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

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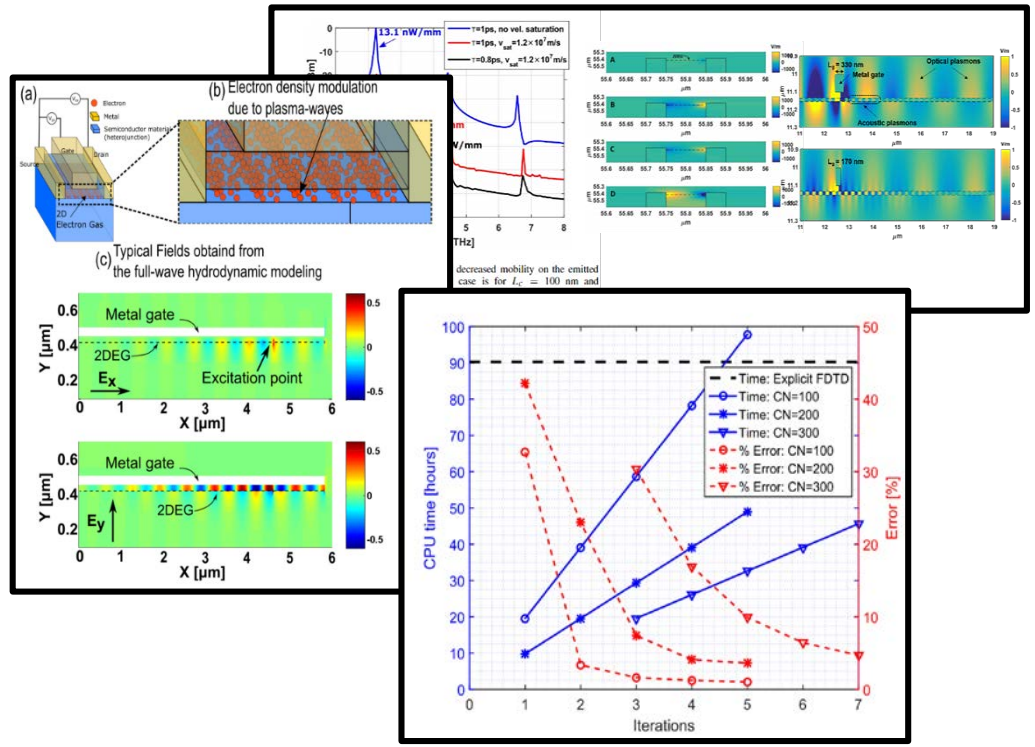
Florida International University,
Miami, FL

Shoe - ben - do

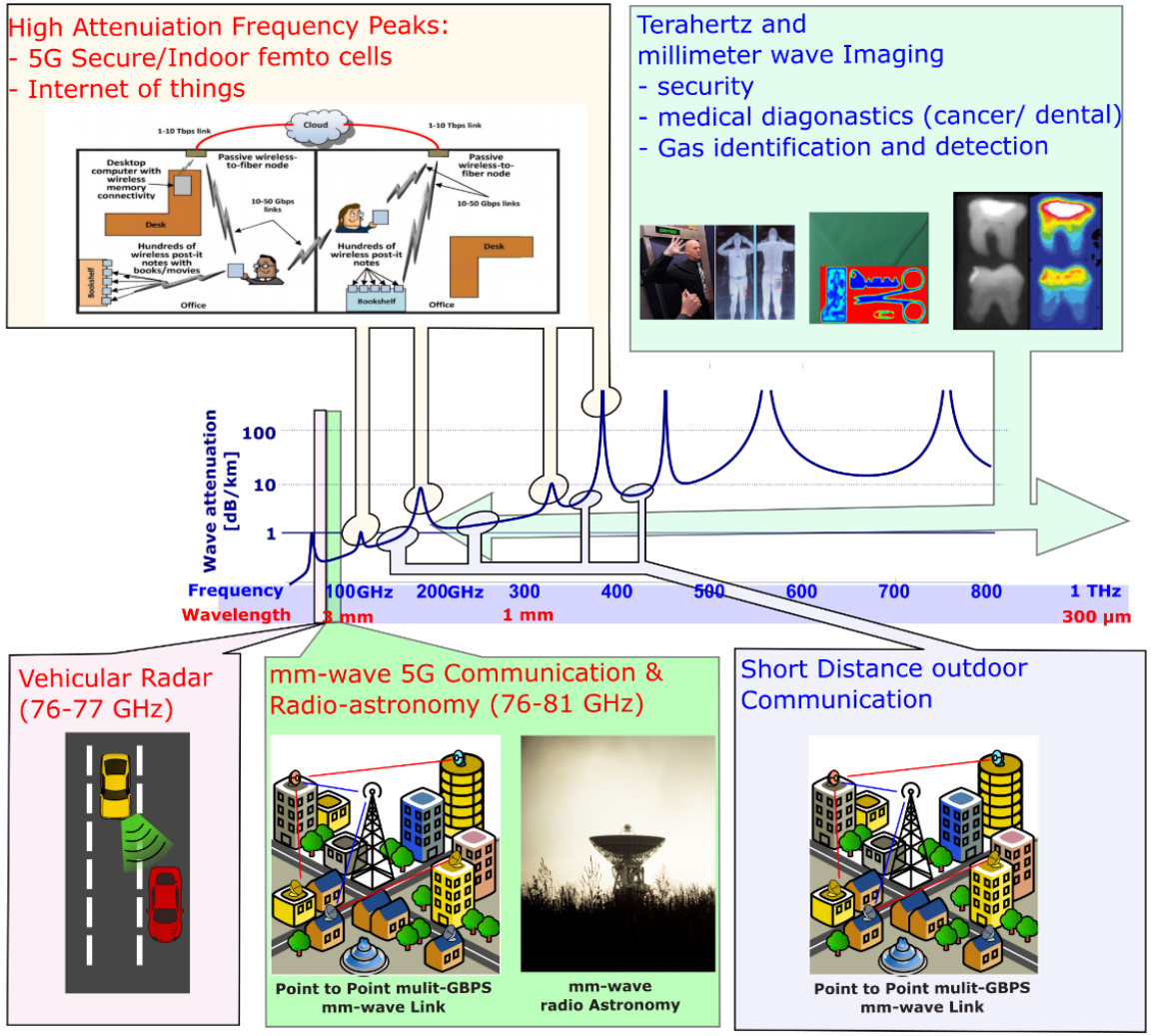
a 'shoe' uncle 'ben' just 'do' it



Collaborators (DATE-MURI, 2012-2017)

- **Ohio State University**
  - John Volakis (now at Florida International University)
  - Fernando Teixeira
  - Siddharth Rajan
- **Cornell University**
  - Huili Grace Xing
- **University of Utah**
  - Berardi Sensale-Rodriguez
- **University of Notre Dame**
  - Patrick Fay

Background: Terahertz Technology



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

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Forms of Plasma-oscillations

Governing Equations Equations

Gauss Law

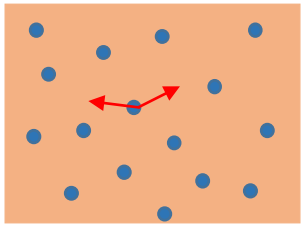
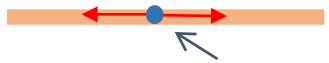
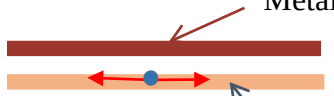
$$\frac{\partial E}{\partial x} = \frac{q}{\epsilon_o \epsilon_r} n_o$$

Continuity Eqn.

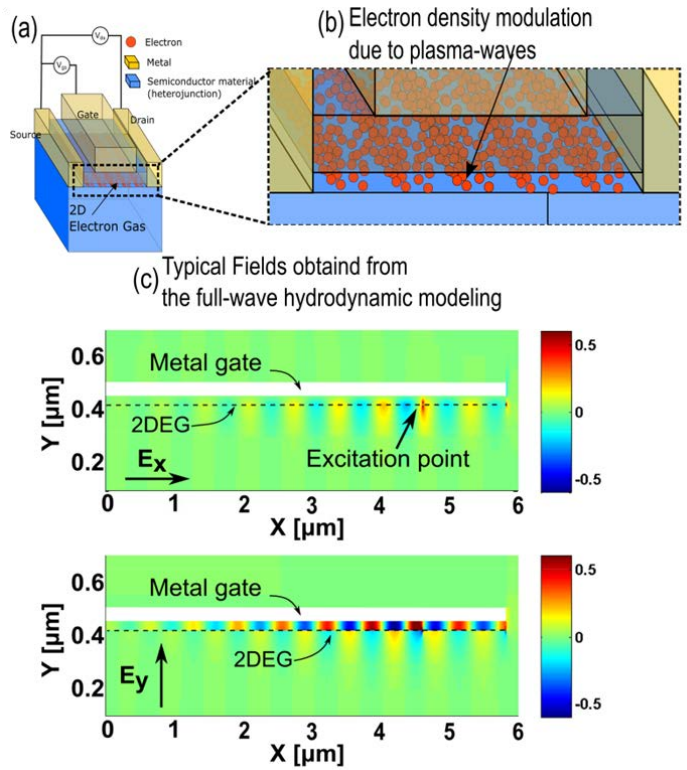
$$\frac{\partial n}{\partial t} + \frac{\partial (nv)}{\partial x} = 0$$

Force Equation

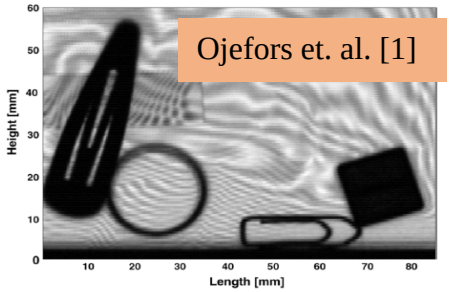
$$\frac{\partial v}{\partial t} = -\frac{qE_x}{m_o}$$

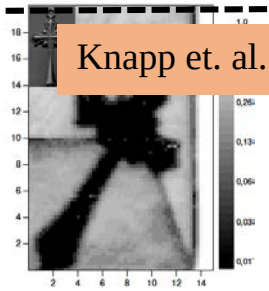
Bulk Plasma Oscillations	2DEG Plasma Oscillations	Gated 2DEG Plasma Oscillations
	 2D confined electron gas	 Metal Gate; 2D confined electron gas
$\omega_p = \sqrt{\frac{nq^2}{m\varepsilon}}$	$\omega_p = \sqrt{\frac{nq^2 k}{2m\varepsilon}}$	$\omega_p = k\sqrt{\frac{eU_o}{m}}$

Graphic showing plasma-Oscillations in FETs/HEMTs



Terahertz Detection using Electron-plasmonics





[1] E. Ojefors, U. R. Pfeiffer, A. Lisauskas and H. G. Roskos, "A 0.65 THz Focal-Plane Array in a Quarter-Micron CMOS Process Technology," in *IEEE Journal of Solid-State Circuits*, vol. 44, no. 7, pp. 1968-1976, July 2009.

[2] W. Knap *et al.*, "Terahertz imaging with GaAs and GaN plasma field effect transistors detectors," *2016 MIXDES - 23rd International Conference Mixed Design of Integrated Circuits and Systems*, Lodz, 2016, pp. 74-77.

Plasma-wave Based Devices at THZ

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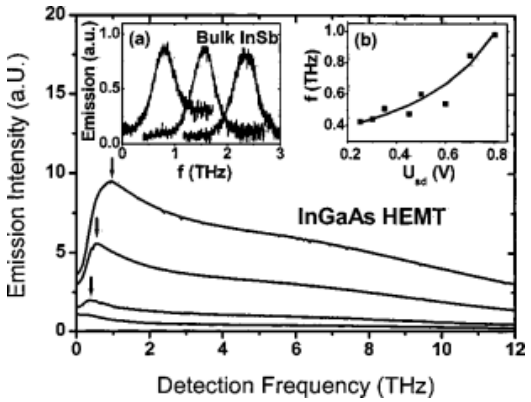
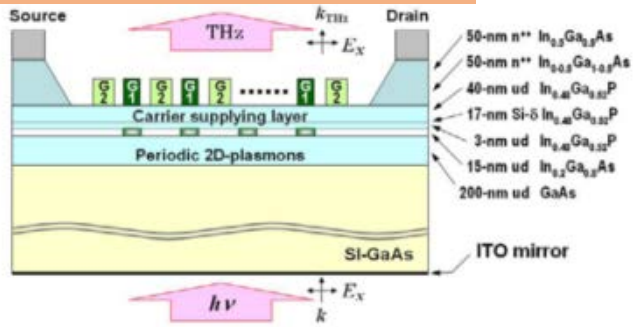
Terahertz emitters / Sources

- 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



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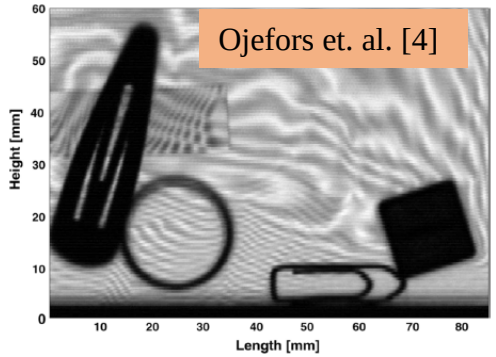

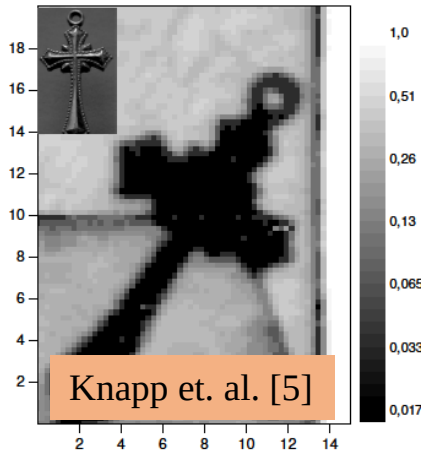

Jessop et. al. [6], Modulator, 2016

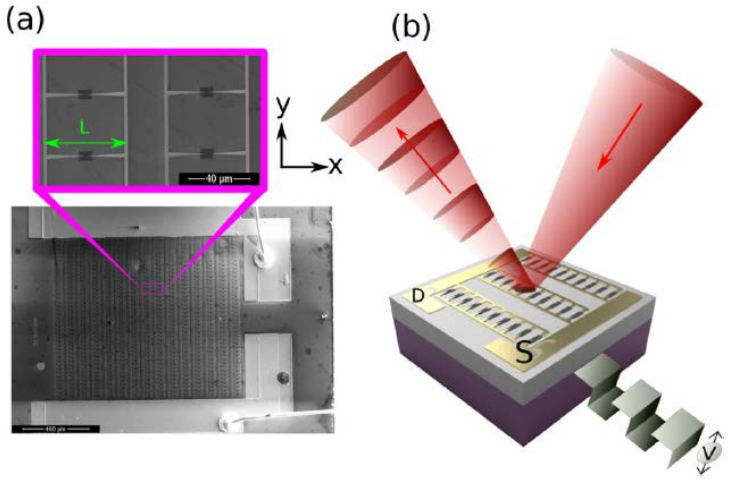

FIG. 1. (a) Scanning electron microscope image of the device. The graphene rectangles are clearly visible between the arms of the antennas. (b) Schematic of the device. A modulating signal to the back gate causes modulation on incoming THz radiation. Source and drain electrodes are grounded.

