Numerical Solution of Initial Boundary Value Problems

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Lecture 4

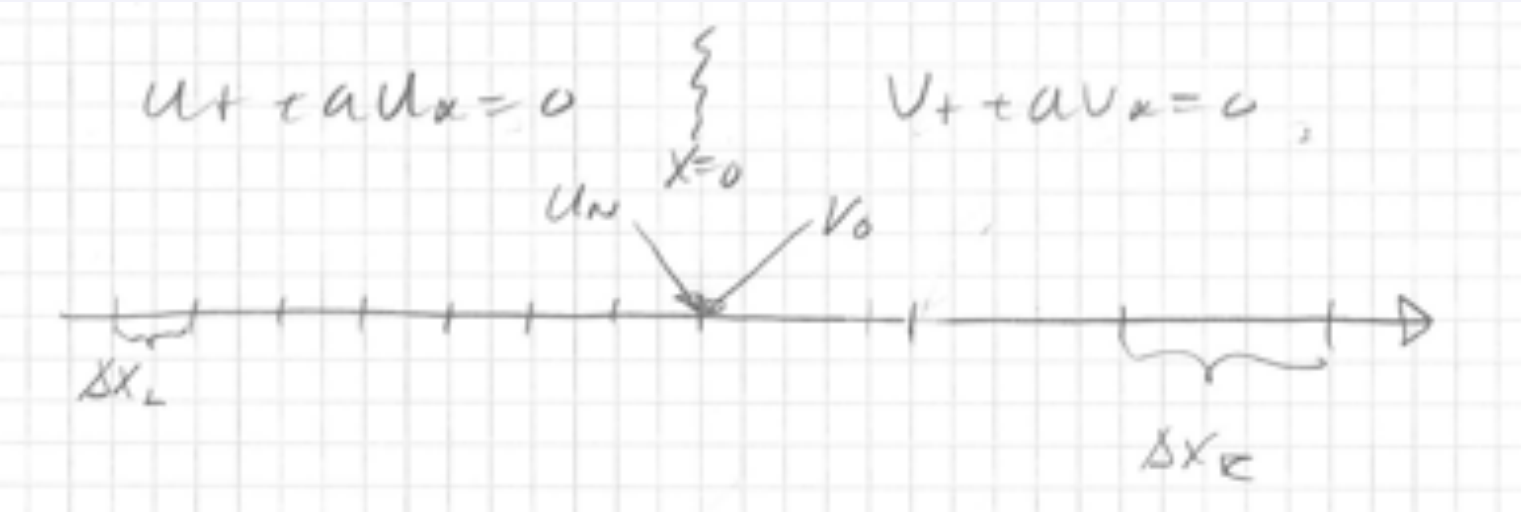
SBP-SAT for multi-block methods

$$u_t + au_x = 0 \quad \wr \quad v_t + av_x = 0$$
$$x = 0$$
$$u = v$$

Multiply with smooth function ($\phi(\pm\infty, t) = 0$) and integrate $\Rightarrow$

$$\int_{-\infty}^{0} \phi u_t + a\phi u_x dx + \int_{0}^{\infty} \phi v_t + a\phi v_x dx = 0 \Rightarrow$$
$$= \int_{-\infty}^{0} \phi u_t dx + \int_{0}^{\infty} \phi v_t dx - \int_{-\infty}^{0} a\phi_x u dx - \int_{0}^{-\infty} a\phi_x v dx$$
$$+ \underbrace{a\phi_0(u - v)_0}_{=0} = 0$$

No remaining terms at the interface $\Rightarrow$ conservation.



$$u_t + aP_L^{-1}Q_L u = \sigma_L P_L^{-1}(u_N - v_0)e_N,$$
$$v_t + aP_R^{-1}Q_R v = \sigma_R P_R^{-1}(v_0 - u_N)e_0.$$

Note that u_N, v_0 are located at the same position in space.

<u>Conservation</u>: Multiply with smooth function ϕ and integrate.

$$\phi^T P_L u_t + a\phi^T Q_L u = \sigma_L \phi_N (u_N - v_0)$$
$$\phi^T P_R v_t + a\phi^T Q_R v = \sigma_R \phi_0 (v_0 - u_N)$$

Numerical integration using SBP operators: $Q \to -Q^T + B \Rightarrow$

$$\underbrace{\phi^T P_L u_T + \phi^T P_R v_t - a(P_L^{-1} Q_L \phi^T) P_L u - a(P_R^{-1} Q_R \phi)^T P_R u +}_{\text{mimic PDE terms}}$$

$$\underbrace{-a\phi_N u_N + \sigma_R \phi_N (u_N - v_0) + a\phi_0 v_0 + \sigma_R \phi (v_0 - u_N)}_{\text{IT=interface terms that should vanish}}$$

Since ϕ smooth, we can factor out $\phi_0 = \phi_N \Rightarrow$

$$\text{IT} = \phi_0(-au_N + \sigma_N(u_N - v_0) + av_0 + \sigma_0(v_0 - u_N)) = \phi_0(u_N - v_0)(\sigma_L - \sigma_R - a).$$

$\therefore$ We have a conservative scheme if $\sigma_L = \sigma_R + a$.

