Homework Set 5

Numerical Initial Value Problems

Revision: 26–Mar–2020

5.1 Stability

Analyze the stability of the following methods applied to the standard linear differential equation

$$\dot{x} = \lambda x \tag{5.1}$$

Also, plot the region of stability.

1. Trapezoidal rule

$$x_{n+1} = x_n + \frac{h}{2}\left(f(t_n,\, x_n) + f(t_{n+1},\, x_{n+1})\right) \tag{5.2}$$

2. Runge-Kutta 2 for $\alpha \in \{1/4,\, 1/2,\, 2/3\}$

$$\begin{array}{c|cc} 0 & & \\ \alpha & \alpha & \\ \hline & 1-\frac{1}{2\alpha} & \frac{1}{2\alpha} \end{array} \tag{5.3}$$

5.2 Estimating an upper bound on the time step

If we are given a differential equation

$$\dot{x} = Ax \tag{5.4}$$

what is an estimate for the maximum time step allowed if we use

- the two-stage Adams–Basthforth scheme
- the implicit midpoint method

for the following two cases of A:

$$\text{case 1: } A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{5.5}$$

$$\text{case 2: } A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -23 & -304 & -732 \end{bmatrix} \tag{5.6}$$

Numerically verify your analysis. Compare this maximum time step with one that ensures a usably accurate solution.

5.3 Variable time-step

The explicit two-stage Adams–Bashforth method has the form

$$x_{i+1} = x_i + b_2 f(t_i,\, x_i) + b_1 f(t_{i-1},\, x_{i-1}) \tag{5.7}$$

If the time step is not uniform ($\Delta t_i \neq$ constant), derive the values of b_2 and b_1. Show that if the time step is uniform, your expression collapses back to the classic formula.

5.4 Predictor–Corrector

Consider the non-dimensional damped oscillator

$$\ddot{x} + 2\zeta\dot{x} + x = 0 \tag{5.8}$$

that has already been normalized by natural frequency. Let $\zeta = 0.02$, and consider the initial values $x(0) = 1$, $\dot{x}(0) = 0$.

1. Implement the 3 stage Adams-Bashforth method and integrate the equations for $t \in [0, 100]$. Compare the results to the analytic solution. Comment on what you find.
2. Implement the 4 stage Adams-Moulton method in a predictor-corrector scheme with your previously made AB3 routine. Integrate the equation of motion for the same time interval as before. Compare to your AB3 results and the analytic solution. Comment on your observations.

5.5 Classical Runge-Kutta

Implement the classic 4th order Runge-Kutta method called the "The 3/8 Rule" (Hairer, Nørsett, and Wanner, 1993, p. 138)

$$\begin{array}{c|cccc} 0 & 0 & & & \\ 1/3 & 1/3 & & & \\ 2/3 & -1/3 & 1 & & \\ 1 & 1 & -1 & 1 & \\ \hline & 1/8 & 3/8 & 3/8 & 1/8 \end{array} \tag{5.9}$$

and use it to solve (5.8) and the same initial conditions as P5.4. Compare the results with the results of P5.4. Investigate the error and relative costs compared to the Adams method.

5.6 Implicit Runge-Kutta

Consider the method shown in the Butcher tableau (Butcher, 2016, p. 232)

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{5.10}$$

known as the two-stage Gauss-Legendre Runge-Kutta method. This is a 4th-order implicit Runge-Kutta (IRK) method, that is A-stable, L-stable, and B-stable. It is also symplectic, but rather expensive to use for large systems since k_1 and k_2 must be found simultaneously. This means if we have an n-th order differential equation, we need to solve $2n$ simultaneously (nonlinear) equations during each time step.

5.6.1 A simple pendulum

Consider a simple planar pendulum that has the Hamiltonian

$$\mathcal{H} = \frac{p^2}{2} - \cos q \tag{5.11}$$

where p is the nondimensional momentum, and q is the angle.

1. Derive Hamilton's equation of this system.
2. For a range of initial conditions, integrate this system using
   - Implicit Euler
   - Adams-Bashforth 2
   - The IRK method of (5.10)
3. Provide discussion on the following points comparing each solver and its results:
   (a) Compare what happens to the energy and other conserved quantities of the system. Some ideas to show these are shown in Figures 5.1 and 5.2. The phase space shows how the solution should remain on a constant contour of $\mathcal{H}$, while the energy plot shows how the energy is changing in the solution.
   (b) Discuss the complexity of the implementations of the solvers and compare the relative computation times.
   (c) Does the long term behavior of IRK method of (5.10) remain well behaved?