- In-spite of developments in plasmonic devices, their modeling methods, so far, are only analytical.
- Rigorous and accurate, Computational Modeling

In This Presentation

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Introduction to Terahertz Plasmonic Devices

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Integrating Hydrodynamic and Electrodynamic Solution: FDTD-HD modeling

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Fast and Accurate?
ADI and iterative ADI methods

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Plasma waves in Single and Multiple 2DEG systems

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Conclusions and Summary

Hybrid Full-Wave Hydrodynamic Modeling

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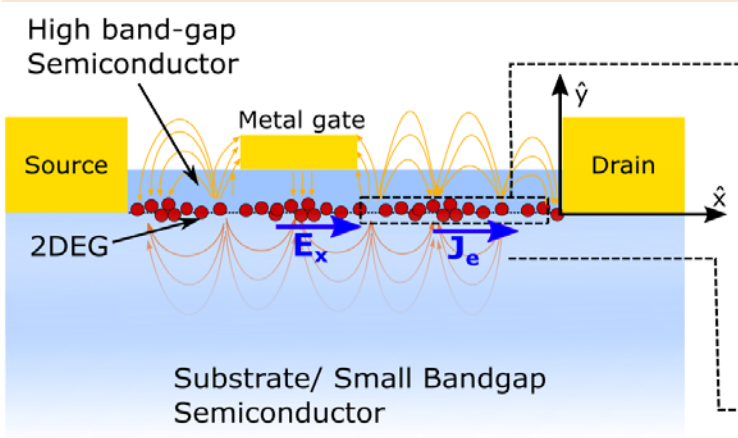
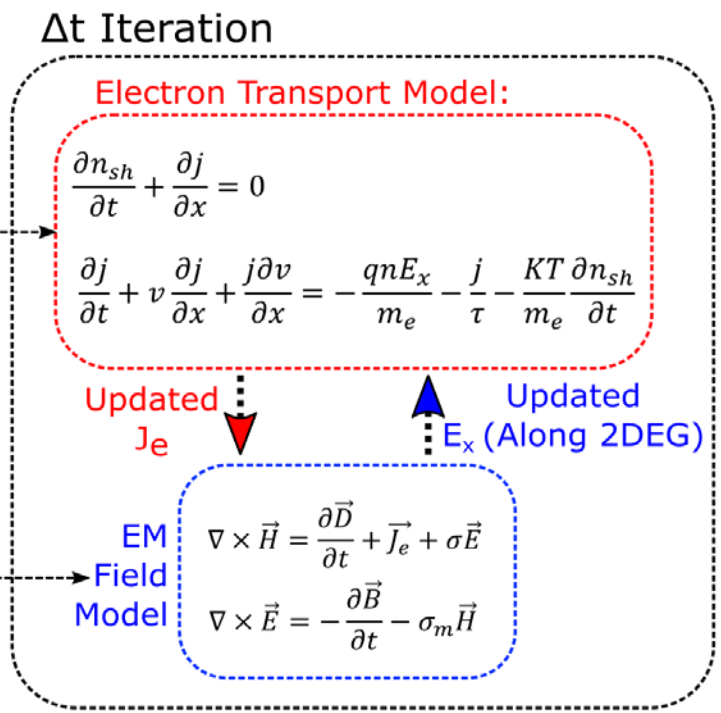
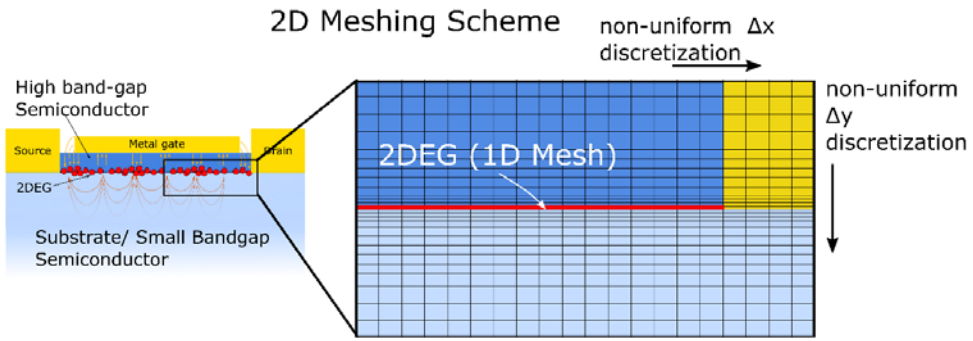
- **Typical Device, Equation-solution and Discretization Scheme.**
- **FDTD-HD model**







n_{sh}: Sheet electron density;
v: electron velocity;
$j = n_{sh}v$ is the sheet current in the channel;
E_x: Longitudinal field in the Channel;

1. Modeling the EM media using Maxwell's equations and electron-transport using Hydrodynamic Equations.
2. Self-consistency achieved using updating HD and FDTD solver with Ex and Je within each time -iterations

3. Shubhendu Bhardwaj, Siddharth Rajan, and John L. Volakis. Analysis of plasma-modes of a gated bilayer system in high electron mobility transistors. *Journal of Applied Physics*, 119(19), 2016
4. Shubhendu Bhardwaj, Berardi Sensale-Rodriguez, Huili Grace Xing, Siddharth Rajan, and John L. Volakis. Resonant tunneling assisted propagation and amplication of plasmons in high electron mobility transistors. *Journal of Applied Physics,* 119(1):013102, 2016
5. Shubhendu Bhardwaj, N. K. Nahar, Siddharth Rajan, and John L. Volakis. Numerical Analysis of Terahertz Emissions From an Ungated HEMT Using Full-Wave Hydrodynamic Model. IEEE Transactions on Electron Devices, 63(3):990 996, March 2016K
6. Khorrami, M.A.; El-Ghazaly, S.; et.al. Global Modeling of Active Terahertz Plasmonic Devices," IEEE THz Sci &Tech – Jan 2014

Difference Equations for the FDTD-HD model

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ME Equation time/space discretization-

$$E_y|_{i+1/2,j}^{n+1} = E_y|_{i+1/2,j}^{n}\left(\frac{1-\sigma_x\Delta t/2\epsilon}{1+\sigma_x\Delta t/2\epsilon}\right) - \left(\frac{1}{1+\sigma_x\Delta t/2\epsilon}\right)\frac{\Delta t}{\Delta x\epsilon}\left[H_z|_{i+1,j}^{n+1/2} - H_z|_{i,j}^{n+1/2}\right] \tag{2.10}$$

$$E_x|_{i,j+1/2}^{n+1} = E_x|_{i,j+1/2}^{n}\left(\frac{1-\sigma_y\Delta t/2\epsilon}{1+\sigma_y\Delta t/2\epsilon}\right) + \left(\frac{1}{1+\sigma_y\Delta t/2\epsilon}\right)\frac{\Delta t}{\Delta y\epsilon}\left[H_z|_{i,j+1}^{n+1/2} - H_z|_{i,j}^{n+1/2}\right] - \frac{\Delta t J_e}{\epsilon} \tag{2.11}$$

$$H_{zx}|_{i,j}^{n+1/2} = H_{zx}|_{i,j}^{n-1/2}\left(\frac{1-\sigma_{xm}\Delta t/2\mu}{1+\sigma_{xm}\Delta t/2\mu}\right) - \left(\frac{1}{1+\sigma_x^*\Delta t/2\mu}\right)\frac{\Delta t}{\Delta x\mu}\left[E_y|_{i+1/2,j}^{n} - E_y|_{i-1/2,j}^{n}\right] \tag{2.12}$$

$$H_{zy}|_{i,j}^{n+1/2} = H_{zy}|_{i,j}^{n-1/2}\left(\frac{1-\sigma_{ym}\Delta t/2\mu}{1+\sigma_{ym}\Delta t/2\mu}\right) + \left(\frac{1}{1+\sigma_y^*\Delta t/2\mu}\right)\frac{\Delta t}{\Delta y\mu}\left[E_x|_{i,j+1/2}^{n} - E_x|_{i,j-1/2}^{n}\right] \tag{2.13}$$

Upwind Scheme for Hydrodynamic Equations-

$$n_{sh}|_i^{n+1} = n_{sh}|_i^n - \frac{\Delta t}{\Delta x}[j|_{i+1/2}^n - j|_{i-1/2}^n], \tag{2.6}$$

$$j|_{i+1/2}^{n+1} = j|_{i+1/2}^n - \Delta t\frac{q n_{sh}|_{i+1/2}^n E_{ch}|_{i+1/2}^n}{m_e} - \Delta t\frac{j|_{i+1/2}^n}{\tau_n} - \Delta t\frac{KT}{m_e}\frac{\left[n_{sh}|_{i+1}^n - n_{sh}|_i^n\right]}{\Delta x} - Conv|_{i+1/2}^n \tag{2.7}$$

Convective Term Definition for Upwind-

For $v|_{i+1/2}^n > 0$, we define

$$Conv|_{i+1/2}^n = \frac{\Delta t}{\Delta x}j|_{i+1/2}^n\left[v|_{i+1/2}^n - v|_{i-1/2}^n\right] + \frac{\Delta t}{\Delta x}v|_{i+1/2}^n\left[j|_{i+1/2}^n - j|_{i-1/2}^n\right] \tag{2.8}$$

and for $v|_{i+1/2}^n < 0$, we define

$$Conv|_{i+1/2}^n = \frac{\Delta t}{\Delta x}j|_{i+1/2}^n\left[v|_{i+3/2}^n - v|_{i+1/2}^n\right] + \frac{\Delta t}{\Delta x}v|_{i+1/2}^n\left[j|_{i+3/2}^n - j|_{i+1/2}^n\right] \tag{2.9}$$

Hybrid Full-wave Hydrodynamic Modeling: Typical Solution

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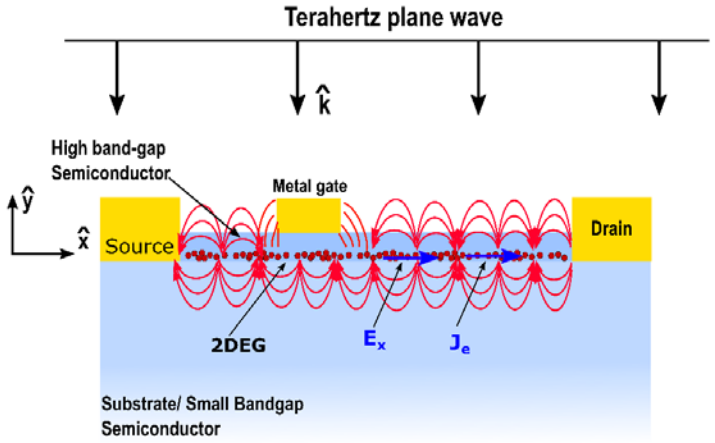
1. A plane wave of freq.= 3 THz is incident on the HEMT structure with small gate discontinuity.
2. The diffracted wave couples to plasmonic modes within 2DEG and propagates away from the channel.
3. The phenomenon was modeled using the developed solver to understand and verify its operation.

Simulation Schematic

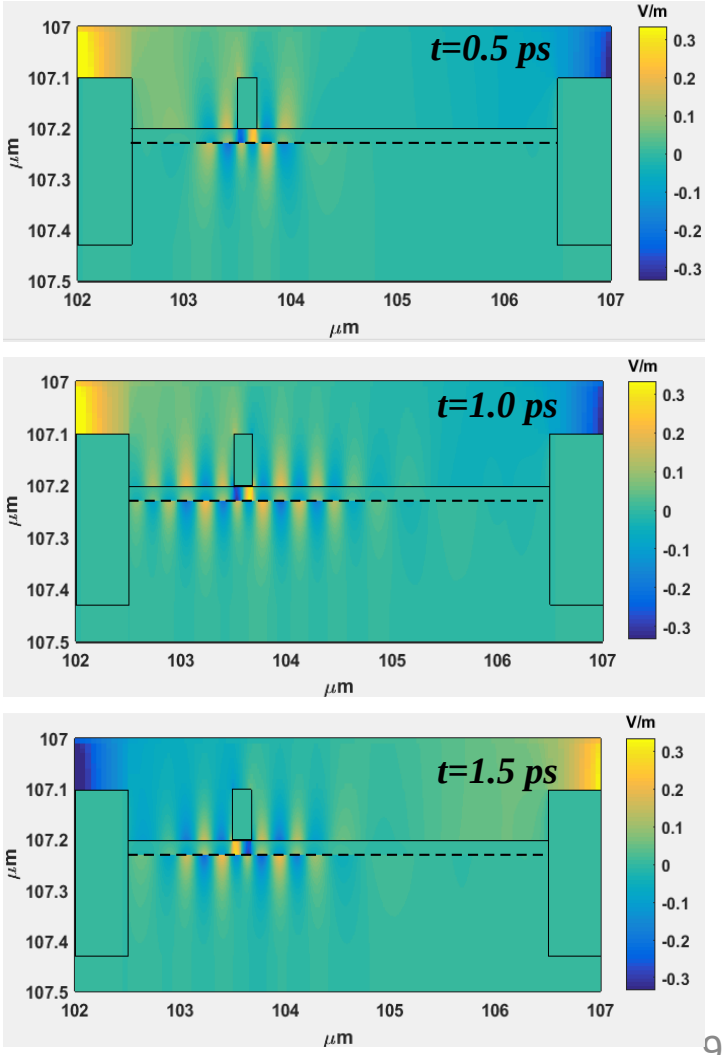


2DEG / material Properties chosen:

Electron Sheet Concentration, (n_{sh})	5e12 cm^{-2}
Effective electron mass, (m_e)	0.2 m_o
Momentum Relaxation time (τ)	1.14 ps
Dielectric Constant (ε_r)	9.5

✓ Tool can become powerful method for visualizing fields and phenomenology within HEMTs.

Simulation results (E-field profiles)



Model Validation using Classical Analytical Results

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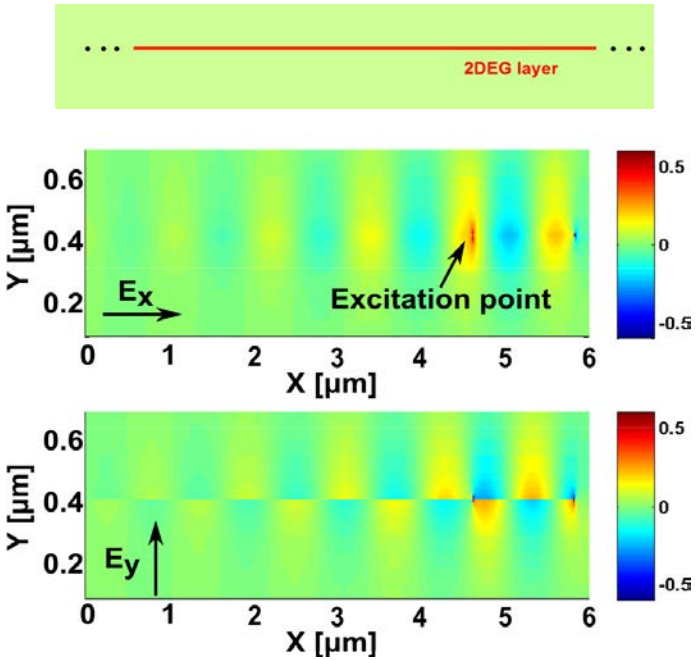
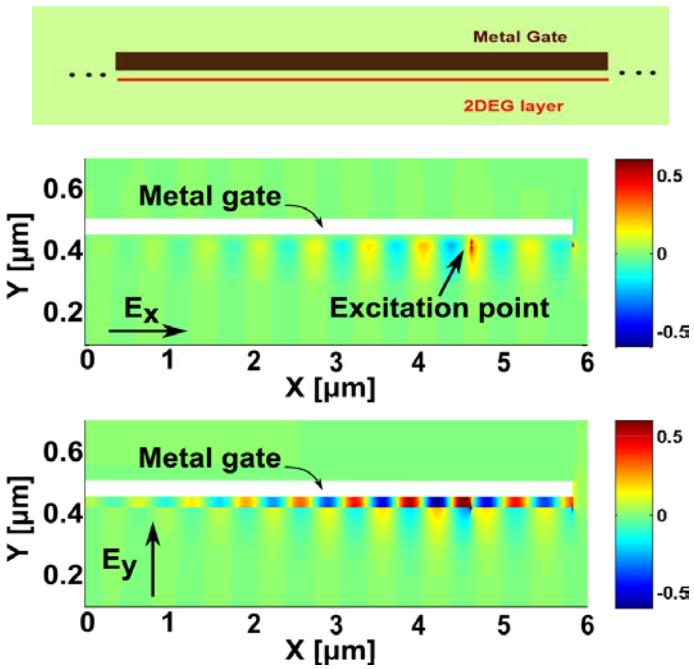
Validation by Simulation of Classically known cases

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

Case 1: 2DEG in bulk dielectric



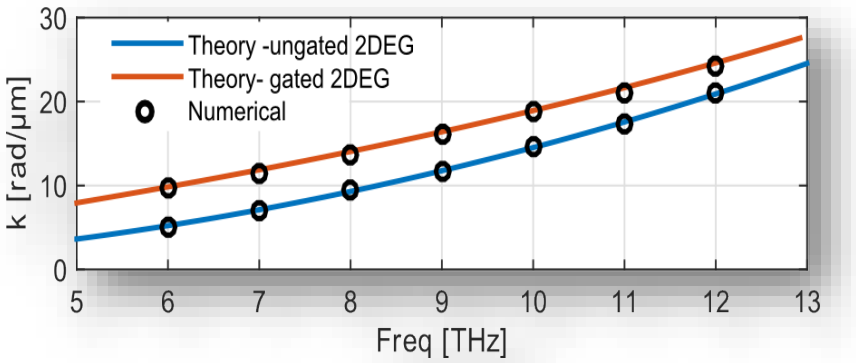
Case-2: Gated- 2DEG in bulk dielectric



ϵ_r=13.9, $m_e = 0.042m_o$, $n_{sh} = 1 \times 10^{13} cm^{-2}$, for gated case d_{barr}=38 nm, μ=10,000 cm²/(V.s)

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

- Comparison of Dispersion curve with classical formulae:



