PFURO 2023

Research Project: 1D Initial Plasma Formation Modeling
Objective: implement a wave-based approach to model light wave propagation in materials
Plans:

- June 5 - June 11 (1st - 2nd weeks)
    - attend online classes
    - write a finite difference scheme for EM wave propagation
- June 18 (3rd week)
    - a python module to model EM wave propagation
- June 25 (4th week)
    - implement the python module into the original 1D-IPF code
- July 2 (5th week)
    - test the code for metals: Aluminum
- July 9 (6th week)
- July 16 (7th week)
- July 23 (8th week)
- July 30 (9th week)
- Aug 6 (10th week)

Numerical Method

In this project, both **explicit** and **implicit** Finite-Difference Time-Domain (FDTD) schemes will be implemented to model the electromagnetic wave propagation in medium. The word “explicit” means that the time-step size “dt” is strictly controlled by Courant–Friedrichs–Lewy (CFL) condition so that the wave propagation distance within a allowed time-step size cannot exceed the grid size “dx”. Any form of **hyperbolic PDEs** are updated explicitly such as Euler equations in the computational fluid dynamics (CFD). The allowed wave propagation step size within a grid size “dx” is controlled by the CFL number. Typically, CFL ~ 0.5.

$$v_{\text{wave}} \times dt < \text{CFL} \times dx \quad \text{… Eq. (0)}$$

An implicit FDTD has the advantage to treat large time-step size with unconditional numerical stability. Any form of **parabolic PDEs** are updated implicitly, in which they have infinite characteristic wave speeds. The goal of this project is to model the laser absorption phenomenon in one dimensional. Because of the fast light signal, the allowed time-step size given by Eq. (0) is very small, compared to other time scales in ICF plasma. Hence, implicit FDTD relieves the harsh condition on the time-step size problem in modeling EM waves.

Task 0 in PFURO program

- Report and compare the numerical stability between explicit and implicit FDTD schemes in modeling EM wave propagation for the initial plasma formation process.

Conventional inertial confinement fusion (ICF) codes adopt the geometric ray trace approach to model the light wave propagation in ICF plasma. The ray trace approach in 2D or 3D simulations are highly noisy in modeling the laser energy deposition, because light wave

energies are dumped along their geometric paths. A wave-based approach, on the other hand, provides a smooth laser energy deposition modeling in multi-dimensional simulations, as well as the capability to model the initial plasma formation process consistently during the solid-to-plasma transition.

The modeling equation in this project is defined below. It is the electromagnetic (EM) wave equation in nonlinear optical media.

$$\nabla^2 E - \frac{n^2}{c^2}\frac{\partial^2 E}{\partial t^2} = \frac{1}{\epsilon_0 c^2}\frac{\partial^2 P_{\mathrm{NL}}}{\partial t^2} + \mu\sigma\frac{\partial E}{\partial t}$$ ... Eq. (1)

Here P_NL is the nonlinear polarization in media. As EM waves propagate into a matter, molecules are polarized and oscillate along the direction of the electric field vector “E”. Depending on crystalline structure, the induced polarization can react with electric fields linearly or nonlinearly. In Eq. (1.0), χ_1 is known as the linear susceptibility, while χ_2 means for the second order susceptibility.

$$P = \epsilon_0(\chi_1 E + \chi_2 E^2 + ...) = \epsilon_0\chi_1 E + P_{\mathrm{NL}}$$ ... Eq. (1.0)

The light speed c and the complex refractive index n relate to the permittivity of free space “ϵ_0”, the permeability of free space μ_0, as well as their correspondence in matter.

$$c = \frac{1}{\sqrt{\mu_0\epsilon_0}}, \quad n = \sqrt{\frac{\mu\epsilon}{\mu_0\epsilon_0}}$$ … Eq. (1.1)

In this project, a non-magnetized plasma is assumed such that

$$\mu \approx \mu_0$$ … Eq. (1.2)

The **complex** refractive index in Eq. (1) is

$$n \approx \sqrt{\epsilon/\epsilon_0} = \sqrt{1+\chi_1} = \sqrt{\epsilon_\mathrm{r}}$$ … Eq. (1.3)

where the linear susceptibility χ_1 is defined in Eq. (1.0). The refractive index is a complex number. Its real part accounts for reflections while the imaginary part accounts for absorptions. For Aluminium at 300 K, its refractive index is,

$$n(\mathrm{Al}; 300K) = n_\mathrm{r} + in_\mathrm{i} = 0.85 + i6.48$$ … Eq. (1.3.0)

The term ϵ_r is known as the relative permittivity. It can be represented by a classical Lorentz model analytically.

$$\epsilon_\mathrm{r} \equiv 1 + \chi_1$$ … Eq. (1.4)

The last term in Eq. (1) refers to the formation of transient current characterized by the electric conductivity σ. The induced current is damped by the material resistance.

Task 1 during the first two weeks in PFURO program

- Derive an explicit finite scheme to discretize Eq. (1) using the second-order central finite differencing in time and space.
- Assume a **linear susceptibility** in Eq. (1) so that $P_NL = 0$
- Ignore the transient current term in Eq. (1).
- Assume a room-temperature complex refractive index for Aluminum in Eq. (1.3.0)

$$\nabla^2 E - \frac{n^2}{c^2}\frac{\partial^2 E}{\partial t^2} = 0 \quad \text{… Eq. (2)}$$

Using the central differencing, the first-order spatial derivative, the second-order spatial derivative and the second-order time derivative are

$$\frac{\partial E(t^n)}{\partial x} \approx \frac{E^n(x_{i+1/2}) - E^n(x_{i-1/2})}{\Delta x} = \frac{E^n_{i+1/2} - E^n_{i-1/2}}{\Delta x} \quad \text{… Eq. (3.0)}$$

$$\frac{\partial^2 E(t^n)}{\partial x^2} = \frac{E^n_{i+1} - 2E^n_i + E^n_{i-1}}{\Delta x^2} \quad \text{… Eq. (3.1)}$$

$$\frac{\partial^2 E(x_i)}{\partial t^2} = \frac{E^{n+1}_i - 2E^n_i + E^{n-1}_i}{\Delta t^2} \quad \text{… Eq. (3.2)}$$

Substituting Eqs. (3.1)-(3.2) into Eq. (2), the explicit update for the electric field is

$$E^{n+1}_i = \left(\frac{\Delta t}{\Delta x}\frac{c}{n}\right)^2 (E^n_{i+1} - 2E^n_i + E^n_{i-1}) - (-2E^n_i + E^{n-1}_i) \quad \text{… Eq. (4.0)}$$

The first bracket in Eq. (4) is required to satisfy Courant condition as stated in Eq. (0)

$$\frac{\Delta t}{\Delta x}\frac{c}{n} < 1 \quad \text{… Eq. (4.1)}$$

5/26/2023 Meeting

- use Google Doc for research communication
- give a tutorial for the IPF code in the next meeting

5/30/2023 Meeting

- not sure for virtual in APS DPP
- begin deriving an explicit finite difference scheme to solve Eq. (2)

- send 1D-IPF code to Nick
- next meeting during the week of June 5
- 27 hours driving from May 31 to June 4