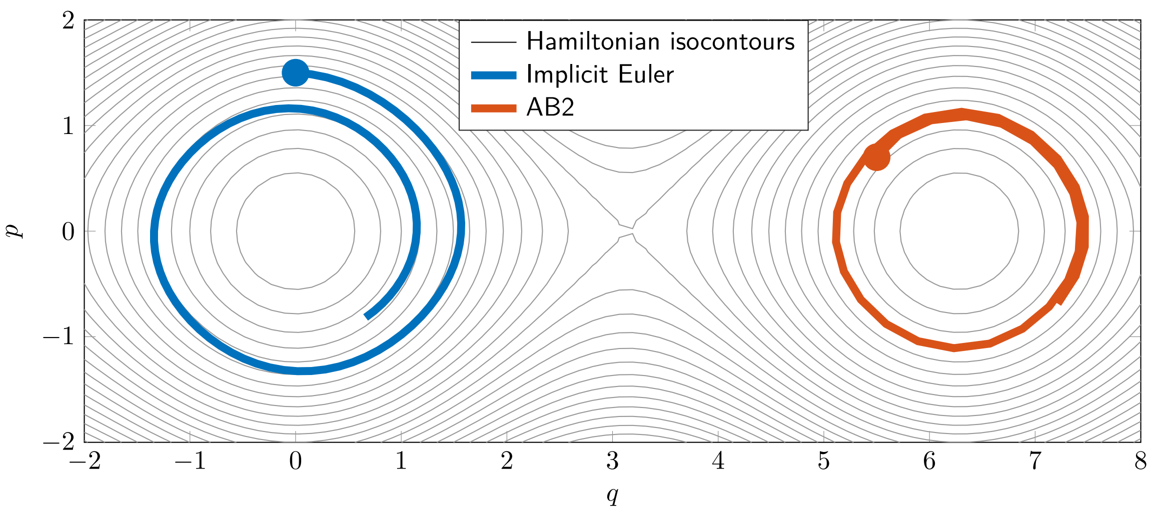

Figure 5.1: Phase-space

5.6.2 Euler equations

The motion of a free rigid body, whose center of mass is at the origin, is described by the Euler equations

$$\dot{y}_1 = a_1 y_2 y_3, \qquad a_1 = (I_2 - I_3)/(I_2 I_3) \tag{5.12a}$$
$$\dot{y}_2 = a_2 y_3 y_1, \qquad a_2 = (I_3 - I_1)/(I_3 I_1) \tag{5.12b}$$
$$\dot{y}_3 = a_3 y_1 y_2, \qquad a_3 = (I_1 - I_2)/(I_1 I_2) \tag{5.12c}$$

