Numerical Methods for Physics: Exercises

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Listed below are the exercises that have been assigned during the course and collected according to the lecture in which they were assigned. Solutions to these exercises need to be handed in to claim the credit points.

Lecture I

- **Root Finding**

  A completely ionized, homogeneous hydrogen plasma is irradiated by X-rays and the electron scattering optical depth is very large. The electrons at temperature T_e are exchanging energy with protons at temperature T_p via Coulomb collisions and with photons at temperature T_γ via Compton scattering. The magnetic fields and all other radiative processes are negligible. Under these conditions the energy balance equation for the electron plasma can be written as

  $$Q \frac{U}{\rho c^2}(T_e - T_\gamma) = \frac{\Lambda}{c^3}\left(\frac{T_p}{T_e} - 1\right)\frac{1}{\sqrt{T_e}}\,, \tag{1}$$

  where $Q := 4\kappa_{es} K_B / m_e c^2 = 2.7{\times}10^{-10}\,\mathrm{cm^2\,g^{-1}\,K^{-1}}$ (with $\kappa_{es} = 0.4\,\mathrm{cm^2\,g^{-1}}$ being the electron scattering opacity), $U/(\rho c^2)$ is the ratio between the radiation energy density and the rest-mass energy density of the electron-positron plasma, and $\Lambda = 4.4 \times 10^{30}$ is a constant.

  (i) Consider the case in which the electrons are heated by Coulomb collisions with the protons at temperature $T_p = 10^9$K and cooled via inverse Compton scattering with photons at temperature $T_\gamma = 10^7$K. Solve equation (1) with $U/(\rho c^2) = 1$ and find the equilibrium temperature for the electrons T_e. The bracketing interval can be found after plotting (1) as a function of T_e.

  (ii) Consider now the case in which the electrons are cooled by Coulomb collisions with the protons at temperature $T_p = 10^7$K and heated via Compton scattering with photons at temperature $T_\gamma = 10^9$K. Solve equation (1) with $U/(\rho c^2) = 8 \times 10^{-5}$ and find the equilibrium temperature for the electrons using as bracketing interval $T_1 = 10^7$K and $T_2 = 10^9$K. Is the Newton-Raphson method efficient? If not explain why.

NOTE

- *Use both the bisection and the Newton-Raphson methods concentrating on the number of iterations necessary to reach the desidered accuracy of* $\epsilon = 10^{-7}$.
- *To make results comparable use as speed of light* $c = 2.99 \times 10^{10}\ \mathrm{cm\,s^{-1}}$.

Lecture II

- **Linear Algebra**

  Consider the following set of linear algebraic equations

$$\boldsymbol{A} \cdot \boldsymbol{x} = \boldsymbol{b} \,, \tag{2}$$

where $\boldsymbol{A}$ is a square matrix of $(n \times n)$ coefficients and $\boldsymbol{x}$, $\boldsymbol{b}$ are the vectors [i.e. $(n \times 1)$ matrices] of unknowns and "right-hand-side" quantities, respectively.

Fill now the matrices $\boldsymbol{A}$ so that its elements a_{ij} are

$$a_{ij} = \frac{1}{\cos(i+\epsilon) + \sin(j+\epsilon)} \,, \tag{3}$$

where $\epsilon = 10^{-5}$ is a small constant number. Similarly, fill the vector $\boldsymbol{b}$ so that its elements b_i are

$$b_i = \frac{1}{i} - \epsilon \,. \tag{4}$$

(i) Solve the system (2) using Cramer's rule when $n = 3$. Compute the number of operations made to obtain the solution.

(ii) Solve the system (2) using a LU-decomposition when $n = 10$. Compute the number of operations made to obtain the solution.

(iii) Compute, both for *(i)* and *(ii)*, the residual vector $\boldsymbol{R}$

$$\boldsymbol{R} = \boldsymbol{A} \cdot \boldsymbol{x} - \boldsymbol{b} \,. \tag{5}$$

Lecture III

- **Polynomial Interpolation**

  Consider the function

$$y(x) = 3 + 200x - 30x^2 + 4x^3 - x^4 \ . \tag{6}$$

  and evaluate it at $N = 100$ points equally spaced in the interval $I: \ x \in [-10, \ 10]$.

  (i) Find its roots in I if they exist.

  (ii) Interpolate the value of the function at $x = -5$ and $x = 5$ using a linear, a quadratic and a cubic interpolating polynomial. Calculate the error made in each case.

