Skewed World of Plasma-wave Modeling: Challenges and Solutions using Unconditionally Stable FDTD Methods

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Shoe - ben - do
a ‘shoe’ uncle ‘ben’ just ‘do’ it
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1. Efficient utilization of millimeter-wave and terahertz bands is one of the most challenging areas of the modern electronics.

2. Innovations in these frequency bands will impact wide array of technologies:
   - high-data rate wireless-communication,
   - security and medical imaging,
   - sensing and vehicular radar.

3. They also exhibit unique spectrum to various gases and materials and are used for detection of explosives and poisonous gases.

4. High attenuation bands in this spectrum (183 GHz, 325 GHz, 380 GHz). At lower attenuation bands- 77 and 240 GHz, cellular, backhaul, fiber-replacement, sensing, and vehicular radar will be viable.

There is growing need for developing components and devices in the area of terahertz electronics. These devices should be 1) compact for ubiquitous and mobile application 2) Operational at room-temperature.
Electronic Plasma-wave: Basics

Forms of Plasma-oscillations

- Bulk Plasma Oscillations
- 2DEG Plasma Oscillations
- Gated 2DEG Plasma Oscillations

Governing Equations Equations

\[
\begin{align*}
\text{Gauss Law} & : \quad \frac{\partial E}{\partial x} = \frac{q}{\epsilon_0 \epsilon_r} n_o \\
\text{Continuity Eqn.} & : \quad \frac{\partial n}{\partial t} + \frac{\partial (nv)}{\partial x} = 0 \\
\text{Force Equation} & : \quad \frac{\partial v}{\partial t} = -\frac{q E_x}{m_o}
\end{align*}
\]

2DEG Plasma Oscillations

- 2D confined electron gas

\[
\omega_p = \sqrt{\frac{nq^2}{m \epsilon}}
\]

Gated 2DEG Plasma Oscillations

- 2D confined electron gas

\[
\omega_p = \sqrt{\frac{nq^2k}{2m \epsilon}}
\]

- Metal Gate

\[
\omega_p = k \sqrt{\frac{eU_o}{m}}
\]

Graphic showing plasma-Oscillations in FETs/HEMTs

- (a) Typical Fields obtained from the full-wave hydrodynamic modeling
- (b) Electron density modulation due to plasma-waves
- (c) 2DEG Plasma Oscillations

Terahertz Detection using Electron-plasmonics


Plasma-wave Based Devices at THZ

Terahertz emitters / Sources

- Plasma-resonances within short gate channel.
- Asymmetrical boundary conditions gives instability

Grating gated plasma mode HEMT (T Otsuji et al 2008)

- Grating Gates, along with optical pumping causes THz emissions

Terahertz Detection using Electron-plasmonics

- Ojefors et. al. [4]
- Knapp et. al. [5]

- Jessop et. al. [6], Modulator, 2016

In-spite of developments in plasmonic devices, their modeling methods, so far, are only analytical.

- Rigorous and accurate, Computational Modeling

FIG. 1. (a) Scanning electron microscope image of the device. The graphene rectangles are clearly visible between the arms of the antennas. (b) Schematic of the device. A modulating signal to the back gate causes modulation on incoming THz radiation. Source and drain electrodes are grounded.
In This Presentation

1. Introduction to Terahertz Plasmonic Devices
2. Integrating Hydrodynamic and Electrodynamics Solution: FDTD-HD modeling
3. Fast and Accurate? ADI and iterative ADI methods
4. Plasma waves in Single and Multiple 2DEG systems
5. Conclusions and Summary
Hybrid Full-Wave Hydrodynamic Modeling


2. Self-consistency achieved using updating HD and FDTD solver with $E_x$ and $J_e$ within each time -iterations


$n_{\text{sh}}$: Sheet electron density; $v$: electron velocity; $j = n_{\text{sh}}v$ is the sheet current in the channel; $E_x$: Longitudinal field in the Channel;
Difference Equations for the FDTD-HD model

ME Equation time/space discretization-

\[
E_{yi,i+1/2,j}^{n+1} = E_{yi,i+1/2,j}^n \left( \frac{1 - \sigma_y \Delta t/2\varepsilon}{1 + \sigma_y \Delta t/2\varepsilon} \right) - \frac{1}{1 + \sigma_y \Delta t/2\varepsilon} \frac{\Delta t}{\Delta x \varepsilon} \left[ H_{zi,i+1,j}^{n+1/2} - H_{zi,i,j}^{n+1/2} \right]
\]

