Numerical Solution of Initial Boundary Value Problems

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Lecture 2

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Initial Boundary Value Problems (IBVPs)



Figure: Boundary conditions: Where? How many? What form?

$$U_t + P(U, \frac{\partial}{\partial x})U = F(x, t), \quad x \in \Omega, \ t \ge 0$$
$$LU = g(x, t) \quad x \in \delta\Omega, \ t \ge 0$$
$$u = f(x) \quad x \in \Omega, \ t = 0$$

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BVPs "Roughly Speaking"

$$P + (L) \rightarrow \tilde{P}, \quad F + (g) \rightarrow \tilde{F}$$

 \Rightarrow
 $U_t + \tilde{P}U = \tilde{F}$
 $U(x, 0) = f$

 \tilde{P} = generalized operator, \tilde{F} = generalized data. Eigenvalue analysis. $\tilde{P} = X(\Lambda^R + i\Lambda^I)X^{-1}$

- Hyperbolic: $\Lambda^R \approx 0$ (Euler, Maxwell, Wave propagation)
- Parabolic: $\Lambda^R > 0$ (damping, heat, diffusion)
- Incompletely Parabolic: $\Lambda^R \ge 0$ (N-S, mixed systems)
- Well-posed: $|\Lambda^R| < \infty$

- (i) Must choose *L* such that $P + L = \tilde{P}$ = bounded operator.
- (ii) Must choose *L* such that we have data LU g = 0.

 \rightarrow (i) and (ii) often in conflict \leftarrow

 $Ex: \quad U=U_{\infty}, \quad U_{x}=0, \quad \alpha U+\beta U_{x}=\alpha U_{\infty}$



Figure: Examples of boundary conditions that could be chosen.

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IVPs	IBVPs	
Continuos + Semi-discrete both on ODE form	Continuous not on ODE form, Semi-discrete on ODE form.	
$\begin{aligned} (\hat{U}_{\omega})_t &= \hat{P}(i\omega)\hat{U}_{\omega} + \hat{F} \\ \hat{U}_{\omega}(0) &= \hat{f} \end{aligned}$	$U_t + AU = F$ $U(0) = f$	
$\hat{P}(i\omega)$ "small" matrix Fourier modes decouple problem Detailed knowledge of eigenvalues/vectors within reach	A "large" matrix All gridpoints included/coupled No detailed knowledge of eigenvalues/vectors	
Knowledge about $\hat{P}(i\omega)$ + Parseval's relation	Energy-method informs us about $A + A^T \ge 0 \Rightarrow A$ ok.	

 \Rightarrow well-posedness/stabilty

 \Rightarrow stabilty

The IBVP

Example

$$u_t = (au_x)_x, \ 0 \le x \le 1, t \ge 0$$

$$u(0, t) = 0$$

$$u(1, t) = 0$$

$$u(x, 0) = f(x), \ a = a(x, t) \ge \delta > 0$$

Scalar product, norm: $(u, v) = \int_0^1 uv \, dx$, $||u||^2 = (u, u)$ Energy method: "multiply with solution, integrate by parts."

$$\int_{0}^{1} uu_{t} dx = (u, Pu) = \int_{0}^{1} u(au_{x})_{x} dx = u(au_{x}) \Big|_{0}^{1} - \int_{0}^{1} au_{x}^{2} dx \Rightarrow$$
$$\frac{d}{dt} ||u||^{2} = 2auu_{x}|_{1} - 2auu_{x}|_{0} - 2\int_{0}^{1} au_{x}^{2} dx \leq -2\delta ||u_{x}||^{2}$$
$$\therefore ||u||^{2} + 2\delta \int_{0}^{t} ||u_{x}||^{2} d\tau \leq ||f||^{2}$$

Note 1: The operator $P = \frac{\partial}{\partial x} a \frac{\partial}{\partial x}$ with boundary conditions is semi-bounded, i.e.

$$(u, Pu) \le -\delta ||u_x||^2 \le 0$$

Note 2: The estimate leads to a decaying solution if $u_x \neq 0$. Typical for parabolic problems.



Figure: Decaying parabolic solutions

Note 3.: For variable viscosity, a conservative formulation as $P = \frac{\partial}{\partial x} a \frac{\partial}{\partial x}$ is necessary. $P = a \frac{\partial^2}{\partial x^2}$ does not lead to an estimate.

