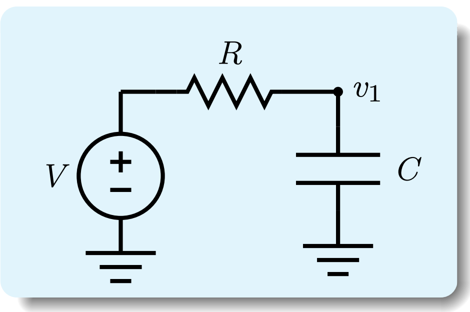
Unit 8.4. Variable Step Methods

Numerical Analysis

June 16, 2015

ODE with Fixed Time Steps

- Fixed time step provide simple and accurate solution in solving ordinary differential equations.
- Time step is dominated by the largest change in solution vector.
- But solution vector is not changing rapidly all the time, can we explore variable steps for better efficiency?



$$V(t) = 1, \quad t \geq 0,$$
$$v_1(0) = 0.$$

Analytical solution:
$$v_1(t) = 1 - \exp(\frac{-t}{RC})$$

- Nodal equation:

$$\frac{dv_1}{dt} = \frac{V - v_1}{RC}$$

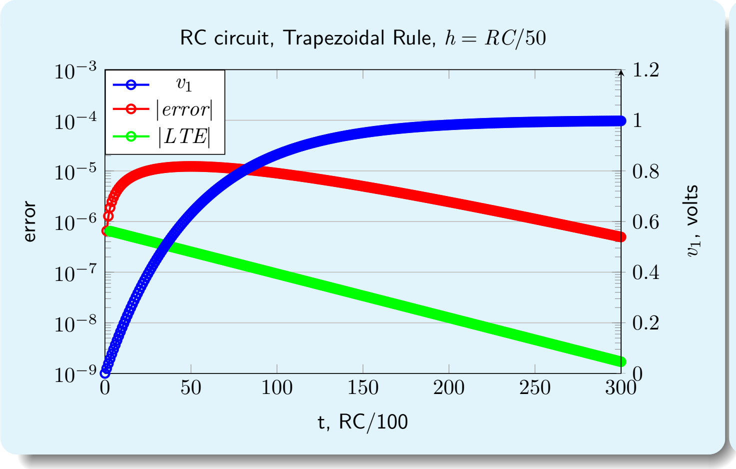
Let $x = v_1$, then

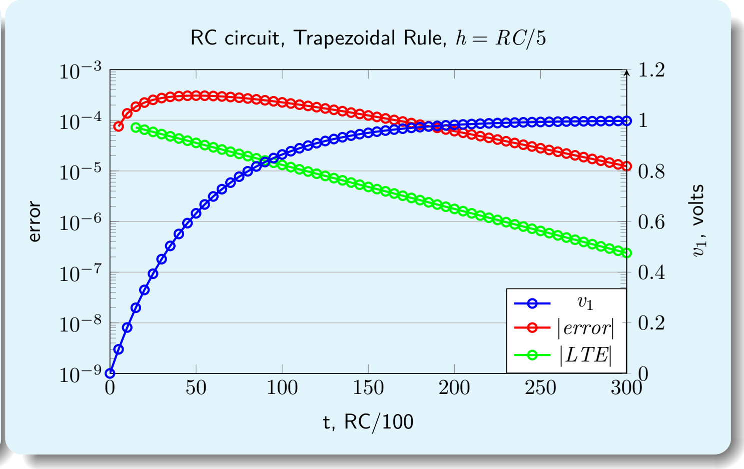
$$\frac{dx}{dt} = f(x, t)$$
$$f = \frac{V - x}{RC}$$

- Trapezoidal rule:

$$x(t+h) = x(t) + \frac{f(t+h) + f(t)}{2}$$
$$LTE = \frac{h^3}{2} a_3 = \frac{h^3}{12} \frac{d^3 x}{dt^3}$$

ODE with Fixed Time Steps, II





- Trapezoidal rule with smaller time steps has better accuracy.
- LTE is a good indicator of the solution accuracy.
- When the solution is saturating, the error and the LTE is becoming smaller.
- Solution accuracy is dominated by the largest error.
- Can we explore variable time step to improve the solution efficiency while maintaining the largest error.