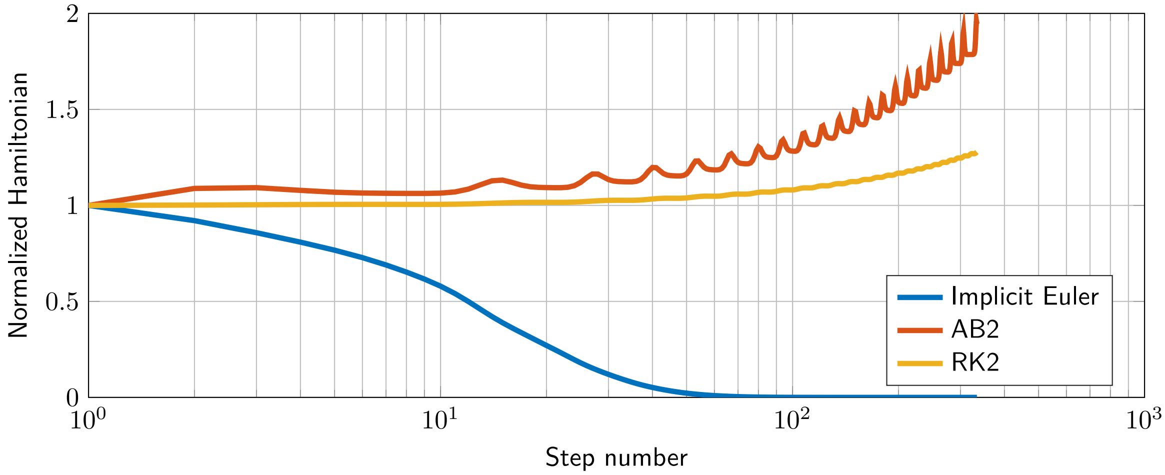

Figure 5.2: Relative Hamiltonian $\frac{\mathcal{H}(q(t),p(t))+1}{\mathcal{H}(q(0),p(0))+1}$

where the tuple $y = (y_1, y_2, y_3)^T$ represents the angular momentum in the body frame, and I_1, I_2, I_3 are the principal moments of inertia. A historical account of the development of these equations is provided in Hairer, Lubich, and Wanner (2006, Sec. VII.5). For this system, the kinetic energy (it's also the Hamiltonian in this case) is a conserved quantity

$$\mathcal{H} = \frac{1}{2}\left(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3}\right) \tag{5.13}$$

It can be shown geometrically that $y_2^2 + y_2^2 + y_3^2$ is also conserved. Therefore we can view solutions to the Euler equations as living on the intersection of the ellipsoid described by the Hamiltonian and the sphere.

Consider the case where $I_1 = 2$, $I_2 = 1$, $I_3 = 2/3$, and $y(0) = (\cos(1.1), 0, \sin(1.1))^T$. Compute the solution using the following methods:

- Explicit Euler
- The implicit midpoint rule
- The IRK method of (5.10)

Plot the solution in 3D: $y_1(t)$ vs $y_2(t)$ vs $y_3(t)$. Do the trajectories remain on $\mathcal{H}$?

5.7 Adaptive step size Runge-Kutta

Consider the Butcher tableau

$$\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{3}{4} & 0 & \frac{3}{4} & & \\
1 & \frac{2}{9} & \frac{1}{3} & \frac{4}{9} & \\
\hline
 & \frac{2}{9} & \frac{1}{3} & \frac{4}{9} & 0 \\
 & \frac{7}{24} & \frac{1}{4} & \frac{1}{3} & \frac{1}{8}
\end{array} \tag{5.14}$$

first provided by Bogacki and Shampine (1989). This is the basis for `ode23`[1] in Matlab. The extra row at the bottom corresponds to a 2nd order method, while the row above that is 3rd order. This provides a way to estimate the local error. Written out, this looks like

$$\begin{aligned}
k_1 &= f(t_n, x_n) \\
k_2 &= f(t_n + \tfrac{1}{2}h_n,\, x_n + \tfrac{1}{2}h_n k_1) \\
k_3 &= f(t_n + \tfrac{3}{4}h_n,\, x_n + \tfrac{3}{4}h_n k_2) \\
x_{n+1} &= x_n + h_n\left(\tfrac{2}{9}k_1 + \tfrac{1}{3}k_2 + \tfrac{4}{9}k_3\right) \\
k_4 &= f(t_n + h_n,\, x_{n+1}) \\
z_{n+1} &= x_n + h_n\left(\tfrac{7}{24}k_1 + \tfrac{1}{4}k_2 + \tfrac{1}{3}k_3 + \tfrac{1}{8}k_4\right)
\end{aligned}$$

where $h_n = t_{n+1} - t_n$. The error is approximately

$$e_{n+1} = |x_{n+1} - z_{n+1}| \tag{5.15}$$

If the error is greater than a tolerance ε, then the step is rejected, the time step is halved, and we try to compute the step again. If the error is less than ε, then we conservatively grow the time step.

$$h_{n+1} = 0.9 h_n \min\left(\max\left(\frac{\varepsilon}{e_{n+1}},\, 0.3\right),\, 2\right) \tag{5.16}$$

5.7.1 Sample problem

Consider the initial value problem

$$\dot{x} = 4e^{0.8t} - 0.5x, \quad x(0) = 2 \tag{5.17}$$

over the time interval $t \in [0, 2]$. Implement the adaptive method of 5.14 to solve this problem to a relative error of $\epsilon = 10^{-8}$. Check $x(2)$ compared to the exact solution.

