Wakefield Excitation in Carbon Nanotubes and Graphene Layers: Hydrodynamic Approach and PIC Simulations

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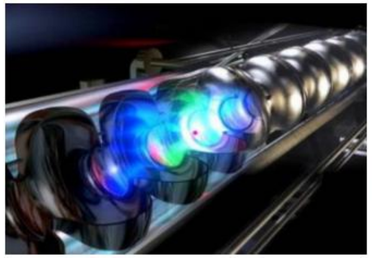
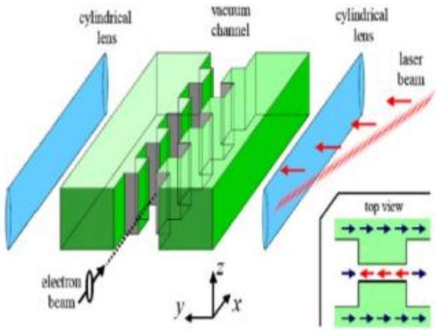
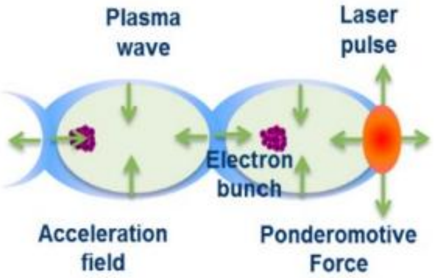
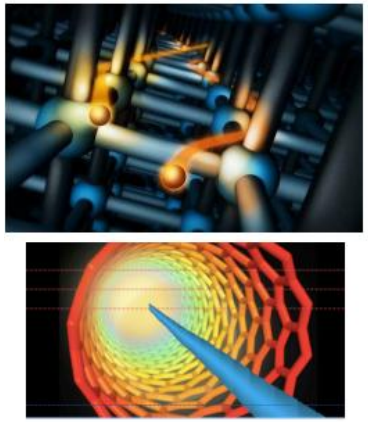
1. Introduction

- The current state-of-the-art of the RF techniques for particle acceleration is limited to gradients on the order of 100 MV/m
- To obtain higher energies, we can increase the length of the accelerators... or use new techniques of acceleration with higher gradients







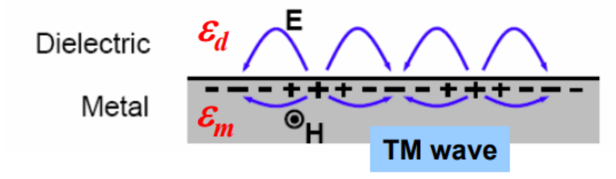


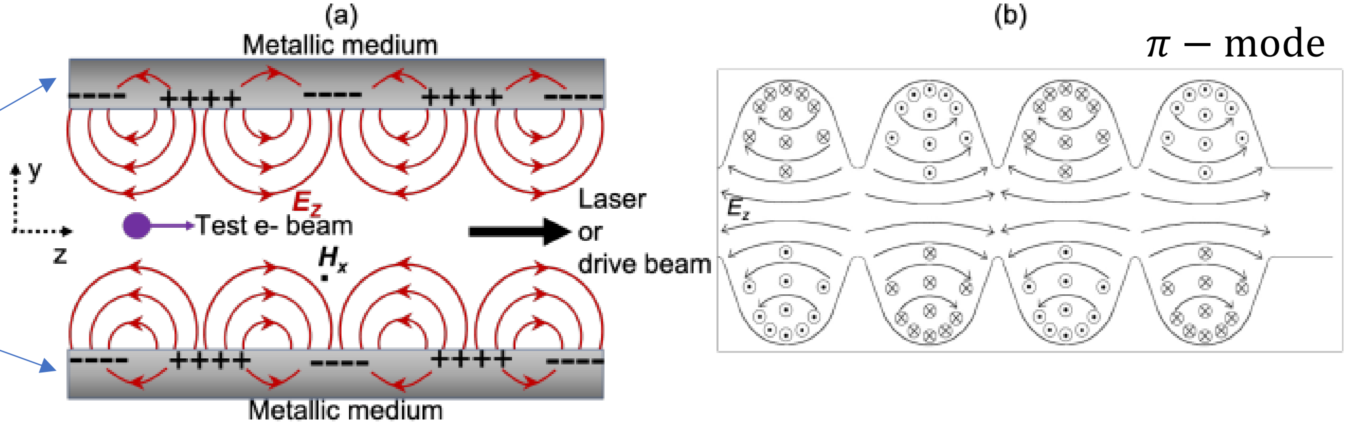
	Conventional RF cavities	Dielectric laser – driven acceleration (DLA)	Plasma / Laser wakefield acceleration (PWFA / LWFA)	Solid-state plasma wakefield acceleration
Based on	Normal / superconducting cavities	Quartz / silicon structure	Gaseous plasma	Crystals, nano-channels, CNTs
Max. longitudinal electric field	$\sim 100\ \mathrm{MV/m}$	$\sim 10\ \mathrm{GV/m}$	$\sim 100\ \mathrm{GV/m}$	$\sim 1 - 100\ \mathrm{TV/m}$ (prediction)
Limitation	Surface breakdown	Damage threshold	Wave breaking	Atomic lattice dissociation

1. Introduction

- **Plasmonic acceleration**
  - Excitation of surface plasmonic modes by laser (laser-driven) or charged particle beam (beam-driven)
  - Collective motion of wall electrons acting like a structured plasma
  - To properly excite wakefields laser or beam driving parameters need to be in the time and space scale of the plasmon wave

