Mathematical Modeling I, Fall 2018: Assignment 2
Due Monday Oct 8
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This homework covers Lagrangian mechanics, numerical methods for ODEs, and stiff problems. For the computer problems, please attach your computer codes to the homework as well. You can work in teams of up to three people. Submit one report per team.

1. [10 points] A mass M is free to slide along a frictionless rail. A pendulum of length l and mass m hangs from M; see Figure 1 (left). The goal is to use the Lagrangian approach to find the equations of motion.

   Let x be the position of M, and let θ be the angle of the pendulum with the vertical; see Figure 1 (left). The overall kinetic energy of the system is sum of the kinetic energy of M, easily seen to be $\frac{1}{2}M\dot{x}^2$, and kinetic energy of m. Noting that the position of the mass m in cartesian coordinates is given by

$$\boldsymbol{r}(t) = \begin{bmatrix} x + l\sin\theta \\ -l\cos\theta \end{bmatrix},$$

   find the kinetic energy of m and subsequently the overall kinetic energy of the system. Then, find the potential energy and write down the Lagrangian, and using principle of stationary action, find the equations governing time evolution of $x(t)$ and $\theta(t)$.

   Since $\nabla r = \begin{bmatrix} \dot{x} + l\cos(\theta)\dot{\theta} \\ l\sin(\theta)\dot{\theta} \end{bmatrix}$, the kinetic energy of m is given by

$$T_m = \frac{1}{2}m\Big[\big(\dot{x} + l\cos(\theta)\dot{\theta}\big)^2 + \big(l\sin(\theta)\dot{\theta}\big)^2\Big].$$

   Thus the overall kinetic energy of the system is

$$\begin{aligned} T &= \frac{1}{2}M\dot{x}^2 + \frac{1}{2}m\Big[\big(\dot{x} + l\cos(\theta)\dot{\theta}\big)^2 + \big(l\sin(\theta)\dot{\theta}\big)^2\Big] \\ &= \frac{1}{2}(M+m)\dot{x}^2 + ml\dot{x}\dot{\theta}\cos(\theta) + \frac{1}{2}ml^2\dot{\theta}^2. \end{aligned}$$

   Taking the vertical position of M to be at height zero, the height h of m is $h = -l\cos(\theta)$. Since potential energy is equal to mgh, the potential energy of the system is

$$V = -mgl\cos(\theta).$$

   Then the Lagrangian is

$$L = T - V = \frac{1}{2}(M+m)\dot{x}^2 + ml\dot{x}\dot{\theta}\cos(\theta) + \frac{1}{2}ml^2\dot{\theta}^2 + mgl\cos(\theta).$$

   The principle of stationary action states that the path taken will be one which is a stationary point of the integral

$$\int_{t_0}^{t_f} T - V \ \mathrm{d}t.$$

   We will find necessary conditions for the stationary point using the Euler-Lagrange equations.

$$L_{\dot{x}} = M\dot{x} + \frac{1}{2}m\big[2\dot{x} + 2l\dot{\theta}\cos(\theta)\big]$$

$$\frac{\mathrm{d}}{\mathrm{d}t}L_{\dot{x}} = (M+m)\ddot{x} + ml\ddot{\theta}\cos(\theta) - ml\dot{\theta}^2\sin(\theta)$$

   $L_x = 0$, so

$$(M+m)\ddot{x} + ml\ddot{\theta}\cos(\theta) - ml\dot{\theta}^2\sin(\theta) = 0.$$

$$L_{\dot\theta} = ml\cos(\theta)\dot x + ml^2\dot\theta$$

$$\frac{\mathrm{d}}{\mathrm{d}t}L_{\dot\theta} = ml\big[\ddot x\cos(\theta) - \dot x\dot\theta\sin(\theta) + l\ddot\theta\big]$$

$$L_\theta = -ml\sin(\theta)\big(\dot x\dot\theta + g\big)$$

So

$$\ddot x\cos(\theta) - \dot x\dot\theta\sin(\theta) + l\ddot\theta = -\sin(\theta)\big(\dot x\dot\theta + g\big).$$

Thus the equations governing the time evolution of $x(t)$ and $\theta(t)$ are

$$(M+m)\ddot x + ml\ddot\theta\cos(\theta) - ml\dot\theta^2\sin(\theta) = 0$$

$$\ddot x\cos(\theta) - \dot x\dot\theta\sin(\theta) + l\ddot\theta = -\sin(\theta)\big(\dot x\dot\theta + g\big).$$

