Self-Consistent Simulations of Beam and Plasma Systems
Final Exam ("take-home")

S. M. Lund, J.-L. Vay, R. Lehe, and D. Winklehner

Thursday, June 16^{th}, 2016

Problem 1 - Maxwell's equations and redundant information.

a) Show that the relativistic Vlasov equation

$$\left\{ \frac{\partial}{\partial t} + \boldsymbol{v} \cdot \frac{\partial}{\partial \boldsymbol{x}} + q\left[\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\right] \cdot \frac{\partial}{\partial \boldsymbol{p}} \right\} f(\boldsymbol{x}, \boldsymbol{p}, t) = 0$$

with

$$\boldsymbol{v} = \frac{\boldsymbol{p}}{\gamma m} = \frac{\boldsymbol{p}/m}{\left[1 + \boldsymbol{p}^2/(mc)^2\right]^{1/2}}$$

implies conservation of charge with

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial \boldsymbol{x}} \cdot \mathbf{J} = 0$$

where

$$\rho = q \int d^3p\, f$$
$$\mathbf{J} = q \int d^3p\, \boldsymbol{v} f$$

Hint 1: Use the same steps as in Monday's problem 3 a).

Hint 2: You are permitted to do this non-relativistically if you want. The result holds either way.

b) The 3D Maxwell equations are linear, 1^{st}-order-in-time, kinematic equations for $\boldsymbol{E}(\boldsymbol{x}, t)$, $\boldsymbol{B}(\boldsymbol{x}, t)$ if $\rho(\boldsymbol{x}, t)$ and $\mathbf{J}(\boldsymbol{x}, t)$ are regarded as prescribed sources.

1) How many field components are in $\boldsymbol{E}$, $\boldsymbol{B}$?

2) How many equations are in the standard set of Maxwell equations?

$$\nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0}$$
$$\nabla \times \boldsymbol{E} = -\frac{\partial}{\partial t}\boldsymbol{B}$$
$$\nabla \cdot \boldsymbol{B} = 0$$
$$\nabla \times \boldsymbol{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial}{\partial t}\boldsymbol{E}$$

3) What initial ($t = 0$) values are required for $\boldsymbol{E}$ and $\boldsymbol{B}$ to solve the Maxwell equations for $\boldsymbol{E}(\boldsymbol{x}, t)$ and $\boldsymbol{B}(\boldsymbol{x}, t)$ for all times t with $\rho(\boldsymbol{x}, t)$ and $\mathbf{J}(\boldsymbol{x}, t)$ specified?

c) To better understand the situation in b), show that the Maxwell equations imply that

$$\begin{aligned} \nabla \times (\nabla \times \boldsymbol{E}) + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\boldsymbol{E} &= -\mu_0 \frac{\partial}{\partial t}\mathbf{J} \\ \nabla \times (\nabla \times \boldsymbol{B}) + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\boldsymbol{B} &= \mu_0 \nabla \times \mathbf{J} \end{aligned}$$

where

$$\mu_0 \epsilon_0 = \frac{1}{c^2}.$$

$\rightarrow$ 6 2^{nd}-order-in-time equations for 6 field components $\boldsymbol{E}$, $\boldsymbol{B}$.

d) Show that

$$\nabla \times \boldsymbol{E} = -\frac{\partial}{\partial t}\boldsymbol{B}$$

implies that

$$\frac{\partial}{\partial t}\nabla \cdot \boldsymbol{B} = 0.$$

Does this imply that $\nabla \cdot \boldsymbol{B}(\boldsymbol{x}, t) = 0$ for all times t if $\nabla \cdot \boldsymbol{B}(\boldsymbol{x}, t = 0) = 0$?

e) Show that

$$\nabla \times \boldsymbol{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial}{\partial t}\boldsymbol{E} \qquad \text{and} \qquad \frac{\partial}{\partial t}\rho + \frac{\partial}{\partial \boldsymbol{x}} \cdot \mathbf{J} = 0$$

imply that

$$\frac{\partial}{\partial t}\left(\nabla \cdot \boldsymbol{E} - \rho/\epsilon_0\right) = 0.$$

Does this imply that $\nabla \cdot \boldsymbol{E} = \rho/\epsilon_0$ for all times t if $\nabla \cdot \boldsymbol{E} = \rho/\epsilon_0$ at $t = 0$?

