The summation-by-parts framework: An abstract matrix-analysis approach to the development of discrete schemes with provable properties

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Interest and objective

Interest: Problems that are
- Time-dependent
- Nonlinear
- Complex geometries

Objective: Provably robust hpc efficient schemes
- Ideal: provably convergent schemes
- Provable stability is a good starting point

Context:
- Novel schemes that show promise for hpc
- Minimally invasive modification of existing codes
Interest and objective

Requirements: Abstract analysis framework

• Discretization agnostic
• Applicable to a wide range of PDEs
• On hardware algorithm

This talk: review the summation-by-parts (SBP) framework as a good starting point
SBP Framework: A matrix analysis methodology

- Systematic approach to the design of new schemes that are: Stable, conservative, and accurate
- Simple: requires basic linear algebra/calculus to do proofs
- Discretization agnostic (FD, FV, DG, CG, FR/CPR, etc.)
- Design order correction of existing schemes
- Easily handles variational crimes

This framework partially answers my requirements
The summation-by-parts (SBP) framework

Core concept: Prove stability at the continuous level
   • Mimic in a one-to-one fashion at the semi/fully-discrete level

Stability: Norm of the solution is bounded by the data of the problem

Outline:
   • Part I: Linear PDEs
   • Part II: Nonlinear PDEs
Pat I: Linear PDEs
Well-posed continuous problems

Well-posed linear IBP:

\[
\frac{\partial u}{\partial t} + Pu + F = 0, \quad t \geq 0, \quad x \in \Omega \\
Bu = G, \quad t \geq 0, \quad x \in \partial \Omega = \Gamma, \\
\mathcal{U}(x, 0) = \mathcal{I}, \quad t = 0, \quad x \in \Omega,
\]

1. A solution exists
2. The solution is unique
3. The solution depends continuously on the data of the problem \((\mathcal{F}, \mathcal{G}, \mathcal{I})\)

We need a mathematical definition for three

\[
|||\mathcal{U}|||_i^2 \leq |||\mathcal{F}|||_{II}^2 + |||\mathcal{G}|||_{III}^2 + |||\mathcal{I}|||_{IV}^2
\]

where the norms could be different
The energy method

Simple approach to construct such estimates

**Example:** consider the linear advection equation

\[
\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad t \geq 0, \quad x \in [x_L, x_R], \quad a > 0,
\]

\[
U(x_L, t) = G, \quad t \geq 0,
\]

\[
U(x, 0) = I, \quad t = 0, \quad x \in [x_L, x_R],
\]
Stability analysis of the convection equation

1) Multiply the PDE by the solution $u$ and integrate in space

$$
\int_{x_L}^{x_R} u \frac{\partial u}{\partial t} \, dx + a \int_{x_L}^{x_R} u \frac{\partial u}{\partial x} \, dx = 0
$$

2) Use integration by parts (IBP) on the spatial term

$$
\int_{x_L}^{x_R} u \frac{\partial u}{\partial t} \, dx + \left[ \frac{a}{2} u^2 \right]_{x_L}^{x_R} = 0
$$

3) Chain rule and Leibniz rule on the temporal term

$$
\frac{1}{2} \frac{d ||u||^2}{dt} + \frac{a}{2} u^2 \bigg|_{x_L}^{x_R} = 0, \quad ||u||^2 \equiv \int_{x_L}^{x_R} u^2 \, dx
$$
4) Integrating in time and applying IC and BC

\[ \| \mathcal{U} \|^2 = \| \mathcal{I} \|^2 - a \int_0^T \mathcal{U}^2(x_R, t)\,dt + a \int_0^T \mathcal{G}^2 \,dt \]

\[ \| \mathcal{U} \|^2 \leq \| \mathcal{I} \|^2 + a \int_0^T \mathcal{G}^2 \,dt \]

Thus, stable

Discussion:
- The energy method is simple
- Integration by parts (IBP) was the key

**Question:** If we can mimic IBP at the discrete level can we follow this analysis?
Goal: mimic IBP

\[
\int_{x_L}^{x_R} \nu \frac{\partial u}{\partial x} \, dx + \int_{x_L}^{x_R} u \frac{\partial \nu}{\partial x} \, dx = \nu u|_{x_L}^{x_R}
\]

Some notation:

