Working with Finite Difference Time Domain for Electromagnetic Simulation

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PROBLEM

- Optoelectronic devices are fundamental to many modern technologies and has great potential for future development.
- Computational modelling is a vital step in research and development, allowing for exploration and optimisation with minimal cost.
- However, existing computational methods model electromagnetic (EM) fields and materials separately.
- The functioning of optoelectronics cannot be modelled accurately without dynamic modelling of light-matter interaction.

Figure 1: Solar Panels (Optoelectronic Device)

PROPOSED SOLUTION

- Existing Particle-In-Cell (PIC) methods successfully model electromagnetic (EM) fields and matter simultaneously for plasma systems.
- Particle-In-Cell (PIC) has been adapted to capture light-matter interactions and thus model optoelectronic devices more accurately.
- Specifically lorentzian-bound particles have been implemented to model bound material response.
- Here we compare the performance of the novel algorithm with a traditional method for electomagnetic simulations.

BACKGROUND

Finite Difference Time Domain (FDTD)

- Simulates Electric and Magnetic Fields
  - Evolved using Maxwell's equations
  - Evolved in turn at staggered, discrete time steps
- Yee grid is used
  - Staggers E-Field and B-field in space
  - Simplifies calculation of curl
  - Naturally results in staggered timesteps
- Staggering allows for use of central difference instead of forward difference
  - Minimises error: second order with respect to time step

$$f'(t) \approx f_{forward}(x, t, \Delta t) + O(\Delta t)$$
$$f'(t) \approx f_{central}(x, t, \Delta t) + O(\Delta t^2)$$

$$\frac{\partial B}{\partial t} = -\nabla \times E \qquad \frac{\partial E}{\partial t} = \frac{1}{\varepsilon_0 \mu_0}(\nabla \times B - \mu_0 J)$$

Figure 2: Maxwell's Curl Equations

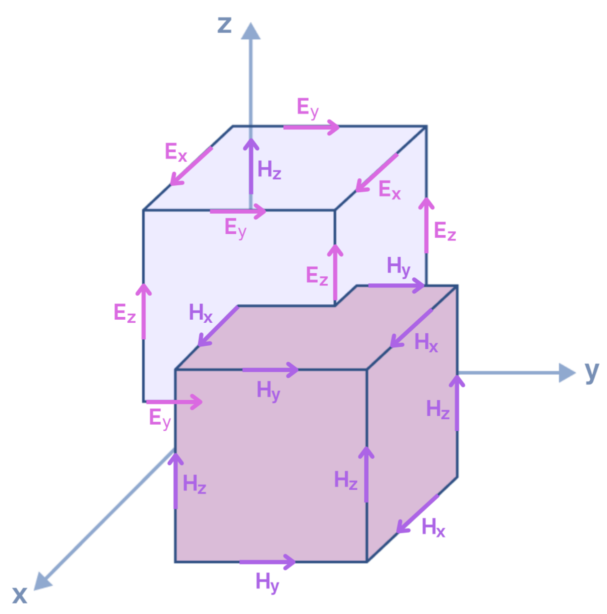


Figure 3: Yee Grid

Particle in Cell (PIC)

- Also simulates (macro) particles
  - Evolved using Newton-Lorentz equations
- Calculates current density based on particles
- Interpolates fields onto particles for the next particle push
- Novel algorithm: particles simulate lorentzian oscillators

$$\frac{\partial x}{\partial t} = v \qquad \frac{\partial v}{\partial t} = \frac{q}{m}(E + v \times B)$$

