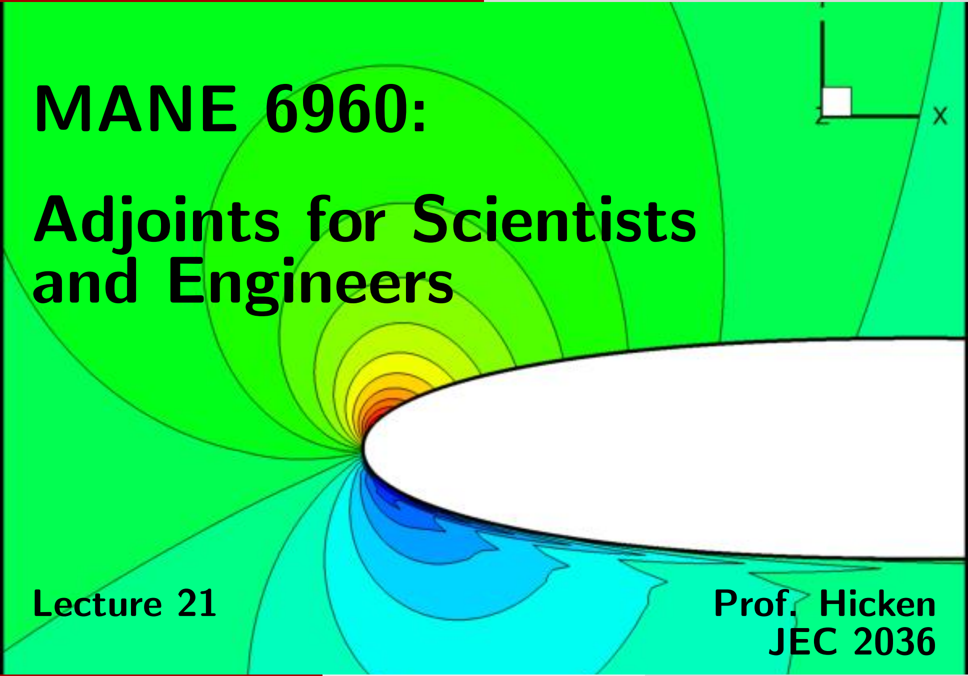


MANE 6960:

Adjoints for Scientists and Engineers

Lecture 21

Prof. Hicken
JEC 2036

Unsteady Adjoint Numerical Studies

Model Problem

I will now present some results of using the two time-marching methods analyzed earlier. To keep visualization simple, I will consider the scalar IVP

$$\frac{du}{dt} = -u, \qquad \forall t \in [0,1], \tag{$\star$}$$
$$u(0) = 1. \tag{IC}$$

- Thus, the exact solution is $u(t) = e^{-t}$
- Note that $T = 1$.

Model Problem (cont.)

The functional considered is

$$J(u) = \int_0^1 \sin(\pi t) u(t)\, dt + u(1).$$

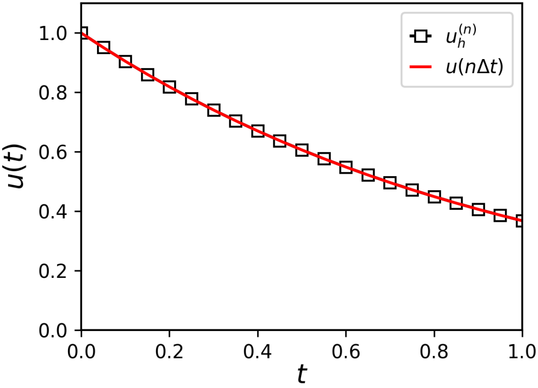
- We have $g(t) = \sin(\pi t)$ and $g_T = 1$.

Based on the above IVP and functional, the exact adjoint is

$$\psi(\tau) = e^{-\tau} \left[g_T + \frac{e^{\tau}}{1+\pi^2} \left(\sin(\pi\tau) - \pi \cos(\pi\tau) \right) + \frac{\pi}{1+\pi^2} \right]$$