Stability: Multiply with the solutions u, v and integrate $\Rightarrow$

$$u^T P_L u_T + v^T P_R v_t = -a u_N^2 + a v_0^2 + 2 u_N \sigma_L (u_N - v_0) + 2 v_0 \sigma_R (v_0 - u_N)$$

$$= \begin{bmatrix} u_N \\ v_0 \end{bmatrix} \begin{bmatrix} -a + 2\sigma_L & -(\sigma_L + \sigma_R) \\ -(\sigma_L + \sigma_R) & a + 2\sigma_R \end{bmatrix} \begin{bmatrix} u_N \\ v_0 \end{bmatrix}$$

$$\lambda_{1,2} = \sigma_L + \sigma_R \pm \sqrt{(\sigma_L + \sigma_R)^2 + (\sigma_L - \sigma_R - a)^2}.$$

We have eigenvalues $\lambda_{1,2} \leq 0$ if

$$\begin{aligned} \sigma_L + \sigma_R \leq 0, &\quad \text{the stability condition } \sigma_R \leq -a/2. \\ \sigma_L - \sigma_R - a = 0, &\quad \text{the conservation condition.} \end{aligned}$$

Note that the conservation condition is necessary for stability.

Summary of multi-block coupling

- Conservation is a natural component of a scheme, if the PDE is conservative (necessary for correct shock speed).
- SBP-SAT + demand of conservation $\Rightarrow$ provide relation between penalty coefficients.
- Conservation necessary for stability (and dual consistency).
- Check for conservation first, next step stability.
- References
  - M.H. Carpenter, J. Nordström, D. Gottlieb JCP 1999.
  - J. Nordström et al JCP 2009.
  - C. La Cognata & J. Nordström BIT 2016.
  - J. Nordström & A. Ruggiu, JCP 2017.
  - J. Nordström & F. Ghasemi, JCP 2017.

Accuracy and error estimates

$$u_t + u_x = 0, \quad u(0,t) = g, \quad u(x,0) = f$$

Semi-discrete

$$v_t + P^{-1}Qv = \sigma P^{-1}(v_0 - g)e_0 \tag{1a}$$
$$v(0) = f \tag{1b}$$

Insert analytical solution u into (1)

$$u_t + P^{-1}Qu = \sigma P^{-1}(u_0 - g)e_0 + T_e \tag{2a}$$
$$u(0) = f \tag{2b}$$

T_e = truncation error from $P^{-1}Qu = u_x + O(h^p)$

Note: <u>No error</u> from penalty term (with Dirichlet b.c.).

(2)-(1) with $u - v = e =$ error $\Rightarrow$

$$e_t + P^{-1}Qe = \sigma P^{-1}e_0 e_0 + T_e \tag{3a}$$

$$e(0) = 0 \tag{3b}$$

Solve (3) and the exact error is known.

Note: $e \neq T_e$. $T_e =$ source of error only, <u>not the error itself</u>.

Energy:

$$e^T P e_t + e^T Q e = \sigma e_0^2 + e_0^T P T_e \Rightarrow$$

$$(\|e\|_P^2)_t = e_0^2(1 + 2\sigma) - e_N^2 + 2e^T P T_e$$

Stability demands that $\sigma \leq -1/2$. Choose $\sigma = -1 \Rightarrow$

$$\frac{d}{dt}\|e\|^2 = -(e_0^2 + e_N^2) + 2(e, T_e). \tag{4}$$

A first crude estimate

$$\frac{d}{dt}||e||^2 = -(e_0^2 + e_N^2) + 2(e, T_e) \leq \eta||e||^2 + \frac{1}{\eta}||T_e||^2 \tag{5}$$

Multiply with integrating factor $e^{-\eta t}$ and integrate $\Rightarrow$

$$||e||^2 =\leq \frac{1}{\eta}e^{-\eta t}\int_0^t e^{-\xi t}||T_e||^2 d\xi = O(||T_e||^2) \tag{6}$$

- The error is equal to the size of the truncation error.
- The truncation error large at boundaries and interface. SBP(S,2S) indicates error of order S.
- Laplace transform technique show that error often of order S+R, where R=order of highest derivative in the IBVP.
- M. Svärd & J. Nordström, JCP 2006.

