Nonlinear Stability of Comp. Navier-Stokes; Discretizations for non-confo SAND2017-13693C (Entropy's not what it used to be!)

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"Nonlinear stability is the holy grail of numerical analysis . . . and has eluded researcher for many years." Marshal L. Merriam, NASA TM 101086 (1989)

Entropy:
"A thermodynamic state function that measures the disorder of a system"

Entropy => Lyapunov function:
"Convex function governing the stability of a nonlinear dynamical system"

The Wild World of Discretization Stability

Motivation

- High-Order spatial operators
  - Well suited for time-dependent simulations with scale separation
  - Informal poll: Fragile in real world applications
  - Incomplete nonlinear stability theory to guide development
    - Use without stabilization: Compromised Robustness
    - Adopt low-order stabilization techniques (Compromised Accuracy)
    - Filter, de-aliasing, over-integeration, spectral hyper-viscosity, entropy viscosity . . .
  - Move from experimentation to mathematics!
- Entropy conservation/stability theory (2013 Fisher, WENO FD)
  - Three decades development for low-order methods (e.g., Tadmor)
  - Summation-by-parts - SAT operators: All Diagonal Norm operators
    - Nonlinear Stability of Navier-Stokes equations
    - Arbitrary order of accuracy
    - Complex Geometries via mapped hexahedral multi-domains
    - Strong Conservation Form (amenable to shock capturing)

Progress Toward an SS Framework: Past, Present, Future

- Past accomplishments
  - Entropy stable multi-block finite-difference WENO4(6) (2013)
  - Entropy stable spectral elements: recent work (2014)
    - Curvilinear mapped hexa elements (Legendre-Gauss-Lobatto)
    - Strong Conservation Form (amenable to shock capturing)
    - Comparison approach (e.g., Nodal DG and entropy stable operators)
  - Solid Wall Boundary Conditions that preserve SS estimate (2015)
  - Staggered grid operators (2015-2016)
    - Broader selection of collocation points (Legendre-Gauss vs. LGL)
    - Data movement in element while maintaining Entropy stability
  - Symplex Operators: Multi-dimensional SBP (2017)
    - Triangle - Tetrahedra: Hicken et al, Shu et al.
- Current
  - Non-conforming interfaces
    - Stability and Accuracy
    - *p*-refinement ; *h*-refinement
- Future . . . Cut-Cell, Overset, Modal

Summation-by-parts Operators

Mimetic Operators

SBP derivative operators discretely mimic the integration-by-parts

$$\int_{x_L}^{x_R} \phi q_x \, \mathrm{d}x = \phi q|_{x_L}^{x_R} - \int_{x_L}^{x_R} \phi_x q \, \mathrm{d}x$$

Mimetic form for first derivative $\mathcal{D}\phi$ is

$$\mathcal{D} = \mathcal{P}^{-1} \mathcal{Q}, \quad \mathcal{P} = \mathcal{P}^T, \quad \zeta^T \mathcal{P} \zeta > 0, \quad \zeta \neq \mathbf{0},$$
$$\mathcal{Q}^T = \mathcal{B} - \mathcal{Q}, \quad \mathcal{B} = \mathrm{diag}\left(-1, 0, \ldots, 0, 1\right)$$

Semi-Discrete:

$$\phi^T \mathcal{P} \mathcal{P}^{-1} \mathcal{Q} \mathbf{q} = \phi^T \left(\mathcal{B} - \mathcal{Q}^T\right) \mathbf{q} = \phi_N q_N - \phi_1 q_1 - \phi^{\boldsymbol{T}} \mathcal{D}^T \mathcal{P} \mathbf{q}$$

Lemma

All SBP derivatives are discretely conservative in the $\mathcal{P}$-norm.

Telescoping Flux Form

$$f_x(\mathbf{q}) = \mathcal{P}^{-1}\mathcal{Q}\mathbf{f} + \mathcal{T}_{p+1} \; = \; \mathcal{P}^{-1}\Delta\bar{\mathbf{f}} + \mathcal{T}_{p+1}$$

$N \times (N+1)$ matrix Δ is defined as

$$\Delta = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

Calculates undivided difference of adjacent fluxes

Lemma

All SBP differentiation matrices are telescoping operators in the norm $\mathcal{P}$ and may be expressed as above.

Calorically perfect Navier-Stokes Equations

$$q_t + (f^i)_{x_i} = (f^{(v)i})_{x_i}, \quad x \in \Omega, \quad t \in [0, \infty),$$
$$Bq = g_b, \quad x \in \partial\Omega, \quad t \in [0, \infty),$$
$$q(x, 0) = g_0(x), \quad x \in \Omega,$$

