Numerical Solution of Initial Boundary Value Problems

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Lecture 3

High Order Finite Difference Approximations, Summation-by-Parts Operators and Weak Boundary Procedures

Pros and Cons for High Order Finite Difference Methods:

- + efficient
- + scales well in multiple dimensions
- + easy to program
- + easy to modify locally (shocks)
- - not trivial to capture complex geometry
- - stability at boundaries and interfaces

Can we get rid of the last drawback?

Stability problems

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

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

$\therefore$ We need a modified formulation.

Summation-By Parts (SBP) operators for FEM-dG-spectral 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

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

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

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

Taking a closer look at what we did. Comparing

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

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

We have derived Ps and Qs by using basis functions and integration by parts.

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

Later, we will do it without basis functions, directly, for finite differences.

Energy estimates

Continuous

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

Semi-discrete

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

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

- We will derive P and Q for high order finite difference methods.

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

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

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

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

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

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

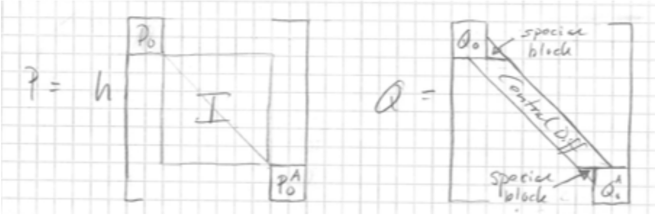
$$
Q + Q^T = \begin{bmatrix} -1 & 0 & 0 & & \\ 0 & 0 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & 0 & 0 \\ & & 0 & 0 & 1 \end{bmatrix}.
$$

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



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.
  - $u_x \approx P^{-1}Qu$, $P = P^T > 0$, $Q + Q^T = B$
  - $u_{xx} \approx (P^{-1}Q)^2 u$, (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.

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

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

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

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" $\alpha_0 \to g(t)$.

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

- 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 ?

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

How do we mimic this discretely ?

$$u_t + a P^{-1} Q u = B(u_0 - g), \quad \text{RHS is accurate, but what is } B?$$

Energy

$$u^T P u_t + a u^T Q u = u^T P B(u_0 - g), \;\Rightarrow\; \frac{d}{dt}\|u\|_P^2 = a u_0^2 + 2u^T P B(u_0 - g) - a u_N^2$$

We need

$$BT = a u_0^2 + 2u^T P B(u_0 - g) \leq a g^2.$$

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 $\sigma = -a$.

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

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

SBP-SAT for advection-diffusion problems

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

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

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

$\therefore$ 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

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

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

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

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

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

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

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

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

$$\begin{aligned} RHS &= -au_0^2 + 2u_0g_0 - au_N^2 + 2u_Ng_1 \\ &= \frac{g_0^2}{a} \underbrace{-\frac{g_0^2}{a} - au_0^2 + 2u_0g_0}_{-a^{-1}(au_0 - g_0)^2} + \frac{g_1^2}{a} \underbrace{-\frac{g_1^2}{a} - au_N^2 + 2u_Ng_1}_{-a^{-1}(au_N - g_1)^2} \end{aligned}$$

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

$\therefore$ Similar to 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.
- 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

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

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:

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

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 problems for N-S equations since two different first derivatives appear.

The second order accurate operator is

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

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

Exercises/Seminars

- Construct 2nd order SBP operator explicitly
- Prove that a diagonal P is a 2S order accurate integration operator (hint: find the compatibility conditions).
- Derive boundary conditions for the wave equation.
- Show energy-estimates for the semi-discrete wave equation, using the boundary conditions above.