

Coupled Solution of Boltzmann Transport Equation Maxwell's and Navier Stokes equations

Rajveer S. Yaduvanshi, Harish Parthasarathy
AIT Delhi, India

Abstract

Investigations on coupled solution for electromagnetic wave transport taking Boltzmann transport equation integrated with Maxwell's equation and Navier Stokes have been formulated and simulated for solutions. We have proposed this solution with iterative approach in finite difference numerical method. We have evaluated V and A are electric and magnetic potentials, E and B are electric and magnetic, ρ and J are charge density and current density respectively.

1. Introduction

Evolution of distribution function is governed with BTE. It means information about flow of gas can be known by solving BTE with proper initial and boundary conditions [1-5]. One could describe a gas flow in classical physics by giving position and velocity of all molecules at any instant of time. BTE can be used to study the non-equilibrium behaviour of a collection of particles i.e. transport parameters. In a state of equilibrium a gas of particles has uniform composition with constant temperature and density. If the gas is subjected to a temperature difference or disturbed by externally applied electric, magnetic, or mechanical forces, it will be set in motion and the temperature, density, and composition may become functions of position and time, in other words, the gas moves out of equilibrium [6-9]. The Boltzmann Equation applies to a quantity known as the distribution function, which describes this non-equilibrium state mathematically and specifies how quickly and in what manner the state of the gas changes when the disturbing forces are varied. The distribution function carries information about the positions and velocities of the particles at any time [10-13].

This would require computing of six parameters (three position and three velocity coordinates) per particle as function of time. This approach is not feasible in practical as number of molecules in gas flow is extremely large. A statistical approach can be taken instead of defining position and velocity of each molecule [14-17]. Using the construct of ensemble, a large number of independent systems evolving independently but under same dynamics can be characterized by density function, which gives out the probability that an ensemble member can be found in some elemental volume in phase space [1]. Here distribution function is function of 7 variables (three physical spaces, three volume space and one time) and it provides complete description of the state of gas.

This method can be used to find probabilities for use in an iterative scheme which iterates to find collision rates in cells. 3D iterative solution using finite difference method, for this problem is formulated and simulations for getting transport parameters have been proposed [18]. The method is based on an exact expansion of the distribution function (solution of the BTE).

This paper is divided into five main sections. Introductory part is placed in section one. Formulations developed are placed at section two.

2. Transport Model and BTE formulations

Let the probable number of particles N at the time t within the spatial element $dx dy dz$ located at (x, y, z) and with velocities in the element $dv_x dv_y dv_z$ at the point (v_x, v_y, v_z) [4-8].

The Boltzmann equation in the relaxation-time approximation [5] is given by, where $f(x, v, t)$ is the particle distribution function, t is the time, x is the spatial coordinate, v is the particle velocity, F is the external force field per unit mass and τ is the relaxation time.

BTE under Steady State Conditions

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{F}{m} \frac{\partial f}{\partial v} = 0 \quad (1)$$

BTE under Equilibrium conditions [2]

$$f(\vec{x}, \vec{v}, t) \left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla_{\vec{x}} + \frac{F}{m} \Delta_{\vec{v}} \right) = 0 \quad (2)$$

3 D representation of BTE under RTA

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{F}{m} \frac{\partial f}{\partial v} = -\frac{f-f_c}{\tau} \quad (3)$$

BTE when collision term is accounted for

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} + \frac{F}{m} \frac{\partial f}{\partial v} = \left(\frac{\partial f}{\partial t} \right) coll \quad (4)$$

The equations mention from (15-21) are very important to realize coupled solution of Boltzmann Transport Equation with Maxwell's equation. The solution of BTE is distribution function which is represented in the results obtained in figures. 1-4, f is the PDF, which is a function of position and velocity of particles and the time variables. The PDF changes or 'evolves' over time according to the above given equation and computes possible convergences, due to the presence of initial velocity, which ultimately affects the mean position of the particle. The affect of external force which might produce

acceleration of the particles can be considered .The initial PDF of the system is considered to be Gaussian, both w.r.t to position x and velocity v. The PDF evolves with time according to BTE. The results of the evolution are presented in a position-velocity mu space at different times using MATLAB. The output is the PDF w. r .t position and velocity, represented in a so-called mu space. Equations 1-17 presents the formulation based on the subject. Figures1-4 presents PDF simulation results.

