EAD 115

Numerical Solution of Engineering and Scientific Problems

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Transient Response of a Chemical Reactor

- Concentration of a substance in a chemical reactor can change during transient periods after startup or change in conditions.
- Accumulation = inputs – outputs.
- $V = \text{volume of the reactor, assumed constant.}$
- $c = \text{concentration of the substance, which can change.}$
Accumulation \( = V \frac{dc}{dt} \)
\( = Qc_{in} - Qc \)
\( c = c_{in} \left(1 - e^{-\left(\frac{Q}{V}\right)t}\right) + c_0 e^{-\left(\frac{Q}{V}\right)t} \)
\( c_{in} = 50\text{mg/m}^3 \)
\( Q = 5\text{m}^3/\text{min} \)
\( V = 100\text{m}^3 \)
\( c_0 = 10\text{mg/m}^3 \)
\( c = 50\left(1 - e^{-0.05t}\right) + 10e^{-0.05t} \)
\[
\frac{dc_1}{dt} = -0.12c_1 + 0.02c_3 + 1
\]
\[ V_1 \frac{dc_1}{dt} = Q_{01} c_{01} + Q_{31} c_3 - Q_{12} c_1 - Q_{15} c_1 \]
\[ \frac{dc_1}{dt} = -0.12 c_1 + 0.02 c_3 + 1 \]
\[ \frac{dc_2}{dt} = 0.15 c_1 - 0.15 c_2 \]
\[ \frac{dc_3}{dt} = 0.025 c_2 - 0.225 c_3 + 4 \]
\[ \frac{dc_4}{dt} = 0.1c_3 - 0.1375 c_4 + 0.025 c_5 \]
\[ \frac{dc_5}{dt} = 0.3c_1 + 0.01c_2 - 0.04c_5 \]
\[ c_1(0) = c_2(0) = c_3(0) = c_4(0) = c_5(0) = 0 \]
Solution using a fourth-order Runge-Kutta method.

We can describe the response in terms of the time to 90% of the equilibrium concentration.

This varies from about 12 for $c_3$ to over 70 for $c_5$. 
\[
\frac{dc_1}{dt} = -0.12c_1 + 0.02c_3 + 1
\]
Predator-Prey Models

• Volterra-Lotka describe the reaction dynamics in an ecosystem

• In the simplest case, we let $x$ represent the number of prey animals (rabbits) and $y$ the number of predator animals (foxes).

• Rabbits naturally increase, and are assumed to have an adequate food supply, but are reduced by predation.

• Foxes increase only if there is adequate prey.
\[
\frac{dx}{dt} = ax - bxy \\
\frac{dy}{dt} = -cy + dxy
\]

Rabbits increase at a natural (birth – death) rate \(a\). Rabbits are reduced by a percentage \(b\) by that depends on the number of foxes. Foxes reproduce at a rate \(dx\) dependent on the food supply. Foxes die at a rate \(c\).
State-Space Representation

- The previous plot showed x and y against t.
- The state-space plot shows y against x.
- This shows the stability, or lack of it, and the dynamics in a more concrete way.
\[ \frac{dx}{dt} = ax - bxy = 0 \]

\[ \frac{dy}{dt} = -cy + dxy = 0 \]

\[ x = 0 \text{ or } a = by \]

\[ y = 0 \text{ or } c = dx \]

\[ (0,0) \text{ or } (c/d, a/b) \]
Stochastic version

\[
\frac{dx}{dt} = ax - bxy + \varepsilon
\]

\[
\frac{dy}{dt} = -cy + dxy + \eta
\]