SBP operators and equivalent telescoping form for N-S yields

$$\mathbf{q}_t \ = \ -\mathcal{D}_i[\mathbf{f}^i(\mathbf{q})] + \mathcal{D}_i[c]_{ij}\mathcal{D}_j\mathbf{q} + \mathcal{P}^{-1}\mathbf{g}_b \ = \ \mathcal{P}^{-1}\Delta_i\left(-\bar{\mathbf{f}}^i + \bar{\mathbf{f}}^{(v)i}\right) + \mathcal{P}^{-1}\mathbf{g}_b$$
$$\mathbf{q}(x, 0) = g_0(x), \quad x \in \Omega$$

with $\mathbf{g}_b$ containing BC data

Entropy Stability

The Stability of High-Order Schemes: Navier-Stokes

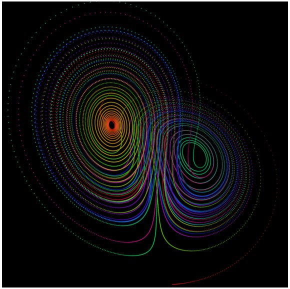
- Mathematical Entropy (Continuous: Discrete)
  - Convex extension of original equations (Friedrichs / Lax)
  - Formed by contracting N-S Eqns. with entropy variables
  - Bounded physical quantity. (N-S Eqns. -> thermodynamic entropy)
- What does it buy you?
  - L2 Stability
    - Entropy is bounded from above in an integral sense
    - Entropy Convexity $\rightarrow$ integral bounds on conserved variables
  - The Nonlinear Stability Plateau for N.S.Eqns.
  - The code doesn't "blow up" (well, usually. . . see below)
- What it doesn't guarantee
  - Stable boundary conditions (Svärd, Parsani)
  - No bounds on derivatives; (e.g., KE stability)
  - Positivity (negative temperatures: Shu's limiters)

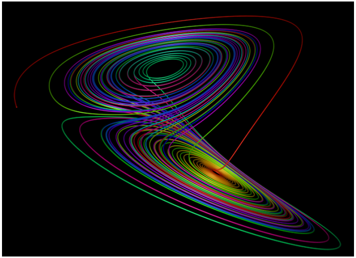
But First a Digression: Lorenz Attractor

- The Lorenz System (Entropy, entropy variables, Convex)

$$\begin{aligned} x_t &= \sigma(y - x) \\ y_t &= rx - y - xz \\ z_t &= xy - bz, \quad \sigma > 1, r > 0, b > 0 \end{aligned}$$

- Models 2D fluid flow in the atmosphere (1963)





Lyapunov function: A Trapping Region (Entropy!)

$$\frac{\partial \mathbf{X}}{\partial t} = F(\mathbf{X}) \quad \mathbf{X} = [x, y, z]$$

$$\begin{aligned} x_t &= \sigma(y - x) \\ y_t &= r\,x - y - xz \\ z_t &= xy - b\,z, \quad \sigma > 1, r > 0, b > 0 \end{aligned}$$

- Lyapunov function: $S = (rx^2 + \sigma y^2 + \sigma(z - 2r)^2)$
  - Convexity: Hessian $H = 2Diag[r, \sigma, \sigma]$
- Entropy Variables $W = \frac{\partial S}{\partial \mathbf{X}} = 2[rx, \sigma y, \sigma(-2r + z)]$
- Total Derivative $\frac{\partial S}{\partial \mathbf{X}} \frac{\partial \mathbf{X}}{\partial t} = \frac{\partial S}{\partial t} = -2\sigma(rx^2 + y^2 + b[(z - r)^2 - r^2])$
  - Stable: $-\infty < x, y < \infty$; $z \leq 0$; $z \geq 2r$
  - UnStable: $0 \leq z \leq 2r$

The Continuous Entropy Equation

Consider entropy S with entropy variables S_q and contract N-S eqns with S_q. Result: differential form of entropy equation

$$S_q q_t + S_q f(q)_{x_i} \;=\; S_t + F_{x_i} \;=\; S_q f^{(v)}_{x_i} \;=\; \left(w^T f^{(v)}\right)_{x_i} - w^T_{x_i} \hat{c}_{ij} w_{x_i}$$

Necessary conditions: 1) convex $S(q) \;=\; w^T$, and 2) S_q simultaneously contracts all (inviscid and viscous) spatial fluxes

$$S_q f^i_{x_i} \;=\; S_q f^i_q q_{x_i} \;=\; F^i_q q_{x_i} \;=\; F^i_{x_i} \quad ; \quad i = 1, \cdots, d$$

Global integration: conservation of entropy

$$\frac{d}{dt} \int_\Omega S \, \mathrm{d}x_i = \left[w^T f^{(v)} - F \right]_{\partial\Omega} - \int_\Omega w^T_{x_j} \hat{c}_{ij} w_{x_i} \, \mathrm{d}x_i$$

The matrix $\hat{c}$ is symmetric positive definite (S.P.D.) and dissipative

Semi-Discrete Analysis: Inviscid Fluxes

$$\mathbf{w}^T \mathcal{P} \mathbf{q}_t + \mathbf{w}^T \Delta_i \bar{\mathbf{f}}_i = \mathbf{w}^T \Delta_i \bar{\mathbf{f}}^{(v)i} + \mathbf{w}^T \mathbf{g}_b, \quad i = 1, 3$$

Inviscid Fluxes

$$\mathbf{w}^T \Delta \bar{\mathbf{f}} = F(q_N) - F(q_1) = \mathbf{1}^T \Delta \overline{\mathbf{F}}$$

