Numerical Methods for Civil Engineers

Lecture Notes
CE 311K - McKinney
Introduction to Computer Methods
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Numerical Solution of Ordinary Differential Equations

Problems involving ordinary differential equations (ODEs) fall into two general categories:

(1) Initial value problems (IVPs), and

(2) Boundary value problems (BVPs).

Introduction

Initial value problems are those for which conditions are specified at only one value of the independent variable. These conditions are termed the *initial conditions*, whether or not they are specified at the point where the independent variable is actually equal to zero. A typical initial value problem might be of the form

$$a\frac{d^2x}{dt^2} + b\frac{dx}{dt} + cx = g(t)$$

with initial conditions

$$x(t_0) = x_0$$

$$\frac{dx}{dt}\bigg|_{t=0} = V_0$$

(a)

or

$$p \frac{dx}{dt} + qx = h(t)$$

with initial conditions
$$x(t_0) = x_0 \tag{b}$$

The variable which is being differentiated is called the dependent variable, x in this case, and the variable with respect to which the dependent variable is differentiated is called the independent variable, t in this case. When the problem involves one independent variable, the equation is called an *ordinary differential equation*. Differential equations are classified as to the highest order derivative appearing in them. In the case of Equation (a), the differential equation is of second order; Equation (b) is of first order. Equation (a) could describe the forced response of a simple harmonic oscillator with time. Since Equation (a) is a second-order differential equation, two conditions have been specified at $t = 0$.

Boundary value problems are those for which conditions are specified at two values of the independent variable. A typical boundary value problem might be of the form

$$a \frac{d^2 y}{dx^2} + b \frac{dy}{dx} + cy = g(y)$$

with boundary conditions
$$y(x_0) = y_0, \quad y(x_L) = y_L$$

This problem could describe the steady-state temperature distribution in a rod of length L with temperature $y(x_0) = y_0$ at $x = x_0$ and $y(x_L) = y_L$ at $x = x_L$. These are called the *boundary conditions*.

Initial Value Problems

Any initial value problem can be represented by a set of one or more coupled first-order ordinary differential equations, each with an initial condition. For example, Equation (a) can be restated by making the substitution

$$z = \frac{dx}{dt}$$

The differential equation is then written as

$$a\frac{dz}{dt} + bz + cx = g(t)$$

With some rearrangement, the problem can now be written as

$$\frac{dx}{dt} = z$$
$$\frac{dz}{dt} = \frac{g(t)}{a} - \frac{b}{a}z - \frac{c}{a}x$$

with initial conditions (one for each equation in the set):

$$x(t_0) = x_0$$
$$z(t_0) = V_0$$

Since any initial value problem can be reduced to a set of first-order ordinary differential equations, we shall concentrate on numerical methods for the solution of first-order differential equations Thus, we consider an initial value problem of the form

$$\frac{dx}{dt} = f(x,t)$$

with initial conditions
$$x(t_0) = x_0$$

Suppose that we know the solution to this equation over the interval $0 \le t \le t_i$. The next step is to advance the solution to $t_{i+1} = t_i + \Delta t$ by extrapolation. We will consider techniques of the *Runge-Kutta* type, where the desired solution x_{i+1} is obtained in terms of x_i, $f(x_i,t_i)$, and $f(x,t)$ evaluated for various estimated values of x between t_i and t_{i+1}. The first such technique is Euler's method and is discussed in the next section.
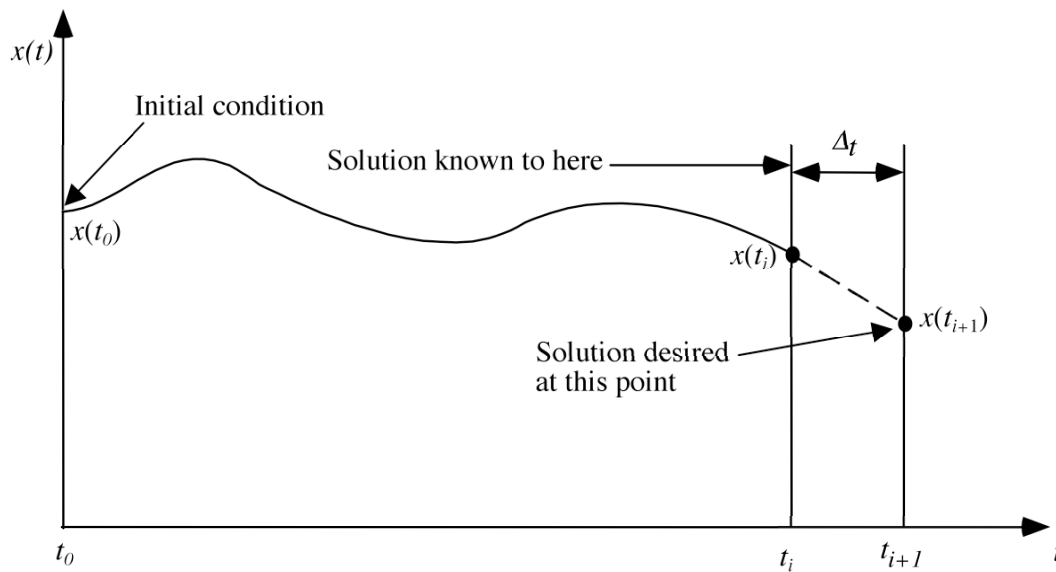

Figure 3. Initial value problem intermediate solution. Solution is known to t_i solution is desired at t_{i+1}.

Euler's Method

Consider the first-order initial value problem

$$\frac{dx}{dt} = f(x,t)$$

with initial conditions

$$x(t_0) = x_0$$

One solution method is to replace the derivative $\frac{dx}{dt}$ by a simple forward finite difference

approximation

$$\frac{dx}{dt} \approx \frac{x_{i+1} - x_i}{\Delta t} = f(x_i, t_i)$$

Solving for x_{i+1} yields

$$x_{i+1} = x_i + \Delta t f(x_i, t_i)$$

Given an initial condition, $x(t_0) = x_0$, it is possible to proceed forward in time from t_0, to obtain a value of x at each new value of t. The slope at the beginning of an interval, $f(x_i, t_i)$, is taken as an approximation of the average slope over the whole interval as shown in Figure 2. The new value of x, at x_{i+1}, is predicted using the slope at the old point, x_i, to extrapolate linearly over the step size Δt.
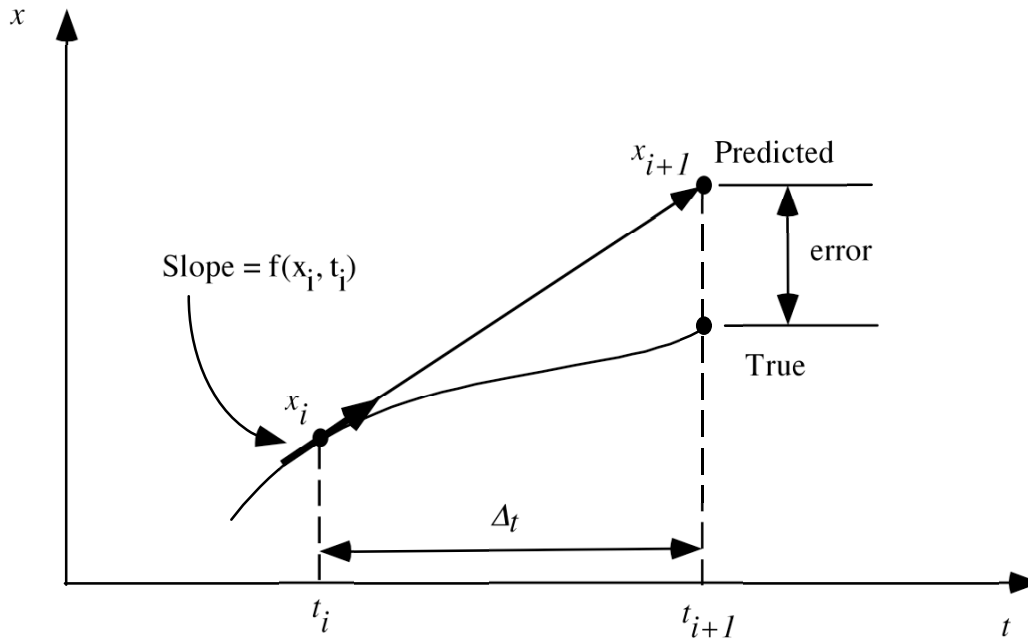
Figure 4. Illustration of Euler's method.

Example: Use Euler's method to find a numerical approximation for *x(t)* where

$$\frac{dx}{dt} = f(x,t) = -2t^3 + 12t^2 - 20t + 8.5$$

$$\text{Initial conditions}: \quad x(0) = 1$$

from $t = 0$ to $t = 4$ using a step size of $\Delta t = 0.5$.

