LECTURE 4:

PRACTICAL TIME STEPPING FOR QUANTUM GRAPH PDE

$$u_t = \alpha \Delta u + f(u) \quad \text{ON } G$$

WE HAVE A FEW COMPETING GOALS

- WANT HIGH-ORDER METHODS SO WE CAN TAKE LARGE TIME STEPS
- WANT TO HANDLE LAPLACIAN TERMS IMPLICITLY, ALSO TO ALLOW LARGE TIME STEPS
- DO NOT WANT TO DO NEWTON ITERATIONS

SOLUTION: IMPLICIT-EXPLICIT (IMEX) SPLITTING RUNGE-KUTTA (RK) METHODS (ASCHER-RUTH-SPITERI 1997)

REVIEW HOW RK METHODS WORK

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

SUPPOSE $x_n = x(t_n)$ known, want to approximate $x(t_{n+1}) = x(t_n + h)$

$$x(t_{n+1}) = x(t_n + h) = x(t_n) + \int_{t_n}^{t_{n+1}} f(x(s),s)\,ds$$

$$= x(t_n) + \frac{h}{2}\left[f(x(t_n),t_n) + f(x(t_{n+1}),t_{n+1})\right] + O(h^3)$$

DEFINE IMPLICIT TRAPEZOIDAL RULE

$$x_{n+1} = x_n + \frac{h}{2}\left(f(x_n,t_i) + f(x_{n+1},t_{n+1})\right)$$

LOCAL TRUNCATION ERROR $= O(h^3)$

TO REACH A FIXED TIME t_{end} need $O(\frac{1}{h})$ STEPS

SO GLOBAL ERROR $\propto h^2$

MODIFY THIS TO MAKE EXPLICIT

$$\text{let } \overline{X} = x_n + h f(x_n, t_n) \quad \text{i.e. a FWD EULER STEP}$$

THEN LET

$$x_{n+1} = x_n + \frac{h}{2}\left(f(x_n, t_n) + f(\overline{X}, t_{n+1})\right)$$

BY EXPANDING EVERYTHING IN TAYLOR SERIES, CAN SHOW

$|x_{n+1} - x(t_{n+1})| \propto h^3$, KEEP SAME ORDER OF ACCURACY

Q: HOW MANY TIMES DO WE EVALUATE $f(x,t)$ / STEP?

WRITE $k_1 = f(x_n, t_n)$

$k_2 = f(x_n + h k_1, t_n + h)$

THEN $x_{n+1} = x_n + \frac{h}{2}(k_1 + k_2)$ A: 2 EVALUATIONS

THIS IS A 2ND ORDER EXPLICIT RK METHOD

CAN WRITE IMPLICIT TRAPEZOIDAL AS AN IMPLICIT RK METHOD, GOOD FOR STIFF PROBLEMS

MOST COMMONLY USED METHOD IS RK4.

$$k_1 = f(x_n, t_n)$$
$$k_2 = f\left(x_n + \frac{h k_1}{2}, t_n + \frac{h}{2}\right)$$
$$k_3 = f\left(x_n + \frac{h k_2}{2}, t_n + \frac{h}{2}\right)$$
$$k_4 = f(x_n + h k_3, t_n + h)$$

$$x_{n+1} = x_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

RECALL HOW RK METHOD'S ARE DEFINED

S-STAGE EXPLICIT METHOD

$$x_{n+1} = x_n + h\sum_{i=1}^{s} b_i k_i$$

$$k_1 = f(x_n, t_n)$$

$$k_2 = f(x_n + (a_{21}k_1)h, t_n + c_2 h)$$

$$k_3 = f(x_n + (a_{31}k_1 + a_{32}k_2)h, t_n + c_3 h)$$

$$\vdots$$

$$k_s = f(x_n + h\sum_{j=1}^{s-1} a_{sj} k_j, t_n + c_s h)$$

SUMMARIZED BY BUTCHER TABLEAU

$$\begin{array}{c|ccccc}
0 & & & & & \\
c_2 & a_{21} & & & & \\
c_3 & a_{31} & a_{32} & & & \\
\vdots & \vdots & & \ddots & & \\
c_s & a_{s,1} & a_{s2} & \cdots & a_{s,s-1} & \\
\hline
 & b_1 & b_2 & \cdot & b_{s-1} & b_s
\end{array}$$