Theorem

The local conditions, (e.g., Tadmor for 2nd-order)

$$(w_{i+1} - w_i)^T \,\bar{\mathbf{f}}^{(S)}_{i+1/2} = \tilde{\psi}_{i+1} - \tilde{\psi}_i, \quad i = 1, 2, \ldots, N-1; \tilde{\psi}_1 = \psi_1, \quad \tilde{\psi}_N = \psi_N$$

when summed, telescope across domain conserving entropy

Semi-Discrete Analysis: Generalized Inviscid Fluxes

Theorem

A two-point high-order entropy conservative flux satisfying $\left(w_{i+1} - w_i\right)^T \bar{f}_i^{(S)} = \tilde{\psi}_{i+1} - \tilde{\psi}_i$ *may be constructed as*

$$\bar{f}_i^{(S)} = \sum_{k=i+1}^{N} \sum_{\ell=1}^{i} 2q_{(\ell,k)} \bar{f}_S\left(q_\ell, q_k\right), \quad 1 \leq i \leq N-1$$

$\bar{f}_S(q_\ell, q_k)$*: a two-point function that satisfies entropy conservation*

$$\left(w_\ell - w_k\right)^T \bar{f}_S\left(q_\ell, q_k\right) = \psi_\ell - \psi_k$$

High-order entropy conservative flux satisfies

$$\mathbf{w}^T \mathcal{P}^{-1} \Delta \bar{\mathbf{f}}^{(S)} = \mathcal{P}^{-1} \Delta \bar{\mathbf{F}} = F_x(\mathbf{q}) + \mathcal{T}_d$$

Design order for all variables

Theorem: Cartesian Tensor-product entropy stability

The discrete operator $\mathcal{D}_x^S$ given by the expression

$$\mathcal{D}_x^S f \;=\; \mathcal{P}^{-1}[\mathcal{Q}_x \circ f_s]\mathbf{1} \;=\; \frac{\partial f}{\partial x} + \mathcal{O}\left((\delta x)^p\right),$$

is entropy conservative provided fluxes $f_S(u_\ell, u_k)$ satisfy

$$(w_i - w_j)\bar{f}_S\left(u_i, u_j\right) = \psi_i - \psi_j.$$

Operator satisfies additional local entropy consistency property,

$$2[W]\mathcal{P}^{-1}[\mathcal{Q}_x \circ f_S(u_i, u_j)]\mathbf{1} \;=\; 2\mathcal{P}^{-1}[\mathcal{Q}_x \circ F_S]\mathbf{1} \;=\; F_x + \mathcal{O}\left((\delta x)^p\right),$$

where

$$2\mathcal{P}^{-1}[\mathcal{Q}_x \circ F_S]\mathbf{1} = \mathcal{P}_{ii}^{-1} \sum_{j=1}^{N} 2q_{(i,j)} \left[\frac{(w_i + w_j)}{2} f_S\left(u_i, u_j\right) - \frac{(\psi_i + \psi_j)}{2}\right], 1 \leq i \leq N.$$

Entropy Stability: SBP-SAT VS. FEM

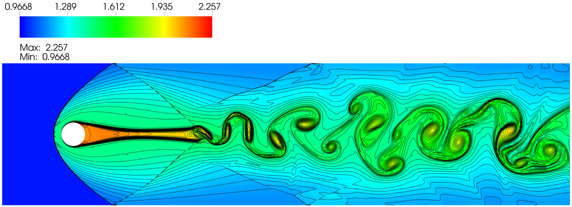
- SBP-SAT
  - Strong conservation form operator
  - Summation of magic dyadic entropy fluxes
  - Stability ensured by entropy flux conservation across domain
  - aliasing does not induce instability
- FEM
  - Typically weak form operator
  - Stability ensured by integral exactness
    - Integration of rational polynomials over element ($p \leq 3$)
    - Inexactness -> aliasing -> instability
    - Additional work on integrals stabilizes formulation
    - Estimate error and added viscosity

A recent history of the entropy world

Flavors of high-order entropy stability

- Multi-block (conforming interface) Finite-Difference WENO
- Spectral Collocation on curvilinear brick elements
- Staggered grid operators (distinct solution / flux pts)
- Extension to general symplices (triangle / tets)

Entropy-Stable WENO4 - Multi-Block Finite-Diff (Fisher)



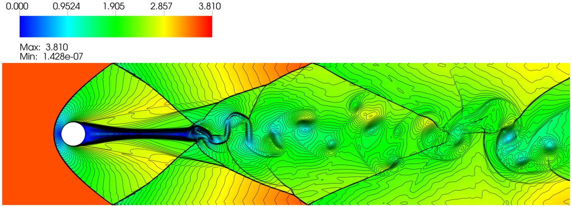
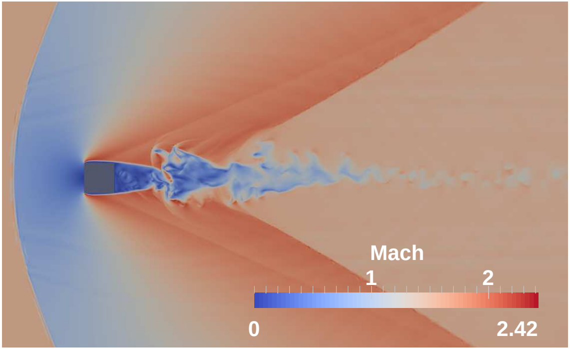


