Superconvergent functional estimates from summation-by-parts finite difference discretizations

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Outline

1. Motivation
2. Preliminaries
3. Theory
4. Practical issues
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1 Motivation

2 Preliminaries

3 Theory

4 Practical issues
The finite difference method is quite efficient in many PDEs and straightforward to derive and implement.
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- Constructing high-order finite difference schemes that are provably time-stable is quite difficult.
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- SBP operators mimic the stability of Galerkin finite-element methods.
- SAT penalties offer time-stability.
- SBP-SAT discretizations achieve both stability and high-order accuracy, but on boundaries that accuracy is decreased.
The finite difference method is quite efficient in many PDEs and straightforward to derive and implement.

Constructing high-order finite difference schemes that are provably time-stable is quite difficult.

SBP operators mimic the stability of Galerkin finite-element methods.

SAT penalties offer time-stability.

SBP-SAT discretizations achieve both stability and high-order accuracy, but on boundaries that accuracy is decreased.

Discretizations based on diagonal-norm SBP-SAT operators produce superconvergent functional estimates.
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Notation

- Uniformly spaced mesh grid on $[0, 1]$:
  \[ x_k = kh, \text{ with } k = 0, 1, \ldots, n \text{ for } h = 1/n \]

- $\mathcal{U} \in C^p([0, 1])$

- $u = \begin{pmatrix} \mathcal{U}(x_0) & \mathcal{U}(x_1) & \ldots & \mathcal{U}(x_n) \end{pmatrix}^T \in \mathbb{R}^{n+1}$

- $u_h \in \mathbb{R}^{n+1}$

- $e_0 = \begin{pmatrix} 1 & 0 & \ldots & 0 & 0 \end{pmatrix}^T \in \mathbb{R}^{n+1}$

- $e_n = \begin{pmatrix} 0 & 0 & \ldots & 0 & 1 \end{pmatrix}^T \in \mathbb{R}^{n+1}$

- $A \otimes B$: Kronecker product

- $A \circ B$: elementwise product
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Summation-by-parts operators

SBP operator

The matrix \( D \in \mathbb{R}^{(n+1) \times (n+1)} \) is a summation-by-parts operator for the first derivative if it has the form

\[
D = H^{-1} Q
\]

where \( H \in \mathbb{R}^{(n+1) \times (n+1)} \) is a symmetric-positive-definite weight matrix with entries \( H_{ij} = \mathcal{O}(h) \) and \( Q \in \mathbb{R}^{(n+1) \times (n+1)} \) satisfies

\[
Q + Q^T = \text{diag}(-1, 0, \ldots, 0, 1) = e_n e_n^T - e_0 e_0^T
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Summation-by-parts operators

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**Remark:** $D$ is a $2s$-order approximation to $d/dx$ at the $n + 1 - 2r$ interior nodes and a $\tau$-order accurate approximation at the $r + r$ boundary nodes.
Summation-by-parts operators

We will consider SBP operators such that:

\[
H = h \begin{pmatrix}
H_L & 0 & 0 \\
0 & I & 0 \\
0 & 0 & H_R
\end{pmatrix}
\]

where \( H_L = \text{diag}(\rho_0, \rho_1, \ldots, \rho_{r-1}) \) and \( H_R = \text{diag}(\rho_{r-1}, \ldots, \rho_1, \rho_0) \).

It is symmetric and positive-definite. It defines an inner product and a norm for vectors in the grid:

\[
(u, z)_H := u^T H z \quad \|u\|_H := (u, u)_H
\]

Functional estimates based on these discretizations are 2\(s\)-accurate.
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Remember:
Due to the truncation error at the boundary, the solution error is \(O(h^{s+1})\).

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- It is symmetric and positive-definite.
- It defines an inner product and a norm for vectors in the grid:
  \[ (u, z)_H := u^T Hz \quad \|u\|_H^2 := (u, u)_H \]
- Functional estimates based on these discretizations are 2s-accurate.
Lemma

Let \( D = H^{-1}Q \) be an SBP first derivative operator. Then

\[
(z, Du)_H = z^T Qu
\]

is a \( 2s \)-order accurate approximation to the integral

\[
\int_0^1 Z \frac{dU}{dx} dx
\]

where \( Z \frac{dU}{dt} \in C^{2s-1}([0, 1]) \).