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

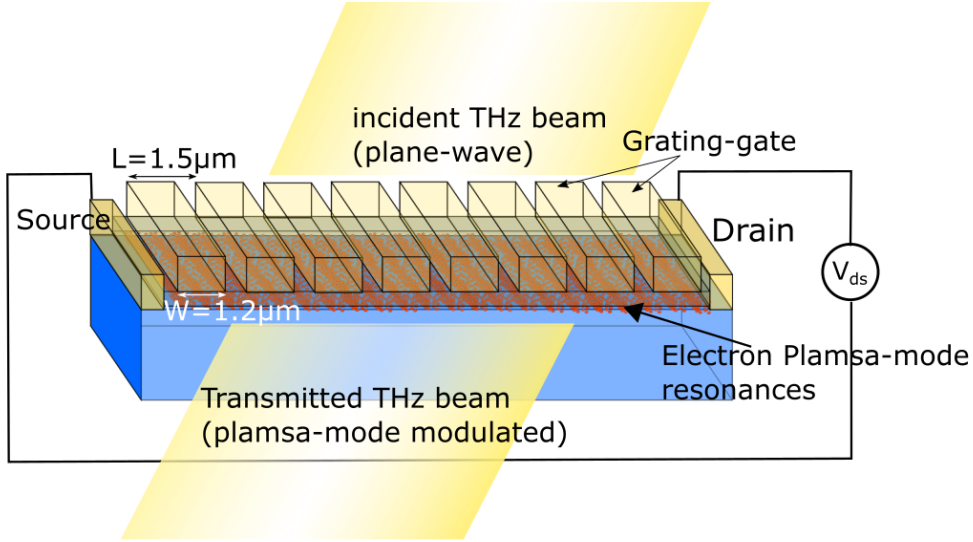
$$\omega = \sqrt{\frac{n_{sh} q^2}{m_e} k \frac{1}{\varepsilon_c + \varepsilon_{ox} \coth(kd)}}$$

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

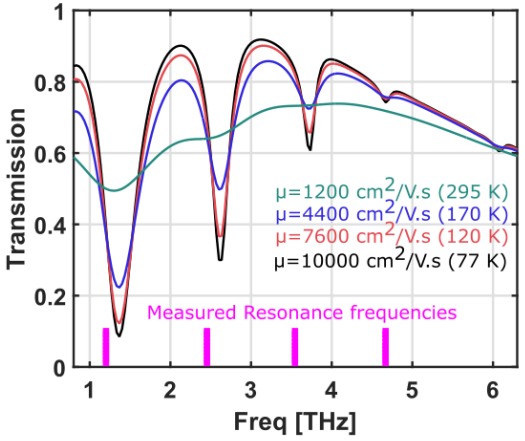
$$k = \frac{\omega^2}{2a}; a = \frac{n_{sh} q^2}{4 m_e \varepsilon_c}$$

[7] A. Eguiluz, T. Lee, J. Quinn, and K. Chiu, "Interface excitations in metal-insulator-semiconductor structures," Physical Review B, vol. 11, no. 12, p. 4989, 1975.
[8] F. Stern, "Polarizability of a two-dimensional electron gas," Physical ReviewLetters, vol. 18, no. 14, p. 546, 1967.

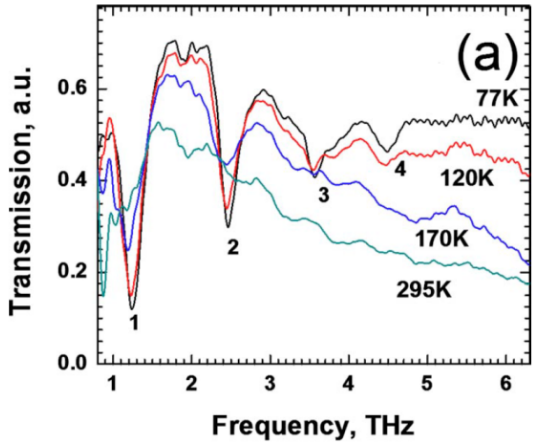
Experimental Validation of Developed Model



Simulated
(Full-wave-hydrodynamic)



Measured
(Muravjov et. al.)



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

[9] Muravjov, A. V. , M.Shur et. Al. "Temperature dependence of plasmonic terahertz absorption in grating-gate gallium-nitride transistor structures" *Applied Physics Letters*, 96, 042105 (2010)

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Conclusions and Summary

Time Limitations in Traditional FDTD-HD Algorithm

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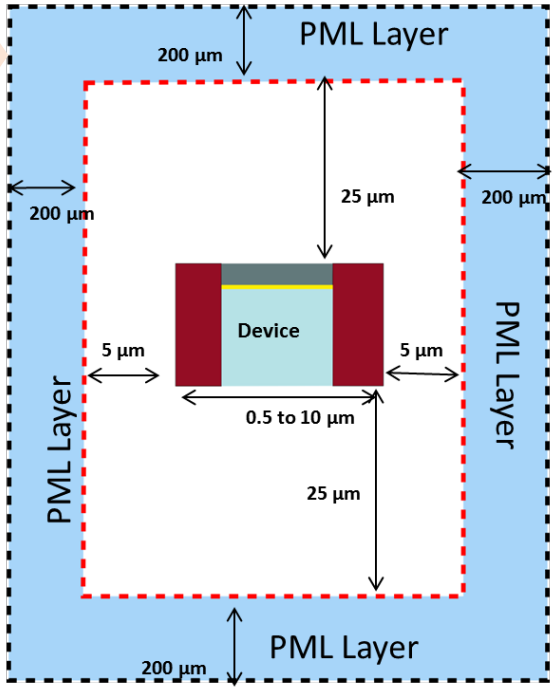
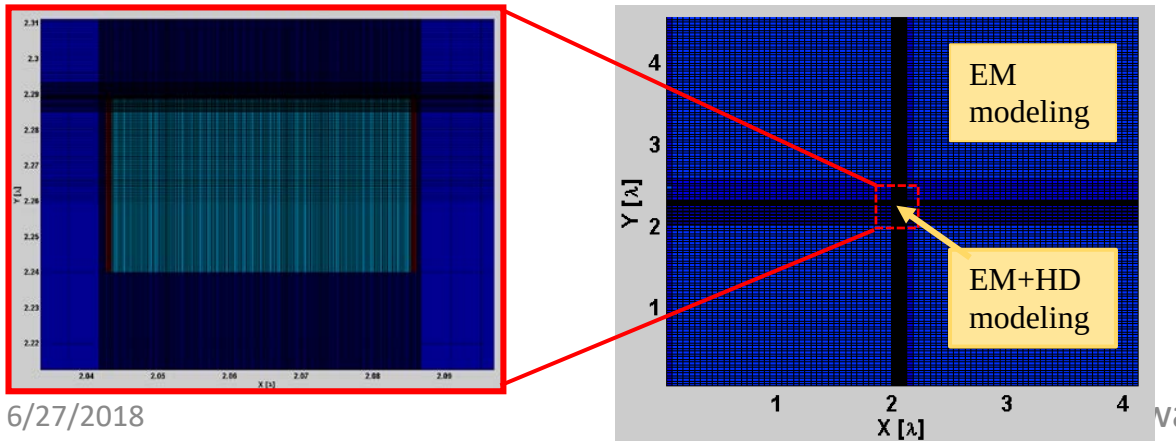
- Typical device model and simulation domain.
- As noted domain is much larger compared 2DEG region.

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 $\lambda/10^4$)

$$L_D = \sqrt{\frac{\varepsilon_r \varepsilon_o K_B T}{q^2 N_D}} \approx 5nm@1e12cm^{-2}$$

- 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)

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Maxwell's Equations for TE_z mode fields: (odd-even splitting: A, B)

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

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

Applying the Crank Nicholson scheme for Δt(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. Δ*t* can be larger than that dictated by Courant Condition). We write them as:

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

Approximation: Remove the Δt^2 term:

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

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

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

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

[13] Shumin Wang, F. L. Teixeira and Ji Chen, "An iterative ADI-FDTD with reduced splitting error," in *IEEE Microwave and Wireless Components Letters*, vol. 15, no. 2, pp. 92-94, Feb. 2005.
[12] T. Namiki, "A new FDTD algorithm based on alternating-direction implicit method," in *IEEE Transactions on Microwave Theory and Techniques*, vol. 47, no. 10, pp. 2003-2007, Oct 1999.

Implicit Equations for ADI-FDTD Method (Step-1)

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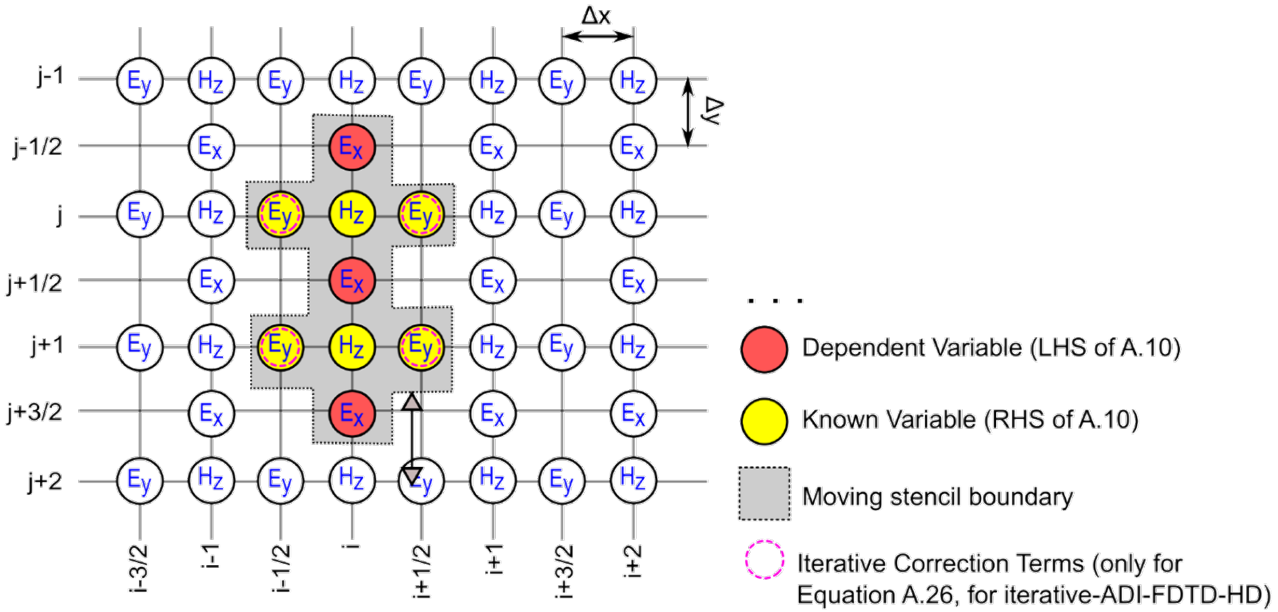
Implicit Equations for E_x determination

$$
\begin{aligned}
&\boxed{E_x|^{tmp}_{i,j+1/2}}\left[1+\Delta t^2\left(\frac{C_{exh}}{2\epsilon\Delta y}\right)_{i,j+1/2}\left(\frac{C_{hzex}}{2\mu\Delta y}\right)_{i,j+1}+\Delta t^2\left(\frac{C_{exh}}{2\epsilon\Delta y}\right)_{i,j+1/2}\left(\frac{C_{hzex}}{2\mu\Delta y}\right)_{i,j}\right]\\
&+\boxed{E_x|^{tmp}_{i,j-1/2}}\left[-\Delta t^2\left(\frac{C_{exh}}{2\epsilon\Delta y}\right)_{i,j+1/2}\left(\frac{C_{hzex}}{2\mu\Delta y}\right)_{i,j+1}\right] \qquad \ldots\\
&+\boxed{E_x|^{tmp}_{i,j+3/2}}\left[-\Delta t^2\left(\frac{C_{exh}}{2\epsilon\Delta y}\right)_{i,j+1/2}\left(\frac{C_{hzex}}{2\mu\Delta y}\right)_{i,j+1}\right]\\
&=C_{exe}|_{i,j+1/2}E_x|^n_{i,j+1/2}+\Delta t\left(\frac{C_exh}{2\epsilon\Delta y}\right)_{i,j+1/2}\Big[C_{hzhy}|_{i,j+1}H_{zy}|^n_{i,j+1}+C_{hzhy}|_{i,j+1}H_{zy}|^n_{i,j+1}\\
&-C_{hzhy}|_{i,j}H_{zy}|^n_{i,j}-C_{hzhy}|_{i,j}H_{zy}|^n_{i,j}\Big]-\Delta t^2\left(\frac{C_{exh}}{2\epsilon\Delta y}\right)_{i,j+1}\Big[\left(\frac{C_{hxex}}{2\mu\Delta x}\right)_{i,j+1}\Big(E_y|^n_{i+1/2,j+1}\\
&-E_y|^n_{i-1/2,j+1}\Big)-\left(\frac{C_{hxey}}{2\mu\Delta y}\right)_{i,j}\Big(E_y|^n_{i+1/2,j}-E_y|^n_{i-1/2,j}\Big)\Big].
\end{aligned}
$$

$$
\begin{aligned}
E_y|^{tmp}_{i-1/2,j} &= C_{eye}|_{i-1/2,j}E^n_y|_{i-1/2,j}\\
&-\Delta t\left(\frac{C_{eyh}}{2\epsilon\Delta x}\right)_{i-1/2,j}\Big[H_{zy}|^n_{i,j}+H_{zy}|^n_{i,j}-H_{zy}|^n_{i-1,j}+H_{zy}|^n_{i-1,j}\Big]
\end{aligned}
\tag{A.11}
$$

$$
H_{zx}|^{tmp}_{i,j}=C_{hzhx}|_{i,j}H^n_{zx}|_{i,j}-\Delta t\left(\frac{C_{hzey}}{2\mu\Delta x}\right)_{i,j}\Big[E_y|^n_{i+1/2,j}-E_y|^n_{i-1/2,j}\Big] \tag{A.12}
$$

$$
H_{zy}|^{tmp}_{i,j}=C_{hzhy}|_{i,j}H^n_{zx}|_{i,j}+\Delta t\left(\frac{C_{hzex}}{2\mu\Delta y}\right)_{i,j}\Big[E_x|^{tmp}_{i,j+1/2}-E_x|^{tmp}_{i,j-1/2}\Big] \tag{A.13}
$$



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.