Figure : The entropy and Mach number on shock-cylinder interaction

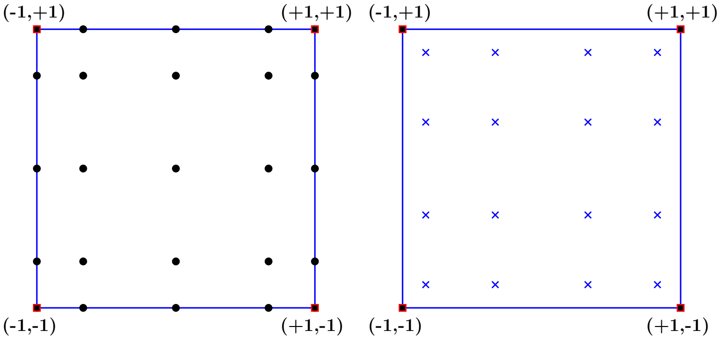
Entropy-Stable Spectral Collocation (Fisher, Parsani, Yamaleev)



(a) Mach number; $\Delta M = 0.0095$.

Figure : Flow past 3D square cylinder at $Re_{\infty} = 10^4$ and $M_{\infty} = 1.5$; fourth-order accurate, no explicit stabilization.

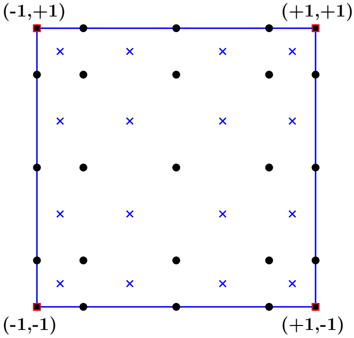
Generalizations of SSDG: Alternative collocation points (Parsani)



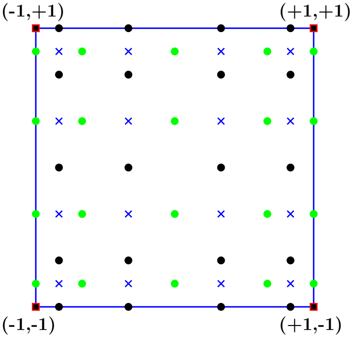
(a) Conventional $LGL \otimes LGL$ (b) Generalized $LG \otimes LG$.

Figure : Conventional LGL and Generalized Gauss 2D tensor product.

Staggered Grid Operators: Extension to 2D



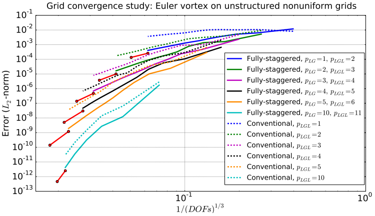
(a) Fully-staggered.



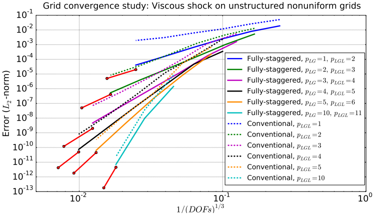
(b) Semi-staggered.

Figure : Fully- and semi-staggered 2D tensor product elements.

Strange Grids: LGL-3D VS. Staggered Gau -> LGL



(a) Euler Vortex



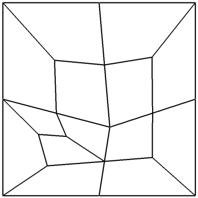
(b) Viscous Shock

Taylor Green 3D Vortex: Staggered Vs. Conventional

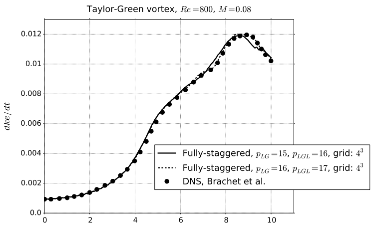
Initial condition:

$$
\begin{aligned}
u_1 &= V_0 \sin\left(\frac{x_1}{L}\right) \cos\left(\frac{x_2}{L}\right) \cos\left(\frac{x_3}{L}\right), \\
u_2 &= -V_0 \cos\left(\frac{x_1}{L}\right) \sin\left(\frac{x_2}{L}\right) \cos\left(\frac{x_3}{L}\right), \qquad u_3 = 0, \\
p &= p_0 + \frac{\rho_0 V_0^2}{16}\left[\cos\left(\frac{2x_1}{L}\right) + \cos\left(\frac{2x_2}{L}\right)\right]\left[\cos\left(\frac{2x_3}{L}\right) + 2\right]
\end{aligned}
\tag{1}
$$

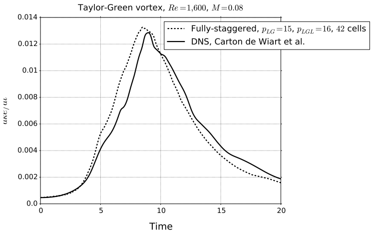
Pathological Grid: (Torture)



Taylor Green 3D Vortex: Staggered/Conventional (cont)