f) Show that the Maxwell equations

$$\nabla \times \boldsymbol{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial}{\partial t}\boldsymbol{E} \qquad \text{and} \qquad \nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0}$$

imply that

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial \boldsymbol{x}} \cdot \mathbf{J} = 0.$$

Does this imply that the Maxwell equations should only be applied to charge ρ and current sources $\mathbf{J}$ which locally conserve charge?

g) Based on a) - f), can we solve Maxwell's equations for $\boldsymbol{E}(\boldsymbol{x}, t)$ and $\boldsymbol{B}(\boldsymbol{x}, t)$ for sources ρ and $\mathbf{J}$ satisfying

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial \boldsymbol{x}} \cdot \mathbf{J} = 0$$

for all times $t \geq 0$ by only solving the two Maxwell equations

$$\nabla \times \boldsymbol{E} = -\frac{\partial}{\partial t}\boldsymbol{B} \qquad \text{and} \qquad \nabla \times \boldsymbol{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial}{\partial t}\boldsymbol{E}$$

provided that

$$\nabla \cdot \boldsymbol{E} = \frac{\rho}{\epsilon_0} \qquad \text{and} \qquad \nabla \cdot \boldsymbol{B} = 0$$

are satisfied at time $t = 0$? If yes, does it matter if we use $\nabla \cdot \boldsymbol{E} = \rho/\epsilon_0$ and $\nabla \cdot \boldsymbol{B} = 0$? Why?

Problem 2 - Extended-stencil Maxwell solver

Let us consider the following scheme for the 1D Maxwell equations in vacuum

$$\frac{{B_y}^{n+1/2}_{\ell+1/2} - {B_y}^{n-1/2}_{\ell+1/2}}{\Delta t} = -\left(\frac{{E_x}^{n}_{\ell+1} - {E_x}^{n}_{\ell}}{\Delta z}\right)$$

$$\frac{{E_x}^{n+1}_{\ell} - {E_x}^{n}_{\ell}}{\Delta t} = -c^2\left((1-\alpha)\frac{{B_y}^{n+1/2}_{\ell+1/2} - {B_y}^{n+1/2}_{\ell-1/2}}{\Delta z} + \alpha\frac{{B_y}^{n+1/2}_{\ell+3/2} - {B_y}^{n+1/2}_{\ell-3/2}}{3\Delta z}\right)$$

where ${B_y}^{n'}_{\ell'}$ and ${E_x}^{n'}_{\ell'}$ represent the fields B_y and E_x at time $n'\Delta t$ and position $\ell'\Delta z$.

a) By performing a Taylor expansion of the B field to order 2 in Δz (i.e. with an error term $O(\Delta z^3)$), show that the expression

$$(1-\alpha)\frac{{B_y}^{n+1/2}_{\ell+1/2} - {B_y}^{n+1/2}_{\ell-1/2}}{\Delta z} + \alpha\frac{{B_y}^{n+1/2}_{\ell+3/2} - {B_y}^{n+1/2}_{\ell-3/2}}{3\Delta z}$$

Is an approximation of $\frac{\partial B}{\partial z}$ at position $\ell\Delta z$ (and time $(n+1/2)\Delta t$) which is accurate to order 2 in Δz.

Hint: remember that ${B_y}^{n+1/2}_{\ell+1/2}$ denotes the B_y field at position $z = (\ell+1/2)\Delta z$. In other words: ${B_y}^{n+1/2}_{\ell+1/2} = {B_y}^{n+1/2}((\ell+1/2)\Delta z)$ (with similar expressions for ${B_y}^{n+1/2}_{\ell-1/2}$, ${B_y}^{n+1/2}_{\ell+3/2}$, ${B_y}^{n+1/2}_{\ell-3/2}$). Then perform a Taylor expansion around $z = \ell\Delta z$.

b) By combining the discrete Maxwell equations, show that the corresponding discrete propagation equation for E_x is of the form:

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

$$+\beta\frac{{E_x}^{n}_{\ell+2} - 4{E_x}^{n}_{\ell+1} + 6{E_x}^{n}_{\ell} - 4{E_x}^{n}_{\ell-1} + {E_x}^{n}_{\ell-2}}{\Delta z^2} \quad (2)$$

and give the expression of β as a function of α.