2D plasmon



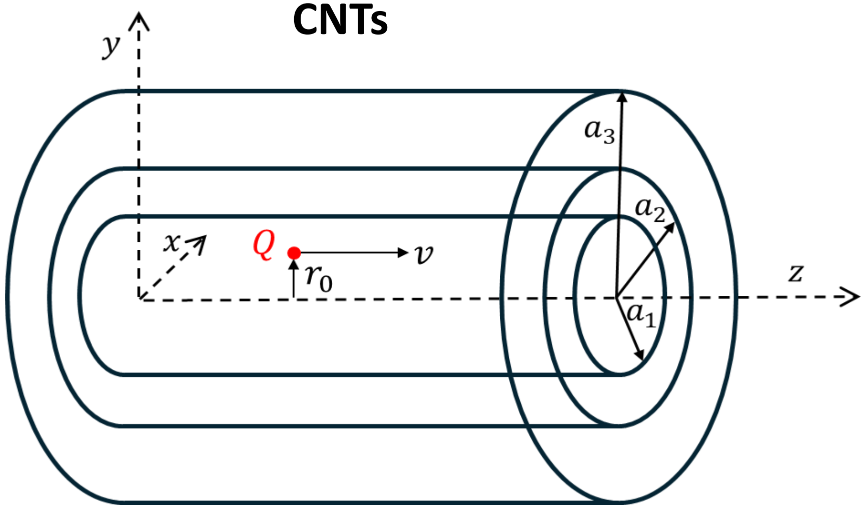


	Plasmonic acceleration	RF cavities
Aperture size	$\sim\mu\text{m}$	$\sim\text{cm}$
Length	$\sim\text{mm}$	$\sim 10\text{cm} - \text{m}$
Longitudinal electric field	$\sim 100\ \text{GV/m}$	$\sim 100\ \text{MV/m}$
Operation	Travelling wave (TW)	Standing Wave (SW) or TW

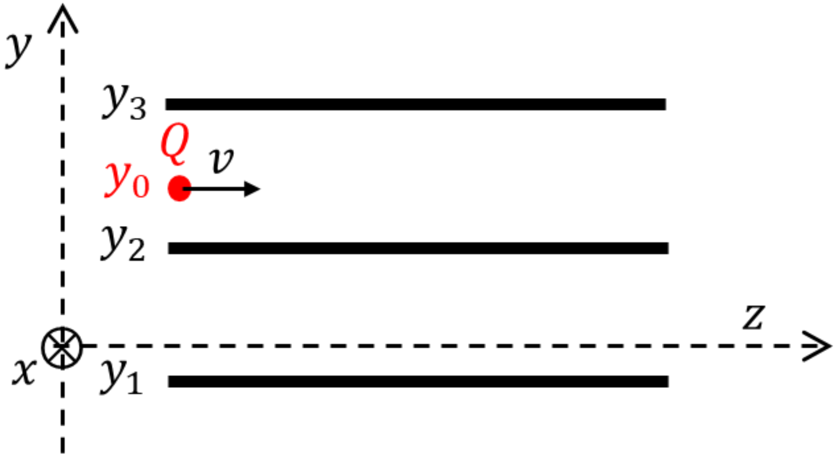
2. Linearized Hydrodynamic Model (LHM)

- In this theory, carbon nanostructures surfaces are modelled as an infinitesimally thin and infinitely long shells with uniform surface density n_0. These electrons are confined in the surfaces
- A driving charge Q travels with velocity v, parallel to the z-axis: $\mathbf{r_0} = (x_0, y_0, vt)$
- Position of electrons excited at the jth surface: $\mathbf{r_j}$

CNTs



Graphene layers



2D density: $n(\mathbf{r_j}, t) = n_0 + n_j(\mathbf{r_j}, t)$

Y-N. Wang, Z. L. Mišković, Phys. Rev. A 69 (2004) 022901
Z. L. Mišković et al., Phys. Lett. A 329 (2004) 94

2. Linearized Hydrodynamic Model (LHM)

- The **electronic excitations** on the surfaces can be described by two differential equations:

(i) the continuity equation

$$\frac{\partial n_j(\mathbf{r}_j, t)}{\partial t} + n_0 \nabla_j \cdot \mathbf{u}_j(\mathbf{r}_j, t) = 0$$

$n_j(\mathbf{r}_j, t)$: perturbed surface density
$\mathbf{u}_j(\mathbf{r}_j, t)$: velocity of the plasma
∇_j differentiates only tangentially to the jth surface

(ii) the momentum-balance equation

$$\frac{\partial \mathbf{u}_j(\mathbf{r}_j, t)}{\partial t} = \nabla_j \cdot \Phi(\mathbf{r}_j, t) - \underbrace{\frac{\alpha}{n_0} \nabla_j \cdot n_j(\mathbf{r}_j, t)}_{\text{Acoustic modes}} + \underbrace{\frac{\beta}{n_0} \nabla_j [\nabla_j^2 n_j(\mathbf{r}_j, t)]}_{\text{Quantum correction}} - \underbrace{\gamma \mathbf{u}_j(\mathbf{r}_j, t)}_{\text{Frictional force}}$$

Acoustic modes: $\alpha = v_F^2/2$, with $v_F = \sqrt{2\pi n_0}$

Quantum correction: $\beta = 1/4$

Frictional force

2. Linearized Hydrodynamic Model (LHM)

- The electric potential is given by $\Phi = \frac{Q}{\|\mathbf{r}-\mathbf{r_0}\|} + \Phi_{ind}$, where

$$\Phi_{ind}(\mathbf{r}, t) = -\sum_j \int d^2\mathbf{r_j} \, \frac{n_j(\mathbf{r_j}, t)}{\|\mathbf{r} - \mathbf{r_j}\|}$$

is the potential resulting from the perturbation of the electron fluids

- The system of partial differential equations can be analytically solved by using **Fourier transforms**
- Induced wakefields:

$$W_x = -\frac{\partial \Phi_{ind}}{\partial x} \qquad W_y = -\frac{\partial \Phi_{ind}}{\partial y} \qquad W_z = -\frac{\partial \Phi_{ind}}{\partial z}$$

