Recent Developments in FUN3D: Entropy Stable DG-FEM

Mark H. Carpenter, Eric J. Nielsen, and Matteo Parsani
Computational AeroSciences Branch
NASA Langley Research Center

http://fun3d.larc.nasa.gov
Acknowledgments

• Bill Jones, NASA Langley Research Center

• Travis Fisher, Sandia National Lab
  • Previously Purdue Univ PhD student in residence at NASA Langley Research Center
Motivation
CFD Vision 2030 Study: A Path to Revolutionary Computational Aero
NASA/CR-2014-218178: Slotnick, Khodadoust, Alonso, Darmofal, Gropp, Lurie, and Mavriplis

Summary

• Applications
  • “Complex flows with BL transition and smooth body separation”
  • Off-design unsteady simulations (stall prediction)
  • LES and Hybrid RANS-LES models
  • Subsonic, transonic, supersonic

• Next generation numerical algorithms
  • High-order (HO) methods**
  • Low dissipation / dispersion
  • Foundational approaches (high risk / high payoff research)

• Robust automation
  • Routine hands-off convergence in all circumstances
  • Novel robust numerical techniques
    • Entropy-preserving schemes offer possibilities of radical advances

** HO spatial operators are well suited for time-dependent simulations. Error accumulates (spatial, temporal, algebraic).
Vision Statement

A brief history of HO methods
- Kreiss-Oliger, 1972; Gottlieb-Orszag, 1977
- Brisk development in 80’s; Canuto-Hussaini-Quarteroni-Zang, 1987

What happened? Instability happened!
- Informal poll of practitioners: Fragile in real world applications
- ICOSAHOM 2014 (Int. Conf. Spectral & High-Order Methods)
  - 200 papers: 20% mentioned “stability” in title
  - Stab(le)(ility)(ilize) (27 papers)
  - Filter/alias/dissipation (12 papers)
  - Move from experimentation to mathematics!

Vision 2019 (August 18)

The nonlinear equations are stable in nature, as should be their discrete representation.

- Maturation of nonlinear stability theory: Turning the corner
- Growing body of schemes with nonlinear stability proofs

Statement: Achieve robustness of current 2\textsuperscript{nd}-order FV schemes
What’s the Plan?

Entropy Stable Spectral Collocation (plus BCs)
- Three pillars: Stability, accuracy, conservation
  - Conservation form operator: Mass, momentum, energy
    - Secondary invariant: Entropy
  - Applicable for capturing shocks (Rankine-Hugoniot via Lax-Wendroff Thm)

Implement in FUN3D
- Established infrastructure and customer base
- Increasing need for HO capability
  - DNS / LES / DES / URANS
  - Aeroacoustics, electromagnetics
  - Rotorcraft
  - Separated flows, stall
  - Mixing
Compressible Navier-Stokes Equations

\[ q_t + \left( f_i^{(I)} \right)_{x_i} = \left( f_i^{(V)} \right)_{x_i}, \quad x \in \Omega, \quad t \in [0, \infty), \]

\[ q|_{\partial \Omega} = g^{(B)}(x, t), \quad x \in \partial \Omega, \quad q(x, 0) = g^{(0)}(x), \quad x \in \Omega \]

Entropy variables: \( S_q \) with \( S = -\rho s \)

Entropy fluxes: \( F_i = -\rho u_i s \)

Entropy equation:

\[ S_q q_t + S_q \left( f_i^{(I)} \right)_{x_i} = S_t + (F_i)_{x_i} = S_q \left( f_i^{(V)} \right)_{x_i} = \left( w^\top f_i^{(V)} \right)_{x_i} - w_{x_i}^\top \hat{c}_{ij} w_{x_j} \]