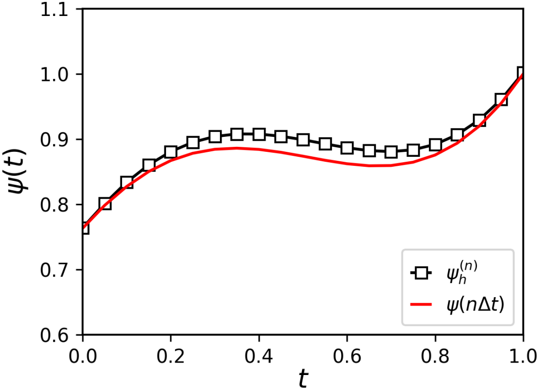
where $\tau = T - t = 1 - t$

RK2 Results



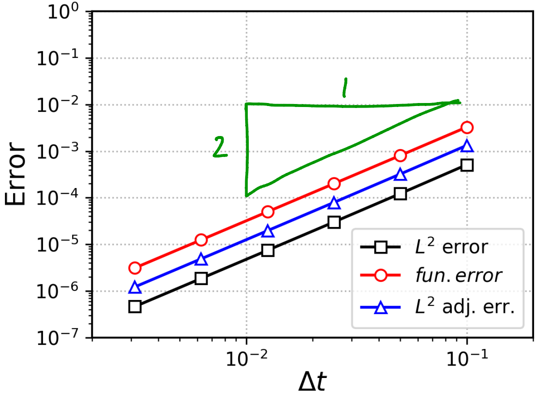
RK2 discrete solution and the exact solution

RK2 Results (cont.)



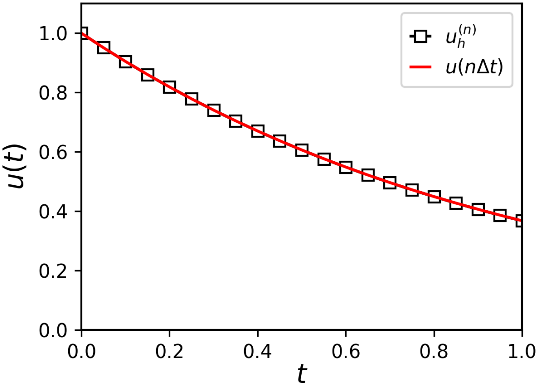
RK2 discrete adjoint and the exact adjoint

RK2 Results (cont.)



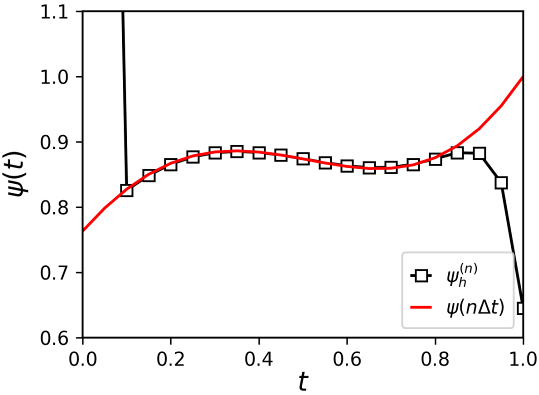
RK2 Solution, adjoint, and functional errors

BDF2 Results



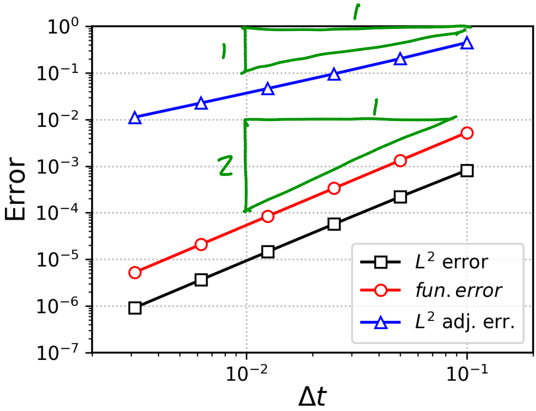
BDF2 discrete solution and the exact solution

BDF2 Results (cont.)



BDF2 discrete adjoint (scaled by 2) and the exact adjoint

BDF2 Results (cont.)



BDF2 Solution, adjoint, and functional errors

RK2 Revisited

The intermediate stage in RK2, $\hat{u}^{(n+1/2)}$, is second-order accurate locally, which suggests that we could use it in the functional.

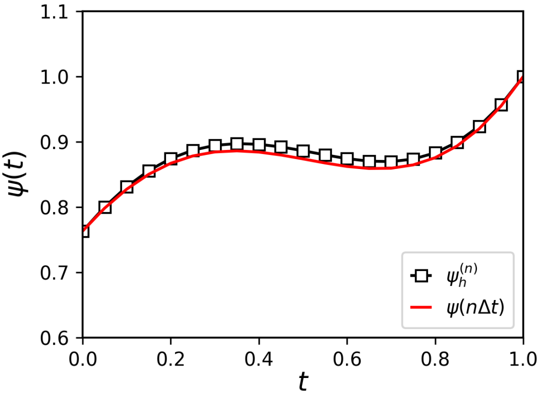
- Indeed, if we include $\hat{u}^{(n+1/2)}$ in the functional, we effectively half the time-step size, so the functional error might reduce by as much as a factor of 4.