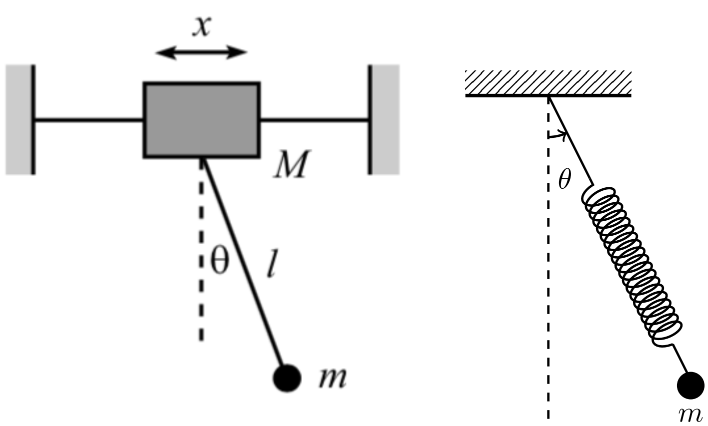


Figure 1: Left: Illustration of a moving pendulum. Right: A spring-pendulum system.

2. [15 points] Recall the spring pendulum problem (see Figure 1 (right)).

> *A mass m is attached to a spring with equilibrium length ℓ. The spring is arranged so that it lies in a straight line. At time t, let the spring have length $\ell + s(t)$; also let its angle with the vertical be $\theta(t)$. We assume the motion takes place in the vertical plane.*

We already derived the following equations of motion for this system, using the Lagrangian approach:

$$m\ddot{s} = m(\ell + s)\dot{\theta}^2 + mg\cos\theta - ks,$$
$$m(\ell + s)\ddot{\theta} + 2m\dot{s}\dot{\theta} = -mg\sin\theta.$$

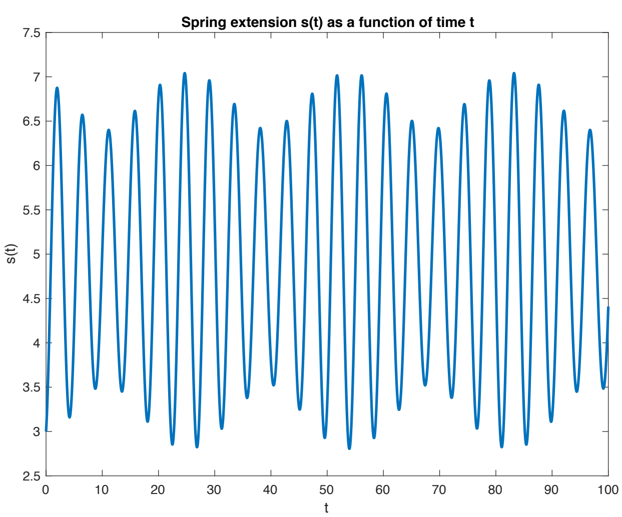
(a) By introducing appropriate notations, write the above system as a first order ODE system. Let $x_1 = s$, $x_2 = \dot{s}$, $x_3 = \theta$, and $x_4 = \dot{\theta}$. Then the above ODE system can be described by

$$\begin{aligned} x_1' &= x_2 \\ x_2' &= (l + x_1)x_4^2 + g\cos(x_3) - \frac{k}{m}x_1 \\ x_3' &= x_4 \\ x_4' &= \frac{-2x_2x_4 - g\sin(x_3)}{l + x_1} \end{aligned}$$

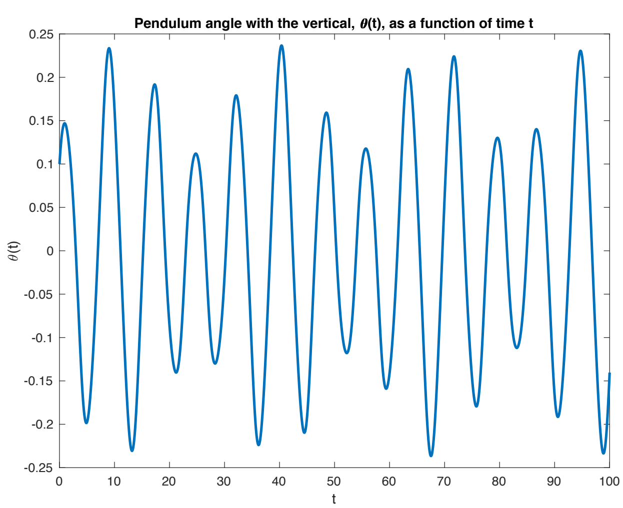
(b) Solve the system numerically using the classical fourth order Runge–Kutta method. (You can build on the RK4 solver I provided in Moodle.) Provide the following plots: $s(t)$ as a function of time, $\theta(t)$ as a function of time, and a plot of $s(t)$ versus $\theta(t)$. Use initial conditions

