NUCL 511
Nuclear Reactor Theory and Kinetics

Lecture Note 9

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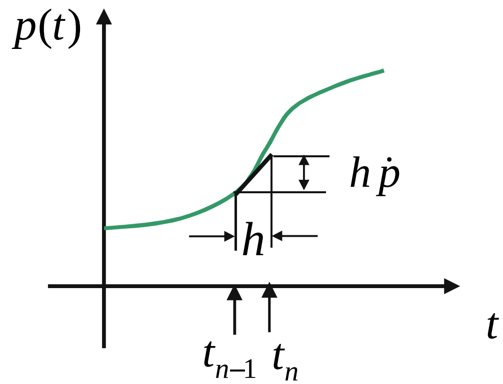
Numerical Solution of PKE

- Prompt kinetics (simplest case)

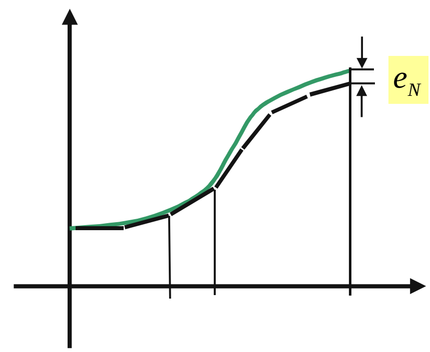
$$\dot{p}(t) = \frac{\rho(t) - \beta}{\Lambda} p(t) = \alpha_p(t) p(t) = f(t, p)$$



- Explicit Euler method
  - Discretize time with a time step size *h*
  - Fine the solution at $t = t_n$ using the solution at $t = t_{n-1}$
    - *Initial condition p0 is known for n = 1*

$$\dot{p}_{n-1} \approx \frac{p_n - p_{n-1}}{h}$$

$$p_n = p_{n-1} + \dot{p}_{n-1} h = p_{n-1} \left(1 + \frac{\rho_{n-1} - \beta}{\Lambda} h \right)$$



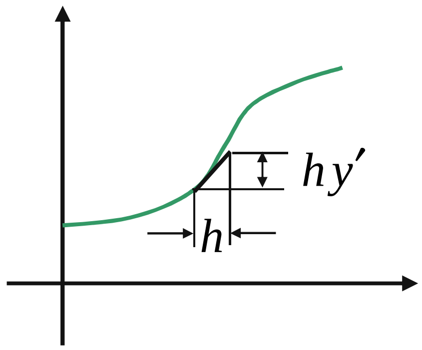
  - Involves errors because the finite difference approximation of the slope cannot be exact
  - The error will be accumulated as well

Euler Method

- Normal form of first order ODE

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0$$

- Explicit Euler Method



$$y_0 = y(x_0)$$
$$y_1 = y_0 + y_0' h = y_0 + f(x_0, y_0)h$$
$$\dots$$
$$y_{n+1} = y_n + y_{n-1}' h = y_n + f(x_{n-1}, y_{n-1})h$$

- Local error of Euler method (single step)
  - Let $\bar{y}(x)$ be the true solution and suppose $y_n = \bar{y}_n$ and $y_n' = \bar{y}_n'$

$$\bar{y}_{n+1} = \bar{y}(x_n + h) = \bar{y}_n + \bar{y}_n' h + \frac{1}{2}\bar{y}''(\xi_n)h^2, \quad x_n \le \xi_n \le x_{n+1}$$

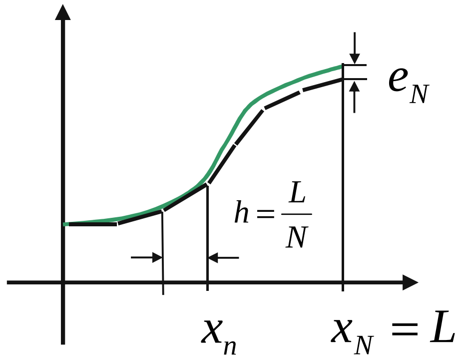
$$y_{n+1} = y_n + y_n' h = \bar{y}_n + \bar{y}_n' h$$