---

Simultaneous approximation term

Let us consider:

\[
\begin{cases}
\frac{\partial U}{\partial t} + a \frac{\partial U}{\partial x} = 0, & x \in \Omega = [0, 1] \ (a > 0) \\
U(x, 0) = U_0(x) \\
U(0, t) = U_L(t)
\end{cases}
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\end{align*}$$

By using a SBP-operator $D$, we obtain the following semidiscretization:

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By using a SBP-operator \( D \), we obtain the following semidiscretization:

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\frac{\partial u_h}{\partial t} + aD u_h = 0
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We can impose boundary conditions in a strong sense. For example, by the injection method:

\[
[I - e_0 e_0^T] \left[ \frac{\partial u_h}{\partial t} + aDu_h \right] + e_0 \left[ e_0^T u_h - U_L(t) \right] = 0
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It can destroy stability properties

Simultaneous approximation term

A SAT is a penalty term used to impose the boundary conditions in a weak sense.


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A SAT is a penalty term used to impose the boundary conditions in a weak sense.

We now obtain the semidiscretization (with SAT):

\[
\frac{\partial u_h}{\partial t} + aDu_h = -\sigma aH^{-1}e_0 \left[ e_0^T u_h - U_L(t) \right]
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where \(\sigma\) is a penalty parameter.
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where \(\sigma\) is a penalty parameter.

**Time-stability**

Using the SAT, the semidiscretization is time-stable; i.e., for \(U_L = 0\) it holds

\[
\|u_h(t)\| \leq C\|u_0\| \text{ for a certain } C \in \mathbb{R}.
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**References**

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where \( \sigma \) is a penalty parameter.

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\[
\frac{d}{dt} \| u_h \|_H^2 = -au_h^T (Q + Q^T) u_h - 2\sigma au_0^2 \\
= -au_n^2 + a(1 - 2\sigma)u_0^2 \leq 0 \iff \sigma \geq \frac{1}{2}
\]
Duality

Let us consider a linear functional \( I(\mathcal{U}) = (\mathcal{G}, \mathcal{U})_\Omega \) where \( \mathcal{U} \) satisfies \( \mathcal{L}\mathcal{U} - \mathcal{F} = 0 \) for a linear differential operator \( \mathcal{L} \) and \( \mathcal{F} \in L^2(\Omega) \). Then, for a generic function \( \mathcal{V} \):

\[
I(\mathcal{U}) = (\mathcal{V}, \mathcal{F})_\Omega - (\mathcal{L}^* \mathcal{V} - \mathcal{G}, \mathcal{U})_\Omega
\]

where \( \mathcal{L}^* \) is such that \( (\mathcal{V}, \mathcal{L}\mathcal{U})_\Omega = (\mathcal{L}^* \mathcal{V}, \mathcal{U})_\Omega \). The associated adjoint problem is:

\[
\mathcal{L}^* \mathcal{V} - \mathcal{G} = 0, \ \forall x \in \Omega
\]
Duality

Let us consider a linear functional $I_h(u_h) = (g, u_h)_h$ where $u_h$ satisfies the associated discretization $\mathcal{L}_h u_h - f = 0$. Then, for a generic vector $v_h \in \mathbb{R}^{n+1}$:

$$I_h(u_h) = (v_h, f)_h - (\mathcal{L}_h^T v_h - g, u_h)_h$$

where $\mathcal{L}_h^T$ is such that $(v_h, \mathcal{L}_h u_h)_h = (\mathcal{L}_h^T v_h, u_h)_h$. The discrete adjoint problem is:

$$\mathcal{L}_h^T v_h - g = 0$$
Duality

Let us consider a linear functional $I_h(u_h) = (g, u_h)_h$ where $u_h$ satisfies the associated discretization $L_h u_h - f = 0$. Then, for a generic vector $v_h \in \mathbb{R}^{n+1}$:

$$I_h(u_h) = (v_h, f)_h - (L_h^T v_h - g, u_h)_h$$

where $L_h^T$ is such that $(v_h, L_h u_h)_h = (L_h^T v_h, u_h)_h$. The discrete adjoint problem is:

$$L_h^T v_h - g = 0$$

Dual-consistency

A discrete operator $L_h$ and functional $J_h$ are dual-consistent of order $q \geq 1$ with respect to a corresponding continuous PDE and functional if

$$L_h^T v - g = O(h^q)$$

where $v$ is the solution to the continuous adjoint problem projected onto the discrete solution space.
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Linear hyperbolic PDEs

Let us consider a scalar hyperbolic PDE:

\[
\begin{cases}
\frac{\partial U}{\partial t} + \frac{\partial}{\partial x}(\lambda U) = F, & x \in \Omega = [0, 1], \ t > 0 \\
U(x, 0) = U_0(x) \\
U(0, t) = U_L(t)
\end{cases}
\]

where \(\lambda(x)\) is the spatially varying wave speed.
Linear hyperbolic PDEs

Let us consider a stationary scalar hyperbolic PDE:

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\begin{aligned}
\frac{\partial}{\partial x}(\lambda U) &= F, \quad x \in \Omega = [0, 1] \\
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\end{cases}
\]

where \( \lambda(x) \) is the spatially varying wave speed. The SBP-SAT discretization is given by:

\[
D(\Lambda u_h) = f - H^{-1}e_0\lambda_0(e_0^T u_h - U_L)
\]

where

\[
\begin{align*}
\lambda_i &= \lambda(x_i), \ i = 0, \ldots, n \\
\Lambda &= \text{diag}(\lambda_0, \ldots, \lambda_n) \\
f &= \begin{bmatrix} F(x_0) \ldots F(x_n) \end{bmatrix}^T
\end{align*}
\]
Linear hyperbolic PDEs

Lemma

Diagonal SBP operators with $s$-accurate boundary closure, the solution error $\|u_h - u\|_p$ is at best $O(h^{s+1})$.