By simple integration, the exact solution to this equation is

$$x(t) = -0.5t^4 + 4t^3 - 10t^2 + 8.5t + 1$$

The Euler formula for this equation is

$$x_{i+1} = x_i + \Delta t f(x,t) = x_i + \Delta t \left(2t_i^3 + 12t_i^2 - 20t_i + 8.5\right)$$

Starting at $t = 0$ ($i = 0$) and using $\Delta t = 0.5$, we find x at $t = 0.5$

$$
\begin{aligned}
x_1 &= x_0 + \Delta t \left(2t_i^3 + 12t_i^2 - 20t_i + 8.5 \right) \\
&= 1.0 + (0.5) \left[2(0)^3 + 12(0)^2 - 20(0) + 8.5 \right] \\
&= 5.25
\end{aligned}
$$

The exact solution at this point is

$$
\begin{aligned}
x_1 &= -0.5(0.5)^4 + 4(0.5)^3 - 10(0.5)^2 + 8.5(0.5) + 1 \\
&= -0.03125 + 0.5 - 2.5 + 4.25 + 1 \\
&= 3.21875
\end{aligned}
$$

Next, we can advance the solution from $t = 0.5$ ($i = 1$) and find x at $t = 1.0$, using the value we just found as an initial condition

$$
\begin{aligned}
x_2 &= x_1 + \Delta t \left(2t_1^3 + 12t_1^2 - 20t_1 + 8.5 \right) \\
&= 5.25 + (0.5) \left[2(0.5)^3 + 12(0.5)^2 - 20(0.5) + 8.5 \right] \\
&= 5.875
\end{aligned}
$$

The exact solution at this point is

$$
\begin{aligned}
x_2 &= -0.5(1)^4 + 4(1)^3 - 10(1)^2 + 8.5(1) + 1 \\
&= -0.5 + 4 - 10 + 8.5 + 1 \\
&= 3
\end{aligned}
$$

The calculations for several steps are plotted in Figure 5. A C program for computing the answer to this problem using Euler's method is presented in Figure 6. The error in the calculations is illustrated in Figure 7. The error in these calculations stems from two factors: (1) the use of finite precision arithmetic in the computer (roundoff error); and (2) the truncation of the Taylor series in the finite difference approximation of the first derivative in Euler's method (truncation error).

Table. Results of Euler Method Calculations.

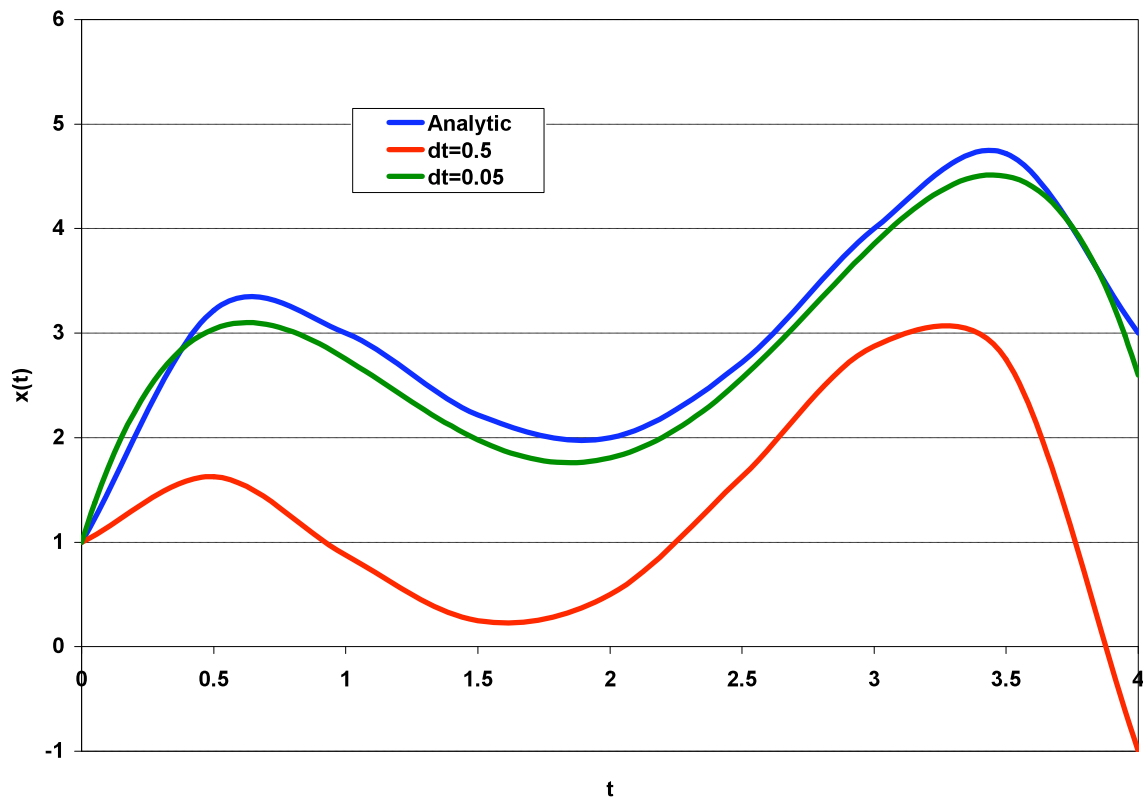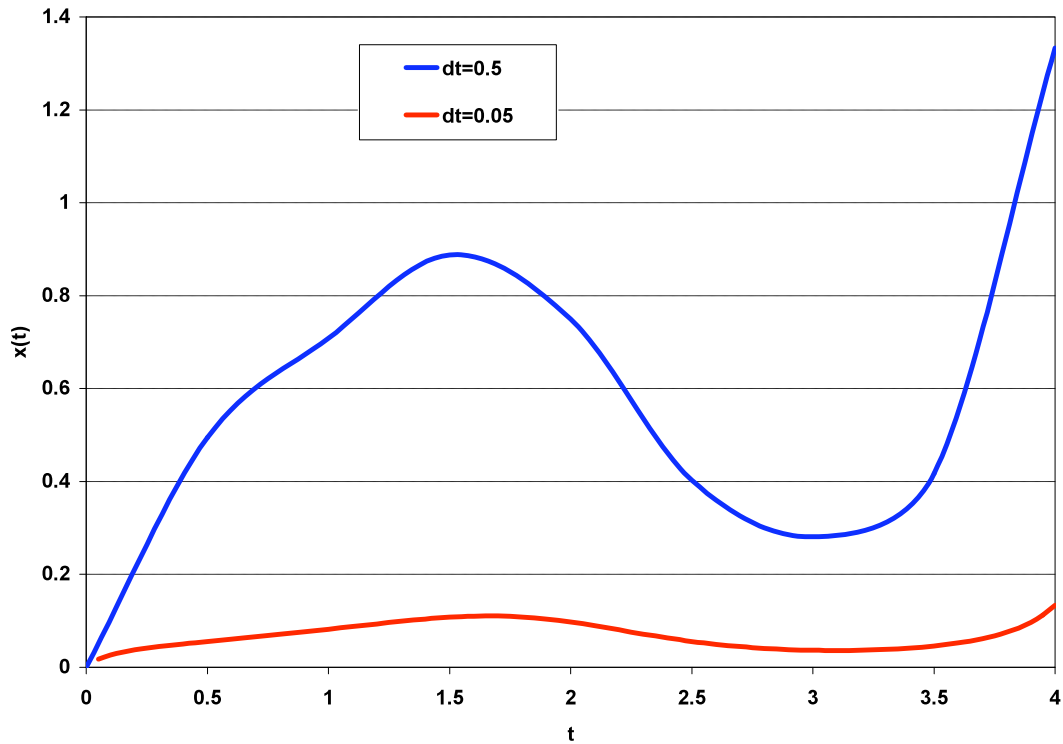|	Analytic		dt=0.50	Error
t	x	t	x	e
0.00	1.00	0.00	1.00	0.00
0.50	3.22	0.50	1.63	0.50
1.00	3.00	1.00	0.88	0.71
1.50	2.22	1.50	0.25	0.89
2.00	2.00	2.00	0.50	0.75
2.50	2.72	2.50	1.63	0.40
3.00	4.00	3.00	2.88	0.28
3.50	4.72	3.50	2.75	0.42
4.00	3.00	4.00	-1.00	1.33

Figure 5. Euler method example

Figure 6. Error in Euler method example.