(2.10)

\[
E_{xi,i,j+1/2}^{n+1} = E_{xi,i,j+1/2}^n \left( \frac{1 - \sigma_x \Delta t/2\mu}{1 + \sigma_x \Delta t/2\mu} \right) + \frac{1}{1 + \sigma_x \Delta t/2\mu} \frac{\Delta t}{\Delta y \mu} \left[ H_{zi,j+1,i}^{n+1/2} - H_{zi,j,i}^{n+1/2} \right] - \frac{\Delta t}{\varepsilon} j_i^{n+1/2}
\]

(2.11)

Upwind Scheme for Hydrodynamic Equations-

\[
n_{sh,i}^{n+1} = n_{sh,i}^n - \frac{\Delta t}{\Delta x} \left[ j_{i+1/2}^{n} - j_{i-1/2}^{n} \right],
\]

(2.6)

\[
j_{i+1/2}^{n+1} = j_{i+1/2}^n - \Delta t \frac{q_{sh,i}^{n+1/2}}{m_c} E_{ci}^{n+1/2} - \frac{\Delta t}{\tau_n} j_{i+1/2}^{n+1}
\]

(2.7)

Convective Term Definition for Upwind-

For \( v_{i+1/2}^n > 0 \), we define

\[
\text{Convec}_{i+1/2}^n = \frac{\Delta t}{\Delta x} \left[ v_{i+1/2}^n - v_{i-1/2}^n \right] + \frac{\Delta t}{\Delta x} \left[ j_{i+1/2}^n - j_{i-1/2}^n \right]
\]

(2.8)

and for \( v_{i+1/2}^n < 0 \), we define

\[
\text{Convec}_{i+1/2}^n = \frac{\Delta t}{\Delta x} \left[ v_{i+1/2}^n - v_{i-1/2}^n \right] + \frac{\Delta t}{\Delta x} \left[ j_{i+1/2}^n - j_{i-1/2}^n \right]
\]

(2.9)
1. A plane wave of freq. = 3 THz is incident on the HEMT structure with small gate discontinuity.

2. The diffracted wave couples to plasmonic modes within 2DEG and propagates away from the channel.

3. The phenomenon was modeled using the developed solver to understand and verify its operation.

**2DEG / material Properties chosen:**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electron Sheet Concentration, ( n_{\text{sh}} )</td>
<td>( 5 \times 10^{12} , \text{cm}^{-2} )</td>
</tr>
<tr>
<td>Effective electron mass, ( m_e )</td>
<td>0.2 ( m_0 )</td>
</tr>
<tr>
<td>Momentum Relaxation time, ( \tau )</td>
<td>1.14 ps</td>
</tr>
<tr>
<td>Dielectric Constant, ( \varepsilon_r )</td>
<td>9.5</td>
</tr>
</tbody>
</table>

✓ Tool can become powerful method for visualizing fields and phenomenology within HEMTs.
Validation by Simulation of Classically known cases

- Propagation fields in infinitely long, thin 2DEG layer
- Calculation of dispersion curves (k-ω curves)

**Case 1: 2DEG in bulk dielectric**

\[ \varepsilon_r = 13.9, \quad m_e = 0.042 m_o, \quad n_{sh} = 1 \times 10^{13} \text{cm}^{-2}, \quad \text{for gated case } d_{barr} = 38 \text{ nm}, \quad \mu = 10,000 \text{ cm}^2/(\text{V.s}) \]

**Case-2: Gated- 2DEG in bulk dielectric**

\[ \omega = \sqrt{\frac{n_{sh} q^2}{m_e} \frac{1}{k \varepsilon + \varepsilon_{ox} \coth(kd)}} \]

**Gated case: Quinn et.al. (1975) [7]**

\[ k = \frac{\omega^2}{2a} \quad ; \quad a = \frac{n_{sh} q^2}{4 m_e \varepsilon_c} \]

**Un-Gated case: Stern et.al. (1967) [8]**

Results Compare well with classical theoretical treatments (within the regime of their approximations).