$$e_{n+1} = y_{n+1} - \bar{y}_{n+1} = -\frac{1}{2}\bar{y}''(\xi_n)h^2 = O(h^2)$$

Global Error of Euler Method

- Error at the end of the problem domain

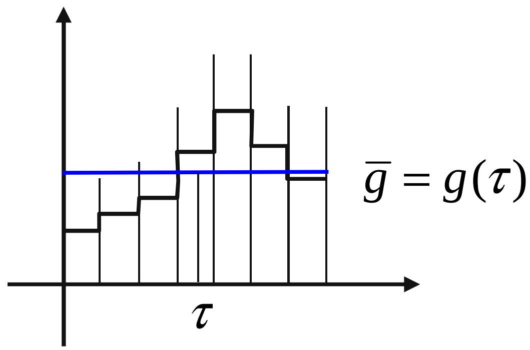
$$e_N = \sum_{n=1}^{N} e_n = -\sum_{n=1}^{N} \frac{1}{2} \bar{y}_n''(\xi_n) h^2, \quad x_{n-1} < \xi_n < x_n$$



$$e_N = \sum_{n=1}^{N} \left[-\frac{1}{2} \bar{y}_n''(\xi_n) h \right] h$$

$$= \sum_{n=1}^{N} g(x_n) h = \bar{g} L = \frac{1}{2} \bar{y}_n''(\tau) h L$$

$$0 < \tau < L$$



$\Rightarrow \quad e_N = O(h)$: First order accuracy

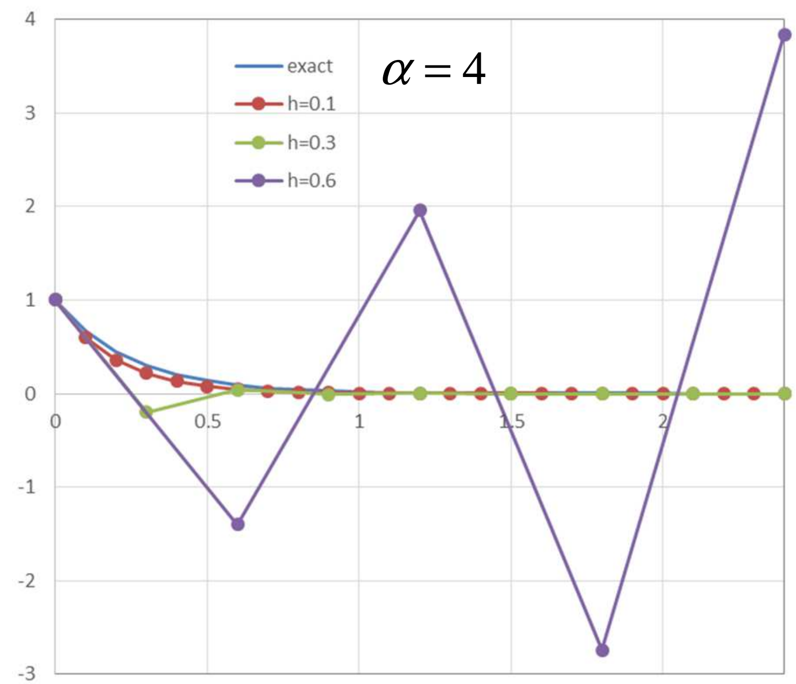
Stability of Explicit Euler Method

- Suppose the following ODE

$$\frac{dy}{dt} = -\alpha y, \quad y(0) = y_0 \quad \Rightarrow \quad y(t) = y_0 e^{-\alpha t}$$

- Explicit Euler method

$$y_{n+1} = y_n - \alpha y_n h = (1-\alpha h) y_n$$



- Solution behavior vs. time step size

$$1-\alpha h > 0 \quad \Rightarrow \quad h < \frac{1}{\alpha}: \ \text{Stable}$$

$$-1 < 1-\alpha h < 0 \quad \Rightarrow \quad \frac{1}{\alpha} < h < \frac{2}{\alpha}: \ \text{Overshoot, Unstable}$$

$$1-\alpha h < -1 \quad \Rightarrow \quad \frac{2}{\alpha} < h: \ \text{Divergent}$$

Unstable behavior is noted if there is fluctuation in the solution (not monotonous increase)

