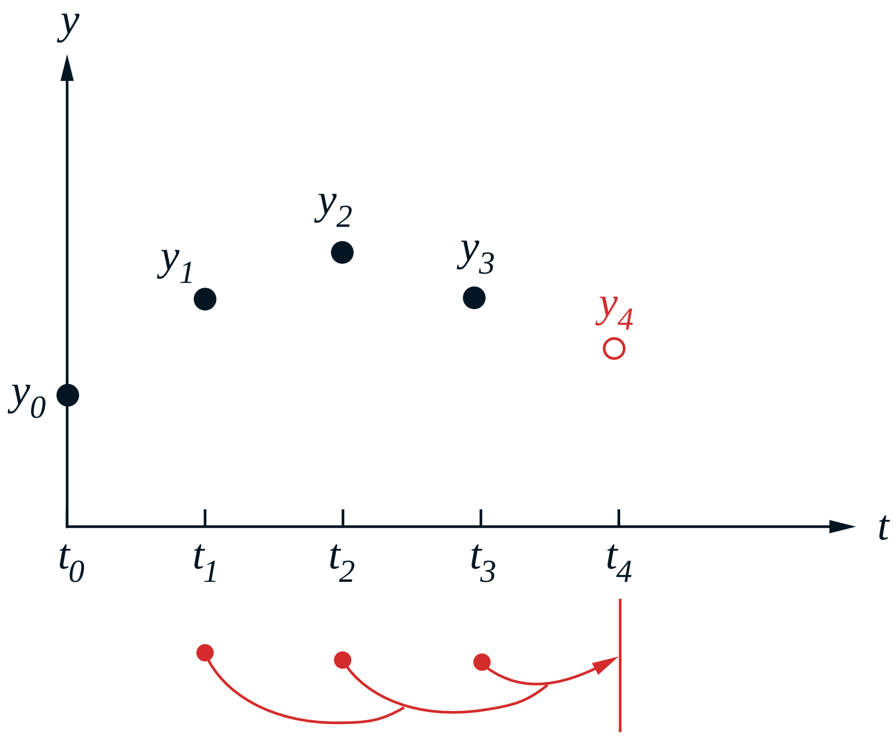
LECTURE 22

MULTI STEP METHODS

- Solve the i.v.p. $\frac{dy}{dt} = f(y, t) \qquad y(t_o) = y_o$

- **Multi step methods use information from several previous or known time levels**



- Open Formulae (Adams-Bashforth)
  - explicit (non-iterative)
  - can have stability problems

- Closed Formulae (Adams-Moulton)
  - implicit (iterative)
  - much better stability properties than open formulae

- Predictor-Corrector Methods
  - 1 cycle predictor → open formula
  - 2-3 cycles corrector → closed formula
  - superior to either open or closed formulae separately

Open Formulae

Derivation

- Develop a forward Taylor series of y about t_j

$$y_{j+1} = y_j + \Delta t\, \dot{y}_j + \frac{(\Delta t)^2}{2!}\ddot{y}_j + \frac{(\Delta t)^3}{3!}\dddot{y}_j + \ldots$$

- However by definition $\dot{y}_j = f_j$ and $\ddot{y}_j = \dot{f}_j$ etc., thus

$$y_{j+1} = y_j + \Delta t\left(f_j + \frac{\Delta t}{2!}\dot{f}_j + \frac{(\Delta t)^2}{3!}\ddot{f}_j + \ldots\right) \qquad (1)$$

- Now replace the various derivatives of f_j with backward difference approximations

1st Order Accurate Adams Open Formula

- Retain only the first two terms in Equation (1)

$$\boldsymbol{y_{j+1} = y_j + \Delta t\ f(y_j, t_j)}$$

- Same as the “explicit” or 1st order Euler method

2nd Order Accurate Adams Open Formula

- Use a backward difference approximation for $\dot{f}_j$

$$\dot{f}_j = \frac{f_j - f_{j-1}}{\Delta t} + \frac{\Delta t}{2}\ddot{f}_j + O(\Delta t)^2$$