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Theorem

Let $I : L^2(\Omega) \rightarrow \mathbb{R}$ be a linear functional defined by:

$$I(\mathcal{U}) = \int_0^1 G\mathcal{U}dx + \alpha(\lambda\mathcal{U})|_{x=1}$$

where $G \in C^{2s}([0, 1])$ and let $H^{-1}A := H^{-1}(Q + e_0e_0^T)\Lambda$ denote the matrix appearing in the linear system ($\star$). Assume that the PDE is well posed and admits solution $\mathcal{U} \in C^{2s}([0, 1])$ and ($\star$) is non-singular. Then, if $\|A^{-T}H\|_{\infty} \leq C$ for some constant $C \in \mathbb{R}$ that does not depend on $n$, the functional estimate:

$$I_h(u_h) = (g, u_h)_H + \alpha\lambda_n(e_n^T u_h)$$

where $g = [G(x_0) \ldots G(x_n)]^T$, is a $2s$-order accurate approximation to $I(\mathcal{U})$. 
Linear hyperbolic PDEs

Proof:
Proof:
Using the SBP norm:

\[ \mathcal{I}(\mathcal{U}) = (g, u)_H + \alpha \lambda_n (e_n^T u) + \mathcal{O}(h^{2s}) \]

\[ = g^T H u + \alpha \lambda_n e_n^T u + \mathcal{O}(h^{2s}) \]

\[ = g^T H u_h - g^T H (u_h - u) + \alpha \lambda_n e_n^T u_h - \alpha \lambda_n e_n^T (u_h - u) + \mathcal{O}(h^{2s}) \]

\[ = \mathcal{I}_h(u_h) - (g^T + \alpha \lambda_n e_n^T H^{-1}) H (u_h - u) + \mathcal{O}(h^{2s}) \]
Linear hyperbolic PDEs

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Using the SBP norm:

\[ \mathcal{I}(U) = (g, u)_H + \alpha \lambda_n (e_n^T u) + \mathcal{O}(h^{2s}) \]
\[ \mathcal{I}(U) = g^T Hu + \alpha \lambda_n e_n^T u + \mathcal{O}(h^{2s}) \]
\[ \mathcal{I}(U) = g^T H u_h - g^T H (u_h - u) + \alpha \lambda_n e_n^T u_h - \alpha \lambda_n e_n^T (u_h - u) + \mathcal{O}(h^{2s}) \]
\[ \mathcal{I}(U) = I_h(u_h) - (g^T + \alpha \lambda_n e_n^T H^{-1}) H(u_h - u) + \mathcal{O}(h^{2s}) \]
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Proof:
Using the SBP norm:

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\[ = I_h(u_h) - (g^T + \alpha \lambda_n e_n^T H^{-1})H(u_h - u) + O(h^{2s}) \]

Left-multiplying (\( \star \)) by \( H \):

\[ Au_h = Hf + \lambda_0 e_0 U_L \]
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\[ Au_h = Hf + \lambda_0 e_0 \mathcal{U}_L \]

In the case that the equation above is applied to the exact solution \(u\):

\[ Au = HD(\Lambda u) + \lambda_0 e_0 \mathcal{U}_L \]
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Using the SBP norm:

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\[ = \mathcal{I}_h(u_h) - (g^T + \alpha \lambda_n e_n^T H^{-1})H(u_h - u) + \mathcal{O}(h^{2s}) \]

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In the case that the equation above is applied to the exact solution \( u \):

\[ Au = HD(\Lambda u) + \lambda_0 e_0 \mathcal{U}_L \]

Using both expressions and \( I = HA^{-1}AH^{-1} \), we obtain:

\[ \mathcal{I}(U) = \mathcal{I}_h(u_h) - (g^T + \alpha \lambda_n e_n^T H^{-1})HA^{-1}AH^{-1}H(u_h - u) + \mathcal{O}(h^{2s}) \]
\[ = \mathcal{I}_h(u_h) - (g^T H + \alpha \lambda_n e_n^T )A^{-1}H(f - D\Lambda u) + \mathcal{O}(h^{2s}) \]
\[ = \mathcal{I}_h(u_h) - v_h^T H(f - D\Lambda u) + \mathcal{O}(h^{2s}) \]
Linear hyperbolic PDEs