Trapezoidal Rule and LTE

- The local truncation error of using trapezoidal method to solve ODE is

$$LTE = \frac{h^3}{2} a_3 = \frac{h^3}{2 \cdot 3!} \frac{d^3 x}{dt^3}$$

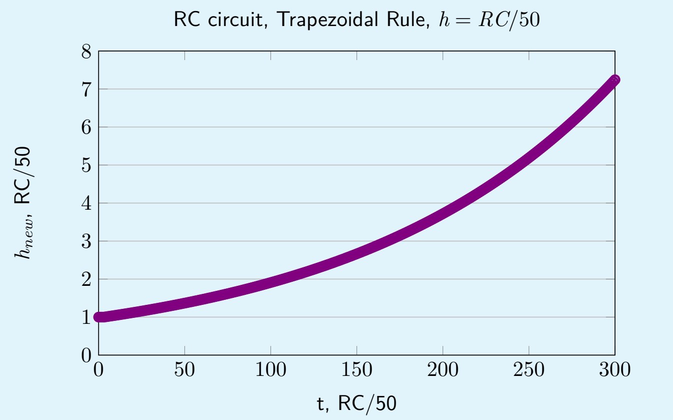
- Note that the derivative $\dfrac{d^k x}{dt^k}$ can be approximated by Eq. (5.1.19), or

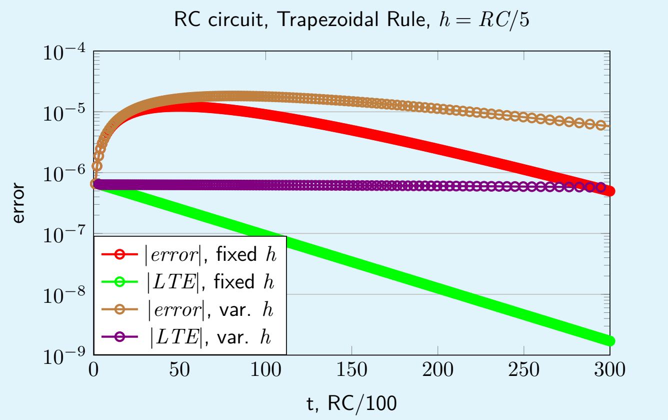
$$\begin{aligned} x[t_i] &= x(t_i), \\ x[t_0, t_1, \cdots, t_k] &= \frac{x[t_1, t_2, \cdots, t_k] - x[t_0, t_1, \cdots, t_{k-1}]}{t_k - t_0} \\ a_k &= \frac{1}{k!} \frac{d^k x}{dt^k} \approx x[t_0, t_1, \cdots, t_k]. \end{aligned} \tag{8.4.1}$$

- Using this equation, once the solution and the derivative are found one can calculate the step size h to keep the LTE constant. For the trapezoidal rule

$$h = \sqrt[3]{\frac{2 \cdot LTE}{a_3}}. \tag{8.4.2}$$

Trapezoidal Rule and LTE, II





- Using equation (8.4.2), time step can be increased when no large changes in solution vector.
  - Solution with similar errors can be obtained more efficiently.
  - For the RC circuit example, number of time steps is reduced from 300 to 136, more than 50% saving.
- Fixed trapezoidal solution method can be modified from fixed time step to variable time step for better efficiency.
  - Note that the LTE is kept the same with similar maximum error.

Variable Time Step Methods

- In general, initial value problem can be solved using variable time step method.

Algorithm 8.4.1. Trapezoidal rule with variable time steps.

Given an ordinary differential equation

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

with initial value $x(0) = x_0$.

let $t = 0$ and select an h,
while $(t \leq t_f)$ {
    $t = t + h$,
    solve $x(t)$ using trapezoidal rule,
    modify h.
}

Variable Time Step Methods, II

- Example of time step selection heuristics.

Heuristic 8.4.2. Iteration based time step selection.

let $\#iter$ be the number of iterations in solving for $x(t)$;
if $(\#iter > iter_{max})$ $h = h/4$;
else if $(\#iter = 1$ and $1.5h \leq h_{max})$ $h = h \times 1.5$;

Heuristic 8.4.3. Δ-V based time step selection.

let $\Delta V = x(t) - x(t-h)$;
if $(|\Delta V| > V_{max})$ $h = h/4$;
else if $(|\Delta V| < V_{min}$ and $1.5h \leq h_{max})$ $h = h \times 1.5$;

- Note that the factors 4 and 1.5 are arbitrary.
- These are heuristics and the solution accuracy (integration error) is not guaranteed.

LTE Based Trapezoidal Rule Method

Algorithm 8.4.4. LTE based trapezoidal rule method.