Important definitions and concepts for an IBVP

$$u_t = Pu + F, \ 0 \le x \le 1, t \ge 0$$

 $Bu = g \ x = 0, 1$ (1)
 $u = f \ 0 \le x \le 1$

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Define scalar products and norms

$$(u, v) = \int_0^1 u^* H v dx, \quad ||u||^2 = (u, u)$$

where H(x) positive definite Hermitian matrix.

<u>Definition</u>: Let *V* be space of differentiable functions satisfying the homogeneous boundary condition Bu = 0. The differential operator *P* is semi-bounded if for all *u* in *V*

$$(u, Pu) \le \alpha ||u||^2, \ \alpha = const.$$

If a solution exists, semi-boundedness guarantees well-posedness since

$$\frac{d}{dt}||u||^2 = 2(u, u_t) = 2(u, Pu) \le 2\alpha ||u||^2$$

Existence?

$$u_t = u_x, \ 0 \le x \le 1, \ t \ge 0$$
$$u(0, t) = u(1, t) = 0$$
$$u(x, 0) = f, \ 0 \le x \le 1$$

 $2(u, Pu) = u^2 |_0^1 = 0, \therefore$ P is a semi-bounded operator

However, the boundary condition at x = 0 is not correct since u = f(x + t) if $x + t \le 1$ and zero otherwise.



:. No existence, we must restrict semi-boundedness.

<u>Definition:</u> P is maximally semi-bounded if it is semi-bounded in *V* but not in any space with less number of boundary conditions.

In our example *V* is too "small" for allowing existence, must be made "bigger" by dropping b.c. at x = 0.

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$$V = \{u(x), u(0) = 0, u(1) = 0\} \Rightarrow (u, Pu) = 0, V \text{ "too small"}.$$
$$V = \{u(x), u(1) = 0\} \Rightarrow (u, Pu) = -\frac{u(0)^2}{2} \le 0, V \text{ "perfect"}.$$
$$V = \{u(x)\} \Rightarrow (u, Pu) = \frac{u(1)^2}{2} - \frac{u(0)^2}{2}, V \text{ "too large"}.$$

Definition: The IBVP (1) is well-posed if for F = g = 0, a unique (i) solution exists (ii) satisfying

$$||u||^2 \le K e^{2\alpha t} ||f||^2$$
(iii)

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K, α are constants independent of the data *f*.

Definition: The IBVP (4) is strongly well-posed if a <u>unique</u> (i) solution <u>exists</u> (ii) satisfying

$$\|u\|_{I}^{2} \leq Ke^{2\alpha t} \left(\|f\|_{I}^{2} + \int_{0}^{t} \left[\|F\|_{I}^{2} + \|g\|_{II}^{2} \right] d\tau \right)$$
(iii)

 k, α are constants independent of the data F, f, g.

Note that different norms exist in (iii).

Symmetrizer and norm for integration-by-parts

$$u_t + Au_x = 0, \ 0 \le x \le 1, \ A \ne A^T$$

Symmetrizer

$$(Su)_t + SAS^{-1}(Su)_x = 0$$

$$(Su)^T (Su)_t + (Su)^T A^s (Su)_x = 0, \quad A^s = SAS^{-1}$$

$$(||u||_S^2)_t + (Su)^T A^s (Su)|_0^1 = 0$$

where $||u||_S^2 = \int_0^1 u^T (S^T S) u dx$ and $(Su)^T A^s (Su) = u^T (S^T S) A u$. Norm

$$u^{T}Pu_{t} + u^{T}PAu_{x} = 0$$
$$(||u||_{P}^{2})_{t} + \int_{0}^{1} u^{T}PAu_{x} + u_{x}^{T}(PA)^{T}udx = 0$$

where $||u||_P^2 = \int_0^1 u^T P u dx$. $PA = (PA)^T$ is satisfied by $P = S^T S$.

Boundary conditions

Where? How many? Of what form?

 $u_t + au_x = 0; \ 0 \le x \le 1; \ t \ge 0$

1. Physical intuition

"Information comes from left." a > 0 b. at x = 0. "Information comes form right." a < 0 b.c. at x = 1.

2. The energy-method

$$\frac{d}{dt}||u||^2 = au_{x=0}^2 - au_{x=1}^2$$

 $a > 0 \Rightarrow$ growth term removed by b.c. at x = 0. $a < 0 \Rightarrow$ growth term removed by b.c. at x = 1.