$$\frac{df}{dx}(x, Vx, t) + Vx \frac{df}{dx} + \frac{fx}{m} \frac{df}{dVx} = 0$$

$$\frac{df}{dx}(x, Vx, t) + Vx \frac{df}{dx} + \frac{e.Eo}{m} \frac{df}{dVx} = 0$$

Now for six space dimensions seven variables are considered. Discretization steps are as follows:

$$\begin{aligned} & \frac{df}{dx}(x, y, z, Vx, Vy, Vz, t) + Vx \frac{df}{dx} + Vy \frac{df}{dy} + Vz \frac{df}{dz} \\ & + \frac{e}{m} (Ex + Vy Bz - Vz By) \frac{df}{dVx} + \frac{e}{m} (Ey + Vx Bx - Vx Bz) \frac{df}{dVy} \\ & + \frac{e}{m} (Ez + Vx By - Vy Bx) \frac{df}{dVz} = 0 \end{aligned} \quad (5)$$

$$\text{Hence } \frac{df}{dx}(x, Vx, t) + Vx \frac{df}{dx} + \frac{e.Eo}{m} \frac{df}{dVx} = 0 \quad (6)$$

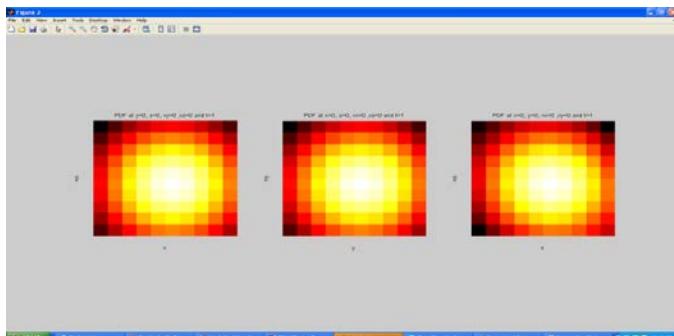


Figure 1. 3D simulation of BTE

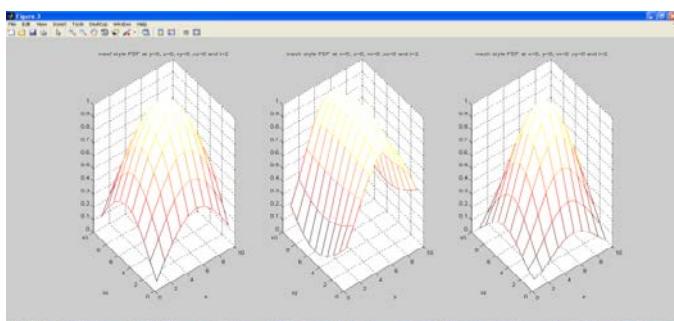


Figure 2. 3D simulation of BTE

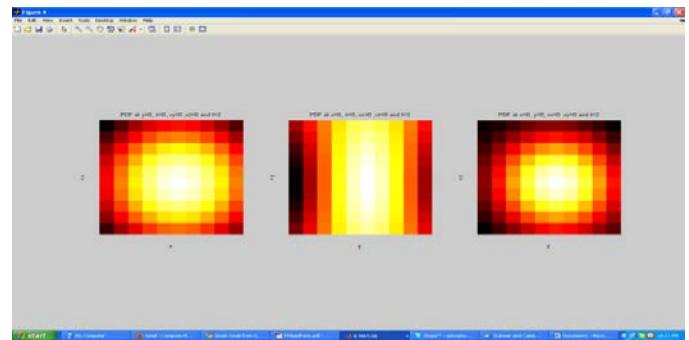


Figure 3.3D simulation of BTE

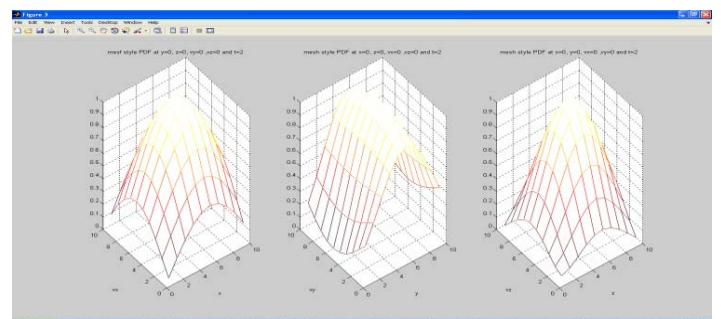


Figure 4. Simulation of BTE in different formats

3. Collision Integral

The distribution function is defined as an expected number of molecules in volume in physical space and in velocity space, distribution function of seven variables (three in physical space and three in velocity space and one in time) which determines elemental volume of phase space. For dilute gas f (distribution function) provides a complete description of the state of the gas .Evolution of distribution function is governed by BTE [6]. Hence information about flow can be obtained by solving BTE with appropriate initial and boundary conditions.PDF Describing position and velocity of molecules by statistical approach by using construct by ensemble approach, we can define macroscopic[7] quantities on interest, an average over all ensemble members . The ensemble is characterized by density function which gives probability that an ensemble member can be found in some elemental volume in phase space. We have taken two particles for considering collision term.

$$\frac{df}{dt} + V \frac{df}{dx} + \frac{f}{m} \frac{df}{dv} = \int \int \int \Omega (f' f_1 - f f_1) v \sigma d^2 \Omega d^3 v \quad (7)$$

Where t= time, v= molecular velocity,v1= Pre Collision
v'=post collision velocity