$$s(0) = 3, \quad \dot{s}(0) = 1, \quad \theta(0) = 0.1, \quad \dot{\theta}(0) = 0.1.$$

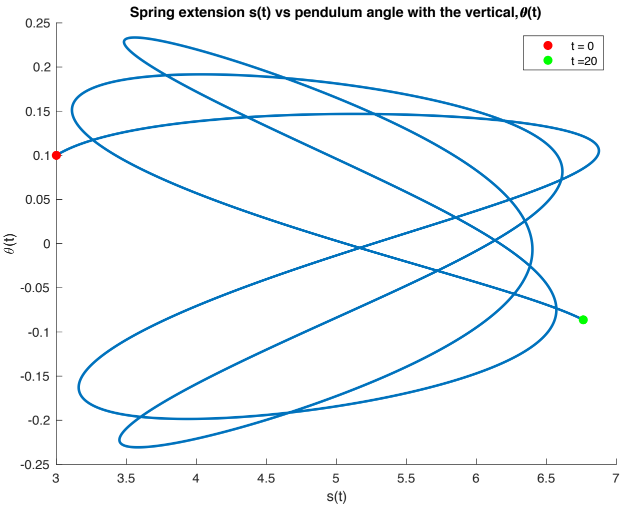
For the model parameters, use $m = 1$, $k = 2$, $\ell = 10$, and use $g = 9.81$.



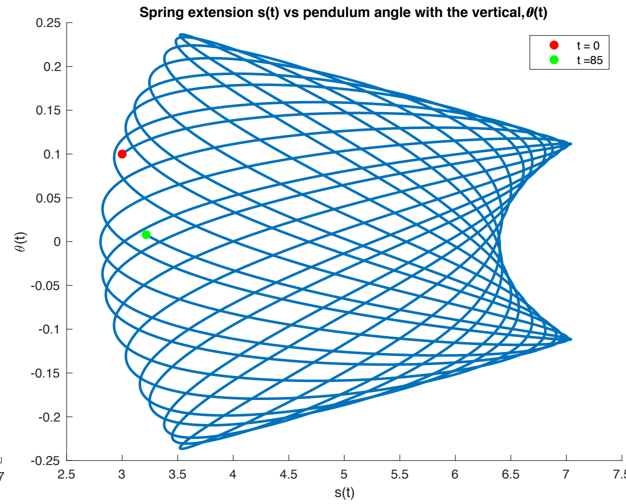
(a) Plot of $s(t)$.



(b) Plot of $\theta(t)$.

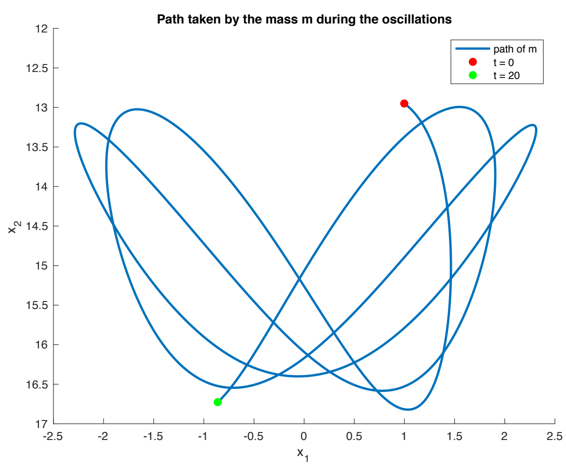


(c) Plot of $s(t)$ vs $\theta(t)$ with final time equal to 20.