3. Carbon nanotubes (CNTs)

- In the LHM, the longitudinal wakefield along the z-axis can be approximated by:

$$W_z \approx W_z^{max} \cos(k_m \zeta)$$

$$W_z^{max} = -4qk_0^3 I_0(|k_0|r_0) I_0(|k_0|r) \Omega_p^2 a^2 K_0^2(|k_0|a) \left|\frac{\partial Z_0}{\partial k}\right|_{k=k_0}^{-1}$$

where k_0 are the positive roots of the condition of the plasma resonance $Z_0(k_0) = (k_0 v)^2 - \omega_0^2(k_0) = 0$, where $\omega_0(k)$ is the dispersion relation for the fundamental mode

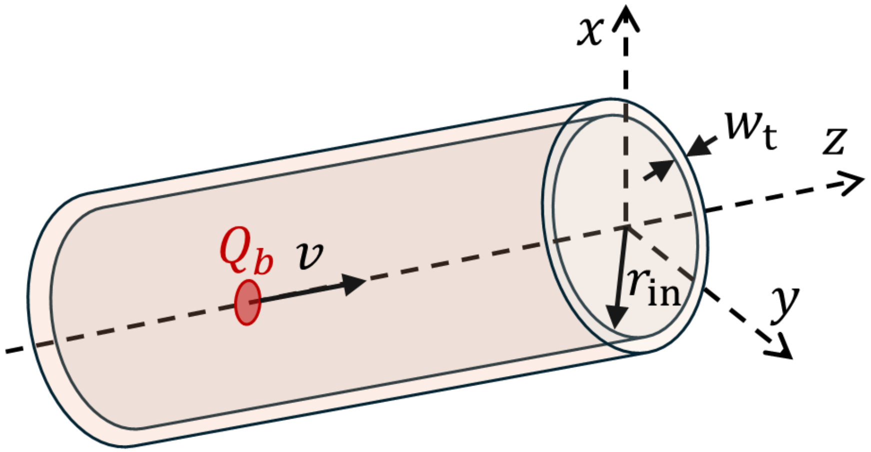
$$\omega_m(k) = \left[\alpha\left(k^2 + \frac{m^2}{a^2}\right) + \beta\left(k^2 + \frac{m^2}{a^2}\right)^2 + \Omega_p^2 a^2 \left(k^2 + \frac{m^2}{a^2}\right) K_m(|k|a) I_m(|k|a)\right]^{1/2}$$

$\Omega_p = \sqrt{4\pi n_0 / a}$ plasma frequency

3. Carbon nanotubes (CNTs)

<u>PIC simulations</u>

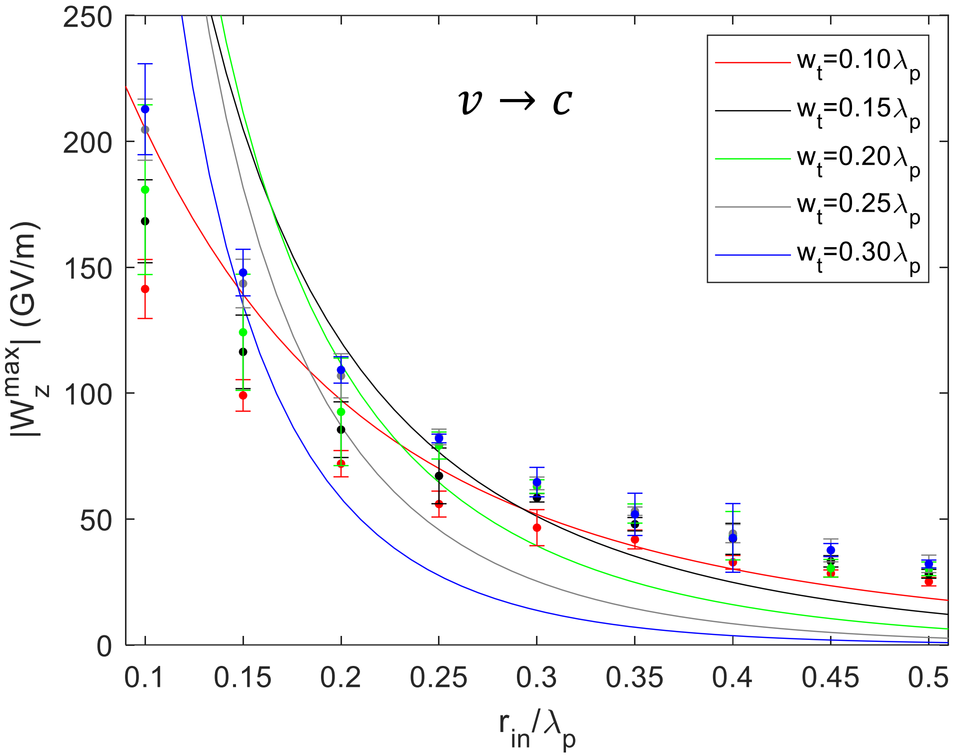
- The Fourier–Bessel Particle-in-Cell **(FBPIC)** code is used to perform the simulations using a cylindrical CNT hollow plasma channel model employing 2D radial grids.
- This code is based on a **collisionless** fluid model which **does not take into account the solid-state properties** related to the ionic lattice.
- We define a hollow plasma channel model with **inner radius** $\boldsymbol{r_{in}}$ and **wall thickness** $\boldsymbol{w_t}$ with a volumetric density $\boldsymbol{n_V = 10^{28}}$ **m**$^{-3}$ of free electrons within this region.
- We will consider a **bi-Gaussian beam driver**, with $\sigma_\zeta = \sigma_r =$ 3.33 nm, and charge $Q_b = -44$ fC travelling **on-axis**. The beam energy follows a Gaussian distribution (mean: 1 GeV, standard deviation: 0.005 GeV).



3. Carbon nanotubes (CNTs)

- To relate the surface density of the LHM and the volumetric density of PIC simulations, we will assume that the **number of free electrons** within the cylindrical surface of radius $a = r_{in}$ is **equal** to the number of free electrons in the wall thickness w_t.

$$n_0 = \frac{n_V w_t}{2r_{in}}(2r_{in} + w_t)$$



$\lambda_p = \frac{2\pi c}{\omega_p}$ is the plasma wavelength, where

$\omega_p = \sqrt{e^2 n_V / \varepsilon_0 m_e}$ is the plasma frequency.