Proof (cont.):
So, we have the discrete adjoint variables \( v_h = A^{-T}(Hg + e_n\lambda_n\alpha) \).
**Linear hyperbolic PDEs**

**Proof (cont.):**
So, we have the discrete adjoint variables $v_h = A^{-T}(Hg + e_n\lambda_n\alpha)$. Now, observe that:

$$A = (Q + e_0 e_0^T)\Lambda = (\lambda_n e_n e_n^T - Q^T \Lambda)$$
Proof (cont.):
So, we have the discrete adjoint variables \( v_h = A^{-T}(Hg + e_n\lambda_n\alpha) \). Now, observe that:
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\]
So, using this and left-multiplying \( v_h \) by \( H^{-1}A^T \), we have:
\[
-\Lambda Dv_h = g - H^{-1}e_n\lambda_n(e_n^Tv_h - \alpha)
\]
which is, exactly, the SBP-SAT discretization of the corresponding adjoint problem of our PDE:
\[
\begin{aligned}
-\lambda \frac{\partial V}{\partial x} &= g, \quad x \in \Omega = [0, 1] \\
V(1) &= \alpha
\end{aligned}
\]
**Linear hyperbolic PDEs**

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So, we have the discrete adjoint variables $v_h = A^{-T}(Hg + e_n\lambda_n\alpha)$. Now, observe that:

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So, using this and left-multiplying $v_h$ by $H^{-1}A^T$, we have:

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which is, exactly, the SBP-SAT discretization of the corresponding adjoint problem of our PDE:

$$\begin{cases} -\lambda \frac{\partial V}{\partial x} = g, \ x \in \Omega = [0, 1] \\ V(1) = \alpha \end{cases}$$

The truncation error is given by $T_h = g + H^{-1}e_n\lambda_n\alpha - H^{-1}A^T v$ and, because it is a SBP discretization, $\|T_h\|_\infty = O(h^s)$. Therefore, $H^{-1}A^T(v_h - v) = T_h$ and, using the hypothesis on $\|A^{-T}H\|_\infty$, we obtain:

$$\|v_h - v\|_\infty \leq C \|T_h\|_\infty = O(h^s)$$
Linear hyperbolic PDEs

Proof (end):
Finally:

\[ \mathcal{I}(U) = \mathcal{I}_h(u_h) - v_h^T H(f - D\Delta u) + O(h^{2s}) \]
\[ = \mathcal{I}_h(u_h) - v^T H(f - D\Delta u) + (v_h - v)^T H(f - D\Delta u) + O(h^{2s}) \]
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Finally:

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Proof (end):
Finally:

\[
\mathcal{I}(U) = I_h(u_h) - v_h^T H(f - DΛu) + O(h^{2s})
\]

\[
= I_h(u_h) - v^T H(f - DΛu) + (v_h - v)^T H(f - DΛu) + O(h^{2s})
\]

\[
\underbrace{O(h^s)}_{\mathcal{O}(h^s)} + \underbrace{O(h^s)}_{\mathcal{O}(h^s)}
\]

Remark: The SBP-SAT discretization of the PDE and the discrete functional estimate lead to a discrete adjoint problem that is a consistent and sufficiently accurate discretization of the adjoint PDE; i.e., it is dual-consistent.
Linear hyperbolic PDEs

Proof (end):
Finally:

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Remark: The SBP-SAT discretization of the PDE and the discrete functional estimate lead to a discrete adjoint problem that is a consistent and sufficiently accurate discretization of the adjoint PDE; i.e., it is dual-consistent.
Proof (end):

Finally:

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Remark: The SBP-SAT discretization of the PDE and the discrete functional estimate lead to a discrete adjoint problem that is a consistent and sufficiently accurate discretization of the adjoint PDE; i.e., it is dual-consistent.
Linear elliptic PDEs

Let us consider a linear elliptic PDE, expressed in the form of first-order system:

\[
\begin{cases}
- \frac{\partial}{\partial x} (\gamma U) = F, \ x \in \Omega = [0, 1] \\
\mathcal{W} = \frac{\partial U}{\partial x}, \ x \in \Omega \\
U(0) = U_L \\
\mathcal{W}(1) = \mathcal{W}_R
\end{cases}
\]

where \( \gamma(x) > 0 \) is the spatially varying diffusion coefficient.
Linear elliptic PDEs

