Nonlinear Stability, Algorithm Optimization, and Monolithic Methods

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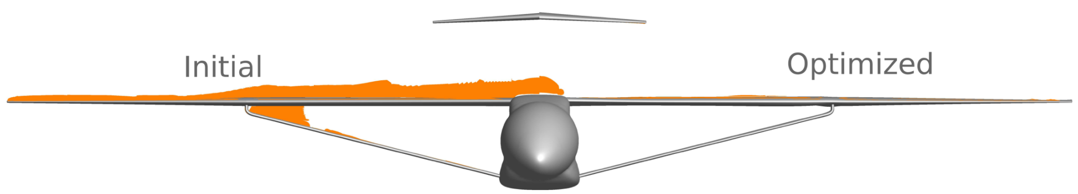
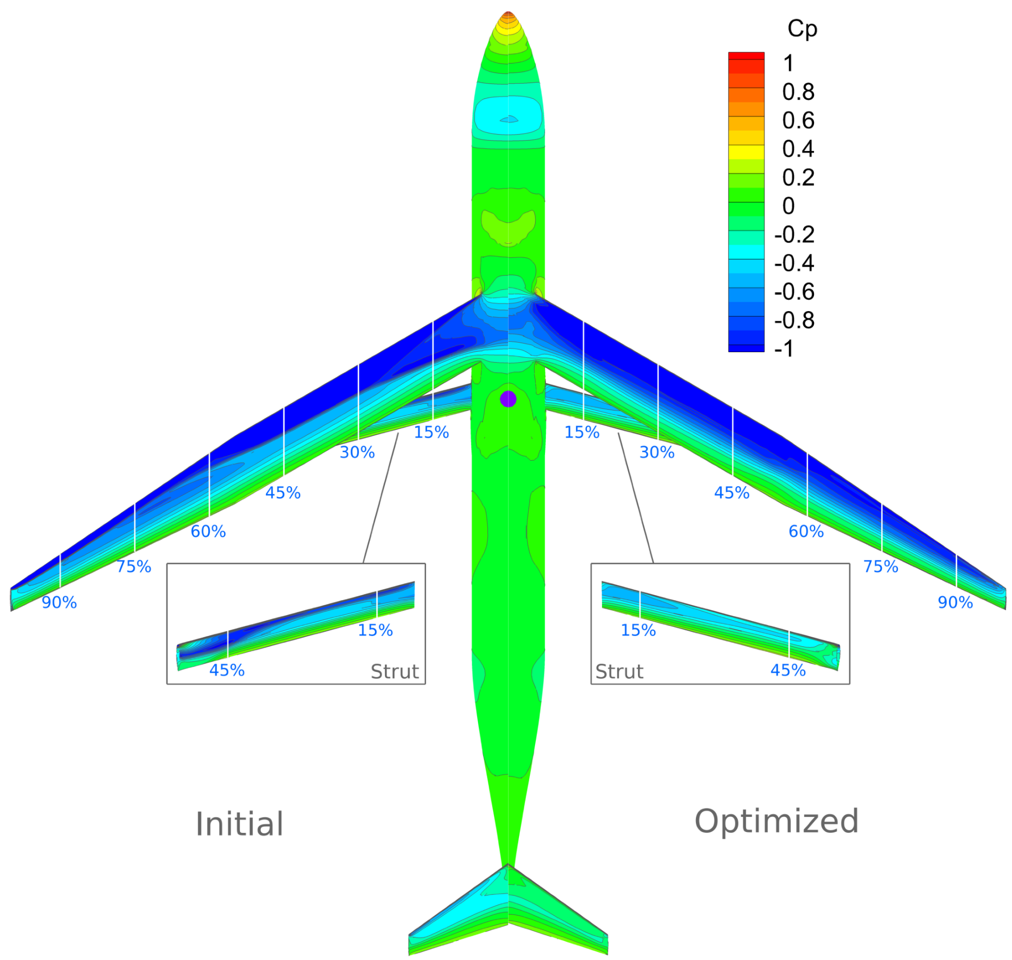
Outline

- Examples of my research
    - aerodynamic shape optimization, turbulent flow control via synthetic jets
- Nonlinearly stable methods
    - multidimensional summation-by-parts operators (Crean et al., JCP 2018)
- Designing an algorithm through numerical optimization
    - implicit Runge-Kutta methods (Boom and Zingg, JCP 2018)
- Monolithic methods for multi-physics analysis and optimization
    - aerostructural analysis and optimization (Zhang and Zingg, AIAA J. 2018)

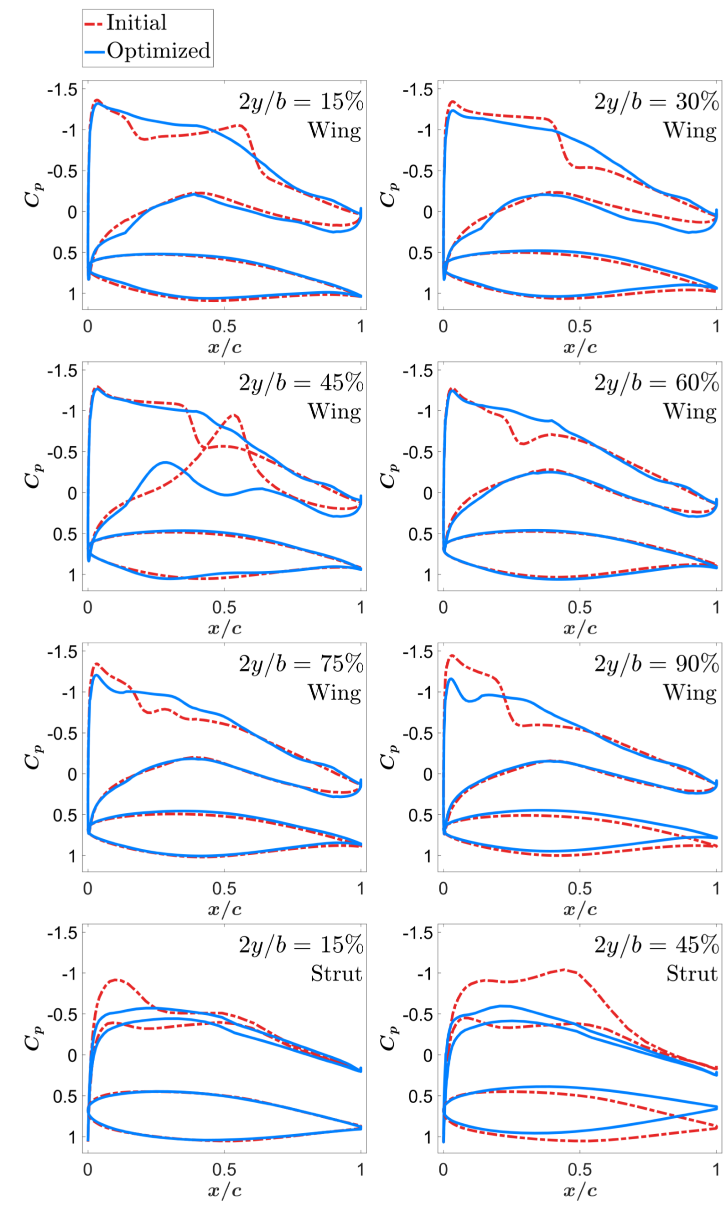
Aerodynamic Shape Optimization of a Regional-Class Strut-Braced Wing Aircraft