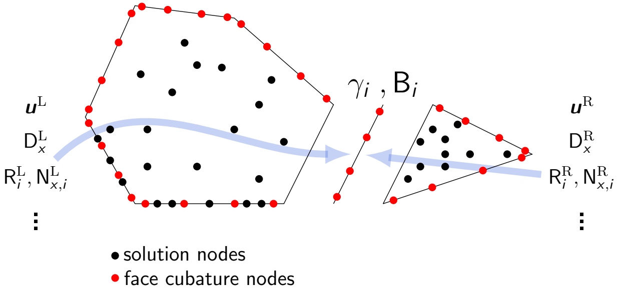


(c) Re=800



(d) Re=1,600

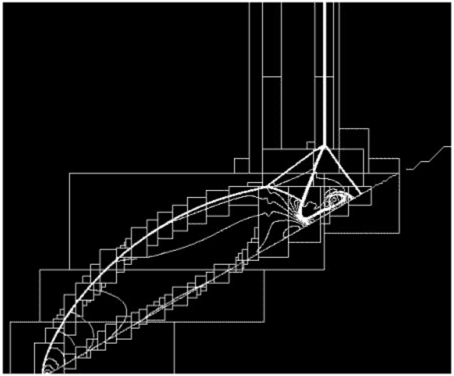
Multi-Dimensional Extensions of SBP (Del Rey Fernandez, Hicken, Crean, Zingg)



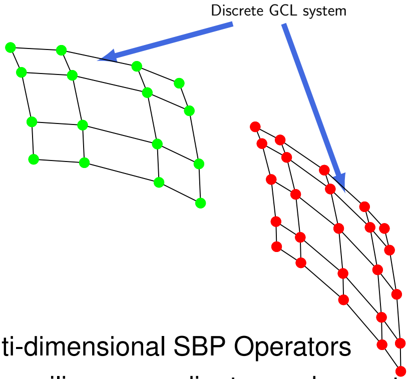
- Distinct volume and surface nodes (in general)
- Interpolate to surfaces, with SAT coupling
- Standard Stability theory with numerical metric terms
- Generalized to any shape (. . .)

Non-Conforming Interfaces

The Target Application: Adaptive Mesh H-Refinement (AMR)



Non-Conforming Interfaces: P-Refinement



- Switch to multi-dimensional SBP Operators
- Transform to curvilinear coordinates and operators
- Construct SBP Operators at Non-Conforming Interface
- Rederive computational metrics
- Prove accuracy and entropy stability

Re-tooling SBP-SAT Entropy Stability

Consider 2D set of points $\mathbf{X}_{xy} \ = \ [(x_i, y_i)]_{i=1}^{N}$, and monomial basis

$$\mathcal{S}_{mn} \ = \ x^m y^n, \quad 0 \leq m+n \leq p$$

and their projection onto the grid $\mathbf{X}_{xy}$ as follows:

$$\mathcal{S}_{mn}(\mathbf{X}_{xy}) = \left(s_{mn}(x_1, y_1), \ldots, s_{mn}(x_N, y_N)\right)^{\top},$$
$$\mathcal{S}'_{mn}(\mathbf{X}_{xy}) = \left(s'_{mn}(x_1, y_1), \ldots, s'_{mn}(x_N, y_N)\right)^{\top}.$$

Definition

$\mathcal{D}_x$ is an SBP approx of $\frac{\partial}{\partial x}$ at $\mathbf{X}_{xy}$ if

- $\mathcal{D}_x \ = \ \mathcal{P}^{-1}\mathcal{Q}_x \ , \ \mathcal{Q}_x + \mathcal{Q}_x \ = \ \mathcal{B}_x \ , \ \mathcal{P} = \mathcal{P}^T \ , \ \zeta^{\top}\mathcal{P}\zeta > 0 \ , \quad \zeta \neq \mathbf{0},$
- $\mathcal{B}_x = {\mathcal{B}_x}^T$ and $\mathcal{S}_{mnk}^{\ T}\mathcal{B}_x\mathcal{S}_{mn\ell} \ = \ \oint_\Gamma \ \mathcal{S}_{mnk}\,\mathcal{S}_{mn\ell}\,\vec{n}_x\, d\Gamma$,
- $\mathcal{D}_x\mathcal{S}_{mn} = \mathcal{S}'_{mn}$, $0 \leq m+n \leq p$ or equivalently $\sum_{\ell=1}^{N} q_{\ell k} x_k^m y_k^n = \mathcal{P}_{(i)(i)}\, m\, x_i^{m-1} y_i^n$, $0 \leq m+n \leq p$.

Curvilinear Transformation: Continuous Coordinates

Transform from physical to computational coordinates

$$J\frac{\partial}{\partial x_\ell} = J\frac{\partial \xi_k}{\partial x_\ell}\frac{\partial}{\partial \xi_k} = J(\xi_k)_{x_\ell}\frac{\partial}{\partial \xi_k} \quad ; \quad J = Det\left(\frac{\partial \mathbf{x}}{\partial \xi}\right) \quad ,$$

with index sums implied on k.