3. Laplace/Normal mode theory (not in this course).

$$u_t = \epsilon u_{xx}, \ 0 \le x \le 1, \ t \ge 0$$

1. Physical intuition "heat everywhere?" \Rightarrow b.c. at x = 0, 1.

2. The energy method

$$\frac{d}{dt}||u||^2 + 2\epsilon||u_x||^2 = 2\epsilon u u_x|_0^1 = \epsilon \begin{bmatrix} u\\ u_x \end{bmatrix}^T \underbrace{\begin{bmatrix} 0 & 1\\ 1 & 0\\ \lambda = \pm 1 \end{bmatrix}}_{\lambda = \pm 1} \begin{bmatrix} u\\ u_x \end{bmatrix}|_0^1$$

Always one negative eigenvalue, always one growth term at each boundary. \Rightarrow b.c. at x = 0, 1.

$$u_t + Au_x = 0, \ 0 \le x \le 1, \ t \ge 0, \ A = \begin{bmatrix} 1 & \alpha \\ \alpha & 1 \end{bmatrix}.$$

- 1. Physical intuition ?
- 2. The energy method

$$\frac{d}{dt} ||u||^2 = u^T A u \Big|_1^0 = (X^T u)^T \Lambda (X^T u) \Big|_1^0$$

$$A = X \Lambda X^T, \quad \Lambda = \begin{bmatrix} 1 + \alpha & 0 \\ 0 & 1 - \alpha \end{bmatrix}, \quad X = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$x = 0 \quad (i) \quad \alpha < -1 \implies 1 \text{ pos. eig.} \implies 1 \text{ b.c.}$$

$$(ii) \quad -1 < \alpha < 1 \implies 2 \text{ pos. eig.} \implies 2 \text{ b.c.}$$

$$(iii) \quad 1 < \alpha \implies 1 \text{ pos. eig.} \implies 1 \text{ b.c.}$$

Minimal nr for maximal semi-boundedness and uniqueness !

The energy-method for Where, How Many and What Kind of boundary conditions



A general conservation law in two dimensions can be written

$$u_{t} + (\underbrace{Au}_{F^{I}})_{x} + (\underbrace{Bu}_{G^{I}})_{y} = \epsilon \left[\underbrace{(C_{11}u_{x} + C_{12}u_{y})_{x}}_{F^{V}} + (\underbrace{C_{21}u_{x} + C_{22}u_{y}}_{G^{V}})_{y} \right]$$
$$u_{t} + (F^{I})_{x} + (G^{I})_{y} = \epsilon (F_{x}^{V} + G_{y}^{V})$$

The matrices A, B, C_{ij} are assumed constant and symmetric.

Energy

$$\underbrace{\int_{\Omega} u^T u_t d\Omega}_{\frac{1}{2} ||u||_t^2} + \underbrace{\int_{\Omega} u^T F_x^I + u^T G_y^V d\Omega}_{\frac{1}{2} (u^T A u)_x + \frac{1}{2} (u^T B u)_y} = \underbrace{\epsilon}_{\Omega} \underbrace{\int_{\Omega} u^T F_x^V + u^T G_y^V d\Omega}_{(u^T F^V)_x + (u^T G^V)_y - (u_x^T F^V + u_y^T G^V)}$$

Green - Gauss \Rightarrow

$$||u||_{t}^{2} + \underbrace{\oint_{\partial\Omega} u^{T}Audy - u^{T}Budx}_{\text{Boundary Terms} = \text{BT}} = \underbrace{\int_{\partial\Omega} (u^{T}F^{V})dy - (u^{T}G^{V})dx}_{\text{Boundary Terms} = \text{BT}}$$

Dissipation = DI

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$$DI = -2\epsilon \int_{\Omega} \begin{bmatrix} u_x \\ u_y \end{bmatrix}^T \underbrace{\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}}_{\text{must be} \ge 0} \begin{bmatrix} u_x \\ u_y \end{bmatrix} d\Omega \le 0$$

$$BT = -\oint u^{T} (Adx - Bdx)u - 2\epsilon u^{T} (F^{V}dy - G^{V}dx) = -\oint u^{T} \tilde{A}u - 2\epsilon u^{T} [\tilde{C}_{x}u_{x} + \tilde{C}_{y}u_{y}] ds$$
$$\tilde{A} = (A, B) \cdot \vec{n}, \quad \tilde{C}_{x} = (C_{11}, C_{21}) \cdot \vec{n}, \quad \tilde{C}_{y} = (C_{12}, C_{22}) \cdot \vec{n}$$