- \( \mathbf{x} \equiv [x_1, \ldots, x_n] \)
- \( \mathbf{u} \equiv [\mathcal{U}(x_1, t), \ldots, \mathcal{U}(x_n, t)]^T \)
- Matrix difference operator: \( D_x f = \frac{\partial \mathcal{F}(\mathbf{x})}{\partial \mathbf{x}} + \mathcal{O}(\Delta x^p) \)

We can exactly capture the RHS with \( E_x = \text{diag}(-1, 0, \ldots, 0, 1) \)

\[
\nu^T E_x \mathbf{u} = \nu_n u_n - \nu_1 u_1 = \nu \mathcal{U}|_{x_L}^{x_R}
\]
We need an approximation to the $L_2$ inner product

$$\tilde{v}^T P_x \tilde{u} \approx \int_{x_L}^{x_R} \tilde{v} \tilde{u} \, dx, \quad P_x = P_x^T, \quad P_x > 0$$

Defining $Q_x \equiv P_x D_x$ we discretize the LHS

$$\approx \int_{x_L}^{x_R} \left[ v \frac{\partial u}{\partial x} \right] \, dx \quad \approx \int_{x_L}^{x_R} \left[ u \frac{\partial v}{\partial x} \right] \, dx$$

$$\underbrace{v^T P_x D_x u} + \underbrace{u^T P_x D_x v} = v^T E_x u$$

$$v^T Q_x u + u^T Q_x v = v^T E_x u$$

$$v^T (Q_x + Q_x^T) u = v^T E_x u$$

$$Q_x + Q_x^T = E_x$$

This is immediate if $Q_x = S_x + \frac{1}{2} E_x$, $S_x = -S_x^T$
SBP operators: Finite-difference origins

Kreiss and Scherer (1974)

$$P_x = \text{diag} \left( p_1, p_2, p_3, p_4, 1, \ldots, 1, p_4, p_3, p_2, p_1 \right)$$

$$Q_x = \begin{bmatrix}
-\frac{1}{2} & q_{12} & q_{13} & q_{14} \\
-q_{12} & 0 & q_{23} & q_{24} \\
-q_{13} & -q_{23} & 0 & q_{34} & \alpha_2 \\
-q_{14} & -q_{24} & -q_{34} & 0 & \alpha_1 & \alpha_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
-q_{14} & -q_{24} & -q_{34} & 0 & \alpha_1 & \alpha_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
-q_{14} & -q_{24} & -q_{34} & 0 & \alpha_1 & \alpha_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\end{bmatrix}$$
SBP operators: Finite-difference origins

Kreiss and Scherer (1974)

- With this form $Q_x + Q_x^T = E_x$
- Now the question is the restriction on the coefficients

Theory of finite-difference SBP operators

- Accuracy constraints and extension to block norm: Bo Strand (1994)
- Weak imposition of boundary conditions: Carpenter and Gottlieb (1994)
- Major contributions from many others: e.g. Jan Nordström, Gunilla Kreiss etc.
Can we go beyond classical finite-differences?

- Collocated DG: Gassner (2013)
- General 1D nodal schemes: DCDRF, Boom, and Zingg (2014)

\[
\begin{align*}
[D_x] & \equiv \begin{pmatrix} 1 & 2 & 3 & \cdots & p \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}, \\
\end{align*}
\]

**DEF:** degree $p$ SBP operator

1. $D_x x^k = k x^{k-1}, \quad k = 0, 1, \ldots, p$
2. $D_x \equiv P_x^{-1} Q_x$
3. $Q_x \equiv S_x + \frac{1}{2} E_x$
4. $E_x \equiv \text{diag}(-1, 0, \ldots, 0, 1)$

This covers a number of nodal based schemes
Why this is useful

Semi-discrete EQ.

\[ \frac{d}{dt} \mathbf{u} + aD_x \mathbf{u} + b \mathbf{c} = 0 \]

1) Multiply by the solution and integrate over the domain

\[ \mathbf{u}^T P_x \frac{d}{dt} \mathbf{u} + a \mathbf{u}^T P_x D_x \mathbf{u} + \mathbf{u}^T P b \mathbf{c} = 0 \]

2) Use IBP on the spatial term

\[ \mathbf{u}^T P_x D_x \mathbf{u} = \mathbf{u}^T Q_x \mathbf{u} = \frac{1}{2} \mathbf{u}^T E_x \mathbf{u} \]

3) Use chain rule and Leibniz’ rule on the temporal term

\[ \frac{1}{2} \frac{d}{dt} \| \mathbf{u} \|_{P_x}^2 = - \frac{a}{2} \mathbf{u}^T E_x \mathbf{u} - \mathbf{u}^T P b \mathbf{c}, \quad \| \mathbf{u} \|_{P_x}^2 \equiv \mathbf{u}^T P_x \mathbf{u} \]
Why this is useful

4) Integrate in time and apply IC and BC

\[ \|u(T)\|_{P_x}^2 = \|I\|_{P_x}^2 - \int_0^T (a u^T E_x u + 2 u^T P bc) \, dt \]

If \(bc\) is constructed appropriately

\[ \|u(T)\|_{P_x}^2 \leq \|I\|_{P_x}^2 + \int_0^T \mathcal{Q}^2 \, dt \]

The semi-discrete form is stable!

What about the fully-discrete case?

- More on this shortly
SBP operators: A second generalization

Previous definition $x(1) = x_L, x(n) = x_R$
Relax restrictions on $E_x$

$$E_x \equiv t_R t_R^T - t_L t_L^T$$
$$t_R^T x^k = x_R^k, \quad t_L^T x^k = x_L^k, \quad k = 0, 1, \ldots, p$$

Now
$$v^T E_x u = v u |_{x_R}^{x_L}, \quad v, u \in \mathbb{P}^p$$
State of the art in SBP operators

Multi-D SBP

- Collocated: Hicken, DCDRF, and Zingg (2017)
- Modal/decoupled: Jesse Chan (2018)
- Staggered: DCDRF, Crean, Hicken, and Carpenter (2019)

- solution nodes/modes
- flux nodes (volume quadrature/cubature nodes)
- surface quadrature/cubature nodes
SBP operators in time

Natural to apply to time-marching
(Boom and Zingg (2015))

\[ \frac{dy}{dt} = \lambda y, \quad y(0) = y_0 \]

SBP-SAT scheme

\[ D_t y = \lambda y - P^{-1} t_L (t_R y - y_0) \]

Many contributions in this area (see the list of papers at the end)
Connection to RK schemes

Butcher tableau:

\[
\begin{array}{c|c}
  c & A \\
  \hline
  b^T & \end{array}
\]

From SBP-SAT scheme:

\[
A = \frac{1}{h} (Q + t_L t_L^T)^{-1} P
\]

\[
b^T = \frac{1}{h} 1^T P
\]

\[
c = \frac{t - 1t_0}{h}
\]

Only captures a subclass of provably stable RK schemes

Enabling technology: RRK methods (David Ketcheson 2:30-3:15)
Summary and discussion

The SBP concept can be applied to a rich set of methods.

The local SBP property is extended to the global SBP property via:

- Appropriate coupling procedures (discontinuous approaches)
- Appropriate imposition of boundary conditions
- Additions such as dissipation are constructed so as not to destroy stability estimates

Results in provably stable schemes whenever the energy method can be used.
Holistic design of time-dependent PDE discretizations

What can the SBP community learn from the time-marching community?

• Generalize the SBP concept
  ▶ what is needed to capture all A-stable, L-stable, etc RK methods
  ▶ what about other modern methods?
  ▶ etc.

• Once it is in SBP form I can apply it to my spatial discretization

How can the time-marching community leverage SBP?

• SBP provides a natural language (rosetta stone)
  ▶ a posterior error estimates etc
Pat II: Non-linear PDEs
Well-posed continuous problems?

No general theory and for NS incomplete

Now a stability estimate is not enough

Necessary but insufficient condition

Fundamental (don’t want the solution to blow up)
Entropy stability analysis

Consider the following hyperbolic PDE:

\[
\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = 0
\]

Equipped with a convex entropy function \( S = f_{nc}(U) \) that satisfies

\[
\frac{\partial S}{\partial u} \frac{\partial F}{\partial x} = W^T \frac{\partial F}{\partial x} = \frac{\partial f}{\partial x}
\]

Integrability condition

where \( f \) is the entropy flux and \( W \) are the entropy variables
Entropy stability analysis

1) Multiply the PDE by $W^T$ and integrate in space

$$\int_{x_L}^{x_R} W^T \frac{\partial U}{\partial t} \, dx + \int_{x_L}^{x_R} W^T \frac{\partial F}{\partial x} \, dx = 0$$

2) Use the IBP rule induced by the integrability condition

$$\int_{x_L}^{x_R} W^T \frac{\partial F}{\partial x} \, dx = \int_{x_L}^{x_R} \frac{\partial f}{\partial x} \, dx = f n_x \bigg|_{x_L}^{x_R}$$

$$\int_{x_L}^{x_R} W^T \frac{\partial U}{\partial t} \, dx + f \bigg|_{x_L}^{x_R} \leq 0$$
3) Use the definition of the entropy variables and Leibniz’ rule

\[
\frac{d}{dt} \int_{x_L}^{x_R} S \, dx + f|_{x_L}^{x_R} \leq 0
\]

4) Integrate in time

\[
\int_{x_L}^{x_R} S(t) \, dx \leq \int_{x_L}^{x_R} S(0) \, dx - \int_0^T f|_{x_L}^{x_R} \, dt
\]

5) Apply data and convert the entropy statement into a stability statement on the solution
Entropy stability analysis: Burgers’ equation

\[ \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( \frac{u^2}{2} \right) = 0, \]

Appropriately formulated BC

\( u(x, 0) = g \)

Entropy function: \( S = \frac{u^2}{2} \)

Entropy variable: \( \mathcal{W} = \frac{\partial S}{\partial u} = \mathcal{U} \)

Flux: \( \mathcal{F} = \frac{u^2}{2} \)

Entropy flux: \( f = \frac{u^3}{3} \)
Entropy stability analysis: Burgers’ equation

1-4) Same as before

5) Apply the data and convert the entropy statement into a stability statement on the solution

\[
\int_{x_L}^{x_R} u^2(T) \, dx \leq \int_{x_L}^{x_R} g^2 \, dx + 2 \int_0^T \beta c dt
\]

\[
\|u(\cdot, T)\|^2 \leq \|g(\cdot)\|^2 + \int_{x_L}^{x_R} g^2 \, dx + 2 \int_0^T \beta c dt
\]

Therefore, assuming appropriate BC, stable
Objective: construct operators that mimic the following IBP rule

$$\int_{x_L}^{x_R} \mathcal{W}^T \frac{\partial \mathcal{F}}{\partial x} \, dx = \int_{x_L}^{x_R} \frac{\partial f}{\partial x} \, dx = f|_{x_L}^{x_R}$$

Approximate inviscid terms using Hadamard formalism

$$2D_x \circ F_x (u, u) 1 \approx \frac{\partial \mathcal{F}}{\partial x} (x)$$

The two-point flux matrix, $F_x$, is constructed from a two-point flux function:

$$f^{sc} (u^{(i)}, u^{(j)}) = \frac{\left\{ (u^{(i)})^2 + u^{(i)}u^{(j)} + (u^{(j)})^2 \right\}}{6}$$

Fisher, Carpenter, and coauthors: Many others have taken up the mantel
An example

\[ D_x = \begin{bmatrix} -\frac{3}{2} & 2 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & -2 & \frac{3}{2} \end{bmatrix}. \]

The two argument Hadamard matrix flux function, \( F(u, u) \) is given as

\[
F(u, u) \equiv \begin{bmatrix}
\frac{(u^{(1)})^2}{2} & \frac{(u^{(1)})^2 + u^{(1)}u^{(2)} + (u^{(2)})^2}{6} & \frac{(u^{(1)})^2 + u^{(1)}u^{(3)} + (u^{(3)})^2}{6} \\
\frac{(u^{(2)})^2 + u^{(2)}u^{(1)} + (u^{(1)})^2}{6} & \frac{(u^{(2)})^2}{2} & \frac{(u^{(2)})^2 + u^{(2)}u^{(3)} + (u^{(3)})^2}{6} \\
\frac{(u^{(3)})^2 + u^{(3)}u^{(1)} + (u^{(1)})^2}{6} & \frac{(u^{(3)})^2 + u^{(3)}u^{(2)} + (u^{(2)})^2}{6} & \frac{(u^{(3)})^2}{2}
\end{bmatrix}. 
\]
Mimetic properties

For $E_x = \text{diag}(-1, 0, \ldots, 0, 1)$ and diagonal $P_x$

$$\approx \int W^T \frac{\partial F}{\partial x} d\Omega$$

$$2w^T P D_x \circ F(u, u) 1 = 1^T E_x \circ F(u, u) w - 1^T E_x \psi = 1^T E_x f$$

