Numerical Solution of Initial Boundary Value Problems

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SBP-SAT for multi-block methods

\[ u_t + au_x = 0 \quad \land \quad v_t + av_x = 0 \]
\[ x = 0 \]
\[ u = v \]

Multiply with smooth function \((\phi(\pm\infty, t) = 0)\) and integrate ⇒
\[
\int_{-\infty}^{0} \phi u_t + a\phi u_x \, dx + \int_{0}^{\infty} \phi v_t + a\phi v_x \, dx = 0 \Rightarrow
\]
\[
\int_{-\infty}^{0} \phi u_t \, dx + \int_{0}^{\infty} \phi v_t \, dx - \int_{-\infty}^{0} a\phi_x u \, dx - \int_{0}^{\infty} a\phi_x v \, dx
\]
\[
+ a\phi_0(u - v)_0 = 0
\]
\[
= 0
\]

No remaining terms at the interface ⇒ conservation.
\begin{align*}
u_t + aP_L^{-1}Q_Lu &= \sigma_L P_L^{-1}(u_N - v_0)e_N, \\
v_t + aP_R^{-1}Q_Rv &= \sigma_R P_R^{-1}(v_0 - u_N)e_0.
\end{align*}

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

**Conservation:** Multiply with smooth function \( \phi \) and integrate.

\begin{align*}
\phi^T P_L u_t + a\phi^T Q_L u &= \sigma_L \phi(u_N - v_0) \\
\phi^T P_R v_t + a\phi^T Q_R v &= \sigma_R \phi_0(v_0 - u_N)
\end{align*}
Numerical integration using SBP operators: $Q \rightarrow -Q^T + B \Rightarrow$

\[
\phi^T P_L u_T + \phi^T P_R v_t - a(P_L^{-1} Q_L \phi^T)P_L u - a(P_R^{-1} Q_R \phi)^T P_R u +
\]

mimic PDE terms

\[
-\alpha \phi_N u_N + \sigma_R \phi_N (u_N - v_0) + \phi_0 v_0 + \sigma_R \phi (v_0 - u_N)
\]

IT=interface terms that should vanish

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

\[
IT = \phi_0 (-\alpha u_N + \sigma_N (u_N - v_0) + \alpha v_0 + \sigma_0 (v_0 - u_N)) = \phi_0 (u_N - v_0) (\sigma_L - \sigma_R - \alpha).
\]

∴ We have a conservative scheme if $\sigma_L = \sigma_R + \alpha$. 
Stability: Multiply with the solutions $u, v$ and integrate $\Rightarrow$

\[ u^T P_L u_T + v^T P_R v_t = -au_N^2 + av_0^2 + 2u_N\sigma_L(u_N - v_0) + 2v_0\sigma_R(v_0 - u_N) \]

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

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

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

\[ \sigma_L + \sigma_R \leq 0, \text{ the stability condition } \sigma_R \leq -a/2. \]

\[ \sigma_L - \sigma_R - a = 0, \text{ the conservation condition.} \]

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 ⇒ provide relation between penalty coefficients.
• Conservation necessary for stability (and dual consistency).
• Check for conservation first, next step stability.

References
Accuracy and error estimates

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

Semi-discrete

\[ v_t + P^{-1}Qv = \sigma P^{-1}(v_0 - g)e_0 \]
\[ v(0) = f \]

(1a)

(1b)

Insert analytical solution \( u \) into (1)

\[ u_t + P^{-1}Qu = \sigma P^{-1}(u_0 - g)e_0 + T_e \]
\[ u(0) = f \]

(2a)

(2b)

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

Note: No error from penalty term (with Dirichlet b.c.).
(2)-(1) with $u - v = e = \text{error} \Rightarrow$

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

$$e(0) = 0 \quad (3b)$$

Solve (3) and the exact error is known.

Note: $e \neq T_e$. $T_e = \text{source of error only, not the error itself.}$

Energy:

$$e^TPe_t + e^TQe = \sigma e_0^2 + e_0^TPTe \Rightarrow$$

$$\left(\|e\|^2_P\right)_t = e_0^2(1 + 2\sigma) - e_N^2 + 2e^TPTe$$

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

$$\frac{d}{dt} \|e\|^2 = -(e_0^2 + e_N^2) + 2(e, T_e). \quad (4)$$
A first crude estimate

\[
\frac{d}{dt} \|e\|^2 = -(e_0^2 + e_N^2) + 2(e, T_e) \leq \eta \|e\|^2 + \frac{1}{\eta} \|T_e\|^2
\]  \hspace{1cm} (5)

Multiply with integrating factor \(e^{-\eta t}\) and integrate ⇒

\[
\|e\|^2 \leq \frac{1}{\eta} e^{-\eta t} \int_0^t e^{-\xi t} \|T_e\|^2 d\xi = O(\|T_e\|^2)
\]  \hspace{1cm} (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.