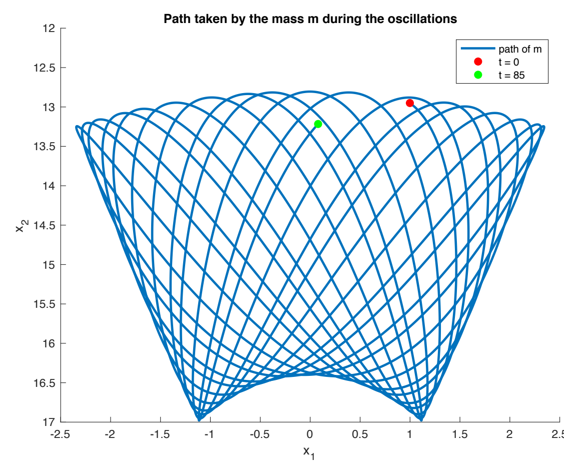


(d) Plot of $s(t)$ vs $\theta(t)$ with final time equal to 85.

(c) Using the solution of the ODE, compute the coordinates of the location of m, $(x_1(t), x_2(t))$, at each time. Then, plot x_1 versus x_2, showing the path taken by m during the oscillations.



(a) Plot of the path taken by the mass m with final time equal to 20.



(b) Plot of the path taken by the mass m with final time equal to 85.

3. [15 points] Consider the following ODE system:

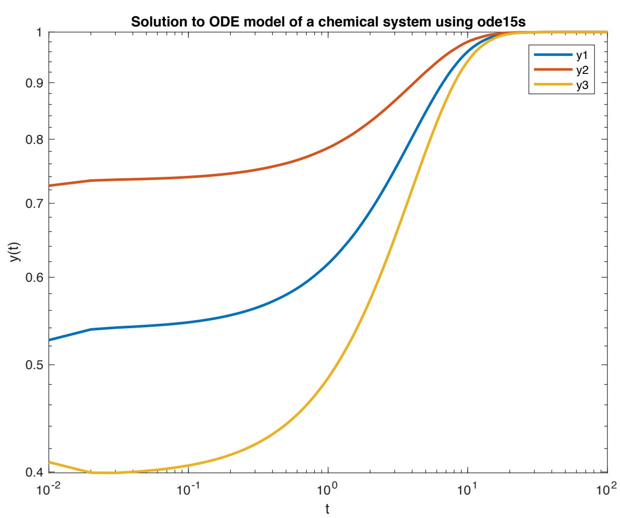
$$\dot{y}_1 = -\frac{5y_1}{\varepsilon} - \frac{y_1 y_2}{\varepsilon} + y_2 y_3 + \frac{5y_2^2}{\varepsilon} + \frac{y_3}{\varepsilon} - y_1,$$
$$\dot{y}_2 = \frac{10y_1}{\varepsilon} - \frac{y_1 y_2}{\varepsilon} - y_2 y_3 - \frac{10y_2^2}{\varepsilon} + \frac{y_3}{\varepsilon} + y_1,$$
$$\dot{y}_3 = \frac{y_1 y_2}{\varepsilon} - y_2 y_3 - \frac{y_3}{\varepsilon} + y_1,$$

with parameter $\varepsilon = 10^{-2}$. The initial conditions are chosen to be

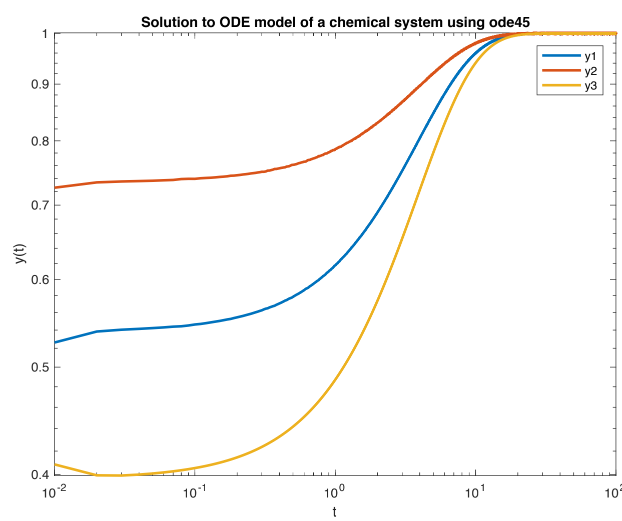
$$y_1(0) = y_2(0) = y_3(0) = 0.5.$$

This is a model of a three-species chemical system, studied in [1].

(a) Compute the solution to this system, on the interval $[0, 100]$, using Matlab's ode45 and ode15s solvers. Provide a loglog plot of y_1, y_2, and y_3 over time, obtained using each of the solvers. Report the number of time-steps taken by each method, and also the computational time (for timing purposes, you can Matlab's `tic` and `toc` commands). Also, report any tolerances/solver options used.