A second crude estimate

$$\frac{d}{dt}||e||^2 = -(e_0^2 + e_N^2) + 2(e, T_e) \leq 2||e||||T_e|| \tag{7}$$

Note now that $\frac{d}{dt}||e||^2 = 2||e||\frac{d}{dt}||e||$ which implies that (7) goes to

$$\frac{d}{dt}||e|| \leq ||T_e||. \tag{8}$$

- The relation (8) indicates a linear growth in time.
- Seemingly, long time integration of hyperbolic problems would lead to large errors.

A third more sharp estimate

$$2\|e\|\,\|e\|_t \leq -(e_0^2 + e_N^2) + 2\|e\|\,\|T_e\| \Rightarrow \|e\|_t \leq \underbrace{-\left(\frac{e_0^2 + e_N^2}{2\|e\|^2}\right)}_{-\eta(t)}\|e\| + \|T_e\|$$

Note that $0 < \eta(t) < 1$. Let $\eta(t) = \text{constant}$ (can be relaxed).

$$\|e(T)\| \leq e^{-\eta T}\int_0^T e^{\eta t}\|T_e\|dt \leq e^{-\eta t}\|T_e\|_{\max}\int_0^T e^{\eta t}dt$$

$$= e^{-\eta t}\|T_e\|_{\max}\frac{(e^{\eta T} - 1)}{\eta} = \|T_e\|_{\max}\frac{(1 - e^{-\eta T})}{\eta} \leq \frac{\|T_e\|_{\max}}{\eta}$$

Summary of error estimates

- The error for finite time is of order S+R, where S=internal accuracy and R= order of highest derivative.
- The standard error estimate give a linear error growth in time.
- A more refined error estimate where boundary effects are included, give a linear error growth in time.
- By mesh refinement, arbitrary accuracy at <u>any future time</u>.
- No linear growth in time for parabolic problems even if boundary procedure not optimal, easier problem.
- Reference: J. Nordström SISC 2007.
- Reference: D. Kopriva, J. Nordström, G. Gassner JSC 2017.
- Reference: J. Nordström, H. Frenander JSC 2018?

Exercises/Seminars

- Show that an errorbound exist for the heat equation, even in the periodic case. Use the Poincare estimate.
- Show that conservation require a modified interface condition if the wave speeds are different in the multi-block problem.
- Derive number and homogenous boundary conditions by using the rotational technique for

$$u_t + au_x = \epsilon u_{xx} = 0, \quad 0 \leq x \leq 1, \quad a, \epsilon > 0.$$

- Derive penalty terms for the above homogenous continuous problem by using the rotational technique.
- Derive penalty terms for the related homogenous semi-discrete problem by using the rotational technique.

Appendix: Old version of "Roadmap"

$$u_t + Au_x = 0, \;\; x \geq 0 \tag{9a}$$

$$Lu = 0, \;\; x = 0 \tag{9b}$$

$$u(x,0) = f(x), \;\; x \geq 0 \tag{9c}$$

The matrix A is symmetric, and it is a model problem for wave propagation (elastic wave, Euler, Maxwell equations).

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

Characteristic boundary conditions: $(X^T u)_i = 0, \;\; \lambda_i > 0 \Rightarrow$

$$\frac{d}{dt}\|u\|^2 = u^T A u \leq 0, \;\; \therefore \text{Maximally semi-bounded operator.}$$

As an example, consider S-W equations in 1D: $A = \begin{bmatrix} \bar{u} & 0 & \bar{c} \\ 0 & \bar{u} & 0 \\ \bar{c} & 0 & \bar{c} \end{bmatrix}$.

$$\frac{d}{dt}\|u\|^2 = u^T A u = W^T \Lambda W = (\bar{u} + \bar{c})w_1^2 + \bar{u}w_2^2 + (\bar{u} - \bar{c})w_3^2,$$

where $W = X^T u$. Well-posed boundary conditions are

$$LW = 0, \quad L = \begin{bmatrix} 1 & 0 & -k \\ 0 & 1 & 0 \end{bmatrix}. \tag{6}$$

We find $\frac{d}{dt}\|u\|^2 = \left[(u + c)k^2 + (u - c)\right] w_3^2 \leq 0$ if $|k| \leq \sqrt{\frac{\bar{c}-\bar{u}}{\bar{c}+\bar{u}}}$.