Let us consider a linear elliptic PDE, expressed in the form of first-order system:

\[
\begin{aligned}
-\frac{\partial}{\partial x} (\gamma u) &= F, \; x \in \Omega = [0, 1] \\
\mathcal{W} &= \frac{\partial u}{\partial x}, \; x \in \Omega \\
U(0) &= U_L \\
\mathcal{W}(1) &= \mathcal{W}_R
\end{aligned}
\]

where $\gamma(x) > 0$ is the spatially varying diffusion coefficient. The SBP-SAT discretization is given by:

\[
-D(\Gamma w_h) = f - H^{-1} e_0 (e_0^T u_h - U_L) - H^{-1} e_n \gamma_n (e_n^T w_h - \mathcal{W}_R)
\]

\[
w_h = Du_h + H^{-1} e_0 (e_0^T u_h - U_L)
\]

where

\[
\begin{align*}
\gamma_i &= \gamma(x_i), \; i = 0, \ldots, n \\
\Gamma &= \text{diag}(\gamma_0, \ldots, \gamma_n) \\
f &= \begin{bmatrix} F(x_0) & \ldots & F(x_n) \end{bmatrix}^T
\]

(\star \star)
**Theorem**

Let $\mathcal{I} : L^2(\Omega) \rightarrow \mathbb{R}$ be a linear functional defined by:

$$
\mathcal{I}(U) = \int_0^1 G_1 U \, dx + \int_0^1 G_2 \frac{\partial U}{\partial x} \, dx + \alpha(U)|_{x=1} + \beta(\gamma \frac{\partial U}{\partial x})|_{x=0}
$$

where $G_1, G_2 \in C^{2s}([0, 1])$. Assume that the PDE is well posed and admits solution $U \in C^{2s}([0, 1])$. Then, the functional estimate:

$$
\mathcal{I}_h(u_h) = (g_1, u_h)_H + (g_2, w_h)_H + \alpha(e_n^T u_h) + \beta \gamma_0 (e_0^T w_h) + \beta(e_0^T u_h - U_L)
$$

where $g_k = [G_k(x_0) \ldots G_k(x_n)]^T$ (with $k = 1, 2$), is a $2s$-order accurate approximation to $\mathcal{I}(U)$. 

---

**Linear elliptic PDEs**
Linear elliptic PDEs

Proof:
Proof:
Using the SBP norm:

\[
\mathcal{I}(U) = (g_1, u)_H + (g_2, w)_H + \alpha (e_n^T u) + \beta \gamma_0 (e_0^T w) + O(h^{2s})
\]

\[
= g_1^T H u_h + g_2^T H w_h + \alpha e_n^T u_h + \beta \gamma_0 (e_0^T w_h) + \beta e_0^T (u_h - u)
\]

\[
- g_1^T H(u_h - u) - g_2^T H(w_h - w) - \alpha e_n^T (u_h - u)
\]

\[
- \beta \gamma_0 e_0^T (w_h - w) - \beta e_0^T (u_h - u) + O(h^{2s})
\]

\[
= \mathcal{I}_h(u_h) - (g_1^T + \alpha e_n^T H^{-1} + \beta e_0^T H^{-1})H(u_h - u)
\]

\[
- (g_2^T + \beta \gamma_0 e_0^T H^{-1})H(w_h - w) + O(h^{2s})
\]
Linear elliptic PDEs

Proof:
Using the SBP norm:

\[ I(U) = (g_1, u)_H + (g_2, w)_H + \alpha (e_n^T u) + \beta \gamma_0 (e_0^T w) + \mathcal{O}(h^{2s}) \]

\[ = g_1^T H u_h + g_2^T H w_h + \alpha e_n^T u_h + \beta \gamma_0 (e_0^T w_h) + \beta e_0^T (u_h - u) \]

\[ - g_1^T H (u_h - u) - g_2^T H (w_h - w) - \alpha e_n^T (u_h - u) \]

\[ - \beta \gamma_0 e_0^T (w_h - w) - \beta e_0^T (u_h - u) + \mathcal{O}(h^{2s}) \]

\[ = I_h(u_h) - (g_1^T + \alpha e_n^T H^{-1} + \beta e_0^T H^{-1}) H (u_h - u) \]

\[ - (g_2^T + \beta \gamma_0 e_0^T H^{-1}) H (w_h - w) + \mathcal{O}(h^{2s}) \]
Linear elliptic PDEs

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\]
\[
- g_1^T H(u_h - u) - g_2^T H(w_h - w) - \alpha e_n^T(u_h - u)
\]
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- \beta \gamma_0 e_0^T(w_h - w) - \beta e_0^T(u_h - u) + \mathcal{O}(h^{2s})
\]
\[
= \mathcal{I}_h(u_h) - (g_1^T + \alpha e_n^T H^{-1} + \beta e_0^T H^{-1})H(u_h - u)
\]
\[
- (g_2^T + \beta \gamma_0 e_0^T H^{-1})H(w_h - w) + \mathcal{O}(h^{2s})
\]