COEFFICIENTS MUST SATISFY CERTAIN ALGEBRAIC CONDITIONS TO HAVE LOCAL TRUNCATION ORDER $(p+1)$, GLOBAL ORDER p

E.G. $$\sum_{i=1}^{s} b_i = 1$$

$$\sum_{j=1}^{i-1} a_{ij} = c_i \qquad i = 2, \ldots, s$$

EG RK4

$$\begin{array}{c|cccc}
0 & & & & \\
1/2 & 1/2 & & & \\
1/2 & 0 & 1/2 & & \\
1 & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}$$

EXPLICIT METHODS GENERALLY HAVE SEVERE STEPSIZE RESTRICTIONS FOR STIFF PROBLEMS

IMPLICIT METHODS

$$k_i = f(t_n + c_i h,\ x_n + \sum_{j=1}^{s} a_{ij} k_j) \qquad i = 1, \dots s$$

TABLEAU

$$\begin{array}{c|cccc}
c_1 & a_{11} & a_{1s} & \cdots & a_{1s} \\
c_2 & a_{21} & \ddots & & \vdots \\
\vdots & \vdots & & \ddots & a_{s-1,s} \\
c_s & a_{s1} & \cdots & \cdots & a_{ss} \\
\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}$$

NOW WE HAVE TO SOLVE A NONLINEAR PROBLEM TO SIMULTANEOUSLY FIND $k_1, \dots, k_s$

THIS IS GENERALLY OVERKILL BUT PRODUCES HIGHEST ORDER + MOST STABLE METHODS FOR GIVEN S

DIAGONALLY - IMPLICIT RK (DIRK) METHODS

$a_{ij} = 0$ FOR $j > i$

THEN

$k_1 = f(x_n + h a_{11} k_1, t_n + c_1 h)$ SOLVE FOR k_1

$k_2 = f(x_n + h(a_{21} k_1 + a_{22} k_2), t_n + c_2 h)$ SOLVE FOR k_2

ETC IF $X \in \mathbb{R}^m$ then s problem in $\mathbb{R}^m$

RATHER THAN ONE PROBLEM in $\mathbb{R}^{ms}$

EG THE IMPLICIT TRAPEZOIDAL METHOD IS DIRK

$k_1 = f(x_n, t_n)$

$k_2 = f(x_n + h k_2, t_n + h)$

$x_{n+1} = x_n + \frac{h}{2}(k_1 + k_2)$

$$\begin{array}{c|cc}
0 & 0 & 0 \\
1 & 0 & 1 \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}$$

ASCHER-RUUTH-SPITERI 1997

CONSIDER AN ODE OF THE FORM (ASSUME AUTONOMOUS)

$$\dot{x} = f(x) + g(x)$$

$f(x)$ contains nonlinear terms with small stiffness, safe to treat by explicit RK methods

$g(x)$ LARGE STIFFNESS BUT LINEAR, THINK $g(x) = Ax$ WHERE A HAS LARGE EIGENVALUES

TO STEP FROM t_n to $t_{n+1} = t_n + h$

DO FOLLOWING

- SET $\hat{k}_1 = f(x_n)$
- FOR $i = 1:s$
  - SOLVE FOR k_i:

$$k_i = g(X_i)$$

$$X_i = x_n + h\sum_{j=1}^{i} a_{ij} k_j + h\sum_{j=1}^{i} \hat{a}_{i+1,j} \hat{k}_j \quad (*)$$

  - SET $\hat{k}_{i+1} = f(X_i)$

FINALLY, EVALUATE

$$x_{n+1} = x_n + h\sum_{j=1}^{s} b_j k_j + h\sum_{j=1}^{s+1} \hat{b}_j \hat{k}_j \quad (**)$$