The B.C.'s can be written

$$LX^T u = 0. \tag{7}$$

Now, how to construct penalty matrices Σ such that

$$W^T(\Lambda + \Sigma L + (\Sigma L)^T)W \leq 0\,? \tag{8}$$

Note: We need ΣL to have same size as Λ and A. This means that $[\Sigma] = L^T$, Try

$$\Sigma L = \begin{bmatrix} \sigma_1 & \sigma_2 \\ \sigma_3 & \sigma_4 \\ \sigma_5 & \sigma_6 \end{bmatrix} \begin{bmatrix} 1 & 0 & -k \\ 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} \sigma_1 & \sigma_2 & -\sigma_1 k \\ \sigma_3 & \sigma_4 & -\sigma_3 k \\ \sigma_5 & \sigma_6 & -\sigma_5 k \end{bmatrix}$$

$$\Sigma L + (\Sigma L)^T = \begin{bmatrix} 2\sigma_1 & \sigma_2 + \sigma_3 & \sigma_5 - \sigma_1 k \\ \sigma_2 + \sigma_3 & 2\sigma_4 & \sigma_6 - \sigma_3 k \\ \sigma_5 - \sigma_1 k & \sigma_5 - \sigma_3 k & -2\sigma_5 k \end{bmatrix}$$

$\Lambda + \Sigma L + (\Sigma L)^T = \text{diagonal} \Rightarrow \sigma_2 + \sigma_3 = \sigma_3 - \sigma_1 k = \sigma_2 - \sigma_3 k = 0.$
$\Lambda + \Sigma L + (\Sigma L)^T \leq 0 \Rightarrow$

$$\begin{aligned} 2\sigma_1 + u + c &\leq 0 \\ 2\sigma_4 + u &\leq 0 \\ -2\sigma_5 k + u - c &\leq 0. \end{aligned}$$

We aim for a "perfect match" such that

$$\frac{d}{dt}\|u\|^2_{P\otimes I} = \left[(\bar{u}+\bar{c})k^2 + (u-c)\right] w_3^2$$

This implies

$$\sigma_1 = -\frac{u+c}{2}, \quad \sigma_4 = -\frac{u}{2}, \quad \sigma_5 = -\frac{u+c}{2}k$$
$$\sigma_2 = 0, \qquad \sigma_3 = 0, \qquad \sigma_6 = 0$$

$$\Sigma = \begin{bmatrix} \frac{u+c}{2} & 0 \\ 0 & -\frac{u}{2} \\ \frac{u+c}{2}k & 0 \end{bmatrix}, \qquad \Sigma L = \begin{bmatrix} \frac{u+c}{2} & 0 & \frac{k(u+c)}{2} \\ 0 & -\frac{u}{2} & 0 \\ \frac{k(u+c)}{2} & 0 & \frac{k^2(u+c)}{2} \end{bmatrix}$$

$$\Lambda + \Sigma L + (\Sigma L)^T = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & k^2(u+c)+u-c \end{bmatrix} \leq 0 \tag{9}$$

$\therefore$ Exactly right! The Σ derived will be used in the SAT term.

$$\Lambda + \Sigma L + (\Sigma L)^T \leq 0 \Rightarrow X(\Lambda + \Sigma L + (\Sigma L)^T)X^T \leq 0 \Rightarrow$$
$$A + \underbrace{X^T \Sigma L X}_{\tilde{\Sigma L}} + \underbrace{X^T (\Sigma L)^T X}_{(\tilde{\Sigma L}^T)} \leq 0 \tag{10}$$

What have we done?

- Found L such that $u^T A u \leq 0$ with minimal number of conditions, maximally semi-bounded operator.
- Formed ΣL = linear combination of boundary conditions.
- Chosen ΣL such that we mimic the continuous estimate.
- Derivation in diagonalised system, easy, not necessary.
- Transformed ΣL in diagonalised system to $\tilde{\Sigma L}$.
- ΣL,$\tilde{\Sigma L}$ penalty matrices in the semi-discrete approximation.

The semi-discrete approximation

We will use so called Kronecker Products, defined below.