The transformed compressible N-S eqns become

$$\begin{aligned}(Jq)_t + \left[J(\xi_k)_{x_\ell}(f_\ell - f_\ell^{(v)})\right]_{\xi_k} = (f_\ell - f_\ell^{(v)})\left[J(\xi_k)_{x_\ell}\right]_{\xi_k} = 0, \\ Bq = g_b, \quad \xi \in \partial\Omega(\xi), \quad t \in [0,\infty), \\ q(x,0) = g_0(x), \quad \xi \in \Omega(\xi),\end{aligned} \tag{2}$$

The GCL terms $\left[J(\xi_k)_{x_\ell}\right]_{\xi_k}, \ell = 1,2,3$ on the right-hand-side of equation (2) are identically zero at the continuous level.

Curvilinear Transformation: Discrete Coordinates

- Thomas(1979),Visbal(2002) construct discrete metric terms as

$$[J(\xi_k)_{x_\ell}]_{\xi_k} \;=\; +\mathcal{D}_{\xi_{\ell+2}}[\mathcal{D}_{\xi_{\ell+1}}(x_{k+1})][x_{k+2}]\mathbf{1} - \mathcal{D}_{\xi_{\ell+1}}[\mathcal{D}_{\xi_{\ell+2}}(x_{k+1})][x_{k+2}]\mathbf{1} \quad , \tag{3}$$

  and discretely satisfy $\mathcal{D}_{\xi_k}[J(\xi_k)_{x_\ell}]\mathbf{1} \;=\; 0 \quad , \quad i = 1,2,3 \quad .$

- Contravariant compressible Navier-Stokes equations become

$$\begin{gathered}\hat{q}_t + \sum_{k=1}^{3} \mathcal{P}_{\xi_k}^{-1}\Delta_{\xi_k}[\hat{\bar{\mathbf{f}}}_k \;-\; \hat{\bar{\mathbf{f}}}_k^{(v)}] \;=\; \sum_{k=1}^{3} \mathcal{P}_{\xi_k}^{-1}[\hat{\mathbf{g}}_k^{(BC)} + \hat{\mathbf{g}}_k^{(Int)}], \quad x \in \Omega, \quad t \in [0,\infty), \\ Bq = g_b, \quad x \in \partial\Omega, \quad t \in [0,\infty), \\ q(x,0) = g_0(x), \quad x \in \Omega,\end{gathered} \tag{4}$$

  with

$$\hat{\mathbf{q}} \;=\; [J]\mathbf{q} \quad ; \quad \hat{\mathcal{D}}_{\xi_1} \;=\; \mathcal{P}^{-1}{}_{\xi_1}\mathcal{Q}_{\xi_1} \;=\; \mathcal{P}^{-1}{}_{\xi_1}\Delta_{\xi_1}\mathcal{I}_{\xi_1}$$

Curvilinear Conservation and Stability: Theorem

- High-order, contravariant, entropy conservative flux $\widehat{\overline{f}}_k^{(S)}$:

$$\widehat{\overline{f}}_k^{(S)}|_i = \sum_{s=i+1}^{N} \sum_{r=1}^{i} 2q_{(r,s)} \sum_{\ell=1}^{3} \overline{f}_S^{\ell}(\mathbf{q}_r, \mathbf{q}_s) \frac{[J(\xi_k)_{x_\ell}]_r + [J(\xi_k)_{x_\ell}]_s}{2} \tag{5}$$

where $\overline{f}_S^{\ell}(\mathbf{q}_\ell, \mathbf{q}_k)$ is two-point non-dissipative function satisfying

$$(w_r^\top - w_s^\top)\overline{f}_S^{\ell}(\mathbf{q}_r, \mathbf{q}_s) = \psi_r^\ell - \psi_s^\ell. \tag{6}$$

- The high-order, contravariant, entropy conservative flux satisfies an additional local entropy consistency property

$$W\mathcal{P}_k^{-1}\Delta_{\xi_k}\widehat{\overline{\mathbf{f}}}_k^{(S)} = \mathcal{P}_k^{-1}\Delta_{\xi_k}\widehat{\overline{\mathbf{F}}}_k^{(S)} = \frac{\partial F(\mathbf{q})}{\partial \xi_k} + \mathcal{T}_p \quad , \tag{7}$$

where p is the order of the truncation error $\mathcal{T}$.

Curvilinear Conservation and Stability: Proof

- Expanding yields

$$\sum_{k=1}^{3} W\mathcal{P}_k^{-1}\Delta_{\xi_k}\widehat{\bar{\mathbf{f}}}_k^{(S)} = \sum_{k=1}^{3}\mathcal{P}_k^{-1}\sum_{j=1}^{N}\sum_{\ell=1}^{3} 2q_{ij}^k w_i^\top \bar{\mathbf{f}}_k^\ell \frac{[J(\xi_k)_{x_\ell}]_i + [J(\xi_k)_{x_\ell}]_j}{2} \quad (8)$$