Experimental Validation of Developed Model

1. Plasmonic resonances have been observed in grating gated 2DEG systems [11].

2. To confirm the model we modeled the same geometry.

3. Resonance frequency and approximate levels of absorptive spectra was confirmed using the model.

4. Some variations arise due to imperfections in the measurement set-up as compared to model.

Overall, the model is validated with previous measurements.

In This Presentation

Introduction to Terahertz Plasmonic Devices

Integrating Hydrodynamic and Electrodynmaic Solution: FDTD-HD modeling

Fast and Accurate? ADI and iterative ADI methods

Plasma waves in Single and Multiple 2DEG systems

Conclusions and Summary
Time Limitations in Traditional FDTD-HD Algorithm

- Typical device model and simulation domain.
- As noted domain is much larger compared 2DEG region.

Scales of mesh and simulation domains are skewed!

- Refined Mesh in the 2DEG region of the device
- Non-uniform meshing

- The mesh size near 2DEG is dictated by the Debye length (of the order $\lambda /10^4$)
  $$L_D = \sqrt{\frac{\varepsilon \varepsilon_0 K_B T}{q^2 N_D}} \approx 5nm @ 1e12 cm^{-2}$$

- Adaptive meshing required to reduce simulation time.
- Due to fine mesh size near the 2DEG, the simulation time-step is small
  $$\Delta t \leq \frac{1}{c} \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}$$

- Typical $\Delta x \sim \lambda /5000$ and $\Delta t=10^{-17}$ s

- There is a need to reduce the simulation times using ‘other’ Improvements
  - ADI-FDTD (improve time)
  - Iterative ADI-FDTD (improve, time and accuracy)
Implicit FDTD Formulation (ADI-FDTD)

Maxwell’s Equations for TE\textsubscript{z} mode fields: (odd-even splitting: A, B)

\[
\frac{\partial \vec{u}}{\partial t} = [A] \vec{u} + [B] \vec{u} \quad \vec{u} = [E_x, E_y, H_z]^T
\]

\[
[A] = \begin{bmatrix}
0 & 0 & \frac{1}{\epsilon} \frac{\partial}{\partial y} \\
0 & 0 & 0 \\
\frac{1}{\mu} \frac{\partial}{\partial y} & 0 & 0
\end{bmatrix} \quad [B] = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & -\frac{1}{\epsilon} \frac{\partial}{\partial x} \\
0 & -\frac{1}{\mu} \frac{\partial}{\partial x} & 0
\end{bmatrix}
\]

Time-Splitting: Allows solution using tridiagonal matrix in two steps.

\[
\left(I - \frac{\Delta t}{2} [A]\right) \vec{u}^{t_{mp}} = \left(I + \frac{\Delta t}{2} [B]\right) \vec{u}^n
\]

\[
\left(I - \frac{\Delta t}{2} [B]\right) \vec{u}^{n+1} = \left(I + \frac{\Delta t}{2} [A]\right) \vec{u}^{t_{mp}}
\]

Approximation: Remove the $\Delta t^2$ term:

\[
\left(I - \frac{\Delta t}{2} [A]\right) \vec{u}^{n+1} = \left(I + \frac{\Delta t}{2} [A]\right) \vec{u}^n
\]

Applying the Crank Nicholson scheme for $\Delta t (1+1/2)$ time step, we get:

\[
\left(I - \frac{\Delta t}{2} [A] - \frac{\Delta t}{2} [B]\right) \vec{u}^{n+1} = \left(I + \frac{\Delta t}{2} [A] + \frac{\Delta t}{2} [B]\right) \vec{u}^n
\]

Above represents set of simultaneous equations (These are unconditionally stable, i.e. $\Delta t$ can be larger than that dictated by Courant Condition). We write them as:

\[
\left(I - \frac{\Delta t}{2} [A]\right) \left(I - \frac{\Delta t}{2} [B]\right) \vec{u}^{n+1} = \left(I + \frac{\Delta t}{2} [A]\right) \left(I + \frac{\Delta t}{2} [B]\right) \vec{u}^n + \frac{\Delta t^2}{4} [A][B](\vec{u}^{n+1} - \vec{u}^n)
\]


