Numerical Solution of Initial Boundary Value Problems

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Stability problems for numerical approximations

Continuous ($\|u\|^2 = \int_0^1 u^2 dx$)

$$u_t + au_x = 0, \quad u(0,t) = g(t) \quad \Rightarrow \quad \frac{d}{dt}\|u\|^2 = \underbrace{ag^2(t)}_{\geq 0} - \underbrace{au(1,t)^2}_{\geq 0}$$

Semi-discrete ($\|u\|_h^2 = \sum_{i=1}^{N-1} u_i u_i \Delta x$)

$$u_{it} + a\left(\frac{u_{i+1} - u_{i-1}}{2\Delta x}\right) = 0, \quad u_0 = g(t), \quad \Rightarrow \quad \frac{d}{dt}\|u\|^2 = \underbrace{ag(t)u_1}_{=?} - \underbrace{au_N u_{N-1}}_{=?}$$

∴ How do we implement boundary conditions for PDE?

∴ How do we choose numerical boundary conditions?

Summation-By Parts (SBP) operators for FE, SE, DG methods

$$u_t + au_x = 0 \tag{1}$$

Let $u = L^T(x)\ \vec{\alpha}(t) = \sum_{i=0}^{N} \alpha_i(t)\phi_i(x)$.

$$L = (\phi_0, \phi_1,\ \dots\ \phi_N)^T, \quad \vec{\alpha} = (\alpha_0, \alpha_1, \dots \alpha_N)^T$$

Insert into (1) $\Rightarrow$

$$L^T\vec{\alpha}_t + aL_x^T\vec{\alpha} = 0 \Rightarrow \underbrace{\int_0^1 LL^T dx}_{P}\,\vec{\alpha}_t + a\underbrace{\int_0^1 LL_x^T dx}_{Q}\,\vec{\alpha} = 0$$

$$P\vec{\alpha}_t + aQ\vec{\alpha} = 0 \tag{2}$$

Intergration-by-parts

$$P\vec{\alpha}_t + aL\,L^T\Big|_0^1 \vec{\alpha} - a\int_0^1 L_x L^T dx\ \ \vec{\alpha} = 0 \Rightarrow P\vec{\alpha}_t + aB\vec{\alpha} - aQ^T\vec{\alpha} = 0$$

$$B = L\,L^T\Big|_0^1 = \begin{bmatrix} \phi_0 \\ \phi_1 \\ \vdots \\ \phi_N \end{bmatrix} [\phi_0\ \phi_1\ \ldots\ \phi_N]\Big|_0^1 = \begin{bmatrix} \phi_0\phi_0 & \phi_0\phi_1 & \ldots & \\ \phi_1\phi_0 & & & \\ & & \ddots & \\ & & & \\ & & & \phi_N\phi_N \end{bmatrix}_0^1$$

For Lagrange polynomials we get

$$B = L\,L^T\Big|_0^1 = \begin{bmatrix} 0 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix} - \begin{bmatrix} 1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{bmatrix} = \begin{bmatrix} -1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}.$$

Summation-By-Parts (SBP) operators

Comparing

$$P\vec{\alpha}_t + aQ\vec{\alpha} = 0 \quad with \quad P\vec{\alpha}_t + aB\vec{\alpha} - aQ^T\vec{\alpha} = 0$$

leads to $Q = B - Q^T$.

We derived P, Q using basis functions and integration by parts.

- P symmetric positive definite: $y^T P y = \int_0^1 (L^T y)^T (L^T y) dx$.
- Q almost skew-symmetric: $Q + Q^T = \int_0^1 L L_x^T + L_x L^T dx = B$

Later, we will do this directly without basis functions and integration by parts.

Energy estimates

Continuous

$$\frac{d}{dt}\|u\|^2 = a\left(u^2(0,t) - u^2(1,t)\right)$$

Semi-discrete

$$\frac{1}{2}\frac{d}{dt}\left(\alpha^T P\alpha\right) + a\vec{\alpha}^T\left(\frac{Q+Q^T}{2} + \frac{Q-Q^T}{2}\right)\vec{\alpha} = 0 \quad \Rightarrow$$

$$\frac{d}{dt}\|\alpha\|_P^2 = a(\alpha_0^2 - \alpha_N^2).$$

- Similar stability results for the different energy rates.
- Quadratic boundary terms appear, no indefinite terms.
- Perfect ”numerical boundary conditions”.