$V'1$ =post collision velocity, F = external force m = mass of the molecule , $f_1=f(x, v_1, t)$ here prime values represents post collision conditions, Due to conservation $V=v - v_1, V=|V'|, \Omega$ Solid angle is deflection angle of relative velocity V' , σ collision cross section will depend on potential , scattering and velocity of particles. Collision cross section is defined by probability that a collision between two molecules will result in a given pair of post collision velocities .The integration over velocity v_1 from $-\infty$ to ∞ in all dimensions while integrating over Ω extends over unit sphere.

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int v_1 \int \Omega (f' f'_1 - f f_1) v \sigma d^2 \Omega d^3 v \quad (8)$$

The term $\int v_1 \int \Omega (f' f'_1 - f f_1) v \sigma d^2 \Omega d^3 v$ represents net rate at which molecular enter the point of interest in phase space due to collision and $\int v_1 \int \Omega (f' f'_1 - f f_1) v \sigma d^2 \Omega d^3 v$ represents the net rate at which molecules are scattered out. Both terms are integrated over all possible pre collision velocity and all possible collision angles. Manifestations of quantum mechanical scattering, chemical reaction dynamics. Molecules makes very important partner compared to atoms. Measurement of relevant parameters of collision has been topics of research. Molecules maybe excited, dissociated or ionized in collision. Application of molecule collision can be applied to know propagation parameters in upper atmosphere. also low temperature plasma processing of material , semiconductor wafer design reactor design .Quantum mechanical[21] scattering is useful to interpret ,predict results of collision .Electron collision probability for various gases can provide transport and reaction in fields such as atmospheric physics and plasma reactor design. Collision probabilities are conventionally expressed as effective areas or cross sections. The cross section depends on the following:

- (a) Size of target
- (b) Collision energy
- (c) Identity of projectile
- (d) Direction of scattering
- (e) Energy transfer

Variational principle for the scattering amplitude whose square modulus gives cross section or probability. Scattering amplitude will provide collision integral and can be evaluated based on Lipmann Schwinger theory. Cross section calculation for larger molecules may require on the order of 10^{13} floating point operations, need s high performance computers for solutions.

As we know

$$\begin{aligned} F_x &= -e. Ex - e. Vy .Bz \\ F_y &= - e. Ey + e. Vx. Bz \\ F_z &= - e .Ez \end{aligned}$$

