Simulation of Beam and Plasma Systems
Homework 5 (Weekend)

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

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Problem 1 - Discrete numerical operations

a) Derive the uniform mesh formulas and error estimates covered in class (3 point centered):

$$\left.\frac{\partial f}{\partial x}\right|_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

$$\left.\frac{\partial^2 f}{\partial x^2}\right|_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2} + \mathcal{O}(\Delta x^2)$$

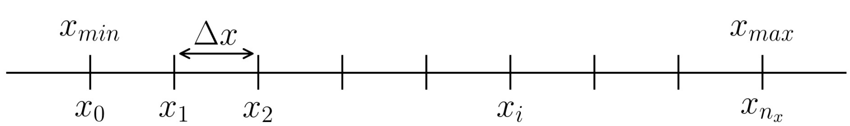
b) Derive the quadrature formulas and error estimates covered in class:

$$\text{Trapezoidal Rule:} \quad \int_{x_{i-1}}^{x_{i+1}} dx f(x) = \frac{f_{i-1} + 2f_i + f_{i+1}}{2}\Delta x + \mathcal{O}(\Delta x^3)$$

$$\text{Simpson's Rule:} \quad \int_{x_{i-1}}^{x_{i+1}} dx f(x) = \frac{f_{i-1} + 4f_i + f_{i+1}}{3}\Delta x + \mathcal{O}(\Delta x^5)$$

Hint: start with a forward approximation for $f(x)$ starting at f_{i-1} and integrate over the half-interval $x_{i-1} - x_i$. The other half interval is analogous.

c) Show that the formulas in b) are consistent with:

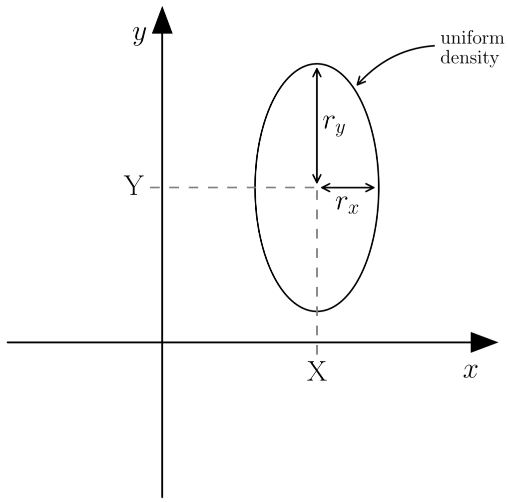


$$\text{Trapezoidal Rule:} \quad \int_{x_{min}}^{x_{max}} dx f(x) = \left\{ \frac{1}{2} f_0 + \sum_{i=1}^{n_x - 1} f_i + \frac{1}{2} f_{n_x} \right\} \Delta x$$

$$\text{Simpson's Rule } (n_x \text{ even}): \quad \int_{x_{min}}^{x_{max}} dx f(x) = \left\{ \frac{1}{3} f_0 + \frac{4}{3} f_1 + \frac{2}{3} f_2 + \frac{4}{3} f_3 + \frac{2}{3} f_4 + \cdots + \frac{2}{3} f_{n_x-2} + \frac{4}{3} f_{n_x-1} + \frac{1}{3} f_{n_x} \right\} \Delta x$$

Problem 2 - Moment formulation of the K-V distribution

The equations of motion for a particle evolving within a K-V beam



with

$$\begin{aligned} \tilde{x} &= x - \mathrm{X} \qquad \mathrm{X} = \langle x \rangle_\perp \\ \tilde{y} &= y - \mathrm{Y} \qquad \mathrm{Y} = \langle y \rangle_\perp \end{aligned}$$

are

$$\begin{aligned} \frac{d}{ds}x' + \kappa_x(s)x - \frac{2Q(x-\mathrm{X})}{r_x(r_x+r_y)} &= 0 \\ \frac{d}{ds}y' + \kappa_y(s)y - \frac{2Q(y-\mathrm{Y})}{r_y(r_x+r_y)} &= 0 \end{aligned}$$

when

$$\left(\frac{\tilde{x}}{r_x}\right)^2 + \left(\frac{\tilde{y}}{r_y}\right)^2 \leq 1.$$

Here

$$Q = \frac{q\lambda}{2\pi\epsilon_0 m\gamma_b^3\beta_b^2 c^2}.$$

a) Show that

$$\begin{aligned} r_x &= 2\langle \tilde{x}^2 \rangle_\perp^{1/2} \\ r_y &= 2\langle \tilde{y}^2 \rangle_\perp^{1/2} \end{aligned}$$