Global conservation statement:

\[ \frac{d}{dt} \int_{\Omega} S \, d\mathbf{x} = \left[ w^\top f_i^{(V)} - F_i \right]_{\partial \Omega} - \int_{\Omega} w_{x_i}^\top \hat{c}_{ij} w_{x_j} \, d\mathbf{x} \]
Semi-Discrete Form

\[ S_q q_t + S_q \left( f^{(I)}_i \right)_{x_i} = S_t + (F_i)_{x_i} = S_q \left( f^{(V)}_i \right)_{x_i} = \left( w^\top f^{(V)}_i \right)_{x_i} - w_{x_i}^\top \hat{c}_{ij} w_{x_j} \]

Summation-by-Parts telescoping form:

\[ q_t = P_{x_i}^{-1} \Delta_{x_i} \left( -\bar{f}^{(I)}_i + \bar{f}^{(V)}_i \right) + P_{x_i}^{-1}(g^{(B)} + g^{(In)}) \]

\[ q(x, 0) = g^{(0)}(x), \quad x \in \Omega \]

- \( g^{(B)} \) contains BC data
- \( g^{(In)} \) interface penalty

Semi-discrete entropy estimate (1D):

\[ 1^\top P S_t = w^\top B \hat{c}_{11} D w - 1^\top \Delta F - (Dw)^\top P \hat{c}_{11} (Dw) \]

\[ \frac{d}{dt} \int_\Omega S \, dx = \left[ w^\top f^{(V)}_i - F_i \right]_{\partial \Omega} - \int_\Omega w_{x_i}^\top \hat{c}_{ij} w_{x_j} \, dx \]
Nonlinearly Stable Wall BCs

Need to design robust, nonlinearly stable wall BCs

\[ \mathbf{g}_1^{(B)} = - \left[ \mathbf{f}_1^{(I)} (\mathbf{q}) - \mathbf{f}_1^{sr} \left( \mathbf{q}, \mathbf{g}^{(E)} \right) \right] + \left[ \mathbf{f}_1^{(V)} - \mathbf{f}_1^{(V,B)} \right] + \mathcal{M} \left( \mathbf{w} - \mathbf{g}^{(NS), Vel} \right) \]

- **No penetration**
- **Thermal**
- **No slip**

Inviscid flux penalty: Flip the sign of the normal velocity component
Viscous flux penalty: Prescribe entropy flow $= T x_1 / T$ scales with $Re$
Interior penalty: No-slip condition on the velocity; scales with $Re$
Current Status of High-Order FUN3D
Integration with FUN3D

- Implemented as optional library built on low-level FUN3D components
- Leverages much of FUN3D infrastructure, including:
  - GNU Autotools build infrastructure
  - Pre-processing, MPI communication
  - Complex variable, operator overloading functionalities
  - Dynamic overset grid infrastructure, extended to HO elements
  - Regression/performance testing infrastructure
  - Distribution, user training, and user support infrastructure
- FUN3D owns primal grid; library constructs and owns necessary HO data
- Extensive development for compatible domain decomposition
- Conventional FUN3D visualization options available on primal grid; additional I/O options for HO solution
- FUN3D controls overall process flow and routes into HO library as needed, e.g.:
  - `call ssdc_initiate()
  - `call ssdc_advance_timestep()
  - `call ssdc_write_soln()`
**FUN3D: FEM Basic Features**

Temporal Integrators
- Explicit: 4\textsuperscript{th}-Order low-storage RK; feedback controller
- Implicit: BDF(1)(2)(3) and BDF2opt (backward difference formulae)

Solvers
- Nonlinear: (In)Exact Newton-Krylov
  - Trust-region dogleg globalization
- Linear: Right-preconditioned GMRES
  - Exact Jacobian
  - (B)ILU(0), (B)ILU(k), (B)ILUTP (lexicographic)
  - Domain decomposition via additive Schwarz (halo: 1 element)

High-Order Definition of Geometry
- Interface with geometry model
- FUN3D elasticity mechanics
Verification and Validation
Interior Operator
3D Viscous Shock

- Exact solution exists for N-S
- Convergence study performed on sequence of nested, highly non-uniform grids
Taylor-Green Vortex
Re=1600, $M_\infty=0.1$