5.7.2 Airfoil

Recall the airfoil of the dynamics HW, shown in Figure 5.3, where we derived Lagrange's equations.

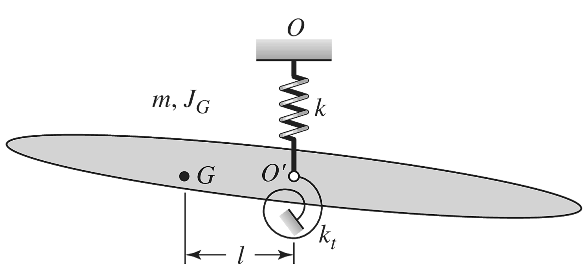

Figure 5.3: Elastically mounted airfoil

Implement the adaptive method of 5.14, and use the equations of motion of the airfoil as the trial problem. Select reasonable values for the parameters. Perform a convergence study to ensure your computed results are reliable.

[1] `https://www.mathworks.com/help/matlab/ref/ode23.html`

5.8 Chemical reactions

Chemical reactions often give rise to stiff systems of coupled rate equations. The time history of a reaction is governed by the following rate equations

$$\dot{C}_1 = -k_1 C_1 + k_2 C_2 C_3 \tag{5.18}$$
$$\dot{C}_2 = k_1 C_1 - k_2 C_2 C_3 - 2k_3 C_2^2 \tag{5.19}$$
$$\dot{C}_3 = 2k_3 C_2^2 \tag{5.20}$$

where k_1, k_2, and k_3 are reaction rate constants given as

$$k_1 = 0.04, \qquad k_2 = 10.0, \qquad k_3 = 1.5 \times 10^3,$$

and the C_i are the concentrations of species A_i in the reaction

$$A_1 \to A_2$$
$$A_2 + A_3 \to A_1 + A_3$$
$$2A_2 \to 2A_3$$

Initially, $C_1(0) = 0.9$, $C_2(0) = 0.1$, and $C_3(0) = 0$.

1. What is the analytical steady state solution? Note that these equations should conserve mass, that is, $C_1 + C_2 + C_3 = 1$.
2. Evaluate the eigenvalues of the Jacobian matrix at $t = 0$. Is the problem stiff?
3. Solve the given system to a steady state solution ($t = 3000$ represents steady state in this problem) using
   (a) Classic Fourth-order Runge–Kutta (Hint: use the stiffness calculation to estimate the maximum time step).
   (b) The Backward Differentiation formula (BDF) method of order 3 (or higher).
   (c) A prepackaged solver for stiff systems, such as MATLAB's `ode23s` or `Rosenbrock23` in Julia.[2]

   Make a log–log plot of the concentrations C_i vs. time. Compare the computer time required for these two methods.
4. Set up the problem with a linearized trapezoidal method. What advantages would such a scheme have over fourth-order RK?

5.9 The Lorenz System

Nonlinear differential equations with several degrees of freedom often exhibit chaotic solutions. Chaos is associated with sensitive dependence to initial conditions and some strange things can happen. In some special circumstances numerical solutions are often confined to what is called a *strange attractor*. It is the sensitive dependence on initial conditions that makes many physical systems (such as weather patterns) unpredictable, and it is the attractor that does not allow physical parameters to get out of hand (e.g., very high or low temperatures, etc.). The classical example of a system that exhibits this behavior is the Lorenz system

$$\dot{x} = \sigma(y - x) \tag{5.21}$$
$$\dot{y} = rx - y - xz \tag{5.22}$$
$$\dot{z} = xy - bz \tag{5.23}$$

[2] This is part of the `DifferentialEquations.jl` package.

The values of σ and b are usually fixed ($\sigma = 10$ and $b = 8/3$ in this problem) leaving r as the control parameter. For low values of r, the stable solutions are stationary. When r exceeds 24.74, the trajectories in xyz space become irregular orbits about two particular points.

1. Solve these equations using $r = 20$. Start from point $(x, y, z) = (1, 1, 1)$, and plot the solution trajectory for $t \in [0, 25]$ in the xy, xz, and yz planes. Also plot x, y, and z versus t. Comment on your plots in terms of the previous discussion.