We define the primal-equation residuals as:
\[
r_u := D(\Gamma w_h) + f - H^{-1}e_0(e_0^T u_h - U_L) - H^{-1}e_n\gamma_n(e_n^T w_h - W_R)
\]
\[
r_w := Du_h - w_h + H^{-1}e_0(e_0^T u_h - U_L)
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Linear elliptic PDEs

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I(U) = (g_1, u)_H + (g_2, w)_H + \alpha(e_n^T u) + \beta\gamma_0(e_0^T w) + \mathcal{O}(h^{2s})
\]

\[
ge_1^T Hu_h + g_2^T Hw_h + \alpha e_n^T u_h + \beta \gamma_0(e_0^T w_h) + \beta e_0^T (u_h - u)
\]

\[
- g_1^T H(u_h - u) - g_2^T H(w_h - w) - \alpha e_n^T (u_h - u)
\]

\[
- \beta \gamma_0 e_0^T (w_h - w) - \beta e_0^T (u_h - u) + \mathcal{O}(h^{2s})
\]

\[
= I_h(u_h) - (g_1^T + \alpha e_n^T H^{-1} + \beta e_0^T H^{-1})H(u_h - u)
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\]

\[
r_w := Du_h - w_h + H^{-1}e_0(e_0^T u_h - U_L)
\]

Noting that \(U_L = e_0^T u\) and \(W = e_n^T w\) and that the residuals are equal to zero, we obtain:

\[
r_u := f + D(\Gamma w) - H^{-1}(e_0 e_0^T H^{-1})H(u_h - u) - H^{-1}(D^T \Gamma^T + e_0 e_0^T \gamma_0 H^{-1})H(w_h - w)
\]

\[
r_w := Du - w - H^{-1}(D^T - e_n e_n^T H^{-1})H(u_h - u) - (w_h - w)
\]
Linear elliptic PDEs

Proof (cont.): Let us take now \( \nu_h, z_h \in \mathbb{R}^{n+1} \) vectors that will behave as Lagrange multipliers associated to \( r_u \) and \( r_w \). If we take the SBP inner product with \( r_u \) and \( r_w \) and subtract the result from the functional, reordering it we obtain:

\[
I(U) = I_h(u_h) - (g_1^T + \alpha e_n^T H^{-1} + \beta e_0^T H^{-1})H(u_h - u)
- (g_2^T + \beta \gamma_0 e_0^T H^{-1})H(w_h - w) - \nu_h^T Hr_u - z_h^T Hr_w + O(h^{2s})
\]
Linear elliptic PDEs

**Proof (cont.):** Let us take now $v_h, z_h \in \mathbb{R}^{n+1}$ vectors that will behave as Lagrange multipliers associated to $r_u$ and $r_w$. If we take the SBP inner product with $r_u$ and $r_w$ and subtract the result from the functional, reordering it we obtain:

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\mathcal{I}(U) = \mathcal{I}_h(u_h) - (g_1^T + \alpha e_n^T H^{-1} + \beta e_0^T H^{-1})H(u_h - u) \\
- (g_2^T + \beta \gamma_0 e_0^T H^{-1})H(w_h - w) - v_h^T H r_u - z_h^T H r_w + \mathcal{O}(h^{2s})
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**Linear elliptic PDEs**

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\]

\[
= \mathcal{I}_h(u_h) - v_h^T H(f + D\Gamma w) - z_h^T H(Du - w) \\
+ [z_h^T D^T - g_1^T - (z_h^T e_n + \alpha) e_n^T H^{-1} + (v_h^T e_0 - \beta) e_0^T H^{-1}] H(u_h - u) \\
+ [v_h^T D^T \Gamma^T - g_2^T + z_h^T + (v_h^T e_0 - \beta) e_0^T \gamma_0 H^{-1}] H(w_h - w) + \mathcal{O}(h^{2s})
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Proof (cont.): Let us take now $v_h, z_h \in \mathbb{R}^{n+1}$ vectors that will behave as Lagrange multipliers associated to $r_u$ and $r_w$. If we take the SBP inner product with $r_u$ and $r_w$ and subtract the result from the functional, reordering it we obtain:

\[
\mathcal{I}(U) = \mathcal{I}_h(u_h) - \left(g_1^T + \alpha e_n^T H^{-1} + \beta e_0^T H^{-1}\right) H(u_h - u) \\
- (g_2^T + \beta \gamma_0 e_0^T H^{-1}) H(w_h - w) - v_h^T H r_u - z_h^T H r_w + O(h^{2s})
\]

\[
= \mathcal{I}_h(u_h) - v_h^T H(f + D\Gamma w) - z_h^T H(Du - w) \\
+ \left[ z_h D^T - g_1^T - (z_h e_n + \alpha) e_n^T H^{-1} + (v_h^T e_0 - \beta) e_0^T H^{-1}\right] H(u_h - u) \\
+ \left[ v_h^T D^T \Gamma^T - g_2^T + z_h^T + (v_h^T e_0 - \beta) e_0^T \gamma_0 H^{-1}\right] H(w_h - w) + O(h^{2s})
\]