Hint: Start by evaluating the quantity

$$\frac{1}{\Delta t}\left(\frac{{E_x}^{n+1}_{\ell} - {E_x}^{n}_{\ell}}{\Delta t} - \frac{{E_x}^{n}_{\ell} - {E_x}^{n-1}_{\ell}}{\Delta t}\right)$$

using the second Maxwell equation from above.

c) By assuming that E_x is of the form

$${E_x}^{n}_{\ell} = E_0 e^{ik\ell\Delta z - i\omega n\Delta t}$$

Show that the discrete dispersion relation is:

$$\frac{1}{c^2\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right) = \frac{1}{\Delta z^2}\sin^2\left(\frac{k\Delta z}{2}\right) - \frac{4\alpha}{3\Delta z^2}\sin^4\left(\frac{k\Delta z}{2}\right)$$

d) For $\alpha < 3/8$, show that the right-hand side of the above equation is a growing function of k, for $k \in [0, \pi/\Delta z]$.

Infer the maximum value that the right-hand takes for $k \in [0, \pi/\Delta z]$, and thus infer that the Courant limit is

$$\Delta t_{CFL} = \frac{\Delta z}{c} \frac{1}{\sqrt{1 - \frac{4\alpha}{3}}}$$

Reminder for standard formulas:

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

Problem 3 - Python ODE solver

Write a python script to advance the moments

$$\frac{d}{ds}\begin{bmatrix} \langle \tilde{x}^2 \rangle_\perp \\ \langle \tilde{x}\tilde{x}' \rangle_\perp \\ \langle \tilde{x}'^2 \rangle_\perp \\ \langle \tilde{y}^2 \rangle_\perp \\ \langle \tilde{y}\tilde{y}' \rangle_\perp \\ \langle \tilde{y}'^2 \rangle_\perp \end{bmatrix} = \begin{bmatrix} 2\langle \tilde{x}\tilde{x}' \rangle_\perp \\ \langle \tilde{x}'^2 \rangle_\perp - \kappa_x(s)\langle \tilde{x}^2 \rangle_\perp + \frac{Q\langle \tilde{x}^2 \rangle_\perp^{1/2}}{2[\langle \tilde{x}^2 \rangle_\perp^{1/2} + \langle \tilde{y}^2 \rangle_\perp^{1/2}]} \\ -2\kappa_x(s)\langle \tilde{x}\tilde{x}' \rangle_\perp + \frac{Q\langle \tilde{x}\tilde{x}' \rangle_\perp}{\langle \tilde{x}^2 \rangle_\perp^{1/2}[\langle \tilde{x}^2 \rangle_\perp^{1/2} + \langle \tilde{y}^2 \rangle_\perp^{1/2}]} \\ 2\langle \tilde{y}\tilde{y}' \rangle_\perp \\ \langle \tilde{y}'^2 \rangle_\perp - \kappa_y(s)\langle \tilde{y}^2 \rangle_\perp + \frac{Q\langle \tilde{y}^2 \rangle_\perp^{1/2}}{2[\langle \tilde{x}^2 \rangle_\perp^{1/2} + \langle \tilde{y}^2 \rangle_\perp^{1/2}]} \\ -2\kappa_y(s)\langle \tilde{y}\tilde{y}' \rangle_\perp + \frac{Q\langle \tilde{y}\tilde{y}' \rangle_\perp}{\langle \tilde{y}^2 \rangle_\perp^{1/2}[\langle \tilde{x}^2 \rangle_\perp^{1/2} + \langle \tilde{y}^2 \rangle_\perp^{1/2}]} \end{bmatrix}$$

with $\kappa_x(s) = -\kappa_y(s) = \hat{\kappa}\cos\left(\frac{2\pi s}{L_p}\right)$. Use a perveance of $\mathrm{Q} = 6 \times 10^{-4}$, focus strength $\hat{\kappa} = \frac{30}{\text{meter}^2}$, and lattice period $\mathrm{L_p} = 0.5$ m.

a) Use a scientific python package with an ODE integrator (e.g. `scipy.integrate.odeint`) to evolve the second order moments from an (arbitrary) initial condition at $s = 0$.