2. Observe the change in the solution by repeating the previous part for $r = 28$. In this case, also plot the trajectory of the solution in the three-dimensional xyz space (let the z axis be in the horizontal plane; hint: use the MATLAB's `plot3(z,y,x)` for this). Compare your plots to the previous part of the problem.

3. Observe the unpredictability at $r = 28$ by over plotting two solutions versus time starting from two initially nearby points: (6, 6, 6) and (6, 6.01, 6).

5.10 Pendulum Absorber

Recall the pendulum attached to a cart from the dynamics HW, as depicted in Figure 5.4. In that previous problem you derived the equations of motion of this system in serval forms, let's simulate these and compare the results. The parameters of the system are given in Table 5.1.

Table 5.1: Parameter values for §5.10

Quantity	**Value**	
m_1	1.0	kg
m_2	1.0	kg
L	0.5	m
k	100	N/m
$f(t)$	0	N
$\theta(0)$	-75	°
$\dot{\theta}(0)$	0	rad/s
$x(0)$	0.1	m
$\dot{x}(0)$	0	m/s

1. If we want a high quality solution, discuss your thought process on the selection of solvers, tolerances, etc.

2. Linearize the system about $(x, \theta) = (0, 0)$, and compute the natural frequencies. Use this info to predict appropriate time-steps for the calculation.

3. Using a solver you implemented, integrate the equations of motions derived by Lagrange's equation (Newton's equations should have matched), and Hamilton's equation. Compare the results and comment on what you find.

4. Derive the equations of motion using the Udwadia-Kalaba equation. Integrate these and compare the results to the previous part. Does the solution qualitatively change? Does it quantitatively change?

5. *Bonus:* Looking at the EOM from Hamilton's equation, use the method of P5.6 and compare to the previous results.

6. *Bonus:* Make an animation of the various results superimposed on the same plot. Vary the initial conditions, and see if anything interesting happens.

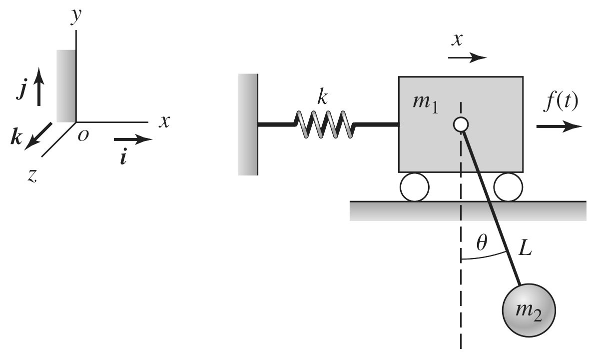

Figure 5.4: A planar pendulum absorber

5.11 The double pendulum

Recall the double-pendulum from the dynamics HW, shown in Figure 5.5. The parameters of this system are

$$\{g, m_1, m_2, l_1, l_2\},$$

and the data are given in Table 5.2.

Table 5.2: Parameter values for §5.11

Quantity	Value	
m_1	1.0	kg
m_2	1.0	kg
l_1	0.5	m
l_2	0.5	m
$\theta_1(0)$	90	°
$\dot{\theta}_1(0)$	0	rad/s
$\theta_2(0)$	90	°
$\dot{\theta}_2(0)$	0	rad/s

5.11.1 Udwadia–Kalaba

Using the Udwadia-Kalabda equations that you (hopefully) derived in the previous homework, determine the following:

1. Integrate these equations using a solver of your choice for at least 5 periods of motion of the top pendulum, and plot some of the solutions.
2. Observe what happens to the constraint equations as well as the energy. Is there drift? Do the lengths change?
3. Animate the solution, or come up with a novel visualization of the result.

5.11.2 Lagrange's equation

Using the equations of motion you (hopefully) derived using Lagrange's equation in terms of θ_1 and θ_2, determine the following:

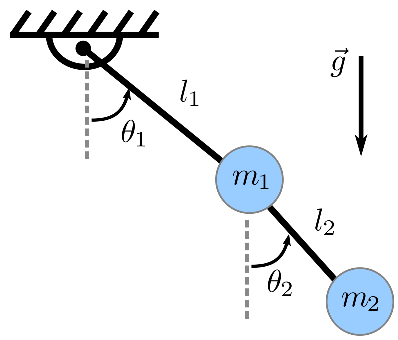

Figure 5.5: A planar lumped-mass ideal double-pendulum.