Now we choose $v_h$ and $z_h$ as the discrete adjoint variables, satisfying:

\[
Dz_h = g_1 + H^{-1} e_n (e_n^T z_h + \alpha) - H^{-1} e_0 (e_0^T v_h - \beta) \\
-z_h = \Gamma Dv_h - g_2 + H^{-1} \gamma_0 e_0 (e_0^T v_h - \beta)
\]
Linear elliptic PDEs

Proof (end):
That is precisely the SBP-SAT discretization of the corresponding continuous adjoint problem:

\[
\begin{align*}
\frac{\partial Z}{\partial x} &= G_1, \quad x \in \Omega \\
-Z &= \gamma \frac{\partial V}{\partial x} - G_2, \quad x \in \Omega \\
V(0) &= \beta \\
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\end{align*}
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Knowing that the truncation error of the SBP-SAT discretization for \( v_h \) is \((s + 1)\)-accurate and for \( z_h \), at least, \( s \)-accurate:

Linear elliptic PDEs

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\[
I(U) = I_h(u_h) - v_h^T H(f + D\Gamma w) - z_h^T H(Du - w) + O(h^{2s})
\]

\[
= I_h(u_h) - v^T H(f + D\Gamma w) - z^T H(Du - w) - (v_h - v)^T H(f + D\Gamma w) - (z_h - z)^T H(Du - w) + O(h^{2s})
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Linear elliptic PDEs

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\[
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I(U) &= I_h(u_h) - v_h^T H(f + D\Gamma w) - z_h^T H(Du - w) + O(h^{2s}) \\
&= I_h(u_h) - \underbrace{v^T H(f + D\Gamma w)}_{O(h^{2s})} - \underbrace{z^T H(Du - w)}_{O(h^{2s})} \\
&\quad - (v_h - v)^T H(f + D\Gamma w) - (z_h - z)^T H(Du - w) + O(h^{2s})
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\]
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\frac{\partial Z}{\partial x} &= G_1, \ x \in \Omega \\
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\mathcal{V}(0) &= \beta \\
Z(1) &= -\alpha
\end{align*}
\]

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\[
\mathcal{I}(U) = \mathcal{I}_h(u_h) - v_h^T H(f + D\Gamma w) - z_h^T H(Du - w) + \mathcal{O}(h^{2s})
\]

\[
= \mathcal{I}_h(u_h) - v^T H(f + D\Gamma w) - z^T H(Du - w) \\
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\]

\[
= \mathcal{I}_h(u_h) + O(h^{2s})
\]
Curvilinear grids

SBP operators can be used in higher dimension applying one-dimensional operators to each spatial direction independently. For example, in the $[0, 1]^3$ cubic domain with a uniform discretization ($x_{ijk} = \frac{1}{h}(i, j, k), \ i, j, k = 0, \ldots, n$), the SBP operator for $\frac{\partial}{\partial x}$ is given by:

$$D_x = I \otimes I \otimes D$$

where $D$ is the one-dimensional SBP operator.
Curvilinear grids

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What happens in general?
SBP operators can be used in higher dimension applying one-dimensional operators to each spatial direction independently. For example, in the $[0,1]^3$ cubic domain with a uniform discretization ($x_{ijk} = \frac{1}{h}(i,j,k), \ i,j,k = 0,...,n$), the SBP operator for $\partial/\partial x$ is given by:

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where $D$ is the one-dimensional SBP operator.

Let us take a compact set $\Omega_x \subset \mathbb{R}^2$ such that there exists an invertible transformation

$$\mathcal{T}(x,y) = (\xi(x,y), \eta(x,y))$$

of class $C^2$ that maps $\Omega_x$ to $\Omega_\xi = [0,1]^2$. 
SBP operators can be used in higher dimension applying one-dimensional operators to each spatial direction independently. For example, in the $[0,1]^3$ cubic domain with a uniform discretization ($x_{ijk} = \frac{1}{h}(i, j, k), \ i, j, k = 0, \ldots, n$), the SBP operator for $\partial/\partial x$ is given by:

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$$\int\int_{\Omega_x} U dx dy = \int\int_{\Omega_\xi} U J d\xi d\eta$$
SBP operators can be used in higher dimension applying one-dimensional operators to each spatial direction independently. For example, in the $[0, 1]^3$ cubic domain with a uniform discretization ($x_{ijk} = \frac{1}{h}(i, j, k)$, $i, j, k = 0, ..., n$), the SBP operator for $\partial / \partial x$ is given by:

