Self-Consistent Simulations of Beam and Plasma Systems
Homework 3

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Wednesday, June 15$^{\text{th}}$, 2016

Problem 1 - Courant limit in 1D

For the Yee scheme in 1D, the discrete propagation equation is:

$$\frac{1}{c^2}\frac{{E_x}_\ell^{n+1} - 2{E_x}_\ell^n + {E_x}_\ell^{n-1}}{\Delta t^2} = \frac{{E_x}_{\ell+1}^n - 2{E_x}_\ell^n + {E_x}_{\ell-1}^n}{\Delta z^2}$$

As explained in class, for $c\Delta t > \Delta z$ this equation has unstable solutions.

a) By assuming that E_x is of the form $E_0 e^{ikz-i\omega t}$, i.e.

$${E_x}_{\ell'}^n = E_0 e^{ik\,\ell'\Delta z - i\omega n\Delta t}$$

rederive the dispersion equation, as done in class.

Hint: Use the Euler formulas:

$$\frac{e^{ix} - e^{-ix}}{2i} = \sin(x) \qquad \frac{e^x + e^{-x}}{2} = \cosh(x)$$

b) In the case $c\Delta t > \Delta z$, what is the maximum value of k (between 0 and $\pi/\Delta z$) for which there is a real solution ω to the dispersion equation?

c) For values of k above this threshold, we will assume that E_x is of the form:

$${E_x}_{\ell'}^n = (-1)^n E_0 e^{ik\,\ell'\Delta z + n\Gamma\Delta t}$$

By inserting this ansatz into the discrete propagation equation, find the corresponding dispersion relation which links Γ and k. From this relation, extract the expression of Γ as a function of k (use the function argch, which is sometimes also denoted as $\cosh^{-1}$).

d) For which value of the wavevector k does the instability growth rate reach its highest value?

e) Download the script `em_unstable.py` from:

`https://raw.githubusercontent.com/RemiLehe/uspas_exercise/master/unstable.py`

As can be seen from the section `if __name__ =='__main__':`, this script is a slight modification of the script `em_pic_1d.py` from previous assignments, where Δt has been set to:

$$\Delta t = 1.01\frac{\Delta z}{c}$$

Run the script and look at plots of the fields in the folder `diagnostics`. Is the observed evolution consistent with the answers to the previous questions? Why?

Problem 2 - Projectional and Sectional Emittance

As discussed in class, the rms emittance

$$\epsilon_{x,rms} = \sqrt{\langle x^2 \rangle_\perp \langle x'^2 \rangle_\perp - \langle xx' \rangle_\perp^2} \qquad [mm\text{-}mrad]$$

is calculated from a projection of the full 4-D trace space into the x-x' plane. Here, the second moments of $f(x, y, x', y')$ are defined as

$$\langle x^2 \rangle = \frac{\iiiint x^2 f(x, y, x', y') dx dy dx' dy'}{\iiiint f(x, y, x', y') dx dy dx' dy'}$$

and similarly for $\langle x'^2 \rangle$ and $\langle xx' \rangle$. An identical treatment holds for the y-y' emittance.
However, many systems we are interested in are cylindrically symmetric and thus it is convenient to run a simulation in a 2D mode with coordinates R and Z. This can speed up the calculation time significantly compared to 3D simulations. Unfortunately, if we just substitute r for x in the above equations for the emittance, we obtain the emittance of a slice and not the projection of the beam (both can be useful, though). It stands to reason that we would like a way to calculate both from the results of a RZ symmetric simulation.
The transformation from cartesian coordinates (x,y,x',y') into polar coordinates (r, θ, r', α') is given by

$$\begin{aligned} r^2 &= x^2 + y^2 \\ r'^2 + \alpha'^2 &= x'^2 + y'^2 \\ x' &= r' \cos\theta - \alpha' \sin\theta \\ y' &= r' \sin\theta + \alpha' \cos\theta \end{aligned}$$

where

$$x' = \frac{\mathrm{d}x}{\mathrm{d}z} = \frac{v_x}{v_z}, \quad r' = \frac{\mathrm{d}r}{\mathrm{d}z} = \frac{v_r}{v_z}, \quad \alpha' = r\frac{\mathrm{d}\theta}{\mathrm{d}z} = \frac{v_\theta}{v_z}.$$

a) In the simple case where the beam has azimuthal symmetry and no azimuthal velocity component ($\alpha' = 0$), transform the above moment equations into polar coordinates to obtain a formula for the projectional emittance $\epsilon_{rms}(x, x')$ that depends only on r and r'.