- Adding / subtracting w_j in equation (8), yields

$$= \sum_{k=1}^{3}\mathcal{P}_k^{-1}\sum_{j=1}^{N}\sum_{\ell=1}^{3} 2q_{ij}^k \left[\frac{(w_i^\top + w_j^\top)}{2} + \frac{(w_i^\top - w_j^\top)}{2}\right] \bar{\mathbf{f}}_k^l \frac{[J(\xi_k)_{x_\ell}]_i + [J(\xi_k)_{x_\ell}]_j}{2}$$

$$= \sum_{k=1}^{3}\mathcal{P}_k^{-1}\sum_{j=1}^{N}\sum_{\ell=1}^{3} 2q_{ij}^k \left[\frac{(w_i^\top + w_j^\top)}{2}\bar{\mathbf{f}}_k^\ell + \frac{(+\psi_i^\ell - \psi_j^\ell)}{2}\right] \frac{[J(\xi_k)_{x_\ell}]_i + [J(\xi_k)_{x_\ell}]_j}{2} \quad (9)$$

- Consistency and GCL terms used to manipulate into final form

$$= \sum_{k=1}^{3}\mathcal{P}_k^{-1}\sum_{j=1}^{N}\sum_{\ell=1}^{3} 2q_{ij}^k \left[\frac{(w_i^\top + w_j^\top)}{2}\bar{\mathbf{f}}_k^\ell - \frac{(\psi_i^\ell + \psi_j^\ell)}{2}\right] \frac{[J(\xi_k)_{x_\ell}]_i + [J(\xi_k)_{x_\ell}]_j}{2}$$

$$= \sum_{k=1}^{3}\mathcal{P}_k^{-1}\Delta_{\xi_k}\widehat{\bar{\mathbf{F}}}_k^{(S)} \quad . \quad (10)$$

"Intuitive" SBP Non-Conforming interface operator

- "Disconnected" $\bar{\mathcal{D}}_x$ on combined domain

$$\bar{\mathcal{D}}_x = \mathcal{P}_x \bar{\mathcal{Q}}_x = \begin{bmatrix} ({\mathcal{P}^L}^{-1} \mathcal{Q}^L) \otimes \mathcal{I}^L & 0 \\ 0 & ({\mathcal{P}^H}^{-1} \mathcal{Q}^H) \otimes \mathcal{I}^H \end{bmatrix} ,$$

- SAT Penalty terms at block 2x2 interface

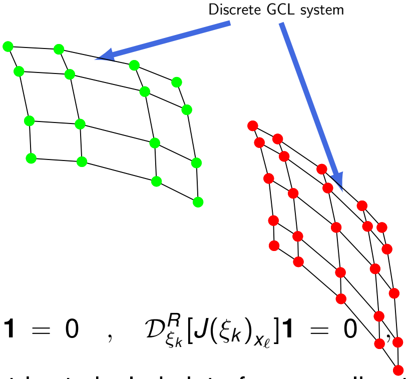
$$\frac{1}{2} \begin{bmatrix} \mathcal{P}^L & 0 \\ 0 & -\mathcal{P}^H \end{bmatrix} + \frac{1}{2} \begin{bmatrix} -\mathcal{P}^L & \mathcal{P}^L \mathcal{I}_{H2L} \\ -\mathcal{P}^H \mathcal{I}_{L2H} & \mathcal{P}^H \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 0 & {\mathcal{I}_{L2H}}^\top \mathcal{P}^H \\ -\mathcal{P}^H \mathcal{I}_{L2H} & 0 \end{bmatrix} .$$

- Combined operator satisfies the following structural constraints

$$\mathcal{D}_x = \mathcal{P}_x \mathcal{Q}_x \quad ; \quad \mathcal{Q}_x + {\mathcal{Q}_x}^T = \mathcal{B}_x .$$

- But in general $\mathcal{D}_{\xi_k}[J(\xi_k)_{x_\ell}]\mathbf{1} \neq 0 \quad , \quad i = 1, 2, 3 \quad .$

Modifying the Metrics



- begin with

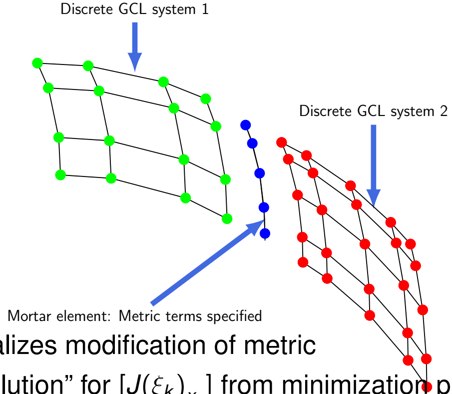
$$\mathcal{D}^L_{\xi_k}[J(\xi_k)_{x_\ell}]\mathbf{1} \;=\; 0 \quad , \quad \mathcal{D}^R_{\xi_k}[J(\xi_k)_{x_\ell}]\mathbf{1} \;=\; 0 \quad , \quad \ell = 1,2,3 \quad (11)$$