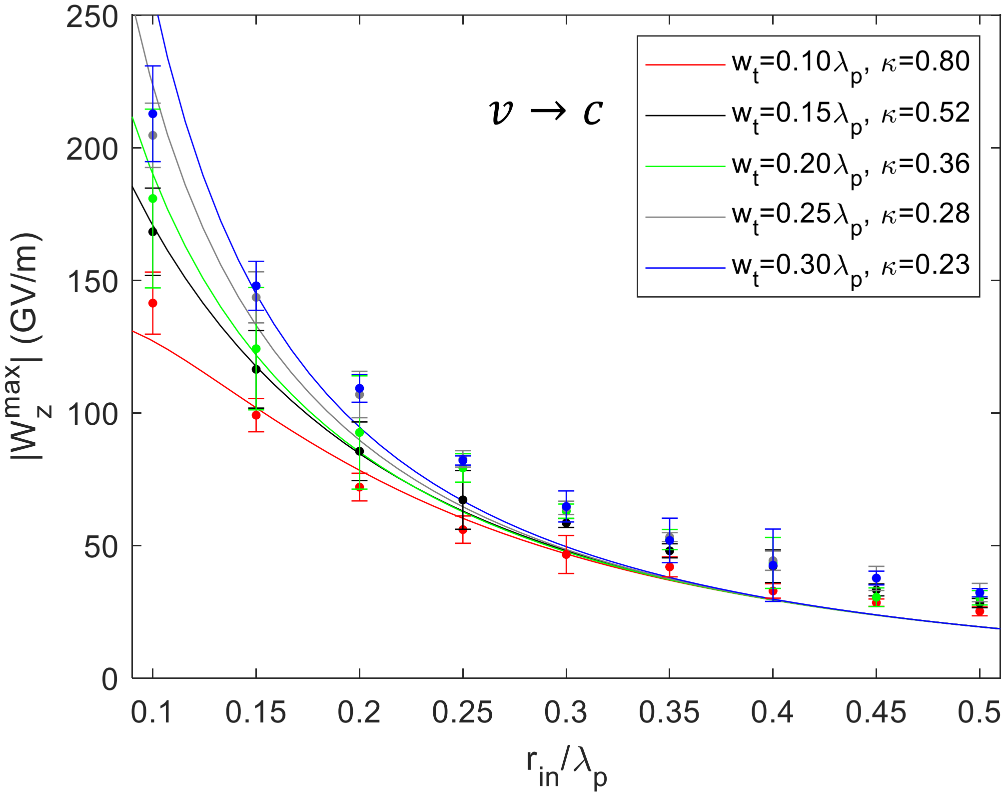
Good qualitative agreement; quantitatively improves if w_t is smaller.

3. Carbon nanotubes (CNTs)

- The comparison is better if we consider an **effective density** to take into account that not all free electrons of the wall thickness excite the wakefield effectively.

$$n_0 = \kappa \frac{n_V w_t}{2r_{in}}(2r_{in} + w_t)$$

$$\kappa \in (0, 1]$$



$\lambda_p = \frac{2\pi c}{\omega_p}$ is the plasma wavelength, where

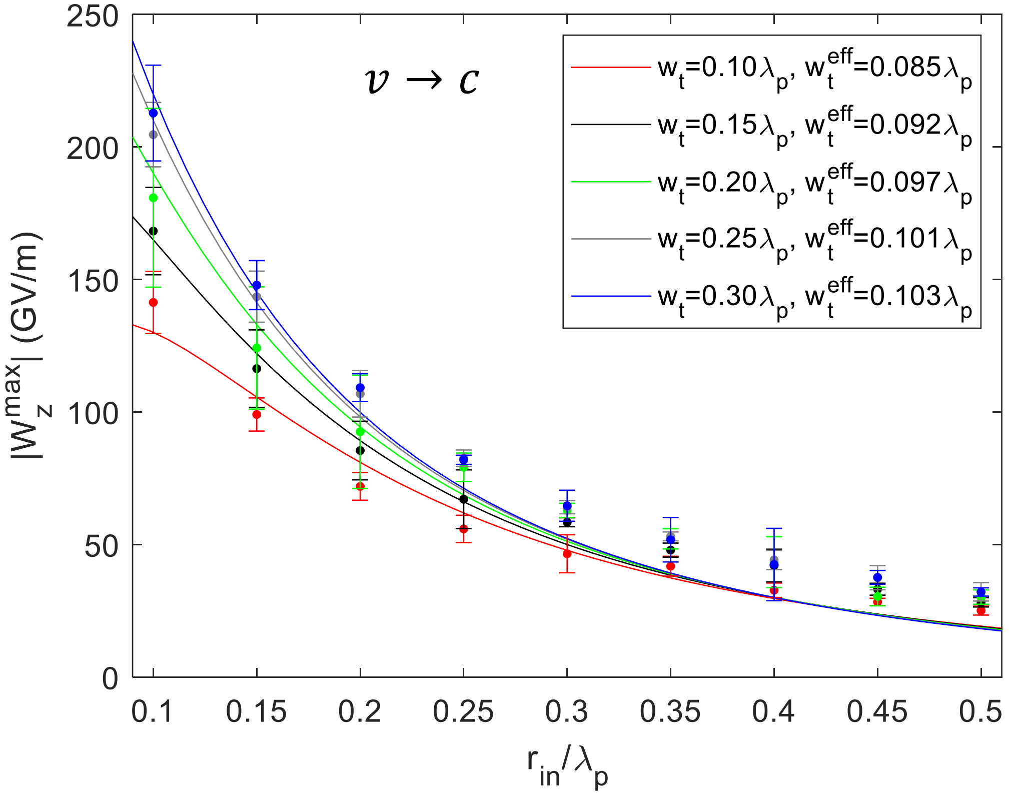
$\omega_p = \sqrt{e^2 n_V/\varepsilon_0 m_e}$ is the plasma frequency.