Hint: use `scipy.integrate.odeint?` in ipython for more information. Ask for help if you are stuck!

b) Apply the result in a) to advance from the initial condition

$$\begin{aligned} \langle \tilde{x}^2 \rangle_\perp = \langle \tilde{y}^2 \rangle_\perp &= \frac{1}{4}\ \text{mm}^2 \\ \langle \tilde{x}\tilde{x}' \rangle_\perp = \langle \tilde{y}\tilde{y}' \rangle_\perp &= 0 \\ \langle \tilde{x}'^2 \rangle_\perp = \langle \tilde{y}'^2 \rangle_\perp &= 25\ \text{mrad}^2 \end{aligned}$$

Use `matplotlib` to plot all 2^{nd} order moments on an axial mesh with at least 10 grid points over 10 lattice periods.

c) Plot the combination of moments corresponding to rms x-emittance

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

vs. s for 10 periods. Should you expect this value to be constant to numerical precision?

d) Show that initial conditions at $s = 0$ can be found for some values of $\langle \tilde{x}^2 \rangle_\perp$ and $\langle \tilde{y}^2 \rangle_\perp$ with initial conditions

$$\begin{aligned} \langle \tilde{x}\tilde{x}' \rangle_\perp = \langle \tilde{y}\tilde{y}' \rangle_\perp &= 0 \\ \langle \tilde{x}'^2 \rangle_\perp = \langle \tilde{y}'^2 \rangle_\perp &= 25 \ \text{mrad}^2 \end{aligned}$$

such that all moments repeat to numeral precision at $s = \mathrm{L_p}$. Is $\epsilon_{x,rms}$ still constant?

Hint: Try numerical root finding from initial guess values of $\langle \tilde{x}^2 \rangle_\perp = \langle \tilde{y}^2 \rangle_\perp$.

Problem 4 - Alternative particle pusher

In order to integrate the continuous equations of motion

$$\frac{d\boldsymbol{x}}{dt} = \frac{\boldsymbol{p}}{\gamma m} \qquad \frac{d\boldsymbol{p}}{dt} = q\left(\boldsymbol{E} + \frac{\boldsymbol{p}}{\gamma m} \times \boldsymbol{B}\right) \quad (\text{with } \gamma = \sqrt{1 + \boldsymbol{p}^2/(mc)^2})$$

we choose to use the following staggered scheme

$$\frac{\boldsymbol{x}^{n+1} - \boldsymbol{x}^n}{\Delta t} = \frac{\boldsymbol{p}^{n+1/2}}{\gamma^{n+1/2} m} \tag{3}$$

$$\frac{\boldsymbol{p}^{n+1/2} - \boldsymbol{p}^{n-1/2}}{\Delta t} = q\left(\boldsymbol{E}^n + \frac{1}{2}\left(\frac{\boldsymbol{p}^{n+1/2}}{\gamma^{n+1/2} m} + \frac{\boldsymbol{p}^{n-1/2}}{\gamma^{n-1/2} m}\right) \times \boldsymbol{B}^n\right) \tag{4}$$

where the superscripts ^{n}, $^{n+1/2}$ and $^{n+1}$ indicates that the corresponding quantity is taken at time $n\Delta t$, $(n+1/2)\Delta t$ and $(n+1)\Delta t$, and where $\gamma^{n+1/2} = \sqrt{1 + (\boldsymbol{p}^{n+1/2})^2/(mc)^2}$ and $\gamma^{n-1/2} = \sqrt{1 + (\boldsymbol{p}^{n-1/2})^2/(mc)^2}$.

While equation (3) is easy to convert into an update equation ($\boldsymbol{x}^{n+1} = \boldsymbol{x}^n + \frac{\boldsymbol{p}^{n+1/2}}{\gamma^{n+1/2} m}\Delta t$), it is more difficult to obtain $\boldsymbol{p}^{n+1/2}$ from $\boldsymbol{p}^{n-1/2}$, since equation (4) is implicit (i.e. it involves $\boldsymbol{p}^{n+1/2}$ in both its right-hand side and left-hand side). The aim of this problem is to obtain the corresponding update equation.

a) Verify that the following scheme

$$\boldsymbol{p}' = \boldsymbol{p}^{n-1/2} + q\boldsymbol{E}^n \Delta t + \boldsymbol{p}^{n-1/2} \times \boldsymbol{s} \qquad \boldsymbol{s} = \frac{q\Delta t \boldsymbol{B}^n}{2\gamma^{n-1/2} m} \tag{5}$$

$$\boldsymbol{p}^{n+1/2} = \boldsymbol{p}' + \boldsymbol{p}^{n+1/2} \times \boldsymbol{t} \qquad \boldsymbol{t} = \frac{q\Delta t \boldsymbol{B}^n}{2\gamma^{n+1/2} m} \tag{6}$$

satisfies equation (4). Which one of the two above equations is implicit?

