10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green
Lecture #14: Implicit Ordinary Differential Equation (ODE) Solvers. Shooting.

Implicit ODE Solvers

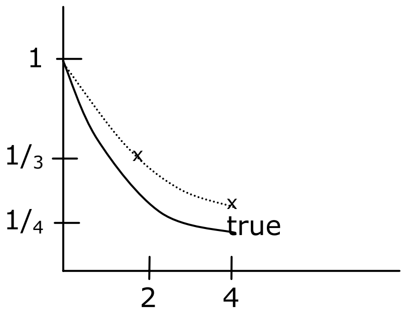
${}^{dy}/_{dt} = -y$ $\quad y(t=0) = 1$ $\quad y_{true} = e^{-t}$

with explicit Euler $\quad \underline{G} = \underline{F}(\underline{Y}(t))$

for this case, instability if $\Delta t > 1$

with implicit Euler $\quad \underline{G} = \underline{F}(\underline{Y}\quad(t+\Delta t))$ $\qquad$ For $\Delta t = 2$,

$$Y_{t+\Delta t}^{new} = Y_t^{old} + \Delta t * F(Y^{\text{new}})$$



$y_{new} = 1+2(-y_{new})$

$3y_{new} = 1 \rightarrow y_{new} = {}^{1}/_{3}$

$e^{-2} = y_{true}$

$y_{new} = {}^{1}/_{3} + 2(-y_{new})$

$3y_{new} = {}^{1}/_{3} \rightarrow y_{new} = {}^{1}/_{9}$

$e^{-4} = y_{true}$

Figure 1. Comparison of implicit Euler to true value.

Accuracy low, but Implicit Euler does not become numerically unstable. Explicit Euler decays too fast. Implicit Euler decays too slow, but it allows one to use larger timesteps.

Stiff Solvers

Stiff: $t_f - t_0 >> \Delta t_{max}$

because of instability (→ Δt_{max})

because of accuracy (→ $t_f - t_0$)

Explicit $|\lambda|_{max}\Delta t \leq 1$ for stability

Stiff solvers:
- ode15s ← usually better
- ode23s ← super stiff

Non-stiff
- ode45 ← explicit method

Example:

$CO + ½O_2 \rightarrow CO_2$

In the presence of H_2, H_2O

$OH + CO \rightarrow H + CO_2$

$H + O_2 \rightarrow OH + O$

$1/\lambda_{OH} \sim 10^{-9}$ s $\qquad$ $1/\lambda_{CO} \sim 1$ s

$\Delta t_{explicit} \leq 10^{-9}$ s

9 orders of magnitude difference in time scales

In diffusion problems $\lambda_{fast}/\lambda_{slow} \sim N_{mesh}^2 \sim 1/(\Delta x)^2$ so a fine mesh makes the problem very stiff.

Shooting

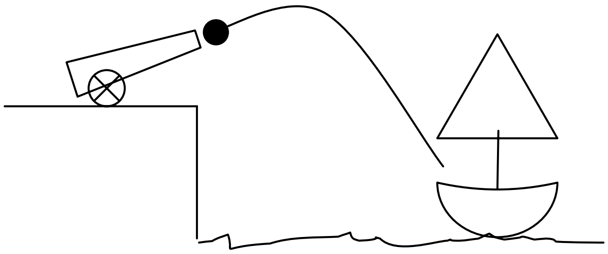


Figure 2.

|-------------------| x

y = height of cannonball

$\underline{Y}(t=0)=\begin{pmatrix} Y_0^{known} \\ Y_0^{guess} \end{pmatrix}$ $\boxed{\underline{Y}_i(t_f) = \underline{Y}_{special}}$

$\underline{Y}(t_f) \leftarrow$ ode15s(…,$\underline{Y}_{os}$,…)

Root-finding (Newton, Broyden)

$g(\underline{Y}^{guess}) = 0 \quad g = \underline{Y}_i(t_f) - \underline{Y}^{special}$

$\underline{Y}_i(t_f) \leftarrow$ ode15s(…, $\underline{Y}^{guess}$,…)

$\underline{Y}_{best}^{guess}$ = bisect(@g, [$\underline{Y}_{low}^{guess}$,$\underline{Y}_{high}^{guess}$],tol)

$|g(\underline{Y}_{best}^{guess})| < ftol$

$|\underline{Y}_{best}^{guess} - \underline{Y}_{true}^{guess}| < xtol$

function error = $g(\underline{Y}^{guess})$

$\underline{Y}_0$ = […, $\underline{Y}^{guess}$]

$\underline{Y}_f$ = ode15s(@F,Yo,tf,tol,options)

error = $\underline{Y}_f(n_{special}) - \underline{Y}_{special}$

inside ode's [events] → stop integrating when something happens