Shock surfaces



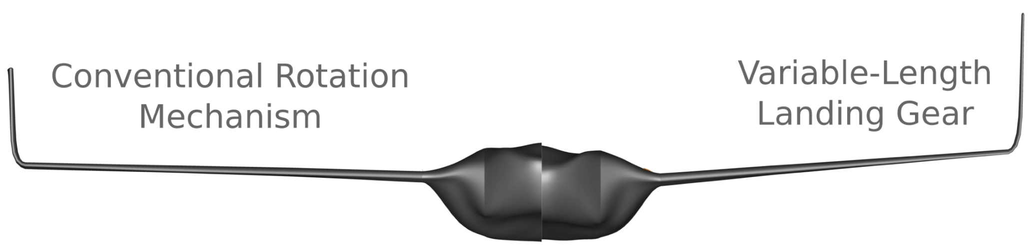
Surface pressure contours



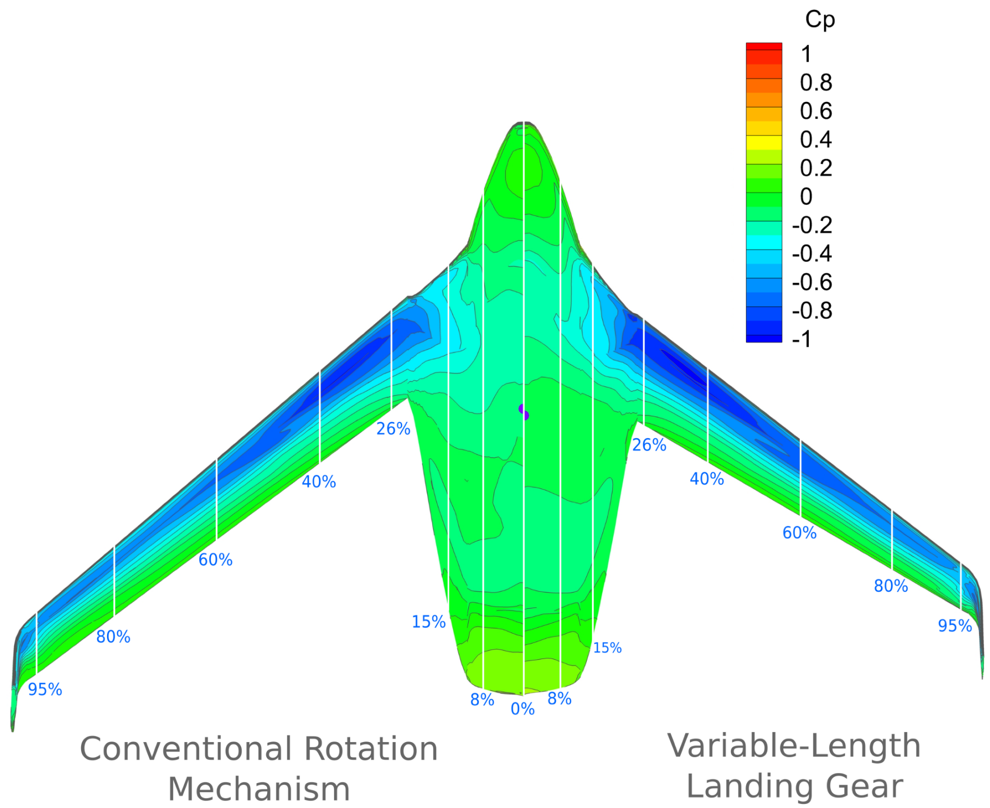
Pressure distributions

- 7.6% block fuel reduction relative to conventional aircraft for 500 nm mission
  - conventional fuselage and empennage reduces risk and development costs

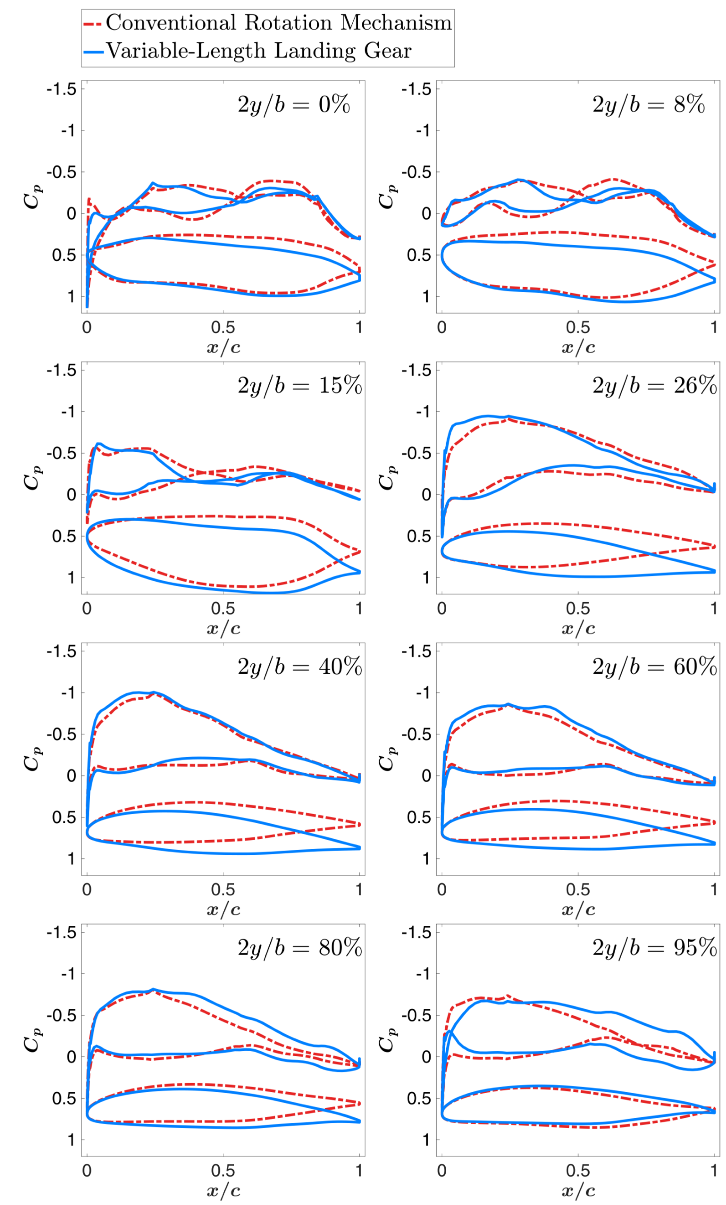
Aerodynamic Shape Optimization of a Regional-Class Hybrid Wing-Body Aircraft