General SBP operators

$$(u, v_x) = \int_0^1 u v_x dx = uv|_1 - uv|_0 - (u_x, v) \tag{3}$$

We want to mimic this discretely such that

$$(u, Dv)_P = u^T P D v = u_N v_N - u_0 v_0 - (Du, v)_P.$$

$$u = (u_0, u_1, \dots u_N)^T, \;\; D \text{ and } P \;\; (N+1) \times (N+1) \text{ matrices}$$

- Does P and D exist ? (Yes, if one uses basis functions)
- What symmetry requirements are needed ?
- How to construct P and D ?

Example:

$$\frac{du_j}{dt} = Du_j, \qquad Du_j = \begin{cases} D_+u_j, & j = 0 \\ D_0u_j, & j \neq 0, N \\ D_-u_j, & j = N \end{cases}$$

Choose scalar product: $(u, v)_h = \frac{h}{2}u_0v_0 + h\sum_{j=1}^{N-1} u_jv_j + \frac{h}{2}u_Nv_N$

$$(u, v)_h = u^T Pv, \quad P = h\,\mathrm{diag}(1/2, 1, 1, ..., 1, 1/2)$$

$$D = \frac{1}{h}\begin{bmatrix} -1 & 1 & 0 & & \\ -1/2 & 0 & 1/2 & & \\ & \ddots & \ddots & \ddots & \\ & & -1/2 & 0 & 1/2 \\ & & & -1 & 1 \end{bmatrix}, \; PD = Q = \frac{1}{2}\begin{bmatrix} -1 & 1 & 0 & & \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ & & & -1 & 1 \end{bmatrix}$$

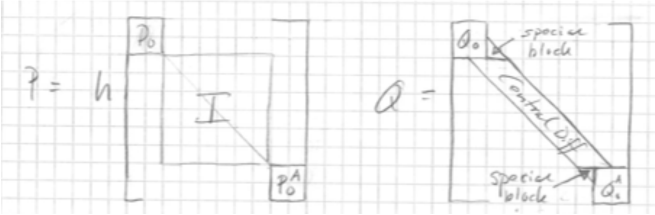
$$Q + Q^T = \begin{bmatrix} -1 & 0 & 0 & & \\ 0 & 0 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & 0 & 0 \\ & & 0 & 0 & 1 \end{bmatrix}.$$

We get

$$(u, Du) = u^T P D u = u^T Q u = u^T (\frac{Q + Q^T}{2}) u = \frac{1}{2}(u_N^2 - u_0^2).$$

- Exactly the analytical result.
- Higher order approximations in the same way, but with more involved algebra.

High order SBP operators for finite differences



P_0^A, Q_0^A are transposed along the anti-diagonal

Theorem ("block norm") For interior order of accuracy $2S$, P, Q exist such that $P = P^T > 0$, $P_0 =$ block matrix and $Q + Q^T = B$ with order $2S - 1$ near boundaries.

Theorem ("diagonal norm") For interior order of accuracy $2S$, $1 \leq S \leq 5$, P, Q exist such that $P = P^T > 0$, $P_0 =$ diagonal matrix, and $Q + Q^T = B$ with order S near boundaries.

The P matrix (or P norm) is an integration operator (both block and diagonal) of order $2S$ = interior accuracy.

Let: ϕ smooth function, $\vec{\phi} = \phi$ injected at the grid points.

Then: $\frac{\partial \phi}{\partial x}$ smooth function, $(\frac{\partial \vec{\phi}}{\partial x}) = \frac{\partial \phi}{\partial x}$ injected at the grid points.

Let $\vec{1} = (1, 1, ..., 1, 1)$. We get

$$\vec{1}^T P(\frac{\partial \vec{\phi}}{\partial x}) = \phi_N - \phi_0 + O(h^{2s}),$$

$$\vec{1}^T P(P^{-1} Q \vec{\phi}) = \vec{1}^T Q \vec{\phi} = \vec{1}^T \left[-Q^T + B \right] \vec{\phi} = -(Q\vec{1})^T \vec{\phi} + \phi_N - \phi_0.$$

- Integration operator of order 2S.
- Exact "integration back" of the numerical derivative.