3. Carbon nanotubes (CNTs)

- Alternatively, we can consider an **effective wall thickness w_t^{eff}**

$$n_0 = \frac{n_V w_t^{eff}}{2r_{in}}(2r_{in} + w_t^{eff})$$

$$w_t^{eff} \leq w_t$$

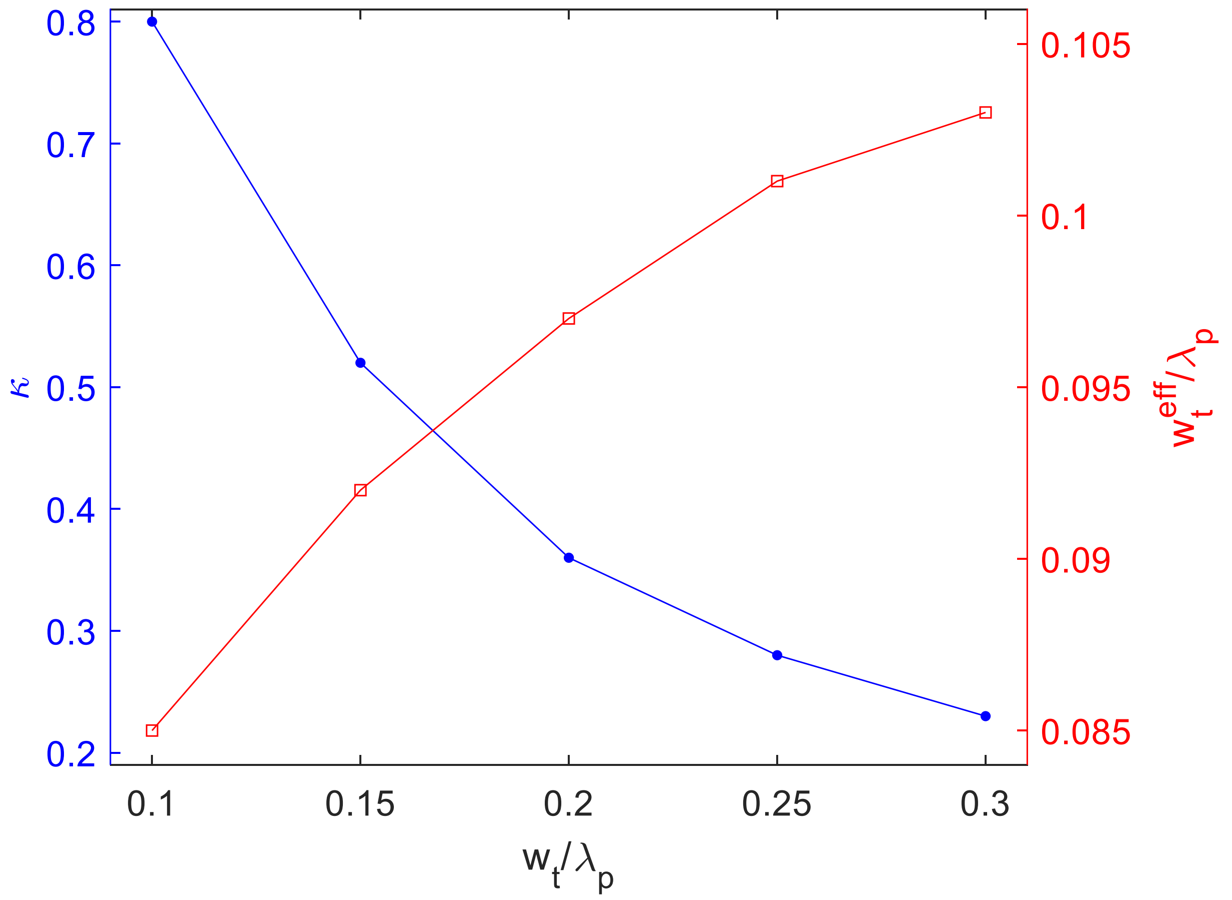


$\lambda_p = \frac{2\pi c}{\omega_p}$ is the plasma wavelength, where

$\omega_p = \sqrt{e^2 n_V/\varepsilon_0 m_e}$ is the plasma frequency.

3. Carbon nanotubes (CNTs)

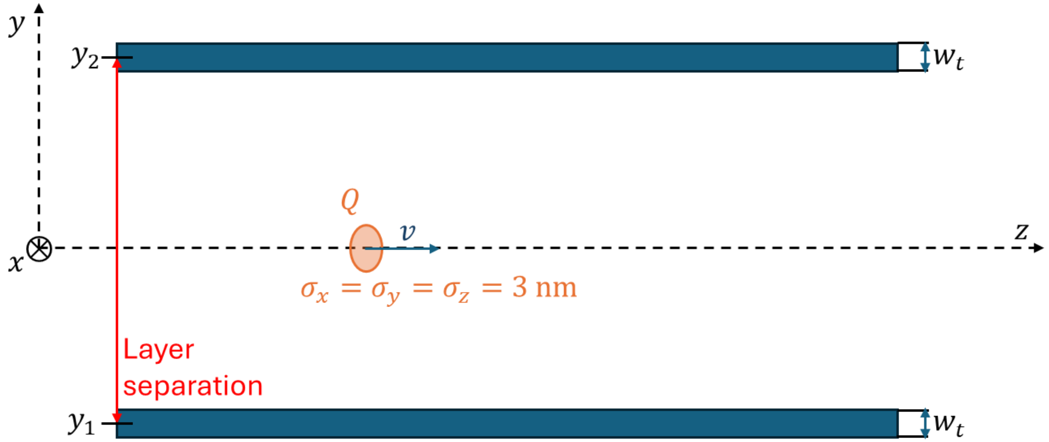
- **Effective parameters.** As it is expected, κ **decreases** and w_t^{eff} **increases** with the wall thickness.



