the time interval $(t_n, t_{n+1}]$ and a relaxation to thermodynamic equilibrium

Step 2b

$$J(f) = 0 \tag{37}$$

at the end of this time interval i.e. at time $t = t_{n+1}$.

Therefore, in the **Step 2a**, we solve (36) in the interval $(t_n, t_{n+1}]$ with initial data (34). From $f(\mathbf{x}, \mathbf{v}, t)$ so obtained we calculate $\rho(\mathbf{x}, t), \mathbf{u}(\mathbf{x}, t), p(\mathbf{x}, t)$ in $(t_n, t_{n+1}]$ from (19) and (20). In the **Step 2b**, we set the value of $f(\mathbf{x}, \mathbf{v}, t)$ at $t = t_n$ to be the Maxwellian corresponding the macrostate $\rho(\mathbf{x}, t_{n+1})$, $\mathbf{u}(\mathbf{x}, t_{n+1})$, $p(\mathbf{x}, t_{n+1})$ obtained from step 2a. Now we denote this Maxwellian by $f_{n+1}(\mathbf{x}, \mathbf{v})$, which forms the initial data

$$f(\mathbf{x}, \mathbf{v}, t = t_{n+1}) = f_n(\mathbf{x}, \mathbf{v}) \tag{38}$$

and then we repeat the whole process again for the time interval $(t_{n+1},\ t_{n+2}]$. These calculations are done numerically i.e. not for $\mathbf{x}\ \epsilon\ R^3$ but at a discrete set of points on macroscale in R^3. Thus, we achieve a numerical method of solution of Euler equations. Note that the mystery "how to follow the evolution of states on the macroscale state by numerically solving microscale BGK equation or a kinetic equation?" no longer remains mysterious since integration with respect to $\mathbf{v}$ in (19) and (20) gives the macrostate at macroscale grid points in $(\mathbf{x}, t)\ \epsilon\ R^3 \times R_+$.

This article does not have the scope of going into more details of the kinetic numerical schemes obtained in the manner described above. We just summarize the above procedure briefly. Problem is to solve numerically the Euler equations (26) - (28) with initial data

$$\rho(\mathbf{x}, 0) = \rho_0(x),\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(x) \text{ and } p(\mathbf{x}, 0) = p_0(x) \tag{39}$$

Step 1 (for $n = 0$). Given (39), we construct the local Maxwellian $M_0(\mathbf{x}, \mathbf{v} - \mathbf{u}_0, t = 0)$ from (21) and set

$$f(\mathbf{x}, \mathbf{v}, 0) \equiv f_0(\mathbf{x}, \mathbf{v}) = M_0(\mathbf{x}, \mathbf{v} - \mathbf{u}_0, 0) \tag{40}$$

Step 2a (for $n = 0$). Solve the linear transport equation (36) with (40). The solution is

$$f(\mathbf{x}, \mathbf{v}, t) = f_0(\mathbf{x} - \mathbf{v}t, \mathbf{v}), \quad t \, \epsilon \, (0, \Delta t] \tag{41}$$

Step 2b (for $n = 0$). On $t \, \epsilon \, (0, \Delta t]$, get $\rho, \mathbf{u}, p$ (or e) from (19) and (20) with f given by (41)

Step 3 (for $n = 0$) or **Step 1** (for $n = 1$). From the values of $\rho, \mathbf{u}$ and p in **Step 2b**, get the initial values $\rho_1, \mathbf{u}_1$ and p_1 at $t = \Delta t$ and construct the local Maxwellian $M_1(\mathbf{x}, \mathbf{u} - \mathbf{u}_1, t = \Delta t)$ and set

$$f(\mathbf{x}, \mathbf{v}, \Delta t) \equiv f_1(\mathbf{x}, \mathbf{v}) = M_1(\mathbf{x}, \mathbf{v} - \mathbf{u}_1, t = \Delta t) \tag{42}$$

Now repeat above the process with $n = 1, \ n = 2, ...$ and get the values of $\rho, \mathbf{u}$ and p for all $t > 0$. We can now prove a theorem (see Godlewski and Raviart, 1996).

Theorem 4: If we start with exact values at t_n, the quantities ρ, u and p (or e), obtained at t_{n+1} after the $(n + 1)$th time step, are first order approximations in Δt of the solution of the initial value problem for Euler equations.

We have described only the time discretization of the kinetic scheme for Euler equations. But this is the basic step. In order to describe a kinetic scheme fully, we must discuss a space discretization, which though complex does not hold much mystery. The details of kinetic schemes are available in many books and articles, for example the book of Godlewski and Raviart.

Reference

1. Bhatnagar, P.L., Gross, E.P and Krook, M., A model for collisional processes in gases I: small amplitude processes in charged and in nutral one-component systems, Phys. Rev. **94**, 1954, 511-525.

2. Phoolan Prasad, A few glimpes of Prof. P.L. Bhatnagar, Mathematics Teachers (India), **14** , 1978, 82-85.

3. Tikekar, V.G., Phoolan Prasad and Renuka Ravindranm, 1989, Prabhu Lal Bhatnagar biographical Memoris-INSA,**14** 116-134.
   Above two articles are avilable at the web page - http://math.iisc.ernet.in/∼prasad/

4. Cercignani, C., The Boltzmann Equation and its Applications, 1987, Springer-Verlag, Heidelberg

5. Godlewski, E and Raviart, P-R, Numerical Approximation of Hyperbolic System of Conservation Laws, 1996, Springer-Verlag, New York.

6. Pullin, D., Direct simulation methods for compressible inviscied ideal gas flow, J. Computational Physics, **34** 1980, 555-574.

7. Deshpande, S.M., A second order accurate kinetic-theory-based method for inviscied compressible flow, NASA Technical paper, 2613, 1986 kinetic theory based new upwind methods for inviscid compressible flows, AIAA 86-0275, 24 Aerospace Sciences Meeting, Reno, 1986

8. Xu, Kun, Gas-Kinetic Schemes for unsteady compressible Flow simulations, von Karman Institute for Fluid Dynamics - Lecture Series: Computational Fluid Dynamics, 1998.