Theory and Features of the SBP-SAT Code ESSENSE

(Code development : Marco Kupianinen SMHI and Peter Eliasson FOI)

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By

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$\vec{H}_2(Lu - h_2)$

LiU expanding reality

Outline

- Theory
  - Key concepts: well-posedness and stability
  - The SBP-SAT technique for an illustrative model problem
- Features
  - Technical details
  - Performance and scalability
  - Some new developments
- Similarities with dG (if time permits)

Theory

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4 building blocks for a stable and high order accurate finite difference scheme

1. The continuous energy method for well-posed boundary or interface condtions that yield an energy estimate.
2. Summation-By-Parts (SBP) operators that mimic integration-by-parts.
3. Weak implementation of boundary/interface conditions using the Simultaneous Approximation Term (SAT) technique.
4. The discrete energy method (DEM) and choice of penalty terms.

Where, how many and what kind of B.C ?

As the most straightforward example, consider the advection equation:

$$u_t + au_x = 0, \quad 0 \le x \le 1.$$

By multiplying with u and integrating over the domain we obtain:

$$\|u\|_t^2 = au_{x=0}^2 - au_{x=1}^2$$

- One boundary condition at x=0 if a>0.
- One boundary condition at x=1 if a<0.
- No boundary condition if a=0.
- Well posed if $u = g(t)$ at appropriate position.

The finite difference SBP operators

Continuous case

$$(u, v_x) = \int_0^1 u v_x dx = (uv)_{x=1} - (uv)_{x=0} - (u_x, v)$$

Discrete case

$$(\vec{U}, \mathcal{D}\vec{V})_P = \vec{U}^T P \mathcal{D}\vec{V} = U_N V_N - U_0 V_0 - (\mathcal{D}\vec{U}, \vec{V})_P$$

$$\mathcal{D}\vec{U} = P^{-1} Q \vec{U}, \quad \underline{P = P^T > 0}, \quad \underline{Q + Q^T = D}, \quad D = diag[-1, 0..0, 1]$$

The finite difference SBP operator

The second order accurate case.

$$Q = \frac{1}{2}\begin{pmatrix} -1 & 1 & & & & \\ -1 & 0 & 1 & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & -1 & 0 & 1 \\ & & & & -1 & 1 \end{pmatrix}, \quad P = \Delta x \begin{pmatrix} \frac{1}{2} & & & & & \\ & 1 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & 1 & \\ & & & & & \frac{1}{2} \end{pmatrix}$$

- For higher orders, more involved closures at the boundaries.
- Almost skew-symmetric, lower accuracy at the boundaries.

The SAT technique and DEM for stability

The continuous problem

$$u_t + u_x = 0, \quad t \geq 0, \quad 0 \leq x \leq 1, \quad u(0,t) = g(t).$$

$$||u||_t^2 = g(t)^2 - u(1,t)^2.$$

The semi-discrete approximation

$$\vec{V}_t + P^{-1}Q\vec{V} = \underline{P^{-1}[\sigma(V_0(t) - g(t))]\vec{e}_0}$$

Stability

$$||\vec{V}||_t^2 = g(t)^2 - V_N(t)^2 + R, \quad R(\sigma = -1) = -(V_0(t) - g(t))^2 \leq 0.$$