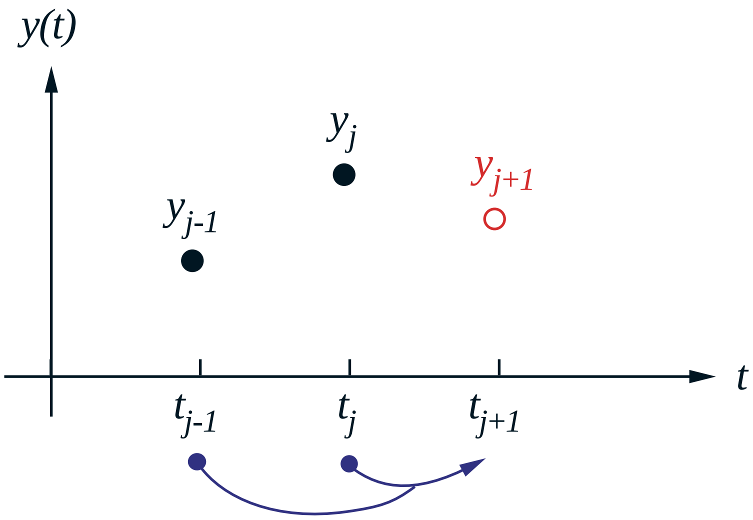
- Substituting we obtain:

$$y_{j+1} = y_j + \Delta t\left\{ f_j + \frac{\Delta t}{2}\left[\frac{f_j - f_{j-1}}{\Delta t} + \frac{\Delta t}{2}\ddot{f}_j + O(\Delta t)^2\right] + \frac{(\Delta t)^2}{3!}\ddot{f}_j \right\} \Rightarrow$$

$$y_{j+1} = y_j + \Delta t\left[\frac{3}{2}f_j - \frac{1}{2}f_{j-1}\right] + \frac{5}{12}(\Delta t)^3\ddot{f}_j + O(\Delta t)^4 \Rightarrow$$

$$y_{j+1} = y_j + \Delta t\left[\frac{3}{2}f_j - \frac{1}{2}f_{j-1}\right] + O(\Delta t)^3 \Rightarrow$$

$$\boldsymbol{y_{j+1} = y_j + \Delta t\left[\frac{3}{2}f(y_j, t_j) - \frac{1}{2}f(y_{j-1}, t_{j-1})\right] + O(\Delta t)^3}$$



- Notes
  - Method is second order since the local truncation term is $O(\Delta t)^3$ (recall the effect of cumulative error during time stepping)
  - Formula was derived by developing a forward Taylor series for y_{j+1} about y_j and using a backward finite difference approximation for the first derivative of $f(y_j, t_j)$
  - Note that the method is ***explicit*** → i.e. the new time level $j+1$ value is computed using the slope at the current and previous time levels j and $j-1$
  - This formula is ***not self starting***! Use 2nd order Runge-Kutta (R.K.) method to start the computations

Example Application of 2nd Order Adams Open Formula

- Problem

$$\frac{dy}{dt} = f(y, t) \quad y(t_o) = y_o$$

- i.c. gives us y_o, t_o

- Apply 2nd order R.K. (Improved Euler) to start the calculations

$$t_1 = t_o + \Delta t$$

$$y_1{}^* = y_o + \Delta t \ f(y_o, t_o)$$

$$y_1 = y_o + \Delta t \ \frac{1}{2}[f(y_o, t_o) + f(y_1{}^*, t_1)]$$

Now we know y_1, t_1

- From time level $j = 1$ to $j+1 = 2$; apply 2nd order Adams Open Formula

$$t_2 = t_1 + \Delta t$$

$$y_2 = y_1 + \Delta t\left[\frac{3}{2}\ f(y_1, t_1) - \frac{1}{2}\ f(y_o, t_o)\right]$$

