Problem Set 3

Exercises for the lecture Fundamentals of Simulation Methods, WS 2020

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Hand in until Wednesday, 25.11., 23:59
Tutorials on Friday, 27.11.
(Group 1, Giovanni Leidi 09:15)
(Group 2, Benedikt Rennekamp 09:15)
(Group 3, Siddhant Deshmukh 11:15)
(Group 4, Fabian Kutzki 14:15)

1. Order of an ODE integration scheme [4 pt.]

Consider the differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(y)$$

for the function $y(t)$ and a general right hand side $f(y)$. This may be integrated discretely with an explicit midpoint method:

$$y^{n+1} = y^n + \Delta t\ f\left\{y^n + \frac{\Delta t}{2} f(y^n, t_n), t_n + \frac{\Delta t}{2}\right\}.$$

Show analytically this scheme is second-order accurate in the time step Δt by calculating the local and global truncation errors.

Hint: Use Taylor expansion.

2. Integration of a stiff equation [8 pt]

Consider an ionized plasma of hydrogen gas that radiatively cools. Its temperature evolution is governed by the equation

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -\frac{2}{3\,k_\mathrm{B}} n_\mathrm{H}\,\Lambda(T) \tag{1}$$

where $\Lambda(T)$ describes the cooling rate as a function of temperature, $k_\mathrm{B} = 1.38 \times 10^{-23}\,\mathrm{J/K}$ is Boltzmann's constant, and n_H is the number density of hydrogen atoms. The cooling rate is a strong function of temperature T, which we here approximate by

$$\Lambda(T) = \begin{cases} \Lambda_0 \left(\frac{T}{T_0}\right)^\alpha & \text{for } T \le T_0 \\ \\ \Lambda_0 \left(\frac{T}{T_0}\right)^\beta & \text{for } T > T_0 \end{cases} \tag{2}$$

with $\Lambda_0 = 10^{-35}\,\mathrm{J\,m^3\,s^{-1}}$, $T_0 = 20000\,\mathrm{K}$, $\alpha = 10.0$, and $\beta = -0.5$. We consider isochoric cooling of gas at density $n_{\mathrm{H}} = 10^6\,\mathrm{m^{-3}}$, with an initial temperature of $T_{\mathrm{init}} = 10^7\,\mathrm{K}$.

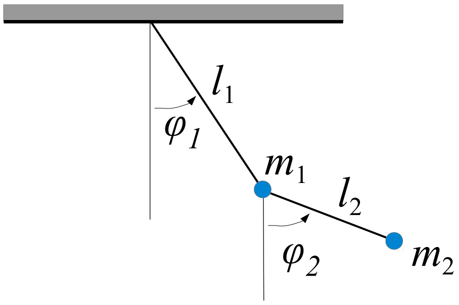
(a) Determine the temperature evolution $T(t)$ by integrating equation (1) with a second-order explicit Runge-Kutta predictor-corrector scheme and a fixed timestep, until the temperature has dropped below 6000 K. Use a timestep size of $\Delta t = 10^{10}\,\mathrm{s}$. Make a plot of the time evolution of the temperature, with a logarithmic scale for temperature and a linear scale for the time.

(b) How many steps do you roughly need in (a) to reach the final temperature? Try to play with the timestep size and see whether you can significantly enlarge the timestep without becoming unstable.

(c) Now implement the second-order integration from (a) with an adaptive step size control, based on estimating the local truncation error by carrying out two half-steps for every step. Use an absolute local error limit $\Delta T_{\mathrm{err}}^{\mathrm{max}} = 50\,\mathrm{K}$ for every step. Overplot your result for the temperature evolution, on the plot for (a), using symbols or a different color. How many steps do you now need? Confirm that your scheme is robust to large changes of the timestep size given as input for the first step.

3. Double pendulum [8 pt.]

We consider a friction-less double pendulum that is constrained to move in one plane. The two masses m_1 and m_2 are connected via massless rods of length l_1 and l_2, respectively, as depicted in the sketch.



The Lagrangian of this system is given by the expression

$$L = \frac{m_1}{2}(l_1\dot{\phi}_1)^2 + \frac{m_2}{2}\left[(l_1\dot{\phi}_1)^2 + (l_2\dot{\phi}_2)^2 + 2l_1l_2\dot{\phi}_1\dot{\phi}_2\cos(\phi_1-\phi_2)\right]$$
$$-m_1 g\, l_1(1-\cos\phi_1) - m_2 g\,[l_1(1-\cos\phi_1) + l_2(1-\cos\phi_2)] \quad (3)$$

(a) Derive the Lagrangian equations of motion,

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{\phi}} - \frac{\partial L}{\partial\phi} = 0, \quad (4)$$

for the angles ϕ_1 and ϕ_2. Hint: Declare conjugate momenta $q \equiv \frac{\partial L}{\partial\dot{\phi}}$ and *do not* explicitly carry out the absolute time derivative; it is sufficient if you give $\frac{\mathrm{d}q_1}{\mathrm{d}t}$ and $\frac{\mathrm{d}q_2}{\mathrm{d}t}$.

(b) Cast the system of equations into 1st-order form, such that the dynamics is described by the ODE

$$\frac{\mathrm{d}\vec{y}}{\mathrm{d}t} = \vec{f}(\vec{y}), \tag{5}$$

where $\vec{y}$ is a four-component vector. Hint: Use the conjugate momenta to eliminate the second derivatives, i.e. adopt $\vec{y} = (\phi_1, \phi_2, q_1, q_2)$ as state vector. Hint 2: When you define f_3, f_4, you can save time/effort if you "re-use" the values of f_1, f_2, no need to plug in their expressions again. You should do so when you are writing the program as well.

(c) Write a computer program that integrates the system with a second-order predictor-corrector Runge-Kutta scheme. Consider the initial conditions $\phi_1 = 50°$, $\phi_2 = -120°$, $\dot{\phi}_1 = \dot{\phi}_2 = 0$, and adopt $m_1 = 0.5$, $m_2 = 1.0$, $l_1 = 2.0$, and $l_2 = 1.0$. For simplicity, we shall use units where $g = 1$. Use a fixed timestep of size $\Delta t = 0.05$, and integrate for the period $T = 100.0$ time units (equivalent to 2000 steps). Plot the relative energy error, $(E_{\mathrm{tot}}(t) - E_{\mathrm{tot}}(t_0))/E_{\mathrm{tot}}(t_0)$, as a function of time.

(d) Produce a second version of your code that uses a fourth-order Runge-Kutta scheme instead. Repeat the simulation from (c) with the same timestep size, and again plot the energy error. How does the size of the error at the end compare, and is this consistent with your expectations?

(e) Let's make a visualization of our double pendulum in order to get a feel for its interesting and quite complex behavior. In fact, this pendulum is one of the simplest systems that shows non-linear chaotic behaviour. To see this, choose two different initial conditions that are very close to each other (e.g. fix one angle and change the other angle just by a bit). Plot how they diverge in phase space: In the angles ϕ_1 vs. ϕ_2 and in the velocities $\dot{\phi}_1$ vs. $\dot{\phi}_2$. Explain what you see.