$$\begin{aligned} \frac{df}{dt} (x, y, z, \mathbf{V}_x, \mathbf{V}_y, \mathbf{V}_z, t) &+ Vx. \frac{df}{dx} + Vy. \frac{df}{dy} + Vz. \frac{df}{dz} + \frac{fx}{m} \cdot \frac{df}{dvx} + \\ \frac{Fy}{m} \cdot \frac{df}{dvy} + \frac{Fz}{m} \cdot \frac{df}{dvz} &= \left(\frac{df}{dt}\right)_{\text{coll}} \\ \text{Also } \frac{df}{dt} (x, y, z, \mathbf{V}_x, \mathbf{V}_y, \mathbf{V}_z, t) &+ vx. \frac{df}{dx} + vy. \frac{df}{dy} + vz. \frac{df}{dz} - \\ \frac{e}{m} (Ex + Vy. Bz) \frac{df}{dvx} - \frac{e}{m} (Ey - Vx. Bz) \frac{df}{dvy} - \frac{e}{m} (Ez) \frac{df}{dvz} &= \left(\frac{df}{dt}\right)_{\text{coll}} \\ \left(\frac{df}{dt}\right)_{\text{coll}} &= \int f(\vec{r}, \vec{v}'_1, t) f((\vec{r}, \vec{v}'_2, t) d^3 v_1' d^3 v_2' \\ &= \int f(\vec{r}, v_1, t) f((\vec{r}, v_2, t) d^3 v_1 d^3 v_2 \end{aligned}$$

$$\begin{aligned} \text{Also due to conservation } |\vec{v}_1|^2 + |\vec{v}_2|^2 &= |\vec{v}'_1|^2 + |\vec{v}'_2|^2 \\ \vec{v}_1 + \vec{v}_2 &= \vec{v}'_1 + \vec{v}'_2 \\ \sum f(r, v, t) d^3 v. d^3 r &= f(r, v, t) d^3 v. d^3 r \\ f(r, v, t) d^3 V. d^3 r &= N \end{aligned}$$

Where N is number of molecules

$f(r, v, t)$ is distribution function

$$\int f(r, v, t) = \frac{N}{V}$$

Incident flux $I = N |v_1 - v_2|$

$v_1, v_2, \theta, v'_1, v'_2$ are five variable for defining collision integral and Scattering angleis θ .

$$\begin{aligned} \text{Magnitude of relative velocity vector } g &= |\vec{v}_1 - \vec{v}_2| \\ \text{Hence } f(\vec{r}, \vec{v}'_1, (\vec{v}_1, \vec{v}_2, \theta)) . f(\vec{r}, \vec{v}'_2, (\vec{v}_1, \vec{v}_2, \theta)) - \\ f(\vec{r}, \vec{v}_1, t) f((\vec{r}, \vec{v}_2, t)) d^3 v_2 d \Omega &= (9) \end{aligned}$$

The distribution function F is defined as $\int d^3 x d^3 v$ is expected number of molecules in volume $d^3 x$ in physical space and $d^3 v$ in velocity space, distribution function of 7 variables (three in physical space and three in velocity space and one in time) which determines elemental volume of phase space . For dilute gas f (distribution function) provides a complete description of the state of the gas. Evolution of distribution function is governed by BTE [6]. Hence information about flow can be obtained by solving BTE with appropriate initial and boundary conditions.PDF Describing position and velocity of molecules by statistical approach by using construct by ensemble approach, we can define macroscopic[7-11] quantities on interest, an average over all ensemble members . The ensemble is characterized by density function which gives probability that an ensemble member can be found in some elemental volume in phase space. We have taken two particles for considering collision term.

$$\begin{aligned} \frac{df}{dt} + v \frac{df}{dx} + \frac{f}{m} \frac{df}{dv} &= \\ \int \int v \int \Omega (f' f'_1 - f f_1) v \sigma d^2 \Omega d^3 v &= (10) \end{aligned}$$

Where t = time , v = molecular velocity, v_1 = Pre Collision

$V'1$ =post collision velocity

F = external force, m = mass of the molecule

$f_1 = f(x, v_1, t)$, $f'_1 = f(x, v_1, t)$ here prime values represents post collision conditions due to conservation $V=v - v_1, V = |V|=|V'|$, Ω Solid angle is deflection angle of relative velocity V' , σ collision cross section will depend on potential , scattering and velocity of particles.

Collision cross section is defined by probability that a collision between two molecules will result in a given pair of post collision velocities. The integration over velocity v_1 from $-\infty$ to ∞ in all dimensions while integrating over Ω extends over unit sphere.