Figure 4: Newton-Lorentz Equations

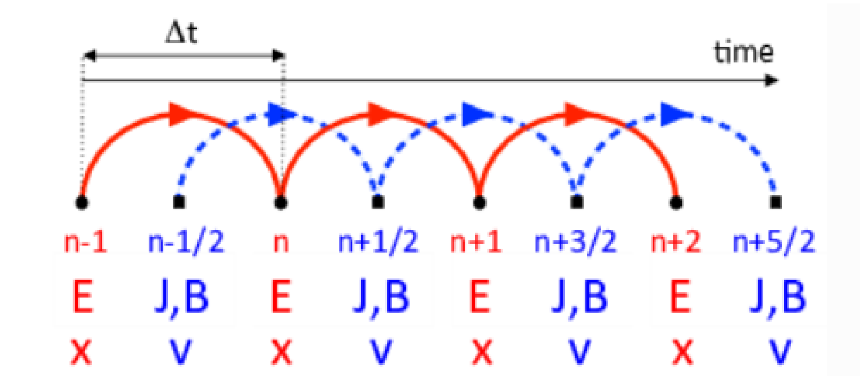
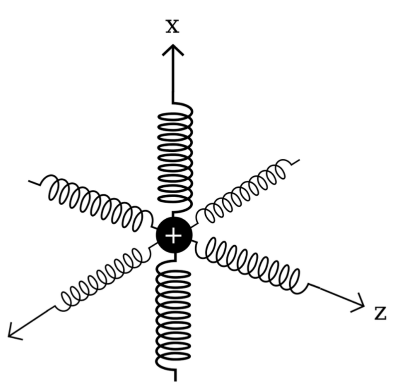


Figure 5: Leapfrog Time-stepping



$$\mathbf{F}_{damping} + \mathbf{F}_{spring} + \mathbf{F}_{driving} = m\frac{d^2\mathbf{r}}{dt^2}$$
$$\frac{-m}{\tau}\frac{d\mathbf{r}}{dt} - k\mathbf{r} - e\mathbf{E}(t) = m\frac{d^2\mathbf{r}}{dt^2}$$

Figure 6: Lorentz Oscillator Model

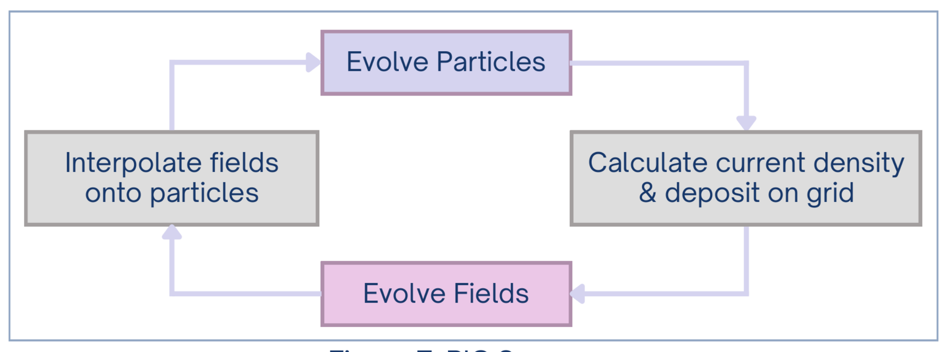


Figure 7: PIC Summary

METHODOLOGY

- Meep and Epoch were used for FDTD and PIC simulations respectively
- Bound material response is simulated using both methods
- Material simulated has a single Lorenztian resonance peak at 364nm
- Time captures were generated for qualitative comparison

RESULTS & ANALYSIS

- No significant difference is observed between the two simulation methods.
- Scattering patterns are similar
  - Reflection observed in both simulations show similar patterns
  - When diffraction is observed (600nm), interference patterns are also consistent.
- Lorentzian behaviour is similar
  - Almost no transmission is observed near (350nm) and below (250nm) the Lorentzian resonance peak.
  - Transmission is observed at frequencies above (600nm) the Lorentzian resonance peak.