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Let us take a compact set $\Omega_x \subset \mathbb{R}^2$ such that there exists an invertible transformation

$$T(x, y) = (\xi(x, y), \eta(x, y))$$

of class $C^{2s}$ that maps $\Omega_x$ to $\Omega_\xi = [0, 1]^2$. We have:

$$\int\int_{\Omega_x} U dx dy = \int\int_{\Omega_\xi} U J d\xi d\eta$$

where

$$J := \left| \frac{\partial(x, y)}{\partial(\xi, \eta)} \right| = \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi} \frac{\partial x}{\partial \eta}$$
Now, we approximate the Jacobian by:

\[ J = (D_{\xi} x) \circ (D_{\eta} y) - (D_{\xi} y) \circ (D_{\eta} x) \]
Curvilinear grids

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Assuming unknowns are ordered first in the \( \xi \) direction and then in the \( \eta \) one, we can use:

\[ D_{\xi} = (I \otimes D) \quad \text{and} \quad D_{\eta} = (D \otimes I) \]
Curvilinear grids

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Approximating \( J \) by \( J \) with SBP operators gives us \( O(h^s) \) error at the boundary, but...
Curvilinear grids

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**Theorem**

Let \( \Omega_x \) and \( \Omega_\xi \) be connected compact subsets of \( \mathbb{R}^2 \). Furthermore, let \( T : \Omega_x \rightarrow \Omega_\xi \) be a \( C^{2s} \) invertible mapping. For grids based on the uniform discretization of \( \Omega_\xi \) and mapped to \( \Omega_x \) using \( T^{-1} \), for \( U \in C^{2s} \) the quadrature

\[ I_h(u) = u(H \otimes H)J \]

is a \( 2s \)-order accurate estimate of the integral \( \int \int_{\Omega_x} U \, dx \, dy \).
Curvilinear grids

We also need to prove $O(h^s)$ truncation error for the discretization of the primal and adjoint equations.
Curvilinear grids

We also need to prove $O(h^s)$ truncation error for the discretization of the primal and adjoint equations. Let us show it with an example:

$$\frac{\partial}{\partial x} (\lambda_x U) + \frac{\partial}{\partial y} (\lambda_y U) = F, \quad \forall (x, y) \in \Omega_x$$
Curvilinear grids

We also need to prove $O(h^s)$ truncation error for the discretization of the primal and adjoint equations. Let us show it with an example:

$$\frac{\partial}{\partial x} (\lambda_x U) + \frac{\partial}{\partial y} (\lambda_y U) = F, \; \forall (x, y) \in \Omega_x$$

Transforming this to $\Omega_\xi$, we obtain:

$$\frac{\partial}{\partial \xi} (\lambda_\xi U) + \frac{\partial}{\partial \eta} (\lambda_\eta U) = FJ, \; \forall (\xi, \eta) \in \Omega_\xi$$

where

$$\lambda_\xi = \frac{\partial y}{\partial \eta} \lambda_x - \frac{\partial x}{\partial \eta} \lambda_y \; \text{and} \; \lambda_\eta = -\frac{\partial y}{\partial \xi} \lambda_x + \frac{\partial x}{\partial \xi} \lambda_y$$
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We approximate the Jacobian as before and velocity by:

$$\Lambda_\xi = \text{diag}(\text{diag}(\lambda_x(x_{ij}, y_{ij})) D_\eta y - \text{diag}(\lambda_y(x_{ij}, y_{ij})) D_\eta x)$$

$$\Lambda_\eta = \text{diag}(-\text{diag}(\lambda_x(x_{ij}, y_{ij})) D_\xi y + \text{diag}(\lambda_y(x_{ij}, y_{ij})) D_\xi x)$$
The SBP-SAT discretizations of the primal and adjoint equations are:

\[
D_\xi(\Lambda_\xi u_h) + D_\eta(\Lambda_\eta u_h) = (J \otimes f) - \left[ I \otimes (H^{-1}e_0e_0^T) \right] \Lambda_\xi(u_h - u)
- \left[ (H^{-1}e_0e_0^T) \otimes I \right] \Lambda_\eta(u_h - u)
\]

\[
- \Lambda_\xi D_\xi v_h - \Lambda_\eta D_\eta v_h = (J \otimes g) - \Lambda_\xi \left[ I \otimes (H^{-1}e_ne_n^T) \right] (v_h - v)
- \Lambda_\eta \left[ (H^{-1}e_ne_n^T) \otimes I \right] (v_h - v)
\]

Repeating the one-dimensional reasoning, it can be shown that both have truncation error of \(O(h^{2s})\) in the interior and \(O(h^s)\) on the boundary, as required for superconvergence of functional estimates.
Semistructured grids

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- Require only $C^0$ grid continuity
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- Lead to a linearly time-stable scheme


Thanks for your attention!