Given an ordinary differential equation

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

with initial value $x(0) = x_0$, final time t_f and a target $LTE = \xi$.

let $t = 0$, $LTE = 1 + \xi$ and select a small h,
while $(LTE > \xi)$ { // initial start up
  $t = h$; using trapezoidal rule to solve for $x(t)$;
  $t = 2h$; using trapezoidal rule to solve for $x(t)$;
  $t = 3h$; using trapezoidal rule to solve for $x(t)$;
  calculate LTE and a_3;
  if $(LTE > \xi)$ $h = h/4$;
}

LTE Based Trapezoidal Rule Method, II

```
while (t < t_f) {              // main solution loop
    h = cbrt(2ξ / a_3);
    t = t + h;
    solve for x(t);
    calculate LTE and a_3;
    while (LTE > ξ) {          // back tracking
        t = t − h;   h = h/4;   t = t + h;
        solve x(t);
        calculate LTE and a_3;
    }
}
```

- For each time point, the local truncation error is maintained to be smaller than ξ
  - Even in start up phase.
- Solution accuracy is quantified by LTE and guaranteed.
- The factor $1/4$ is arbitrary.

Variable Time Step Methods

- Fixed time step methods solve initial value problem accurately provided the time step, h, is small enough.
  - h should be determined by the time points, where the solution vector changes rapidly.
  - Most of the time, this small h is an overkill.
- Variable time step methods can provide much faster solution time with similar integration errors.
  - Heuristics for time step modification.
  - LTE-based time step control.
- SPICE uses variable time step control.
  - Solutions are interpolated if the time point is not calculated.

2nd Order Gear's Method

- Trapezoidal rule method is under-damped.
  - Solution oscillation may happen in case of large time steps.
- Gear's method is stable and can be exploited for large time steps.
- 2nd order Gear's method needs two past times points

$$x(t+h) = \frac{4}{3}x(t) - \frac{1}{3}x(t-h) + \frac{2h}{3}f(t+h).$$

- Need to generalize the formula for variable time step.

$$x(t+h_1) = \alpha_1 x(t) - \alpha_2 x(t-h_2) + \alpha_3 h_1 f(t+h_1). \tag{8.4.3}$$

- Consider

$$\begin{aligned} x(t) &= a_0 + a_1 t + a_2 t^2 \\ f(t) &= a_1 + 2a_2 t \\ x(t+h_1) &= a_0 + a_1(t+h_1) + a_2(t+h_1)^2 \qquad (8.4.4) \\ &= \alpha_1 x(t) + \alpha_2 x(t-h_2) + h_1\alpha_3 f(t+h_1) \\ &= \alpha_1(a_0 + a_1 t + a_2 t^2) + \alpha_2\Big(a_0 + a_1(t-h_2) + a_2(t-h_2)^2\Big) \\ &\quad + h_1\alpha_3\Big(a_1 + 2a_2(t+h_1)\Big) \\ &= a_0(\alpha_1+\alpha_2) + a_1\Big(\alpha_1 t + \alpha_2(t-h_2) + h_1\alpha_3\Big) \\ &\quad + a_2\Big(\alpha_1 t^2 + \alpha_2(t-h_2)^2 + 2h_1\alpha_3(t+h_1)\Big) \qquad (8.4.5) \end{aligned}$$

2nd Order Gear's Method, II

- To match the coefficients of Eqs. (8.4.4) and (8.4.5)

$$\begin{aligned} \alpha_1 + \alpha_2 &= 1 \\ -h_2\alpha_2 + h_1\alpha_3 &= h_1 \\ h_2^2\alpha_2 + 2h_1^2\alpha_3 &= h_1^2 \end{aligned}$$

- Or in matrix-vector form

$$\begin{bmatrix} 1 & 1 & 0 \\ 0 & -h_2 & h_1 \\ 0 & h_2^2 & 2h_1^2 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \begin{bmatrix} 1 \\ h_1 \\ h_1^2 \end{bmatrix}$$

- And the coefficients can be found to be

$$\begin{aligned} \alpha_1 &= \frac{(h_1+h_2)^2}{h_2(2h_1+h_2)} \\ \alpha_2 &= \frac{-h_1^2}{h_2(2h_1+h_2)} \\ \alpha_3 &= \frac{h_1+h_2}{2h_1+h_2} \end{aligned}$$

2nd Order Gear's Method, III

- The coefficients for Gear-2 with variable steps are

$$\alpha_1 = \frac{(h_1+h_2)^2}{h_2(2h_1+h_2)}$$
$$\alpha_2 = \frac{-h_1^2}{h_2(2h_1+h_2)}$$
$$\alpha_3 = \frac{h_1+h_2}{2h_1+h_2}$$

- If $h_1 = h_2$

$$\alpha_1 = \frac{4}{3}, \qquad \alpha_2 = \frac{-1}{3}, \qquad \alpha_3 = \frac{2}{3}.$$