Construction of SBP operators

Symmetry requirements: make ansatz on elements, aim for

$$P = P^T > 0, \;\; Q + Q^T = \mathrm{diag}[-1, 0, 0, ..., 0, 1].$$

Accuracy requirements:

$$\begin{aligned} P^{-1}Q\vec{1} &= 0, & Q\vec{1} &= 0 \\ P^{-1}Q\vec{x} &= \vec{1}, & Q\vec{x} &= P\vec{1} \\ P^{-1}Q\vec{x^2} &= 2\vec{x}, & Q\vec{x^2} &= 2P\vec{x} \\ &\vdots & &\vdots \end{aligned}$$

$$\vec{1} = (1, 1, ..., 1, 1), \quad \vec{x} = (0, \Delta x, 2\Delta x, ...1), \quad \vec{x^2} = (0, \Delta x^2, ..., 1)$$

- Solve for unknowns in P, Q using e.g. Maple.
- Non-unique operators, more unknowns than equations.
- Parameters modify bandwith, errors and spectral radius.

Summary: first derivative SBP operators

- SBP operators mimic Integration-by-Parts.
    - $u_x \approx P^{-1}Qu, P = P^T > 0, Q + Q^T = B$
    - $u_{xx} \approx (P^{-1}Q)^2u$, (wide).
    - $u_{xx} \approx P^{-1}(-A + BD)$, $A + A^T \geq 0$ (compact)
    - Diagonal norm operators most important.
    - Numerical boundary conditions form SBP operators.
    - SBP operators for "all" orders exist.
- References
    - B. Strand, JCP 1994.
    - M.H. Carpenter, J. Nordström & D. Gottlieb JCP 1999.
    - K. Mattsson & J. Nordström, JCP 2004.
    - M. Svärd & J. Nordström, (Review) JCP 2013.

What about boundary conditions?

$$u_t + au_x = 0, \quad u(0,t) = g(t)$$

(i) Multiply with smooth function α and integrate.

$$\int_0^1 \alpha u_t dx + a \int_0^1 \alpha u_x dx = 0 \;\Rightarrow\; \int_0^1 \alpha u_t dx + a\alpha\, u|_0^1 - a \int_0^1 \alpha_x u dx = 0$$

(ii) Change $u(0,t)$ to $g(t)$ (DG procedure) and integrate back.

$$\int_0^1 \alpha u_t dx + a \int_0^1 \alpha u_x = \underbrace{-\alpha(0) a \left(u(0,t) - g\right)}_{\text{penalty term}}$$

(iii) Stability? Change $\alpha \rightarrow u$ and integrate.

$$\frac{d}{dt}\|u\|^2 = ag^2 - au^2(1,t) - a\left(u(0,t) - g\right)^2$$

More on boundary conditions

$$P\vec{\alpha}_t + aQ\vec{\alpha} = 0, \quad Q + Q^T = B \quad \Rightarrow \quad P\vec{\alpha}_t + aB\vec{\alpha} - aQ^T\vec{\alpha} = 0.$$

DG trick: replace "what you have with what you like"
$\alpha_0 \rightarrow g(t)$.

$$P\vec{\alpha}_t + a\begin{bmatrix} -g(t) \\ 0 \\ \vdots \\ \alpha_N \end{bmatrix} - aQ^T\vec{\alpha} = 0, \quad \Rightarrow \quad P\vec{\alpha}_t + aQ\vec{\alpha} = \begin{bmatrix} -a(\alpha_0 - g(t)) \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

- DG uses a weak penalty formulation.

$$\frac{1}{2}\frac{d}{dt}\left(\alpha^T P\alpha\right) + a\vec{\alpha}^T\left(\frac{Q+Q^T}{2} + \frac{Q-Q^T}{2}\right)\vec{\alpha} = -a\alpha_0(\alpha_0 - g(t)) \quad \Rightarrow$$

$$\frac{d}{dt}\|\alpha\|_P^2 = a(g(t)^2 - \alpha_N^2) - a(\alpha_0 - g(t))^2.$$

- DG is energy stable with optimally sharp energy estimates.

Weak boundary procedure - SAT

"Simultaneous Approximation Term"

How do we impose boundary conditions that lead to stability ?

$$u_t + au_x = 0, \quad u(0,t) \quad = g, \quad \Rightarrow \quad \frac{d}{dt}\|u\|^2 = ag^2 - au^2(1,t)$$

How do we mimic this discretely ?

$$u_t + aP^{-1}Qu = B(u_0 - g), \text{ RHS is accurate, but what is } B?$$

Energy

$$u^T Pu_t + au^T Qu = u^T PB(u_0 - g), \Rightarrow \frac{d}{dt}\|u\|_P^2 = au_0^2 + 2u^T PB(u_0 - g) - au_N^2$$