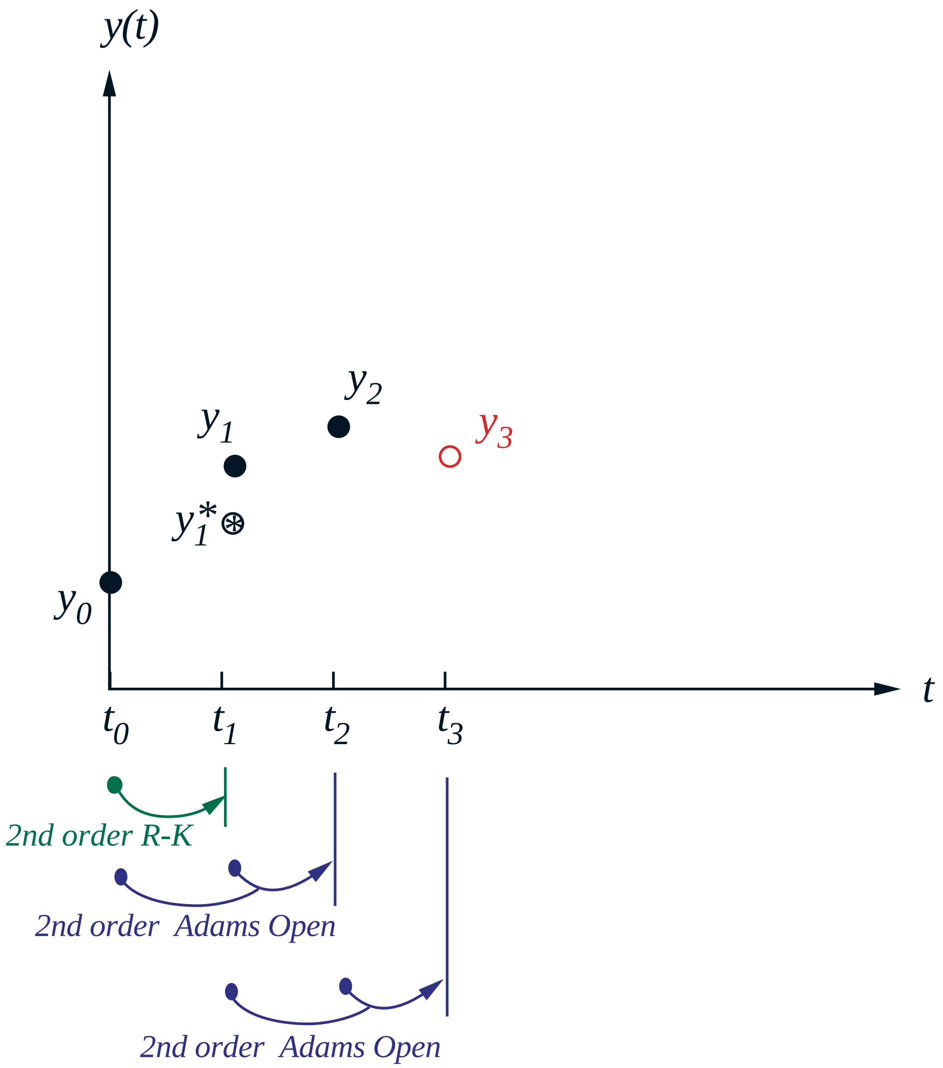
Now we know y_2, t_2

- From time level $j = 2$ to $j+1 = 3$; apply 2nd order Adams Open Formula

$$t_3 = t_2 + \Delta t$$

$$y_3 = y_2 + \Delta t\left[\frac{3}{2}\ f(y_2, t_2) - \frac{1}{2}\ f(y_1, t_1)\right]$$

Now we know y_3, t_3


$y(t)$
t
y_0
y_1
y_1^*
y_2
y_3
t_0
t_1
t_2
t_3
2nd order R-K
2nd order Adams Open
2nd order Adams Open

3rd Order Accurate Adams Open Formula

- Substitute into Equation (1) for $\dot{f}_j$ and $\ddot{f}_j$ using first order accurate approximations carrying a sufficient number of truncation terms as