- If $h_1 \ll h_2$

$$\alpha_1 \to 1, \qquad \alpha_2 \to 0, \qquad \alpha_3 \to 1,$$
$$x(t+h_1) = x(t) + h_1 f(t+h_1).$$

  - Gear-2 approaches backward Euler method.
- If $h_1 \gg h_2$

$$\alpha_1 \to 1 + \frac{h_1}{2h_2}, \qquad \alpha_2 \to \frac{-h_1}{2h_2}, \qquad \alpha_3 \to \frac{1}{2},$$
$$x(t+h_1) = x(t) + \left(\frac{x(t)-x(t-h_2)}{h_2} + f(t+h_1)\right)\frac{h_1}{2}.$$

  - Gear-2 approaches trapezoidal rule.

LTE for 2nd Order Gear's Method

- 2nd order Gear's method

$$x(t+h_1) = \alpha_1 x(t) + \alpha_2 x(t-h_2) + h_1\alpha_3 f(t+h_1).$$

- For LTE consider t^3 term

$$\begin{aligned}
x(t) &= a_0 + a_1 t + a_2 t^2 + a_3 t^3 \\
f(t) &= a_1 + 2a_2 t + 3a_3 t^2 \\
x(t+h) &= a_0 + a_1(t+h) + a_2(t+h)^2 + a_3(t+h)^3 \qquad (8.4.6) \\
&= \alpha_1 x(t) + \alpha_2 x(t-h) + h_1\alpha_3 f(t+h_1) \\
&= \alpha_1(a_0 + a_1 t + a_2 t^2 + a_3 t^3) \\
&\quad + \alpha_2\left(a_0 + a_1(t-h_2) + a_2(t-h_2)^2 + a_3(t-h_2)^3\right) \\
&\quad + h_1\alpha_3\left(a_1 + 2a_2(t+h_1) + 3a_3(t+h_1)^2\right) \qquad (8.4.7)
\end{aligned}$$

In (8.4.6) : $\quad a_3(t+h_1)^3 = a_3(t^3 + 3t^2h_1 + 3th_1^2 + h_1^3)$

In (8.4.7) : $\quad a_3\left(\alpha_1 t^3 + \alpha_2(t-h_2)^3 + 3h_1\alpha_3(t+h_1)^2\right)$

$$= a_3\Big(t^3(\alpha_1+\alpha_2) + t^2(-3\alpha_2 h_2 + 3h_1\alpha_3) + t(3\alpha_2 h_2^2 + 6h_1\alpha_3) - \alpha_2 h_2^3 + 3\alpha_3 h_1^3\Big)$$

LTE for 2nd Order Gear's Method, II

- Thus, we have

$$LTE = a_3(-\alpha_2 h_2^3 + 3\alpha_3 h_1^3 - h_1^3) \tag{8.4.8}$$

- Or in matrix-vector form

$$\begin{bmatrix} 1 & 1 & 0 \\ 0 & -h_2 & h_1 \\ 0 & h_2^2 & 2h_1^2 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \begin{bmatrix} 1 \\ h_1 \\ h_1^2 \end{bmatrix}$$

  LTE is the next row of the system of equations.
- Solving LTE explicitly in h's

$$\begin{aligned} LTE =& a_3(-\alpha_2 h_2^3 + 3\alpha_3 h_1^3 - h_1^3) \\ =& a_3 h_1^3(-\alpha_2 \frac{h_2^3}{h_1^3} + 3\alpha_3 - 1) \\ =& a_3 h_1^3(\frac{h_2^2}{h_1(2h_1 + h_2)} + \frac{h_1 + 2h_2}{2h_1 + h_2}) \\ =& a_3 h_1^2 \frac{(h_1 + h_2)^2}{2h_1 + h_2} \end{aligned}$$

LTE for 2nd Order Gear's Method, III

- LTE for Gear-2 method

$$LTE = a_3 h_1^2 \frac{(h_1 + h_2)^2}{2h_1 + h_2} \tag{8.4.9}$$

- If $h_1 = h_2 = h$

$$LTE = \frac{4}{3} a_3 h^3$$

- If $h_1 \ll h_2$

$$LTE = a_3 h_1^2 h_2$$

  - Gear-2 approaches backward Euler with LTE multiplied by h_2.
- If $h_1 \gg h_2$

$$LTE = \frac{a_3}{2} h_1^3$$

  - Gear-2 approaches trapezoidal rule.