- **Cubic Spline**

  Consider the function

$$y(x) = \sum_i A_i \cos\left(2\pi \frac{m_i}{L} x\right) \ , \tag{7}$$

  in the interval $I: \ x \in [0, \ 20]$, where $A_i = (1, 1/2, -1/2)$, $m_i = (8, 24, 8/3)$, $L = 64$.

  (i) Interpolate the value of the function at $x = 12$ using a linear, a quadratic and a cubic interpolating polynomial. Calculate the error made in each case.

  (ii) Interpolate the value of the function at $x = 12$ using now a cubic spline. Compare with the results obtained before.

- **Bilinear Interpolation**

  Consider the function

$$z(x, y) = x^2 - y^2 + 1 \tag{8}$$

  in the interval $I: \ x, \ y \in [-10, \ 10]$.

  (i) Interpolate the value of the function at the point $(5, 0)$ using a bilinear interpolation method. Calculate the error made and its scaling with the size of the interpolating grid.

Lecture IV

- **Closed Quadratures**

  Consider the following integral

$$I_1 = \int_0^{\pi/2} \sin^{2m-1}\theta \cos^{2n-1}\theta d\theta \tag{9}$$

where $m > 0,\ n > 0$.

(i) Calculate I_1 numerically using the trapezoidal extended closed formula (cf. your lecture notes).

(ii) Calculate I_1 numerically using Simpson's extended closed formula (cf. your lecture notes).

(iii) Compare the results obtained in *(i)* and *(ii)* validating the scaling of the two formulas in terms of the number of points N.

- **Open Quadratures**

  Consider the following integral

$$I_2 = \int_0^{\infty} \frac{x^{p-1}}{1+x} dx \tag{10}$$

where $0 < p < 1$.

(i) Calculate I_2 numerically using the following extended open formula of order $\mathcal{O}\left(1/N^2\right)$

$$\int_{x_1}^{x_N} f(x)dx = h\left[\frac{3}{2}f_2 + f_3 + f_4 + \ldots + f_{N-2} + \frac{3}{2}f_{N-1}\right] + \mathcal{O}\left(\frac{1}{N^2}\right) \tag{11}$$

(ii) Calculate I_2 numerically using the following extended open formula of order $\mathcal{O}\left(1/N^4\right)$

$$\begin{aligned}\int_{x_1}^{x_N} f(x)dx = h\Bigg[&\frac{27}{12}f_2 + 0 + \frac{13}{12}f_4 + \frac{4}{3}f_5 + \ldots \\ &+\frac{4}{3}f_{N-4} + \frac{13}{12}f_{N-3} + 0 + \frac{27}{12}f_{N-1}\Bigg] + \mathcal{O}\left(\frac{1}{N^4}\right)\end{aligned} \tag{12}$$

where the coefficients of the interior points are $4/3$ and $2/3$, alternatively.

(iii) Compare the results obtained in *(i)* and *(ii)* validating the scaling of the two formulas in terms of the number of points N.

NOTES

- *I suggest to use* $p = 0.5$ *and to try first using* $m = 1$, $n = 1$ *and then* $m = 2$, $n = 4$. *What are the differencese found?*
- *Plotting the integrand is always a good idea.*
- *Both* I_1 *and* I_2 *can be calculated analytically. A good investment of your time is in reading that book of tabulated integrals you never use...*
- *You don't really want to calculate* I_2 *between* 0 *and* ∞*! Think about a useful variable transformation that would make the integration between* 0 *and* 1.
- *The scaling of the error with* N *in the open formulas is derived for continuous functions. Do not expect miracles.*

Lecture V

- **Non-Uniform Deviates**

  An astrophysicist has developed a code to evolve the trajectories of photons produced by a perfect black-body at a temperature $T = 6 \times 10^3$ K. As initial conditions she will need to specify for each photon its energy and direction of propagation. Provide her with the initial distribution of 10^4 black-body photons with ν between 0 and 5×10^4 K, to which she will then assign a random initial direction of propagation. [Hint: Recall that the number density of photons $\mathcal{N}(\nu, T)$ at temperature T and with frequencies between ν and $\nu + \mathrm{d}\nu$ is

  $$\mathrm{d}\mathcal{N}(\nu, T) = \frac{8\pi\nu^2}{c^3}\left[\exp\left(\frac{h\nu}{kT}\right) - 1\right]^{-1}\mathrm{d}\nu \ . \tag{13}$$

  and where you can set $h = c = k = 1$.] Produce a plot of the photon distribution function.