Shock surfaces (absent)



Surface pressure contours

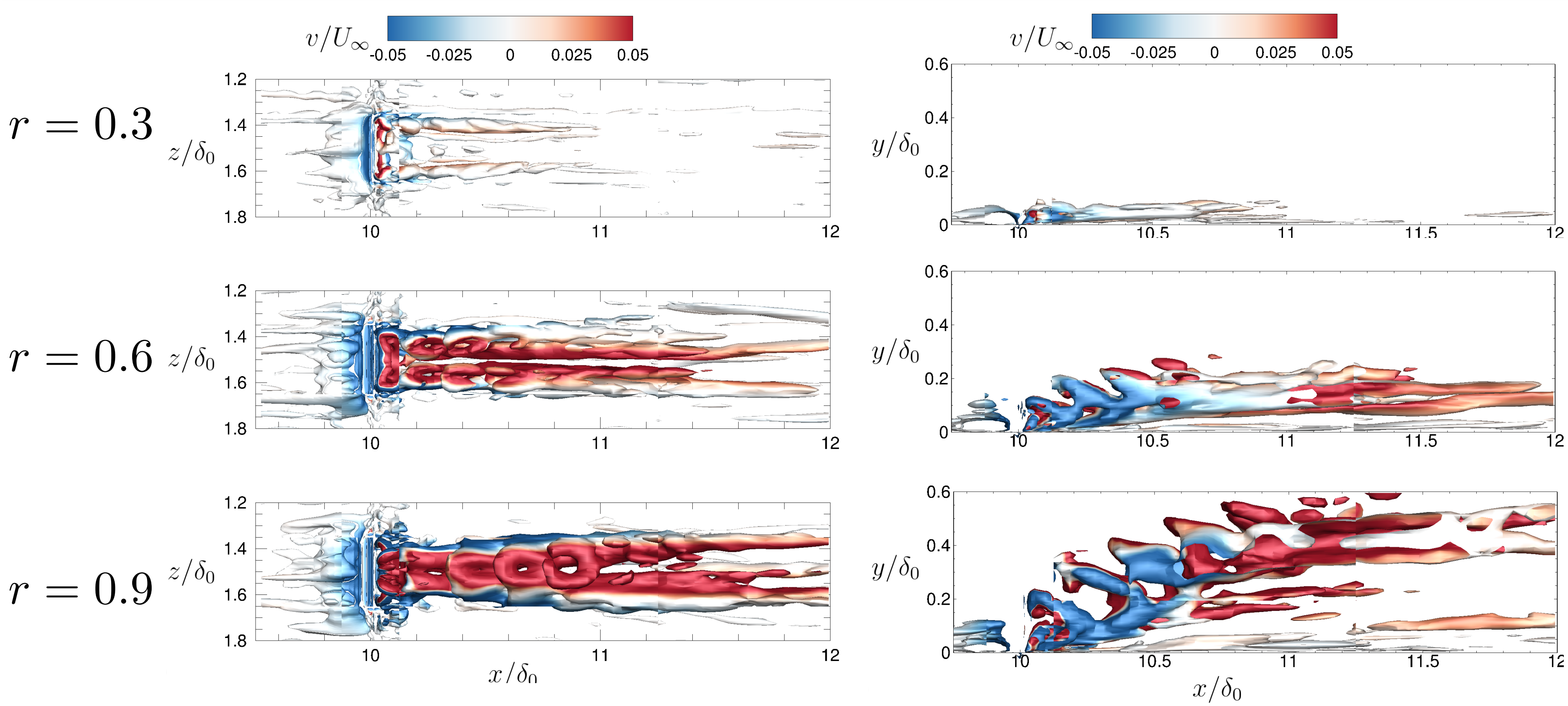


Pressure distributions

- Substantial improvement in energy efficiency relative to conventional aircraft
    - 11-16% block fuel burn improvement for 500 nm mission

Simulation of Synthetic Jet in Crossflow

Vortical Structures in Crossflow – $\mathrm{St}_\infty = 0.1$



- Quasi-steady streamwise vortices far downstream
- Double and single declined vortex rings with increasing r
- Penetrate deeper than $\mathrm{St} = 0.05$ only at $r = 0.9$

CFD in Aeronautics: Future Needs

- Extensive use of multidisciplinary analysis and optimization in design and development
  - requires efficient and robust methods for solving the steady Reynolds-averaged Navier-Stokes equations coupled to FEM structural model
  - increasing need for time-accurate simulations for off-design conditions such as buffet and flutter
  - scale-resolving simulations needed for some conditions
- Increasing need for scale resolving simulations for research into advanced concepts such as active flow control
  - intriguing drag reduction results have been obtained at low Reynolds numbers
  - scale-resolving simulations of comparable physical phenomena at flight Reynolds numbers requires substantial improvements in algorithms

Nonlinear stability, algorithm optimization, and monolithic methods

- Nonlinear stability
  - potential for improved robustness of algorithms for CFD
  - particularly relevant for high-order methods and scale-resolving simulations
- Algorithm optimization
  - enables improvements in efficiency
  - enables trade-off studies and tailoring of algorithms to application classes
- Monolithic methods
  - enable improved robustness and efficiency for coupled multi-physics problems in analysis and optimization

Nonlinear Stability: Importance of Provable Stability

- Most numerical algorithms for CFD today are not provably stable for the problems to which they are applied
- When a solution diverges it can be difficult to ascertain why
- Numerical dissipation is typically added to overcome any instabilities
- The amount of dissipation needed can be difficult to ascertain - hence excessive dissipation is often used
- Provably stable methods have the potential to improve reliability & robustness and reduce the degree of user expertise needed to solve complex problems

Nonlinear Stability — Entropy Stability

- Entropy stability provides one approach to developing nonlinearly stable schemes
  - Second Law of Thermodynamics
- Numerous researchers have contributed to the development of entropy stable methods (Tadmor, Carpenter, Fisher, Chan, and many more)
- Considerable progress has been made, but further advances are needed:
  - completely general boundary conditions
  - positivity preservation
  - convergence
  - time-marching methods (relaxation Runge-Kutta methods)
- Entropy stability is not a panacea
  - does not directly address monotonicity preservation (oscillations)
  - importance to solution of steady problems not yet clear
  - balance between robustness and cost

Linear Stability - Continuous PDE

Linear convection equation:

$$\frac{\partial \mathcal{U}}{\partial t} + a\frac{\partial \mathcal{U}}{\partial x} = 0 \,, \qquad x \in [x_L, x_R] \,, \quad t \geq 0$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}||\mathcal{U}||^2 = -a\left[\mathcal{U}^2(x_R,t) - \mathcal{U}^2(x_L,t)\right]$$