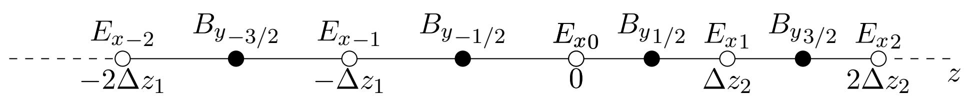
b) Implement both ways of calculating $\epsilon_{x,rms}$ (from x, x' and from r, r') as functions in a python script.

c) Use the random number generator `numpy.random` to generate a round, azimuthally symmetric particle distribution with no azimuthal velocity component in polar coordinates. Transform the distribution into cartesian coordinates and confirm your calculations in a) by calculating $\epsilon_{x,rms}$ from either distribution using the appropriate function.

Note: A more rigorous treatment of the dynamics of skew beams in an R-Z simulation can be found in [Chan et al., NIM A, 1991].

Problem 3 - Reflection between two grids with different resolution

We consider a grid which has a different resolution for $z > 0$ and $z < 0$:



In the area $z < 0$, the discretized Maxwell equations are:

$$\frac{{B_y}_{\ell+1/2}^{n+1/2} - {B_y}_{\ell+1/2}^{n-1/2}}{\Delta t} = -\left(\frac{{E_x}_{\ell+1}^{n} - {E_x}_{\ell}^{n}}{\Delta z_1}\right) \qquad \text{for any } \ell < 0 \tag{1}$$

$$\frac{{E_x}_{\ell}^{n+1} - {E_x}_{\ell}^{n}}{c^2\Delta t} = -\left(\frac{{B_y}_{\ell+1/2}^{n+1/2} - {B_y}_{\ell-1/2}^{n+1/2}}{\Delta z_1}\right) \qquad \text{for any } \ell < 0 \tag{2}$$

and in the area $z > 0$, the discretized Maxwell equations are:

$$\frac{{B_y}_{\ell+1/2}^{n+1/2} - {B_y}_{\ell+1/2}^{n-1/2}}{\Delta t} = -\left(\frac{{E_x}_{\ell+1}^{n} - {E_x}_{\ell}^{n}}{\Delta z_2}\right) \qquad \text{for any } \ell \geq 0 \tag{3}$$

$$\frac{{E_x}_{\ell}^{n+1} - {E_x}_{\ell}^{n}}{c^2\Delta t} = -\left(\frac{{B_y}_{\ell+1/2}^{n+1/2} - {B_y}_{\ell-1/2}^{n+1/2}}{\Delta z_2}\right) \qquad \text{for any } \ell > 0 \tag{4}$$

and finally, at the boundary between the two domains ($\ell = 0$) the equation for the field E_x is:

$$\frac{{E_x}_{0}^{n+1} - {E_x}_{0}^{n}}{c^2\Delta t} = -\left(\frac{{B_y}_{1/2}^{n+1/2} - {B_y}_{-1/2}^{n+1/2}}{\frac{\Delta z_1 + \Delta z_2}{2}}\right) \qquad \text{for any } \ell > 0 \tag{5}$$

We will look for a solutions of these equations, in the form:

$${E_x}_{\ell}^{n} = E e^{ik_1\Delta z_1 \ell - i\omega n\Delta t} - RE e^{-ik_1\Delta z_1 \ell - i\omega n\Delta t} \qquad \text{for any } \ell \leq 0 \tag{6}$$

$${E_x}_{\ell}^{n} = TE e^{ik_2\Delta z_2 \ell - i\omega n\Delta t} \qquad \text{for any } \ell \geq 0 \tag{7}$$

$${B_y}_{\ell+1/2}^{n+1/2} = \frac{E}{c} e^{ik_1\Delta z_1(\ell+1/2) - i\omega(n+1/2)\Delta t} + R\frac{E}{c} e^{-ik_1\Delta z_1(\ell+1/2) - i\omega(n+1/2)\Delta t} \qquad \text{for any } \ell < 0 \tag{8}$$

$${B_y}_{\ell+1/2}^{n+1/2} = T\frac{E}{c} e^{ik_2\Delta z_2(\ell+1/2) - i\omega(n+1/2)\Delta t} \qquad \text{for any } \ell \geq 0 \tag{9}$$

where R and T are unknown complex coefficients.