- **Monte Carlo Integrals: 1D**

  Given the function $f(x) = (1 + x^2)^{-1}$, consider its definite integral

  $$I = \int_0^1 \frac{1}{1 + x^2}dx = \frac{\pi}{4} \ . \tag{14}$$

  (i) Evalute I numerically through a Monte Carlo integration using $N = 10, 20, 50, 100, 200, 500, 1000, 2000, 5000$ random points. For the same number of points calculate also the variance

  $$S = \langle f^2 \rangle - \langle f \rangle^2 \ , \tag{15}$$

  where

  $$\langle f^2 \rangle := \frac{1}{N}\sum_{i=1}^{N}(f(x_i))^2 \ , \qquad \langle f \rangle^2 := \left(\frac{1}{N}\sum_{i=1}^{N} f(x_i)\right)^2 \ . \tag{16}$$

  Plot both I and S versus N and discuss whether your results are in accordance with what you expect.

  (ii) Consider the new function $w(x) = (4 - 2x)/3$ which has a definite integral $\int_0^1 w(x)dx = 1$. Using $w(x)$ we can rewrite the integral I as

  $$I = \int_0^1 \frac{f(x)}{w(x)}w(x)dx = \int_0^1 \frac{f(y)}{w(y)}dy \ , \tag{17}$$

  where the new variable y is defined so that

  $$\frac{dy}{dx} = w(x) \qquad y = \frac{1}{3}x(4 - x) \ . \tag{18}$$

[You are encouraged to prove (17)]. Use now the Monte Carlo integration techniques to calculate the integral (17) ans show that this transformation reduces the variance and thus increases the accuracy for the same number of random points.

- **Monte Carlo Integrals: 3D (Optional)**

  The coordinates of the center of mass of an object with uniform density ρ can be written as

$$x^i_{_{CM}} = \frac{\int_V \rho x^i dxdydz}{\int_V \rho dxdydz} \tag{19}$$

  (i) Calculate the $x^i_{_{CM}}$ and their variances for the portion of the torus of equation

$$z^2 + \left(\sqrt{x^2+y^2} - 3\right)^2 \leq 1 \;, \tag{20}$$

  limited by

$$1 \leq x \leq 4 \qquad -3 \leq y \leq 4 \qquad -1 \leq z \leq 1 \tag{21}$$

  [see "Numerical Recipes", §7.6 for the figure of the truncated torus.]

Lecture VI

Integration of ODEs: bound particle-orbits around a Schwarzschild black hole
Consider a massive test-particle moving in a generic bound orbit around a Schwarzschild black hole of mass $M = 5M_\odot$ (hereafter we will assume $G = c^2 = M_\odot = 1$). The equations of motion will be the geodesic equations for that spacetime and these can be recast in a convenient form in terms of the *periastron* r_1 and of the *eccentricity* $0 \leq e < 1$ as

$$\frac{dt}{d\chi} = \frac{p^2 M}{(p-2-2e\cos\chi)(1+e\cos\chi)^2}\left[\frac{(p-2-2e)(p-2+2e)}{p-6-2e\cos\chi}\right]^{1/2}, \tag{22}$$

$$\frac{d\phi}{d\chi} = \left(\frac{p}{p-6-2e\cos\chi}\right)^{1/2}, \tag{23}$$

where

- t is the time coordinate
- $\chi \in [0, 2\pi]$ is a single-valued, cyclic parameter along the orbit related to the radial coordinate through the expression

  $$r(\chi) = \frac{pM}{1+e\cos\chi}, \tag{24}$$

  so that $r \in [pM/(1+e), pM/(1-e)]$.
- ϕ is the azimuthal coordinate (the trajectory is in the plane $\theta = \pi/2$)
- p is a constant of the orbit, usually referred to as the *latus rectum* and defined as

  $$p := \frac{(1+e)r_1}{M}, \tag{25}$$

In practice, the radial coordinate r will oscillate during the orbit between the minimum value at the periastron r_1 and the maximum value at the apoastron $r_2 := pM/(1-e)$.