The SBP-SAT technique in multiple dimensions

$$w_t + \bar{D}_x F + \bar{D}_y G = SAT$$

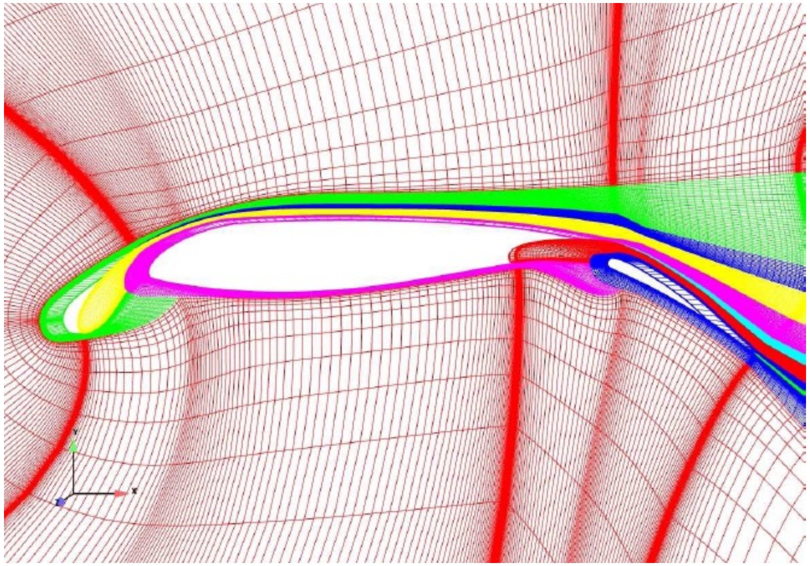
Tensor product form using Kronecker products

$$\bar{D}_x = (D_x \otimes I_y \otimes I_4) \qquad \bar{D}_y = (I_x \otimes D_y \otimes I_4)$$

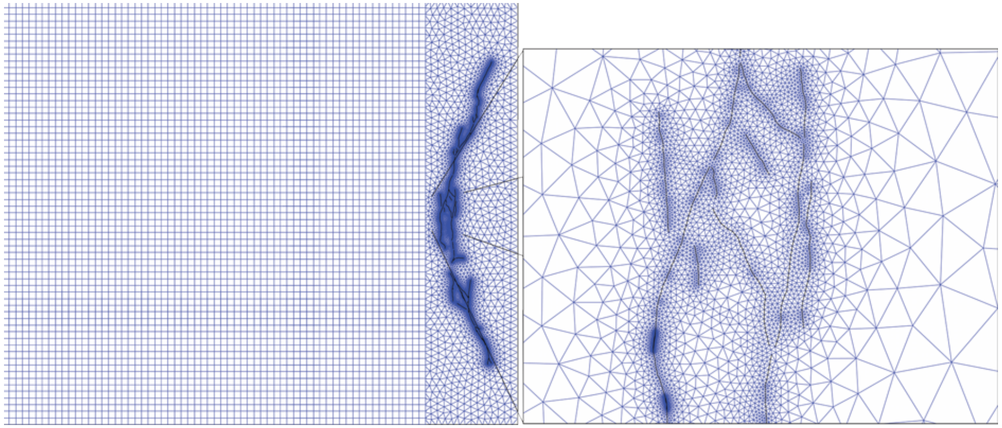
The SAT term imposes the boundary conditions $u = g_2, v = g_3, T_y = g_4$ weakly

$$SAT = \bar{P}_y^{-1} \bar{E}_0 \left[\left(H_2 w - g_2 \right) + \left(H_3 w - g_3 \right) + \left(D_y H_4 w - g_4 \right) \right]$$

Complex Geometries



Landers fault



<u>Complex geometry</u>: Multiblock method, curvilinear mesh, smooth transform to cube, weak interface conditions.

<u>Nasty geometry:</u> Hybrid structured-unstructured method, weak interface conditions.

The ”BIG PICTURE”

- Make sure PDE is well posed and have an energy estimate (boundary/interface conditions).
- Make a curvilinear multi-block mesh. Transform curvilinear blocks to cubes.
- Discretize each coordinate direction using SBP operators and SAT boundary/interface conditions.
- Semi-discrete ODE: $U_t + A(U)U = F, \quad t \geq 0$
- Energy stability guarantee all eigenvalues to A ok.
- Time-integration, RK4 standard.