Runge Kutta Formulas

Among the most widely used formulas for numerically solving ordinary differential equations are the Runge-Kutta techniques. High-order accuracy can be obtained by evaluating the righ-hand-side function at selected points within the interval rather than at just the end points of the interval. Consider again the first-order initial value problem

$$\frac{dx}{dt} = f(x,t)$$

with initial conditions
$$x(t_0) = x_0$$

In the development of the Runge Kutta formulas, we assume that the estimate of the solution $x(t)$ is

$$x_{n+1} = x_n + \Delta x$$
$$= x_n + \sum_{i=1}^{p} w_i k_i$$

where

$$k_i = \Delta t f(x_n + \sum_{j=1}^{i-1} a_{ij} k_j, t_n + c_i \Delta t), \qquad c_1 = 0$$

That is, the increment Δx is a weighted sum of function evaluations at points within the interval $[x_i, x_{i+1}]$. If we cut this estimate off after the first term, we have

$$x_{n+1} = x_n + \Delta x$$
$$= x_n + w_1 k_1$$

where

$$k_1 = \Delta t f(x_n, t_n)$$

Now, if we set $w_1 = 1$, the result is Euler's method (first-order Runge Kutta)

$$x_{n+1} = x_n + \Delta t f(x_n, t_n)$$

If, instead, we cut the estimate off after the second term, we have

$$x_{n+1} = x_n + \Delta x$$
$$= x_n + w_1 k_1 + w_2 k_2$$

where

$$k_1 = \Delta t f(x_n, t_n)$$
$$k_2 = \Delta t f(x_n + a_{21}k_1, t_n + c_2\Delta t)$$

Now, if we set $w_1 = w_2 = \frac{1}{2}$ and $c_2 = a_{21} = 1$, the result is the modified Euler's method (second-order Runge Kutta)

$$x_{n+1} = x_n + \frac{\Delta t}{2}\left[f(x_n, t_n) + f(x_n + \Delta t f(x_n, t_n), t_n + \Delta t)\right]$$

This method is implemented as

$$x_{i+1}^* = x_i + \Delta t f(x_i, t_i)$$
$$x_{i+1} = x_i + \frac{\Delta t}{2}\left[f(x_i, t_i) + f(x_{i+1}^*, t_{i+1})\right]$$
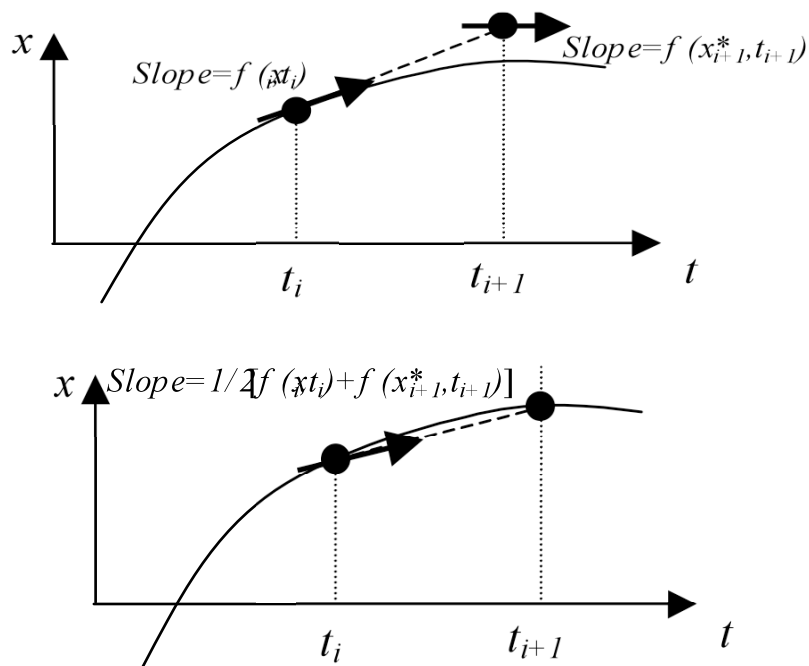

Figure 7. Modified Euler method.

The most widely used Runge-Kutta method is the fourth-order method, where we cut the estimate off after the fourth term

$$x_{n+1} = x_n + \Delta x$$
$$= x_n + w_1 k_1 + w_2 k_2 + w_3 k_3 + w_4 k_4$$

where

$$k_1 = \Delta t f(x_n, t_n)$$
$$k_2 = \Delta t f(x_n + a_{21}k_1, t_n + c_2\Delta t)$$
$$k_3 = \Delta t f(x_n + a_{31}k_1 + a_{32}k_2, t_n + c_3\Delta t)$$
$$k_4 = \Delta t f(x_n + a_{41}k_1 + a_{42}k_2 + a_{43}k_3, t_n + c_4\Delta t)$$

and

$$w_1 = w_4 = 1/6,$$
$$w_2 = w_3 = 1/3 \text{ and}$$
$$c_2 = c_3 = a_{21} = a_{32} = 1/2, c_4 = 1, \text{ and}$$
$$a_{31} = a_{41} = a_{42} = 0$$

The computational formula for the Fourth-order Runge-Kutta method is

$$x_{n+1} = x_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}$$

where

$$k_1 = \Delta t f(x_n, t_n)$$
$$k_2 = \Delta t f(x_n + \frac{k_1}{2}, t_n + \frac{\Delta t}{2})$$
$$k_3 = \Delta t f(x_n + \frac{k_2}{2}, t_n + \frac{\Delta t}{2})$$
$$k_4 = \Delta t f(x_n + k_3, t_n + \Delta t)$$

Example:

$$\frac{dx}{dt} = -(x)^2$$

with initial conditions
$$x(t = 1) = 1$$

Analytical solution:

$$x(t) = \frac{1}{t}$$

Euler method:

$$x_{i+1} = x_i - \Delta t x_i^2$$

Modified Euler (second-order Runge-Kutta) method:

$$x_{i+1}^* = x_i - \Delta t x_i^2$$

$$x_{i+1} = x_i - \frac{\Delta t}{2}\left[x_i^2 + x_{i+1}^{*2} \right]$$

Fourth-order Runge-Kutta method:

$$x_{n+1} = x_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}$$

where

$$k_1 = \Delta t f(x_i, t_i) = -\Delta t(x_i^2)$$

$$k_2 = \Delta t f(x_i + \frac{k_1}{2}, t_i + \frac{\Delta t}{2}) = \Delta t \left(x_i + \frac{k_1}{2} \right)^2$$

$$k_3 = \Delta t f(x_i + \frac{k_2}{2}, t_i + \frac{\Delta t}{2}) = \Delta t \left(x_i + \frac{k_2}{2} \right)^2$$

$$k_4 = \Delta t f(x_i + k_3, t_i + \Delta t) = \Delta t \left(x_i + k_3 \right)^2$$
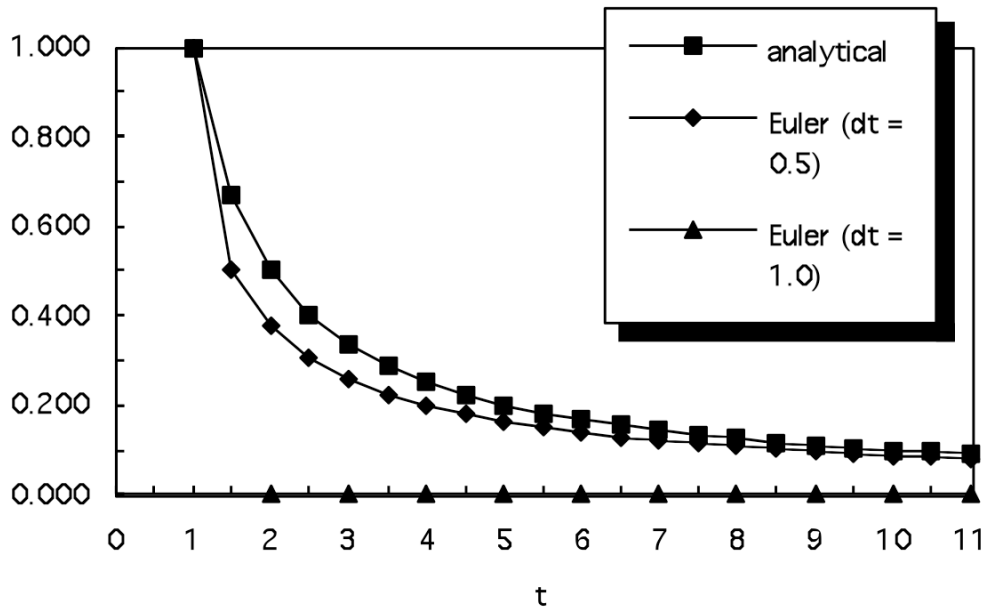
Figure 8. Analytical solution versus Euler method approximation for two levels of discretization ($\Delta t = 0.5$ and $\Delta t = 1.0$).