$a > 0$

$$\frac{\mathrm{d}}{\mathrm{d}t}||\mathcal{U}||^2 = -a\left[\mathcal{U}^2(x_R,t) - \mathcal{G}^2(t)\right] \leq a\mathcal{G}^2(t)$$

Linear Stability - Semi-Discrete Form Summation-by-Parts Property

$$\mathsf{D} = \mathsf{H}^{-1}\mathsf{Q} \qquad \mathsf{Q} + \mathsf{Q}^T = \mathsf{E} = \begin{bmatrix} -1 & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & 1 \end{bmatrix}$$

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} + a\mathsf{H}^{-1}\mathsf{Q}\boldsymbol{u} = 0 \qquad \boldsymbol{u}^T\mathsf{H}\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = -a\boldsymbol{u}^T\mathsf{Q}\boldsymbol{u}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}||\boldsymbol{u}||_{\mathsf{H}}^2 = -a(u_N^2 - u_1^2)$$

With a SAT to enforce the boundary condition ($a > 0$):

$$\frac{\mathrm{d}||\boldsymbol{u}||_{\mathsf{H}}^2}{\mathrm{d}t} \leq a\mathcal{G}^2$$

Consistent with continuous result

Inviscid Burgers Equation

conservative form:

$$\frac{\partial \mathcal{U}}{\partial t} + \frac{\partial}{\partial x}\left(\frac{1}{2}\mathcal{U}^2\right) = 0\,, \qquad x \in [x_L, x_R]\,, \quad t \geq 0$$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}||\mathcal{U}||^2 = -\frac{1}{3}\mathcal{U}^3|_{x_L}^{x_R} \quad = 0$$

= 0 for periodic boundary conditions

SBP discretization of conservative form:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}||\boldsymbol{u}||_{\mathsf{H}}^2 = -\boldsymbol{u}^T\left[\frac{\mathsf{QU} + \mathsf{UQ}^T}{2}\right]\boldsymbol{u}$$

U and Q do not commute so stability cannot be proven

Inviscid Burgers Equation
Skew-Symmetric (Split) Form

$$\frac{\partial \mathcal{U}}{\partial t} + \frac{1}{3}\frac{\partial}{\partial x}\left(\mathcal{U}^2\right) + \frac{1}{3}\mathcal{U}\frac{\partial \mathcal{U}}{\partial x} = 0$$

SBP discretization of skew-symmetric form:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}||\boldsymbol{u}||_{\mathrm{H}}^2 = -\frac{u_N^3}{3} + \frac{u_1^3}{3}$$

with suitable SAT

$$\frac{\mathrm{d}}{\mathrm{d}t}||\boldsymbol{u}||_{\mathrm{H}}^2 = 0$$

for periodic boundary conditions

Mimics continuous result and provably stable

Euler Equations - Entropy Conservation (Smooth Solutions)

thermodynamic entropy: $s = \ln(p/\rho^{\gamma})$

mathematical entropy: $\mathcal{S} \equiv -\rho s/(\gamma - 1)$

entropy variables: $\mathcal{W} \equiv \dfrac{\partial \mathcal{S}}{\partial \mathcal{U}} = \left[\frac{\gamma - s}{\gamma - 1} - \frac{1}{2}\frac{\rho}{p}(u^2 + v^2), \quad \frac{\rho u}{p}, \quad \frac{\rho v}{p}, \quad -\frac{\rho}{p} \right]^T$

entropy fluxes: $\mathcal{W}^T \dfrac{\partial \mathcal{F}_x}{\partial \mathcal{U}} \equiv \dfrac{\partial \mathcal{G}_x}{\partial \mathcal{U}}, \qquad \text{and} \qquad \mathcal{W}^T \dfrac{\partial \mathcal{F}_y}{\partial \mathcal{U}} \equiv \dfrac{\partial \mathcal{G}_y}{\partial \mathcal{U}}$

$$\int_{\Omega} \mathcal{W}^T \left[\frac{\partial \mathcal{U}}{\partial t} + \frac{\partial \mathcal{F}_x}{\partial x} + \frac{\partial \mathcal{F}_y}{\partial y} \right] d\Omega = 0$$

smooth solutions: $\Rightarrow$ $\dfrac{d}{dt}\displaystyle\int_{\Omega} \mathcal{S}\, d\Omega + \int_{\partial\Omega} \left(\mathcal{G}_x n_x + \mathcal{G}_y n_y\right) d\Gamma = 0.$

Entropy Conservation and Entropy Stability

in general including shock waves (physically relevant solutions):

$$\int_{\Omega} \frac{\partial \mathcal{S}}{\partial t} \, \mathrm{d}\Omega + \sum_{i=1}^{d} \int_{\partial\Omega} \mathcal{G}_{x_i} n_{x_i} \, \mathrm{d}\Gamma \leq 0$$

A bound on entropy ensures an L^2 bound on the solution given that density, pressure, and temperature are all positive (Dafermos, Svard).

An entropy-conservative scheme ensures that entropy is conserved in the interior of the domain, e.g. with periodic boundary conditions.

An entropy-stable scheme ensures that the mathematical entropy is nonincreasing in the interior of the domain, e.g. with periodic boundary conditions.

Ingredients of entropy-conservative and entropy-stable schemes (Fisher & Carpenter, Crean et al.):

- SBP property
- dyadic or two-point entropy-conservative flux functions (e.g. Ismail & Roe)

Entropy-Stable Schemes for Unstructured Grids (Crean et al. 2018)

Extended the work of Fisher and Carpenter to general curved elements building on the multidimensional SBP operators of Hicken et al. (2016)

Entropy-conservative scheme gives (with periodic boundary conditions):

$$\sum_{\kappa=1}^{K} \mathbf{1}^T \mathsf{H}_\kappa \frac{\mathrm{d}\boldsymbol{s}_\kappa}{\mathrm{d}t} = 0.$$

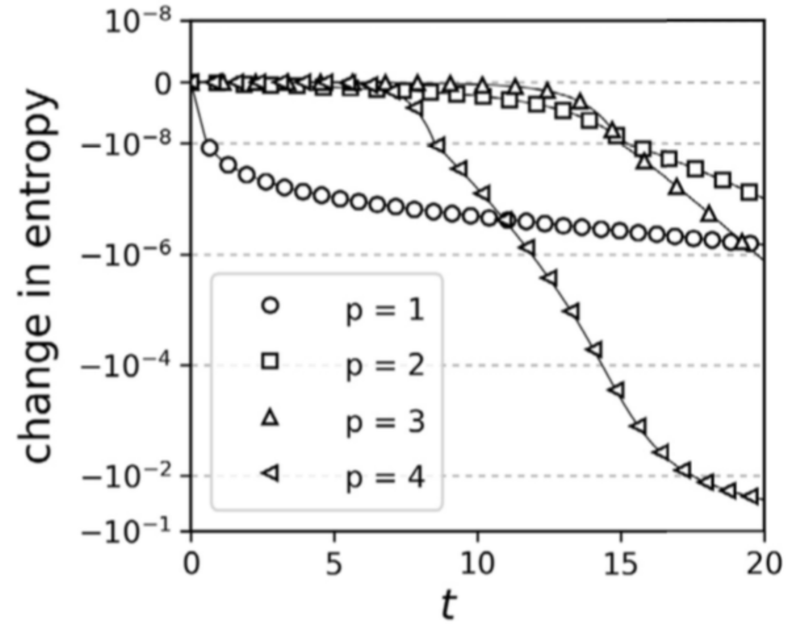
Entropy-stable scheme provides (through dissipative interior penalties):