Features

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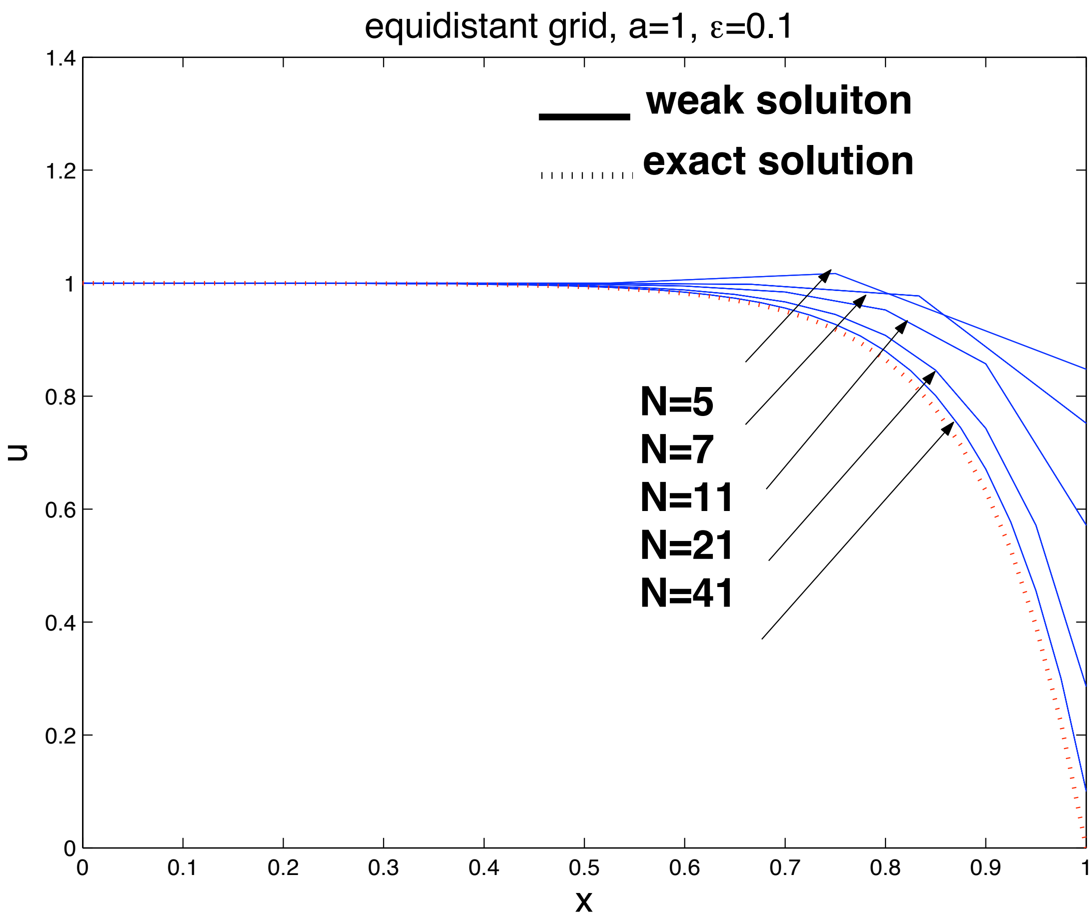
Technical details

- Main characteristics
  - Energy stable SBP/SAT/FDM of orders 2, 3, 4, 5 and 6.
  - Multi-block structured grids, no differentiation across blocks.
  - Both classical and DRP SBP operators available.
  - RK4 in time, SBP-SAT in time and multi-grid for time-space soon.
- Details
  - MPI-parallell, Fortran 2003
  - Intel Math Kernel library (MKL) for linear algebra (BLAS) operations.
  - Reproducable results: binary and output files are 'tagged' with relevant info (compiler, flags/options, date, host, etc.).