Table 1. Analytical solution versus Euler method approximation for three levels of discretization ($\Delta t = 0.5$, $\Delta t = 1.0$, and $\Delta t = 2.0$).

t	analytical	Euler ($\Delta t = 0.5$)	Euler ($\Delta t = 1.0$)	Euler ($\Delta t = 2.0$)
1	1.000	1.000	1.000	1.000
1.5	0.667	0.500		
2	0.500	0.375	0.000	
2.5	0.400	0.305		
3	0.333	0.258	0.000	-1.000
3.5	0.286	0.225		
4	0.250	0.200	0.000	
4.5	0.222	0.180		
5	0.200	0.164	0.000	-3.000
5.5	0.182	0.150		
6	0.167	0.139	0.000	
6.5	0.154	0.129		
7	0.143	0.121	0.000	-21.000
7.5	0.133	0.114		
8	0.125	0.107	0.000	
8.5	0.118	0.101		
9	0.111	0.096	0.000	-903.000
9.5	0.105	0.092		
10	0.100	0.087	0.000	
10.5	0.095	0.084		
11	0.091	0.080	0.000	-1.63E+06

Table 2. Modified Euler method (2-nd order Runge Kutta) approximation ($\Delta t = 0.5$).

t	x_i^* ($\Delta t = 0.5$)	Modified Euler
1	1	1.000
1.5	0.500	0.688
2	0.451	0.518
2.5	0.384	0.414
3	0.329	0.344
3.5	0.285	0.294
4	0.251	0.257
4.5	0.224	0.228
5	0.202	0.205
5.5	0.184	0.186
6	0.169	0.170
6.5	0.156	0.157
7	0.145	0.145
7.5	0.135	0.136
8	0.126	0.127
8.5	0.119	0.119
9	0.112	0.113
9.5	0.106	0.107
10	0.101	0.101
10.5	0.096	0.096
11	0.092	0.092

Table 3. Fourth order Runge Kutta approximation ($\Delta t = 0.5$).

| t	K_1	K_2	K_3	K_4	x_{i+1}
1					1.000
1.5	-0.500	-0.281	-0.369	-0.199	0.667
2	-0.222	-0.154	-0.174	-0.121	0.500
2.5	-0.125	-0.096	-0.102	-0.079	0.400
3	-0.080	-0.065	-0.068	-0.055	0.333
3.5	-0.056	-0.047	-0.048	-0.041	0.286
4	-0.041	-0.035	-0.036	-0.031	0.250
4.5	-0.031	-0.027	-0.028	-0.025	0.222
5	-0.025	-0.022	-0.022	-0.020	0.200
5.5	-0.020	-0.018	-0.018	-0.017	0.182
6	-0.017	-0.015	-0.015	-0.014	0.167
6.5	-0.014	-0.013	-0.013	-0.012	0.154
7	-0.012	-0.011	-0.011	-0.010	0.143
7.5	-0.010	-0.009	-0.010	-0.009	0.133
8	-0.009	-0.008	-0.008	-0.008	0.125
8.5	-0.008	-0.007	-0.007	-0.007	0.118
9	-0.007	-0.007	-0.007	-0.006	0.111
9.5	-0.006	-0.006	-0.006	-0.006	0.105
10	-0.006	-0.005	-0.005	-0.005	0.100
10.5	-0.005	-0.005	-0.005	-0.005	0.095
11	-0.005	-0.004	-0.004	-0.004	0.091
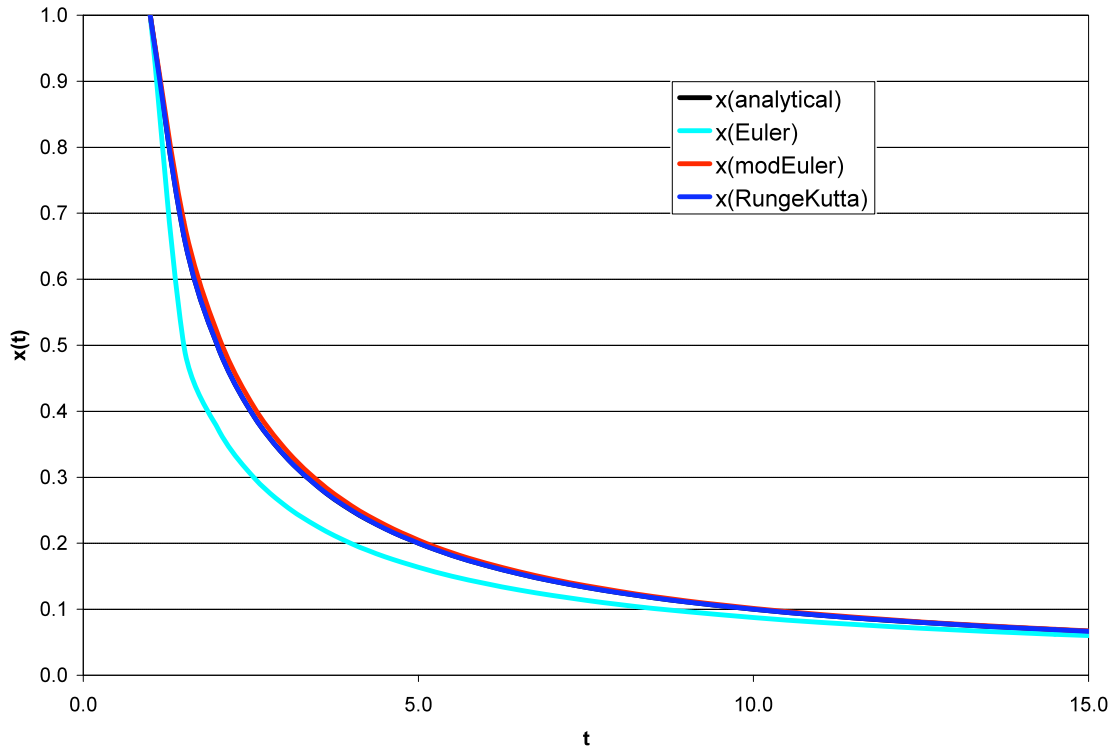
Figure 9. Comparison of analytical, Euler (1-st order RK), modified Euler (2-nd order RK), and 4-th order Runge Kutta approximation ($\Delta t = 0.5$).

Table 4. Comparison of analytical, Euler (1-st order RK), modified Euler (2-nd order RK), and 4-th order Runge Kutta approximation ($\Delta t = 0.5$).

t	analytical	Euler	Mod. Euler	4-th Order RK
1	1.000	1.000	1.000	1.000
1.5	0.667	0.500	0.688	0.667
2	0.500	0.375	0.518	0.500
2.5	0.400	0.305	0.414	0.400
3	0.333	0.258	0.344	0.333
3.5	0.286	0.225	0.294	0.286
4	0.250	0.200	0.257	0.250
4.5	0.222	0.180	0.228	0.222
5	0.200	0.164	0.205	0.200
5.5	0.182	0.150	0.186	0.182
6	0.167	0.139	0.170	0.167
6.5	0.154	0.129	0.157	0.154
7	0.143	0.121	0.145	0.143
7.5	0.133	0.114	0.136	0.133
8	0.125	0.107	0.127	0.125
8.5	0.118	0.101	0.119	0.118
9	0.111	0.096	0.113	0.111
9.5	0.105	0.092	0.107	0.105
10	0.100	0.087	0.101	0.100

| 10.5 | 0.095 | 0.084 | 0.096 | 0.095 |
| 11 | 0.091 | 0.080 | 0.092 | 0.091 |

Boundary Value Problems

Recall that boundary value problems are those for which conditions are specified at two values
of the independent variable. A typical boundary value problem might be of the form

$$\frac{d^2x}{dt^2} + a(x,t)\frac{dx}{dt} + b(x,t) = 0$$

with boundary conditions

(1) $x(t = 0) = x_0, \quad x(t = L) = x_L,$ or

(2) $\left.\frac{dx}{dt}\right|_{t=0} = V_0, \quad x(t = L) = x_L,$ or

(3) $x(t = 0) = x_0, \quad \left.\frac{dx}{dt}\right|_{t=L} = V_L$

Two methods are commonly used to solve boundary value problems: (1) the shooting method,
and (2) finite-difference methods.

Section under construction

Example: Flow in a leaky confined aquifer

Consider the steady flow from left to right in the semi-confined aquifer shown in Figure 2. The
aquitard is leaky. Determine the head in the aquifer.

Figure. Flow in a leaky-confined aquifer.

The governing equation for flow in the aquifer can be written as

$$\nabla \cdot K\nabla h + \frac{K'}{b'}(h_0 - h) = 0$$

If the aquifer is considered to be homogeneous and isotropic, we can write this equation as

$$\nabla^2 h + \frac{h_0 - h}{\lambda^2} = 0$$

where $\lambda^2 = bKb'/K'$. Now for one-dimensional flow, we have

$$\lambda^2 \frac{d^2 h}{dx^2} - h = h_0$$

a second-order ordinary differential eqation with constant coefficients which has the solution

$$h(x) = h_0 - \frac{(h_A - h_0)\sinh(\frac{L-x}{\lambda}) + (h_B - h_0)\sinh(\frac{x}{\lambda})}{\sinh(\frac{L}{\lambda})}$$

Consider the values $L = 1000$ m, $H_A = 100$ m, $H_b = 80$ m, $K = 20$ m/day (clean sand), $B = 50$ m, $B' = 2$ m, $K' = 0.10$ m/day (silt), n = 0.35. The head distributions for the values of h_0 are shown in Table 1 and plotted in Figure 3.