Using the trapezoid rule on each step, we have the following expression for the discrete functional that includes $\hat{u}_h^{(n+1/2)}$:

$$J_{h,\Delta t} = \sum_{n=0}^{N-1} \frac{\Delta t}{4} \left[\left(g^{(n)}\right)^T u_h^{(n)} + 2 \left(g^{(n+1/2)}\right)^T \hat{u}_h^{(n+1/2)} \right.$$

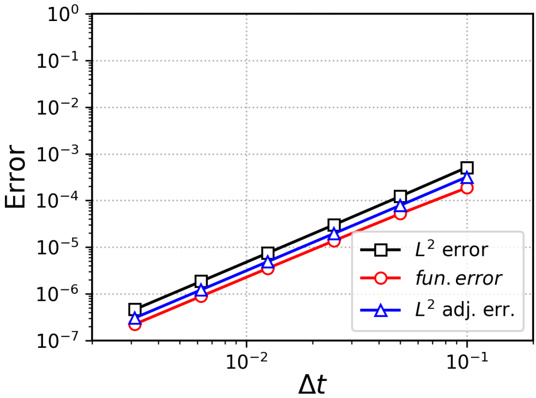
$$\left. + \left(g^{(n+1)}\right)^T u_h^{(n+1)} \right] + g_T^T u_h^{(N)}$$

RK2 Revisited (cont.)



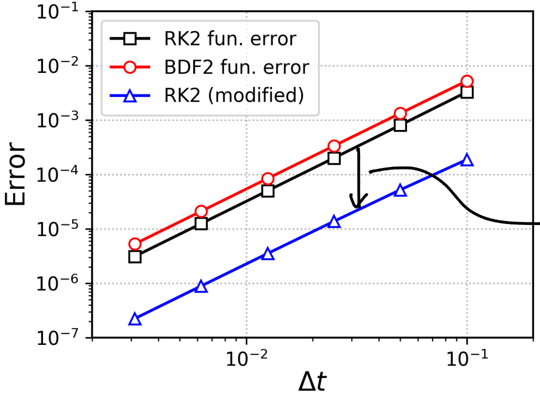
modified RK2 discrete adjoint and the exact adjoint

RK2 Revisited (cont.)



modified RK2 Solution, adjoint, and functional errors

RK2 Revisited (cont.)



factor of 15 improvement

Comparison of functional errors

Deriving the Adjoint IBVP for Nonlinear Problems

Model Nonlinear IBVP

Before deriving the adjoint IBVP for nonlinear problems, we make the following observation:

- Most nonlinear IBVP have linear temporal operators, such as $\partial u/\partial t$ and $\partial^2 u/\partial t^2$.

If the above assumption is not met, one can always apply Fréchet differentiation to the space-time operator, and derive the space-time extended Green's identity.

We will, furthermore, only consider $\partial u/\partial t$.

- $\partial^2 u/\partial t^2$ can be handled as in the linear IBVP described earlier

Model Nonlinear IBVP (cont.)

Therefore, we will focus on nonlinear IBVPs of the form

$$\begin{aligned} \frac{\partial u}{\partial t} + N(u) &= 0, && \forall x \in \Omega, t \in [0,T], \\ B(u) &= 0, && \forall x \in \Gamma, t \in [0,T], \\ u &= u_0, && \forall x \in \Omega, t = 0. \end{aligned} \qquad (\star)$$

- note that the initial condition is also a linear operator
- if this is not the case, it is best to first derive the extended Green's identity to check for compatibility.

Model Nonlinear IBVP (cont.)

The generic, nonlinear functional is given by

$$J(u) = \int_0^T \int_\Omega g(u)\, d\Omega\, dt + \int_0^T \int_\Gamma c(C(u))\, d\Gamma\, dt + \int_\Omega g_T\left(u\big|_{t=T} \right)\, d\Omega$$

Recycling Adjoint BVP Theory

Recall the compatibility condition (i.e. Green's extended identity) for a nonlinear BVP:

$$(\psi, N'[u]v)_\Omega - (v, N'[u]^*\psi)_\Omega =$$
$$(C[u]'v, B'[u]^*\psi)_\Gamma - (B'[u]v, C'[u]^*\psi)_\Gamma, \qquad \forall v, \psi \in \mathcal{U},$$

By including the temporal derivative in the PDE and integrating over the time domain, we can "recycle" the above expression to get the space-time generalization, just as we did for the linear IBVP.