Implicit Equations for $E_x$ determination

\[
E_{x\mid i,j+1/2}^{\text{tmp}} = 1 + \Delta t^2 \left( \frac{C_{eh}^{\text{ex}}}{2\varepsilon \Delta y} \right)_{i,j+1/2} \left( \frac{C_{hxx}^{\text{ex}}}{2\mu \Delta y} \right)_{i,j+1} + \Delta t^2 \left( \frac{C_{eh}^{\text{ex}}}{2\varepsilon \Delta y} \right)_{i,j+1/2} \left( \frac{C_{hxx}^{\text{ex}}}{2\mu \Delta y} \right)_{i,j} \\
+ E_{x\mid i,j-1/2}^{\text{tmp}} \left[ - \Delta t^2 \left( \frac{C_{eh}^{\text{ex}}}{2\varepsilon \Delta y} \right)_{i,j+1/2} \left( \frac{C_{hxx}^{\text{ex}}}{2\mu \Delta y} \right)_{i,j+1} \right] \\
+ E_{x\mid i,j+3/2}^{\text{tmp}} \left[ - \Delta t^2 \left( \frac{C_{eh}^{\text{ex}}}{2\varepsilon \Delta y} \right)_{i,j+1/2} \left( \frac{C_{hxx}^{\text{ex}}}{2\mu \Delta y} \right)_{i,j+1} \right] \\
= C_{ex}^{\text{ex}} \varepsilon_{i,j+1/2} E_{x\mid i,j+1/2}^n + \Delta t \left( \frac{C_{eh}^{\text{ex}}}{2\varepsilon \Delta y} \right)_{i,j+1/2} \left[ C_{hxx}^{\text{ex}} \mu_{i,j+1} H_{y\mid i,j+1}^n + C_{hxx}^{\text{ex}} \mu_{i,j+1} H_{y\mid i,j+1}^n \right] \\
- C_{hx}^{\text{ex}} \mu_{i,j} H_{y\mid i,j}^n + C_{hx}^{\text{ex}} \mu_{i,j} H_{y\mid i,j}^n \\
- \Delta t^2 \left( \frac{C_{eh}^{\text{ex}}}{2\varepsilon \Delta y} \right)_{i,j+1/2} \left[ C_{hxx}^{\text{ex}} \mu_{i,j+1} E_{y\mid i,j+1/2}^n \right] \\
- E_{y\mid i-1/2,j-1/2}^{\text{tmp}} = C_{eh}^{\text{ex}} \varepsilon_{i-1/2,j} E_{x\mid i-1/2,j}^n - \Delta t \left( \frac{C_{eh}^{\text{ex}}}{2\varepsilon \Delta x} \right)_{i-1/2,j} \left[ H_{x\mid i,j}^n + H_{x\mid i,j}^n - H_{y\mid i-1,j}^n + H_{y\mid i-1,j}^n \right] \quad (A.11)
\]

\[
H_{x\mid i,j}^{\text{tmp}} = C_{hx}^{\text{ex}} \mu_{i,j} H_{x\mid i,j}^n - \Delta t \left( \frac{C_{hx}^{\text{ex}}}{2\mu \Delta x} \right)_{i,j} \left[ E_{y\mid i+1/2,j}^n - E_{y\mid i-1/2,j}^n \right] \quad (A.12)
\]

\[
H_{y\mid i,j}^{\text{tmp}} = C_{hx}^{\text{ex}} \mu_{i,j} H_{x\mid i,j}^n + \Delta t \left( \frac{C_{hx}^{\text{ex}}}{2\mu \Delta y} \right)_{i,j} \left[ E_{x\mid i,j+1/2}^n - E_{x\mid i,j-1/2}^n \right] \quad (A.13)
\]

1. Fields are calculated at an intermediate time step using n time step values.
2. By moving the stencil along the vertical grid, we obtain the Simultaneous Tridiagonal System of equations.
3. Above represents ADI-FDTD solution.
1. In second step fields are calculated for \( n+1 \) using fields-values at the intermediate time step.

2. This time stencil moves horizontally making system of trigonal equations.
Flowcharts for ADI Methods

### Explicit FDTD-HD Method

- **Maxwell’s Equations: FDTD**
  - \( \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}_e + \sigma \vec{E} \)
  - \( \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} - \sigma_m \vec{H} \)

- **Calculation of Field values using time-marching algorithm:**
  - Calculation of Ex for \( t+\Delta t \)
  - Calculation of Ey for \( t+\Delta t \)
  - Calculation of Hz for \( t+\Delta t \)

- **Electron-Transport in channel**
  - Hydrodynamic: Upwind Scheme
  - \( \frac{\partial n_{sh}}{\partial t} + \frac{\partial j}{\partial x} = 0 \)