Figure. Semi-confined aquifer head values for various overlying aquifer head levels.

Table. Semi-confined aquifer head values for various overlying aquifer head levels.

X	$h_0=110$	$h_0=105$	$h_0=100$	$h_0=95$	$h_0=90$
0.00	100.00	100.00	100.00	100.00	100.00
100.00	105.03	102.50	99.97	97.45	94.92
200.00	107.47	103.70	99.93	96.17	92.40
300.00	108.59	104.23	99.86	95.49	91.13
400.00	108.98	104.35	99.71	95.08	90.45
500.00	108.84	104.13	99.42	94.71	90.00
600.00	108.08	103.45	98.82	94.19	89.55
700.00	106.33	101.97	97.60	93.24	88.87
800.00	102.67	98.91	95.14	91.37	87.60
900.00	95.19	92.67	90.14	87.61	85.08
1000.00	80.00	80.00	80.00	80.00	80.00

Systems of Ordinary Differential Equations

Consider the system of ordinary differential equations

$$\frac{dy_1}{dx} = f_1(x, y_1, y_2, ..., y_n)$$
$$\frac{dy_2}{dx} = f_2(x, y_1, y_2, ..., y_n)$$
$$\vdots$$
$$\frac{dy_n}{dx} = f_n(x, y_1, y_2, ..., y_n)$$

Example: Find a solution to the following system of two ODE's using fourth-order Runge-Kutta on the interval $0 \le x \le 2$, $\Delta x = 0.5$

$$\frac{dy_1}{dx} = -0.5y_1$$

$$\frac{dy_2}{dx} = 4 - 0.3y_2 - 0.1y_1$$

with initial conditions

$$y_1 = 4 \quad @\, x = 0$$
$$y_2 = 6 \quad @\, x = 0$$

The formulas for fourth-order Runge-Kutta method are

$$y_{1,i+1} = y_{1,i} + \frac{1}{6}\left(K_{1,1} + 2K_{2,1} + 2K_{3,1} + K_{4,1}\right)\Delta x$$

$$y_{2,i+1} = y_{2,i} + \frac{1}{6}\left(K_{1,2} + 2K_{2,2} + 2K_{3,2} + K_{4,2}\right)\Delta x$$

where

$$K_{1,1} = f_1(x_i, y_{1i}, y_{2i})$$

$$K_{2,1} = f_1\left(x_i + \frac{\Delta x}{2}, y_{1i} + \frac{\Delta x}{2}K_{1,1}, y_{2i} + \frac{\Delta x}{2}K_{1,1}\right)$$

$$K_{3,1} = f_1\left(x_i + \frac{\Delta x}{2}, y_{1i} + \frac{\Delta x}{2}K_{2,1}, y_{2i} + \frac{\Delta x}{2}K_{2,1}\right)$$

$$K_{4,1} = f_1\left(x_i + \Delta x, y_{1i} + \Delta x K_{3,1}, y_{2i} + \Delta x K_{3,1}\right)$$

and

$$K_{1,2} = f_2(x_i, y_{1i}, y_{2i})$$

$$K_{2,2} = f_2\left(x_i + \frac{\Delta x}{2}, y_{1i} + \frac{\Delta x}{2}K_{1,2}, y_{2i} + \frac{\Delta x}{2}K_{1,2}\right)$$

$$K_{3,2} = f_2\left(x_i + \frac{\Delta x}{2}, y_{1i} + \frac{\Delta x}{2}K_{2,2}, y_{2i} + \frac{\Delta x}{2}K_{2,2}\right)$$

$$K_{4,2} = f_2\left(x_i + \Delta x, y_{1i} + \Delta x K_{3,2}, y_{2i} + \Delta x K_{3,2}\right)$$

For the example problem:

1) Compute some *K* values:

$$K_{1,1} = f_1(0,4,6) = -0.5(4) = -2$$

$$K_{1,2} = f_2(0,4,6) = 4 - 0.3(6) - 0.1(4) = 1.8$$

2) Compute some intermediate y values

$$y_1^* = y_{1,i} + \frac{\Delta x}{2} K_{1,1} = 4 + 0.5(0.5)(-2) = 3.5$$

$$y_2^* = y_{2,i} + \frac{\Delta x}{2} K_{1,2} = 6 + 0.5(0.5)(1.8) = 6.45$$

and some K values

$$K_{2,1} = f_1(0.25,3.5,6.45) = -0.5(3.5) = -1.75$$

$$K_{2,2} = f_2(0.25,3.5,6.45) = 4 - 0.3(6.45) - 0.1(3.5) = 1.715$$

3) Compute some more intermediate y values

$$y_1^{**} = y_{1,i} + \frac{\Delta x}{2} K_{2,1} = 4 + 0.5(-1.75) = 3.563$$

$$y_2^{**} = y_{2,i} + \frac{\Delta x}{2} K_{2,2} = 6 + 0.5(1.715) = 6.43$$

and some K values

$$K_{3,1} = f_1(0.25,3.563,6.43) = -1.78125$$

$$K_{3,2} = f_2(0.25,3.563,6.43) = 1.715125$$

4) Compute some more intermediate y values

$$y_1^{***} = y_{1,i} + \Delta x K_{3,1} = 4 + 0.5(-1.78125) = 3.1094$$

$$y_2^{***} = y_{2,i} + \Delta x K_{3,2} = 6 + 0.5(1.715125) = 6.8576$$

and some K values

$$K_{4,1} = f_1(0.25,3.1094,6.8576) = -1.5547$$

$$K_{4,2} = f_2(0.25,3.1094,6.8576) = 1.6318$$

5) Now, compute the next y values

$$y_{1,i+1} = 4 + \frac{1}{6}\left[-2 + 2(-1.75) + 2(-1.78125) - 1.5547\right] * (0.5)$$
$$= 3.1152$$

$$y_{2,i+1} = 6 + \frac{1}{6}\left[1.8 + 2(1.715) + 2(1.715) + 1.63179\right] * (0.5)$$
$$= 6.857$$

Repeat steps (1) - (5) for $i = 1,2,3,4$.

Example: Predator - Prey models (Ricklefs, p. 536)

In an ecosystem, the size (number) of the prey population is H and the rate of growth of the prey population ($\frac{dH}{dt}$) is comprised of two components:

1) Unrestricted reproductive rate (growth rate) of prey population $= g_1H$, where g_1 is the growth rate of an individual in the population.

2) Removal of prey from the population by predators (death rate). This is assumed to be proportional to the product of the prey and predator population sizes (PH, this term is proportional to the probability of an encounter between predator and prey) times a coefficient of predation d_1.

Thus, the overall increase in the size of the prey population is given by

$$\frac{dH}{dt} = g_1H - d_1PH$$

The growth rate of the predator population is proportional to the number of prey that the predator succeeds in capturing (d_1PH) minus the death rate (d_2) times the number of predators (P)

$$\frac{dP}{dt} = g_2 PH - d_2 P$$

where $g_2 = ad_1$, and a is the efficiency with which predators convert food (prey) into offspring.

When the predator and prey populations are in equilibrium

$$\frac{dH}{dt} = 0, \qquad g_1 H - d_1 PH = 0, \qquad P* = \frac{g_1}{d_1}$$

where P* is the greatest number of predators that the prey population can sustain, and

$$\frac{dP}{dt} = 0, \qquad g_2 PH - d_2 P = 0, \qquad H* = \frac{d_2}{g_2}$$

where H* is the minimum level of prey population required to sustain the predators.

Example: (Chapra and Canale, prob. 22.20)

If $P(0) = 5, H(0) = 20, g_1 = 1, g_2 = 0.02, d_1 = 0.1, d_2 = 0.5$, compute $P(t)$ and $H(t)$ from $t = 0$ to 10 using the fourth-order Runge-Kutta technique and $\Delta t = 0.5$.

Reactor Mass Balance

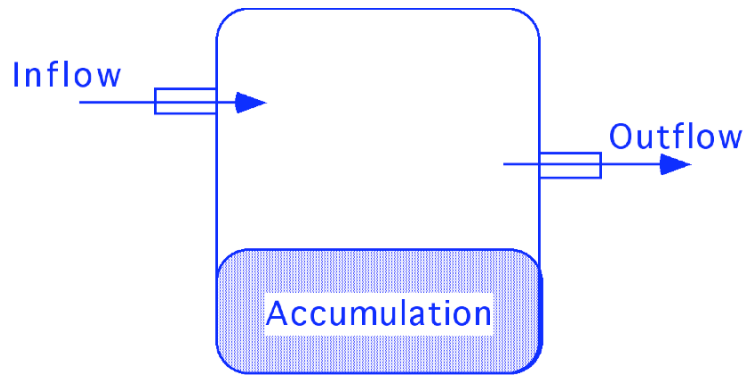Consider the conservation of mass in a fully mixed reactor vessel as shown in the following Figure.

