LECTURE 3: APPLYING THE DISCRETIZATIONS

OUR BASIC SET UP

- EACH EDGE e_j DISCRETIZED THE <u>EXTENDED</u> GRID OF (N_j+2) POINTS
- THE DISCRETE 2ND DERIVATIVE OPERATOR IS A RECTANGULAR $N_j \times (N_j+2)$ MATRIX L_j^{int} WHICH MAPS TO THE INTERIOR GRID, WHERE ALL EQUATIONS ARE SATISFIED EXCEPT VERTEX CONDITIONS
- AN INTERPOLATION MATRIX $P_{INT}^{(j)}$ MAPS VALUES DEFINED ON EXTENDED GRID TO INTERIOR POINT
- THE VERTEX CONDITIONS AT VERTEX V_k GIVEN BY A WIDE MATRIX OF d_k ROWS $M_{VC}^{(k)}$ ($N_{EXT} = \sum_{e_j \in \mathbb{E}_G} (N_j+2)$ COLUMNS WIDE

SOME NOTATION:

$$L_{INT} = \begin{bmatrix} L_{INT}^{(1)} & & & \\ & L_{INT}^{(2)} & & \\ & & \ddots & \\ & & & L_{INT}^{(|\mathbb{E}_G|)} \end{bmatrix}$$

= WIDE LAPLACIAN

EACH BLOCK HAS TWO MORE COLUMNS THAN ROWS

$$P_{INT} = \begin{bmatrix} P_{INT}^{(1)} & & & \\ & P_{INT}^{(2)} & & \\ & & \ddots & \\ & & & P_{INT}^{(|\mathbb{E}_G|)} \end{bmatrix}$$

= MATRIX INTERPOLATING FROM <u>EXT</u>ENDED GRID TO <u>INT</u>ERIOR GRID

$$\underbrace{M_{VC} = \begin{bmatrix} M_{VC}^{(1)} \\ \vdots \\ M_{VC}^{(|\mathbb{V}_G|)} \end{bmatrix}}_{N_{EXT}} \left.\vphantom{\begin{bmatrix} M \\ \vdots \\ M \end{bmatrix}}\right\} 2|\mathbb{E}_G|$$

= DISCRETIZED VERTEX CONDITION

$\mathbb{O} = 2|E_G| \times N_{EXT}$ MATRIX OF ZEROES

TO SOLVE PROBLEMS UNIQUELY, NEED SQUARE MATRIX

DEFINE $L_0 = \left[\begin{array}{c} L_{INT} \\ \hline \mathbb{O} \end{array}\right]$, $L_{VC} = \left[\begin{array}{c} L_{INT} \\ \hline M_{VC} \end{array}\right]$

$P_0 = \left[\begin{array}{c} P_{INT} \\ \hline \mathbb{O} \end{array}\right]$, $P_{VC} = \left[\begin{array}{c} P_{INT} \\ \hline M_{VC} \end{array}\right]$

WILL USE THESE FOUR MATRICES TO DISCRETIZE A VARIETY OF PROBLEMS

TO SOLVE $\Delta u = f$ ON G

SUBJECT TO HOMOGENEOUS VERTEX CONDITIONS

LET $\vec{f}$ = VECTOR OF f VALUES ON X_{EXT}

$\vec{u}$ = (UNKNOWN) VECTOR OF u VALUES ON X_{EXT}

SOLVE BOTH

$L_{INT}\vec{u} = P_{INT}\vec{f}$ — N_{INT} EQNS IN N_{EXT} VARIABLES

& $M_{VC}\vec{u} = \vec{0}$ — $2|E_G|$ EQNS IN N_{EXT} VARIABLES

N_{EXT} EQNS IN N_{EXT} VARS

CONCATENATE

$L_{VC}\vec{u} = P_0\vec{f}$

EXAMPLE IN SLIDES

EIGENVALUE PROBLEMS ARE VERY SIMILAR

$$L_{INT}\vec{u} = \lambda P_{INT}\vec{u} \quad \text{ON} \quad X_{EXT}$$

$$M_{VC}\vec{u} = \vec{0}$$

CONCATENATE

$$L_{VC}\vec{u} = \lambda P_0 \vec{u}$$

THIS IS A GENERALIZED EIGENVALUE PROBLEM

$$A\vec{v} = \lambda B\vec{v}$$

P_0 IS SINGULAR, SO WE CAN'T JUST LEFT MULTIPLY BY P_0^{-1} TO GET A STANDARD EIGENVALUE PROBLEM.