(a) Solution obtained using Matlab's ode15s.



(b) Solution obtained using Matlab's ode45.

The method ode15s used 75419 time-steps and took 1.9508 seconds. The method ode45 used only 69 time-steps and took 0.0937 seconds. The default tolerances and solver options were used.

(b) Compute the eigenvalues of the system Jacobian[1] at each of the time-steps of the simulation. Plots these eigenvalues over time. Comment on what you see; what are the implications of the observed magnitudes of the eigenvalues? If you were going to integrate this system using forward Euler, can you estimate the order of the step-size required?

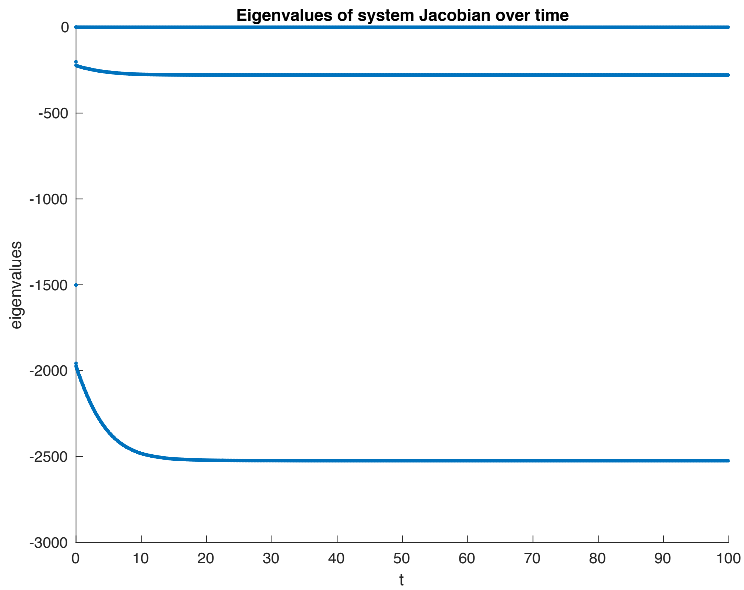


Figure 6: Eigenvalues of the system Jacobian over time.

The eigenvalues of this system indicate that this ODE system is stiff. We observe some eignvalues which have negative real parts of large magnitude, along with other eigenvalues of moderate magnitude. This is characteristic of stiff problems. If we were to integrate this system with forward Euler, we would need $|1 + h\lambda| < 1$. Since we have λ with values around -2500, we require $-1 < 1 - 2500\ h < 1$; i.e., $0 < h < 2/2500 = 8 \times 10^{-4}$. Thus the step-size required to solve this system using forward Euler would be around 10^{-5}.

[1]For an ODE system $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$, by the system Jacobian, we mean the matrix $\mathbf{J}$ with entries $J_{ij} = \frac{\partial f_i}{\partial y_j}$.

4. [10 points]

(a) Consider the Crank–Nicolson method (trapezoidal rule),

$$y_{n+1} = y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_{n+1}, y_{n+1})\right),$$

used for solving the IVP $y' = f(x, y)$, $y(0) = y_0$. Find the stability function of the method, find its stability region, and show that the method is A-stable.

Applying this method to the IVP $y' = \lambda y$, $y(0) = 1$, we get

$$y_{n+1} = y_n + \frac{h}{2}[\lambda y_n + \lambda y_{n+1}]$$

$$y_{n+1}(1 - \frac{h}{2}\lambda) = y_n(1 + \frac{h}{2}\lambda)$$

$$y_{n+1} = y_n \frac{1 + (h/2)\lambda}{1 - (h/2)\lambda}$$

Since $y_0 = 1$, we have

$$y_n = \left(\frac{1 + (h/2)\lambda}{1 - (h/2)\lambda}\right)^n$$

For this problem, we should have $y(t) \to 0$ as $t \to \infty$, so for convergence, we require