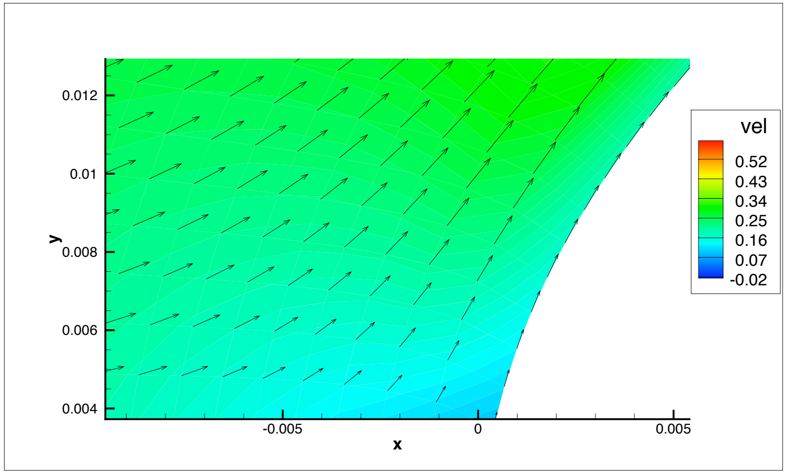
Performance and scalability

- Strong scaling when coarse grained i.e. many gridpoints/core (twice as fast with twice the number of cores).
- Weak scaling when fine-grained i.e. few gridpoints/core (same time for twice as large problem with twice the number of cores).
- Tested for 2048 cores and still scaling well (10^7 gridpoints).
- 3rd order method costs 2.5% more than 2nd order method.
- 4th order method costs 11% more than 2nd order method.