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int v_1 \int \Omega (f' f'_1 - f f_1) v \sigma d^2 \Omega d^3 v \quad (11)$$

Collision integral is five dimensional integral that must be evaluated for every point in physical space, every point in time and every point velocity space. Collision cross section σ will depend on intermolecular potential and pre and post collision velocities and scattering angle Ω [17-19] , though it is constant for hard sphere molecules.

The term $\int v_1 \int \Omega (f' f'_1 - f f_1) v \sigma d^2 \Omega d^3 v$ represents net rate at which molecular enter the point of interest in phase space due to collision and $\int v_1 \int \Omega (f' f'_1 - f f_1) v \sigma d^2 \Omega d^3 v$ represents the net rate at which molecules are scattered out . Both terms are integrated over all possible pre collision velocity and all possible collision angles.

Solving Boltzmann transport equation governing drift and diffusion of the particles rate of the arrival, time, spectrum etc can be predicted .Ionic flux density is given by Flick's law. Study of collision between electrons. Collision kernels can be useful tool for carrying simulations. Relaxation time approximation (RTA) is simplification to BTE Integral .We can determine friction and diffusion coefficients that that are due to collisions. Here friction term represents drag or slow down of particles due to collision and diffusion term producing a spreading of distribution function.

$$f_i(t, \vec{r}, \vec{v}) \text{ where } i = 1, 2, 3, 4, \dots, N$$

m_i = Mass, e_i = Charge

Distribution function and derivation of collision integral of multi species taking non reactive pairs into consideration has been worked and can be written as follows:

$$\frac{\partial f_i}{\partial t} + (v, \nabla_r) f_i + \frac{e_i}{m_i} (\mathbf{E} + \vec{V} \vec{B}) \nabla_v \cdot f_i = \sum_{j=1}^N I_{ij} \quad (12)$$

i species colliding with j species and evaluating collision integral as below:

$$I_{ij} = \sum_j \int (-f_i(t, \vec{r}, \vec{v}) \cdot f_j(t, \vec{r}, \vec{v}) + f_i(t, \vec{r}, \vec{v}') \cdot f_j(t, \vec{r}', v_i)) \sigma_{ij}(v, v_i, v', v') \delta^3 v_i \quad (13)$$

4. Coupled model of Electromagnetic Wave

Flow of EM through plasma can be analyzed as follows:

$$\frac{\partial f_i}{\partial t} + (v, \nabla_r) f_i + \frac{e_i}{m_i} (\mathbf{E} + \vec{V} \vec{B}) \nabla_v \cdot f_i = -\frac{f - f_c}{\tau} \quad (14)$$

Here we have simulated the above equation formed by recursive method. We have solved E & B. For solving these values we have evaluated V & A .Again for solution of A and V we need to compute the values of J and p. After computing all the above values we need to substitute all values obtained thus to the given master or coupled equation by iterative method. For computing coupled solution we have assumed Gaussian as initial function. Results of simulations are presented in fig 4 which gives us total insight of for possible solution of coupled Boltzmann Transport Equation.

$$\vec{E}(\vec{r}, t) = -\vec{\nabla}_v v(\vec{r}, t) - \frac{d}{dt} \vec{A}(\vec{r}, t) \quad (15)$$