Iso-surface of the z-component of vorticity

$t = 0$
$t = 20$
Taylor-Green Vortex
Evolution of Kinetic Energy and Enstrophy

Evolution of the time derivative of the kinetic energy

Evolution of the enstrophy

- $p = 2$ with $128^3$ elements
- $p = 3$ with $96^3$ elements
- $p = 4$ with $64^3$ elements
- Hillewaert et al.; spectral method with $512^3$ elements
• Standard benchmark test case for 2nd high-order workshop (C3.3, “difficult”)

• $M_\infty = 0.1$, $\alpha = 8^\circ$, $Re_c = 60,000$

• Should show small region of laminar separation on upper surface followed by transition to turbulent flow downstream

• Grid is 179 x 55 x 15: 134,568 hexes with periodic sidewalls

• BDF2opt run from freestream to approximately 8 convection times

• FUN3D solutions shown are isosurfaces of velocity magnitude colored by pressure
• \( p = 4 \) solution points shown: surface points are projected to the geometry
• Mesh interior is deformed using existing FUN3D linear elasticity mechanics
**SD7003 Test Case**

*Finite Volume Scheme vs Entropy-Stable Scheme with p = 1*

---

**Standard FUN3D**

*Second-Order Finite Volume Scheme*

- 147,675 DOFs
- Shows mild spanwise variations very late

---

**Entropy-Stable Scheme with p = 1 (second order)**

- 134,568 DOFs
- Does not develop spanwise variations
- Discontinuities at element interfaces clearly visible
**SD7003 Test Case**

*Entropy-Stable Scheme with $p = 2, 3$*

**Entropy-Stable Scheme with $p = 2$ (third order)**
- 3,633,336 DOFs
- Shows spanwise breakdown and develops expected behavior

**Entropy-Stable Scheme with $p = 3$ (fourth order)**
- 8,612,352 DOFs
- Fine-scale features start to appear, transition shifts downstream
Entropy-Stable Scheme with $p = 4$ (fifth order)

- 16,821,000 DOFs
- Good qualitative resolution of expected flow physics
Supersonic Flow Past 3D Square Cylinder

\[ Re = 10,000 \quad M_\infty = 1.5 \quad p = 3 \text{ (fourth order)} \]

- 2,048,000 DOFs
- No dealiasing, artificial dissipation, or filtering
Conclusions

_Raising the bar on high-order CFD: Building a firm mathematical foundation for nonlinear stability_

- If the code blows up, there’s a bug
- Entropy conservation and stability using DG-FEM SBP operator
- First known nonlinearly stable no-slip wall BCs at any order
- All test cases demonstrate design order accuracy for smooth flows
- Noteworthy robustness for shocks even without additional dissipation or limiting
Foundational Algorithmic Development

- Entropy stability of all boundary conditions
- Entropy stability of turbulence equations including source terms
- Entropy stability for all schemes on all element types
- Provable stability of nonlinear iteration operator
- Prove stability of regularized reverse time adjoint operator
- DONE: August 18, 2019
Mathematical entropy (Continuous $\rightarrow$ Discrete)
- Convex extension of original equations (Friedrichs / Lax)
- Formed by contracting N-S equations with entropy variables
- Bounded physical quantity (N-S equations $\rightarrow$ thermodynamic entropy)

What does it buy you?
- Nonlinear stability in $L^2$
  - Entropy is bounded from above in an integral sense
  - The code doesn’t “blow up” (well, usually…see below)
- The nonlinear stability plateau for N-S equations