Hint: This is easier if you take

$$\int_{ellipse} d\tilde{x} \int d\tilde{y} \cdots = r_x r_y \int_0^1 d\rho\rho \int_{-\pi}^{\pi} d\theta \cdots$$

$$\begin{aligned}\tilde{x} &= r_x \rho \cos\theta \\ \tilde{y} &= r_y \rho \sin\theta\end{aligned}$$

with

$$\rho \in [0,1], \quad \theta \in [-\pi, \pi], \quad \textbf{and} \quad d\tilde{x}d\tilde{y} = r_x r_y \rho d\rho d\theta.$$

b) Derive the equations of motion summarized in class as:

$$\frac{d}{ds}\begin{bmatrix}\langle x\rangle_\perp \\ \langle x'\rangle_\perp \\ \langle y\rangle_\perp \\ \langle y'\rangle_\perp\end{bmatrix} = \begin{bmatrix}\langle x'\rangle_\perp \\ -\kappa_x(s)\langle x\rangle_\perp \\ \langle y'\rangle_\perp \\ -\kappa_y(s)\langle y\rangle_\perp\end{bmatrix}$$

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

Moments not shown are zero. $\langle \tilde{x}\tilde{y}\rangle = 0$ is obvious and $\langle \tilde{x}\tilde{y}'\rangle = \langle \tilde{x}'\tilde{y}\rangle = 0$ follows from the kinetic distribution.

c) Show from the results in part b) that

$$\epsilon_x = \text{const.} \qquad \text{with} \qquad \epsilon_x = 4[\langle \tilde{x}^2\rangle_\perp \langle \tilde{x}'^2\rangle_\perp - \langle \tilde{x}\tilde{x}'\rangle_\perp^2]^{1/2}$$

d) Show from the results in part b) and c) that

$$\frac{d^2}{ds^2}r_x + \kappa_x(s)r_x - \frac{2Q}{r_x + r_y} - \frac{\epsilon_x^2}{r_x^3} = 0$$

This is the "standard" form of the K-V envelope equation.

Problem 3 - Parallel Computing

Important: This problem requires you to install mpi4py. This is notably difficult to install, and thus it is strongly recommended to use the classroom computers. If you use the classroom computers, install `mpi4py` by typing:

```
conda install -c conda-forge mpi4py
```

Then download the code at: `http://raw.githubusercontent.com/RemiLehe/uspas_exercise/master/em_pic_1d_mpi.py`. This is a version of the previous script `em_pic_1d.py`, where we increased the number of grid points and modified the script so that it can run with MPI, using domain decomposition. However, the update of the guard cells has only partially been implemented in the code.

Note: Read the following carefully and make sure you answer all the questions!

a) Search for the group of lines that starts with `INITIALIZATION:`. Why do we initialize the arrays `self.Ex` and `self.By` by using `Nz_local` and not `Nz_global`?

b) Search for the line `PLOTTING: NEW LINES RELATED TO MPI`. Can you explain (briefly) why we need to use `mpi_comm.gather` here? Why is the rest of the code of this function included in an `if mpi_comm.rank == 0:` clause?

c) Run the code using

```
mpirun -np 4 python em_pic_1d_mpi.py
```

(You may have to wait 20-40 seconds for it to complete.) Look at the plots in the `diagnostics/` folder. Does the pulse behave as expected? Why?

d) Look for the lines that start with `ASSIGNMENT: Set the guard cells with the correct value` (There are 2 places in the code with these lines.) Modify the lines below to correctly set the guard cells. Run the code again and check that the pulse propagates correctly. (Then send your script to Daniel.)

e) Run the code several times by using different numbers of MPI ranks, measure the execution time (on Linux, you can use the `time` command ; the execution time is the one labeled with `real`):

```
time mpirun -np 1 python em_pic_1d_mpi.py
time mpirun -np 2 python em_pic_1d_mpi.py
time mpirun -np 4 python em_pic_1d_mpi.py
time mpirun -np 8 python em_pic_1d_mpi.py
```

How does the execution time scale with the number of processors? Does this correspond to the ideal scaling? If not, can you suggest possible reasons for why the ideal scaling is not obtained?

Problem 4 - Sirepo/Elegant - Use case: fs diagnostic

a) During today's lecture and computer lab, you were asked to create a Sirepo/elegant simulation from scratch, which implements a laser modulator and an rf deflecting cavity, based on an active "attoscope" experiment at the Accelerator Test Facility (ATF) at Argonne National Lab.

   Create a document with plots of final longitudinal phase space, consider several 2D phase space projections: (t, x), (t,x'), (t,y), (t,y'), (x,y), (x,x'), (y,y'), (t,p). Write 2 or 3 sentences for each plot, explaining what you see.

b) Create additional beam lines on the "Lattice" tab as follows:

   - One where you increase the length of the laser modulator by 2x
   - One where you increase the strength of the laser modulator by 2x
   - One where you make the modulator twice as long, but half as strong.
   - One where you increase the length of the rf cavity by 2x
   - One where you increase the strength of the rf cavity by 2x
   - One where you make the rf cavity twice as long, but half as strong.

   In each case, give the beam line a reasonable name. Make sure you are using a good choice for the numerical integrator and the number of steps. For two of the phase space plots that you find interesting, copy them into your document and discuss how they differ from the original plots of problem a) above.

c) What wavelength do thing is being used for the laser in the laser modulator? How did you get this value?