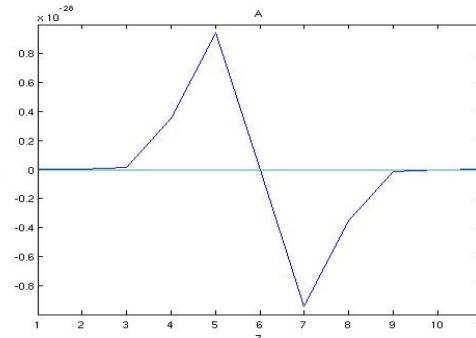


Fig 4(a). A vs Z at specific value x, y, t mid points

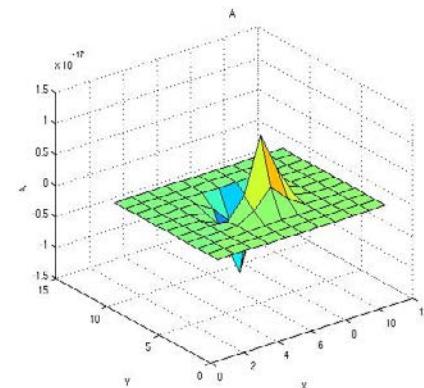


Fig 4(b). A vs X, Y at specific value z, t mid points

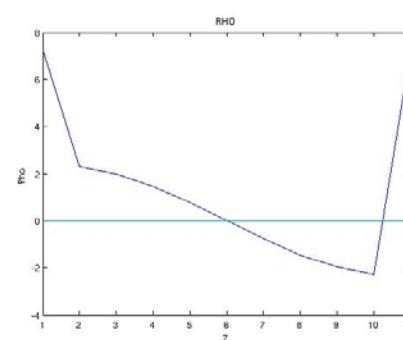


Fig 4(c). $\rho(\vec{r}, t)$ charge density rho vs. Z at specific mid points x, y, t