$$\left|\frac{1 + (h/2)\lambda}{1 - (h/2)\lambda}\right| < 1$$

Thus the stability function $\phi(z)$ where $z = h\lambda$ is

$$\phi(z) = \frac{1 + z/2}{1 - z/2}$$

Thus the stability region of the function is $z \in \mathbb{C}$ such that

$$\left|\frac{1 + z/2}{1 - z/2}\right| < 1$$

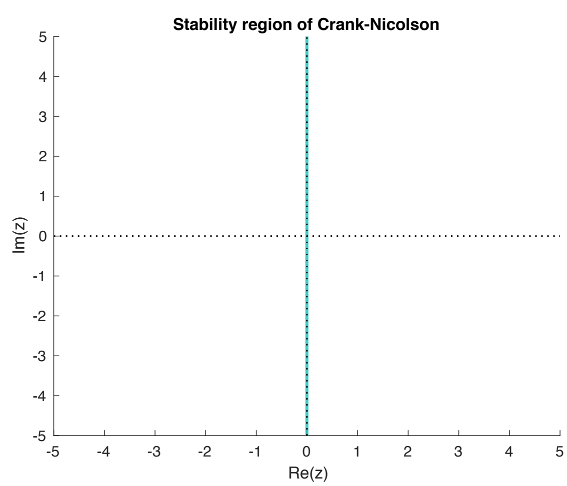


Figure 7: Stability region of the Crank–Nicolson method. The shaded area is the stability region.

Note that the stability region encompasses the entire negative real half of of complex plane, thus the Crank–Nicolson method A-stable.

(b) Find the stability region of the 2nd order Runge–Kutta method

$$y_{n+1} = y_n + \frac{h}{2}\Big[f(x_n, y_n) + f\big(x_{n+1}, y_n + hf(x_n, y_n)\big)\Big].$$

Is this method A-stable?

Applying this method to the IVP $y' = \lambda y$, $y(0) = 1$, we get

$$\begin{aligned} y_{n+1} &= y_n + \frac{h}{2}[\lambda y_n + \lambda(1 + h\lambda)y_n] \\ &= y_n + h\lambda/2 \; y_n(2 + h\lambda) \\ &= y_n[1 + h\lambda + 1/2 \; (h\lambda)^2] \end{aligned}$$

Since $y_0 = 1$, we have

$$y_n = (1 + h\lambda + 1/2 \; (h\lambda)^2)^n$$

For this problem, we should have $y(t) \to 0$ as $t \to \infty$, so for convergence, we require

$$|1 + h\lambda + 1/2 \; (h\lambda)^2| < 1$$

Thus the stability function $\phi(z)$ where $z = h\lambda$ is

$$\phi(z) = 1 + z + \frac{z^2}{2}$$

Thus the stability region of the function is $z \in \mathbb{C}$ such that

$$\left|1 + z + \frac{z^2}{2}\right| < 1$$

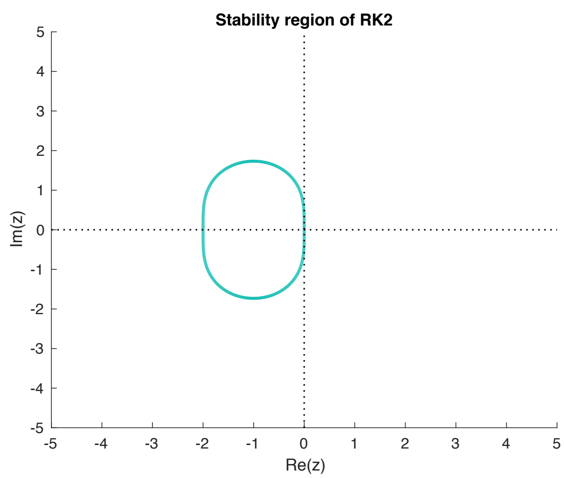


Figure 8: Stability region of the 2nd order Runga–Kutta method. The shaded area is the stability region.

Since the stability region does not encompass the entire negative real half of the complex plane, the RK2 method is not A-stable. A simpler way to show this is by considering the point $z = -4$. Then $\phi(z) = \phi(-4) = 1 - 4 + \frac{(-4)^2}{2} = 5$. Since $|\phi(-4)| = |5| = 5 \geq 1$, $z = -4$ is not in the stability region. However, $z = -4$ lies in the negative real half of complex plane, so the RK2 method is not A-stable.

Note: for finding the stability regions, follow the approach of applying the numerical scheme to the model initial value problem $y' = \lambda y$, $y(0) = 1$, with $\lambda \in \mathbb{C}$, as done in class.

References

[1] Valorani, M., Goussis, D. A., Creta, F., & Najm, H. N. (2005). Higher order corrections in the approximation of low-dimensional manifolds and the construction of simplified problems with the CSP method. Journal of Computational Physics, 209(2), 754-786.