a) Show that the expressions in equations (6) to (9) are solutions of the discrete Maxwell equations for $z < 0$ and $z > 0$ (i.e. equations (1) to (4)), provided that:

$$\frac{1}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right) = \frac{1}{\Delta z_1}\sin\left(\frac{k_1\Delta z_1}{2}\right) \qquad \text{and} \qquad \frac{1}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right) = \frac{1}{\Delta z_2}\sin\left(\frac{k_2\Delta z_2}{2}\right) \tag{10}$$

b) From the fact that equation (6) and (7) are both valid for $\ell = 0$, deduce that

$$R + T = 1$$

c) By inserting the expressions (7) to (9) into (5), and by using the relation $R+T=1$, show we obtain the following equation for R:

$$(e^{-i\omega\Delta t/2} - e^{i\omega\Delta t/2})(1-R) = -\beta[(1-R)e^{ik_2\Delta z_2/2} - e^{-ik_1\Delta z_1/2} - Re^{ik_1\Delta z_1/2}]$$

with $\beta = \frac{2c\Delta t}{\Delta z_1+\Delta z_2}$. (Note that, from equations (7) to (9) and $R+T=1$, one has $E_{x\,0}^{\,n+1} = E(1-R)e^{-i\omega\Delta t}$, $E_{x\,0}^{\,n} = E(1-R)$, $B_{y\,1/2}^{\,n+1/2} = \frac{E}{c}(1-R)e^{ik_2\Delta z_2/2-i\omega\Delta t/2}$, $B_{y\,-1/2}^{\,n+1/2} = \frac{E}{c}e^{ik_1\Delta z_1/2-i\omega\Delta t/2} + \frac{RE}{c}e^{-ik_1\Delta z_1/2-i\omega\Delta t/2}$.)

Conclude that the reflection coefficient $|R|$ is

$$|R| = \left|\frac{(e^{-i\omega\Delta t/2} - e^{i\omega\Delta t/2}) + \beta(e^{ik_2\Delta z_2/2} - e^{-ik_1\Delta z_1/2})}{(e^{-i\omega\Delta t/2} - e^{i\omega\Delta t/2}) + \beta(e^{ik_2\Delta z_2/2} + e^{ik_1\Delta z_1/2})}\right|$$

d) We wish to plot $|R|$ as a function ω. In order to do so, we first need to express $e^{ik_1\Delta z_1/2}$ and $e^{ik_2\Delta z_2/2}$ as a function of ω.

From equation (10), using $\sin(k_1\Delta z_1/2) = \frac{e^{ik_1\Delta z_1/2} - e^{-ik_1\Delta z_1/2}}{2i}$, show that $e^{ik_1 z_1/2}$ satisfies the equation

$$(e^{ik_1\Delta z_1/2})^2 - 2i\frac{\Delta z_1}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)e^{ik_1\Delta z_1/2} - 1 = 0$$

and by remarking that this is a second-order polynomial equation, show that the expression of $e^{ik_1\Delta z_1/2}$ as a function of ω is:

$$e^{ik_1\Delta z_1/2} = i\frac{\Delta z_1}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right) + (1 - \left(\frac{\Delta z_1}{c\Delta t}\right)^2\sin^2\left(\frac{\omega\Delta t}{2}\right))^{1/2} \tag{11}$$

(where the sign + is chosen from knowing the solution for $\Delta z_1 = c\Delta t$)

e) Download the file from

`https://raw.githubusercontent.com/RemiLehe/uspas_exercise/master/plot_reflection.py`. This script plots $|R|$ as a function of ω (and of $\lambda/\Delta z_2$, where λ is the wavelength of the incident wave), using the above formula. In the case of the script, the resolution of the second grid is 5 times coarser than that of the first grid.

Run the script and interpret the evolution of the reflection coefficient: what happens when the wave is not resolved anymore by the second grid (i.e. when $\lambda < 3\Delta z_2$)?

f) What is the value of the coefficient $|R|$ when $\Delta z_2 = \Delta z_1$? Is this to be expected?

g) Download the file from

`https://raw.githubusercontent.com/RemiLehe/uspas_exercise/master/em_pic_1d_mr.py`.

The script simulates the propagation of electromagnetic fields in 1D on a succession of 2 grids that can be set a different resolutions and are linked by an algorithm selected by the user. The code prints the coefficients of reflection and transmission, and can perform scans on the wavelength and the method used to connect the grids.

Set l_scan=0, l_method=1, Nz=300, lw=25., and run. Repeat for lw=15., lw=10. and lw=5. Repeat for method=2 and method=3. Observe how for all the tested methods, the reflection is total for wavelengths that are below the cutoff of the coarser grid.

Then, set l_scan=1, Nz=500, and run the script. After some time, the run concludes and you have a file coef_refl.pdf that you may open. The plot shows the coefficient of reflection versus incident wavelength, for three tested methods to connect the two grids, from analysis (solid curves, for methods 1 and 2), and from simulations (crosses, circles and x for methods 1, 2 and 3). Observe that the simulations confirm the theoretical predictions. Also observe that the different algorithms to connect the grids result in widely different coefficient of reflection at long wavelength.

Finally, repeat the scan with Nz=100. What happened to the agreement between theory and simulations? Can you explain why?