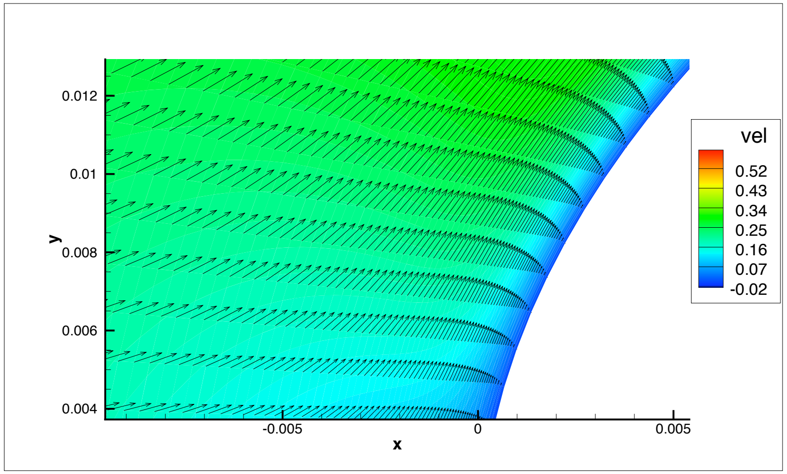
Euler "converges" to Navier-Stokes



Solid boundary, error indicator



N points normal

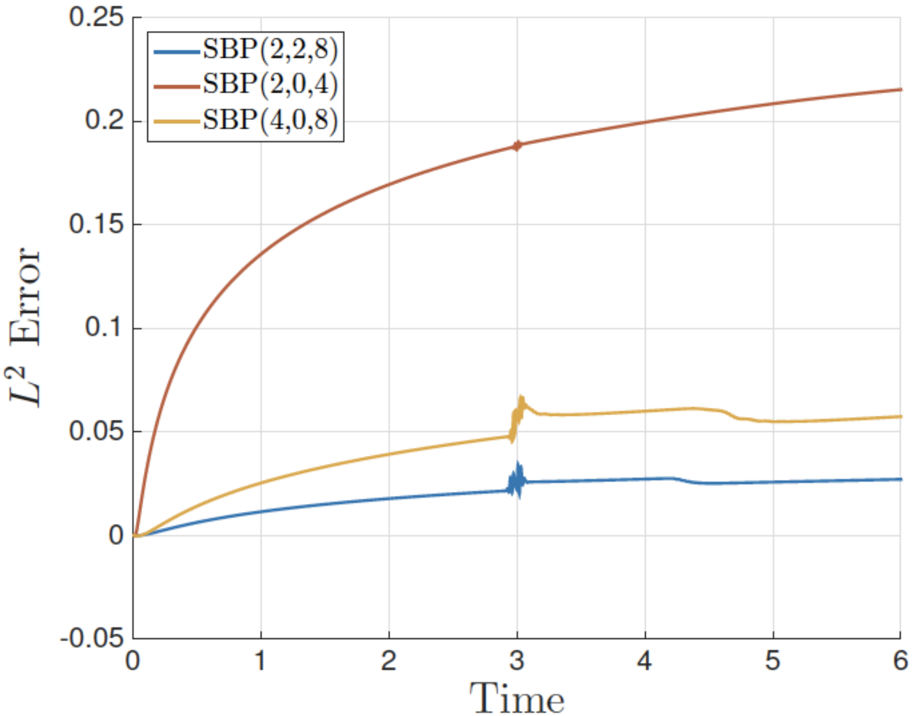


16N points normal

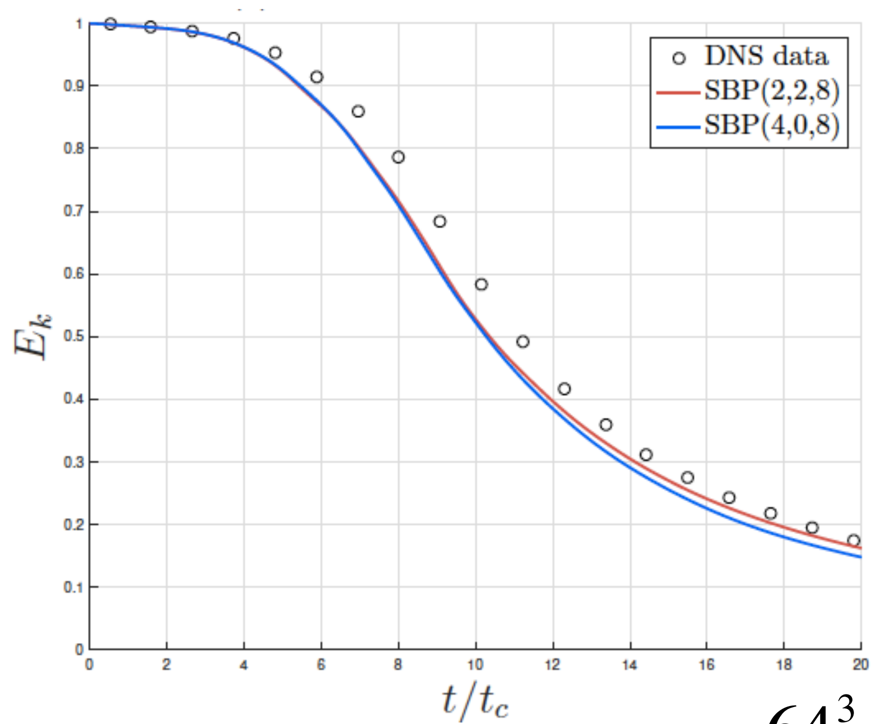
JCP 2008, 2012, Comp. Fluids 2010

Dispersion Relation Preserving SBP Operators

(PhD student Viktor Linders)