Figure 10. Conceptual diagram of a reactor vessel with 1 inlet and 1 outlet.

Conservation of mass is a mass balance accounting of the material passing in or out of the reactor vessel, where

Rate of Mass Input - Rate of Mass Output = Change in Mass Storage (Accumulation)

At steady-state, we have

Change in Mass Storage (Accumulation) = 0

or

Rate of Mass Input = Rate of Mass Output

$$\sum_{inlets} Q_i c_i \;=\; \sum_{outlets} Q_o c_o$$

However, if steady-state conditions do not exist in the system, then we must consider the time rate of accumulation of the substance in the reactor

$$Accumulation = \frac{\Delta M}{\Delta t} \;=\; \frac{\Delta(cV)}{\Delta t} \;=\; V\frac{\Delta c}{\Delta t}$$

where

      M is the mass of chemical in the reactor, and

V is the (constant) volume of the reactor

So that

$$V\frac{dc}{dt} = \sum_{inlets} Q_i c_i - \sum_{outlets} Q_o c_o$$

For example, if the vessel has is a single inlet and a single outlet, then

$$V\frac{dc}{dt} = Q_i c_i - Qc$$

If $c = c_0$ @ $t = 0$, then the solution of this ODE is

$$c(t) = c_{IN}(1 - e^{-\frac{Q}{V}t}) + c_0 e^{-\frac{Q}{V}t}$$

If $c_{IN} = 50$ mg/m³, $Q = 5$ m³/min, $V = 100$ m³, and $c_0 = 10$ mg/m³, we have

$$c(t) = 50(1 - e^{-0.05t}) + 10e^{-0.05t}$$

Euler's method can be used to approximate the solution to the ODE.

$$\frac{c_{i+1} - c_i}{\Delta t} = \frac{Q_{IN}}{V}c_{IN} - \frac{Q_o}{V}c_i$$

or

$$c_{i+1} = c_i + \Delta t(\frac{Q_{IN}}{V}c_{IN} - \frac{Q_o}{V}c_i)$$

Now, plugging in the numerical values, we have

$$c_{i+1} = c_i + \Delta t(\frac{Q_{IN}}{V}c_{IN} - \frac{Q_o}{V}c_i)$$

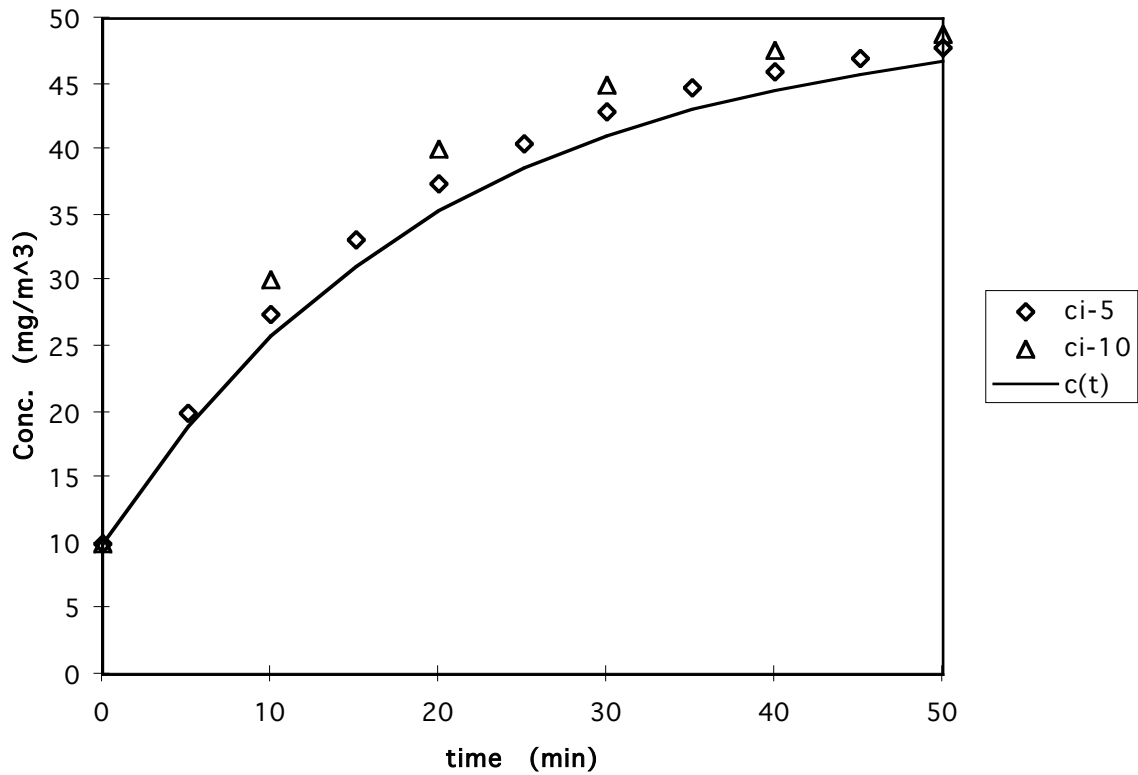Question: What would the formulas for the modified Euler method look like?

Figure 11. Comparison of analytical solution and Euler approximation.

System of Coupled Reactors

Consider the 5 interconnected reactors shown in the Figure. We can write 5 simultaneous mass-balance equations, one for each reactor,

$$V_1 \frac{dc_1}{dt} = Q_{01}c_{01} + Q_{31}c_3 - Q_{12}c_1 - Q_{15}c_1$$

$$V_2 \frac{dc_2}{dt} = Q_{12}c_1 - Q_{25}c_2 - Q_{24}c_2 - Q_{23}c_2$$

$$V_3 \frac{dc_3}{dt} = Q_{03}c_{03} + Q_{23}c_2 - Q_{31}c_3 - Q_{34}c_3$$

$$V_4 \frac{dc_4}{dt} = Q_{24}c_2 + Q_{54}c_5 + Q_{34}c_3 - Q_{44}c_4$$

$$V_5 \frac{dc_5}{dt} = Q_{15}c_1 + Q_{25}c_2 - Q_{55}c_5 - Q_{54}c_5$$

Now we must solve a system of ODE's instead of a single ODE. We can still apply the Euler method to this system.

$$c_{1,i+1} = c_{1,i} + \Delta t \frac{50 - 6c_{1,i} + c_{3,i}}{50}$$

$$c_{2,i+1} = c_{2,i} + \Delta t \frac{3c_{1,i} - 3c_{2,i}}{20}$$

$$c_{3,i+1} = c_{3,i} + \Delta t \frac{160 + c_{2,i} - 9c_{3,i}}{40}$$

$$c_{4,i+1} = c_{4,i} + \Delta t \frac{c_{2,i} + 8c_{3,i} - 11c_{4,i} + 2c_{5,i}}{80}$$

$$c_{5,i+1} = c_{5,i} + \Delta t \frac{3c_{1,i} + c_{2,i} - 4c_{5,i}}{100}$$

Which may be written in a matrix-vector notation as

$$
\begin{bmatrix} c_{1,i+1} \\ c_{2,i+1} \\ c_{3,i+1} \\ c_{4,i+1} \\ c_{5,i+1} \end{bmatrix}
=
\begin{bmatrix} c_{1,i} \\ c_{2,i} \\ c_{3,i} \\ c_{4,i} \\ c_{5,i} \end{bmatrix}
+ \Delta t
\begin{bmatrix}
-6/50 & & 1/50 & & \\
3/20 & -3/20 & & & \\
& 1/40 & -9/40 & & \\
& 1/80 & 8/80 & -11/80 & 2/80 \\
3/100 & 1/100 & & & -4/100
\end{bmatrix}
\begin{bmatrix} c_{1,i} \\ c_{2,i} \\ c_{3,i} \\ c_{4,i} \\ c_{5,i} \end{bmatrix}
+ \Delta t
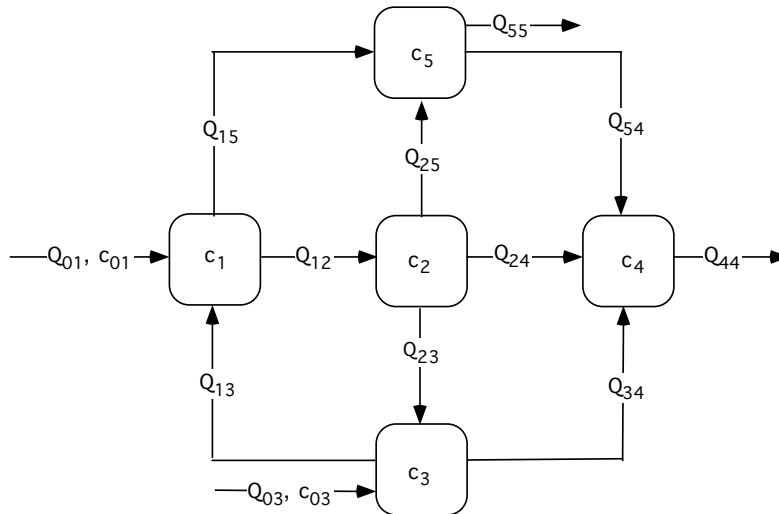\begin{bmatrix} 1 \\ 0 \\ 4 \\ 0 \\ 0 \end{bmatrix}
$$

Figure 12. System of 5 interconnected reactors.