- **Calculations of n at \( t+\Delta t/R \)**
  - **Calculations of J at \( t+\Delta t/R \)**

- **Update Ex**

- **Update Jx**

- **Update Jy**

- **Update Jz**

- **Update Jt**

- **End**

- **Time-step Limited by**
  \[ \Delta t \leq \frac{1}{c} \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}} \]

\[ \approx 10^{-17} \text{s} \]

### ADI-FDTD-HD Method

- **Maxwell’s Equations: ADI-FDTD**
  - \( \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}_e + \sigma \vec{E} \)
  - \( \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} - \sigma_m \vec{H} \)

- **Calculation of Ex for \( t+\Delta t/2 \)** using tridiagonal system of linear equation
  - Calculate Hz for \( t+\Delta t/2 \) using update equation
  - Calculate Ey for \( t+\Delta t/2 \) using update equation

- **Electron-Transport in channel**
  - Hydrodynamic: Upwind Scheme
  - \( \frac{\partial n_{sh}}{\partial t} + \frac{\partial j}{\partial x} = 0 \)

- **Calculations of n at \( t+\Delta t/R \)**

- **Calculations of J at \( t+\Delta t/R \)**

- **Update Ex**

- **Update Jx**

- **Update Jy**

- **Update Jz**

- **End**

- **Unconditionally stable: \( \Delta t \) can be arbitrarily large, with stability.**
Time-Improvements Using ADI-FDTD-HD Method

Simulation Set-up:

Performance for increasing $CN$ ($\Delta t_{\text{ADI}} = CN \times \Delta t_{\text{FDTD}}$)

Simulation time reduction:

<table>
<thead>
<tr>
<th></th>
<th>Min. $\Delta x$, $\Delta y$</th>
<th>$\Delta T$ (s)</th>
<th>CPU-time per time-step (s.)</th>
<th>CPU-TIME total (Hrs.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDTD-HD</td>
<td>4 nm, 1 nm</td>
<td>$3.24 \times 10^{-18}$</td>
<td>0.35</td>
<td>90</td>
</tr>
<tr>
<td>ADI-FDTD-HD, CN=100</td>
<td>4 nm, 1 nm</td>
<td>$3.24 \times 10^{-16}$</td>
<td>7.59</td>
<td>19.57</td>
</tr>
<tr>
<td>ADI-FDTD-HD, CN=200</td>
<td>4 nm, 1 nm</td>
<td>$6.48 \times 10^{-16}$</td>
<td>7.59</td>
<td>9.79</td>
</tr>
<tr>
<td>ADI-FDTD-HD, CN=300</td>
<td>4 nm, 1 nm</td>
<td>$9.72 \times 10^{-16}$</td>
<td>7.59</td>
<td>6.52</td>
</tr>
</tbody>
</table>

Thus, using ADI-FDTD, we decrease the simulation-times, but as the time reduces errors increase.

To improve accuracy we pursue Iterative-ADI-FDTD.

Field Accuracy Performance of ADI-FDTD-HD
Iterative-ADI-FDTD Method - Overview

**ADI-FDTD Scheme**

\[
(I - \frac{\Delta t}{2} [A])(I - \frac{\Delta t}{2} [B])\bar{u}^{n+1} = (I + \frac{\Delta t}{2} [A])(I + \frac{\Delta t}{2} [B])\bar{u}^n + \frac{\Delta t^2}{4} [A][B](\bar{u}^{n+1} - \bar{u}^n)
\]

**Approximation:** Remove the \(\Delta t^2\) term:

\[
(I - \frac{\Delta t}{2} [A])(I - \frac{\Delta t}{2} [B])\bar{u}^{n+1} = (I + \frac{\Delta t}{2} [A])(I + \frac{\Delta t}{2} [B])\bar{u}^n
\]

**Time-Splitting:** Allows solution using tridiagonal matrix in two steps.

\[
(I - \frac{\Delta t}{2} [A])\bar{u}^{tmp} = (I + \frac{\Delta t}{2} [B])\bar{u}^n
\]

\[
(I - \frac{\Delta t}{2} [B])\bar{u}^{n+1} = (I + \frac{\Delta t}{2} [A])\bar{u}^{tmp}
\]