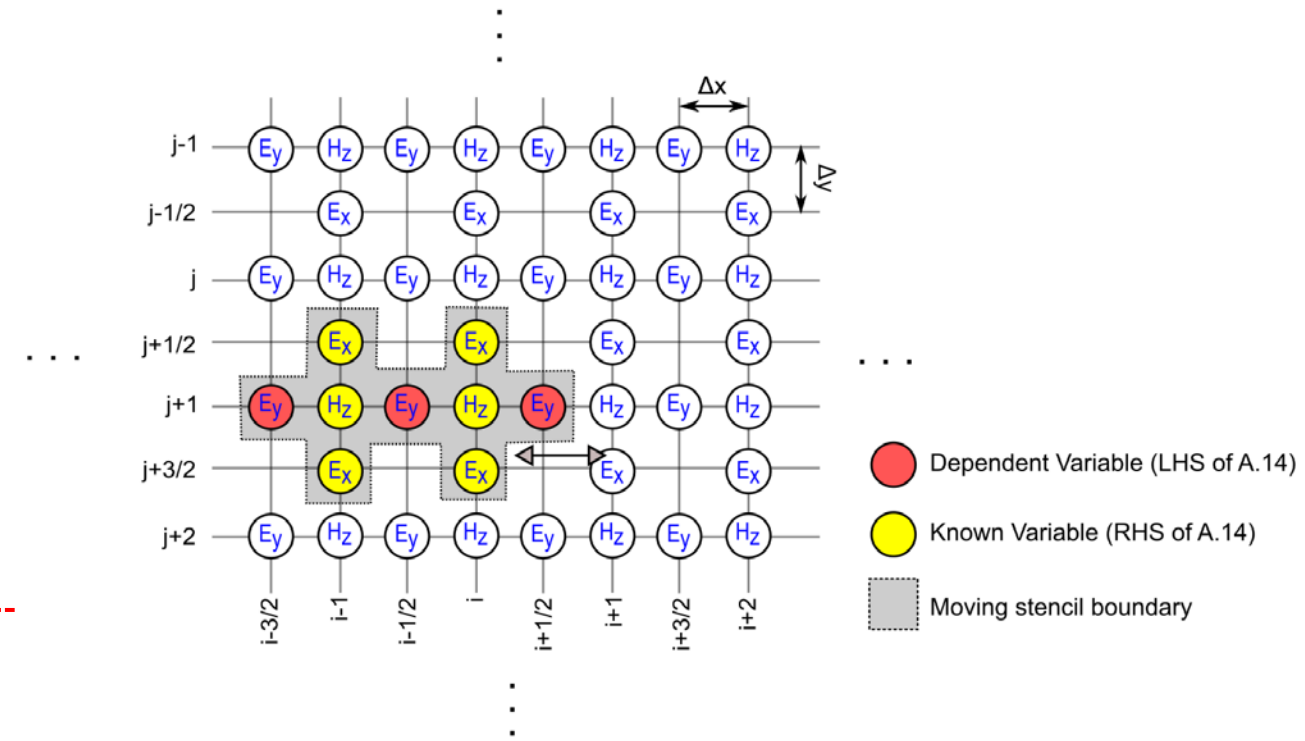
Implicit Equations ADI-FDTD Step-2

$$
\begin{aligned}
&E_y|^{n+1}_{i-1/2,j}\left[1+\Delta t^2\left(\frac{C_{eyh}}{2\epsilon\Delta x}\right)_{i-1/2,j}\left(\frac{C_{hzey}}{2\mu\Delta x}\right)_{i,j}+\Delta t^2\left(\frac{C_{eyh}}{2\epsilon\Delta x}\right)_{i-1/2,j}\left(\frac{C_{hzey}}{2\mu\Delta x}\right)_{i-1,j}\right]\\
&+E_y|^{n+1}_{i+1/2,j}\left[-\Delta t^2\left(\frac{C_{eyh}}{2\epsilon\Delta x}\right)_{i-1/2,j}\left(\frac{C_{hzey}}{2\mu\Delta x}\right)_{i,j}\right]\\
&+E_y|^{n+1}_{i-3/2,j}\left[-\Delta t^2\left(\frac{C_{eyh}}{2\epsilon\Delta x}\right)_{i-1/2,j}\left(\frac{C_{hzey}}{2\mu\Delta x}\right)_{i-1,j}\right]\\
&=C_{eye}|_{i-1/2,j}E_y|^{tmp}_{i-1/2,j}-\Delta t\left(\frac{C_{eyh}}{2\epsilon\Delta x}\right)_{i-1/2,j}\left[C_{hzhx}|_{i,j}H_{zy}|^{tmp}_{i,j}+C_{hzhy}|_{i,j}H_{zy}|^{tmp}_{i,j}\right.\\
&\left.-C_{hzhy}|_{i-1,j}H_{zy}|^{tmp}_{i-1,j}-C_{hzhy}|_{i-1,j}H_{zy}|^{tmp}_{i-1,j}\right]-\Delta t^2\left(\frac{C_{eyh}}{2\epsilon\Delta y}\right)_{i-1/2,j}\left[\left(\frac{C_{hzex}}{2\mu\Delta y}\right)_{i,j}\left(E_x|^{tmp}_{i,j+1/2}\right.\right.\\
&\left.\left.-E_x|^{tmp}_{i,j-1/2}\right)-\left(\frac{C_{hzex}}{2\mu\Delta y}\right)_{i-1,j}\left(E_x|^{tmp}_{i-1,j+1/2}-E_x|^{tmp}_{i-1/2,j-1/2}\right)\right].
\end{aligned}
\tag{A.14}
$$

$$
\begin{aligned}
E_x|^{n+1}_{i,j+1/2}&=C_{exe}|_{i,j+1/2}E_x|^{tmp}_{i,j+1/2}\\
&-\Delta t\left(\frac{C_{exh}}{2\epsilon\Delta y}\right)_{i,j+1/2}\left[H_{zx}|^{tmp}_{i,j+1}+H_{zy}|^{tmp}_{i,j+1}-H_{zx}|^{tmp}_{i,j}-H_{zy}|^{tm}_{i,j}\right]
\end{aligned}
$$

$$
H_{zx}|^{n+1}_{i,j}=C_{hzhx}|_{i,j}H_{zx}|^{tmp}_{i,j}-\Delta t\left(\frac{C_{hzey}}{2\mu\Delta x}\right)_{i,j}\left[E_y|^{n+1}_{i+1/2,j}-E_y|^{n+1}_{i-1/2,j}\right]
$$

$$
H_{zy}|^{n+1}_{i,j}=C_{hzhy}|_{i,j}H_{zx}|^{tmp}_{i,j}+\Delta t\left(\frac{C_{hzex}}{2\mu\Delta y}\right)_{i,j}\left[E_x|^{tmp}_{i,j+1/2}-E_x|^{tmp}_{i,j-1/2}\right]
$$



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

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Explicit FDTD-HD Method

Maxwell's Equations: ADI FDTD

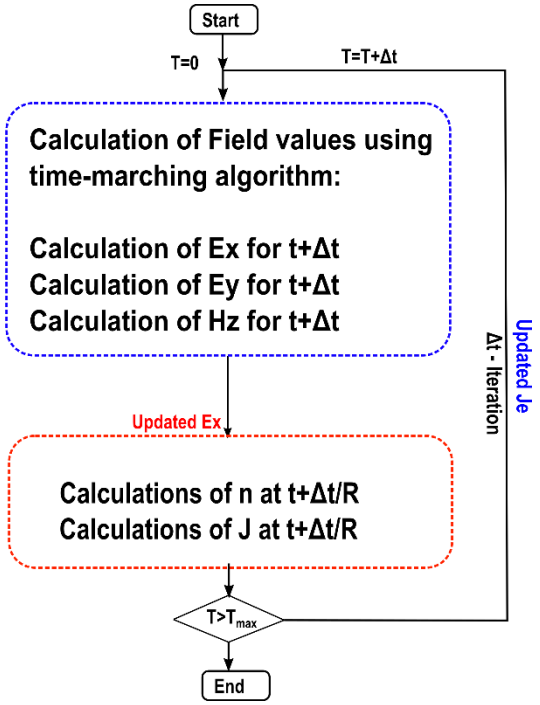
$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J_e} + \sigma \vec{E}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} - \sigma_m \vec{H}$$

Electron-Transport in channel
Hydrodynamic: Upwind Scheme

$$\frac{\partial n_{sh}}{\partial t} + \frac{\partial j}{\partial x} = 0$$

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



- Time-step Limited by $\Delta t \leq \frac{1}{c} / \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}$ $\approx 10^{-17}$s

ADI-FDTD-HD Method

Maxwell's Equations: ADI-FDTD

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J_e} + \sigma \vec{E}$$

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Electron-Transport in channel
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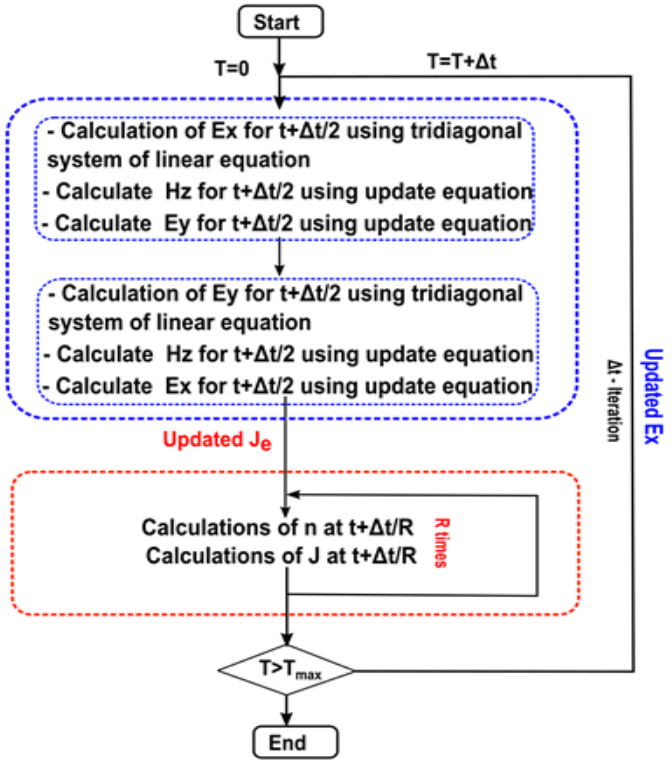
$$\frac{\partial j}{\partial t} + v\frac{\partial j}{\partial x} + \frac{j\partial v}{\partial x} = -\frac{qnE_x}{m_e} - \frac{j}{\tau} - \frac{KT}{m_e}\frac{\partial n_{sh}}{\partial t}$$



- ✓ Unconditionally stable: Δt can be arbitrarily large, with stability.

Time-Improvements Using ADI-FDTD-HD Method

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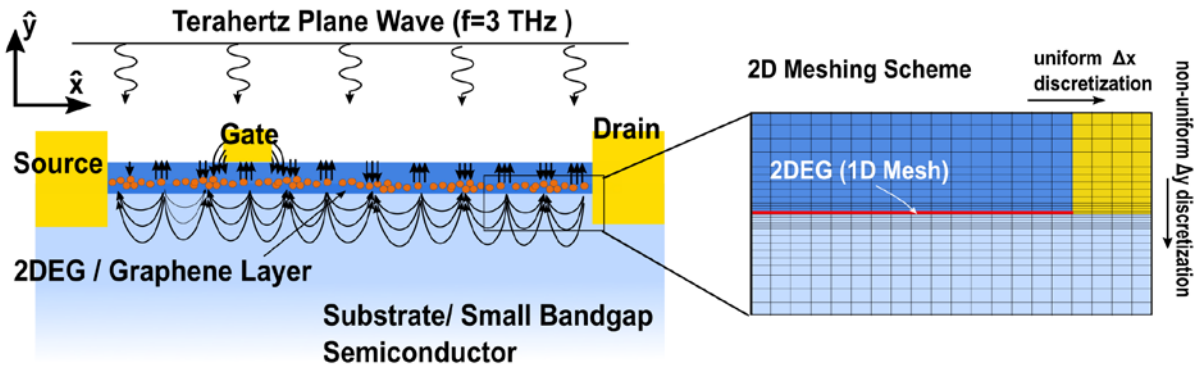
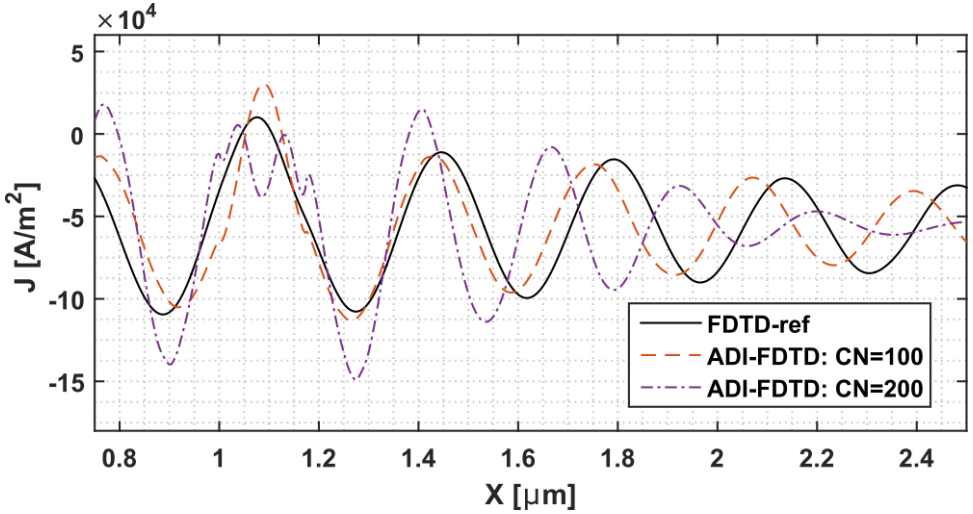
Simulation Set-up:



Simulation time reduction:

	Min. Δx, Δy	ΔT (s)	CPU-time per time-step (s.)	CPU-TIME total (Hrs.)
FDTD-HD	4 nm, 1nm	3.24×10^{-18}	0.35	90
ADI-FDTD-HD, CN=100	4 nm, 1nm	3.24×10^{-16}	7.59	19.57
ADI-FDTD-HD, CN=200	4 nm, 1nm	6.48×10^{-16}	7.59	9.79
ADI-FDTD-HD, CN=300	4 nm, 1nm	9.72×10^{-16}	7.59	6.52

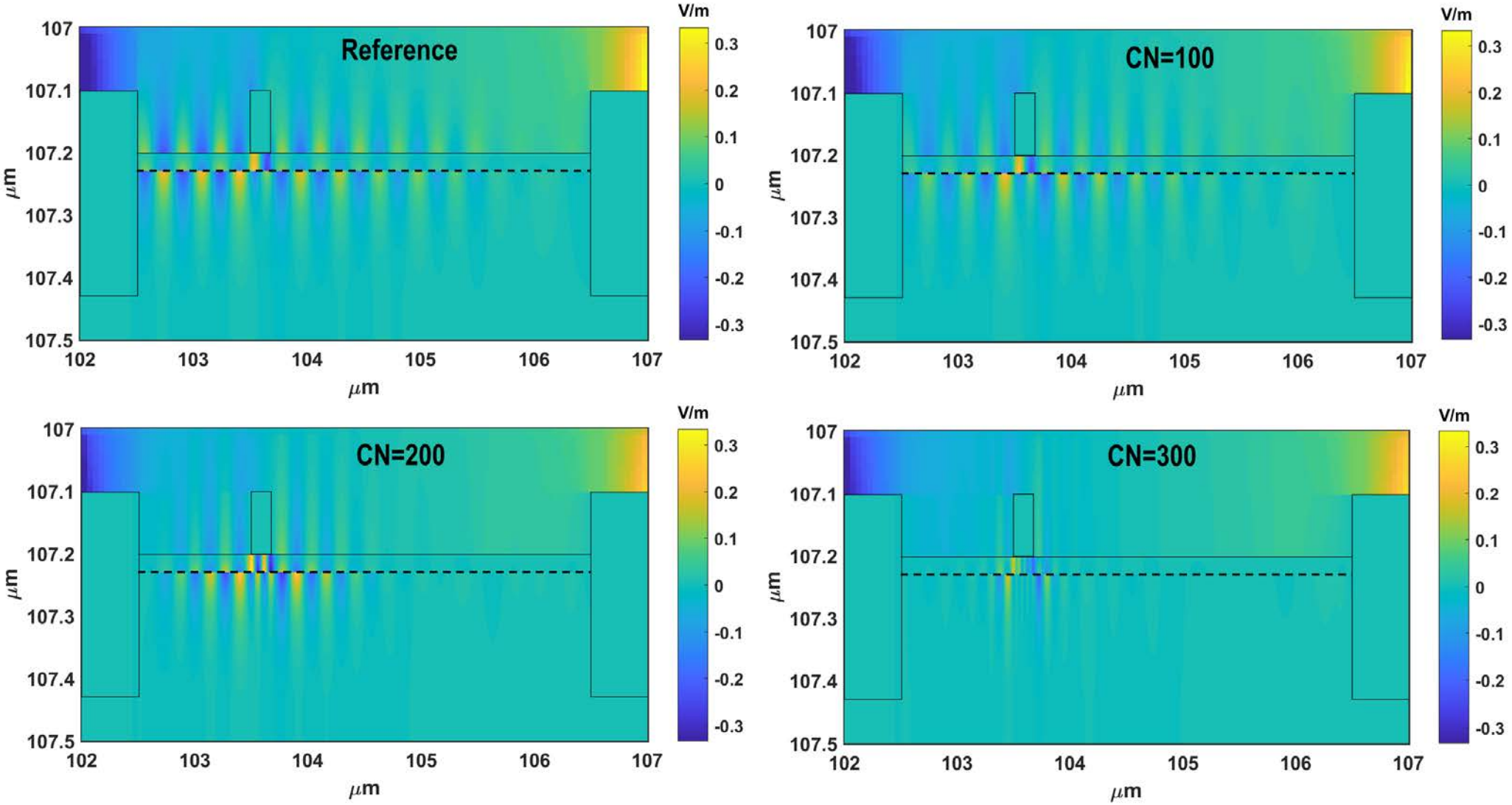
Performance for increasing *CN* ($\Delta t_{ADi} = CN \times \Delta t_{FDTD}$)



- Thus, using ADI-FDTD, we decrease the simulation-times, but as the time reduces errors increase
- To improve accuracy we pursue Iterative-ADI-FDTD

[10] T. Namiki, "A new FDTD algorithm based on alternating-direction implicit method," in *IEEE Transactions on Microwave Theory and Techniques*, vol. 47, no. 10, pp. 2003-2007, Oct 1999.