We need

$$BT = au_0^2 + 2u^T PB(u_0 - g) \le ag^2.$$

Let

$$B(u_0 - g) = \sigma P^{-1}(u_0 - g)e_0, \;\; e_0 = (1, 0, 0, ..., 0)^T, \sigma = \text{unknown.}$$

This leads to

$$\begin{aligned} BT = au_0^2 + 2\sigma u_0(u_0 - g) = ag^2 + \begin{bmatrix} u_0 \\ g \end{bmatrix}^T \begin{bmatrix} a + 2\sigma & -\sigma \\ -\sigma & -a \end{bmatrix} \begin{bmatrix} u_0 \\ g \end{bmatrix} \\ = g^2 - a(u_0 - g)^2 \end{aligned}$$

if $\sigma = -a$.

$$\therefore \tfrac{d}{dt}\|u\|_P^2 = ag^2 - au_N^2 - a(u_0 - g)^2$$

$\therefore$ "More stable than the IBVP".

SBP-SAT for advection-diffusion problems

$$u_t + au_x = \epsilon u_{xx} \;; \qquad 0 \le x \le 1, t \ge 0 \qquad (4a)$$
$$L_0 u = g_0 \qquad x = 0, t \ge 0 \qquad (4b)$$
$$L_1 u = g_1 \qquad x = 1, t \ge 0 \qquad (4c)$$
$$u(x,0) = f(x) \qquad 0 \le x \le 1, t = 0 \qquad (4d)$$

Energy method for determining L_0, L_1. We consider $a, \epsilon > 0$.

$$\int_0^1 uu_t + auu_x dx = \epsilon \int_0^1 uu_{xx} dx \Rightarrow \left(\|u\|^2 = \int_0^1 u^2 dx \right)$$

$$\frac{d}{dt}\|u\|^2 + 2\epsilon\|u_x\|^2 = (au^2 - 2\epsilon u\, u_x)_0 - (au^2 - 2\epsilon uu_x)_1.$$

Note that

$$BT = au^2 - 2\epsilon uu_x = a^{-1}\left[(au - \epsilon u_x)^2 - (\epsilon u_x)^2\right].$$

$$BT = a^{-1}\left[(au - \epsilon u_x)^2 - (\epsilon u_x)^2\right]$$

At $x = 0$, let

$$L_0 = a - \epsilon\frac{\partial}{\partial x}$$

At $x = 1$, let

$$L_1 = \epsilon\frac{\partial}{\partial x}$$

This leads to

$$BT_0 = a^{-1}\left[g_0^2 - (\epsilon u_x)^2\right], \quad BT_1 = a^{-1}\left[(au - \epsilon u_x)^2 - g_1^2\right],$$

or formulated in another way

$$BT_0 = \frac{g_0^2}{a} - a^{-1}(au_0 - g_0)^2, \quad BT_1 = \frac{g_1^2}{a} - a^{-1}(au_N - g_1)^2.$$

$\therefore$ Well-posed boundary conditions with a bounded energy.

$$
\begin{aligned}
u_t + aP^{-1}Qu = \epsilon P^{-1}Qu_x + P^{-1}\sigma_0(au_0 - \epsilon(u_x)_0 - g_0)e_0 + \\
+ P^{-1}\sigma_1(\epsilon(u_x)_N - g_1)e_N \qquad (5) \\
u(0) = f
\end{aligned}
$$

The parameters σ_0, σ_1 will be determined by stability requirements. We also used $u_x = P^{-1}Qu$, $e_0 = (1, 0, 0, ..., 0)^T$, $e_N = (0, 0, ..., 0, 1)^T$.

Energy

$$
u^T Pu_t + au^T Qu = \epsilon u^T Qu_x + \sigma_0 u_0(au_0 - \epsilon(u_x)_0 - g_0) + \sigma_1 u_N(\epsilon(u_x)_N - g_1) \qquad (6)
$$