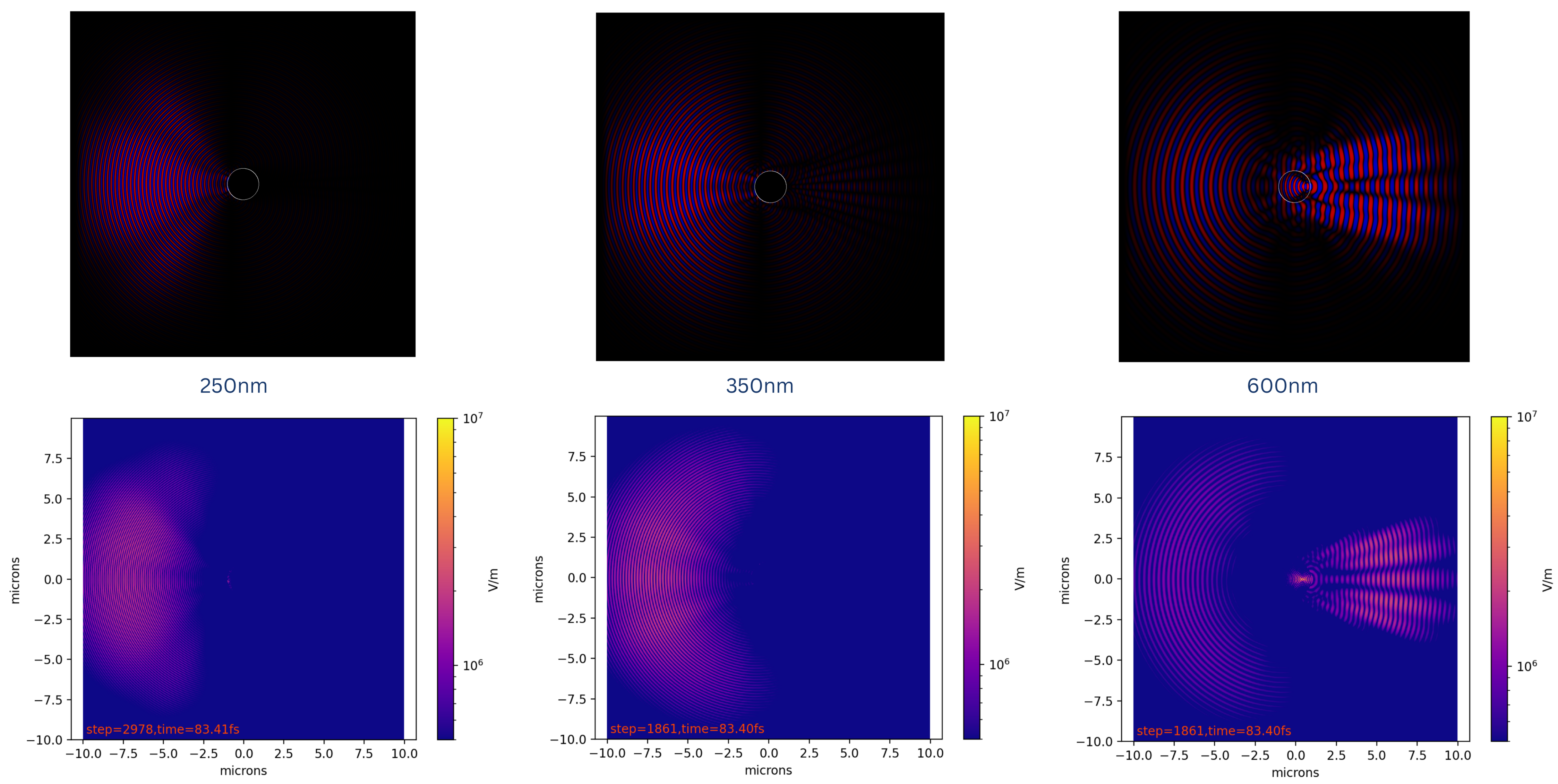


Figure 8: Comparison Between PIC (below) and MEEP (above) Simulations

FUTURE RESEARCH

- Conduct a comparison with 3D Mie Scattering using National super computer resources.
- Conduct a quantitative analysis by comparing absorption spectrums.
- Evaluate ability to simulate optoelectronic devices such as photodetectors or free electron driven light source.

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