Field Accuracy Performance of ADI-FDTD-HD



Iterative-ADI-FDTD Method- Overview

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ADI-FDTD Scheme

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

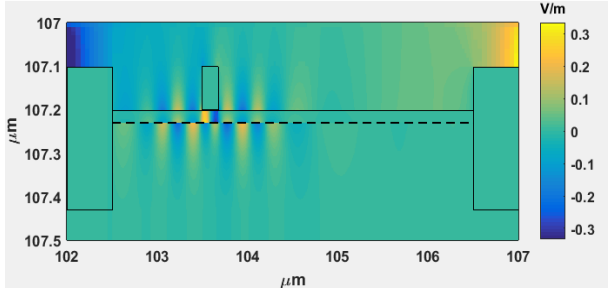
Approximation: Remove the Δt^2 term:

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

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

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

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



Iterative ADI-FDTD Scheme

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

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

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

Implementing ADI Methods

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ADI-FDTD-HD Method

Maxwell's Equations: ADI-FDTD

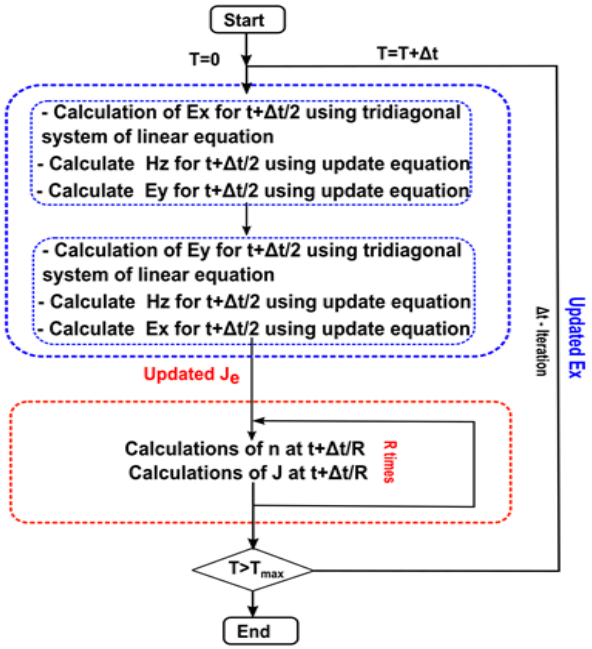
$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J_e} + \sigma \vec{E}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} - \sigma_m \vec{H}$$

Electron-Transport in channel Hydrodynamic: Upwind Scheme

$$\frac{\partial n_{sh}}{\partial t} + \frac{\partial j}{\partial x} = 0$$

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



✓ Unconditionally stable: Δt can be arbitrarily large

Iterative-ADI-FDTD-HD Method

Maxwell's Equations: it-ADI-FDTD

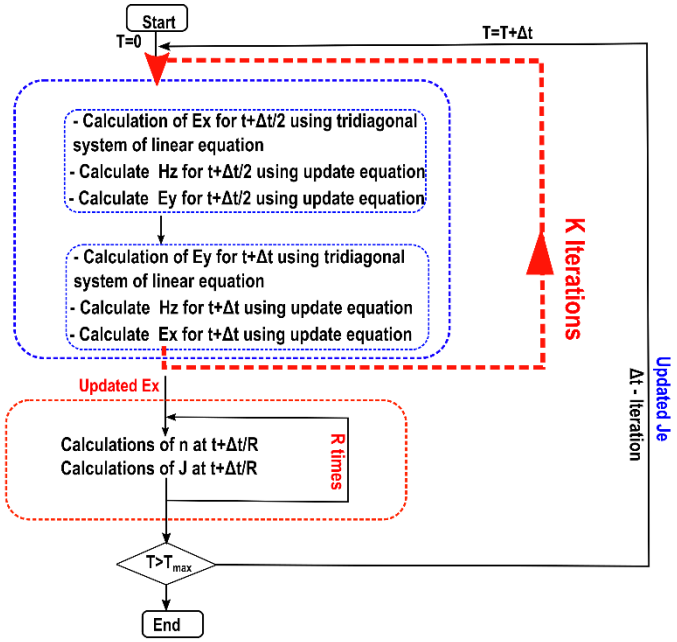
$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J_e} + \sigma \vec{E}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} - \sigma_m \vec{H}$$

Electron-Transport in channel Hydrodynamic: Upwind Scheme

$$\frac{\partial n_{sh}}{\partial t} + \frac{\partial j}{\partial x} = 0$$

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



✓ Unconditionally stable: Δt can be arbitrarily large
✓ Accuracy recovered by iterative method

Iterative ADI-FDTD-HD

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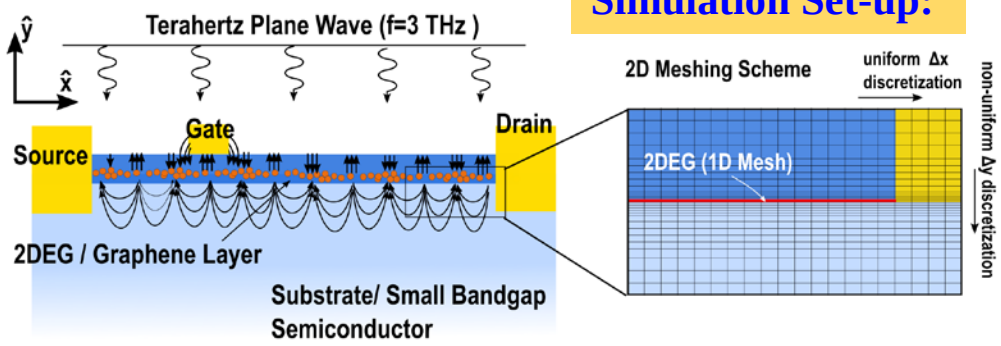
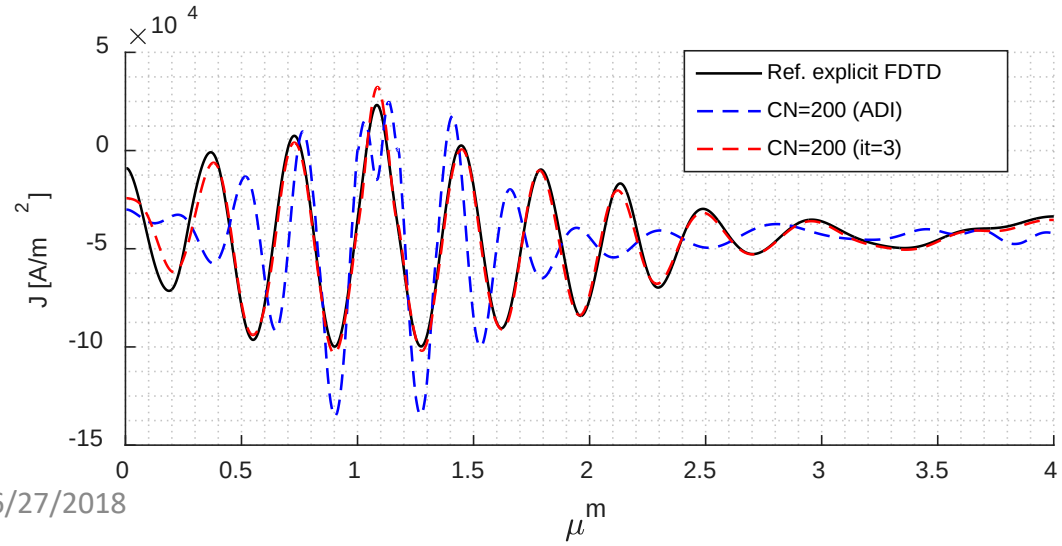
Simulation Set-up:

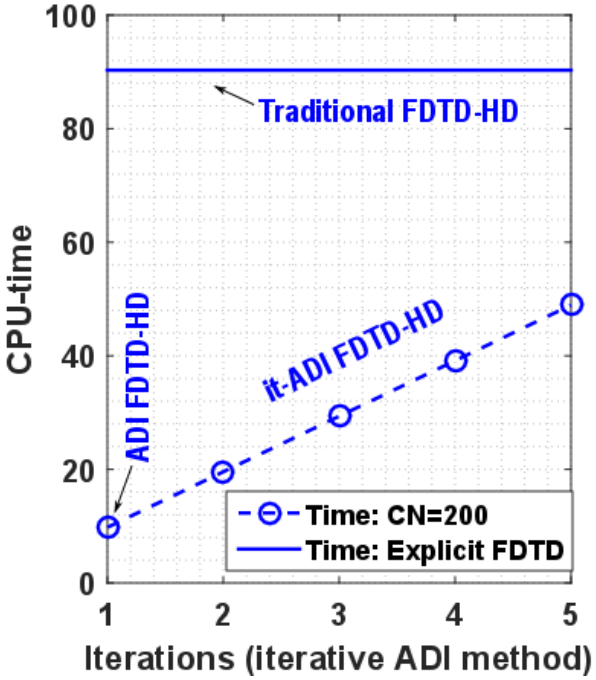


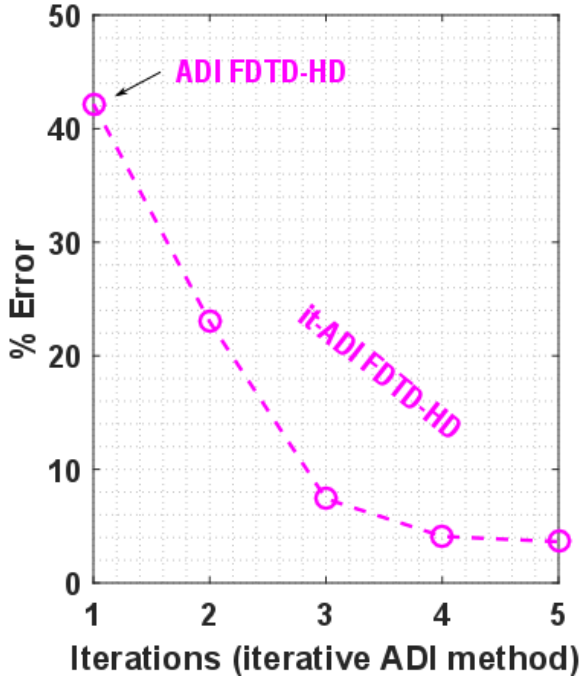
Similar to ADI method, we develop iterative ADI method, that uses corrective iterations as per [11] to fix the accuracy issues with the ADI method.

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

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







[11] Shumin Wang, F. L. Teixeira and Ji Chen, "An iterative ADI-FDTD with reduced splitting error," in *IEEE Microwave and Wireless Components Letters*, vol. 15, no. 2, pp. 92-94, Feb. 2005.

Field Correction using Iterative Method

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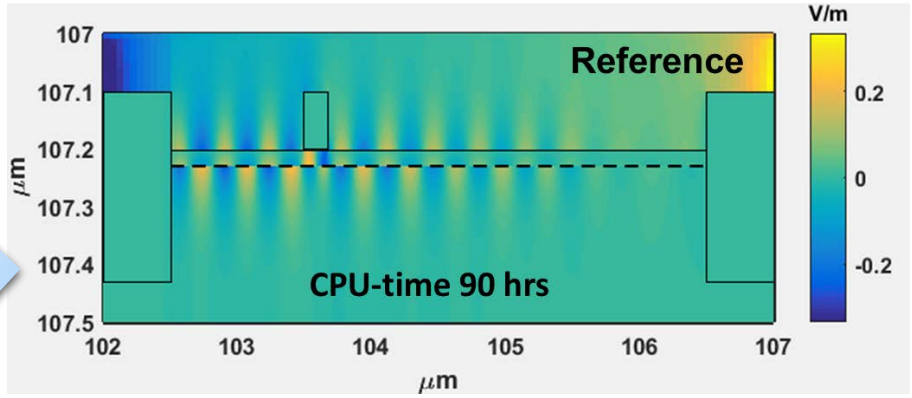
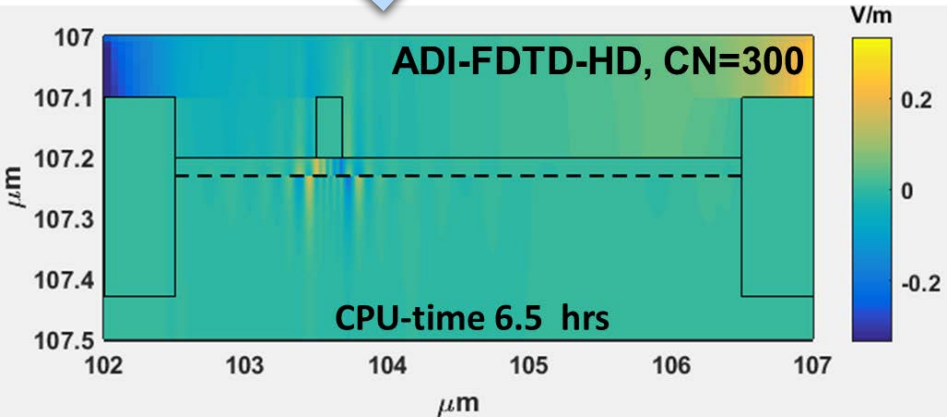
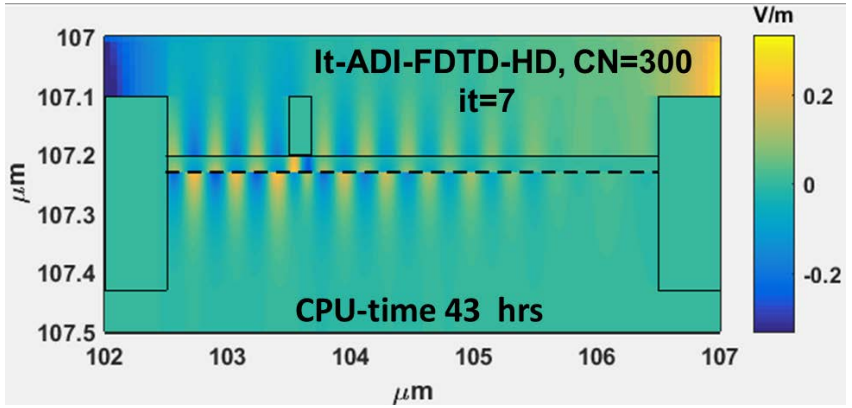


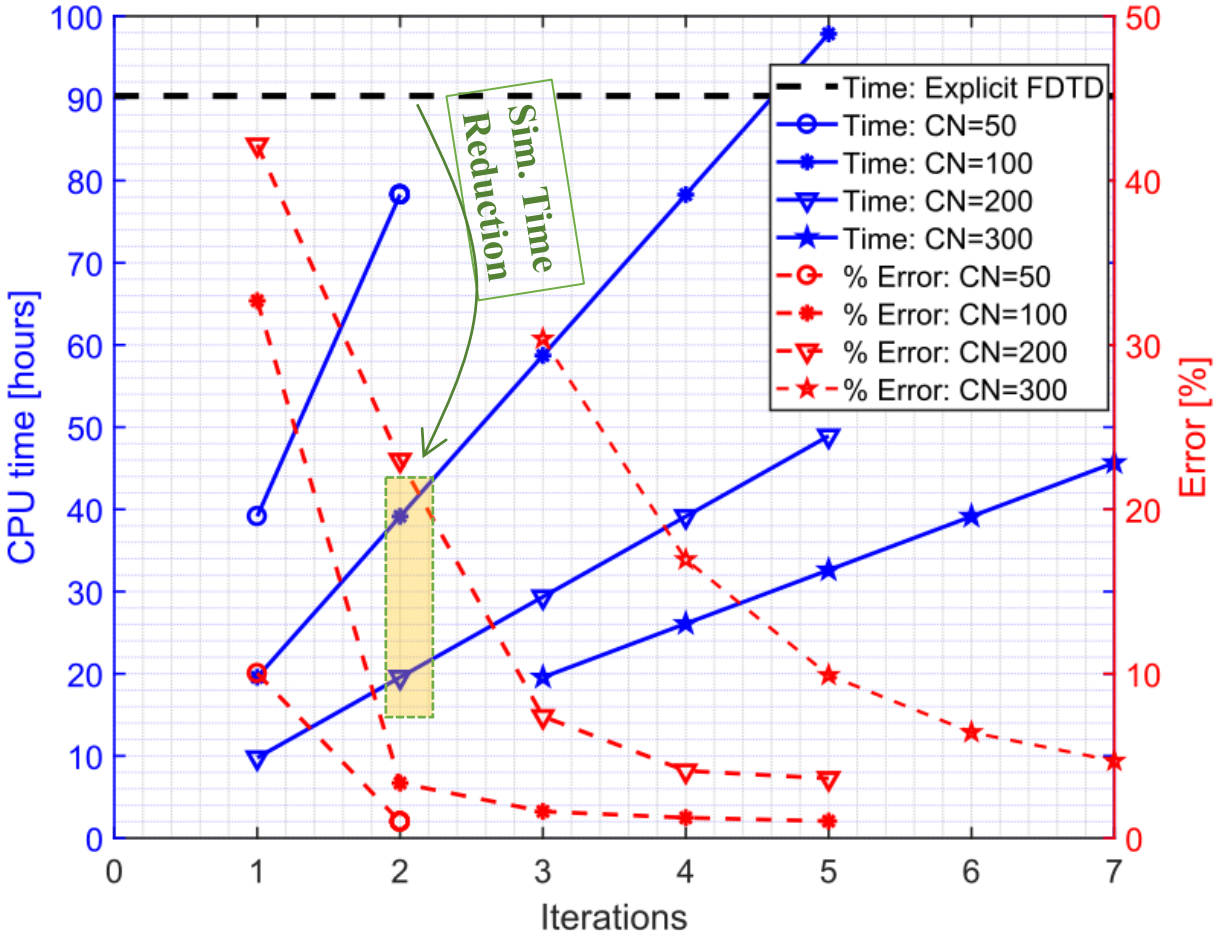
ADI-FDTD-HD method
- **Very fast,**
- **qualitative solution**