**Iterative ADI-FDTD Scheme**

1. The two split equations are solved K times.
2. Added term ~ \(\Delta t^2\) is responsible for iterative correction.
3. Max. iteration number K can be fine-tuned for time/error compromise.

\[
(I - \frac{\Delta t}{2} [A])\bar{u}^{k+1}_{tmp} = (I + \frac{\Delta t}{2} [B])\bar{u}^n + \frac{\Delta t^2}{8} [A][B](\bar{u}^{k+1}_{n+1} - \bar{u}^n)
\]

\[
(I - \frac{\Delta t}{2} [B])\bar{u}^{n+1}_{k+1} = (I + \frac{\Delta t}{2} [A])\bar{u}^{k+1}_{tmp} + \frac{\Delta t^2}{8} [A][B](\bar{u}^{n+1}_{k+1} - \bar{u}^n)
\]
Implementing ADI Methods

**ADI-FDTD-HD Method**

Maxwell’s Equations: ADI-FDTD

\[ \mathbf{v} \times \mathbf{H} = \frac{\partial \mathbf{E}}{\partial t} + j \sigma \mathbf{E} \]
\[ \mathbf{v} \times \mathbf{E} = - \frac{\partial \mathbf{H}}{\partial t} - \sigma_m \mathbf{H} \]

- Calculation of Ex for t+Δt/2 using tridiagonal system of linear equation
- Calculate Hx for t+Δt/2 using update equation
- Calculate Ey for t+Δt/2 using update equation
- Calculation of Ey for t+Δt/2 using tridiagonal system of linear equation
- Calculate Hx for t+Δt/2 using update equation
- Calculate Ex for t+Δt/2 using update equation

Electron-Transport in channel
Hydrodynamic: Upwind Scheme

\[ \frac{\partial j}{\partial t} + v \frac{\partial j}{\partial x} + j \frac{\partial v}{\partial x} = \frac{qnE_x - j}{m_e} - \frac{KT}{m_e} \frac{\partial n_{sh}}{\partial t} \]

Calculations of n at t+Δt/2
Calculations of J at t+Δt/2

End

**Iterative-ADI-FDTD-HD Method**

Maxwell’s Equations: t-ADI-FDTD

\[ \mathbf{v} \times \mathbf{H} = \frac{\partial \mathbf{E}}{\partial t} + j \sigma \mathbf{E} \]
\[ \mathbf{v} \times \mathbf{E} = - \frac{\partial \mathbf{H}}{\partial t} - \sigma_m \mathbf{H} \]

- Calculation of Ex for t+Δt/2 using tridiagonal system of linear equation
- Calculate Hx for t+Δt/2 using update equation
- Calculate Ey for t+Δt/2 using update equation
- Calculation of Ey for t+Δt/2 using tridiagonal system of linear equation
- Calculate Hx for t+Δt/2 using update equation
- Calculate Ex for t+Δt/2 using update equation

Electron-Transport in channel
Hydrodynamic: Upwind Scheme

\[ \frac{\partial j}{\partial t} + v \frac{\partial j}{\partial x} + j \frac{\partial v}{\partial x} = \frac{qnE_x - j}{m_e} - \frac{KT}{m_e} \frac{\partial n_{sh}}{\partial t} \]

Calculations of n at t+Δt/R
Calculations of J at t+Δt/R

\[ \frac{\partial n_{sh}}{\partial t} + \frac{\partial J}{\partial x} = 0 \]

Iterations

K

Updated J

Refine

End

✓ Unconditionally stable: Δt can be arbitrarily large
✓ Accuracy recovered by iterative method
Iterative ADI-FDTD-HD

Simulation Set-up:

The channel oscillation currents for several cases- For CN=200, we consider it=3, 5:

Similar to ADI method, we develop iterative ADI method, that uses corrective iterations as per [11] to fix the accuracy issues with the ADI method.

Accuracy is improved using iterative ADI method at some computational cost, overall time still smaller than traditional methods.

Field Correction using Iterative Method

**ADI-FDTD-HD method**
- Very fast
- Qualitative solution

**Iterative ADI-FDTD-HD method**
- 50% Faster
- Accurate Solution
The developed method provide a way of fine-tuning the simulation-times and accuracy using CN-it combinations.

Specifically, for $CN=100$, $it=2$, we obtain time-cost reduction by factor of 0.42 with 3% error in calculations.