4. Graphene layers

PIC simulations

- **WarpX** [14] has been chosen to perform the simulations of the graphene layers
- Graphene layers are modelled as layers filled with a uniformly distributed, pre-ionized cold plasma of carbon ions and electrons
- Graphene layers will be centered at plane $y = y_j$ with a wall thickness w_t and a volumetric density $n_j = n_0/w_t$ in order to ensure that the number of free electrons within the jth layer with surface density $n_0 = 1.53 \times 10^{20}$ m^{-2} in the LHM is equal to the number of free electrons in the wall thickness w_t
- We will consider a Gaussian proton beam as a driver, with $\sigma_x = \sigma_y = \sigma_z =$ 3 nm, and charge $Q = 1000e$ travelling between the graphene layers
- The simulations span a total duration of 9.5 fs, which is sufficient for wakefield excitation to occur



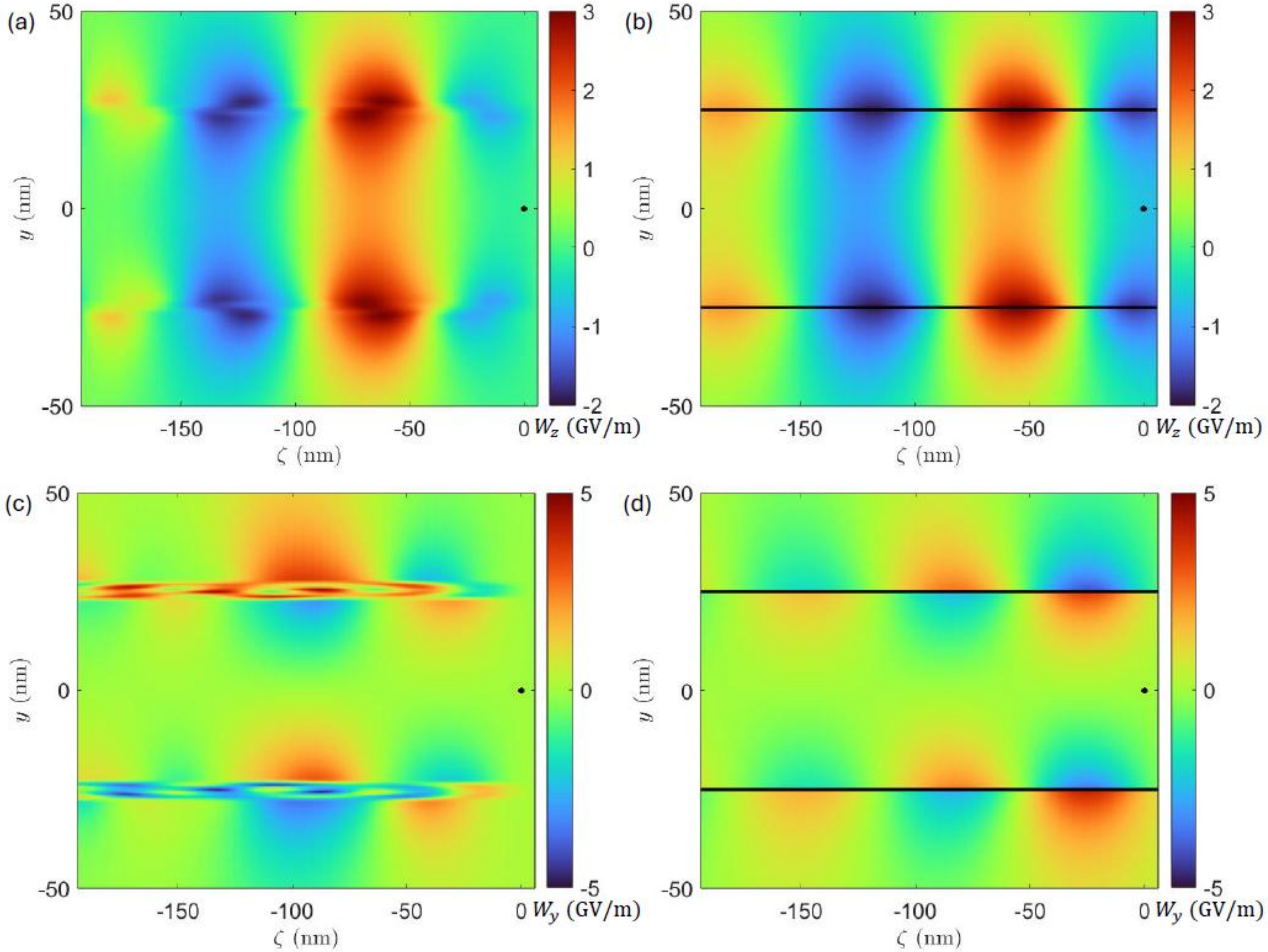
4. Graphene layers

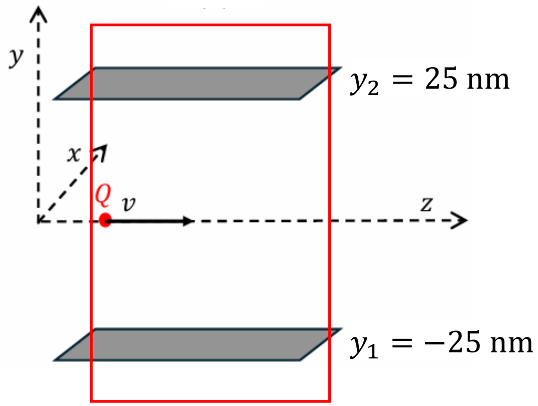
Comparison

PIC simulations | Linearized hydrodynamic model

Longitudinal wakefield

Transverse wakefield





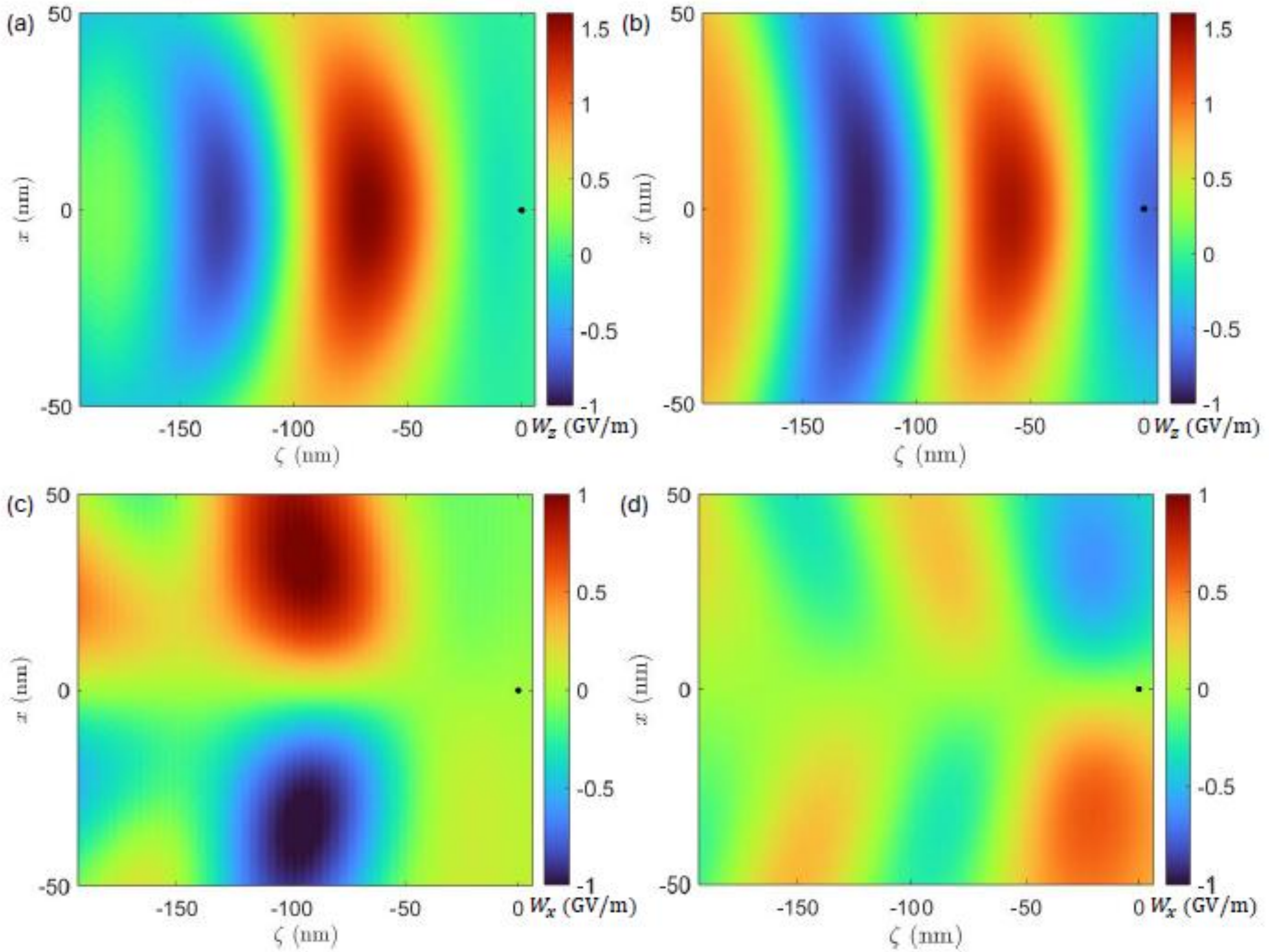
4. Graphene layers

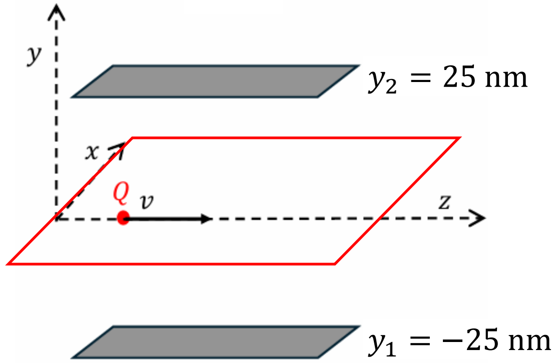
<u>Comparison</u>