IN FACT, WE ASSUME $b_{s+1} = 0$, SO WE CAN SKIP THE LAST EVALUATION $\hat{k}_{s+1} = f(X_s)$

FURTHER, SET THE COEFFICIENTS TO

$$a_{js} = b_j, \quad \hat{a}_{s+1,j} = \hat{b}_j$$

THEN $(*)$ WITH $i=s$ AND $(**)$ ARE SAME EQN AND $x_{n+1} = X_s$

EXAMPLE APPLYING THIS WITH

FORWARD EULER FOR $f(x)$

BACKWARD EULER FOR $g(x)$

YIELDS: $x_{n+1} = x_n + h(f(x_n) + g(x_{n+1}))$

MORE SLOWLY $\hat{k}_1 = f(x_n)$ (A)

$$k_1 = g(\bar{X}_1)$$

WHERE $\bar{X}_1 = x_n + h(\hat{k}_1 + k_1)$

SO $k_1 = g(x_n + h(\hat{k}_1 + k_1))$

$$x_{n+1} = x_n + h(\hat{k}_1 + k_1)$$

NOW ADAPT THIS FOR QUANTUM GRAPH.

RECALL FROM LAST TIME, EXPLICIT STEPS PICK UP IMPLICITNESS FOR ENFORCING VERTEX CONDITIONS

$$u_t = \underbrace{\alpha \Delta u}_{g(u)} + f(u)$$

$$u_{n+1} = u_n + h(\alpha \Delta u_{n+1} + f(u_n))$$

$$u_{n+1} - h\alpha \Delta u_{n+1} = u_n + hf(u_n)$$

DISCRETIZE ON INTERIOR

$$(P_{INT} - h\alpha L_{INT})\vec{u}_{n+1} = P_{INT}(\vec{u}_n + hf(\vec{u}_n))$$

ADD VERTEX CONDS

$$M_{VC}\vec{u}_{n+1} = \vec{0}$$

$$(1 - h\alpha)M_{VC}\vec{u}_{n+1} = 0$$

CONCATENATE

$$(P_{vc} - h\alpha L_{vc})\vec{u}_{n+1} = P_0\left(\vec{u}_n + h f(\vec{u}_n)\right)$$

QGLAB USES A 3RD ORDER 4-STAGE DIRK METHOD

$$
\underbrace{
c_i \;
\begin{array}{c|cccc}
\multicolumn{5}{c}{a_{ij}} \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\
\frac{2}{3} & \frac{1}{6} & \frac{1}{2} & 0 & 0 \\
\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\
1 & \frac{3}{2} & -\frac{3}{2} & \frac{1}{2} & \frac{1}{2} \\
\hline
 & \frac{3}{2} & -\frac{3}{2} & \frac{1}{2} & \frac{1}{2} \\
\multicolumn{5}{c}{b_j}
\end{array}
}_{\text{IM}}
\qquad
\underbrace{
\hat{c}_i \;
\begin{array}{c|ccccc}
\multicolumn{6}{c}{\hat{a}_{ij}} \\
0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\
\frac{2}{3} & \frac{11}{18} & \frac{1}{18} & 0 & 0 & 0 \\
\frac{1}{2} & \frac{5}{6} & -\frac{5}{6} & \frac{1}{2} & 0 & 0 \\
1 & \frac{1}{4} & \frac{7}{4} & \frac{3}{4} & -\frac{7}{4} & 0 \\
\hline
 & \frac{1}{4} & \frac{7}{4} & \frac{3}{4} & -\frac{7}{4} & 0 \\
\multicolumn{6}{c}{\hat{b}_j}
\end{array}
}_{\text{EX}}
$$

SAME TYPE OF MODIFICATIONS ARE MADE TO EQUATIONS DEFINING TH $\hat{k}_i$ & $\hat{k}_i$

$$u_{n+1} = u_n + h\left(\alpha \Delta u_{n+1} + f(u_n)\right)$$

$$u_{n+1} - h\alpha \Delta u_{n+1} = u_n + h f(u_n)$$

DISCRETIZE ON INTERIOR

$$\left(P_{INT} - h\alpha L_{INT}\right)\vec{u}_{n+1} = P_{INT}\left(\vec{u}_n + hf(\vec{u}_n)\right)$$

ADD VERTEX CONDS

$$M_{VC}\,\vec{u}_{n+1} = \vec{0}$$

$$(1 - h\alpha) M_{VC}\,\vec{u}_{n+1} = 0$$

CONCATENATE

$$\left(P_{VC} - h\alpha L_{VC}\right)\vec{u}_{n+1} = P_0\left(\vec{u}_n + h f(\vec{u}_n)\right)$$