AME 60614: Numerical Methods
Fall 2021

Problem Set 3
Due: November 4, 2021

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Submission guidelines: A hard copy of written work is due in class. Additionally, submit through Sakai an archive (`tar` or similar) of all files requested in this assignment. Place files from individual problems into separate folders within your archive, *i.e.*, `p1/`, `p2/`, etc. Please give this archive a name of the form `lastname_firstname_ps3.tar`.

Contact `jmacart@nd.edu` with any questions.

1 Iteratively Implicit Methods

For nonlinear problems, fully implicit methods require the solution of a nonlinear set of equations, which can be costly and not guaranteed to converge. As an alternative to fully implicit methods, iteratively implicit methods do not require the solution of a nonlinear system of equations. However, the stability properties of these schemes often only approximate fully implicit stability.

With iteratively implicit methods, an estimated solution y_{n+1}^* is initially "predicted" using an explicit scheme. A nominally implicit scheme is then applied in one or more "corrector" steps, in which the right-hand-side of the "corrector" is evaluated using the best estimate for the solution at the current time level, either from the "predictor" step or the previous "corrector" step.

Consider a predictor-corrector algorithm based on a first-order Adams–Bashforth "predictor" and a second-order Adams–Moulton "corrector":

$$\text{Predictor:} \qquad y_{n+1}^* = y_n + hy_n' + O(h^2) \tag{1}$$

$$\text{Corrector:} \qquad y_{n+1} = y_n + \frac{h}{2}\left(y_{n+1}'^* + y_n'\right) + O(h^3) \tag{2}$$

where the intermediate solution is indicated by $(\cdot)^*$. Further corrections are possible by iterating on (2). These steps form the Adams–Bashforth–Moulton (ABM) algorithm.

a. After the first corrector step, what is the order of accuracy of the numerical approximation at the next time step? From an accuracy standpoint, is there any reason for additional corrector steps? *(Note: This determination should be made for a general f.)*

b. Determine and plot the linear stability diagram after the first corrector step. What method is this? How does this stability diagram compare to the stability of the first-order Adams–Bashforth and fully implicit second-order Adams–Moulton methods alone?

c. Determine and plot the linear stability diagram after one, two, three, and four corrector steps. What is the real-axis stability limit?

d. Obtain the stability diagram in the limit of an infinite number of corrector steps (i.e., as the semi-implicit scheme converges? *(Hint: It is probably easier to answer this from the amplification factor directly rather than the linear stability diagram.)*

2 Harmonically Forced Undamped Oscillator

In dynamical systems, a Hamiltonian $H = \lambda^2/2 - \cos\theta$ is a physically-conserved quantity, where λ is a characteristic frequency and θ is a phase angle. ODEs governing the phase and frequency may be expressed, respectively, as

$$\begin{aligned} \frac{d\theta}{dt} &= \frac{\partial H}{\partial \lambda} = \lambda, \\ \frac{d\lambda}{dt} &= -\frac{\partial H}{\partial \theta} = -\sin\theta. \end{aligned} \tag{3}$$

Conservation of a Hamiltonian can be recast as satisfying Liouville's Theorem expressed in terms of the Jacobian of the (θ, λ) phase space, such that

$$|J| = \left| \frac{\partial(\theta, \lambda)}{\partial(\theta_0, \lambda_0)} \right| = 1.$$

Consider a forward-Euler solution of the system (3):

$$\begin{aligned} \theta_{n+1} &= \theta_n + h\lambda_n \\ \lambda_{n+1} &= \lambda_n - h\sin\theta_n. \end{aligned} \tag{4}$$

The Jacobian of the (θ, λ) phase space for the solution (4) is

$$|J| = \begin{vmatrix} 1 & h \\ -h\cos\theta_n & 1 \end{vmatrix} \neq 1,$$

from which it is evident that the explicit Euler solution does not conserve the Hamiltonian. Now consider a modification of the Euler method that uses the updated value of θ:

$$\begin{aligned} \theta_{n+1} &= \theta_n + h\lambda_n \\ \lambda_{n+1} &= \lambda_n - h\sin\theta_{n+1}. \end{aligned} \tag{5}$$

This is known as the *modified* or *symplectic Euler* method.

a. Derive the order-of-accuracy of the symplectic Euler method.

b. Show that the symplectic Euler method conserves the Hamiltonian defined above.

Now, let the displacement $x(t)$ of a harmonically forced undamped oscillator be described by the initial value problem

$$mx'' + kx = F\cos\omega t,$$

where m is the mass of the oscillator, k is the spring constant, and F and ω are the magnitude and frequency, respectively, of the harmonic forcing. If we define the *natural frequency* of the oscillator as $\omega_n \equiv \sqrt{k/m}$, then the governing equation can be rewritten as:

$$x'' + \omega_n^2 x = \frac{F}{m}\cos\omega t. \tag{6}$$

With $m = F = 1$, $\omega = 0.1$, $\omega_n = 5$, and the initial conditions $x(0) = 0$ and $x'(0) = 0$, solve (6) over $t \in [0, 100]$ using each of the following methods:

c. Forward Euler,

d. Modified (symplectic) Euler,

e. Fourth-order Runge–Kutta.

How do you expect the response of this system to look? What about the solution is implied by the relatively fast and slow frequencies?

Plot the following for each solution method. Combine them into one plot for (i), one plot for (ii), and one plot for (iii).

i. The system response ($x(t)$ vs. t),

ii. The phase portrait ($x'(t)$ vs. $x(t)$),

iii. The error (L_2 norm) of the numerical solution compared to the analytical solution at each point in time (ε vs. t, semilog-y plot).

