Lecture 13: Numerical Solution of ODE Initial Value Problems

Outline

1) Motivation and examples
2) Basic Stepping schemes and errors (relationship to quadrature)
   A) Euler
   B) Mid-point
   C) 4th order Runge-Kutta Schemes
3) Example and Comparison of Schemes
4) Adaptive Stepping schemes and embedded RK
5) Intro to Matlabs ODE suite

Systems of ODE's (Initial value problems):

Many useful (or at least interesting) models of physical, biological, societal systems can be written as systems of ordinary differential equations (ODE's). If, in addition, the initial state is known, then all of these problems can be written as

\[ \frac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}) \quad \mathbf{u}(0) = \mathbf{u}_0 \]

where:
- \( \mathbf{u}(t) \) is a state vector
- \( \mathbf{f}(t, \mathbf{u}) \) is a vector-valued function that controls how \( \mathbf{u} \) changes with time
- \( \mathbf{u}(0) \) is the initial condition at time \( t=0 \)
Examples:
Simple Radioactive decay (1-nuclide)

\[ \frac{dC}{dt} = -\lambda C \]
\[ C(t) = C_0 e^{-\lambda t} \]

Radioactive decay Chains (n-nuclides)

\[ ^{238}\text{U} \rightarrow ^{230}\text{Th} \rightarrow ^{226}\text{Ra} \]

\[ t_{1/2}^{^{238}\text{U}} = 4\text{Gyr} \]
\[ t_{1/2}^{^{230}\text{Th}} = 75,000\text{ yr} \]
\[ t_{1/2}^{^{226}\text{Ra}} = 1600\text{ yr} \]
Examples:
Radioactive decay Chains (n-nuclides)

Examples:
Higher order ODE's (e.g. van der pol oscillator)

\[ y'' - \mu (1-y^2)y' + y = 0; \quad y(0)=y_0, \ y'(0)=v_0 \]
Examples:
Higher order ODE's (e.g. van der pol oscillator)

\( y_0 = 0.1, v_0 = 0 \)

Examples:
Particle tracking in a flow

Ocean model results for the Southern California coastal ocean (3 km resolution):
velocity field at \( \sigma = 26.6 \text{ km/m}^3 \) shows the meandering southward California Current, the nearshore northward Davison Current, and the cyclonic circulation within the Bight.

General form of dynamical systems
(all can be thought of as tracking states through a flow)

\[ \frac{du}{dt} = f(t,u) \quad u(0) = u_0 \]

Example: simple radioactive decay and direction sets

\[ \frac{dc}{dt} = -c \quad c(0) = 1 \]
\[ f(t,c) = c \]

\[ c(t) = e^{-t} \]
Basic Stepping Schemes: relationship to Quadrature

\[ \frac{dx}{dt} = f(t,x) \]
\[ x(t+h) = x(t) + h f(t,x) \]
\[ u_{n+1} = u_n + h f(t_n, u_n) + O(h^2) \]
\[ u_{n+1} - u_n = \int_{t_n}^{t_{n+1}} f(t,x) dt \]

Basic Stepping Schemes: Euler's method

\[ k_1 = h f(t_n, u_n) \]
\[ u_{n+1} = u_n + k_1 \]
\[ u_{n+1} = u_n + h f + E \]
\[ u(t+h) = u(t) + h \frac{du}{dt} + \frac{h^2}{2} \frac{d^2u}{dt^2} + O(h^3) \]

First order scheme

\[ C_{n+1} = (1 - \lambda h) C_n \]
\[ k_1 = (1 - \lambda h) C_0 \]
\[ C_k = e^{-\lambda t} C_0 \]
Stability:

\[ \frac{\partial C}{\partial t} = -\lambda C \]

Euler Scheme

\[ C_{n+1} = (1-\lambda h)C_n \]

Stability: \(|1-\lambda h| < 1\)

\[ C_k = (1-\lambda h)^k C_0 \]

Stability: \(h > \frac{1}{\lambda} < \frac{3}{\lambda}\)

Basic Stepping Schemes: Mid-point method

\[ k_1 = h f(t_n, C_n) \]

\[ k_2 = h f(t_n + \frac{h}{2}, C_n + k_1) \]

\[ C_{n+1} = C_n + k_2 + O(h^3) \]
Basic Stepping Schemes: 4th order Runge-Kutta Scheme

\[ u_{n+1} = u_n + \frac{k_1}{6} + \frac{(k_2 + k_3)}{3} + \frac{k_4}{6} + O(h^5) \]

Comparison of Errors and Accuracy:
Adaptive Time stepping:
Step doubling RK4

Relative truncation error

\[
\begin{align*}
\Delta_0 & \propto h_0^5 \\
\Delta_1 & \propto h_1^5 \\
h_1 &= h_0 \left( \frac{\Delta_1}{\Delta_0} \right)^{1/5} \\
\Delta_0 & \leq \max \left( \text{RelTol}\times h_{\text{max}}, \text{AbsTol} \times 10^{-8} \right)
\end{align*}
\]

Adaptive Time stepping:
Embedded Runge-Kutta Schemes and Matlab’s ODE45