EXAMPLE IN SLIDES

STATIONARY NLS

$$\Delta\psi + \Lambda\psi + 2\psi^3 = 0 \qquad \text{NOTE } \psi : G \to \mathbb{R}$$

ASSUME $\Lambda \in \mathbb{R}$ IS GIVEN

RECALL NEWTON'S METHOD $f: \mathbb{R}^n \to \mathbb{R}^n$

GIVEN A GUESS x_n s.t $f(x_n) \neq 0$

Let $x_{n+1} = x_n + \delta$

$$f(x_{n+1}) = f(x_n + \delta)$$

$$\approx f(x_n) + Df\big|_{x_n} \cdot \delta$$

let δ SOLVE $Df\big|_{x_n} \delta = -f(x_n)$

SET $x_{n+1} = x_n + \delta$

FOR OUR PROBLEM

$$f(\psi;\lambda) = \Delta\psi + \Lambda\psi + 2\psi^3$$

$$Df(\psi,\lambda) = \Delta + \Lambda + 6\psi^2$$

OF COURSE δ IS SUBJECT TO VERTEX CONDITIONS

$$(\Delta + \Lambda + 6\psi_n^2)\,\delta = -(\Delta\psi_n + \Lambda\psi_n + 2\psi_n^3)$$

DISCRETIZE TO THE INTERIOR POINSTS

$$(L_{INT} + P_{INT}\cdot(6\,\mathrm{diag}\,\psi_n^2 + \Lambda I))\,\delta = -L_{INT}\psi_n - P_{INT}(\Lambda I + 2\,\mathrm{DIAG}\,\psi_n^3)$$

+ VERTEX CONDITIONS

$$M_{VC}\,\delta = 0$$

EXTEND L_{INT} ON LEFT WITH M_{VC}, ALL OTHER MATRICES WITH ZEROES

$$\underbrace{(L_{VC} + P_0(6\,\mathrm{Diag}\,\psi_n^2 + \Lambda I))}_{\text{myMatrix}(\psi_n,\Lambda)}\,\delta = \underbrace{-L_0\psi_n - P_0(\Lambda\psi_n + 2\,\mathrm{DIAG}\,\psi_n^3)}_{\text{myFunction}(\psi_n,\Lambda)}$$

TIME-STEPPING FOR EVOLUTIONARY PDE ON QUANTUM GRAPHS

RECALL SOME BASIC TIME-STEPPING ALGORITHMS FOR $\begin{cases} \frac{du}{dt} = f(u) \\ u(0) = u_0 \end{cases}$

FIX $h \ll 1$. LET $t_n = nh$, $n = 0, 1, 2, \ldots$

$u_n \approx u(t_n)$

FORWARD EULER

$$\frac{d}{dt}\Big|_{t=t_n} = \frac{u(t_{n+1}) - u(t_n)}{h} + O(h)$$

Let x_{n+1} solve

$$\frac{u_{n+1} - u_n}{h} = f(x_n)$$

$$\left. u_{n+1} = u_n + h f(u_n) \right\} \text{ AN EXPLICIT METHOD}$$

LOCAL TRUNCATION ERROR $O(h^2) \rightarrow$ GLOBAL $O(h)$

LET'S TAKE $f(u) = \mu \Delta u$ ON A QUANTUM GRAPH G

CONTINUOUS IN SPACE $u_{n+1} = u_n + h\mu \Delta u_n$

NOW DISCRETIZE. THIS MUST HOLD ON THE INTERIOR GRID.