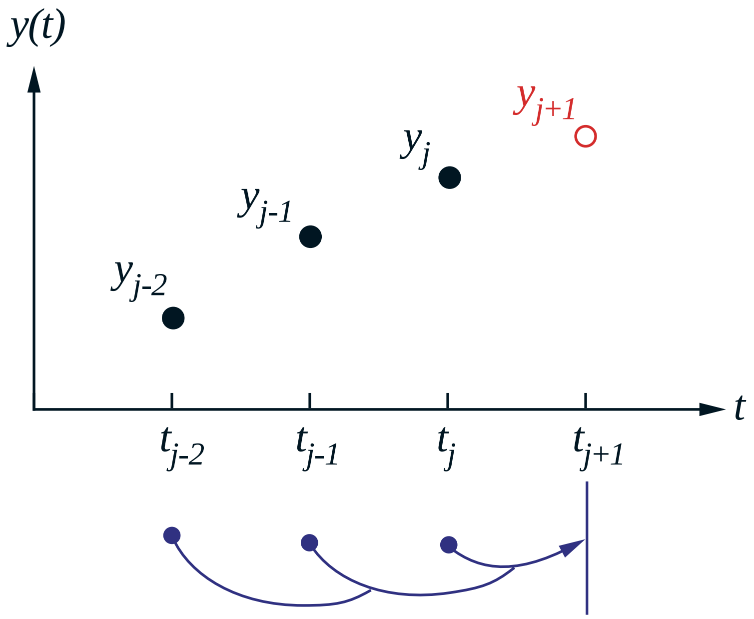
$$\dot{f}_j = \frac{f_j - f_{j-1}}{\Delta t} + \frac{\Delta t}{2}\ddot{f}_j + O(\Delta t)^2$$

$$\ddot{f}_j = \frac{f_j - 2f_{j-1} + f_{j-2}}{(\Delta t)^2} + O(\Delta t)$$

  - Note that the local truncation term for equation (1) must be $O(\Delta t)^4$
    - If you use first order accurate approximations, you must carry a sufficient number of truncation terms in each approximation to the derivatives of f, i.e. $\dot{f}_j$, $\ddot{f}_j$, etc.
    - Alternatively you must use an approximation which in of itself is accurate enough such that the leading order truncation term substituted into equation (1) leads to a $O(\Delta t)^4$ truncation term.

- Collecting terms we have:

$$\boldsymbol{y_{j+1} = y_j + \Delta t\left[\frac{23}{12}f(y_j, t_j) - \frac{16}{12}f(y_{j-1}, t_{j-1}) + \frac{5}{12}f(y_{j-2}, t_{j-2})\right] + O(\Delta t)^4}$$



- Method is third order accurate
- Need to start this method with 2 steps of a 3rd order accurate R.K. method
    - i.c. gives y_o, t_o
    - R.K. starter gives y_1, t_1 and y_2, t_2
    - Now we can use the 3rd order Adams Open Formula

Summary of Adams Open Formulae

- General form of all Adams Open formulae

$$y_{j+1} = y_j + \Delta t[\alpha\ f(y_j, t_j) + \beta\ f(y_{j-1}, t_{j-1}) + \gamma\ f(y_{j-2}, t_{j-2}) + \delta\ f(y_{j-3}, t_{j-3}) + \ldots]$$

- Formulae are explicit: y_{j+1} is computed in terms of slope at t_j, t_{j-1}, $t_{j-2}, \ldots$

- All higher order Adams formulae are not self starting (don't know f_{-1}, f_{-2}, etc.).
    - Must start method with an appropriate order Runge-Kutta formula.

- Open formulae are more efficient than R.K. methods of the same order since slope calculations $f(y, t)$ at a given point are re-used for at least several time steps.

- Open formulae are very easy to implement

- Open formulae ***may*** have stability problems

Closed Formulae

Derivation

- Use a backward Taylor Series expansion for $y(t)$ about $y(t+\Delta t)$. Hence

$$y_j = y_{j+1} - \Delta t \left.\frac{dy}{dt}\right|_{j+1} + \frac{(\Delta t)^2}{2!} \left.\frac{d^2y}{dt^2}\right|_{j+1} - \frac{(\Delta t)^3}{3!} \left.\frac{d^3y}{dt^3}\right|_{j+1} + \dots$$

- Noting that $\left.\frac{dy}{dt}\right|_{j+1} = f_{j+1}$, $\left.\frac{d^2y}{dt^2}\right|_{j+1} = \dot{f}_{j+1}$, $\left.\frac{d^3y}{dt^3}\right|_{j+1} = \ddot{f}_{j+1}$, etc.

$$y_j = y_{j+1} - \Delta t\ f_{j+1} + \frac{(\Delta t)^2}{2!} \dot{f}_{j+1} - \frac{(\Delta t)^3}{3!} \ddot{f}_{j+1} + \dots \quad \Rightarrow$$

$$y_{j+1} = y_j + \Delta t \left[f_{j+1} - \frac{\Delta t}{2} \dot{f}_{j+1} + \frac{\Delta t^2}{3!} \ddot{f}_{j+1} - \dots \right] \tag{2}$$

- Now substitute in backward difference approximations for the various derivatives $\dot{f}_{j+1}$, $\ddot{f}_{j+1}$, etc.