PIC simulations | Linearized hydrodynamic model

Longitudinal wakefield

Transverse wakefield

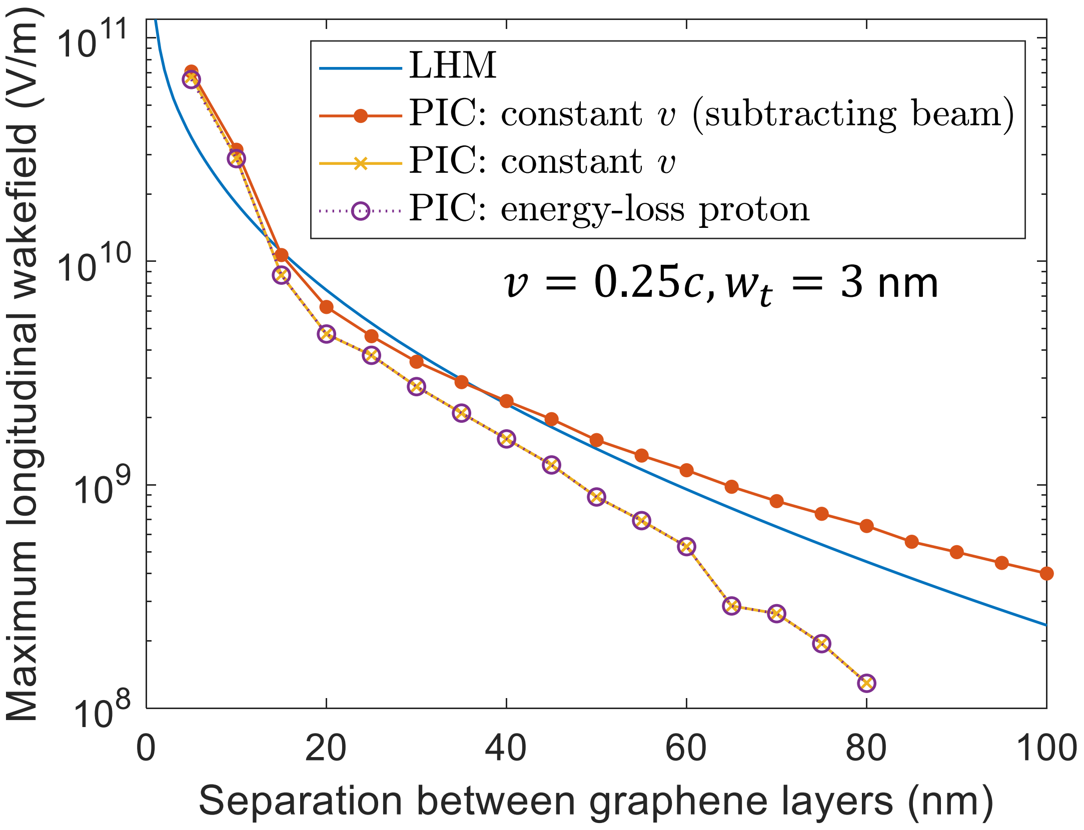


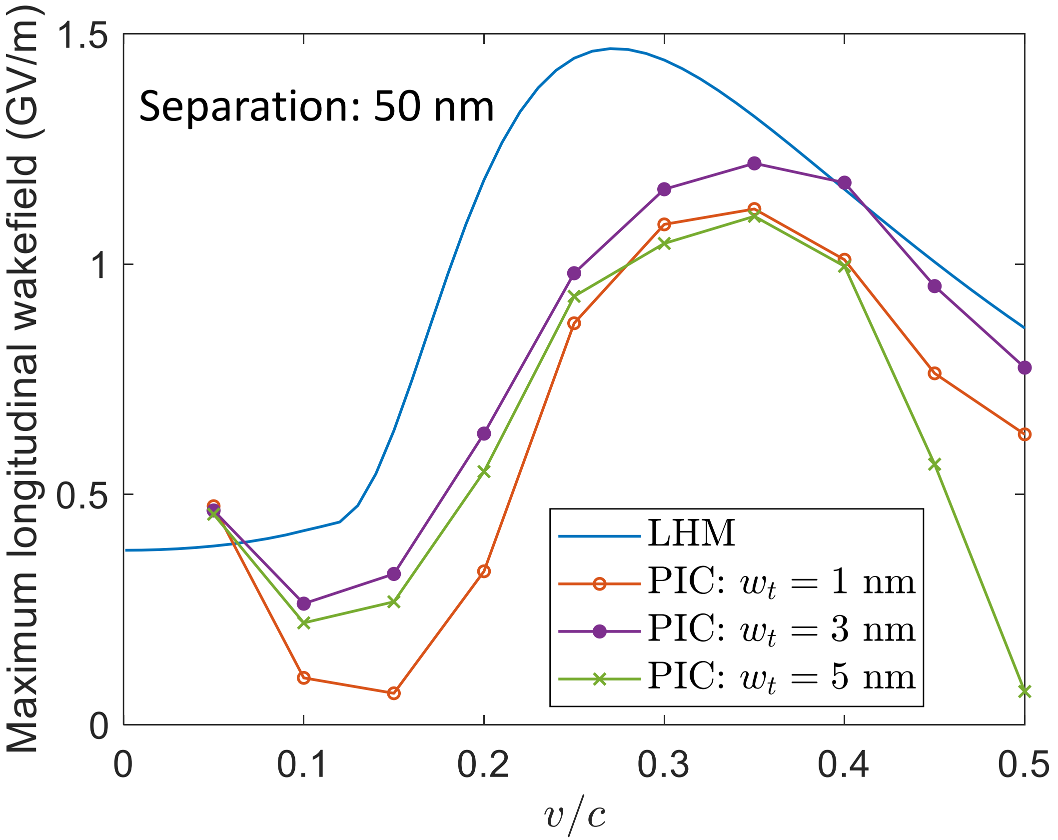


Decay due to spread in the plane

4. Graphene layers

Comparison





- In general, there is a good agreement between the PIC simulations and the linearized hydrodynamic model

5. Discussion

The discrepancies obtained between the linearized hydrodynamic model and the PIC simulations can be explained due to the differences between both approximations, such as:

- The **solid-state properties** cannot be taken into account in PIC codes, whereas these properties may be modelled with the parameters α, β, and γ in the linearized hydrodynamic model
- We are comparing a **3D region** with free electrons in PIC simulations with a **2D surface** in the linearized hydrodynamic model
- The electrons and carbon ions comprising the CNT can **move in 3D in PIC simulations**, whereas they are assumed to be confined over the surface in the linearized hydrodynamic model
- The **driver interacts** with the surrounding medium (losing energy) in PIC codes, whereas in the linearized hydrodynamic model we assume a **constant velocity**
- The size of the driver beam in the PIC simulations **is not a point-like charge** as assumed in the linearized hydrodynamic model

	LHM	**PIC**
Solid-state effects	YES (α, β, γ)	NO
Region with free electrons	2D	3D
Movement of CNT particles	2D	3D
Driver interaction	NO (constant v)	YES
Driver beam size	point-like	bi-Gaussian

6. Conclusions and outlook

- We have compared the excited wakefields in carbon nanostructures using the **linearized hydrodynamic model** and PIC simulations
- The **amplitude** of the longitudinal wakefield follows a **similar trend** in the linearized hydrodynamic model and PIC simulations
- The agreement in the amplitude of the wakefield in CNTs is much better if we consider an **effective density**
- The linearized hydrodynamic model can be used to obtain an **estimation** of the amplitude of the wakefield in hollow plasmas with small wall thickness instead of performing time-consuming PIC simulations
- **Further investigations** employing a different approximation to relate the surface and volumetric density and scanning in other key parameters are ongoing

Acknowledgments

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Thank you for your attention