Exercises

1. Solve the following initial value problem analytically over the interval from $x = 0$ to 2:

$$\frac{dy}{dx} = yx^2 - 1.2y$$

where $y(0) = 1$. Plot the solution.

2. Use Euler's method with h = 0.5 and 0.25 to solve Problem 1. Plot the results on the same graph to visually compare the accuracy of the two step sizes.

3. Use the Modified Euler method with h = 0.5 and 0.25 to solve the following initial value problem analytically over the interval from $x = 0$ to 2:

$$\frac{dy}{dx} = yx^2 - 1.2y$$

where $y(0) = 1$. Plot the solution.

4. Use the 4-th Order Runge – Kutta method with h = 0.25 to solve

$$\frac{dy}{dx} = yx^2 - 1.2y$$

where $y(0) = 1$. Plot the solution.

5. (a) What are the advantages and disadvantages of using the Euler method to solve an Ordinary Differential Equation rather than using a 4-th Order Runge-Kutta method? (b) Solve the following Ordinary Differential Equation using the Euler method from $t = 0.0$ to 1.0 with $\Delta t = 0.2$.

$$\frac{dy}{dt} = e^{-t} + y \qquad y(t) = 0.0 \ \ at \ \ t_0 = 0$$

6. Use the Euler method and a step size of $\Delta t = 0.25$, solve the initial value problem on the interval $t = [0, 1]$

$$\frac{dx}{dt} = (1 + t)\sqrt{x} \qquad \text{where } x(0) = 1.$$

7. Population growth of any species is frequently modeled by an ordinary differential equation of the form

$$\frac{dN}{dt} \ = \ aN \ - \ bN^2$$

$$N(0) \ = \ N_0$$

where N is the population size, aN represents the birth rate, and bN^2 represents the death rate due to all causes, such as disease, competition for food supplies, and so on. If $N_0 = 100,000$, $a = 0.1$, and $b = 8 \times 10^{-7}$, calculate $N(t)$ for $t = 0$ to 20 using $\Delta t = 1$.

8. The population of two species competing for the same food supply can be modeled by the pair of ordinary differential equations

$$\frac{dN_1}{dt} \ = \ N_1(A_1 \ - \ B_1 N_1 \ - \ C_1 N_2)$$

$$N_1(0) \ = \ N_{1,0}$$

$$\frac{dN_2}{dt} \ = \ N_2(A_2 \ - \ B2N_2 \ - \ C_2 N_1)$$

$$N_2(0) \ = \ N_{2,0}$$

where AN is the birth rate, and BN^2 represents the death rate due to disease, and CN_1N_2 models the death rate due to competition for the food supply. If $N_{1,0}(0) = N_{2,0}(0) = 100{,}000$, $A_1 = 0.1$, $B_1 = 8 \times 10^{-7}$, $C_1 = 1 \times 10^{-6}$, $A_2 = 0.1$, $B_2 = 8 \times 10^{-7}$, $C_2 = 1 \times 10^{-6}$, calculate $N_{1,0}(t)$, and $N_{2,0}(t)$ for $t = 0$ to 10 years using $\Delta t = 1$.

9. Solve the following pair of ODE's by the Euler method from $t = 0.0$ to 1.0, with $\Delta t = 0.2$:

$$\frac{dy}{dt} = 2y + z + t, \qquad y(0) = 1.0$$

$$\frac{dz}{dt} = y + z + t, \qquad z(0) = 1.0$$

10. The following equation is used to describe the conservation of mass for a reservoir

$$\frac{dS}{dt} \quad = \quad I(t) \; - \; Q(H) \; (1)$$

where S is the volume of water in storage in the reservoir, $I(t)$ is the inflow into the reservoir as a function of time t, and $Q(H)$ is the outflow from the reservoir, which is determined by the elevation H of water in the reservoir. The change in volume S of the water in the reservoir, due to a change in the water depth dH, is expressed as

$$dS \quad = \quad AdH$$

where A is the area of the reservoir (assumed constant in this problem) and H is the elevation of the water surface. Equation (1) can then be written as

$$\frac{dH}{dt} \quad = \quad \frac{1}{A}[I(t) \; - \; Q(H)] \quad (2)$$

Develop the equations necessary to solve Equation (2) using the fourth-order Runge Kutta method (just set up the equations!). Assume that the function $I(t)$ is known and

$$Q(H) \;=\; \alpha H^{\beta}$$

where α and β are constants

$$\frac{dH}{dt} \;=\; f(H,t) \;=\; \frac{1}{A}[I(t) - \alpha H^{\beta}]$$
$$H(t_0) \;=\; H_0$$

11. The following equation describes the steady-state diffusion of a dissolved substance into a quiescent fluid body in which a first-order reaction occurs:

$$D\frac{d^2c}{dx^2} - Kc = 0 \qquad (1)$$

with boundary conditions:

$$c(0) = 0, \, c(1) = C_1$$

where $c(x)$ (M/L^3) is the concentration of the dissolved substance, D (L/T^2) is the diffusion coefficient, K (1/T) is the reaction rate, and C_1 (M/L^3) is a specified concentration on the right boundary of the domain.

(a) Write a finite-difference approximation of Equation (1)

(b) Using 3 evenly spaced nodes with node spacing $\Delta x = 0.5$, write the finite difference equation that you developed in part (a) for each node at which the concentration is unknown in the system.

(c) Solve for the unknown concentration using the numerical values for the coefficients:
$D = 0.01$ cm^2/s, $K = 0.1$ s^{-1}, and $C_1 = 1.0$ g/cm^3.

12. Water quality models can be used to predict the concentration of various constituents in receiving waters (streams, lakes, and rivers). Many of these models are extensions of the two simple equations proposed by Streeter and Phelps (1925)[1] for predicting the biochemical oxygen demand (BOD) of various biodegradable constituents, and the resulting dissolved oxygen (DO) concentration in rivers. The BOD concentration (B) and the dissolved oxygen deficit concentration (D) (i.e., the difference between the water's saturated dissolved oxygen concentration and the actual concentration--see Figure below) in a river are functions of simultaneous reactions which can be described by the equations:

$$\frac{dB}{dt} = -K_d B$$
$$\frac{dD}{dt} = K_d B - K_a D$$
(1)

where K_d is the deoxygenation rate constant (T^{-1}), K_a is the reaeration rate constant (T^{-1}), and t [T] is the time of flow along a section of river. The solution of these equations for a single waste discharge at the beginning of a river section results in the dissolved oxygen sag curve shown in the following Figure.

