Self-Consistent Simulations of Beam and Plasma Systems
Homework 1

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

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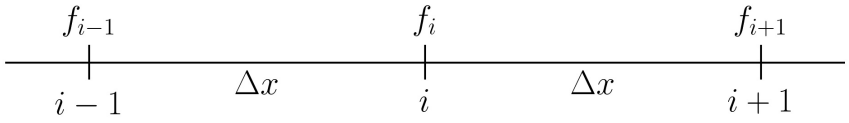
Problem 1 - Derivatives on a non-uniform mesh.

In class, we discretized a first derivative on a uniform grid



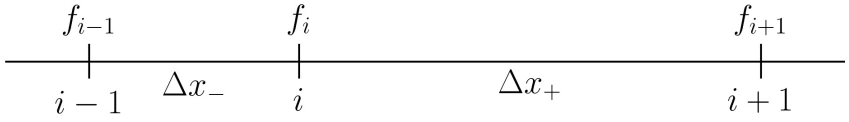
as:

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

whereas a second derivative is discretized as

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

Similarly, discretize the first and second derivative for a non-uniform grid



i.e. find:

$$\begin{aligned}\left.\frac{\partial f}{\partial x}\right|_i &= \cdots + \mathcal{O}(\Delta x_{+,-}^2) \\ \left.\frac{\partial^2 f}{\partial x^2}\right|_i &= \cdots + \mathcal{O}(\Delta x_{+,-})\end{aligned}$$

Notice that we find an $\mathcal{O}(\Delta x_{+,-})$ error term for the second derivative instead of an $\mathcal{O}(\Delta x^2)$ term as we did for the uniform grid. Establish the order of error with your answer!

Problem 2 - Python program for Runge-Kutta order 2

We wish to integrate the differential equation

$$\frac{d\,x(t)}{dt} = x(t)\cos(t) \qquad x(0) = 1$$

with Euler's method and the Runge-Kutta method (order 2), and compare the results.

a) Download the file `euler.py` from:

`http://raw.githubusercontent.com/RemiLehe/uspas_exercise/master/euler.py`.

Copy it to a new name `rungekutta.py` and modify it to implement the Runge-Kutta method, order 2. In particular:

- Change the name of the class from `EulerSolver` to `RKSolver`
- Change the name of the `euler_integration` method to `rk_integration`, and implement the Runge-Kutta method, order 2 (see the presentation *Overview of Basic Numerical Methods*)

b) In `ipython`, import classes `EulerSolver` from `euler.py` and `RKSolver` from `runge_kutta.py`. Evaluate the results of both methods for `N=100` ; what is the RMS error in both cases?

Problem 3 - Computational Reproducibility

a) Read at least one of the technical references (see the lecture slides to refresh your memory) regarding computational reproducibility. Write 3 paragraphs on the subject of computational reproducibility. Be sure to make a connection with at least one of the external references.

- How could improved computational reproducibility benefit your science?
- How could it improve your institution?
- Describe an experience with computational reproducibility (or the opposite).
- Discuss what you think would be most effective for improving reproducibility.
- Discuss pros/cons, trade-offs or how to address cost-benefit concerns.
- $\cdots$ or choose your own theme

b) For the computer lab on computational reproducibility, you were asked to generate three sets of plots from the Jupyter notebook (see the computer lab slides to refresh your memory). Write a paragraph for each of your 3 sets of plots:

- Explain what you did and/or what you learned
- Feel free to comment on the Jupyter notebook experience
- Make plots and text available to instructors (print, PDF, web$\cdots$)