Implicit Euler Method

- Use the endpoint slope of the interval

$$y'_{n+1} = f(x_{n+1}, y_{n+1})$$
$$y_{n+1} = y_n + y'_{n+1}h$$

  - Example for the exponential decay

$$y_{n+1} = y_n - \alpha y_{n+1}h \quad \Rightarrow \quad y_{n+1} = \frac{1}{1+\alpha h} y_n$$

$$0 < \frac{1}{1+\alpha h} < 1 \quad \Rightarrow \quad \text{uncontionally stable}$$

- Unconditionally stable, but may lead to a nonlinear equation

$$y_{n+1} = y_n + f(x_{n+1}, y_{n+1})h$$

- The order of accuracy is a first order like the explicit scheme

$$\dot{p}_{n-1} \cong \frac{p_n - p_{n-1}}{h} = \alpha_p(t_n)p_n = \frac{\rho_n - \beta}{\Lambda} p_n \quad \Rightarrow \quad p_n = \frac{p_{n-1}}{1+\alpha_n h}$$

Euler Methods for 6G PKE

- Point kinetics equation

$$\dot{p} = \frac{\rho(t)-\beta}{\Lambda} p + \frac{1}{\Lambda}\sum_{k=1}^{K} \lambda_k \zeta_k$$

$$\dot{\zeta}_k = \beta_k p - \lambda_k \zeta_k$$

- Explicit method

$$\frac{p_n - p_{n-1}}{h} = \frac{1}{\Lambda}\left[(\rho_{n-1}-\beta)p_{n-1} + \sum_{k=1}^{K}\lambda_k \zeta_k^{(n-1)}\right] \equiv \frac{1}{\Lambda} R_{n-1}$$

$$\frac{\zeta_k^{(n)} - \zeta_k^{(n-1)}}{h} = \beta_k p_{n-1} - \lambda_k \zeta_k^{(n-1)}$$

$\Rightarrow$

$$p_n = p_{n-1} + \frac{h}{\Lambda} R_{n-1}$$

$$\zeta_k^{(n)} = (1-\lambda_k h)\zeta_k^{(n-1)} + \beta_k h p_{n-1}$$

- Implicit method

$$\frac{p_n - p_{n-1}}{h} = \frac{1}{\Lambda}\left[(\rho_n - \beta)p_n + \sum_{k=1}^{K}\lambda_k \zeta_k^{(n)}\right]$$

$$\frac{\zeta_k^{(n)} - \zeta_k^{(n-1)}}{h} = \beta_k p_n - \lambda_k \zeta_k^{(n)}$$

$\Rightarrow$

$$\left[\frac{\Lambda}{h} + (\beta - \rho_n)\right] p_n - \sum_{k=1}^{K}\lambda_k \zeta_k^{(n)} = \frac{\Lambda}{h} p_{n-1}$$

$$-\beta_k p_n + \left(\frac{1}{h} + \lambda_k\right)\zeta_k^{(n)} = \frac{\zeta_k^{(n-1)}}{h}$$

Implicit Euler Method for 6G PKE

- Implicit scheme yields a system of 7 coupled equations

$$\left[\frac{\Lambda}{h}+(\beta-\rho_n)\right]p_n-\sum_{k=1}^{K}\lambda_k\zeta_k^{(n)}=\frac{\Lambda}{h}p_{n-1}$$

$$-\beta_k p_n+(\frac{1}{h}+\lambda_k)\zeta_k^{(n)}=\frac{\zeta_k^{(n-1)}}{h}$$

$$\begin{bmatrix} \Lambda/h+(\beta-\rho_n) & -\lambda_1 & \cdots & -\lambda_6 \\ -\beta_1 & 1/h+\lambda_1 & & \\ & & \ddots & \\ -\beta_6 & & & 1/h+\lambda_6 \end{bmatrix}\begin{bmatrix} p_n \\ \zeta_1^{(n)} \\ \vdots \\ \zeta_6^{(n)} \end{bmatrix}=\begin{bmatrix} \Lambda p_{n-1}/h \\ \zeta_1^{(n-1)}/h \\ \vdots \\ \zeta_6^{(n-1)}/h \end{bmatrix}$$

