1 Pen and paper

1. Consider the ODE

\[ \frac{\partial}{\partial t} \begin{pmatrix} x(t) \\ mv(t) \end{pmatrix} = \begin{pmatrix} -\frac{\partial e}{\partial x}(x(t)) - \gamma v(t) \\ 0 \end{pmatrix} \]

with Hamiltonian \( H(t) = \frac{m}{2} (v(t))^2 + e(x(t)) \).

(a) Let \( \gamma = 0 \) and \( e(x) = \frac{k}{2} x^2 \). Consider a Forward Euler discretization of the problem. Show that \( H^{n+1} \geq H^n \) \( \forall \Delta t \) where \( H^n = \frac{m}{2} (v^n)^2 + e(x^n) \) and \( x^n, v^n \) are the Forward Euler approximations.

(b) Let \( \gamma > 0 \) and \( e(x) = \frac{k}{2} x^2 \). Consider the following discretization

\[
\begin{align*}
x^{n+1} &= x^n + \frac{\Delta t}{2} (v^n + v^{n+1}) \\
v^{n+1} &= v^n - \frac{\Delta t}{m} x^n - \frac{\Delta t \gamma}{m} v^{n+1}
\end{align*}
\]

For which \( \Delta t \) can we say that

\[
\left| \begin{pmatrix} x^{n+1} \\ v^{n+1} \end{pmatrix} \right| \leq \left| \begin{pmatrix} x^n \\ v^n \end{pmatrix} \right| ?
\]

(c) What is the truncation error for the scheme in part (b)?

2. Shooting: Consider the elasticity problem with

\[ \frac{\partial}{\partial X} \left( P(F(X)) \right) = \rho(X) g, \ X \in (0, 1) \]

\[ \phi(0) = \hat{x}_0, \ \phi(1) = \hat{x}_1 \]

where \( \phi : [0, 1] \to \mathbb{R}^2, F(X) = \frac{\partial \phi}{\partial X}(X) \) and \( P : \mathbb{R}^2 \to \mathbb{R}^2 \) with \( \psi : \mathbb{R}^2 \to \mathbb{R} \) and \( P(F) = \frac{\partial \psi}{\partial F}(F) \).

(a) Define \( \hat{\phi}(X; c) \) and \( F(X; c) = \frac{\partial \hat{\phi}}{\partial X}(X; c) \) as the solution of

\[ \frac{\partial}{\partial X} \left( P(F(X; c)) \right) = \rho(X) g, \ X \in (0, 1) \]

\[ \hat{\phi}(0; c) = \hat{x}_0, \ \frac{\partial \hat{\phi}}{\partial X}(0; c) = c \]

Define the function \( h(c) = \hat{\phi}(1; c) - \hat{x}_1 \). If we use Newton’s method to solve for roots \( h(c) \) to develop a shooting algorithm, we will need to know \( \frac{\partial \hat{\phi}}{\partial c}(1; c) \). Derive an IVP for \( \frac{\partial \hat{\phi}}{\partial c}(X; c) \).

(b) Let \( g = \begin{pmatrix} 0 \\ -9.8 \end{pmatrix} \), \( \psi(F) = \frac{k}{2} |F|^2 \), \( \rho(X) = 1 + d(X) \), \( \hat{x}_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \), \( \hat{x}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \) and

\[
d(X) = \begin{cases} C & X \in \left( \frac{1}{2} - l, \frac{1}{2} + l \right) \\
0 & \text{otherwise}
\end{cases}
\]

with \( l < \frac{1}{2} \). Solve for the \( c \) that solves \( h(c) = 0 \) for the \( h(c) \) described in part (a). You will not need to use Newton’s method in this case.
2 Programming