1. *an order h^p approximation to the differential form of the Euler equations;*
2. *discretely conservative of ρ, ρu, ρv, and e, and;*
3. *entropy stable, in that the entropy is non-increasing in time.*

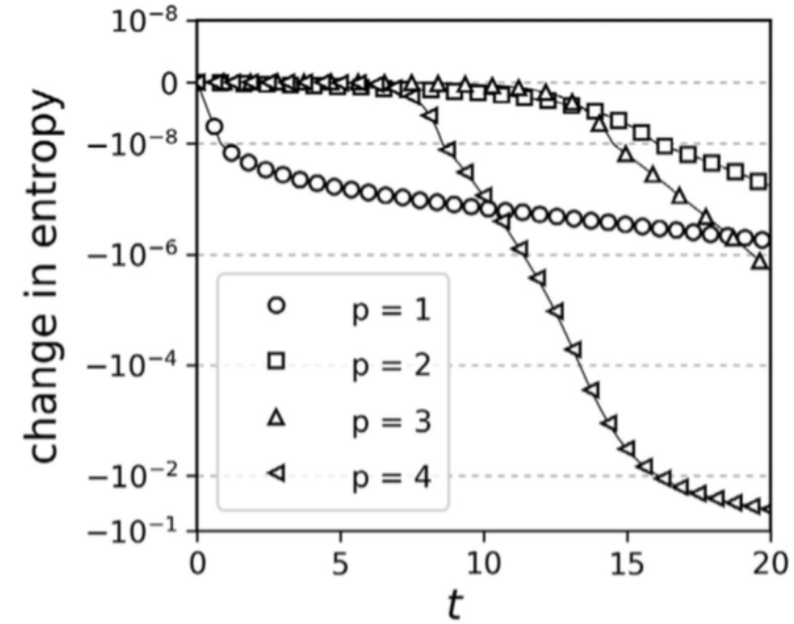
Caveat: requires positivity of thermodynamic quantities

Entropy-Stable Schemes on General Curved Elements: Inviscid Taylor-Green Vortex

Entropy-conservative scheme

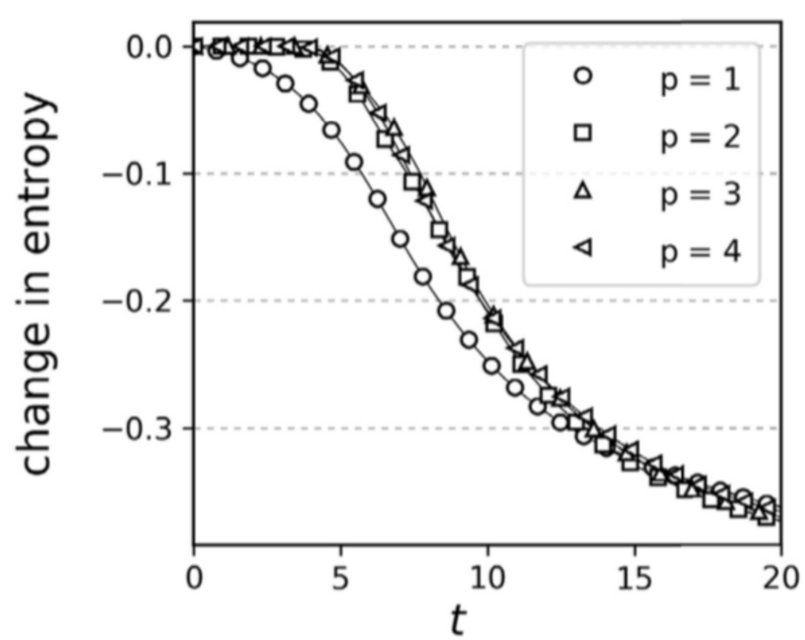


(a) Linear mesh

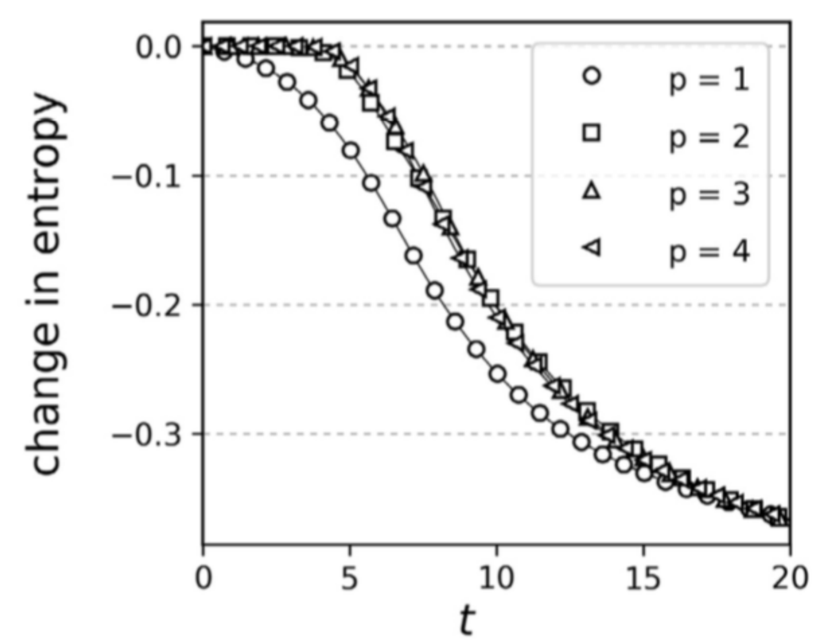


(b) Curvilinear mesh

Entropy-stable scheme



(a) Linear mesh



(b) Curvilinear mesh

“Designing” an Algorithm Through Numerical Optimization

- In engineering design, we typically attempt to find the product that is best in some sense subject to many constraints
  - consequently numerical optimization can play an important role in engineering design, for example in aircraft design
  - the use of optimization enables rigorous trade-off studies
- Why not apply the same approach to the “design” of numerical methods?
  - apply numerical optimization to determine any undetermined coefficients with objective and constraints tailored to a particular application area
  - trade-offs associated with various properties of an algorithm can be evaluated
- From Kennedy and Carpenter’s 2019 review of DIRK methods for ODEs:
  - “Arguably, what is needed are methods that are optimized over a broad spectrum of characteristics. Invariably, requiring one attribute may preclude another; hence, priorities must be established.”