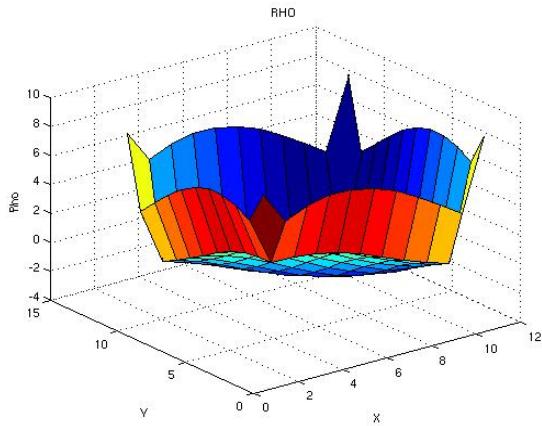


Fig 4(d). Rho vs X,Y at specific value z , t mid points

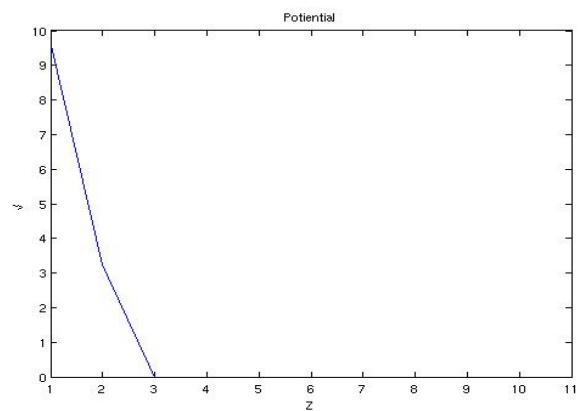


Fig 4(g). V vs Z at specific value x , y ,t mid points

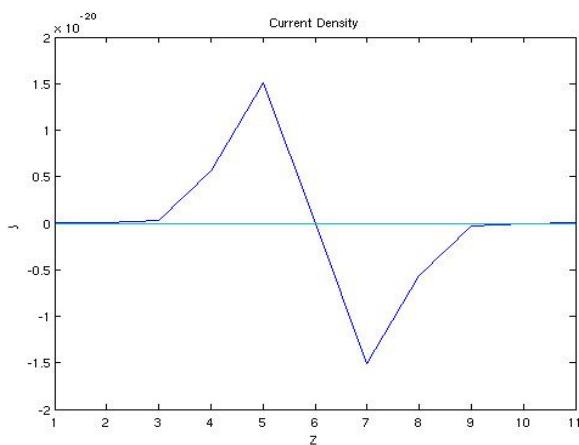


Fig 4(e). J at specific value x ,y ,t mid points w.r.t to Z

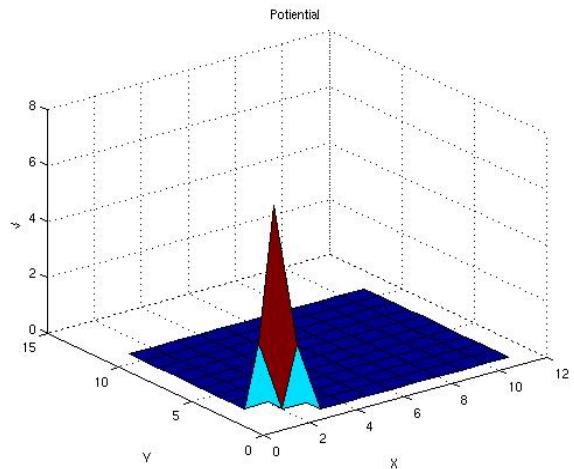


Fig 4(h). V vs X,Y at specific value z, t mid points

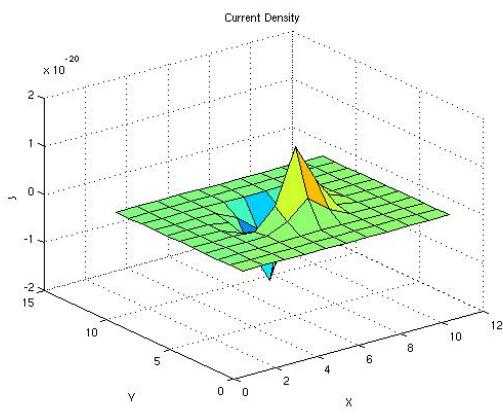


Fig 4(f). J vs X,Y at specific value z, t mid points

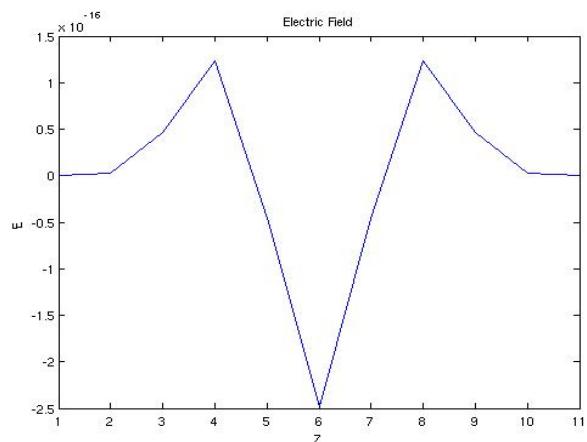


Fig.4(i). E vs Z at specific value x, y, z mid points

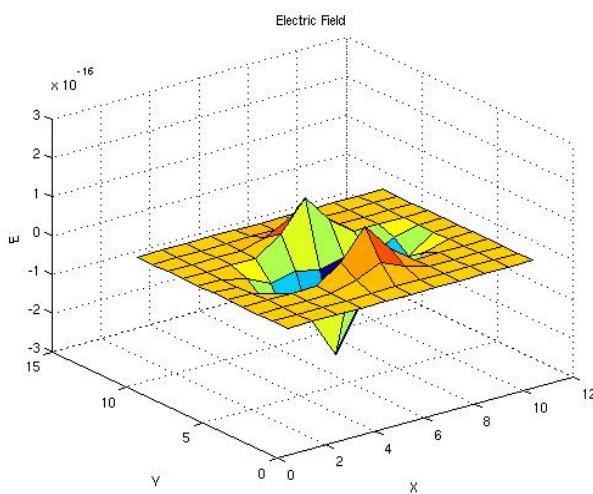


Fig 4(j). E vs X,Y at specific value z,t mid points

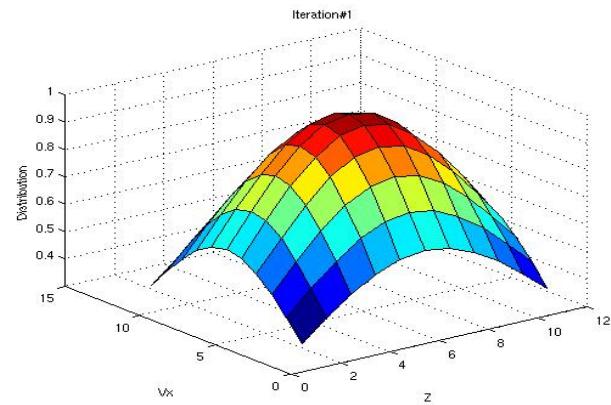


Fig 4(m). PDF vs Vx, Z

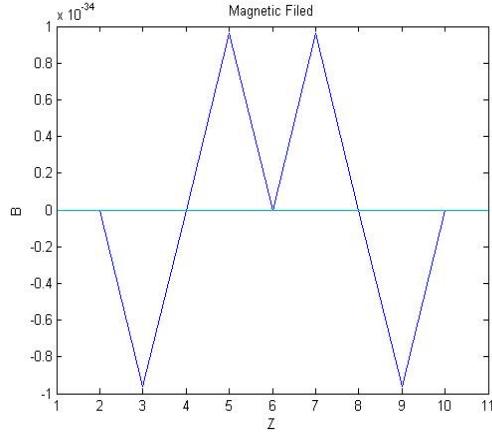


Fig 4(k). B vs Z at specific value x , y , t mid points

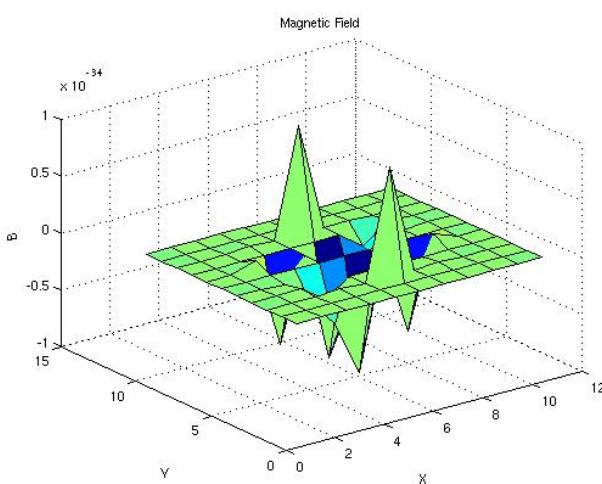


Fig 4(l). B vs X,Y at specific value z, t mid points

$$\vec{B}(\vec{r}, t) = \vec{\nabla}' \times \vec{A}'(\vec{r}, t) \quad (16)$$

Where E and B are electric and magnetic fields.

$$V(\vec{r}, t) = \frac{1}{4\pi\epsilon_0} \int \frac{e^{i(\vec{r}-t-\frac{|\vec{r}-\vec{r}'|}{2})}}{|\vec{r}-\vec{r}'|} d^3 r' \quad (17)$$

$$\vec{A}(\vec{r}, t) = \frac{1}{4\pi} \int \frac{i(\vec{r}-t-\frac{|\vec{r}-\vec{r}'|}{2})}{|\vec{r}-\vec{r}'|} d^3 r' \quad (18)$$

Where V and A are electric and magnetic potentials respectively.

$$\rho(\vec{r}, t) = -e \int f(\vec{r}, \vec{v}, t) d^3 v \quad (19)$$