Further, just qualitative results (for rough estimates) can be calculated at much faster speed using large-CN-small-it combinations.
In This Presentation

- Introduction to Terahertz Plasmonic Devices
- Integrating Hydrodynamic and Electrodynamic Solution: FDTD-HD modeling
- Fast and Accurate? ADI and iterative ADI methods
- Applications of the developed model
  1) 2DEG bilayers
  2) Short Channel HEMTs
- Conclusions and Summary
Origin of Multilayer HEMTs

1. When two 2DEGs are placed in close vicinity, they are electromagnetically coupled.

2. In such scenarios, the plasmonic waves ride along two or more channels.

3. Such 2DEG systems are possible in state-of-the-art HEMTs using a periodic lattice of heterojunctions [16].

4. These devices promise higher conductivity performance.

5. Thus the plasma-wave properties change due to presence of closely spaced 2DEG channels.

The plasma-dynamics in single channel system is well understood using analytical methods. However, there is lack of understanding for the multiple channel systems.

Problem of Plasmonic Modes in Bilayer

1. Our objective in this presentation is to find out the plasma-modes existing in double channel HEMTs.
2. The channels are close to each other ~ mutual coupling?
   1. Two separate modes or single collective modes?
   2. What would be the dispersion relations and field profiles in such two channel systems?
3. We would use analytical and multi-physical simulation methods to find answers to above questions.
Both Acoustic and optical modes are observed.

Acoustic modes are confined between the channel.

Optical modes are outside the channel.
Modeling of Gated-Bilayer

First numerical illustration: Excitation and propagation of Optical Plasmonic and Acoustic Plasmonic Modes in gated-bilayer was demonstrated using multi-physical Models

• Both Acoustic and optical modes are observed.
• Acoustic modes are confined between the channel.
• Optical modes are outside the channel.

Wave numbers for the two modes

Variation of excitation coefficient with change of gap
Summary of Modal Solutions in 2DEG-Bilayers

The two modes in the double channel are due to in-phase and out-of-phase plasmonic oscillations in the two channels. In-phase: Optical modes. Out-of-phase: Acoustic modes.

- Solver has allowed understanding of the two modes within the bilayer strictures.
Verification of the Bilayer Plasma-Waves

- A THz Gaussian pulse was incident on a bilayer structure.
- The excited propagating plasmonic pulse was observed to be moving on bilayer structure.
- FFT was taken to identify the dispersion curves ($\omega - k$) curves.
- Only OP modes were identified, suggesting that in practical scenarios, OP modes are easier to excite.
- OP mode dispersion relation were in agreement with analytical results.
Terahertz Emissions from Small gate-length HEMT

First Reports of Terahertz Emission from sub-micron channel HEMT

QEL, 1997

Emission of THz radiation from optically excited coherent plasmons in a two-dimensional electron gas


JAP, 2005

Voltage tuneable terahertz emission from a ballistic nanometer InGaAs/InAlAs transistor


1. Terahertz Emissions have been observed from Short Channel High Electron Mobility Transistors (Some experimental Observations and analysis available)

2. The analytical models employed have provided qualitative understanding of the phenomenon.

TED, 1993, First Analytical models

Shallow Water Analogy for a Ballistic Field Effect Transistor: New Mechanism of Plasma Wave Generation by dc Current

Michael Dyakonov¹ and Michael Shur²

¹A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia
²Department of Electrical Engineering, University of Virginia, Charlottesville, Virginia 22903
(Received 21 June 1993)

TED, 2016, First Full-wave-hydrodynamic models Numerical Analysis of Terahertz Emissions From an Ungated HEMT Using Full-Wave Hydrodynamic Model

Shubhendu Bhardwaj, Student Member, IEEE, Nitin K. Nandakumar, Senior Member, IEEE, Siddhartha Raja, and John L. Volakis, Fellow, IEEE
Basics of DS instability and THz Emissions

1. Short Channel, terminated by ohmic contacts.
2. The AC boundary conditions cause reflection of AC current.
3. Reflection gain: due to difference in wave numbers in forward & backward directions.
4. This can lead to oscillations and emissions.