(i) Solve the set of coupled ordinary differential equations (22)–(23) for the following choice of initial conditions

(a) $r_1 = 7.0M \ , e = 0.3$

(b) $r_1 = 6.1M \ , e = 0.2$

(c) $r_1 = 5.26M, e = 0.22722$

(ii) Verify that the change in ϕ after one complete revolution in which χ changes by 2π is $2(1+3/p)\pi$ so that the precession of the periastron in one revolution is

$$\Delta\phi = \frac{6\pi}{p} = \frac{6\pi M}{r_1(1+e)} \ . \tag{26}$$

(iii) Plot the following quantities

(a) r vs t

(b) r vs χ

(c) ϕ vs χ

(d) $r\cos\phi$ vs χ

(e) $r\sin\phi$ vs χ

(f) $r\cos\phi$ vs $r\sin\phi$

NOTE

- *Perform the integrations using a 2nd-order and a 4th-order Runge-Kutta algorithm and compare the results*
- *If motivated, implement a 4th scheme with with step-size adjustment. Measure the computational gain.*
- *Note that equation (26) has been derived as a first-order expansion in powers of $1/p$ of the right-hand-side of equation (23). Don't expect it to be valid beyond its range of validity. Consider it also in the case of Mercury.*

Lecture VII

Hyperbolic PDEs: the wave equation in 1D
Given the scalar wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \ , \tag{27}$$

a) Build a numerical code to solve for (27) on a grid with extents $x \in [0, 1]$ and with initial conditions given by

$$u(x) = \exp[-(x - x_0)^2/\sigma^2] \ , \tag{28}$$

with $x_0 = 0.5$ and $\sigma = 0.1$.

b) Perform the time integration of equation (27) implementing the following numerical schemes:

(i) FTCS;

(ii) Lax;

(iii) Leapfrog;

(iv) Lax-Wendroff;

Compare the results obtained with the analytic solution to equation (27) paying attention to the stability, accuracy and dissipation of the scheme used.

c) Impose either *Outgoing wave* or *Periodic* boundary conditions.

Hyperbolic PDEs: the wave equation in 2D (Optional)
Solve the equivalent equation (27) in two dimensions by using a Leapfrog and/or Lax-Wendroff evolution scheme.

NOTE: *You don't need to build four/eight different codes to solve the first problem. Construct a driver routine and four subroutines that update the solution to the new time level.*

Lecture VIII

Parabolic PDEs: the diffusion equation in 1D
Given the scalar diffusion equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \ , \tag{29}$$

where D is a constant diffusion coefficient.

a) Build a numerical code to solve for (29) on a grid with extents $x \in [0, 1]$ and with initial conditions given by

$$u(x) = \exp[-(x - x_0)^2/\sigma^2] \ , \tag{30}$$

with $x_0 = 0.5$ and $\sigma = 0.1$.

b) Perform the time integration of equation (29) implementing the following numerical schemes:

(i) FTCS. Check what happens when the stability condition is violated.

(ii) BTCS. Check what happens when the timestep is changed.

(iii) Dufort-Frankel. Check the accuracy of the solution and compare with the other methods.

Optional

- Perform the time integration of equation (29) implementing a Crank-Nicholson scheme.
- Perform the time integration of equation (29) and compare it with the semi-analytic solution.

NOTE: *You may want to establish first the time at which you want the final solution (e.g. a fraction of the diffusion timescale, with $D = 1$) and then reach that time in the appropriate number of timesteps.*

Lecture IX

Elliptic Partial Differential Equations
In a two-dimensional Cartesian coordinate system $\{x, y\}$ consider the following linear elliptic equation

$$\nabla^2 \phi = -5 \sin(x + 2y) \ , \tag{31}$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \ . \tag{32}$$

a) Solve (31) in a computational domain with $x \in [0, \pi]$ and $y \in [0, \pi]$ using the **Gauss-Seidel** method. Continue your iteration at least until the L_∞ norm of the k-th *residual*

$$L_\infty(\xi^k) := \max \left\{ \xi^{(k)}_{i,j} \right\} = \max \left\{ \left(\nabla^2 \phi\right)^{(k)}_{i,j} + 5 \sin(x + 2y) \right\} \ , \tag{33}$$

is $L_\infty(\xi^k) < 10^{-6}$. Repeat your calculations for three grid resolutions (e.g. using 32^2, 64^2 and 128^2 gridpoints).

b) For each iteration calculate the ratio

$$\frac{L_\infty(\xi^k) - L_\infty(\xi^{k-1})}{L_\infty(\xi^{k-1})} \ , \tag{34}$$

and plot it versus the number of iterations for the different grid resolutions used. Comment on your findings.