$$\vec{J}(\vec{r}, t) = -e \int \vec{V}(\vec{r}, \vec{v}, t) d^3 v \quad (20)$$

Here ρ and J are charge density and current density respectively. We shall evaluate the value of

$E_x(p, q, r, n)$ which can be discretized as

$$E_x(p \Delta, q \Delta, r \Delta, n \tau)$$

$$B_x(\vec{r}, t) = -\frac{\partial A_y(\vec{r}, t)}{\partial x} - \frac{\partial A_z(\vec{r}, t)}{\partial r} \quad (21)$$

$$\frac{\partial f(\vec{r}, t)}{\partial t} + (\vec{V}, \vec{\nabla}) f(\vec{r}, \vec{V}) - \frac{e}{m} (\vec{E} + \vec{V} \times \vec{B}, \vec{\nabla}_V) f(\vec{r}, \vec{v}, t) = \frac{f_0 - f}{\tau} \quad (22)$$

$$\left[\frac{\partial f}{\partial t} \right]_{coll} = \sigma(v, \theta) |V - V'| (-f(\vec{r}, \vec{v}, t) + f(\vec{r}, \vec{v}', t) + f(\vec{r}, \vec{v}, t) f(\vec{r}, \vec{v}', t) d^3 V' \sin \theta d\theta) \quad (23)$$

Taking initial function as $f_0(\vec{r}, \vec{v}, t) = \text{Gaussian function}$.

We have evaluated value of E, B, A, V, J and ρ .

5. Conclusion

We have considered transport equations for linear response to compute distribution function and then non linear response for computing collision integral. Boltzmann transport equation will be very effective application to have better insight about EM transport in upper atmosphere i.e. ionosphere. Results for 3D simulation and coupled solutions have been evaluated. We observed pulse nature in coupled solution which can be best way seen as switching feature for VLSI design.

5. References

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