$$P_{INT} \vec{u}_{n+1} = (P_{INT} + \mu L_{INT}) \vec{u}_n$$

BUT $\vec{u}_{n+1}$ MUST ALSO SATISFY DISCRETIZED VERTEX CONDITITIONS

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

STACK THE TWO EQUATIONS

$$\begin{bmatrix} P_{INT} \\ \hline M_{CV} \end{bmatrix} \vec{u}_{n+1} = \begin{bmatrix} P_{INT} + h\mu L_{INT} \\ \hline 0 \end{bmatrix} \vec{u}_n$$

$$P_{VC} \vec{u}_{n+1} = (P_0 + h\mu L_0) \vec{u}_n$$

- THIS IS <u>IMPLICIT</u>. $\vec{u}_{n+1}$ GIVEN AS THE SOLUTION TO A SYSTEM OF ALGEBRAIC EQNS.
- THE IMPLICITNESS IS LINEAR IN THE UNKNOWN $\vec{u}_{n+1}$
- THE MATRIX P_{VC} IS WELL-CONDITIONED. ALL ITS SINGULAR VALUES ONLY VARY BY A FEW ORDERS OF MAGNITUDE.
- STILL, THE UNDERLYING EQUATION IS STIFF: THE RHS HAS LARGE NEGATIVE EIGENVALUES
- NEED TO TAKE $h \ll 1$ FOR STABILITY

RECALL WHY: SCALAR EXAMPLE

$$\frac{dx}{dt} = \lambda x \qquad \lambda < 0$$

EXACT SOLUTION

$$x = x_0 e^{\lambda t} \xrightarrow[t \to \infty]{} 0$$

FWD EULER

$$x_{n+1} = x_n + \lambda h x_n = (1 + \lambda h) x_n$$

SUM UP: $x_n = (1 + h\lambda)^n x_0$

NEED $\lim_{n \to \infty} x_n = 0 \Rightarrow |1 + h\lambda| < 1$

$$-1 < 1 + h\lambda < 1$$
$$0 < |\lambda| h < 2 \Rightarrow \boxed{h < \frac{2}{|\lambda|}}$$

THE SOLUTION: IMPLICIT METHOD

ON ODE $\quad x_{n+1} = x_n + h f(x_{n+1})$

MODEL PROBLEM $\quad x_{n+1} = x_n + h\lambda x_{n+1}, \quad \lambda < 0$

$$(1-h\lambda)x_{n+1} = x_n$$

$$x_n = \underbrace{(1-h\lambda)}_{1-h\lambda>1}{}^{-n} x_0 \xrightarrow[h\to\infty]{} 0 \quad \forall h>0$$

CONTINUOUS $\quad u_{n+1} = u_n + h\mu \Delta u_{n+1}$

DISCRETIZE TO INTERIOR GRID: $P_{int}\vec{u}_{n+1} = P_{int}\vec{u}_n + h\mu L_{int}\vec{u}_{n+1}$

$$(P_{int} - h\mu L_{int})\vec{u}_{n+1} = P_{int}\vec{u}_n$$

EXTEND WITH VERTEX CONDITIONS ON u_{n+1}

$$\begin{bmatrix} P_{int} - h\mu L_{int} \\ \hline M_{VC} \end{bmatrix} \vec{u}_{n+1} = P_0 \vec{u}_n$$

THIS WON'T HAVE STEPSIZE RESTRICTIONS, BUT IS STILL ONLY FIRST-ORDER IN h.

CRANK-NICHOLSON: 2ND ORDER IN TIME

ON THE QUANTUM GRAPH: EVALUATE AT $t = t_n + \frac{h}{2}$

$$\frac{u_{n+1} - u_n}{h} = \frac{1}{2}(\Delta u_{n+1} + \Delta u_n)$$

$$u_{n+1} - \frac{h}{2}\Delta u_{n+1} = u_n + \frac{h}{2}\Delta u_n$$

DISCRETIZE ON INTERIOR

$$\left(P_{INT} - \frac{h}{2}L_{int}\right)\vec{u}_{n+1} = \left(P_{INT} + \frac{h}{2}L_{int}\right)\vec{u}_n$$

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

$$\begin{bmatrix} P_{INT} - \frac{h}{2}L_{int} \\ \hline M_{VC} \end{bmatrix} \vec{u}_{n+1} = \left(P_0 + \frac{h}{2}L_0\right)\vec{u}_n$$

EQUIVALENTLY

$$\left(P_{VC} - \frac{h}{2} L_{VC}\right) \vec{u}_{n+1} = \left(P_0 + \frac{h}{2} L_0\right) \vec{u}_n$$

QUESTION FOR NEXT TIME

HOW CAN WE EFFICIENTLY SIMULATE

$$i u_t + \Delta u + \sigma |u|^2 u = 0 \, ?$$