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[1] Streeter, H.W., and E.P. Phelps, A study of the pollution and natural purification of the Ohio River, U.S. Public Health Service, Publication Health Bulletin 146, Feb. 1925.
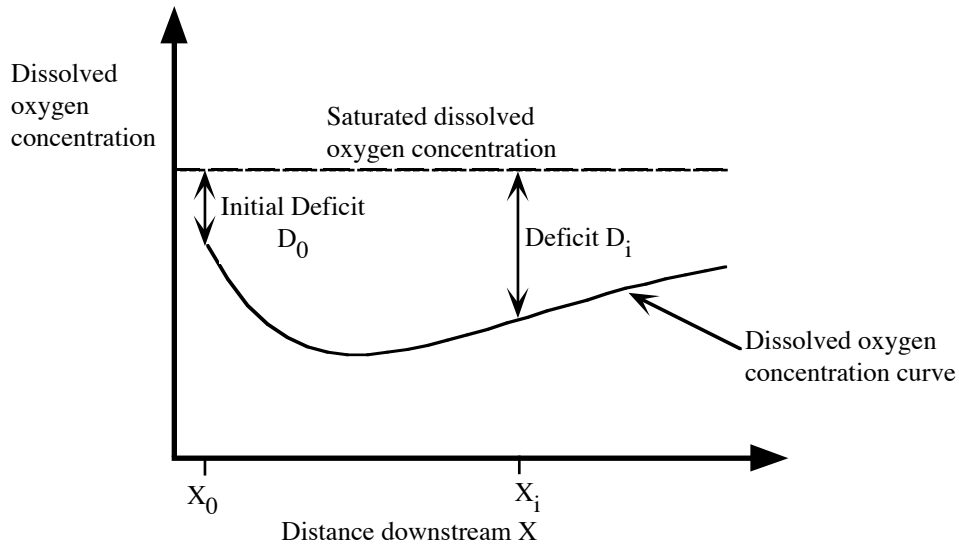
Figure. Dissolved oxygen "sag" curve resulting from single point discharge of BOD and initial oxygen deficit concentration at $X = 0$.
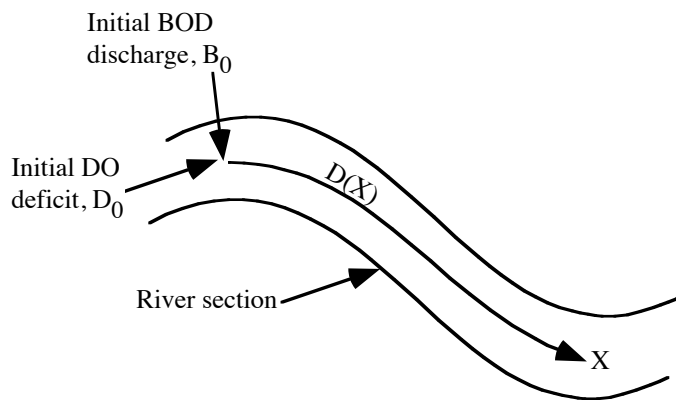

Figure. River section showing initial DO deficit and BOD discharge location.

(a) Develop the equations for applying Euler's method to solve the Streeter-Phelps equations for both BOD, B, and dissolved oxygen deficit, D.

(b) Solve for the BOD, B, and dissolved oxygen deficit, D, in the river using the Euler method equations that you developed in part (a) using the following data:

$K_d = 0.3\ \text{day}^{-1}$ = deoxygenation rate constant

$K_a = 0.4\ \text{day}^{-1}$ = reaeration rate constant

$D_{sat} = 8\ \text{mg/L}$ = Saturated dissolved oxygen concentration

$D_0 = 1.0\ \text{mg/L}$ = Initial dissolved oxygen deficit

$B_0 = 15\ \text{mg/L}$ = Initial BOD concentration at the beginning of the river section

$\Delta t = 3/4\ \text{day}$

Take 3 steps of the method.

13. Using the modified Euler method (second-order Runge Kutta method), take two steps of $\Delta t = 0.1$ for the following initial value problem

$$\frac{dy}{dt} = \frac{4t}{y} + ty, \qquad y(0) = 3$$

a) 13 pts. Solve the following Ordinary Differential Equation using the Euler method from $t = 0.0$ to 1.0 with $\Delta t = 0.2$.

$$\frac{dy}{dt} = e^{-t} + y \quad y(t) = 0.0 \ \ at \ \ t_0 = 0$$

14. **Euler method for systems** In the classic Lokta-Volterra equation of predator - prey modeling, the overall increase in the size of a prey population is given by

$$\frac{dH}{dt} = g_1 H - d_1 PH$$

where H is the size of the prey population, P is the size of the predator population, g_2 is the growth rate of the prey population, and the death rate is d_2. The predator population is governed by the equation

$$\frac{dP}{dt} = g_2 PH - d_2 P$$

where g_2 is the growth rate of the predator population, and the death rate is d_2.

(a) Show the formulas for the Euler method of solving these 2 ordinary differential equations (Don't plug in any numbers yet, just show the formulas.)

(b) Consider the initial conditions

$$P(0) = 5, H(0) = 20$$

and the numerical values

$$g_1 = 1, g_2 = 0.02,$$
$$d_1 = 0.1, d_2 = 0.5$$

Compute P(t) and H(t) from t = 0 - 1.5 using the Euler method and $\Delta t = 0.5$.

(b.1) Show the calculation for the first time step (from 0 to 0.5)

(b.2) Show the calculation for the second time step (from 0.5 to 1)

(b.3) Show the calculation for the third time step (from 1 to 1.5)

(c) Explain the solution of these equations in terms of the sizes and behavior of the populations.

15. **Leaky acres.** Consider the steady flow from left to right in the leaky aquifer shown in the Figure. The aquitard is leaky. If there is no leakage up from below and flow in the aquitard is vertical, and we have another aquifer above the aquitard where the head is h_0 , for one-dimensional flow indicated in the figure, we have

$$\frac{d^2h}{dx^2} - \frac{h}{\lambda^2} = -\frac{h_0}{\lambda^2}$$

where $\lambda^2 = bKb'/K'$ is called the leakage factor, K is the hydraulic conductivity and b is the aquifer thickness, h is the average head at a point in the aquifer, , and K' and b' are the conductivity and thickness, respectively, of the confining layer (aquitard).
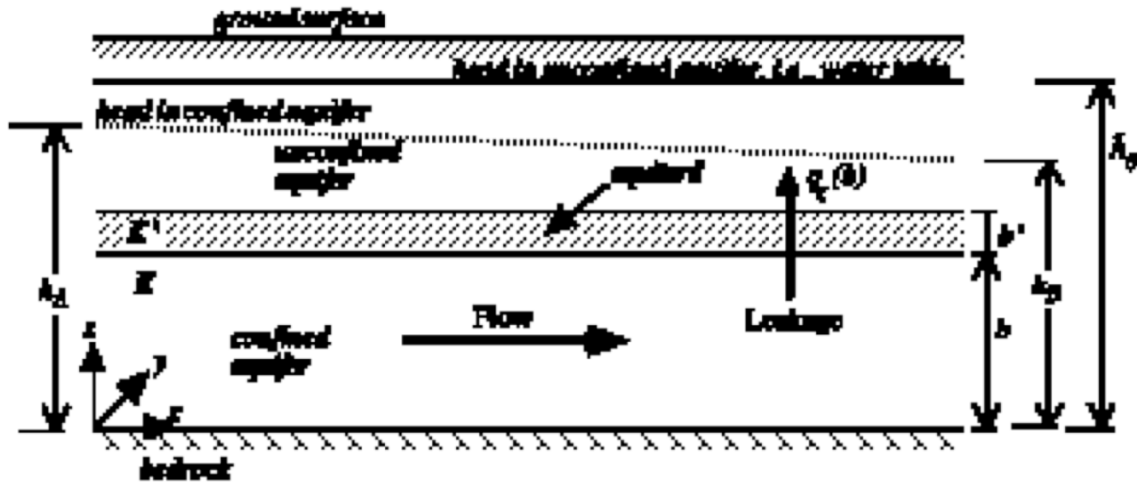

Figure. Flow in a leaky-confined aquifer.

Consider the values $L = 1000$ m, $\Delta x = 200$m, $H_A = 100$ m, $H_B = 80$ m, $K = 20$ m/day (clean sand), $b = 50$ m, $b' = 2$ m, $K' = 0.10$ m/day (silt). The head distributions for values of h_0 (head in the overlying aquifer) are shown in the Table.

(a) Apply a second-order accurate finite-difference approximation to the second derivative and write out the resulting equation.

(b) Write out the finite-difference equation for each node i where the head is unknown, that is, nodes 1 - 4.

(c) Show the resulting system of equations, written in matrix-vector form, if you move all the known values to the right-hand-side of the equation and leave the unknowns on the left.

(d) Discuss how you would solve this system of equations using a computer. Draw a simple flowchart of your method of solution.

16. Use Euler's method to find the solution to the initial value problem:

$$\frac{dy}{dx} = y + 2x - 1 \qquad y(x = 1) = 1 \quad 0 \le x \le 1 \qquad \Delta x = 0.1$$

Compare your result at $x = 1.0$ with the value of the exact solution

$$y(x) = -1 - 2x + 2e^x$$

at the same point.

17. **Modified Euler Method.** a. Solve the following initial value problem analytically over the interval $x = 0$ to 1.

$$\frac{dy}{dx} = (1 + x)\sqrt{y}$$

where $y(0) = 1$.

b. Use the Modified Euler method with $h = 0.5$ to solve the following initial value problem in Part (a) over the interval from $x = 0$ to 1:

18. Consider the following initial value problem:

$$\frac{dx}{dt} = -2t - x \quad x(t = 0) = -1, \quad 0 \le t \le 0.5, \qquad \Delta t = 0.25$$

(a) Use Euler's method to solve the initial value problem.

(b) Use the Modified-Euler method to solve the initial value problem.

(c) Compute the percent relative error from parts (a) and (b) at t = 0.5 by comparing to the value of the exact solution

$$x(t) = -3e^{-t} - 2t + 2$$