First Order Accurate Adams Closed Formula

- Only consider the first two terms in the backward Taylor series, Equation (2)

$$\boldsymbol{y_{j+1} = y_j + \Delta t\ f(y_{j+1}, t_{j+1}) + O(\Delta t)^2}$$

- Notes
  - Hence we are computing our updated point using the slope of our updated point (versus the open formula where we used the old point to compute the slope)!
  - Formula is implicit since computation of y_{j+1} involves evaluating the slope at $f(y_{j+1}, t_{j+1})$
  - First and second order closed formulae are self starting while higher order closed formulae are not
  - If $f(y, t)$ is a linear function of y → we can solve for y directly:
    - e.g. Solve $\frac{dy}{dt} = y + t^3$ using the first order Adams Closed Formula

$$y_{j+1} = y_j + \Delta t(y_{j+1} + t_{j+1}^3) \quad \Rightarrow$$

$$y_{j+1}(1-\Delta t) = y_j + \Delta t\ t_{j+1}^3 \quad \Rightarrow$$

$$y_{j+1} = \frac{1}{(1-\Delta t)}[y_j + \Delta t\ t_{j+1}^3]$$

- If $f(y, t)$ is a ***nonlinear*** function of y → we must iterate to get a solution
  - e.g. Solve $\frac{dy}{dt} = y^2 + t^3$ using the First Order Adams Closed Formula

$$y_{j+1} = y_j + \Delta t(y_{j+1}^2 + t_{j+1}^3)$$

  - Establish an iterative solution

$$y_{j+1}^{(k+1)} = y_j + \Delta t[(y_{j+1}^{(k)})^2 + t_{j+1}^3]$$

  - Note that this 1st order closed formula is self starting

2nd Order Accurate Adams Closed Formulae

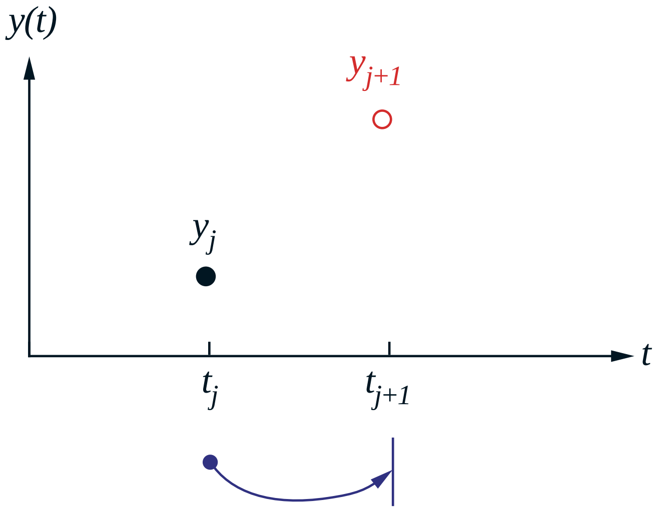
- Approximate $\dot{f}_{j+1}$ using a first order backward difference approximation:

$$\dot{f}_{j+1} = \frac{f_{j+1} - f_j}{\Delta t} + O(\Delta t)$$

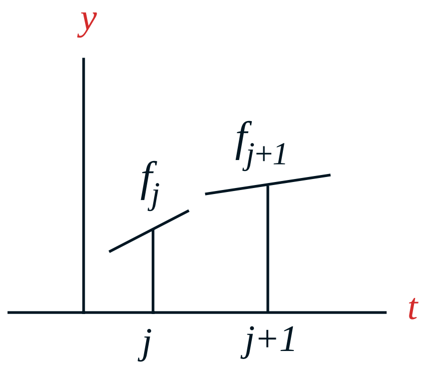
- Substituting into Equation (2) and collecting terms yields a locally 3rd and globally 2nd order method:

$$y_{j+1} = y_j + \frac{\Delta t}{2}[f_{j+1} + f_j] + O(\Delta t)^3 \quad \Rightarrow$$

$$\boldsymbol{y_{j+1} = y_j + \Delta t\, \frac{1}{2}[f(y_{j+1}, t_{j+1}) + f(y_j, t_j)] + O(\Delta t)^3}$$