Boundary Conditions? Where? How many? What form?

$$BT = -\oint \begin{bmatrix} u \\ \varepsilon u_x \\ \varepsilon u_y \end{bmatrix}^T \begin{bmatrix} \tilde{A} & \tilde{C}_x & \tilde{C}_y \\ \tilde{C}_x & 0 & 0 \\ \tilde{C}_y & 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ \varepsilon u_x \\ \varepsilon u_y \end{bmatrix} ds =$$
$$= -\oint \begin{bmatrix} W+ \\ W^0 \\ W^- \end{bmatrix}^T \begin{bmatrix} \Lambda^+ & 0 & 0 \\ & \Lambda^0 & 0 \\ 0 & 0 & \Lambda^- \end{bmatrix} \begin{bmatrix} W^+ \\ W^0 \\ W^- \end{bmatrix} ds.$$

- Number of boundary conditions = Number of negative entries in Λ⁻.
- Where? On all points on boundary where negative eigenvalues exist.
- Form of boundary conditions? $W^- = RW^+ + g$ for a choice of R that leads to a bound. See JNO.

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Summary of well-posedness for IBVP

- A maximally semi-bounded differential operator leads to well-posedness for homogeneous boundary conditions (g = 0) and non-zero initial data *f* and forcing function *F*.
- Strong well-posedness with $(g \neq 0)$ require further analysis. Use the procedure in JNO (or Normal mode analysis).
- The choice of boundary conditions (choice of matrix R) is the crucial part in general.
- For the Euler and compressible Navier-Stokes also problematic to integrate by parts. Splitting, change of variables and a particular choice of norm is probably necessary.

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Semi-discrete approximations of IBVPs

Example:

$$\frac{d}{dt}u_{j} = D_{o}u_{j}, \quad j = 0...N$$

$$u_{-1} = 2u_{0} - u_{1}, \quad u_{N+1} = 0$$

$$u_{j}(0) = f_{j}, \quad j = 0...N$$

The linear extrapolation at j = 0 give a one-sided approximation

$$(u_0)_t = (u_1 - u_0)/h.$$

Define new scalar product:

$$(u, v)_{h} = \delta h u_{0} v_{0} + \sum_{j=1}^{N} u_{j} v_{j} h = u^{T} P v, \quad P = h \text{diag}(\delta, 1, 1, ...1)$$
$$(u, Qu) = \delta u_{0}(u_{1} - u_{0}) + u_{1}(u_{1} - u_{0})/2... = -\delta u_{0}^{2} + u_{0} u_{1}(\delta - 1/2)$$
The choice $\delta = 1/2 \Rightarrow (u, Qu) = -\delta u_{0}^{2}, \quad \therefore \underline{Q} = \text{semi-bounded!}$

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The general formulation

$$\frac{d}{dt}u_j = Qu_j + F_j, \quad j = 0...N$$

$$B_h u = g$$

$$u_j(0) = f_j, \quad j = 0...N$$
(2)

 $B_h u = g$ contains a complete set of boundary conditions, both for the IBVP and purely numerical ones.

The number of bondary conditions is equal to the number of linearly independent conditions. (No problem with existence). The discrete scalar product and norm typically have the form

$$(u, v)_h = \sum_{j=1}^{N+1} \langle u_j, \tilde{H}_j v_j \rangle h, \quad ||u||^2 = (u, u)_h$$

where \tilde{H}_j positive definite symmetric matrix.

<u>Definition</u>: Let V_h be the space of grid-vector functions u that satisfies $B_h u = 0$. The difference operator Q is <u>semi-bounded</u> if for all $u \in V_h$

 $(u, Qu) \le \alpha \|u\|_h^2$

holds. α = bounded constant independent of V_h , h.

<u>Definition</u>: The problem (2) is <u>stable</u> for F = g = 0 if

 $||u||_h \le k e^{\alpha t} ||f||_h$

holds. k, α are constants independent of f, h.

<u>Theorem</u>: If Q is semi-bounded, then (2) is stable.

<u>Note 1:</u> No problem with existence and number of boundary conditions and maximal semi-boundedness.

Note 2: An added forcing function poses no problem.