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots \\ a_{21}B & & \\ & & \ddots \\ & & \end{bmatrix},$$

$$(A \otimes B)(C \otimes D) = AC \otimes BD, \quad (A \otimes B)^T = A^T \otimes B^T, \quad (A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$$

The scheme using SBP-SAT and Kronecker products is

$$\begin{aligned} u_t + (P^{-1}Q \otimes A)u &= (P^{-1}E_o \otimes \tilde{\Sigma L})(u - g) \\ u(0) &= f. \end{aligned} \tag{11}$$

Energy with $g = 0$ leads to

$$u^T(P \otimes I)u_t + u^T(Q \otimes A)U = u_0^T \tilde{\Sigma L} u_0. \tag{12}$$

Add transpose of (12) to itself $\Rightarrow$

$$\underbrace{(u^T(P \otimes I)u)_t}_{\frac{d}{dt}(\|u\|^2_{P\otimes I})} + u^T(\underbrace{Q + Q^T}_{B} \otimes A)u = u_0^T(\tilde{\Sigma L} + (\tilde{\Sigma L})^T)u_0.$$

We find

$$\frac{d}{dt}\left(\|u\|^2_{P\otimes I}\right) = u_0^T(A + \tilde{\Sigma L} + (\tilde{\Sigma L})^T)u_0 \leq 0,$$

by the previous derivation, see (10).

$\therefore$ Energy stability follows automatically from well-posed boundary conditions.

Boundary procedures for parabolic problems

$$
\begin{aligned}
u_t + Au_x &= \epsilon(Bu_x)_x, \;\; x \geq 0 \\
Lu &= 0, \;\; x = 0 \\
u(x,0) &= f(x), \;\; x \geq 0
\end{aligned}
\tag{13}
$$

$$
\frac{d}{dt}\|u\|^2 + 2\epsilon \int_0^\infty u_x^T B u_x dx = u^T A u - \underbrace{\epsilon u^T B u_x - \epsilon u_x^T B u_x}_{\text{indefinite terms}} = BT
$$

All boundary operators L must remove the indefinite terms $\Rightarrow$

$$
Lu = Cu - \epsilon B u_x = 0. \tag{14}
$$

The relation (14) $\Rightarrow$ BT in estimate becomes

$$
BT = u^T(A - C - C^T)u.
$$

C must be determined such that:

- We impose correct nr. of boundary conditions (existence).
- $A - (C + C^T) \leq 0$ (energy estimate).

Assume this is done and that $L = C - \epsilon B \frac{\partial}{\partial x}$ is known.

What are the penalty coefficients such that

$$BT = u^T A u - \epsilon u^T B u_x - \epsilon u_x^T B u + u^T (\Sigma L + (\Sigma L)^T) u \leq 0 \ ?$$

Try $\Sigma = -I \Rightarrow BT = u^T (A - (C + C^T)) u \leq 0$.

<u>Remark:</u> This perfect scaling is due to the fact that i) we replace the indefinite term $u^T B u_x$ exactly by the boundary operator L, and ii) that L is a square matrix.

The SBP-SAT approximation is

$$u_t+(P^{-1}Q\otimes A)u-\epsilon(P^{-1}Q\otimes B)u_x = [P^{-1}E_0\otimes \underbrace{(-I)}_{\Sigma}][\underbrace{(I\otimes C)u-\epsilon(I\otimes B)u_x}_{LU}].$$

Energy:

$$u^T(P\otimes I)u_t + u^T(Q\otimes A)u - \epsilon u^T(Q\otimes B)u_x = -u_0^T(Cu_0+\epsilon B(u_x)_0)u.$$

Same technique as before $\Rightarrow$

$$\begin{aligned}
&(u^T(P\otimes I)u)_t + 2\epsilon(u_x^T(P\otimes I)u_x) = \\
&u_0^T Au_0 - \epsilon u_0^T B(u_x)_0 - (u_x)_0^T Bu_0 - u_0^T Cu_0 + \epsilon u_0^T B(u_x)_0 \\
&\qquad\qquad - u_0^T C^T u_0 + \epsilon (u_x)_0^T Bu_0 \\
&\qquad\qquad = u_0^T(A-(C+C^T))u_0 \le 0.
\end{aligned}$$

$\therefore$ The well-posedness condition leads directly to stability.

Summary of SAT procedure

- Well-posed boundary conditions: LW = 0, that lead to an energy estimate for the PDE is necessary.
- With the boundary operator L known, construct $\tilde{\Sigma L}$ such that $A + \tilde{\Sigma L} + (\tilde{\Sigma L})^T \leq 0$.
- By using $\tilde{\Sigma L}$ as the penalty matrix in the numerical approximation, stability is obtained almost automatically.
- References
  - M.H. Carpenter, J. Nordström, D. Gottlieb JCP 1999.
  - J. Nordström et al JCP 2009.
  - J. Berg, J. Nordström APNUM 2012.