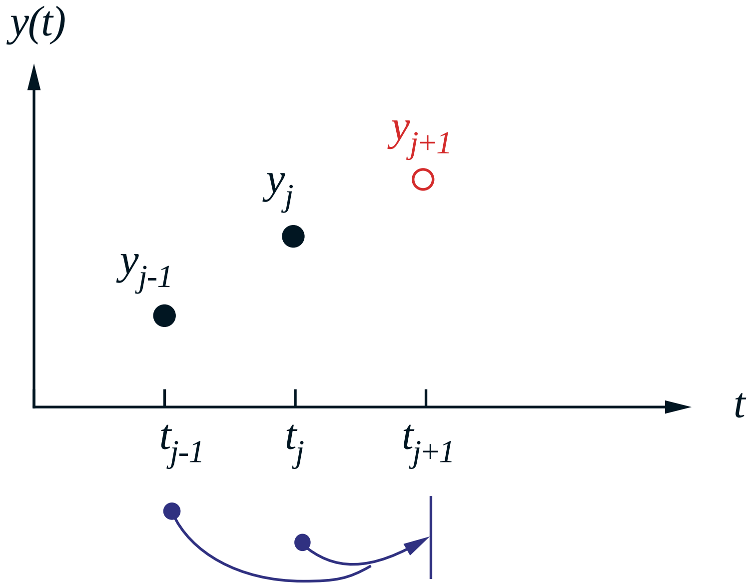
- Notes
  - Formula is implicit, i.e. y_{j+1} involves calculating $f(y_{j+1}, t_{j+1})$
  - Same as “trapezoidal rule” or Crank-Nicolson $\Rightarrow$ Slope is averaged between the old j time level and the new $j+1$ time level



  - Must iterate if $f(y, t)$ is nonlinear in y
  - Formula is ***self*** starting

3rd Order Accurate Adams Closed Formula

$$y_{j+1} = y_j + \Delta t\left[\frac{5}{12}f(y_{j+1}, t_{j+1}) + \frac{8}{12}f(y_j, t_j) - \frac{1}{12}f(y_{j-1}, t_{j-1})\right] + O(\Delta t)^4$$



- Notes
    - Formula derived by taking Equation (2) and substituting backward finite difference approximations for $\dot{f}_{j+1}$ and $\ddot{f}_{j+1}$.

- Difference approximations used in the derivation must be of sufficient accuracy! You can either:
    - Apply first order approximations and carry a sufficient number of truncation terms
    - Apply higher order accurate approximations
    - Either way, all truncated terms ***must*** be consistently $O(\Delta t)^4$!
- Formula is implicit since it involves computing y_{j+1} using the slope $f(y_{j+1}, t_{j+1})$
- Must iterate if $f(y, t)$ is nonlinear
- Formula is third order accurate
- This formula and all closed formulae of 3rd order or higher accuracy are ***not self starting*** → must use R.K. methods of equal or better order accuracy as "starters"
- It can be costly to iterate → try to get a good first guess for $y_{j+1}^{(0)}$
    - try $y_{j+1}^{(0)} \cong y_j$
    - another first estimate could be obtained by using an <u>open</u> formula to compute $y_{j+1}^{(0)}$ → <u>Predictor-Corrector Methods</u>

Predictor-Corrector Methods

- **Provide a first estimate for the new solution $y_{j+1}^{(0)}$ using an open formula → Predictor**
- **Apply a closed formula using $y_{j+1}^{(0)}$ as an initial estimate to start the iteration → Corrector. Only need a few iterations since initial "guess" is very good!**
- Require that order of the corrector $\geq$ the order of the predictor
- Advantages of P-C methods
  - Few iterations are required due to the excellent first guess
  - Stability properties are controlled by the corrector! Correctors or closed formulae have excellent stability properties.
  - Error estimates are easy to obtain
- If needed, use R.K. single step methods as starters
- P-C methods overall are very efficient and are often used in production codes