“Designing” an Algorithm Through Numerical Optimization

- Examples
  - “Optimal Diagonal-Norm SBP Operators,” Mattsson, Almquist, Carpenter 2013
  - Runge-Kutta methods: Ketcheson, Parsani, Kennedy/Carpenter, Tsitouras, Vermeire, Bogey/Bailly, Boom/Zingg
  - various authors have chosen undetermined coefficients in spatial schemes to minimize spectral radius
  - Marchildon and Zingg optimized multidimensional SBP operators
- Boom, P.D., and Zingg, D.W., Optimization of High-Order Diagonally-Implicit Runge-Kutta Time-Marching Methods, J. Comp. Phys., 2018
  - presented constrained numerical optimization of linearly and algebraically stable diagonally-implicit Runge-Kutta methods
  - found several methods with advantageous properties

Boom & Zingg: Optimization of High-Order DIRK Methods

- In the construction of high-order implicit Runge-Kutta methods, several coefficients will often remain undetermined after solving the desired order and stability conditions

- At lower orders, optimization of coefficients can be done analytically, but as order is increased the size and complexity of the expressions grow and analytical solution becomes intractable

- Parameters include
  - order of the method (p), number of stages (s), stage order of individual stages (q_i), stiff accuracy (Y/N)

- Objective function combines
  - L_2 principal error norm, spacing of abscissa values (affects numerical solution efficiency), violation of internal and algebraic stability conditions

- Constraints can be selected from
  - A stability, L stability, algebraic stability, internal stability

Boom & Zingg: Optimization of High-Order DIRK Methods

- SDIRK[p,(q_i)](s)X_SA_i
  - order of the method (p), number of stages (s), stage order of individual stages (q_i), X = A/L/Algebraic (stability), SA = stiffly accurate, i = identifier
  - relative efficiency measure: error norm * number of stages^p
- SDIRK[3,(1,2,2)](3)L_14
  - good balance of properties with slightly reduced error norm compared to comparable 3-stage methods in the literature
- SDIRK[3,1](4)L_SA_5
  - most efficient 3rd-order stiffly accurate method found with error norm less than 50% of that of the reference method
- SDIRK[5,1](5)L_02
  - 40% lower error norm than reference method, which is not L stable, but gives up a small increase in violation of algebraic stability conditions and some stage order compared to reference method

Optimization of High-Order DIRK Methods: Lessons Learned

- Efficient new methods have been found
  - despite long history of research on implicit Runge-Kutta methods
  - benefits realized in simulations
- Design space has many local optima
  - virtually impossible to prove that the global minimum has been found
- Optimization approach can be applied to many aspects of numerical methods, including both time-marching methods and spatial discretizations
  - whenever there are a significant number of undetermined coefficients

Monolithic Approach to Aerostructural Analysis and Optimization

- Aerostructural analysis
  - evaluate the performance of a wing under steady turbulent flow conditions, including loads and deflections
  - external shape determines aerodynamic performance (RANS equations)
  - structural layout and sizing determines deflections (FEM model)
  - coupling via load and displacement transfer
- Aerostructural optimization
  - determines external shape and sizes structural components to minimize an objective function (typically drag while accounting for the impact of weight on the drag) while satisfying constraints (such as lift, maximum stress constraint)
  - drag is generally minimized at cruise conditions, while the structure is sized under critical loading conditions

Partitioned and Monolithic Approaches to Analysis

- Partitioned approach
  - solve the flow and structural equations alternately until a self-consistent solution is obtained
  - straightforward to implement (“black box”, “nonintrusive”)
  - straightforward to use a different flow or structural solver
- Monolithic approach
  - solve the multiple disciplines in a fully coupled manner
  - more complex to program, but potentially more efficient and robust
  - advantageous to retain specialized solvers for each discipline (how?)

Aerostructural Optimization Problem

$$
\begin{aligned}
\min_{\mathbf{v}} \quad & & \mathcal{J}(\mathbf{v}, [\mathbf{q}, \mathbf{b}_\Delta, \mathbf{u}]^T)\,, & & \\
\text{subject to:} \quad & & \mathbf{R}_{\text{AS}}(\mathbf{v}, [\mathbf{q}, \mathbf{b}_\Delta, \mathbf{u}]^T) & = 0\,, & \\
& & \mathcal{C}_{\text{eq},i}(\mathbf{v}, [\mathbf{q}, \mathbf{b}_\Delta, \mathbf{u}]^T) & = 0\,, & i = 1, \cdots, n_{\text{eq}} \\
& l_j \leq & \mathcal{C}_{\text{in},j}(\mathbf{v}, [\mathbf{q}, \mathbf{b}_\Delta, \mathbf{u}]^T) & \leq u_j\,, & j = 1, \cdots, n_{\text{in}}
\end{aligned}
$$

- high-dimensional - gradient-based optimization algorithm preferred
- many more design variables than constraints - adjoint method preferred
    - structural stress constraints are aggregated

Aerostructural Analysis Problem

aerostructural residual, including aerodynamics, mesh movement, and structures

$$\mathbf{R}_{\mathrm{AS}} = \begin{bmatrix} \mathbf{R}_{\mathrm{A}}(\mathbf{q}, \mathbf{b}_{\Delta}) \\ \mathbf{R}_{\mathrm{M}\Delta}(\mathbf{b}_{\Delta}, \mathbf{u}) \\ \mathbf{R}_{\mathrm{S}}(\mathbf{q}, \mathbf{b}_{\Delta}, \mathbf{u},) \end{bmatrix} = 0$$

- inexact Newton method

- solve linear system with FGMRES

$$\frac{\partial \mathbf{R}_{\mathrm{AS}}^{(n)}}{\partial [\mathbf{q}, \mathbf{b}_{\Delta}, \mathbf{u}]^{(n)}} \begin{bmatrix} \Delta \mathbf{q} \\ \Delta \mathbf{b}_{\Delta} \\ \Delta \mathbf{u} \end{bmatrix}^{(n)} = \mathbb{A}^{(n)} \boldsymbol{\delta}^{(n)} = -\mathbf{R}_{\mathrm{AS}}^{(n)}$$

coupled Jacobian matrix

$$\mathbb{A} = \begin{bmatrix} \frac{\partial \mathbf{R}_{\mathrm{A}}}{\partial \mathbf{q}} & \frac{\partial \mathbf{R}_{\mathrm{A}}}{\partial \mathbf{b}_{\Delta}} & 0 \\ 0 & \frac{\partial \mathbf{R}_{\mathrm{M}\Delta}}{\partial \mathbf{b}_{\Delta}} & \frac{\partial \mathbf{R}_{\mathrm{M}\Delta}}{\partial \mathbf{u}} \\ \frac{\partial \mathbf{R}_{\mathrm{S}}}{\partial \mathbf{q}} & \frac{\partial \mathbf{R}_{\mathrm{S}}}{\partial \mathbf{b}_{\Delta}} & \frac{\partial \mathbf{R}_{\mathrm{S}}}{\partial \mathbf{u}} \end{bmatrix}$$