1. Mass/spring: Consider the system

\[ \frac{\partial}{\partial t} \begin{pmatrix} \mathbf{x}(t) \\ \mathbf{v}(t) \end{pmatrix} = \left( \mathbf{M}^{-1} \begin{pmatrix} \mathbf{v}(t) \\ -\frac{\partial e}{\partial \mathbf{x}}(\mathbf{x}(t)) - \gamma \mathbf{v}(t) \end{pmatrix} \right) + \mathbf{g}, \quad t > 0 \]

with \( \mathbf{x} = \begin{pmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{N_p-1} \end{pmatrix} \in \mathbb{R}^{2N_p}, \mathbf{v} = \begin{pmatrix} \mathbf{v}_0 \\ \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_{N_p-1} \end{pmatrix} \in \mathbb{R}^{2N_p}, \mathbf{g} = \begin{pmatrix} 0 \\ \mathbf{g} \end{pmatrix} \in \mathbb{R}^{2N_p} \) with \( \mathbf{g} = \begin{pmatrix} 0 \\ -\mathbf{9.8} \end{pmatrix} \in \mathbb{R}^2, \mathbf{v}_i, \mathbf{x}_i \in \mathbb{R}^2, e(\mathbf{x}) = \sum_{i=1}^{N_p-1} \frac{k}{2(N_p-1)} ((N_p - 1) |\mathbf{x}_i - \mathbf{x}_{i-1}| - 1)^2, \mathbf{M} = \begin{pmatrix} m_0 \mathbf{I}_2 \\ m_1 \mathbf{I}_2 \\ \vdots \\ m_{N_p-1} \mathbf{I}_2 \end{pmatrix} \in \mathbb{R}^{2N_p \times 2N_p}, m_0 = \infty, m_i > 0 \) for \( i > 0, k > 0, \gamma > 0 \) and initial conditions \( \mathbf{x}_i(0) = \left( \frac{N_p-i}{N_p} 0 \right), \mathbf{v}_i(0) = \mathbf{0}. \)

(a) Let \( m_i = \frac{1}{N_p} \) for \( i > 0, k = 100, T = 10 \) and \( \gamma = \frac{1}{4} \sqrt{\frac{4k}{N_p}}. \) Linearize the problem around the initial data and use this to compute a time step \( \Delta t_s \) for absolute stability with \( N_p = 5. \)

(b) Plot the Forward Euler approximation of the problem with \( \Delta t = \frac{3}{2} \Delta t_s \) and \( N_p = 5. \)

(c) Plot the Forward Euler approximation of the problem with \( \Delta t = \frac{2}{3} \Delta t_s \) and \( N_p = 5. \)

2. Repeat problems (b) and (c) with Backward Euler.

3. Shooting: Consider the elasticity problem with

\[ \frac{\partial}{\partial X} (\mathbf{P}(\mathbf{F}(X))) = \rho(X)\mathbf{g}, \quad X \in (0, 1) \]

\[ \phi(0) = \mathbf{x}_0, \quad \phi(1) = \mathbf{x}_1 \]

where \( \phi : [0, 1] \rightarrow \mathbb{R}^2, \mathbf{F}(X) = \frac{\partial \phi}{\partial X}(X) \) and \( \mathbf{P} : \mathbb{R}^2 \rightarrow \mathbb{R}^2 \) with \( \psi : \mathbb{R}^2 \rightarrow \mathbb{R} \) and \( \mathbf{P}(\mathbf{F}) = \frac{\partial \psi}{\partial \mathbf{F}}(\mathbf{F}). \)

(a) Let \( \mathbf{g} = \begin{pmatrix} 0 \\ -\mathbf{9.8} \end{pmatrix}, \psi(\mathbf{F}) = \frac{1}{2} |\mathbf{F}|^2, \rho(X) = 1 + d(x), \mathbf{\hat{x}}_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \mathbf{\hat{x}}_1 = \begin{pmatrix} 1 \\ \frac{1}{3} \end{pmatrix} \) and

\[ d(x) = \begin{cases} C & x \in \left( \frac{1}{2} - l, \frac{1}{2} + l \right) \\ 0 & \text{otherwise} \end{cases} \]

Implement a shooting method to approximate the solution to this problem with \( C = 2 \) and \( l = .1. \) Run with \( k = 100, 10 \) and \( 1. \) Use the IVP approximation (Forward Euler, Backward Euler, Trapezoidal Rule etc.) that you consider most appropriate.

(b) Use the result from part (b) of the last Pen and Paper problem for check your answer.