A second crude estimate

\[
\frac{d}{dt} \|e\|^2 = -(e_0^2 + e_N^2) + 2(e, Te) \leq 2\|e\|\|Te\| \quad (7)
\]

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

\[
\frac{d}{dt} \|e\| \leq \|Te\|. \quad (8)
\]

• 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

\[ 2\|e\|_t \|e\| \leq -(e_0^2 + e_N^2) + 2\|e\|_t \|T_e\| \Rightarrow \|e\|_t \leq -\left( \frac{e_0^2 + e_N^2}{2\|e\|^2} \right) \|e\| + \|T_e\| \]

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

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

\[ = e^{-\eta T} \|T_e\|_{\text{max}} \frac{(e^{\eta T} - 1)}{\eta} = \|T_e\|_{\text{max}} \frac{(1 - e^{-\eta T})}{\eta} \leq \frac{\|T_e\|_{\text{max}}}{\eta} \]
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 gives a linear error growth in time.
- A more refined error estimate where boundary effects are included, gives a linear error growth in time.
- By mesh refinement, arbitrary accuracy at any future time.
- No linear growth in time for parabolic problems even if boundary procedure not optimal, easier problem.
Exercises/Seminars

• Show that an error bound exists 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”

\[ u_t + Au_x = 0, \ x \geq 0 \]  \hspace{1cm} (9a)
\[ Lu = 0, \ x = 0 \]  \hspace{1cm} (9b)
\[ u(x, 0) = f(x), \ x \geq 0 \]  \hspace{1cm} (9c)

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

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

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

\[
\frac{d}{dt} \|u\|^2 = u^T Au \leq 0, \quad \therefore \text{Maximally semi-bounded operator.}
\]
As an example, consider S-W equations in 1D: \( A = \begin{bmatrix} \tilde{u} & 0 & \tilde{c} \\ 0 & \tilde{u} & 0 \\ \tilde{c} & 0 & \tilde{c} \end{bmatrix} \).

\[
\frac{d}{dt} ||u||^2 = u^T Au = W^T \Lambda W = (\tilde{u} + \tilde{c})w_1^2 + \tilde{u}w_2^2 + (\tilde{u} - \tilde{c})w_3^2,
\]

where \( W = X^T u \). Well-posed boundary conditions are

\[
LW = 0, \quad L = \begin{bmatrix} 1 & 0 & -k \\ 0 & 1 & 0 \end{bmatrix}.
\]

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

The B.C.’s can be written

\[
LX^T u = 0.
\]

Now, how to construct penalty matrices \( \Sigma \) such that

\[
W^T (\Lambda + \Sigma L + (\Sigma L)^T) W \leq 0 ?
\]
Note: We need $\Sigma L$ to have same size as $\Lambda$ and $A$. This means that $[\Sigma] = L^T$. Try

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

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

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

$$
\Lambda + \Sigma L + (\Sigma L)^T \leq 0 \Rightarrow
$$

$$
2\sigma_1 + u + c \leq 0
$$

$$
2\sigma_4 + u \leq 0
$$

$$
-2\sigma_5 k + u - c \leq 0.
$$
We aim for a “perfect match” such that

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

This implies

\[
\sigma_1 = -\frac{u + c}{2}, \quad \sigma_4 = -\frac{u}{2}, \quad \sigma_5 = -\frac{u + c}{2}k
\]

\[
\sigma_2 = 0, \quad \sigma_3 = 0, \quad \sigma_6 = 0
\]

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

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

\[\therefore\quad \text{Exactly right! The } \Sigma \text{ derived will be used in the SAT term.}\]
\[ \Lambda + \Sigma L + (\Sigma L)^T \leq 0 \Rightarrow X(\Lambda + \Sigma L + (\Sigma L)^T)X^T \leq 0 \Rightarrow A + X^T\Sigma LX + X^T(\Sigma L)^TX \leq 0 \]

(10)

What have we done?

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

We will use so called **Kronecker Products**, defined below.

\[ A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \ldots \\ a_{21}B & \ldots \end{bmatrix} , \]

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

The scheme using SBP-SAT and Kronecker products is

\[ u_t + (P^{-1}Q \otimes A)u = (P^{-1}E_0 \otimes \tilde{\Sigma}L)(u - g) \]
\[ u(0) = f. \quad (11) \]

Energy with \( g = 0 \) leads to

\[ u^T(P \otimes I)u_t + u^T(Q \otimes A)U = u_0^T\tilde{\Sigma}Lu_0. \quad (12) \]
Add transpose of (12) to itself ⇒

\[
(u^T(P \otimes I)u)_t + u^T(Q + Q^T \otimes A)u = u_0^T(\tilde{\Sigma}L + (\tilde{\Sigma}L)^T)u_0.
\]

\[\frac{d}{dt}(\|u\|^2_{P \otimes I}) + B \leq 0,\]

We find

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

by the previous derivation, see (10).

∴ Energy stability follows automatically from well-posed boundary conditions.
Boundary procedures for parabolic problems

\[ u_t + Au_x = \epsilon (Bu_x)_x, \quad x \geq 0 \]

\[ Lu = 0, \quad x = 0 \quad \text{(13)} \]

\[ u(x,0) = f(x), \quad x \geq 0 \]

\[
\frac{d}{dt} ||u||^2 + 2\epsilon \int_0^\infty u_x^T Bu_x dx = u^T Au - \epsilon u^T Bu_x - \epsilon u_x^T Bu_x = BT
\]

All boundary operators \( L \) must remove the indefinite terms \( \Rightarrow \)

\[ Lu = Cu - \epsilon Bu_x = 0. \quad \text{(14)} \]

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

**Remark:** 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
\[ u_t + (P^{-1} Q \otimes A)u - \epsilon (P^{-1} Q \otimes B)u_x = \left[ P^{-1} E_0 \otimes (-I) \right][(I \otimes C)u - \epsilon (I \otimes B)u_x]. \]

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 \(\Rightarrow\)
\[
(u^T (P \otimes I)u)_t + 2\epsilon (u_x^T (P \otimes I)u_x) = \\
u_0^T Au_0 - \epsilon u_0^T Bu_0 - (u_x)_0^T Bu_0 - u_0^T Cu_0 + \epsilon u_0^T Bu_0 \]
\[
- u_0^T C^T u_0 + \epsilon (u_x)_0^T Bu_0 \]
\[
= u_0^T (A - (C + C^T))u_0 \leq 0. \]

\(\therefore\) 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