Definition: The problem (2) is strongly stable if

$$||u||_{h}^{2} \leq k^{2} e^{2\alpha t} \left(||f||_{h}^{2} + \int_{0}^{t} \left(||F||_{h}^{2} + ||g||_{B}^{2} \right) d\tau \right).$$

 k, α are bounded constants independent of F, f, g, h.

<u>Definition</u>: The problem (2) is <u>time-stable</u> or <u>strictly-stable</u> if the corresponding estimate for (1) with $F = g = \overline{0}$ has the estimate

$$\|u\| \le k_c e^{\alpha_c t} \|f\|$$

and the estimate of (2) with F = g = 0 is

 $||u||_h \le k_d e^{\alpha_d t} ||f||_h$

where $\alpha_d \leq \alpha_c + O(h)$.

Not only the solution but also the time growth converges.

Splitting techniques

Consider the Cauchy ($u(\pm\infty, t) = 0$) problem for

$$u_t + au_x = 0, \ a = a(x, t).$$

The energy method gives

$$\frac{d}{dt}||u||^2 = \int_{-\infty}^{\infty} a_x u^2 dx \le |a_x|_{\infty}||u||^2$$

 $\therefore a \frac{\partial}{\partial x}$ is a semi-bounded operator for a well-posed problem.

A naive discretization using central difference operators yields $u_t + AQu = 0$ and

$$\frac{d}{dt}||u||_h^2 = -u^T (AQ + (AQ)^T)u \neq \int_{-\infty}^{\infty} a_x u^2 dx.$$

The skew-symmetry $Q + Q^T = 0$ does not help.

Go back to PDE

$$au_x = \alpha(au)_x + \beta au_x + \gamma a_x u = (\alpha + \beta)au_x + (\alpha + \gamma)a_x u$$

implies $\beta = 1 - \alpha, \gamma = -\alpha$.

The energy method again following the "advice" above leads to

$$\frac{1}{2}\frac{d}{dt}||u||^2 + \alpha u(au)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} (1-2\alpha)auu_x dx = \int_{-\infty}^{\infty} \alpha a_x u^2 dx.$$

The choice $\alpha = 1/2$ leads to

$$\frac{d}{dt}||u||^2 = \int_{-\infty}^{\infty} a_x u^2 dx,$$

which we of knew already. What about the semi-discrete case ?

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Semi-discrete again (not so naive this time)

$$U_t + \frac{1}{2}Q(AU) + \frac{1}{2}AQU - \frac{1}{2}A_xU = 0.$$

The energy method yields

$$2U^{T}U_{t}\Delta x = -U^{T}(QA + AQ)U\Delta x + U^{T}A_{x}U\Delta x$$
$$= \left[(QU)^{T}(AU) - (AU)^{T}(QU)\right]\Delta x + U^{T}A_{x}U\Delta x$$
$$= U^{T}A_{x}U\Delta x.$$

$$\therefore \left(||U||_h^2 \right)_t = U^T A_x U \Delta x \to \int_{-\infty}^{\infty} a_x u^2 dx$$

: Convergence to the PDE result. (See J. Nordström JSC 2006).

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... The same technique must be used for nonlinear problems.

Summary of the Energy-method		
Continuous		Semi-discrete
$U_t = PU$		$U_t = QU$
LU = g		BU = g
U = f		U = f
	Semi-boundness	
$\frac{1}{2} U _{t}^{2}$		$\frac{1}{2}(U _{h})_{t}$
= (U, PU)		=(U,QU)
$\leq \alpha_c U ^2$		$\leq \alpha_d \ U\ _h^2$
	Well-posedness and Stability	11
$ U \le e^{\alpha_c t} f $		$ U _h \le e^{\alpha_d t} f _h$
	Time/Strict-Stability	
	$\alpha_c \le \alpha_d + O(h)$	

Exercises/Seminars

- Discuss well-posedness and boundary conditions
- Show maximal semi-boundedness and semi-boundedness.
- Discuss splitting techniques.
- Derive the skew-symmetric continuous and semi-discrete approximation (periodic boundary conditions) for the Burger's equation.
- Show that the symmetrizer *S* leads to the norm $P = S^T S$.
- Prove that homogeneous boundary conditions of the form
 W⁻ = RW⁺ lead to a bound. What is the stability condition?
- Prove that the boundary conditions cannot have the form $W^- = RW^+ + CW^0$.