Preconditioning of Linear System

point-Jacobi preconditioner

$$\mathbf{w} = \begin{bmatrix} \mathbf{w}_\mathrm{A} \\ \mathbf{w}_\mathrm{M} \\ \mathbf{w}_\mathrm{S} \end{bmatrix} = \begin{bmatrix} c_{\mathrm{scl,A}}^{-1} \mathbf{M}_\mathrm{A}^{-1} r_{\mathrm{scl,A}}^{-1} \mathbf{z}_\mathrm{A} \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ c_{\mathrm{scl,M}}^{-1} \mathbf{M}_\mathrm{M}^{-1} r_{\mathrm{scl,M}}^{-1} \mathbf{z}_\mathrm{M} \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ c_{\mathrm{scl,S}}^{-1} \mathbf{M}_\mathrm{S}^{-1} r_{\mathrm{scl,S}}^{-1} \mathbf{z}_\mathrm{S} \end{bmatrix}$$

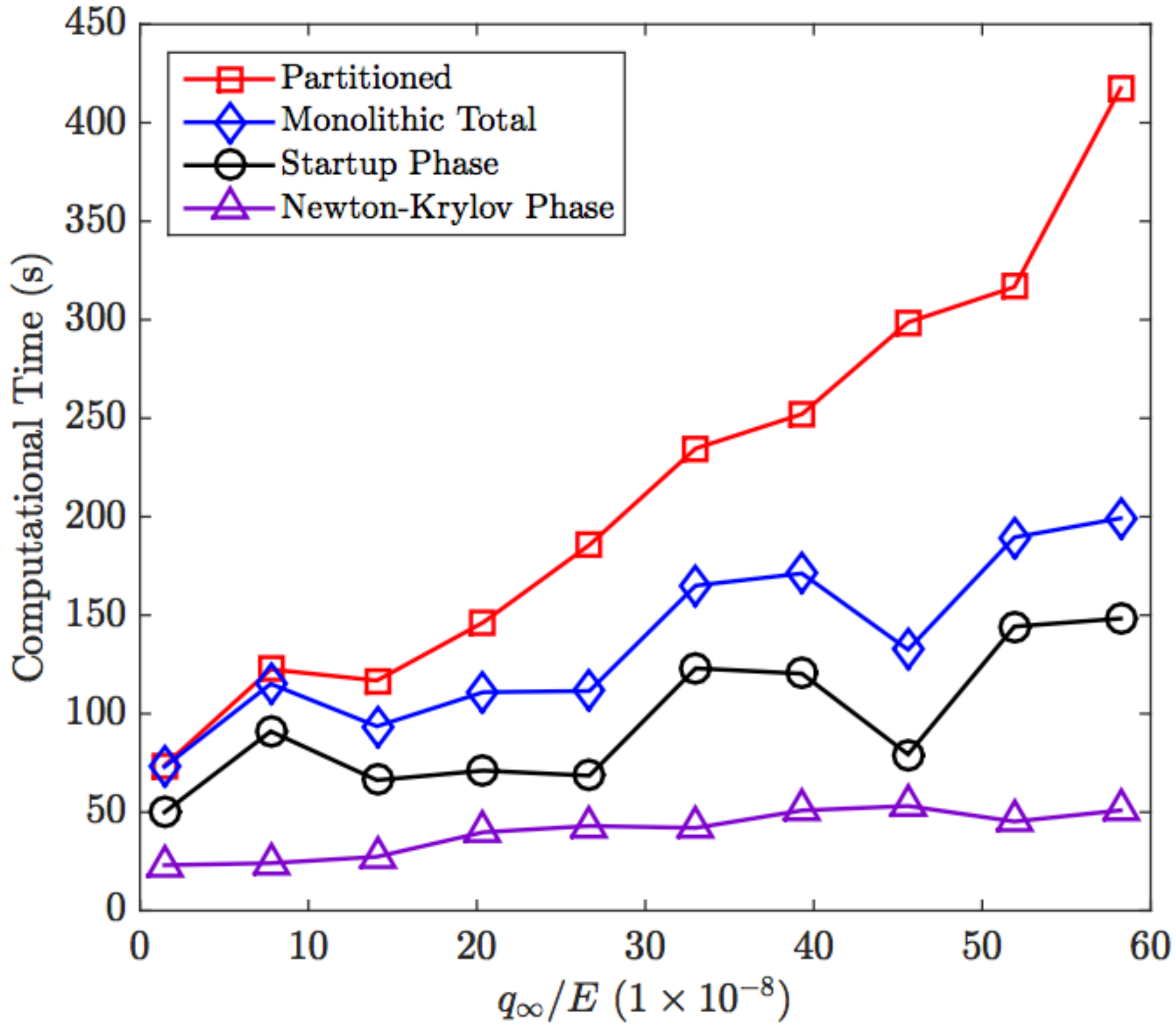
where $$\mathbf{M}_\mathrm{A}^{-1} \approx \left(\frac{\partial \hat{\mathbf{R}}_\mathrm{A}^{(n)}}{\partial \mathbf{q}^{(n)}} \right)^{-1}, \quad \mathbf{M}_\mathrm{M}^{-1} \approx \left(\frac{\partial \hat{\mathbf{R}}_{\mathrm{M}\Delta}^{(n)}}{\partial \hat{\mathbf{b}}_\Delta^{(n)}} \right)^{-1}, \quad \mathbf{M}_\mathrm{S}^{-1} \approx \left(\frac{\partial \mathbf{R}_\mathrm{S}^{(n)}}{\partial \mathbf{u}^{(n)}} \right)^{-1}$$

- use the efficient linear solution technique associated with each discipline as the preconditioner for the associated portion of the system

- the specialization is achieved at the preconditioner level

- Gauss-Seidel approach also possible

Comparison with Partitioned Approach: Analysis



- benefit of monolithic approach increases as the flexibility parameter (coupling) increases