LTE for 2nd Order Gear's Method, IV

- LTE for Gear-2 method
$$LTE = a_3 h_1^2 \frac{(h_1 + h_2)^2}{2h_1 + h_2}$$
- Let $h_1 = \gamma h_2$, then $LTE = a_3 h_2^3 \dfrac{\gamma^2(1+\gamma)^2}{2\gamma + 1}$.
Note that $\gamma > 0$
$$a_3 h_2^3 \frac{\gamma^2(1+\gamma)^2}{2\gamma+1} > a_3 h_2^3 \frac{\gamma^2(1+\gamma)^2}{2\gamma+2} = a_3 h_2^3 \gamma^2 \frac{1+\gamma}{2} > \frac{a_3 h_1^3}{2}.$$
And if $\gamma >= 1$ then
$$a_3 h_2^3 \frac{\gamma^2(1+\gamma)^2}{2\gamma+1} < a_3 h_2^3 \frac{\gamma^2(1+\gamma)^2}{2\gamma} <= a_3 h_2^3 \frac{\gamma^2(\gamma+\gamma)^2}{2\gamma} = a_3 h_2^3 \gamma^3 \cdot 2 = 2a_3 h_1^3.$$
otherwise, $\gamma < 1$
$$a_3 h_2^3 \frac{\gamma^2(1+\gamma)^2}{2\gamma+1} < a_3 h_2^3 \frac{\gamma^2(1+2\gamma)^2}{2\gamma+1} = a_3 h_2^3 \gamma^2(1+2\gamma) < a_3 h_2^3 2\gamma^3 = 2a_3 h_1^3.$$
- Thus,
$$\frac{a_3 h_1^3}{2} < LTE < 2a_3 h_1^3. \tag{8.4.10}$$

LTE for 2nd Order Gear's Method, V

- We treat LTE as a function of h_1^3,
$$LTE(h_1) \sim \Gamma h_1^3.$$
then for h_{new}
$$LTE(h_{new}) \sim \Gamma h_{new}^3 \sim LTE(h_1) \times \left(\frac{h_{new}}{h_1}\right)^3.$$
Or given a target $LTE = \xi$ to be met for h_{new}
$$\xi \sim LTE(h_1) \times \left(\frac{h_{new}}{h_1}\right)^3$$
$$h_{new} \approx h_1 \sqrt[3]{\frac{\xi}{LTE(h_1)}}. \tag{8.4.11}$$
- Using this equation, time step control for Gear-2 method can be developed.
  - Note that, the new LTE will be explicitly calculated and thus the accuracy of this equation does not affect the overall solution error.

Gear-2 with Variable Time Steps

Algorithm. 8.4.5. Gear-2 with variable time steps.

Given the ordinary differential equation

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

with initial condition $x(0) = x_0$, final time t_f and a target $LTE = \xi$.

Let $LTE = 1 + \xi$ and choose a small h_1 ,
while $(LTE > \xi)$ { // initial start up
$t = h_1$; solve for $x(t)$ using backward Euler method;
$t = 2h_1$; solve for $x(t)$ using Gear-2 method;
$t = 3h_1$; solve for $x(t)$ using Gear-2 method;

calculate $LTE = \frac{4}{3} a_3 h_1^3$;

if $(LTE > \xi)$ $h_1 = \sqrt[3]{\frac{\xi}{LTE}}$;
}

Gear-2 with Variable Time Steps, II

while $(t < t_f)$ { // main loop

$h_{new} = h_1 \sqrt[3]{\frac{\xi}{LTE}}$;

$t = t + h_{new}$;
solve for $x(t)$ using Gear-2 with variable steps;
calculate LTE;
while $(LTE > \xi)$ {
$t = t - h_{new}$;

$h_{new} = h_1 \sqrt[3]{\frac{\xi}{LTE}}$;

$t = t + h_{new}$;
solve for $x(t)$ using Gear-2 with variable steps;
calculate LTE;
}
}

Higher Order Gear's Methods

- Higher order Gear's methods with variable steps can be similarly developed.
- Higher order methods have smaller LTE usually,
  - Or can take larger time steps given the same LTE.
- It is stable with large time steps.
  - Compared to trapezoidal rule or similar backward integration methods.
- Thus, Gear's formulas have been popular in circuit simulations.
  - Stiff equations are not uncommon.
  - Order as high as 7 has been offered.
- Dynamic systems with many variables can be solved in the same way.
- Nonlinear dynamic systems are usually solved using Newton's method.

Summary

- Fixed time step methods
  - Time step chosen to ensure small errors
  - Dominated by time steps with rapid solution changes
  - Most of the time steps have small solution changes
- Variable time step methods
  - Maintain same error while exploiting larger time steps when solution is not changing much
  - LTE based algorithms are popular
- Trapezoidal method with variable time steps
- Gear-2 method with variable time steps.