Discuss the strengths and weaknesses of each solution method for this problem. Which method gives the highest degree of accuracy for a given amount of CPU time? Do any of the methods conserve energy?

Be sure to include your codes in your `.tar` archive.

3 Implicit and Explicit Analogs of Common Methods

Two classes of methods were only briefly discussed in class: implicit Runge–Kutta methods and explicit analogs of the Backward Differentiation Formula (BDF) methods. Your task is to explore their stability properties using the analysis tools we have developed.

a. Consider the two-stage implicit Runge–Kutta method given by

$$\begin{aligned} y_{n+1} &= y_n + \frac{1}{2}k_1 + \frac{1}{2}k_2 \\ k_1 &= hf\left(t_n + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h,\ y_n + \frac{1}{4}k_1 + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)k_2\right) \\ k_2 &= hf\left(t_n + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h,\ y_n + \left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)k_1 + \frac{1}{4}k_2\right). \end{aligned}$$

Determine and plot the linear stability diagram of this scheme. Which scheme does its stability diagram resemble? Given its stability properties and high order-of-accuracy, why would this ***fourth-order*** scheme be less likely to be used in practice?

b. Explicit analogs of Backward Differentiation Formulas have the general form

$$y_{n+1} + \sum_{k=0}^{S} \alpha_k y_{n-k} = \beta f_n + O(h^m)$$

Derive second- and third-order methods of this form. What is another name for the second-order method? *Hint: Refer to Moin's book if necessary.* Determine and plot the linear stability characteristics of your second- and third-order explicit BDF schemes, and discuss their stability properties. *(Hint: Be very careful with your stability diagrams. What happens for $\sigma < 1$ and $\sigma > 1$?)* Under what conditions could you use these methods in practice?

4 Stiff Systems of ODEs

Stiff systems of ordinary differential equations are commonly encountered in chemical kinetics. Consider the following set of chemical reactions that describe the formation of nitrous oxide (NO) in combustion systems at high temperature (known as the Zeldovich mechanism or "thermal NO").

$$\mathrm{N_2 + O \leftrightarrow NO + N} \tag{R1}$$

$$\mathrm{N + O_2 \rightarrow NO + O} \tag{R2}$$

From these two reactions, evolution equations for the mole fractions, X_n, of the five species can be written as:

$$\begin{aligned}
X'_{\mathrm{N_2}} &= -k_{1f}X_{\mathrm{N_2}}X_{\mathrm{O}} + k_{1b}X_{\mathrm{NO}}X_{\mathrm{N}},\\
X'_{\mathrm{O_2}} &= -k_{2f}X_{\mathrm{O_2}}X_{\mathrm{N}},\\
X'_{\mathrm{N}} &= k_{1f}X_{\mathrm{N_2}}X_{\mathrm{O}} - k_{1b}X_{\mathrm{NO}}X_{\mathrm{N}} - k_{2f}X_{\mathrm{O_2}}X_{\mathrm{N}},\\
X'_{\mathrm{O}} &= -k_{1f}X_{\mathrm{N_2}}X_{\mathrm{O}} + k_{1b}X_{\mathrm{NO}}X_{\mathrm{N}} + k_{2f}X_{\mathrm{O_2}}X_{\mathrm{N}},\\
X'_{\mathrm{NO}} &= k_{1f}X_{\mathrm{N_2}}X_{\mathrm{O}} - k_{1b}X_{\mathrm{NO}}X_{\mathrm{N}} + k_{2f}X_{\mathrm{O_2}}X_{\mathrm{N}}.
\end{aligned}$$

At a given system condition, the reaction rate coefficients k_i are:

$$\begin{aligned}
k_{1f} &= 2\times 10^{3}\ \mathrm{s}^{-1},\\
k_{1b} &= 3\times 10^{-12}\ \mathrm{s}^{-1},\\
k_{2f} &= 2\times 10^{1}\ \mathrm{s}^{-1}.
\end{aligned}$$

a. Given the initial conditions $X_{\mathrm{N_2}} = 0.75$, $X_{\mathrm{O_2}} = 0.23$, $X_{\mathrm{N}} = 0.01$, $X_{\mathrm{O}} = 0.01$, and $X_{\mathrm{NO}} = 0.0$, compute the eigenvalues of the Jacobian of the system at the initial time. Is the system stiff?

b. Solve the evolution of the system until $t = 40$ s using each of the following methods:

   i. Fourth-order Runge–Kutta (RK4),

   ii. Adams–Moulton (AM) with adaptive time-stepping,

   iii. Backward Differentiation Formulas (BDF) with adaptive time-stepping.[1]

   You should write your own RK4 solver. Utilize "canned" routines for the adaptive AM and BDF solvers from, for example, the Matlab ODE suite, SciPy's `solve_ivp` routine, or the CVODE package (or write your own). Include in your `.tar` archive your solver code and, if necessary, a Makefile and README. (If you use CVODE, then you should tell me how to link against the precompiled library.) A tutorial for using CVODE is posted to Sakai.

   Plot the evolution of the system in time on log-log axes. How do the three methods compare in terms of required computational cost? *(Note: You may need to adjust your tolerances for the adaptive solvers.)* Why would you choose a BDF method over another implicit method like Adams–Moulton?

[1] G.D. Byrne, A.C. Hindmarsh, A polyalgorithm for the numerical solution of ordinary differential equations, *ACM Trans. Math. Soft.* 1 (1975) 71–96.