Iterative ADI-FDTD-HD method
- **50 % Faster**
- **Accurate Solution**



Summary Time-cost / Error for ADI Methods



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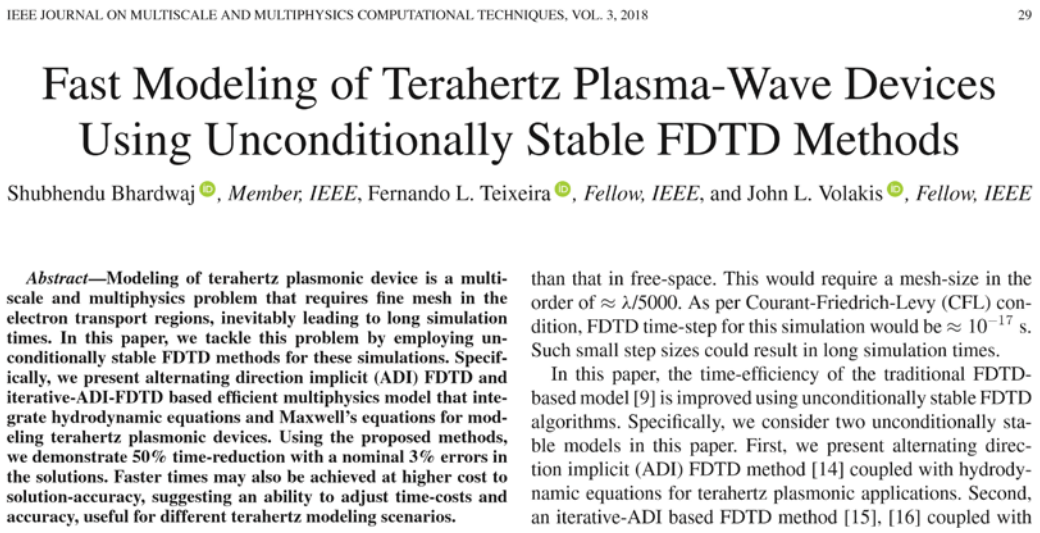

IEEE JOURNAL ON MULTISCALE AND MULTIPHYSICS COMPUTATIONAL TECHNIQUES, VOL. 3, 2018 29

Fast Modeling of Terahertz Plasma-Wave Devices Using Unconditionally Stable FDTD Methods

Shubhendu Bhardwaj, *Member, IEEE*, Fernando L. Teixeira, *Fellow, IEEE*, and John L. Volakis, *Fellow, IEEE*

***Abstract*—Modeling of terahertz plasmonic device is a multi-scale and multiphysics problem that requires fine mesh in the electron transport regions, inevitably leading to long simulation times. In this paper, we tackle this problem by employing unconditionally stable FDTD methods for these simulations. Specifically, we present alternating direction implicit (ADI) FDTD and iterative-ADI-FDTD based efficient multiphysics model that integrate hydrodynamic equations and Maxwell's equations for modeling terahertz plasmonic devices. Using the proposed methods, we demonstrate 50% time-reduction with a nominal 3% errors in the solutions. Faster times may also be achieved at higher cost to solution-accuracy, suggesting an ability to adjust time-costs and accuracy, useful for different terahertz modeling scenarios.**

than that in free-space. This would require a mesh-size in the order of $\approx \lambda/5000$. As per Courant-Friedrich-Levy (CFL) condition, FDTD time-step for this simulation would be $\approx 10^{-17}$ s. Such small step sizes could result in long simulation times.

In this paper, the time-efficiency of the traditional FDTD-based model [9] is improved using unconditionally stable FDTD algorithms. Specifically, we consider two unconditionally stable models in this paper. First, we present alternating direction implicit (ADI) FDTD method [14] coupled with hydrodynamic equations for terahertz plasmonic applications. Second, an iterative-ADI based FDTD method [15], [16] coupled with

- 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

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Introduction to Terahertz Plasmonic Devices

↓

Integrating Hydrodynamic and Electrodynamic Solution: FDTD-HD modeling

↓

Fast and Accurate?
ADI and iterative ADI methods

↓

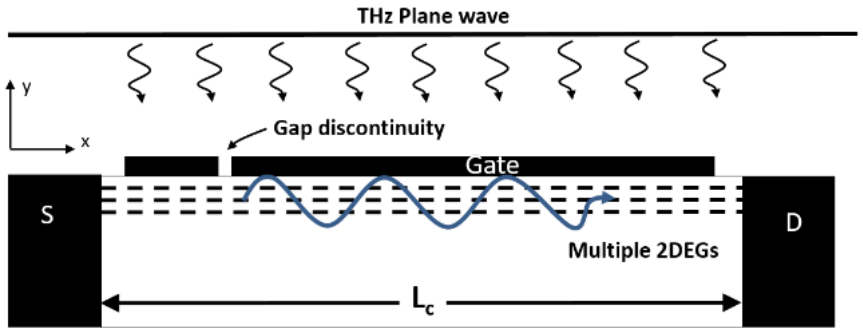
Applications of the developed model
1) 2DEG bilayers 2) Short Channel HEMTs

↓

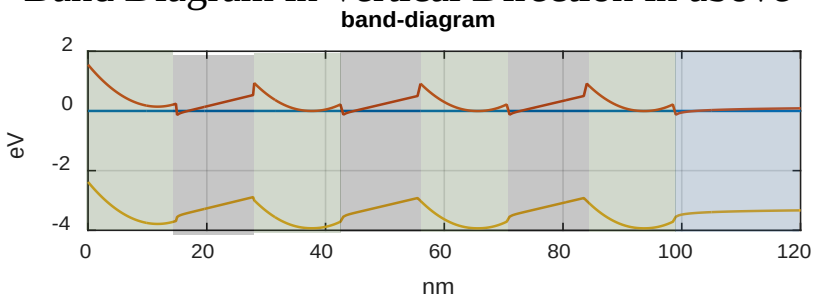
Conclusions and Summary

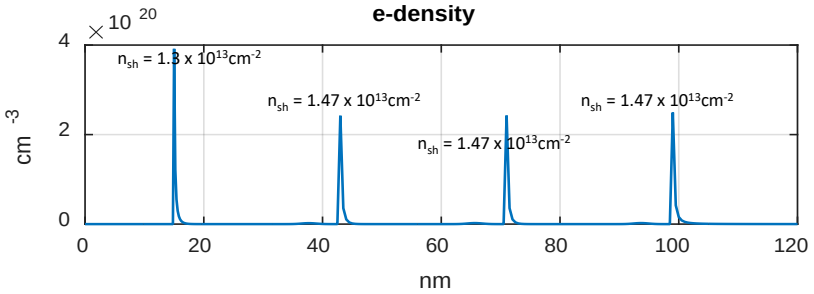
Origin of Multilayer HEMTs

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.



Band Diagram in Vertical Direction in above





AlGaN x=0.22 N_d=1.03e19 cm^{-3}

GaN

GaN Buffer N_d=1e16 cm^{-3}

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

[12] S. Heikman, S. Keller, D. S. Green, S. P. DenBaars, and U. K. Mishra, "High conductivity modulation doped AlGaN/GaN multiple channel heterostructures,"Journal of Applied Physics, vol. 94, no. 8, 2003.

Problem of Plasmonic Modes in Bilayer

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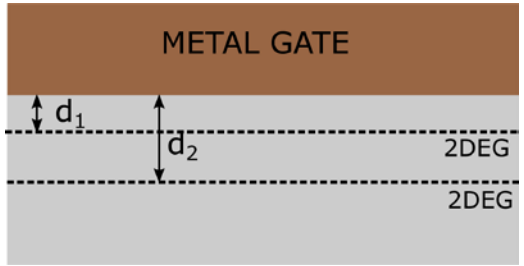
Simplified Geometry Under Consideration:

1. Gated- double 2DEGs



2. Un-gated- double 2DEGs

JOURNAL OF APPLIED PHYSICS **119**, 193102 (2016)

Analysis of plasma-modes of a gated bilayer system in high electron mobility transistors

Shubhendu Bhardwaj, Siddharth Rajan, and John L. Volakis
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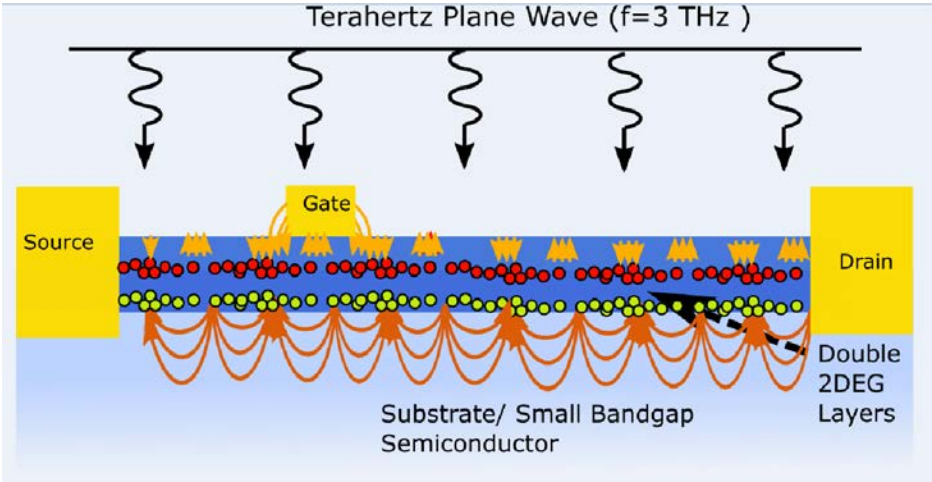
(Received 16 March 2016; accepted 5 May 2016; published online 17 May 2016)

We present rigorous analytical and computational models to study the plasma-waves in a gated-bilayer system present in a double-channel high electron mobility transistor. By analytically deriving the dispersion relations, we have identified the optical and acoustic modes in such systems. We find that the presence of the metal gate selectively modifies the optical plasmons of an ungated-bilayer, while the acoustic plasmons remain largely unchanged. Analysis shows that these modified optical plasmons could be advantageous for resonant and non-resonant plasma-wave devices. The paper further serves to verify our analytical formulae using a full-wave hydrodynamic numerical solver, based on finite difference time domain algorithm. Using the solver, we examine these modes in the gated/ungated bilayers under a plane wave excitation. We observe that, most incident power couples to the optical mode for such an excitation. Nevertheless, acoustic modes can also be excited, if the discontinuity dimensions are optimized accordingly. These observations are also explained using 2D field-plots for the first time, thus providing intuitive understanding of the plasmon excitation in the bilayers. *Published by AIP Publishing.* [http://dx.doi.org/10.1063/1.4950795]

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.

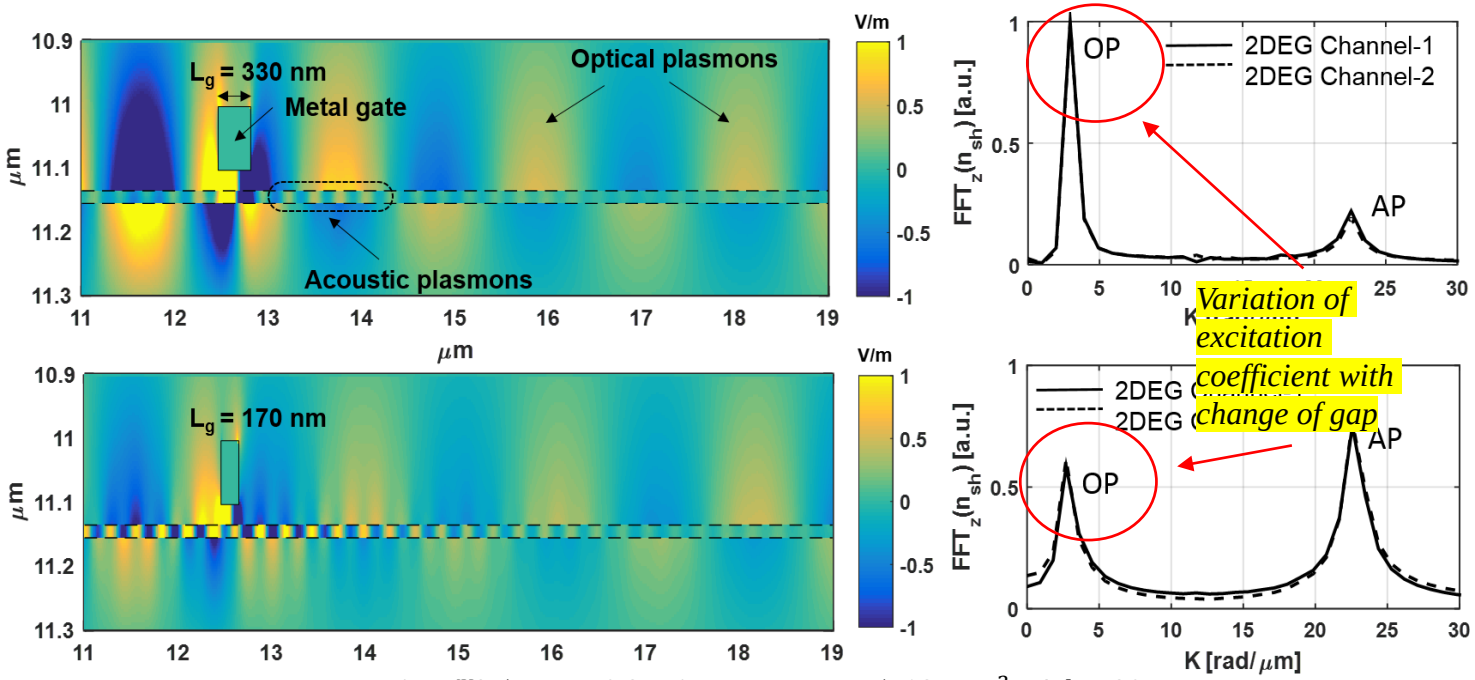
Full-wave Multiphysics modeling of Bilayer



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

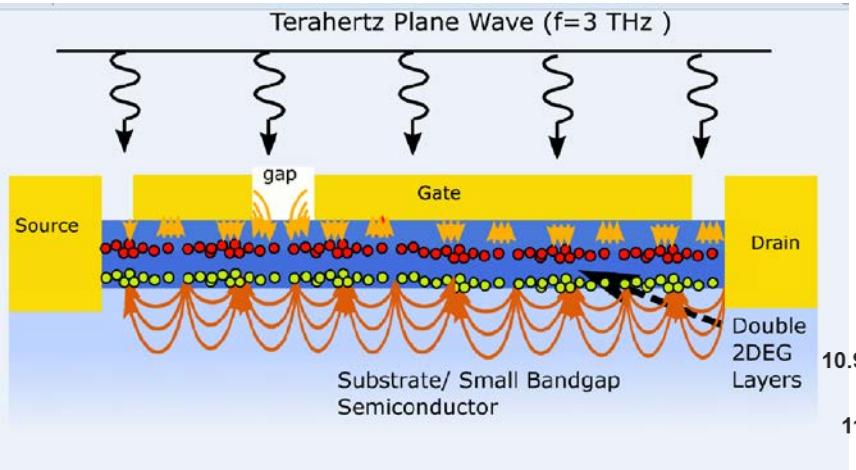
- Both Acoustic and optical modes are observed.
- Acoustic modes are confined between the channel.
- Optical modes are outside the channel.