The advection equation



Navier-Stokes, TGV, 64^3

JCP 2015, AIAA 2016

SBP-SAT in time

$$u_t = \lambda u, \quad u(0) = f \text{ and } 0 \leq t \leq T$$

The numerical approximation using SBP-SAT is

$$P^{-1}Q\vec{U} = \lambda\vec{U} + P^{-1}(\sigma(U_0 - f))\vec{e_0}.$$

Continuous estimate

$$|u(T)|^2 - 2Re(\lambda)||u||^2 = |f|^2$$

Discrete estimate

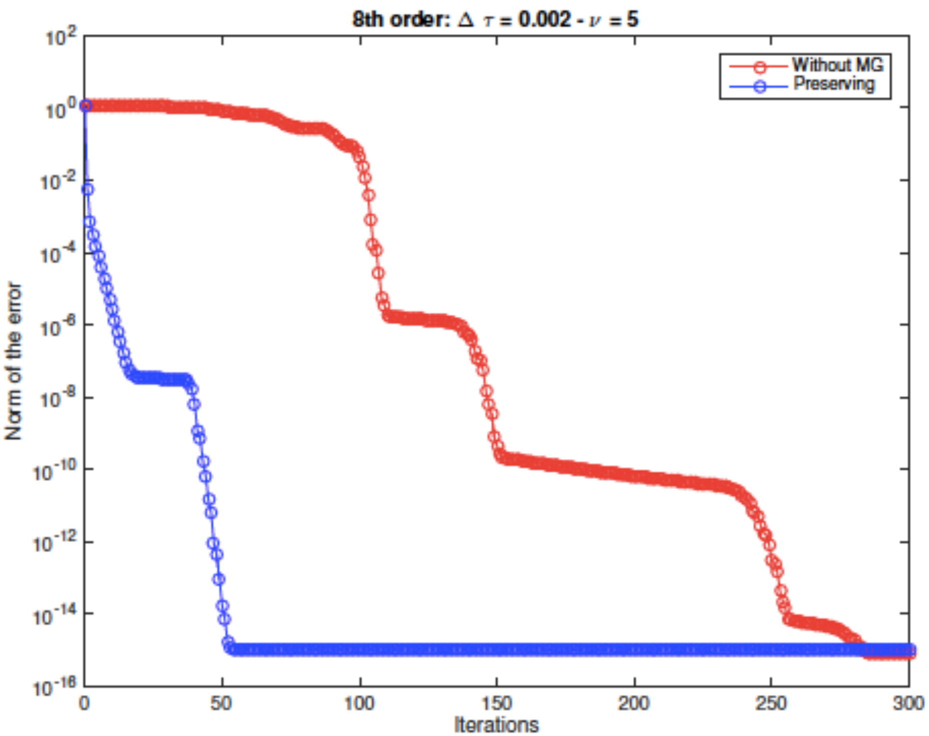
$$|\vec{U}_N|^2 - 2Re(\lambda)||\vec{U}||_P^2 = |f|^2 - |U_0 - f|^2$$

- Almost identical and optimally sharp estimates.
- Unconditional stabillity, up to 10th order accurate.

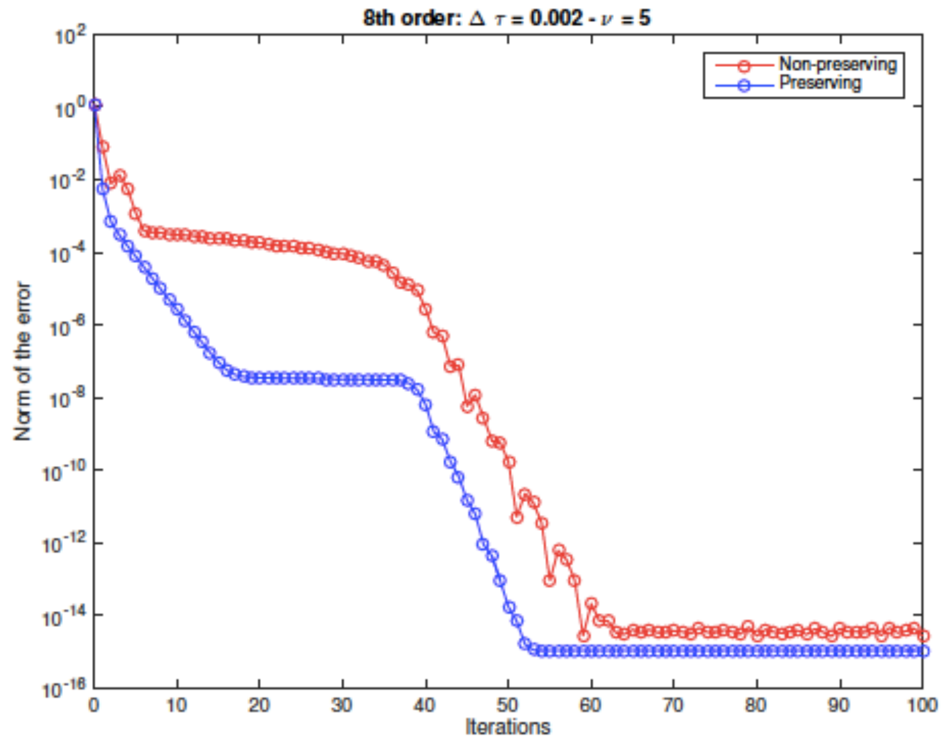
JCP 2013, 2014

Multi-grid with SBP Preserving Restriction and Prolongation Operators

(PhD student Andrea Ruggio)



8th order, with and without multi-grid



8th order, SBP preserving and conventional

Thank you for listening !

$$\vec{H}_2(Lu - h_2)$$