Example

- Predictor: 4th order Adams Open

$$y_{j+1}^{(0)} = y_j + \Delta t\left[\frac{55}{24} f(y_j, t_j) - \frac{59}{24} f(y_{j-1}, t_{j-1}) + \frac{37}{24} f(y_{j-2}, t_{j-2}) - \frac{9}{24} f(y_{j-3}, t_{j-3})\right]$$

- Corrector: 4th order Adams Closed

$$y_{j+1}^{(k+1)} = y_j + \Delta t\left[\frac{9}{24} f(y_{j+1}^{(k)}, t_{j+1}) + \frac{19}{24} f(y_j, t_j) - \frac{5}{24} f(y_{j-1}, t_{j-1}) + \frac{1}{24} f(y_{j-2}, t_{j-2})\right]$$

  - When $y_{j+1}^{(k+1)}$ has converged $\Rightarrow y_{j+1}^{(k+1)} - y_{j+1}^{(k)} \leq$ specified value $\Rightarrow$ $\boldsymbol{y_{j+1}^{(k+1)}} \rightarrow \boldsymbol{y_{j+1}}$

- Must start the method if higher than 2nd order → starter
  - Accuracy of the starter must be equal or better than the corrector
  - Need to obtain values of y and f for the first three steps beyond the i.c. (y_o, y_1, y_2, y_3 with corresponding f's such that the predictor can be used)
  - Thus, in this case we would have taken 3 starter steps to obtain y_1, y_2 and y_3 using at least a 4th order accurate R.K.

- Improve the initial value for the corrector by estimating the truncation error of the predictor → modifier

$$\tilde{y}^{(0)}_{j+1} = y^{(0)}_{j+1} + \lambda(y_j - y^{(0)}_j)$$

where

$\tilde{y}^{(0)}_{j+1}$ will be the value used to start the corrector

$y^{(0)}_{j+1}$ = the value from the predictor

y_j = the final solution (converged corrector solution) for the previous time step

$y^{(0)}_j$ = the unmodified predictor value from the previous time step

- Estimate of the error in predictor comes from comparing the error series for the predictor and the corrector

- The λ varies depending on the method!

- Estimate for the truncation error of the corrector → total truncation error per time step (not total solution error)

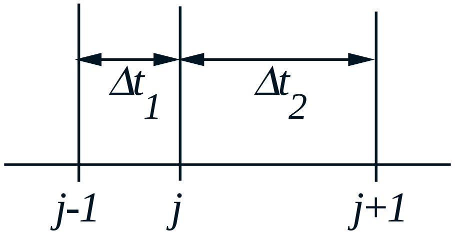
$$E_{j+1} = (1-\lambda)(y_{j+1} - y_{j+1}^{(0)})$$

  - allows modification of time step Δt to obtain the desired accuracy
  - i.e. you can estimate whether to increase/decrease Δt)

- Summary of the steps in a P-C procedure
  - (1) Use Starter for only the first few time steps
  - (2) Apply the Predictor
  - (3) Apply the Modifier
  - (4) Apply the Corrector and iterate to a specified tolerance
  - (5) Repeat step (2)

Implementation of Changes in Time Step

- Change time step from Δt_1 to Δt_2



- If the formula contains only j and $j+1$ → no problem

- If formula contains $j-1$ → there is a problem since you don't know the value of the solution y at t_{j-1}

- Options:
  - Use R.K. method to start up method from the time level where you change the time step, i.e. time level t_j
  - Use a polynomial interpolator to get an actual continuous function of functional values behind j for some distance

Comments Predictor-Corrector Methods

- For most problems P-C method uses less computer time than R.K. methods of the same order

- Many predictors have poor stability characteristics
  - Unstable predictor → stability has only one time step to be unstable before it is improved by the corrector
  - Hence it is important to have a stable corrector → however many of the correctors have very good stability characteristics!