1. Setup these equations to be solved for at least 5 periods of motion of the top pendulum.
2. Solve the equations using the following solvers: `ode45`, `ode23`, `ode113`, `ode15s`, `ode23t`, `ode23tb`. *Bonus:* Add some additional solvers that you implement by hand to this list. Take note of the computation time for each method. Superimpose the solutions of each method on a plot of the system, and discuss what you see.
3. Using the computed solutions from the previous step, compute the energy (Hamiltonian) of the system. Compare how the energy changes (or not) in time for the various solvers.
4. Animate the solutions from multiple solvers on top of one another. Comment on when the solutions diverge.

5.11.3 Bonus – Twitter

Make an animated gif of your results. Post it online and tweet it to `@FitzgeraldLab`.

5.12 The Pleiades

Let's consider a simplified celestial mechanics problem called "The Pleiades Problem." Here, there are seven stars in the plane with coordinates (x_i, y_i) and each has mass $m_i = i$, where $i \in \{1, 2, \ldots, 7\}$. The equations of motion for each body are simplified to be

$$\ddot{x}_i = \sum_{j \neq i} m_j \left(x_j - x_i\right)/r_{ij} \tag{5.24a}$$

$$\ddot{y}_i = \sum_{j \neq i} m_j \left(y_j - y_i\right)/r_{ij} \tag{5.24b}$$

where

$$r_{ij} = \left((x_i - x_j)^2 + (y_i - y_j)^2\right)^{3/2} \tag{5.24c}$$

The initial values are given in Table 5.3. We want to determine the solution for time $t \in [0, 3]$.

1. Select an appropriate method to compute the solution. A couple notes on this: (1) there is no damping in this system, (2) the rate at which things change can be large, so the method should be adaptive.
2. Implement your chosen method on (5.24), and test it out on the given initial conditions from Table 5.3.
3. Note the largest and smallest time step taken over the simulation. How much does it vary?
4. Build a plot of the $x - y$ positions. Hint: this should look like Figure 5.6.
5. Build a plot of the speed of each particle vs time. Hint: this should look like Figure 5.7.
6. Bonus: make an animation of the results.

Table 5.3: Parameter values for §5.12

i	$x_i(0)$	$y_i(0)$	$\dot{x}_i(0)$	$\dot{y}_i(0)$
1	3	3	0	0
2	3	−3	0	0
3	−1	2	0	0
4	−3	0	0	−1.25
5	2	0	0	1
6	−2	−4	1.75	0
7	2	4	−1.5	0