c) Using the analytic solution to (31)

$$\phi_\mathrm{A} = \sin(x + 2y) \ , \tag{35}$$

calculate the following norms of ϕ in terms of the analytic solution

$$L^\mathrm{A}_\infty(\phi^k) \quad := \quad \max \left\{ \phi^{(k)}_{i,j} - \phi_\mathrm{A} \right\} \ , \tag{36}$$

$$L^\mathrm{A}_2(\phi^k) \quad := \quad \frac{1}{N_x N_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \left[\phi^{(k)}_{i,j} - \phi_\mathrm{A} \right]^2 \ , \tag{37}$$

where N_x and N_y are the number of gridpoints in the two directions. Plot the results versus the number of iterations for the different grid resolutions used; comment your findings.

d) Extend the calculations made in *a)* until $L_\infty(\xi^k)$ reaches the roundoff error. Can you reach machine accuracy also for $L^\mathrm{A}_\infty(\phi^k)$? Explain why.

NOTES

- *Initial Data*: initial data close to the correct solutions are always a good way to achieve rapid convergence. This exercise, however, is sufficiently simple that the convergence will be reached even if you start from trivial initial data such as $\phi = 1 \ \forall \, (x, y)$.
- *Boundary Conditions*: most of the times the boundary conditions are not known and need to be deduced either from the behaviour of the solution or from the form of the equation. In this exercise the analytic solution is known and the boundary conditions to be imposed can be that $\phi = \phi_{\rm A}$ at the boundaries.

Optional

i) Recalculate points *a)*, *b)*, and *c)* using the **SOR** iteration procedure. Compare the results with those obtained using the **Gauss-Seidel** iteration procedure.

ii) Do not impose analytic boundary conditions but deduce the value of ϕ at the boundaries from the values it assumes in the interior of the grid, using high order extrapolation routines.

Lecture X

Numerical Fourier Transforms

Consider the function $h(t)$ defined in the domain $t \in [0, 1]$, as

$$h(t) := \sum_{i=1}^{3} A_i \cos(\omega_i t) \tag{38}$$

where $A_i = (-0.5, 0.5, 0.75)$ and $\omega_i = 2\pi f_i$ with $f_i = (2.0, 3.0, 9.0)$.

a) Discretize $h(t)$, i.e. consider N evaluations of $h(t)$ at fixed values of t

$$h_n(t) := h(t = n\Delta) \,, \qquad n = 0, 1, \ldots N - 1. \tag{39}$$

b) Add a random noise at each discrete value of h, i.e.

$$h_n(t_n) \to h_n(t_n) + a\xi \tag{40}$$

with $a = 0.5$ and ξ is a uniform random number in the interval $[-1, 1]$.

c) Calculate a discrete Fourier transform of h_n, with $N = 128$ (you can use also a pre-packaged routine, e.g. `four1` of the Numerical Recipe book).

d) Remove the noise from $H(f)$ by setting to zero all the $\mathfrak{Re}\{|H(f)|\}$ with $\mathfrak{Re}\{|H(f)|\} < 3\langle H(f)\rangle$, where $\langle H(f)\rangle$ is the mean value of $\mathfrak{Re}\{|H(f)|\}$. Call the "cleaned" Fourier transform $H_c(f)$.

e) Convolve the cleaned Fourier transform $H_c(f)$ with a filter F_c, i.e. $H_c(f) \to H_c(f) \times F_c(f)$ to remove any spurious high frequency peaks, e.g.

$$F_c(f) = \begin{cases} 1 & \text{for } f \le f_{\rm N} \\ 0 & \text{for } f > f_{\rm N} \end{cases}$$

where $f_{\rm N} := 1/(2\Delta)$ is the Nyquist frequency and f is always positive.

f) Calculate the inverse Fourier transform of the new $H_c(f)$ and compare it with the original data $h(t)$. Use Parseval's theorem to obtain the right amplitude.

g) Repeat the exercise changing the amplitudes A_i and frequencies ω_i. Comment on your results.

h) Repeat the exercise convolving the cleaned Fourier transform $H_c(f)$ with a filter preserving only the peak with the largest power. Compare the inverse Fourier transform obtained in this way with the original data $h(t)$.

i) Repeat the exercise with now $t \in [0, 10]$ and $N = 1280$. Compare the results to when $t \in [0, 1]$ and $N = 128$ and express your conclusions.