E_y Fields at (t=12 ps)



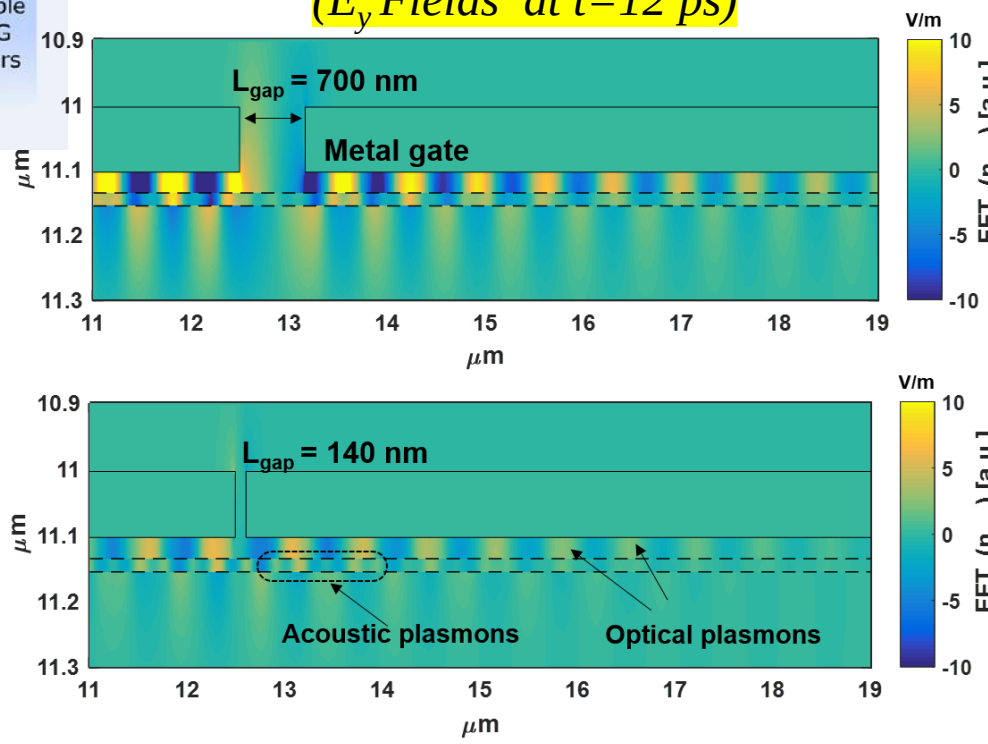
GaN material System ($\epsilon_r = 9.5, m_e = 0.2m_o$), $n_{o1} = n_{o2} = 5e12\ cm^{-2}$, $\Delta d = 20\ nm, \mu = 10{,}000\ cm^2/(V.s)$

Modeling of Gated-Bilayer

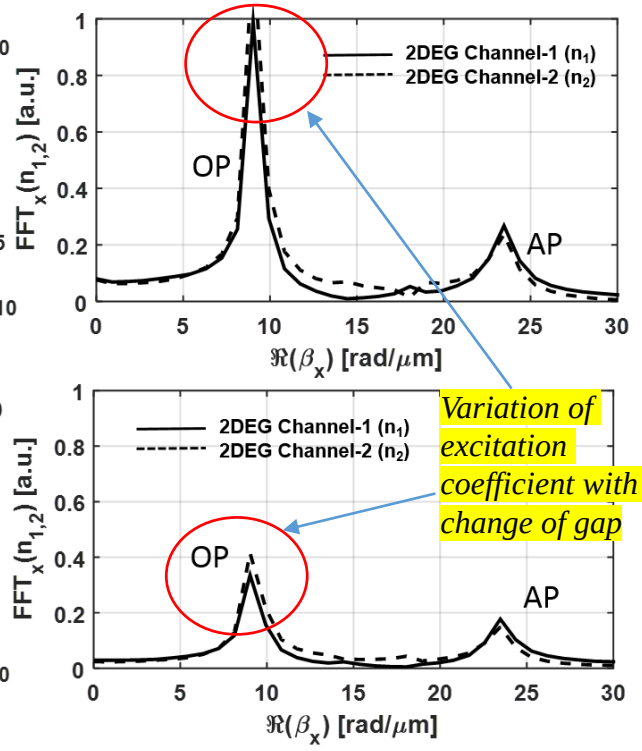


First numerical illustration: Excitation and propagation of Optical Plasmonic and Acoustic Plasmonic Modes in gated-bilayer was demonstrated using multi-physical Models

(E_y Fields at t=12 ps)



Wave numbers for the two modes



Variation of excitation coefficient with change of gap

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

Summary of Modal Solutions in 2DEG-Bilayers

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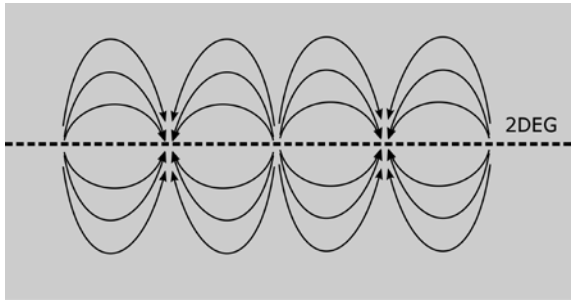
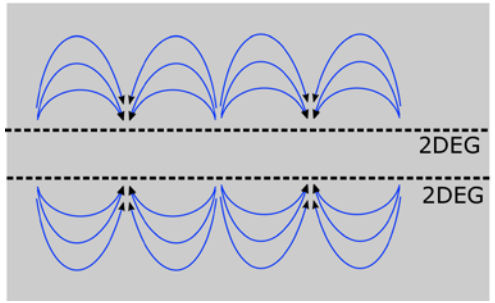
Single Channel

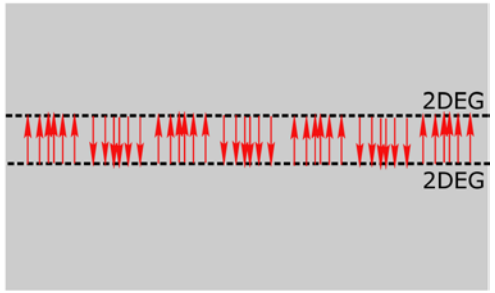


Double Channel

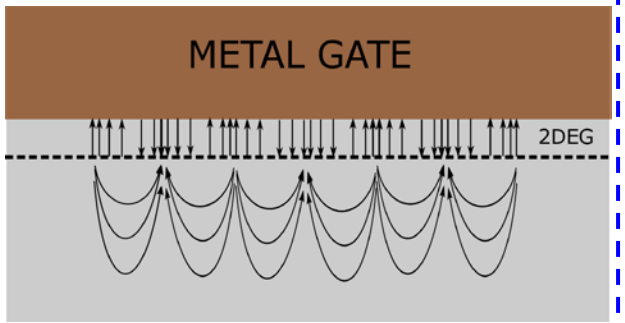
OPTICAL MODES



ACOUSTIC MODES

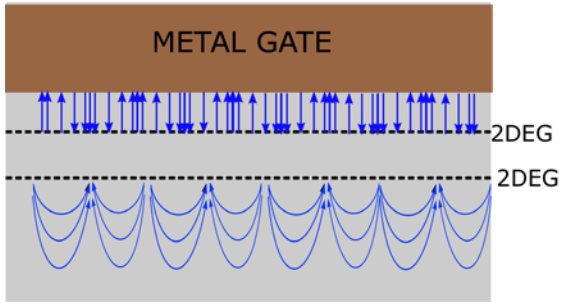


Single Channel With Gate

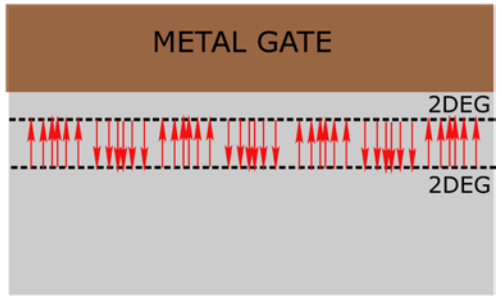


Double Channel with Gate

OPTICAL MODES



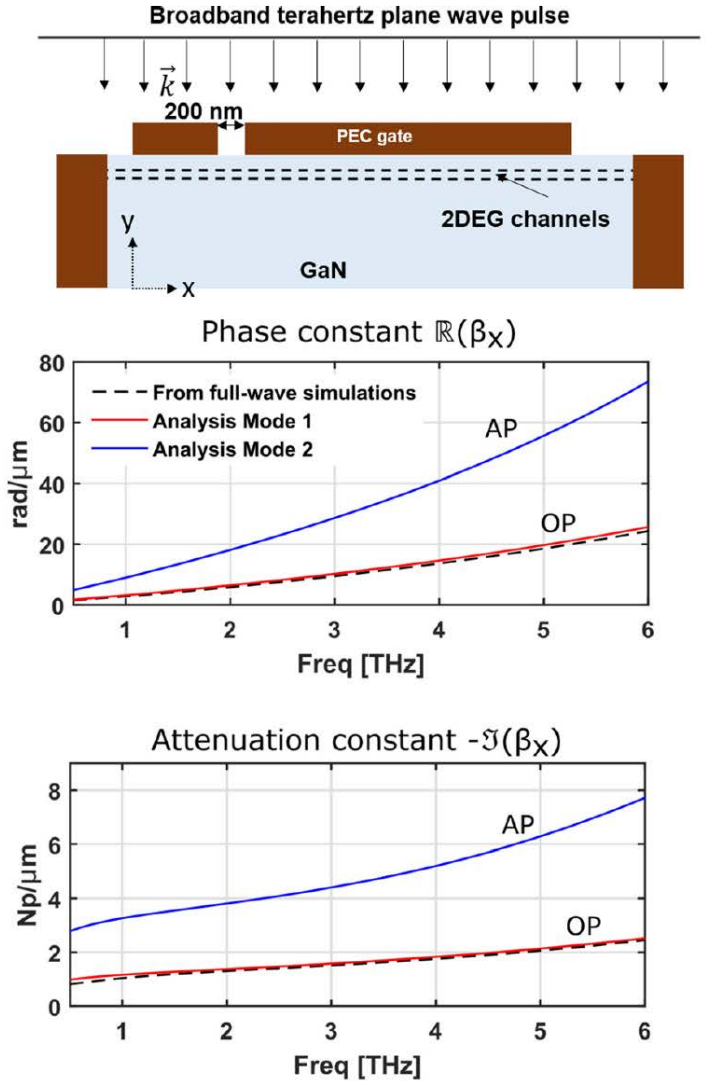
ACOUSTIC MODES

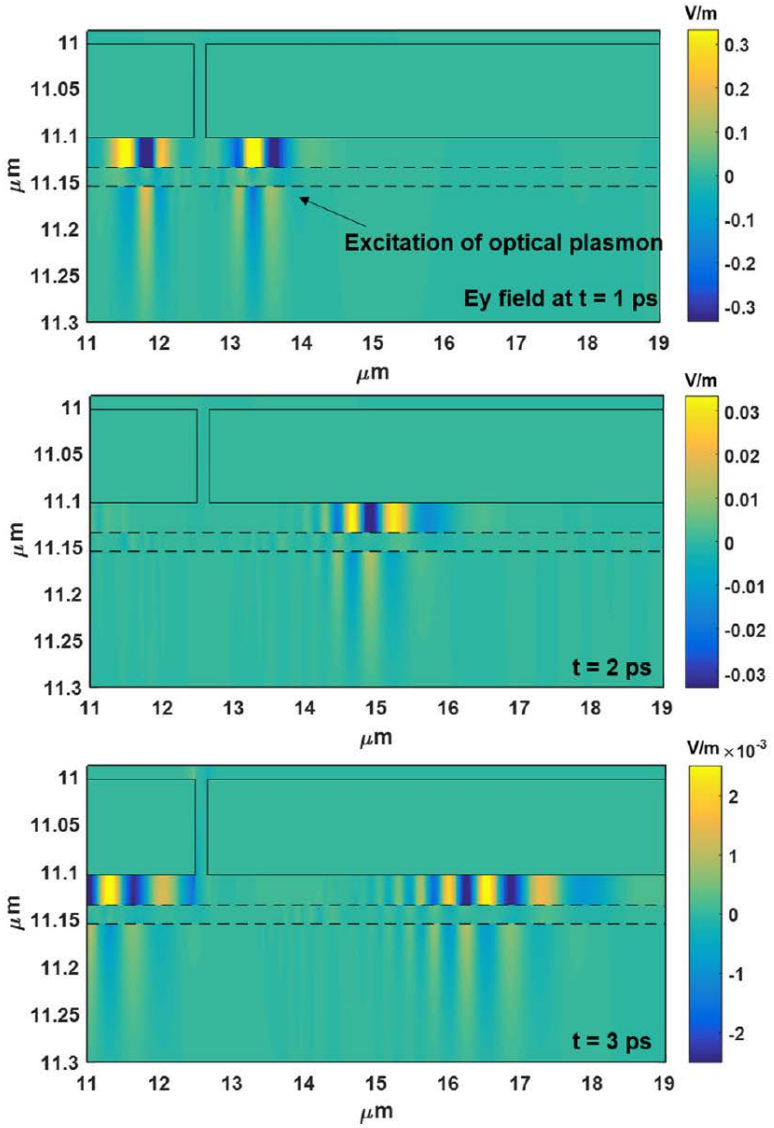


- Solver has allowed understanding of the two modes within the bilayer strictures.

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

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

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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

M. Voßebürger, H. G. Roskos, F. Wolter, C. Waschke, H. Kurz, K. Hirakawa,* I. Wilke,* K. Yamanaka,* *Institut für Halbleitertechnik, RWTH Aachen, D-52056 Aachen, Germany*

JAP, 2005

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

J. Lusakowski, W. Knap, N. Dyakonova, L. Varani, J. Mateos, T. Gonzalez, Y. Roelens, S. Bollaert, A. Cappy, and K. Karpierz

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 Dyakonov[1] and Michael Shur[2]

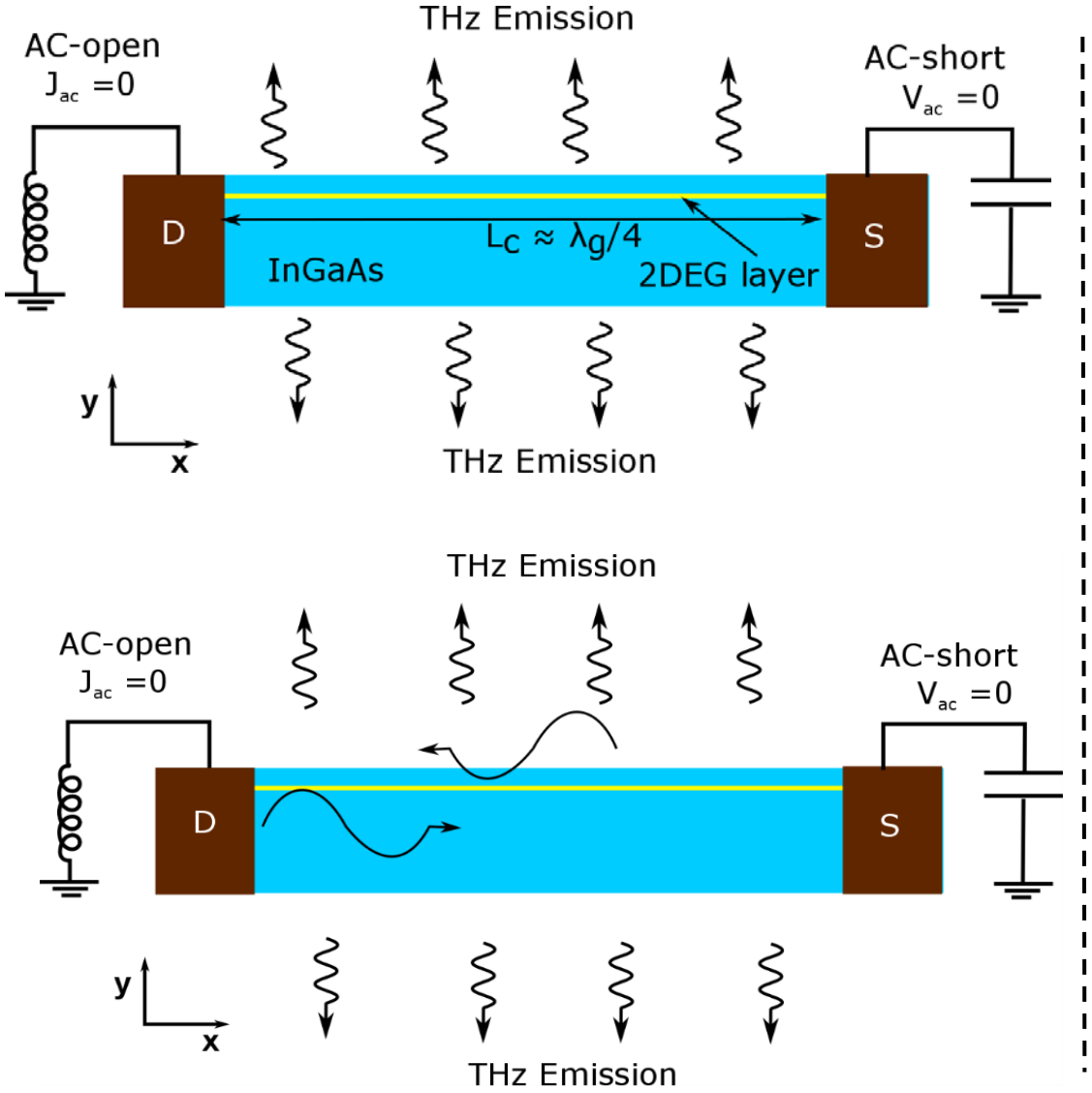
[1]*A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia*
[2]*Department of Electrical Engineering, University of Virginia, Charlottesville, Virginia 22903*
(Received 21 June 1993)