- At drain we see oscillating interference of upstream and downstream plasmon.
- The 2 DEG channel acts like a quarter wave cavity.
- Frequency $\sim 1/\text{travel time}$
First Numerical Verifications

Phenomenological Verifications via Full-wave Multiphysical Solution

1. Left, Top: Reflection of plasma-wave from constant Current boundary conditions.
2. Left, Below: Field profile at different time instant- dipole like oscillation is observed.
3. Right, top: Emitted Spectra from the device.
4. Right, Below: Relation between channel electron density and power of the emitted spectra

Model Allows ‘Physical Simulation’ for the plasma-wave emissions from Short-channel ungated HEMT.
Conclusions and Summary

1. Modeling of Graphene and 2DEG systems is a Multi-physical problem requiring solution of electron transport and electromagnetics.

2. Tradition FDTD-HD methods require high computational time ‘skewed’ mesh dimensions.

3. ADI-FDTD-HD methods show significant reduction in simulation times with some cost to accuracy (CN<200).

4. It-ADI-FDTD-HD methods overcome accuracy issue, with some time compromise, still better than traditional FDTD-HD method. (50 % reduction in time, with nominal 3% error)
Publications/Awards (2012-2017)

Publications

Awards
Student Paper
1. Best student paper award- iWaT-2017
2. Best student paper award-AMTA-2015
3. Best student paper award, second prize, AMTA-2014

Others
1. Early Career Scientist, GASS-2017
2. Presidential Fellowship-2016
3. Louis B. Vetter Award-2016
4. ESL student of the Year -2016
To the Office of Naval Research for providing support for this work under Devices and Architectures for Terahertz Electronics Multidisciplinary University Research Initiative (DATE MURI), Grant N00014-11-1-0721
Comparison of Three Approaches

Particle Transport Models

Particle Approach:
Here, we solve the Vlasov Equation;
\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + q m_e \left( \mathbf{E} + \mathbf{v} \times \mathbf{B} \right) \nabla_k f = 0
\]
\( f \) is the distribution functions
- Calculates flight of each particle under external force.
- Most rigorous form of solution
- Number of particles can be defined
- Implementation algorithms:
  - Particle in Cell
  - Monte Carlos (includes Collision)
- Time Consuming

BTE (Kinetic Approach)
Boltzmann equation
\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + q m_e \left( \mathbf{E} + \mathbf{v} \times \mathbf{B} \right) \nabla_k f = \left. \frac{\partial f}{\partial t} \right|_{\text{coll}}
\]
f is the distribution functions
- Intermediate level description of particle dynamic – between HD and particle approach
- Assumes the parameters as distribution function
- BTE as such is quite complex to solve, since its 7 dimensional equation
- Provides lot of information but as a distribution of \( v, k, n \) etc.
- Free to chose he distribution function, and non-equilibrium cases may be described by this
- Complicated to solve

Hydrodynamic Approach

\[
\frac{\partial n}{\partial t} + \frac{\partial j}{\partial x} = 0
\]
\[
\frac{\partial j}{\partial t} + v \frac{\partial j}{\partial x} + j \frac{\partial v}{\partial x} = - \frac{q n E_x}{m_e} - \frac{j}{\tau} - \frac{K T}{m_e} \frac{\partial n}{\partial x}
\]
- Derived from moments of BTE.
- Macroscopic observation distances are longer than the mean free path.
- Macroscopic observation times are longer than the mean free flight time.
- Assumes local bulk parameters (in stead of particles)
- Valid when time and space variations are small, i.e. equilibrium particle distribution is maintained.
- Requires closure equations, i.e. assumes parabolic bands
Regimes of Applications

Molecular dynamics (Monte Carlo solution, Particle in Cell approach)

Boltzmann transport Equation

Hydrodynamic Model

1. Number of particles $\rightarrow \infty$
2. Only 2 particle collisions assumed

1. Mean free path $\ll$ macroscopic observation length
2. Mean free time $\ll$ macroscopic observation time step
3. Parabolic bands are assumed
4. Thermal equilibrium assumed (small fluctuations around Maxwellian)
Limitations and advantages for Semiconductor Simulations

Vasileska, Goodnick et. al., “Monte Carlo Device Simulations” online:

**Hydrodynamic Model**

$L_g \geq 0.1$ µm
- Hot carrier effects, such as velocity overshoot, included in the model
- Overestimates the velocity at high fields

**Particle Based Simulation**

$L_g < 0.1$ µm
- Accurate up to classical limits
- Allows proper treatment of discrete impurity effects
- Time consuming

Vasileska, Goodnick, “Computation Electronics”: