# 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

# The summation-by-parts (SBP) framework

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:

$$\begin{aligned}
&\frac{\partial \mathcal{U}}{\partial t} + \mathrm{P}\mathcal{U} + \mathcal{F} = 0, \quad t \geq 0, \quad \boldsymbol{x} \in \Omega \\
&\mathrm{B}\mathcal{U} = \mathcal{G}, \quad t \geq 0, \quad \boldsymbol{x} \in \partial\Omega = \Gamma, \\
&\mathcal{U}(\boldsymbol{x}, 0) = \mathcal{I}, \quad t = 0, \quad \boldsymbol{x} \in \Omega,
\end{aligned}$$

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

Simple approach to construct such estimates

Example: consider the linear advection equation

$$\frac{\partial \mathcal{U}}{\partial t} + a\frac{\partial \mathcal{U}}{\partial x} = 0, \quad t \geq 0, \quad x \in [x_L, x_R], \quad a > 0,$$
$$\mathcal{U}(x_L, t) = \mathcal{G}, \quad t \geq 0,$$
$$\mathcal{U}(x, 0) = \mathcal{I}, \quad t = 0, \quad x \in [x_L, x_R],$$

# Stability analysis of the convection equation

1) Multiply the PDE by the solution $\mathcal{U}$ and integrate in space

$$\int_{x_L}^{x_R} \mathcal{U}\frac{\partial \mathcal{U}}{\partial t}\mathrm{d}x + a\int_{x_L}^{x_R} \mathcal{U}\frac{\partial \mathcal{U}}{\partial x}\mathrm{d}x = 0$$

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

$$\int_{x_L}^{x_R} \mathcal{U}\frac{\partial \mathcal{U}}{\partial t}\mathrm{d}x + \frac{a}{2}\,\mathcal{U}^2\Big|_{x_L}^{x_R} = 0$$

3) Chain rule and Leibniz rule on the temporal term

$$\frac{1}{2}\frac{\mathrm{d}||\mathcal{U}||^2}{\mathrm{d}t} + \frac{a}{2}\,\mathcal{U}^2\Big|_{x_L}^{x_R} = 0, \quad ||\mathcal{U}||^2 \equiv \int_{x_L}^{x_R} \mathcal{U}^2\mathrm{d}x$$

4) Integrating in time and applying IC and BC

$$||\mathcal{U}||^2 = ||\mathcal{I}||^2 - a\int_0^T \mathcal{U}^2(x_R, t)\mathrm{d}t + a\int_0^T \mathcal{G}^2\mathrm{d}t$$

$$||\mathcal{U}||^2 \leq ||\mathcal{I}||^2 + a\int_0^T \mathcal{G}^2\mathrm{d}t$$

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?

# SBP operators: Finite-difference origins

Goal: mimic IBP

$$\int_{x_L}^{x_R} \mathcal{V}\frac{\partial \mathcal{U}}{\partial x}\mathrm{d}x + \int_{x_L}^{x_R} \mathcal{U}\frac{\partial \mathcal{V}}{\partial x}\mathrm{d}x = \mathcal{V}\mathcal{U}|_{x_L}^{x_R}$$

Some notation:

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

We can exactly capture the RHS with $\mathrm{E}_x = \mathrm{diag}(-1, 0, \ldots, 0, 1)$

$$\boldsymbol{v}^T \mathrm{E}_x \boldsymbol{u} = v_n u_n - v_1 u_1 = \mathcal{V}\mathcal{U}|_{x_L}^{x_R}$$

# SBP operators: Finite difference origins

We need an approximation to the $L_2$ inner product

$$\tilde{\boldsymbol{v}}^T \mathrm{P}_x \tilde{\boldsymbol{u}} \approx \int_{x_L}^{x_R} \tilde{\mathcal{V}}\tilde{\mathcal{U}} \mathrm{d}x, \quad \mathrm{P}_x = \mathrm{P}_x^T, \quad \mathrm{P}_x > 0$$

Defining $\mathrm{Q}_x \equiv \mathrm{P}_x \mathrm{D}_x$ we discretize the LHS

$$\overbrace{\approx \int_{x_L}^{x_R} \mathcal{V} \frac{\partial \mathcal{U}}{\partial x} \mathrm{d}x}^{\boldsymbol{v}^T \mathrm{P}_x \mathrm{D}_x \boldsymbol{u}} + \overbrace{\approx \int_{x_L}^{x_R} \mathcal{U} \frac{\partial \mathcal{V}}{\partial x} \mathrm{d}x}^{\boldsymbol{u}^T \mathrm{P}_x \mathrm{D}_x \boldsymbol{v}} = \boldsymbol{v}^T \mathrm{E}_x \boldsymbol{u}$$

$$\boldsymbol{v}^T \mathrm{Q}_x \boldsymbol{u} + \boldsymbol{u}^T \mathrm{Q}_x \boldsymbol{v} = \boldsymbol{v}^T \mathrm{E}_x \boldsymbol{u}$$

$$\boldsymbol{v}^T \left( \mathrm{Q}_x + \mathrm{Q}_x^T \right) \boldsymbol{u} = \boldsymbol{v}^T \mathrm{E}_x \boldsymbol{u}$$

$$\mathrm{Q}_x + \mathrm{Q}_x^T = \mathrm{E}_x$$

This is immediate if $\mathrm{Q}_x = \mathrm{S}_x + \frac{1}{2}\mathrm{E}_x$, $\mathrm{S}_x = -\mathrm{S}_x^T$

# SBP operators: Finite-difference origins

Kreiss and Scherer (1974)

$$\mathsf{P}_x = \operatorname{diag}\left(p_1, p_2, p_3, p_4, 1, \ldots, 1, p_4, p_3, p_2, p_1\right)$$

$$\mathsf{Q}_x = \begin{bmatrix}
-\frac{1}{2} & q_{12} & q_{13} & q_{14} & & & & & & & & & \\
-q_{12} & 0 & q_{23} & q_{24} & & & & & & & & & \\
-q_{13} & -q_{23} & 0 & q_{34} & \alpha_2 & & & & & & & & \\
-q_{14} & -q_{24} & -q_{34} & 0 & \alpha_1 & \alpha_2 & & & & & & & \\
 & & -\alpha_2 & -\alpha_1 & 0 & \alpha_1 & \alpha_2 & & & & & & \\
 & & & -\alpha_2 & -\alpha_1 & 0 & \alpha_1 & \alpha_2 & & & & & \\
 & & & & \ddots & \ddots & \ddots & \ddots & \ddots & & & & \\
 & & & & & -\alpha_2 & -\alpha_1 & 0 & \alpha_1 & \alpha_2 & & & \\
 & & & & & & -\alpha_2 & -\alpha_1 & 0 & \alpha_1 & \alpha_2 & & \\
 & & & & & & & -\alpha_2 & -\alpha_1 & 0 & -q_{34} & q_{24} & q_{14} \\
 & & & & & & & & -\alpha_2 & -q_{34} & 0 & -q_{23} & q_{13} \\
 & & & & & & & & & -q_{24} & -q_{23} & 0 & q_{12} \\
 & & & & & & & & & -q_{14} & -q_{13} & -q_{12} & \frac{1}{2}
\end{bmatrix}$$

# 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

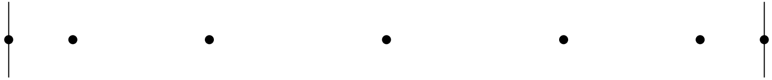
- Accuracy constraints and extension to block norm: Bo Strand (1994)
- Weak imposition of boundary conditions: Carpenter and Gottlieb (1994)
- Projection method for BC: Olsson (1995)
- Major contributions from many others: e.g. Jan Nordström, Gunilla Kreiss etc.

  ⋮

# SBP operators: A first generalization

Can we go beyond classical finite-differences?

- Yes: Spectral Methods: Carpenter and Gottlieb (1995)
- Collocated DG: Gassner (2013)
- General 1D nodal schemes: DCDRF, Boom, and Zingg (2014)



DEF: degree $p$ SBP operator

1. $D_x \boldsymbol{x}^k = k\boldsymbol{x}^{k-1}, \quad k = 0, 1, .., p$
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.

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + a\mathrm{D}_x\boldsymbol{u} + \boldsymbol{bc} = 0$$

1) Multiply by the solution and integrate over the domain

$$\boldsymbol{u}^T\mathrm{P}_x\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + a\boldsymbol{u}^T\mathrm{P}_x\mathrm{D}_x\boldsymbol{u} + \boldsymbol{u}^T\mathrm{P}\boldsymbol{bc} = 0$$

2) Use IBP on the spatial term

$$\boldsymbol{u}^T\mathrm{P}_x\mathrm{D}_x\boldsymbol{u} = \boldsymbol{u}^T\mathrm{Q}_x\boldsymbol{u} = \frac{1}{2}\boldsymbol{u}^T\mathrm{E}_x\boldsymbol{u}$$

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

$$\frac{1}{2}\frac{\mathrm{d}||\boldsymbol{u}||^2_{\mathrm{P}_x}}{\mathrm{d}t} = -\frac{a}{2}\boldsymbol{u}^T\mathrm{E}_x\boldsymbol{u} - \boldsymbol{u}^T\mathrm{P}\boldsymbol{bc}, \quad ||\boldsymbol{u}||^2_{\mathrm{P}_x} \equiv \boldsymbol{u}^T\mathrm{P}_x\boldsymbol{u}$$

# Why this is useful

4) Integrate in time and apply IC and BC

$$||\boldsymbol{u}(T)||^2_{\mathrm{P}_x} = ||\boldsymbol{I}||^2_{\mathrm{P}_x} - \int_0^T \left( a\boldsymbol{u}^T \mathrm{E}_x \boldsymbol{u} + 2\boldsymbol{u}^T \mathrm{P}\boldsymbol{bc} \right) \mathrm{d}t$$

If $\boldsymbol{bc}$ is constructed appropriately

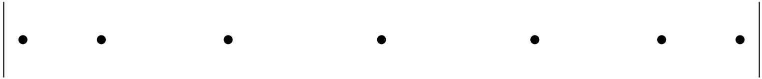
$$||\boldsymbol{u}(T)||^2_{\mathrm{P}_x} \leq ||\boldsymbol{I}||^2_{\mathrm{P}_x} + \int_0^T \mathcal{G}^2 \mathrm{d}t$$

The semi-discrete form is stable!

What about the fully-discrete case?

- More on this shortly

# SBP operators: A second generalization



Previous definition $\boldsymbol{x}(1) = x_L$, $\boldsymbol{x}(n) = x_R$
Relax restrictions on $\mathrm{E}_x$

$$\mathrm{E}_x \equiv \boldsymbol{t}_R \boldsymbol{t}_R^T - \boldsymbol{t}_L \boldsymbol{t}_L^T$$
$$\boldsymbol{t}_R^T \boldsymbol{x}^k = x_R^k, \quad \boldsymbol{t}_L^T \boldsymbol{x}^k = x_L^k, \quad k = 0, 1, \ldots, p$$

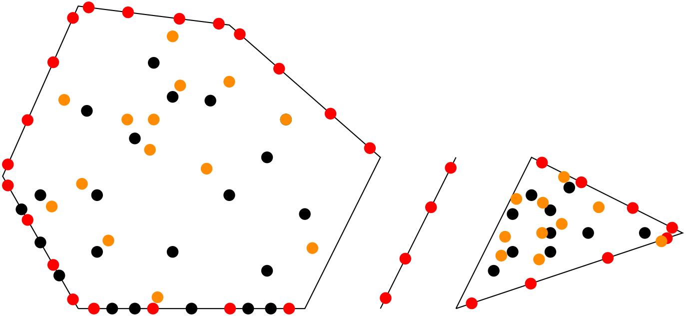
Now

$$\boldsymbol{v}^T \mathrm{E}_x \boldsymbol{u} = \mathcal{V}\mathcal{U}\Big|_{x_L}^{x_R}, \quad \mathcal{V}, \mathcal{U} \in \mathbb{P}^p$$

# 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))

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \lambda y, \quad y(0) = y_0$$

SBP-SAT scheme

$$\mathrm{D}_t \boldsymbol{y} = \lambda \boldsymbol{y} - \mathrm{P}^{-1} \boldsymbol{t}_L \left( \boldsymbol{t}_{\boldsymbol{R}} \boldsymbol{y} - y_0 \right)$$

Many contributions in this area (see the list of papers at the end)

# Connection to RK schemes

Butcher tableau:

$$\begin{array}{c|c} \boldsymbol{c} & \mathsf{A} \\ \hline & \boldsymbol{b}^T \end{array}$$

From SBP-SAT scheme:

$$\mathsf{A} = \frac{1}{h}\left(\mathsf{Q} + \boldsymbol{t}_L \boldsymbol{t}_L^T\right)^{-1}\mathsf{P}$$

$$\boldsymbol{b}^T = \frac{1}{h}1^T\mathsf{P}$$

$$\boldsymbol{c} = \frac{\boldsymbol{t} - 1t_0}{h}$$

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:

$$\frac{\partial \mathcal{U}}{\partial t} + \frac{\partial \mathcal{F}}{\partial x} = 0$$

Equipped with a convex entropy function $\mathcal{S} = \mathrm{fnc}(\mathcal{U})$ that satisfies

$$\frac{\partial \mathcal{S}}{\partial \mathcal{U}} \frac{\partial \mathcal{F}}{\partial x} = \mathcal{W}^{\mathrm{T}} \frac{\partial \mathcal{F}}{\partial x} = \frac{\partial f}{\partial x}$$

Integrability condition

where $f$ is the entropy flux and $\mathcal{W}$ are the entropy variables

# Entropy stability analysis

1) Multiply the PDE by $\mathcal{W}^{\mathrm{T}}$ and integrate in space

$$\int_{x_L}^{x_R} \mathcal{W}^{\mathrm{T}} \frac{\partial \mathcal{U}}{\partial t} \mathrm{d}x + \int_{x_L}^{x_R} \mathcal{W}^{\mathrm{T}} \frac{\partial \mathcal{F}}{\partial x} \mathrm{d}x = 0$$

2) Use the IBP rule induced by the integrability condition

$$\int_{x_L}^{x_R} \mathcal{W}^{\mathrm{T}} \frac{\partial \mathcal{F}}{\partial x} \mathrm{d}x = \int_{x_L}^{x_R} \frac{\partial f}{\partial x} \mathrm{d}x = f n_x \Big|_{x_L}^{x_R}$$

$$\int_{x_L}^{x_R} \mathcal{W}^{\mathrm{T}} \frac{\partial \mathcal{U}}{\partial t} \mathrm{d}x + f \Big|_{x_L}^{x_R} \leq 0$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{x_L}^{x_R} \mathcal{S}\,\mathrm{d}x + f\big|_{x_L}^{x_R} \leq 0$$

4) Integrate in time

$$\int_{x_L}^{x_R} \mathcal{S}(t)\mathrm{d}x \leq \int_{x_L}^{x_R} \mathcal{S}(0)\mathrm{d}x - \int_0^T f\big|_{x_L}^{x_R}\,\mathrm{d}t$$

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

# Entropy stability analysis: Burgers' equation

$$\frac{\partial \mathcal{U}}{\partial t} + \frac{\partial}{\partial x}\left(\frac{\mathcal{U}^2}{2}\right) = 0,$$

Appropriately formulated BC

$$\mathcal{U}(x, 0) = \mathcal{I}$$

Entropy function: $\mathcal{S} = \frac{\mathcal{U}^2}{2}$ Entropy variable: $\mathcal{W} = \frac{\partial \mathcal{S}}{\partial \mathcal{U}} = \mathcal{U}$

Flux: $\mathcal{F} = \frac{\mathcal{U}^2}{2}$ Entropy flux: $f = \frac{\mathcal{U}^3}{3}$

# 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

$$\int_{x_L}^{x_R} \mathcal{U}^2(T)\mathrm{d}x \leq \int_{x_L}^{x_R} \mathcal{I}^2\mathrm{d}x + 2\int_0^T \mathcal{b}c\,\mathrm{d}t$$

$$||\mathcal{U}(\cdot, T)||^2 \leq ||\mathcal{I}(\cdot)||^2 + \int_{x_L}^{x_R} \mathcal{I}^2\mathrm{d}x + 2\int_0^T \mathcal{b}c\,\mathrm{d}t$$

Therefore, assuming appropriate BC, stable

Objective: construct operators that mimic the following IBP rule

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

Approximate inviscid terms using Hadammard formalism

$$2\mathrm{D}_x \circ \mathrm{F}_x \left(\boldsymbol{u}, \boldsymbol{u}\right) 1 \approx \frac{\partial \mathcal{F}}{\partial x}(\boldsymbol{x})$$

The two-point flux matrix, $\mathrm{F}_x$, is constructed from a two-point flux function:

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

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

# An example

$$\mathrm{D}_x = \begin{bmatrix} -\frac{3}{2} & 2 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & -2 & \frac{3}{2} \end{bmatrix}.$$

The two argument Hadammard matrix flux function, $\mathrm{F}(\boldsymbol{u},\boldsymbol{u})$ is given as

$$\mathrm{F}(\boldsymbol{u},\boldsymbol{u}) \equiv$$

$$\begin{bmatrix} \frac{\left(\boldsymbol{u}^{(1)}\right)^2}{2} & \frac{\left(\boldsymbol{u}^{(1)}\right)^2+\boldsymbol{u}^{(1)}\boldsymbol{u}^{(2)}+\left(\boldsymbol{u}^{(2)}\right)^2}{6} & \frac{\left(\boldsymbol{u}^{(1)}\right)^2+\boldsymbol{u}^{(1)}\boldsymbol{u}^{(3)}+\left(\boldsymbol{u}^{(3)}\right)^2}{6} \\ \frac{\left(\boldsymbol{u}^{(2)}\right)^2+\boldsymbol{u}^{(2)}\boldsymbol{u}^{(1)}+\left(\boldsymbol{u}^{(1)}\right)^2}{6} & \frac{\left(\boldsymbol{u}^{(2)}\right)^2}{2} & \frac{\left(\boldsymbol{u}^{(2)}\right)^2+\boldsymbol{u}^{(2)}\boldsymbol{u}^{(3)}+\left(\boldsymbol{u}^{(3)}\right)^2}{6} \\ \frac{\left(\boldsymbol{u}^{(3)}\right)^2+\boldsymbol{u}^{(3)}\boldsymbol{u}^{(1)}+\left(\boldsymbol{u}^{(1)}\right)^2}{6} & \frac{\left(\boldsymbol{u}^{(3)}\right)^2+\boldsymbol{u}^{(3)}\boldsymbol{u}^{(2)}+\left(\boldsymbol{u}^{(2)}\right)^2}{6} & \frac{\left(\boldsymbol{u}^{(3)}\right)^2}{2} \end{bmatrix}.$$

# Mimetic properties

For $\mathsf{E}_x = \mathrm{diag}(-1, 0, \ldots, 0, 1)$ and diagonal $\mathsf{P}_x$

$$\overbrace{2\boldsymbol{w}^{\mathrm{T}}\mathsf{P}\mathsf{D}_x \circ \mathsf{F}\left(\boldsymbol{u},\boldsymbol{u}\right)\mathbf{1}}^{\approx \int \mathcal{W}^{\mathrm{T}} \frac{\partial \mathcal{F}}{\partial x} \mathrm{d}\Omega} = \overbrace{\mathbf{1}^{\mathrm{T}}\mathsf{E}_x \circ \mathsf{F}\left(\boldsymbol{u},\boldsymbol{u}\right)\boldsymbol{w} - \mathbf{1}^{\mathrm{T}}\mathsf{E}_x\boldsymbol{\psi} = \mathbf{1}^{T}\mathsf{E}_x\boldsymbol{f}}^{\left(\mathcal{W}^{\mathrm{T}}\mathcal{F} - \Psi\right)\big|_{x_L}^{x_R} = f\big|_{x_L}^{x_R}}$$

Nonlinear SBP property: Mimetic term by term

Extension to various generalizations of the SBP concept follow

Discretization:

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + 2\mathsf{D}_x \circ \mathsf{F}\left(\boldsymbol{u}, \boldsymbol{u}\right) 1 + \boldsymbol{bc} = 0$$

1) Multiply through by $\boldsymbol{w}^{\mathrm{T}}\mathsf{P}_x$

$$\boldsymbol{w}^{\mathrm{T}}\mathsf{P}_x\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + 2\boldsymbol{w}^{\mathrm{T}}\mathsf{P}_x\mathsf{D}_x \circ \mathsf{F}\left(\boldsymbol{u}, \boldsymbol{u}\right) 1 + \boldsymbol{w}^{T}\mathsf{P}_x\boldsymbol{bc} = 0$$

2) Use the nonlinear SBP property

$$\boldsymbol{w}^{\mathrm{T}}\mathsf{P}_x\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + 1\mathsf{E}_x\boldsymbol{f} + \boldsymbol{w}^{T}\mathsf{P}_x\boldsymbol{bc} = 0$$

# Semidiscrete analysis: Burgers' equation

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

$$\frac{\mathrm{d}1^{\mathrm{T}}\mathsf{P}_x\boldsymbol{s}}{\mathrm{d}\boldsymbol{t}} = -1\mathsf{E}_x\boldsymbol{f} - \boldsymbol{w}^T\mathsf{P}_x\boldsymbol{bc}$$

4) Integrate in time

$$1^{\mathrm{T}}\mathsf{P}_x\boldsymbol{s}(T) = 1^{\mathrm{T}}\mathsf{P}_x\boldsymbol{s}(0) - \int_0^T \left(1\mathsf{E}_x\boldsymbol{f} + \boldsymbol{w}^T\mathsf{P}_x\boldsymbol{bc}\right)\mathrm{d}t$$

5) Apply the data and convert the entropy statement into a stability statement on the solution: Using $\boldsymbol{s} = \frac{1}{2}\left[\boldsymbol{u}\right]\boldsymbol{u}$ and $\mathsf{P}_x$ is diagonal

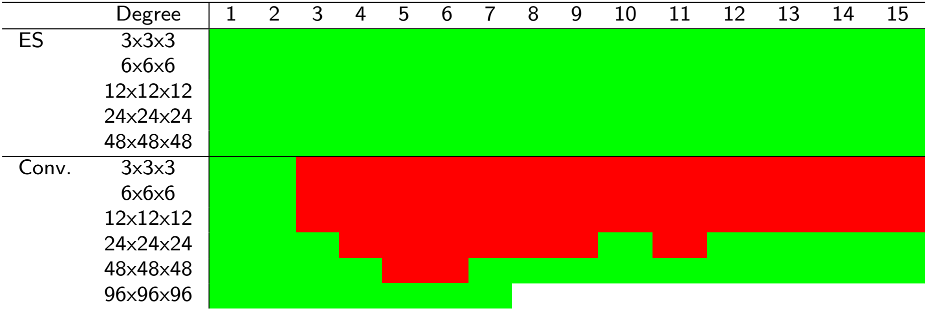
$$\|\boldsymbol{u}\|^2_{\mathsf{P}_x} = \|\boldsymbol{I}\|^2_{\mathsf{P}_x} - 2\int_0^T \left(1\mathsf{E}_x\boldsymbol{f} + \boldsymbol{w}^T\mathsf{P}_x\boldsymbol{bc}\right)\mathrm{d}t$$

The remainder of the analysis follows the continuous analysis with appropriate $\boldsymbol{bc}$

What about the fully discrete case?

# Why entropy-stability?

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




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))

$$2\mathrm{D}_t \circ \mathrm{U}\left(\boldsymbol{u}, \boldsymbol{u}\right)\mathbf{1} \approx \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t}$$

Continuous problem

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

Discrete

$$\boldsymbol{w}^T \mathrm{P} \mathrm{D}_t \circ \mathrm{U}\left(\boldsymbol{u}, \boldsymbol{u}\right)\mathbf{1} = \mathbf{1}^T \mathrm{P}_\Omega \boldsymbol{s}^{[T]} - \mathbf{1}^T \mathrm{P}_\Omega \boldsymbol{s}^{[0]}$$

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

$$\underbrace{\frac{\mathrm{d}\boldsymbol{u}_H}{\mathrm{d}t} = RHS_H(\boldsymbol{u}_H)}_{\text{entropy stable}}, \qquad \underbrace{\boldsymbol{u}_H^{n+1} = \boldsymbol{u}_H^n + RHS_H(\boldsymbol{u}_H^n)}_{\text{not positivity preserving}}$$

Special low-order scheme

$$\underbrace{\frac{\mathrm{d}\boldsymbol{u}_L}{\mathrm{d}t} = RHS_H(\boldsymbol{u}_L)}_{\text{entropy stable}}, \qquad \underbrace{\boldsymbol{u}_L^{n+1} = \boldsymbol{u}_L^n + RHS_L(\boldsymbol{u}_L^n)}_{\Delta t \text{ s.t. positivity preserving}}$$

Positivity-preservation achieved via sub-cell dissipation $(\boldsymbol{f}^{EC} - \boldsymbol{f}^{ED})$

# The last piece: positivity

## HO positivity preserving via flux limiting

$$\tilde{\boldsymbol{u}}_H = \boldsymbol{u}_L^{n+1} + \theta\left(\boldsymbol{u}_H^{n+1} - \boldsymbol{u}_L^{n+1}\right), \quad \exists \theta \in [0,1] \text{ s.t. positivity preserving}$$

- 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

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# References and questions


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