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*, Niru K. Nahar, *Senior Member, IEEE*, Siddharth Rajan, and John L. Volakis, *Fellow, IEEE*

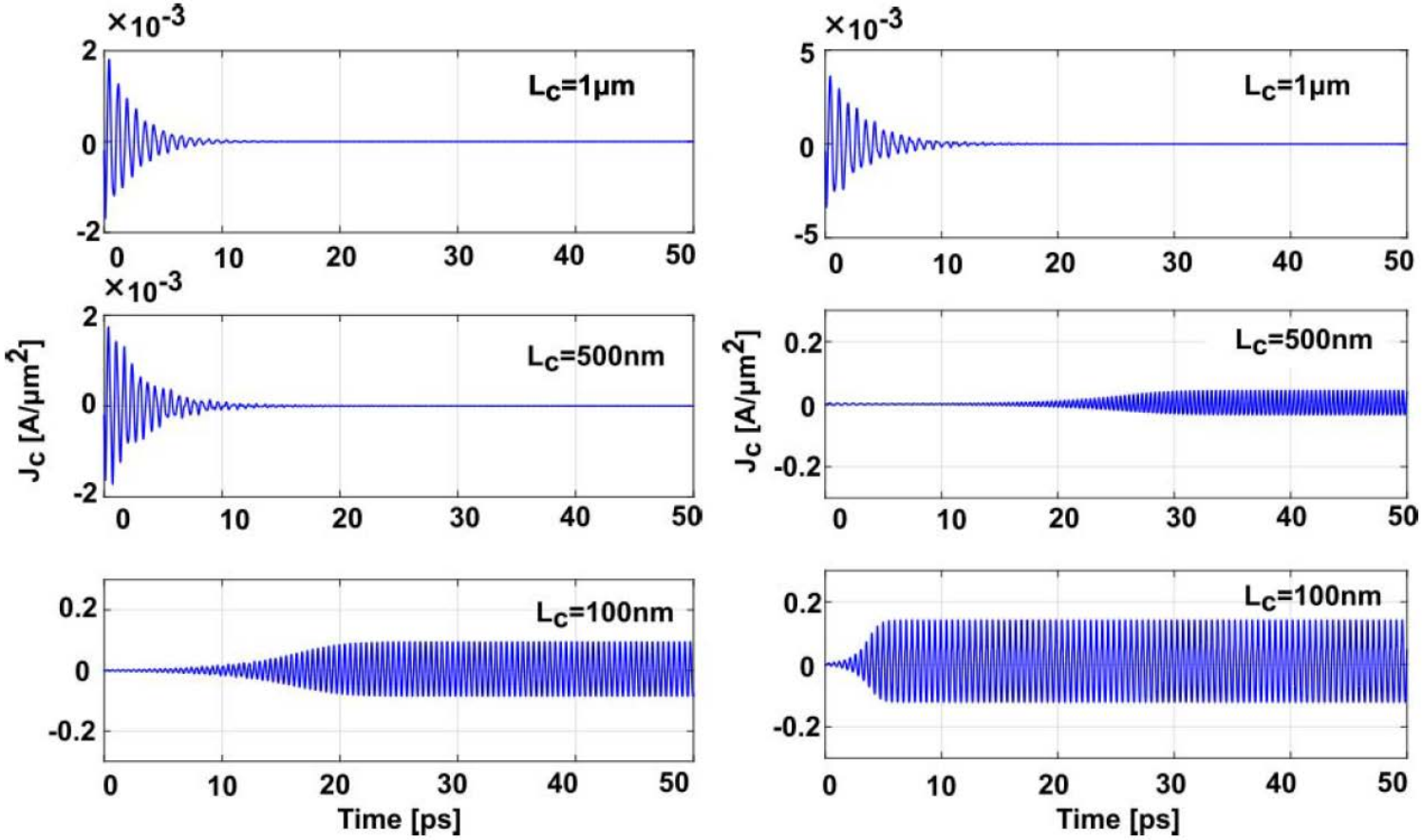
Basics of DS instability and THz Emissions



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 ~ 1/travel time

First Numerical Verifications



S. Bhardwaj, N. K. Nahar, S. Rajan, and J. L. Volakis, "Numerical Analysis of Terahertz Emissions from an Ungated HEMT Using Full-Wave Hydrodynamic Model" *IEEE Transactions on Electron Devices*, vol. 63, no. 3, pp. 990–996, March 2016

Phenomenological Verifications via Full-wave Multiphysical Solution

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Understanding the mechanism of instability

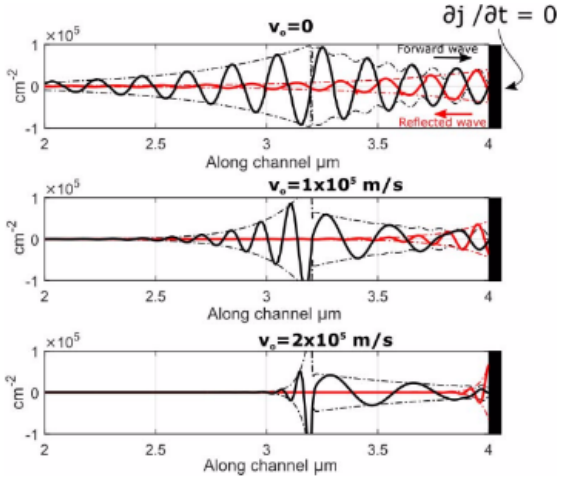
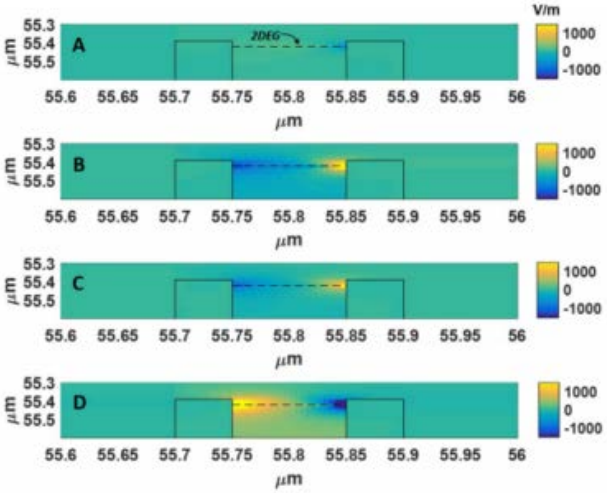


Fig. 3. Numerical modeling of wave propagation in the 2DEG terminated by ac-open conditions. Black curves: forward/backward waves. Red curves: reflected waves. Dashed-dotted curves: envelop of the fluctuations. The parameters used are $n_{sh} = 1 \times 10^{12}$, $\tau = 1$ ps, $\epsilon_r = 13.9$, and $m_e = 0.042\ m_o$. The drift velocity v_o is toward the right.



Estimation of power levels

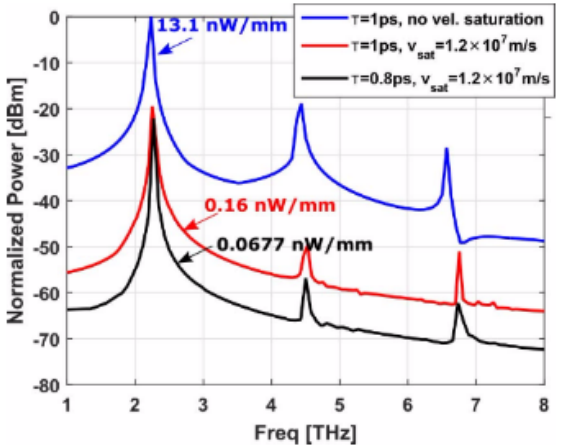


Fig. 7. Effect of velocity saturation and decreased mobility on the emitted power from the device. The considered case is for $L_c = 100$ nm and $n_{sh} = 1 \times 10^{12}$ cm^{-2}.

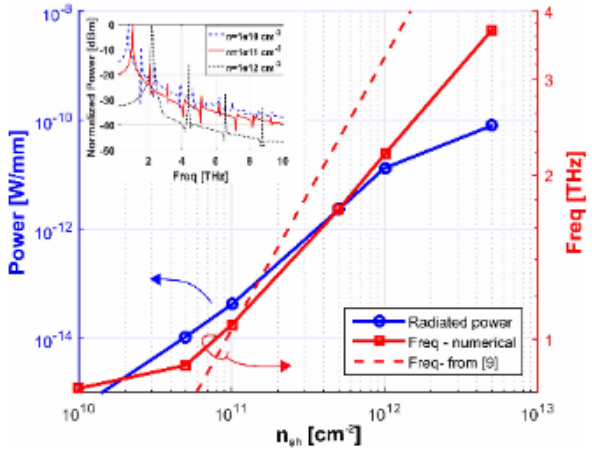


Fig. 6. Frequency and power dependence on channel carrier density, n_{sh}, in the 2DEG layer ($L_c = 100$ nm and $v_o = 2\times10^5$ m/s). Theoretical calculations as per [8].

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)

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Publications

1. S. Bhardwaj, F. L. Teixeira and J. L. Volakis, "Fast Modeling of Terahertz Plasma-Wave Devices Using Unconditionally Stable FDTD Methods," *in IEEE Journal on Multiscale and Multiphysics Computational Techniques*, vol. 3, pp. 29-36, 2018.
2. S. Bhardwaj, and J. L. Volakis, “Hexagonal Waveguide based Circularly-Polarized Horn Antennas for Sub-mm-wave / Terahertz Band” IEEE Transactions on Antennas and Propagation, Early Access March 2018.
3. S. Bhardwaj, N. K. Nahar and J. L. Volakis, "A Cost-Effective Phaseless Pattern Measurement Method for a CP Antenna in a Submillimeter-Wave Band," in *IEEE Antennas and Wireless Propagation Letters*, vol. 16, no. , pp. 1683-1686, 2017.
4. Shubhendu Bhardwaj, Niru K. Nahar, and John L. Volakis. All electronic propagation loss measurement and link budget analysis for 350 GHz communication link. *Microwave and Optical Technology Letters*, 59(2):415{423, 2017
5. Shubhendu Bhardwaj, Siddharth Rajan, and John L. Volakis. Analysis of plasma-modes of a gated bilayer system in high electron mobility transistors. *Journal of Applied Physics*, 119(19), 2016
6. Shubhendu Bhardwaj, Berardi Sensale-Rodriguez, Huili Grace Xing, Siddharth Rajan, and John L. Volakis. Resonant tunneling assisted propagation and amplification of plasmons in high electron mobility transistors. *Journal of Applied Physics*, 119(1):013102, 2016
7. Shubhendu Bhardwaj, N. K. Nahar, Siddharth Rajan, and John L. Volakis. Numerical Analysis of Terahertz Emissions From an Ungated HEMT Using Full-Wave Hydrodynamic Model. *IEEE Transactions on Electron Devices*, 63(3):990-996, March 2016
8. Shubhendu Bhardwaj, Niru K. Nahar, and John L. Volakis. Novel phaseless gain characterization for circularly polarized antennas at mm-wave and thz frequencies. IEEE Transactions on Antennas and Propagation, 63(10):4263{4270, Oct 2015
9. Shubhendu Bhardwaj, Niru K. Nahar, and John L. Volakis. Radial line slot array antenna with vertical waveguide feed for F-band communication. *Microwaves, Antennas & Propagation, IET*, 9(3):193-199, 2014

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

Acknowledgement

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

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Particle Transport Models

Particle Approach:

Here, we solve the Vlasov Equation;

$$\frac{\partial f}{\partial t} + \vec{v}\nabla_x f + qm_e\left(\vec{E} + \vec{v} \times \vec{B}\right)\nabla_k f = 0$$

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

$$\frac{\partial f}{\partial t} + \vec{v}\nabla_x f + qm_e\left(\vec{E} + \vec{v} \times \vec{B}\right)\nabla_k f = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

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

$$\frac{\partial n}{\partial t} + \frac{\partial j}{\partial x} = 0$$

$$\frac{\partial j}{\partial t} + v\frac{\partial j}{\partial x} + \frac{j\partial v}{\partial x} = -\frac{qnE_x}{m_e} - \frac{j}{\tau} - \frac{KT}{m_e}\frac{\partial n}{\partial x}$$

- 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)

1. Number of particles → ∞
2. Only 2 particle collisions assumed

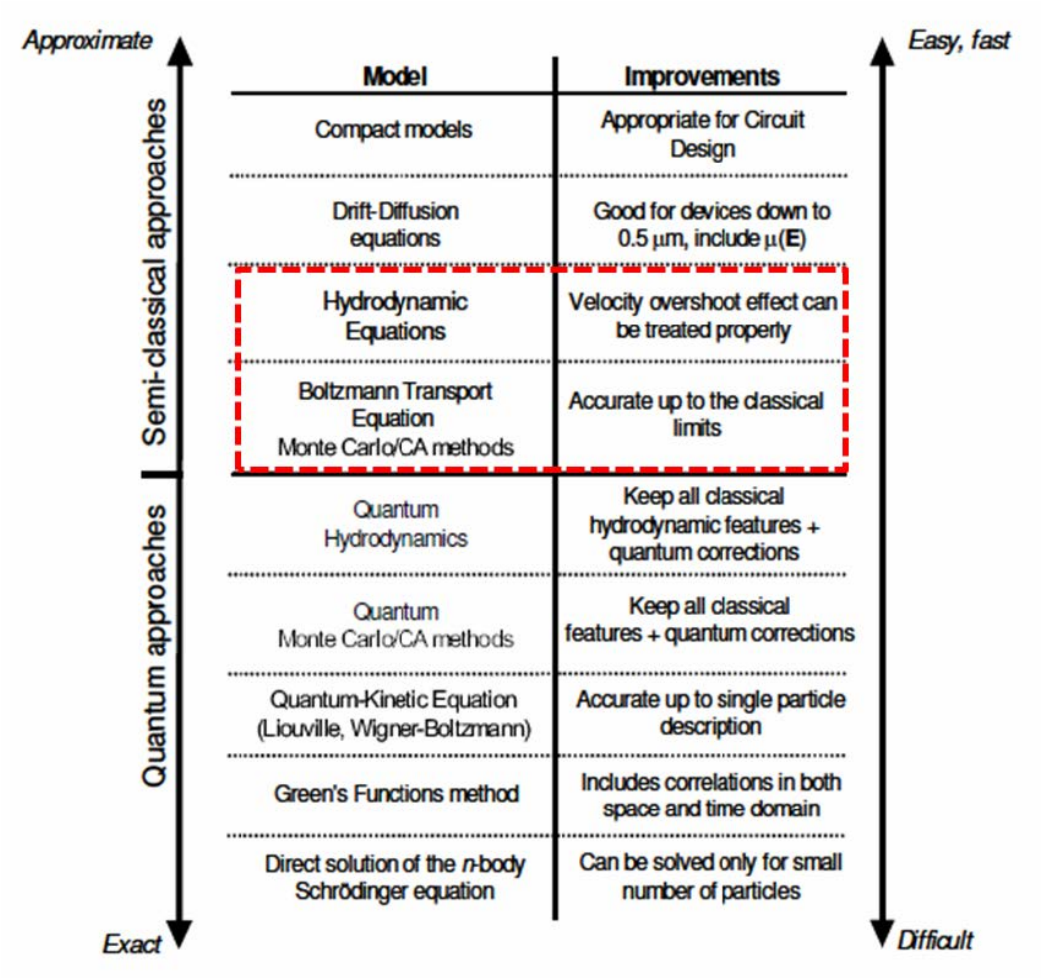
Boltzmann transport Equation

1. Mean free path << macroscopic observation length
2. Mean free time << macroscopic observation time step
3. Parabolic bands are assumed
4. Thermal equilibrium assumed
(small fluctuations around Maxwellian)

Hydrodynamic Model

Limitations and advantages for Semiconductor Simulations

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



Model	Improvements
Compact models	Appropriate for Circuit Design
Drift-Diffusion equations	Good for devices down to 0.5 μm, include μ(E)
Hydrodynamic Equations	Velocity overshoot effect can be treated properly
Boltzmann Transport Equation Monte Carlo/CA methods	Accurate up to the classical limits
Quantum Hydrodynamics	Keep all classical hydrodynamic features + quantum corrections
Quantum Monte Carlo/CA methods	Keep all classical features + quantum corrections
Quantum-Kinetic Equation (Liouville, Wigner-Boltzmann)	Accurate up to single particle description
Green's Functions method	Includes correlations in both space and time domain
Direct solution of the *n*-body Schrödinger equation	Can be solved only for small number of particles

Vasileska, Goodnick, "Computation Electronics":

Particle Based Simulation

L_g<0.1 μm

- Accurate upto classical limits
- Allows proper treatment of discrete impurity effects
- Time consuming

Hydrodynamic Model

L_g≥0.1 μm

- Hot carrier effects, such as velocity overshoot, included in the model
- Overestimates the velocity at high fields