Add transpose of equation (6) to itself $\Rightarrow$

$$
\underbrace{u^T Pu_t + u_t^T Pu}_{(1)} + \underbrace{au^T(Q + Q^T)u}_{(2)} - \underbrace{\epsilon(u^T Qu_x + u_x^T Q^T u)}_{(3)} + 2BT. \qquad (7)
$$

$$(1) = \frac{d}{dt}(u^T P u) = \frac{d}{dt}(\|u\|_P^2)$$
$$(2) = a u^T (Q + Q^T) u = a u^T B u = a(u_N^2 - u_0^2)$$
$$(3) = \epsilon(u^T Q u_x + u_x^T Q^T u) = \epsilon(u^T(-Q^T + B)u_x + u_x^T(-Q + B)u)$$
$$= -\epsilon(u^T Q^T u_x + u_x^T Q u) + \epsilon(u^T B u_x + u_x^T B u)$$

$$u^T Q^T u_x + u_x^T Q u = 2u_x^T Q u = 2u_x^T P P^{-1} Q u = 2u_x^T P u_x = 2\epsilon\|u_x\|_P^2$$

$$u^T B u_x + u_x^T B u = 2u^T B u_x = 2u_N (u_x)_N - 2u_0 (u_x)_0$$

$$\therefore \quad \frac{d}{dt}\|u\|^2 + 2\epsilon\|u_x\|^2 = \underbrace{(a u_0^2 - 2\epsilon u_0 (u_x)_0) - (a u_N^2 - 2\epsilon u_N (u_x)_N)}_{\text{from equation}}$$
$$= \underbrace{2\sigma_0 u_0 (a u_0 - \epsilon (u_x)_0 - g_0) + 2\sigma_1 u_N (\epsilon (u_x)_N - g_1)}_{\text{from penalty terms}}$$

Choose $\sigma_0 = -1, \sigma_1 = -1$ such that mixed the uu_x terms cancel.

$$
\begin{aligned}
RHS &= -au_0^2 + 2u_0 g_0 - au_N^2 + 2u_N g_1 \\
&= \frac{g_0^2}{a} \underbrace{- \frac{g_0^2}{a} - au_0^2 + 2u_0 g_0}_{-a^{-1}(au_0 - g_0)^2} + \frac{g_1^2}{a} \underbrace{- \frac{g_1^2}{a} - au_N^2 + 2u_N g_1}_{-a^{-1}(au_N - g_1)^2}
\end{aligned}
$$

$$
\frac{d}{dt}(\|u\|_P^2) + 2\epsilon \|u_x\|_P^2 = \frac{g_0^2}{a} - a^{-1}(au_0 - g_0)^2 + \frac{g_1^2}{a} - a^{-1}(au_N - g_1)^2
$$

$\therefore$ Exactly the same form as the continuous energy estimate.

Summary of SAT procedure

- Find well-posed boundary conditions that lead to an energy estimate.
- Construct penalty/forcing terms that impose these boundary conditions.
- Choose penalty coefficient such that indefinite terms are removed.
- Aim for the same/similar estimate as in the continuous case, possibly with a small damping term added.
- References
  - JNO
  - M. H. Carpenter, D. Gottlieb & S. Abarbanel JCP 1994.
  - M. H. Carpenter, J. Nordström & D. Gottlieb JCP 1999.

Second derivative SBP operators

$$(u, u_{xx}) = \int_0^1 u u_{xx} dx = u u_x|_1 - u u_x|_0 - \|u_x\|^2 \qquad (8)$$

Can we construct operators that mimics (8)?

Yes, by for example using the first derivative twice.

$$(u, (P^{-1}Q)^2 u) = u^T Q u_x = u^T(-Q^T + B)u_x = u_N (u_x)_N - u_0 (u_x)_0 - \|u_x\|_P^2$$

since

$$-u^T Q^T u_x = -u^T Q^T P^{-1} P u_x = -(P^{-1}Qu)^T P u_x = -u_x^T P u_x.$$

Drawbacks with wide operator $(P^{-1}Q)^2$

- Unnecessary wide which leads to large error constant.
- Bad damping of high wave-numbers, which the PDE have.

$$u_t = u_{xx} \quad u = \hat{u}e^{i\omega x} \Rightarrow \hat{u}_t = -\omega^2 \hat{u}$$

$$\hat{u}_{jt} = D_0 D_0 u_j \quad \hat{u} = \hat{u}e^{i\omega x_j} \Rightarrow \hat{u}_t = -\frac{1}{h^2}\sin^2(\xi)\hat{u}$$

$$u_{jt} = D_+ D_- u_j \quad u = \hat{u}e^{i\omega x_j} \Rightarrow \hat{u}_t = -\frac{4}{h^2}\sin^2(\xi/2)\hat{u}$$

For $\xi_{\max} = \pi$, there is no damping with the wide operator.