Nonlinear SBP property: Mimetic term by term

Extension to various generalizations of the SBP concept follow
Semidiscrete analysis: Burgers’ equation

Discretization:

\[
\frac{du}{dt} + 2D_x \circ F(u, u) 1 + bc = 0
\]

1) Multiply through by \( w^T P_x \)

\[
w^T P_x \frac{du}{dt} + 2w^T P_x D_x \circ F(u, u) 1 + w^T P_x bc = 0
\]

2) Use the nonlinear SBP property

\[
w^T P_x \frac{du}{dt} + 1E_x f + w^T P_x bc = 0
\]
Semidiscrete analysis: Burgers’ equation

3) Use the definition of the entropy variables and Leibniz’ rule

\[ \frac{d1^T P_x s}{dt} = -1E_x f - w^T P_x bc \]

4) Integrate in time

\[ 1^T P_x s(T) = 1^T P_x s(0) - \int_0^T (1E_x f + w^T P_x bc) \, dt \]
5) Apply the data and convert the entropy statement into a stability statement on the solution: Using $s = \frac{1}{2} \begin{bmatrix} u \end{bmatrix} u$ and $P_x$ is diagonal

$$\|u\|_{P_x}^2 = \|l\|_{P_x}^2 - 2 \int_0^T (1E_x f + w^T P_x bc) \, dt$$

The remainder of the analysis follows the continuous analysis with appropriate $bc$

What about the fully discrete case?
Why entropy-stability?

3D Taylor-Green vortex: Successful (green) and failure (red)

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Matteo Parsani, Lisandro Dalcin, and coauthors (pushing hard on HPC/practical demonstrations)
SBP operators in time

Linear IBP property is not enough: Solution (Friedrich et al. (2019))

\[ 2D_t \circ U(u, u) 1 \approx \frac{d u}{d t} \]

Continuous problem

\[
\int_0^T \int_{\Omega} \mathcal{W}^T \frac{\partial U}{\partial t} d\Omega dt = \int_{\Omega} s(T) d\Omega - \int_{\Omega} s(0) d\Omega
\]

Discrete

\[
\mathbf{w}^T \mathbf{PD}_t \circ U(u, u) 1 = 1^T P_{\Omega} s^T - 1^T P_{\Omega} s^0
\]

Enabling technology: RRK methods (David Ketcheson 2:30-3:15)
Holistic design of time-dependent PDE discretizations

As before, there is a two way street: some thoughts

Extension from linear operators

- Can we insert into the SBP two-point flux framework?
- Might destroy the delicate balance
- Might need retooling of entropy-stability

Instinct: there is something more than the above, especially outside of the NS context
The last piece: positivity preservation

Entropy stability proof assumes positivity

- Recent work by Yamaleev and Upperman (2021)

High-order scheme

\[
\frac{du_H}{dt} = RHS_H(u_H), \quad \text{entropy stable}
\]

\[
u_H^{n+1} = u_H^n + RHS_H(u_H^n)
\]

not positivity preserving

Special low-order scheme

\[
\frac{du_L}{dt} = RHS_H(u_L), \quad \text{entropy stable}
\]

\[
u_L^{n+1} = u_L^n + RHS_L(u_L^n)
\]

\[\Delta t \text{ s.t. positivity preserving}\]

Positivity-preservation achieved via sub-cell dissipation \((f^{EC} - f^{ED})\)
The last piece: positivity

HO positivity preserving via flux limiting

\( \tilde{u}_H = u_L^{n+1} + \theta (u_H^{n+1} - u_L^{n+1}) , \quad \exists \theta \in [0, 1] \) s.t. positivity preserving

- Fully discrete scheme:
- Positivity preserving
- High-order
- Conservative

Practical considerations:

- High-order in time: SSP
- Entropy stable velocity and temperature limiters
- RRK (work in progress): positivity preserving and
  - Euler: entropy conservative for smooth flows
  - NS: entropy stable
Collaborators

University of Manchester
  • Dr. Pieter D. Boom
NASA Langley Research Center
  • Dr. Mark H. Carpenter
Rice University
  • Prof. Jesse Chan
KAUST
  • Dr. Lisandro Dalcin
NASA Langley Research Center
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References and questions

SBP: general


SBP: time


SBP: entropy stability


SBP: positivity preservation