Critical point is not stable.
Extinction can occur
Stochastic dynamics after 5 time periods
Stochastic dynamics after 10 time periods
Stochastic dynamics after 30 time periods
Simulating Transient Current in an Electric Circuit
\[ L \frac{di}{dt} + Ri + \frac{q}{C} - E(t) = 0 \] (Kirkoff's Law)

\[ L \frac{di}{dt} = \text{voltage drop across the inductor} \]

\[ L = \text{inductance} \]

\[ R = \text{resistance (of the resistor)} = 0 \]

\[ q = \text{charge on the capacitor} \]

\[ C = \text{capacitance (of the capacitor)} \]

\[ E(t) = \text{time-varying voltage source} = E_0 \sin \omega t \]

\[ i = \frac{dq}{dt} \]

\[ q(t) = \frac{-E_0}{L(p^2 - \omega^2)} \frac{\omega}{p} \sin pt + \frac{E_0}{L(p^2 - \omega^2)} \sin \omega t \text{ where } p = 1/\sqrt{LC} \]
Capacitor

Current

Time

0 20 40 60 80 100
• Assume \( L = 1\text{H}, E_0 = 1\text{V}, C = 0.25\text{C, } \omega^2 = 3.5\text{s}^2 \), so that \( p = 2 \).

• \( q(t) = -1.8708 \sin(2t) + 2 \sin(1.8708t) \)

• Although an analytical solution exists, try integration with Euler and RK 4 methods

• Use \( h = 0.1\text{s} \), evaluate accuracy at \( t = 10\text{s} \).

• \( q(t) = -1.996\text{C} \) (exact)

• \( q(t) \approx -6.638 \) (Euler)

• \( q(t) \approx -1.9897 \) (RK4)
The Swinging Pendulum

• The usual analysis of a swinging pendulum is an approximation which is valid for small arcs.

• We compare the exact solution of the approximate problem with an approximate solution of a more realistic model.

• We do still model this as a point mass on a weightless, inextensible rod, so it is not completely realistic.
The force on the weight in the direction $x$ tangent to the path is

$$F = -W \sin \theta = \frac{W}{g} a$$

The angular acceleration in terms of the length $l$ of the rod is

$$\alpha = \frac{d^2 \theta}{dt^2} = a/l$$

$$-W \sin \theta = \frac{Wl}{g} \alpha = \frac{Wl}{g} \frac{d^2 \theta}{dt^2}$$

$$\frac{d^2 \theta}{dt^2} + \frac{g}{l} \sin \theta = 0$$
Exact solution to an approximation when $\theta$ is small

\[
\sin \theta = \theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \frac{\theta^7}{7!} + \cdots \approx \theta
\]

\[
\frac{d^2 \theta}{dt^2} + \frac{g}{l} \theta = 0
\]

\[
\theta(t) = \theta_0 \cos \sqrt{\frac{g}{l}} t
\]

The period of the pendulum is then

\[
T = 2\pi \sqrt{\frac{l}{g}}
\]
\[ T = 2\pi \sqrt{\frac{l}{g}} \]

\[ l = 2\text{ft} \]

\[ \theta_0 = \frac{\pi}{4} \quad (45^\circ) \]

\[ T = 1.5659\text{s} \]
An approximate (numerical) solution to a more accurate physical model

\[
\frac{d^2 \theta}{dt^2} + \frac{g}{l} \sin \theta = 0
\]

\[
\frac{d \theta}{dt} = v
\]

\[
\frac{dv}{dt} = -\frac{g}{l} \sin \theta = -16.1 \sin \theta \quad \text{(for } l = 2\text{ft)}
\]

Approximate with Euler method and standard order 4 Runge-Kutta method
Standard Fourth-Order Method