- modify the metrics to include interface coupling terms

$$\mathcal{D}^L_{\xi_k}[J(\xi_k)_{x_\ell}]\mathbf{1} \;=\; \phi^{L-R} \,,\; \mathcal{D}^R_{\xi_k}[J(\xi_k)_{x_\ell}]\mathbf{1} \;=\; \phi^{R-L} \,,\; \ell = 1,2,3 \quad (12)$$

with ϕ the appropriate interface coupling terms

Simplifying My Life



- Mortar localizes modification of metric
- “optimal solution” for $[J(\xi_k)_{x_\ell}]$ from minimization problem
  $a_m^k \;=\; a_{m,target} - (\mathcal{M}^k)^\dagger(\mathcal{A}a_{m,target}^k - b_m^k) \quad , \quad m = 1,2,3 \quad \forall k$
- Moore-Penrose pseudo inverse $(\mathcal{M}^k)^\dagger \;=\; \mathcal{V}(\Sigma^k)^\dagger(\mathcal{U})^\top$

Legendre Spectral Collocation: Interpolation

On interval $-1 \le x \le 1$, define discrete points

$$\tilde{\mathbf{x}} = \left(\widetilde{x}_1, \widetilde{x}_2, \cdots, \widetilde{x}_{M-1}, \widetilde{x}_M\right)^\top, \; \widetilde{x}_0 \le \widetilde{x}_1, \widetilde{x}_2, \cdots, \widetilde{x}_{M-1}, \widetilde{x}_M \le \widetilde{x}_{M+1};$$

$$\mathbf{x} = \left(x_1, x_2, \cdots, x_{N-1}, x_N\right)^\top, \; -1 \le x_1, x_2, \cdots, x_{N-1}, x_N \le 1.$$

- Recall form of interface terms (Mortar or otherwise)

$$\frac{1}{2}\begin{bmatrix} \mathcal{P}^L & 0 \\ 0 & -\mathcal{P}^H \end{bmatrix} + \frac{1}{2}\begin{bmatrix} -\mathcal{P}^L & \mathcal{P}^L\mathcal{I}_{H2L} \\ -\mathcal{P}^H\mathcal{I}_{L2H} & \mathcal{P}^H \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 0 & {\mathcal{I}_{L2H}}^\top\mathcal{P}^H \\ -\mathcal{P}^H\mathcal{I}_{L2H} & 0 \end{bmatrix}$$

- “Magic” interpolation operators exchanging data

$$\begin{aligned} \mathcal{P}^L\mathcal{I}_{H2L} &= \mathcal{R}, \\ \mathcal{P}^H\mathcal{I}_{L2H} &= \mathcal{R}^\top, \\ \mathcal{P}^L\mathcal{I}_{H2L} &= {\mathcal{I}_{L2H}}^\top\mathcal{P}^H, \end{aligned} \tag{13}$$

- Suboptimal; p-1

Accuracy: Curvilinear Non-Conforming Operators

Supersonic Vortex with measure zero interface

- Measure zero set? Gustafsson?
- testing continues

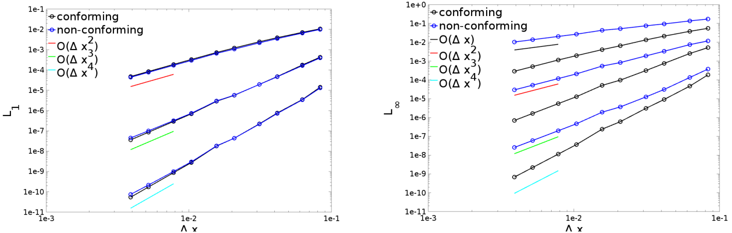


Figure : Convergence in L_1 and L_∞.

Conclusions

- Four classes of entropy stable algorithms Compressible NS
  - Finite-Difference: WENO4
  - Spectral collocation (LGL) on hexahedral Brick elements
  - Spectral collocation (Gau-LGL) on hexahedral Brick elements
  - Extension to arbitrary simplices (Tet, polygon, . . .)
- Wrapping up non-conforming interface theory
  - p-refinement -> h-refinement
  - Requires precise restriction/prolongation interpolation pair
  - Modification of GCL terms simplifed via Mortar
  - Sub-optimal convergence $p + \frac{1}{2}$ in L_2
- Future: Petsc
  - Mesh handling infrastructure (DMPLEX)
  - Load balanced AMR through P4est
- Almost there Marshal!
  - Semi-discrete and continuous stability theory (nearly) equivalent

Thank you for your attention.

PETSC

PETSc: Portable, Extensible Toolkit for Scientific computations

- Mesh handling infrastructure (DMPLEX)
  - Load balanced AMR through P4est
  - Interfaces with many different mesh formats
  - Handling of mesh ghost cells transparent to the user
- Non-Conformal interfaces:
  - tree structure for subset-superset relationships with “reference tree”
  - hanging nodes handled “under the hood”
- ODE solvers (TS)
  - Implicit and explicit Runge-Kutta
  - Adaptive time stepping
- Nonlinear solvers (SNES)
- Krylov solvers (KSP)

High performance implementation of the algorithm

- Higher order methods are cache-friendly and compute bound, suitable for future exascale architectures
- Exploit all levels of parallelism
  - Distributed memory inter-node parallelization
  - Shared memory intra-node parallelization
  - Exploit vector units in modern processors and co-processors
- Separate user-defined physics from lower level computational kernels associated with the discretization scheme
- Reuse the infrastructure to perform acoustics (CAA) and CEM simulations
- Open source distribution