Monolithic Coupled Adjoint Solution

adjoint system

$$\underbrace{\begin{bmatrix} \frac{\partial \mathbf{R}_\mathrm{A}}{\partial \mathbf{q}}^T & 0 & \frac{\partial \mathbf{R}_\mathrm{S}}{\partial \mathbf{q}}^T \\ \frac{\partial \mathbf{R}_\mathrm{A}}{\partial \mathbf{b}_\Delta}^T & \frac{\partial \mathbf{R}_{\mathrm{M}\Delta}}{\partial \mathbf{b}_\Delta}^T & \frac{\partial \mathbf{R}_\mathrm{S}}{\partial \mathbf{b}_\Delta}^T \\ 0 & \frac{\partial \mathbf{R}_{\mathrm{M}\Delta}}{\partial \mathbf{u}}^T & \frac{\partial \mathbf{R}_\mathrm{S}}{\partial \mathbf{u}}^T \end{bmatrix}}_{\mathbb{A}^T} \begin{bmatrix} \mathbf{\Psi}_\mathrm{A} \\ \mathbf{\Psi}_{\mathrm{M}\Delta} \\ \mathbf{\Psi}_\mathrm{S} \end{bmatrix} = \begin{bmatrix} -\frac{\partial \mathcal{J}}{\partial \mathbf{q}}^T \\ -\frac{\partial \mathcal{J}}{\partial \mathbf{b}_\Delta}^T \\ -\frac{\partial \mathcal{J}}{\partial \mathbf{u}}^T \end{bmatrix}$$

- again reuse the efficient linear solution technique associated with each discipline

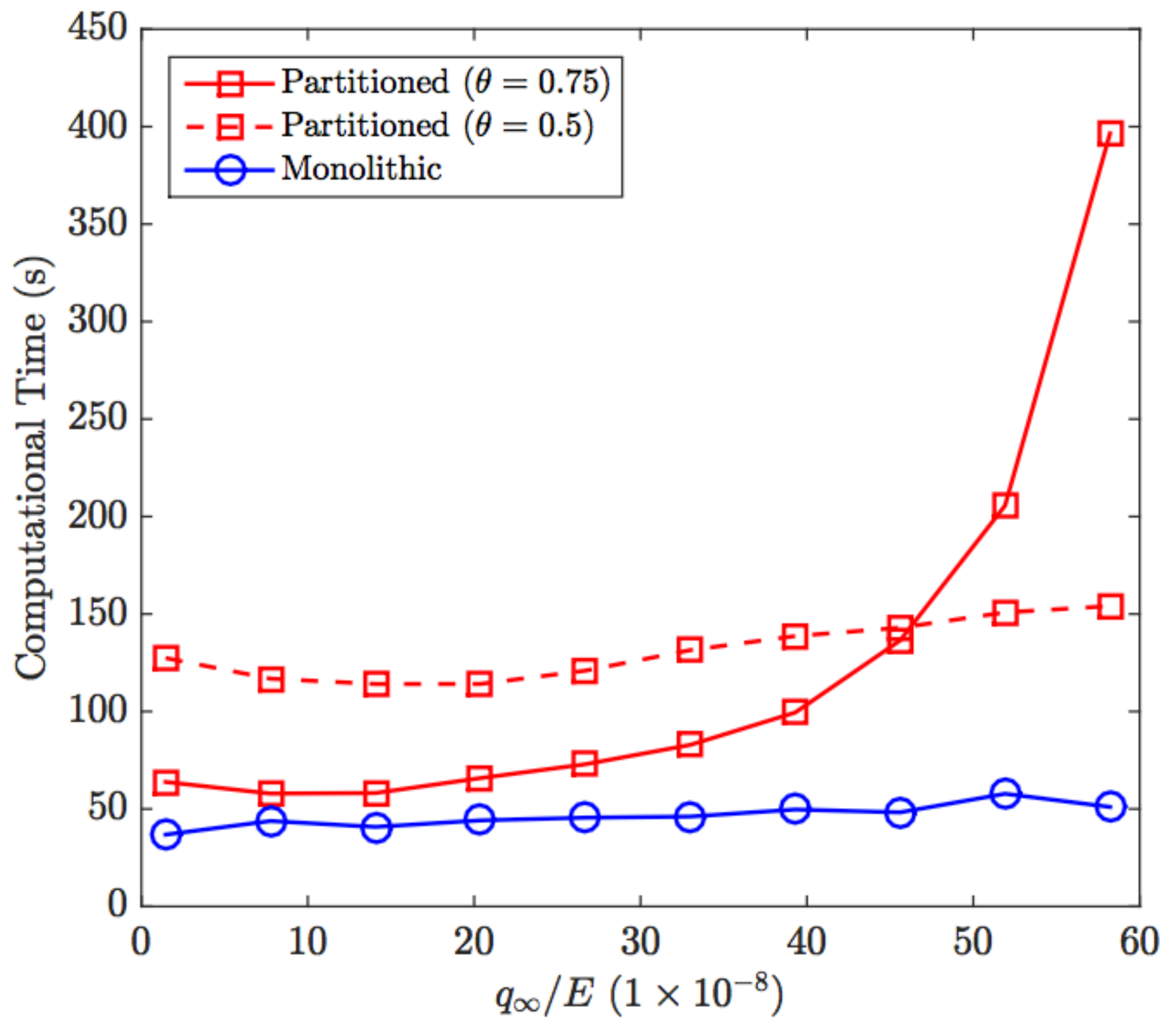
- Gauss-Seidel variant shown

$$\frac{\partial \mathbf{R}_\mathrm{A}}{\partial \mathbf{q}}^T (c_{\mathrm{scl,A}} \mathbf{w}_\mathrm{A}) = r^{-1}_{\mathrm{scl,A}} \mathbf{z}_\mathrm{A} = \hat{\mathbf{z}}_\mathrm{A}$$

$$\frac{\partial \hat{\mathbf{R}}_{\mathrm{M}\Delta}}{\partial \hat{\mathbf{b}}_\Delta}^T (c_{\mathrm{scl,M}} \mathbf{w}_\mathrm{M}) = r^{-1}_{\mathrm{scl,M}} \mathbf{z}_\mathrm{M} - \frac{\partial \mathbf{R}_\mathrm{A}}{\partial \hat{\mathbf{b}}_\Delta}^T (c_{\mathrm{scl,A}} \mathbf{w}_\mathrm{A}) = \hat{\mathbf{z}}_\mathrm{M}$$

$$\mathbf{M}_\mathrm{S} (c_{\mathrm{scl,S}} \mathbf{w}_\mathrm{S}) = r^{-1}_{\mathrm{scl,S}} \mathbf{z}_\mathrm{S} - \frac{\partial \hat{\mathbf{R}}_{\mathrm{M}\Delta}}{\partial \mathbf{u}}^T (c_{\mathrm{scl,M}} \mathbf{w}_\mathrm{M}) = \hat{\mathbf{z}}_\mathrm{S}$$

Comparison with Partitioned Approach: Adjoint Solution



- benefit of monolithic approach again increases as the flexibility parameter (coupling) increases

- monolithic approach is more robust as well

Concluding Remarks

- Nonlinearly stable schemes
  - can potentially greatly improve the robustness of flow solvers
  - many open questions remain to be addressed
- Algorithm optimization
  - can be applied in many contexts to design algorithms for specific properties and to find new and improved algorithms
- Monolithic approach to coupled analysis and optimization problems
  - apply the discipline-specific methods in the preconditioning of the linear system
  - very effective for tightly coupled problems