\[ k_1 = f(x_i, y_i) \]
\[ k_2 = f(x_i + h/2, y_i + k_1 h/2) \]
\[ k_3 = f(x_i + h/2, y_i + k_2 h/2) \]
\[ k_4 = f(x_i + h, y_i + k_3 h) \]
\[ y_{i+1} = y_i + \frac{(k_1 + 2k_2 + 2k_3 + k_4)h}{6} \]
\[k_{11} = f_1(t_0, \theta_0, v_0) = v_0 = 0\]
\[k_{12} = f_2(t_0, \theta_0, v_0) = -16.1 \sin \theta_0 = -16.1 \sin \pi / 4\]
\[= -16.2 \sin 0.785398 = -11.38441918\]
\[\theta^*_1 = \theta_0 + 0.005 k_{11} = \theta_0 + 0.005(0) = \pi / 4 = 0.785398163\]
\[v^*_1 = v_0 + 0.005 k_{12} = 0 + 0.005(-11.38441918) = -0.056922096\]
\[k_{21} = f_1(t^*_1, \theta^*_1, v^*_1) = v^*_1 = -0.056922096\]
\[k_{22} = f_2(t^*_1, \theta^*_1, v^*_1) = -16.1 \sin \theta^*_1 = -11.38441918\]
\[\theta^*_2 = \theta_0 + 0.005 k_{21} = 0.785113553\]
\[v^*_2 = v_0 + 0.005 k_{22} = -0.056922096\]
\[ \theta_2^* = \theta_0 + 0.005k_{21} = 0.785113553 \]
\[ v_2^* = v_0 + 0.005k_{22} = -0.056922096 \]
\[ k_{31} = f_1(t_2^*, \theta_2^*, v_2^*) = v_2^* = -0.056922096 \]
\[ k_{32} = f_2(t_2^*, \theta_2^*, v_2^*) = -16.1\sin\theta_2^* = -11.38117859 \]
\[ \theta_3^* = \theta_0 + 0.01k_{31} = 0.784828942 \]
\[ v_3^* = v_0 + 0.01k_{32} = -0.113811786 \]
\[ k_{41} = f_1(t_3^*, \theta_3^*, v_3^*) = v_3^* = -0.113811786 \]
\[ k_{42} = f_2(t_3^*, \theta_3^*, v_3^*) = -16.1\sin\theta_3^* = -11.37793708 \]
\[ \phi_1 = k_{11} + 2k_{12} + 2k_{13} + 2k_{14} = -0.056916695 \]
\[ \phi_2 = k_{21} + 2k_{22} + 2k_{23} + 2k_{24} = -11.38225863 \]
\[ \theta_1 = \theta_0 + 0.01\phi_1 = 0.784828996 \]
\[ v_1 = v_0 + 0.01\phi_2 = -0.113822586 \]
<table>
<thead>
<tr>
<th>Time</th>
<th>Linear</th>
<th>Euler h=0.05</th>
<th>RK 4 h=0.05</th>
<th>RK 4 h=0.01</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.785398</td>
<td>0.785398</td>
<td>0.785398</td>
<td>0.785398</td>
</tr>
<tr>
<td>0.2</td>
<td>0.545784</td>
<td>0.615453</td>
<td>0.566582</td>
<td>0.566579</td>
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<td>0.4</td>
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<td>0.050228</td>
<td>0.021895</td>
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<tr>
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<td>-0.784242</td>
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<tr>
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<td>1.2</td>
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<td>-0.065611</td>
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<tr>
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<tr>
<td>1.6</td>
<td>0.778062</td>
<td>1.316795</td>
<td>0.780762</td>
<td>0.780777</td>
</tr>
</tbody>
</table>
Analysis of Numerical Solutions

• The Euler method with \( h = 0.05 \) generates impossible results at times \( t = 0.8, 1.0, \) and 1.6.

• The RK4 solutions with \( h = 0.05 \) and \( h = 0.01 \) are the same to 4 decimal places, suggesting the accuracy of the latter is at least that good.

• The RK4 \( h = 0.01 \) solution attains a max of 0.785385 at \( t = 1.63 \) compared to 0.785398 at the initial conditions.

• Thus the difference between the linear approximation and the RK 4 solution can safely be interpreted.
<table>
<thead>
<tr>
<th>Initial Displacement</th>
<th>Linear Model Exact</th>
<th>Nonlinear Model RK4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi/16$</td>
<td>1.5659</td>
<td>1.57</td>
</tr>
<tr>
<td>$\pi/4$</td>
<td>1.5659</td>
<td>1.63</td>
</tr>
<tr>
<td>$\pi/2$</td>
<td>1.5659</td>
<td>1.85</td>
</tr>
</tbody>
</table>
An approximate solution to the exact problem is often better in a practical sense than the exact solution to an approximate problem.

The art is in knowing how much to include in the model, and how accurate an approximate solution is required.