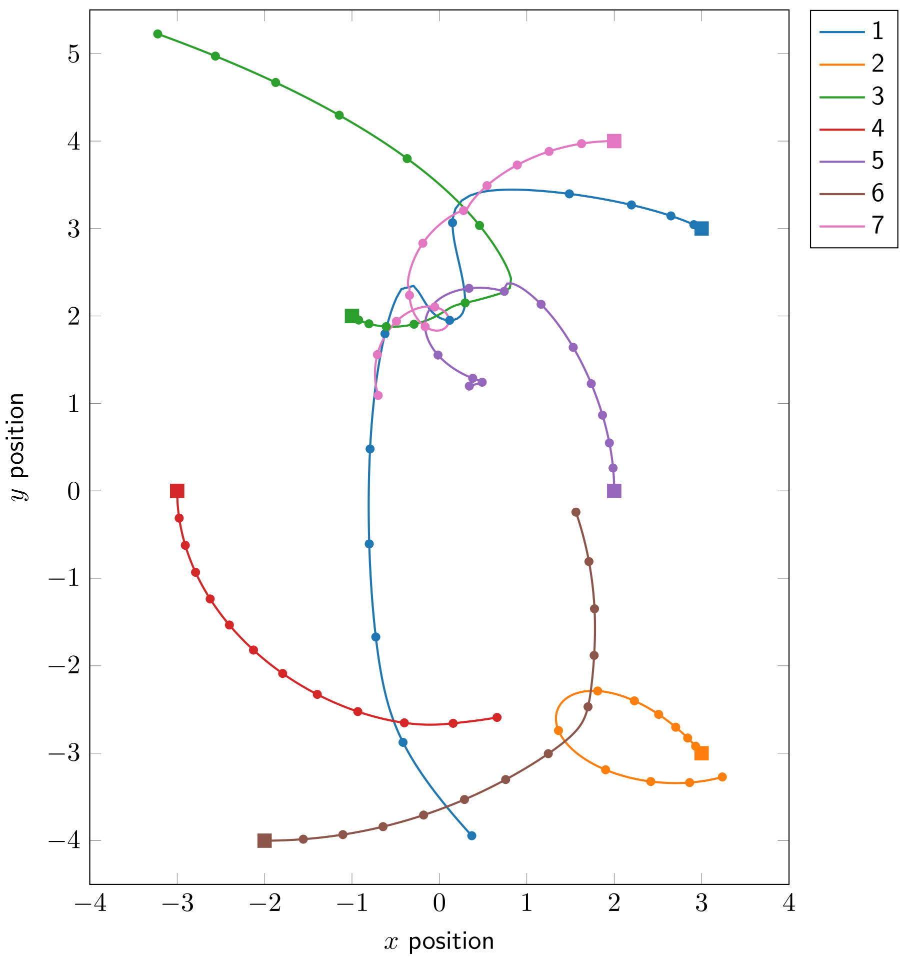

Figure 5.6: Solutions to (5.24), the dots indicate even time increments of 0.25 units. The squares are the starting locations for each body.

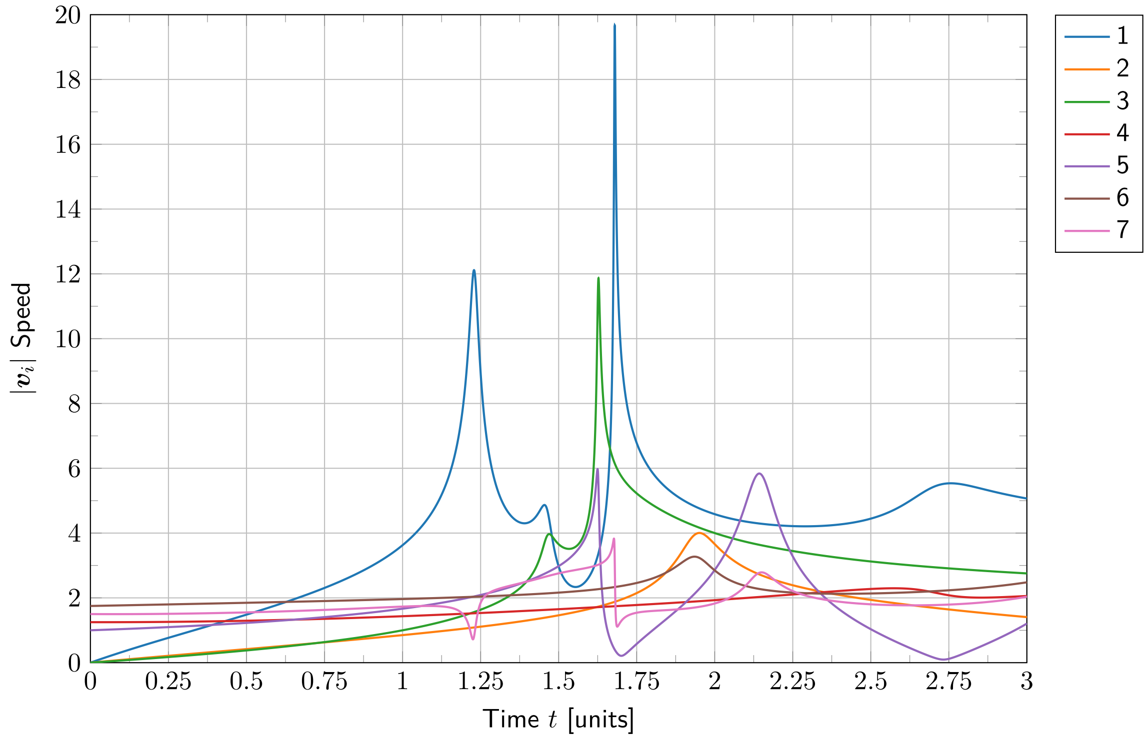

Figure 5.7: Speeds of each body as a function of time.

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