PHYS 410: Computational Physics
Solving Ordinary Differential Equations (ODEs)

1. Introduction

- Numerical solution of ODEs is a huge subject that has been studied for many decades
- The state-of-the-art in packaged routines is thus very high, and for many applications it is certainly not necessary to code solvers one's self
- Will study a little of the theory underlying simple methods and will also discuss some techniques which are actually used in practice
- In our discussion of applications will generally rely on MATLAB built-in solvers which will be used more or less as black boxes
- In that context will emphasize techniques that can be used to assess reliability and accuracy of the computed results
- Innumerable applications in virtually every subfield of physics; we will focus in the first instance on problems in mechanics and related fields

1.1 Casting Systems of ODEs in First Order Form

- Can *always* reduce a system of ODEs to set of first order DEs by introducing appropriate new (auxiliary) variables.

Example 1

$$y''(x) + q(x)y'(x) = r(x) \qquad ' \equiv \frac{d}{dx} \tag{1}$$

- Introduce new variable $z(x) \equiv y'(x)$, then (1) becomes

$$\begin{aligned} y' &= z \\ z' &= r - qz \end{aligned}$$

Example 2

$$y''''(x) = f(x) \tag{2}$$

- Introduce new variables

$$\begin{aligned} y_1(x) &\equiv y'(x) \\ y_2(x) &\equiv y''(x) \\ y_3(x) &\equiv y'''(x) \end{aligned}$$

then (2) becomes

$$
\begin{aligned}
y' &= y_1 \\
y_1' &= y_2 \\
y_2' &= y_3 \\
y_3' &= f
\end{aligned}
$$

- Thus, the generic problem in ODEs is reduced to study of a set of N coupled, *first-order* DEs for the functions, $y_i, i = 1, 2, \ldots, N$

$$
y_i'(x) \equiv \frac{dy_i}{dx}(x) = f_i(x, y_1, y_2, \cdots, y_N) \qquad i = 1, 2, \ldots N \tag{3}
$$

  where the $f_i(\cdots)$ are *known functions* of x and y_i

- *Equivalent forms:* $\mathbf{y} \equiv (y_1, y_2, \cdots, y_N)$

$$
\mathbf{y}'(x) = \mathbf{f}(x, \mathbf{y})
$$
$$
\dot{\mathbf{y}}(t) = \mathbf{f}(t, \mathbf{y})
$$

1.2 Boundary / Initial Conditions

- ODE problem not completely specified by DEs themselves
- Nature of boundary conditions is crucial aspect of problem
- Generally, BCs are *algebraic* conditions on certain of the y_i in (3) that are to be satisfied at discrete specified points.
- Generally will need N conditions for N-th order system
- BCs divide ODE problems into 2 broad classes

1.2.1 Initial Value Problems

- All the y_i are given at some starting (initial) value, $t_{\min}$ and we wish to find the y_i at some final value, $t_{\max}$, or at some *set* of values

$$
t_n, \qquad t_{\min} \le t_n \le t_{\max} \qquad n = 1, 2, \cdots
$$

1.2.2 (Two-point) Boundary Value Problems

- BCs are specified at more than one value of x. Typically some will be specified at $x = x_{\min}$, the remainder at $x = x_{\max}$.

- We will begin with a discussion of some basic methods of solution that are most applicable to initial value problems

- We also note that the reduction of an arbitrary system of ODEs to a first order system is most relevant to initial value problems

2. Solution of ODEs (initial value problems): Basic Methods

2.1 Euler Methods

- Consider the basic ODE
$$y'(x) = f(x, y)$$
which is to be solved on some interval $[x_0, x]$ where $y(x_0)$ is given
- One approach: Taylor series
$$y(x) = y(x_0) + (x - x_0)y'(x_0) + \frac{(x - x_0)^2}{2!}y''(x_0) + \cdots$$
- Higher derivatives get messy:
$$\begin{aligned} y''(x) &= \frac{\partial}{\partial x}f(x,y) + \frac{dy}{dx}\frac{\partial}{\partial y}f(x,y) \\ &= \frac{\partial}{\partial x}f(x,y) + f(x,y)\frac{\partial}{\partial y}f(x,y) \end{aligned}$$
- For this and other reasons, Taylor series technique tends not to be used, but for our purposes is still useful for derivation of other schemes
- To second order we have
$$\begin{aligned} y(x) &= y_0 + (x - x_0)f(x_0, y_0) + \frac{(x - x_0)^2}{2!} \\ &\times \left[\frac{\partial f(x_0, y_0)}{\partial x} + f(x_0, y_0)\frac{\partial f(x_0, y_0)}{\partial y}\right] + O(x - x_0)^3 \end{aligned}$$
- Truncate the series at two terms:
$$y(x) \approx y(x_0) + (x - x_0)y'(x_0) = y(x_0) + (x - x_0)f(x_0, y_0)$$
- Define $x - x_0 =$ step size $= h$
- Gives us the *(forward) Euler method*
$$\boxed{y(x_0 + h) = y(x_0) + hf(x_0, y_0) = y_0 + hf_0}$$
- Or in terms of finite difference notation previously introduced
$$\boxed{y_{n+1} = y_n + hf_n}$$
- Basic algorithm for *any* ODE integrator. Take repeated steps, possibly adjusting step size as we will later see, until integration limit has been achieved.
- Forward Euler is only $O(h)$ accurate, useful only for pedagogy. Should essentially never be used in practice.
- Intuitively, could improve accuracy of method by using value of y' at midpoint of interval, rather than start.
- That is, want estimate of $f(x_0 + h/2, y(x_0 + h/2))$