Compact second derivative SBP operator

Consider:

$$\begin{aligned}
D^{(2)} &= (P^{-1}Q)^2 = P^{-1}(QP^{-1}Q) = P^{-1}((-Q^T + B)P^{-1}Q) = \\
&= P^{-1}(-Q^T P^{-1}Q + BP^{-1}Q) \\
u^T PD^{(2)}u &= u^T(-Q^T P^{-1}Q + BP^{-1}Q) = -(Qu)^T P^{-1}Qu + u^T BDu \\
&= -(P^{-1}Qu)^T P(P^{-1}Qu) + u^T BDu = \\
&= -\|Du\|_P^2 + u^T BDu. \quad \text{A perfect stability result.}
\end{aligned}$$

Can we make a compact version of this?

Yes! It has the structure:

$$D^{(2)} = P^{-1}(-A + BD)$$

Observations regarding $D^{(2)} = P^{-1}(-A + BD)$

- Compact, occupies same space as $P^{-1}Q$.
- $A + A^T \geq 0$ for stability.
- Clumsy to use for flux-based equations.
  $F = AU - \epsilon(B_{11}D_x u + B_{12}D_y u);\ F_x = D_x F$.
- Certain stability complications for N-S equations since two different first derivatives appear.

The second order accurate operator is

$$D^{(2)} = \frac{1}{h^2}\begin{bmatrix} 1 & -2 & 1 & 0 & \\ 1 & -2 & 1 & 0 & \\ 0 & 1 & -2 & 1 & \\ & & & \ddots & \end{bmatrix},$$

$$A = \frac{1}{h}\begin{bmatrix} 1 & -1 & 0 & 0 & \\ -1 & 2 & 1 & 0 & \\ 0 & 1 & -2 & 1 & \\ & & & \ddots & \end{bmatrix}, \quad D = \frac{1}{h}\begin{bmatrix} \frac{3}{2} & -2 & \frac{1}{2} & 0 & \\ 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & \\ & & & \ddots & \end{bmatrix}.$$

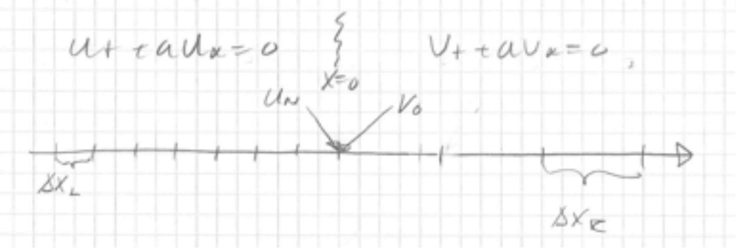
SBP-SAT for multi-block methods

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

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 $\Rightarrow$

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

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

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

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

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

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 ⇒ 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

$$v_t + P^{-1}Qv = \sigma P^{-1}(v_0 - g)e_0 \tag{9a}$$
$$v(0) = f \tag{9b}$$

Insert analytical solution u into (1)

$$u_t + P^{-1}Qu = \sigma P^{-1}(u_0 - g)e_0 + T_e \tag{10a}$$
$$u(0) = f \tag{10b}$$

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 $u - v = e = \text{error} \Rightarrow$

$$e_t + P^{-1}Qe = \sigma P^{-1}e_0 e_0 + T_e \tag{11a}$$
$$e(0) = 0 \tag{11b}$$

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 $\sigma = -1 \Rightarrow$

$$\frac{d}{dt}\|e\|^2 = -(e_0^2 + e_N^2) + 2(e, T_e). \tag{12}$$

A first crude estimate

$$\frac{d}{dt}||e||^2 = -(e_0^2 + e_N^2) + 2(e, T_e) \leq \eta||e||^2 + \frac{1}{\eta}||T_e||^2 \qquad (13)$$

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

$$||e||^2 =\leq \frac{1}{\eta}e^{-\eta t}\int_0^t e^{-\xi t}||T_e||^2 d\xi = O(||T_e||^2) \qquad (14)$$

- 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

$$\frac{d}{dt}||e||^2 = -(e_0^2 + e_N^2) + 2(e, T_e) \leq 2||e||||T_e|| \quad (15)$$

Note now that $\frac{d}{dt}||e||^2 = 2||e||\frac{d}{dt}||e||$ which implies that (15) goes to

$$\frac{d}{dt}||e|| \leq ||T_e||. \quad (16)$$

- The relation (16) indicates a linear growth in time.
- Seemingly, long time integration of hyperbolic problems would lead to large errors, rendering the solution useless.

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 $\eta(t) =$ 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, lead to an error bound.
- 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?

End of Lecture 2