  - Arrow head form

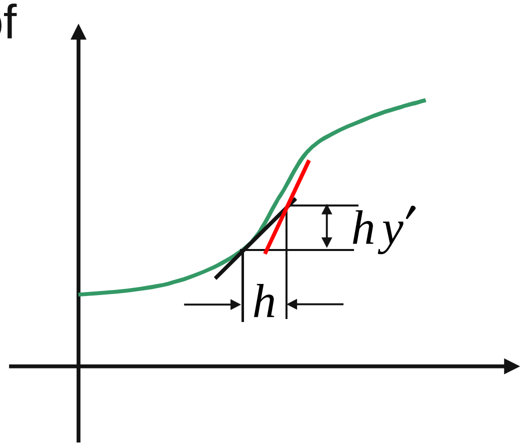
$$\begin{bmatrix} 1/h+\lambda_1 & & & -\beta_1 \\ & \ddots & & \\ & & 1/h+\lambda_6 & -\beta_6 \\ -\lambda_1 & \cdots & -\lambda_6 & \Lambda/h+(\beta-\rho_n) \end{bmatrix}\begin{bmatrix} \zeta_1^{(n)} \\ \vdots \\ \zeta_6^{(n)} \\ p_n \end{bmatrix}=\begin{bmatrix} \zeta_1^{(n-1)}/h \\ \vdots \\ \zeta_6^{(n-1)}/h \\ \Lambda p_{n-1}/h \end{bmatrix}$$

Predictor-Corrector Method

- Predictor step
  - Determine the new provisional value by the use of the explicit Euler method

$$y'_n = f(x_n, y_n)$$

$$\tilde{y}_{n+1} = y_n + h\, y'_n$$



  - Determine the slope at the new point

$$\tilde{y}'_{n+1} = f(x_{n+1}, \tilde{y}_{n+1}) = f(x_n + h, y_n + hy'_n)$$

- Corrector step
  - Determine the interval average slope using the beginning and end point slopes

$$\hat{y}'_n = \frac{1}{2}(y'_n + \tilde{y}'_{n+1})$$

  - Obtain the final value using the average slope

$$y_{n+1} = y_n + h\hat{y}'_n$$

$$= y_n + \frac{1}{2}[y'_n + f(x_n + h, y_n + hy'_n)]h$$

Predictor-Corrector Method

- Error of Predictor-Corrector Method
  - Predictor-corrector solution

$$\begin{aligned}
\tilde{y}'_{n+1} &= f(x_n + h, y_n + hy'_n) \\
&= f(x_n, y_n) + \frac{\partial f}{\partial x} h + \frac{\partial f}{\partial y} h y'_n + O(h^2) \\
&= f(x_n, y_n) + \left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} y'_n \right) h + O(h^2) \quad \Leftarrow \quad \frac{df}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{dy}{dx} = \frac{dy'}{dx} = y'' \\
&= y'_n + y''_n h + O(h^2)
\end{aligned}$$

$$\begin{aligned}
y_{n+1} &= y_n + \frac{1}{2}\left[y'_n + \left\{ y'_n + y''_n h + O(h^2) \right\} \right] h \\
&= y_n + y'_n h + \frac{1}{2} y''_n h^2 + O(h^3)
\end{aligned}$$

  - Taylor series expansion of true solution

$$\bar{y}_{n+1} = \bar{y}_n + \bar{y}'_n h + \frac{1}{2} \bar{y}''_n h^2 + \frac{1}{6} \bar{y}'''_n h^3 + O(h^4)$$

Predictor-Corrector Method

- One step error
  - Assume the solution is exact at x_n

$$y'_n = f(x_n, y_n) = \bar{y}'_n$$

$$y''_n \equiv \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} y'_n = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} \bar{y}'_n = \bar{y}''_n$$

  - Then the error at x_{n+1} becomes

$$e_{n+1} = y_{n+1} - \bar{y}_{n+1} = -\frac{1}{6} \bar{y}'''_n h^3 + O(h^3) - O(h^4) = O(h^3)$$

  - Third order accurate local error
  - Second order accurate global error