b) By taking the vector product and scalar product of (6) by $\boldsymbol{t}_+$, show that $\boldsymbol{p}^{n+1/2}$ can be extracted from this equation and reads

$$\boldsymbol{p}^{n+1/2} = \frac{1}{1 + \boldsymbol{t}^2}\left(\boldsymbol{p}' + \boldsymbol{p}' \times \boldsymbol{t} + (\boldsymbol{p}' \cdot \boldsymbol{t})\boldsymbol{t}\right) \tag{7}$$

Reminder: For any set of 3 vectors $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$, one has $(\boldsymbol{a} \times \boldsymbol{b}) \times \boldsymbol{c} = (\boldsymbol{a} \cdot \boldsymbol{c})\boldsymbol{b} - (\boldsymbol{b} \cdot \boldsymbol{c})\boldsymbol{a}$

c) In fact, equation (7) is still not explicit, since the expression of $\boldsymbol{t}$ (in equation (3)) depends on $\boldsymbol{p}^{n+1/2}$, through $\gamma^{n+1/2}$.

Thus, in order to extract $\boldsymbol{p}^{n+1/2}$ explicitly from equation (7), take the following steps:

- From equation (7), show that the expression of $(\boldsymbol{p}^{n+1/2})^2$ is:

$$(\boldsymbol{p}^{n+1/2})^2 = \frac{(\boldsymbol{p}')^2 + (\boldsymbol{p}' \cdot \boldsymbol{t})^2}{1 + \boldsymbol{t}^2} \tag{8}$$

  Reminder: For any set of two vectors $\boldsymbol{a}$, $\boldsymbol{b}$, one has $(\boldsymbol{a} \times \boldsymbol{b}) \cdot (\boldsymbol{a} \times \boldsymbol{b}) = \boldsymbol{a}^2\boldsymbol{b}^2 - (\boldsymbol{a} \cdot \boldsymbol{b})^2$

- Using the notation

$$\boldsymbol{\tau} = \frac{q\boldsymbol{B}\Delta t}{2m} = \gamma^{n+1/2}\boldsymbol{t} \tag{9}$$

  show that equation (8) leads to

$$(\gamma^2)^2 + [\tau^2 - (\gamma')^2]\gamma^2 - [(u^*)^2 + \tau^2] = 0 \tag{10}$$

  where γ is a short-hand notation for $\gamma^{n+1/2}$ (in other words $\gamma^2 = 1 + (\boldsymbol{p}^{n+1/2})^2/(mc)^2$) and where the following notations where used

$$\tau^2 = \boldsymbol{\tau}^2 \qquad u = \frac{\boldsymbol{p}' \cdot \boldsymbol{\tau}}{mc} \qquad (\gamma')^2 = 1 + \frac{(\boldsymbol{p}')^2}{(mc)^2} \tag{11}$$

- By remarking that equation (10) is a second-order polynomial in γ^2, show that its solution is:

$$\gamma = \frac{1}{\sqrt{2}}\sqrt{(\gamma')^2 - \tau^2 + \sqrt{[(\gamma')^2 - \tau^2]^2 + 4u^2 + 4\tau^2}} \tag{12}$$

d) Summing up all the previous step, in an actual algorithm (e.g. in Python) that computes $\boldsymbol{p}^{n+1/2}$ from $\boldsymbol{p}^{n-1/2}$, in **which order** should the following steps be executed?

i) Compute $\gamma^{n+1/2}$ (also denoted here as γ) using equation (12) and equation (11).

ii) Compute $\boldsymbol{s}$ using equation (3), and $\boldsymbol{\tau}$ using equation (11)

iii) Compute $\boldsymbol{p}^{n+1/2}$ using equation (7)

iv) Compute $\boldsymbol{p}'$ from $\boldsymbol{p}^{n-1/2}$ using equation (5)

v) Compute $\boldsymbol{t}$ from $\boldsymbol{\tau}$ and $\gamma^{n+1/2}$ (using equation (9))

e) Download the script `particle_pusher.py` from

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

This is an incomplete script that implements the solver considered here. Find the lines tagged by `## ASSIGNEMENT` and complete them with the appropriate code.

f) Run the script (`python particle_pusher.py`). It integrates the equations of motion for a relativistic electron ($\gamma \simeq 100$), in a magnetic field of 1 Tesla.

What do you expect the motion to be? Are the results from the code quantitatively consistent with the expected Larmor period of $\tau = \frac{2\pi\gamma m_e}{eB_0}$ (with $B_0 = 1\ T$, $m_e = 0.9 \times 10^{-30}\ kg$ and $e = 1.6 \times 10^{-19}\ C$) ?