Recycling Adjoint BVP Theory (cont.)

First, we Fréchet differentiate the adjoint-weighted residual with respect to u in the direction v to get

$$D_v \left\{ \int_0^T \int_\Omega \psi \left[\frac{\partial u}{\partial t} + N(u) \right] \, d\Omega \, dt \right\}$$

$$= \int_0^T \int_\Omega \psi \left[\frac{\partial v}{\partial t} + N'[u] v \right] d\Omega \, dt$$

We also need the Fréchet derivative of the functional:

$$J'[u]v = \int_0^T \int_\Omega g'[u] \, v \, d\Omega \, dt$$

$$+ \int_0^T \int_\Gamma c'[Cu] \, C'[u] \, v \, d\Gamma \, dt + \int_\Omega g_T'[u(T)] \, v \Big|_{t=T} d\Omega$$

Recycling Adjoint BVP Theory (cont.)

Next, we recall from the linear IBVP analysis that

$$\int_\Omega \int_0^T \psi \frac{\partial v}{\partial t}\, dt\, d\Omega = -\int_\Omega \int_0^T \frac{\partial \psi}{\partial t} v\, dt\, d\Omega + \int_\Omega (\psi v)\big|_{t=0}^{t=T}\, d\Omega. \quad (\ddagger)$$

To put all the pieces together, we form the following Lagrangian, Fréchet differentiate, and set the result to zero:

$$L(u,\psi) = J(u) - \int_0^T \int_\Omega \psi \left[\frac{\partial u}{\partial t} + N(u) \right] d\Omega\, dt$$

$$L'[u]v = J'[u]v \overbrace{- \int_\Omega \int_0^T \psi \frac{\partial v}{\partial t}\, dt\, d\Omega}^{(\ddagger)} \overbrace{- \int_0^T \int_\Omega \psi\, N'[u]v\, d\Omega\, dt}^{\text{BVP compatibility}}$$

Recycling Adjoint BVP Theory (cont.)

$$L'[u]v = \overbrace{\int_0^T\int_\Omega g'[u]\,v\,d\Omega\,dt}^{\text{PDE}} + \overbrace{\int_0^T\int_\Gamma c'[C(u)]\,C'[u]\,v\,d\Gamma\,dt}^{\text{adj B.C.}}$$

$$+ \overbrace{\int_\Omega g_T'[u(T)]\,v\Big|_{t=T}\,d\Omega}^{\text{adj T.C}} - \overbrace{\int_\Omega\int_0^T -\frac{\partial\psi}{\partial t}\,v\,dt\,d\Omega}^{\text{PDE}} - \overbrace{\int_\Omega (\psi v)\Big|_{t=0}^{T}\,d\Omega}^{\text{adj. T.C. and linearized dual fun.}}$$

$$- \overbrace{\int_0^T\int_\Omega v\,N'[u]^*\,\psi\,d\Omega\,dt}^{\text{PDE}} - \overbrace{\int_0^T\int_\Gamma (C'[u]v)\,B'[u]^*\,\psi\,d\Gamma\,dt}^{\text{adj B.C.}}$$

$$+ \overbrace{\int_0^T\int_\Gamma (B'[u]v)(C'[u]^*\psi)\,d\Gamma\,dt}^{\text{linearized dual functional}}$$

Recycling Adjoint BVP Theory (cont.)

Definition: Adjoint Problem (nonlinear IBVP)

Let u be the solution to the nonlinear IBVP ($\star$), and consider the nonlinear functional $J(u)$ defined earlier. Then the associated adjoint initial-boundary-value problem is

$$\begin{aligned} -\frac{\partial \psi}{\partial t} + N'[u]^* \psi &= g'[u], && \forall x \in \Omega, t \in [0,T] \\ B'[u]^* \psi &= c'[Cu], && \forall x \in \Gamma, t \in [0,T], \\ \psi &= g'_T\left[u(T)\right], && \forall x \in \Omega, t = T. \end{aligned} \tag{Adj}$$

Exercise

Consider the IVPs

$$\frac{du}{dt} = -u, \qquad u(0) = u_0 \tag{1}$$
$$\frac{du}{dt} = -u^3, \quad u(0) = u_0. \tag{2}$$

If you had to implement an adjoint based on the IVPs (1) and (2), how would the implementations differ?

need to save u in order to compute $N'[u]^*$

References