What it doesn’t guarantee
- Positivity (e.g., negative temperatures)
  - Shu’s limiter (RCA NRA with Brown Univ)
Telescopic Flux Form

\[ f_x(q) = Df + T_{p+1} = P^{-1} \Delta\bar{f} + T_{p+1}, \quad T_{p+1} = \text{trunc. error} \]

\[
\Delta = \begin{pmatrix}
-1 & 1 & 0 & 0 & 0 & 0 \\
0 & -1 & 1 & 0 & 0 & 0 \\
0 & 0 & \ddots & \ddots & 0 & 0 \\
0 & 0 & 0 & -1 & 1 & 0 \\
0 & 0 & 0 & 0 & -1 & 1 \\
\end{pmatrix} \rightarrow [\mathcal{N} \times (\mathcal{N} + 1)]
\]

\( \Delta \): calculates undivided difference of adjacent fluxes

\[
\begin{array}{ccccccc}
f_0 & f_1 & f_2 & f_3 & f_4 & f_5 \\
\hline
f_1 & f_2 & f_3 & f_4 & f_5 \\
u_0 & u_1 & u_2 & u_3 & u_4 \\
x_1 & x_2 & x_3 & x_4 & x_5 \\
\bar{x}_0 & \bar{x}_1 & \bar{x}_2 & \bar{x}_3 & \bar{x}_4 & \bar{x}_5 \\
-1 & \frac{-9}{10} & -\sqrt{\frac{3}{7}} & -\frac{16}{45} \frac{16}{45} & \pm\frac{9}{10} + 1
\end{array}
\]
A Quick Review of Stability Proofs

Linear advection equation

\[
u \left[ \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \right]; \quad \int_{-1}^{1} \left( \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \right); \quad \frac{1}{2} \frac{\partial}{\partial t} \| u \|^2 = \left( -a \frac{\partial u^2}{2} \right) \right]_{-1}^{+1}
\]

Burgers’ equation

\[
u \left[ \frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u^2}{\partial x} = \epsilon \frac{\partial^2 u}{\partial x^2} \right]; \quad \frac{1}{2} \frac{\partial}{\partial t} \| u \|^2 + \epsilon \left\| \frac{\partial u}{\partial x} \right\|^2 = \left( \epsilon \frac{\partial u^2}{\partial x} - \frac{2u}{3} \frac{u^2}{2} \right) \right]_{-1}^{+1}
\]

Incompressible Navier-Stokes equations

\[
u_i \left[ \rho \frac{\partial u_i}{\partial t} + \rho \frac{\partial u_i u_i}{\partial x_j} + \frac{\partial \rho \delta_{ij}}{\partial x_j} = \frac{\partial}{\partial x_j} \epsilon \frac{\partial u_i}{\partial x_j} \right]; \quad \frac{\partial u_i}{\partial x_i} = 0 \right]; \quad \rho \frac{\partial}{\partial t} \left\| \frac{1}{2} u_k u_k \right\|^2 + \epsilon \left\| \frac{\partial u_i}{\partial x_j} \right\|^2 = \left( \epsilon \frac{\partial^2 u_k u_k}{\partial x_j} - u_j \left( \frac{1}{2} u_k u_k + \rho \right) \delta_{ij} \right) \right]_{\partial S}
\]

Compressible Navier-Stokes?
**Summation-by-Parts Operators**

Integration by parts:

\[
\int_{x_L}^{x_R} \phi q_x \, dx = \phi q|_{x_L}^{x_R} - \int_{x_L}^{x_R} \phi_x q \, dx
\]

Semi-discrete:

\[
\phi^\top \mathcal{P} \mathcal{P}^{-1} Q \mathbf{q} = \phi^\top \left( \mathcal{B} - Q^\top \right) \mathbf{q} = \phi_N q_N - \phi_1 q_1 - \phi^\top \mathcal{D}^\top \mathcal{P} \mathbf{q}
\]

Mimetic form for first derivative \( \mathcal{D} \phi \) if:

\[
\mathcal{D} = \mathcal{P}^{-1} Q, \quad \mathcal{P} = \mathcal{P}^\top, \quad \zeta^\top \mathcal{P} \zeta > 0, \quad \zeta \neq \mathbf{0},
\]

\[
Q^\top = \mathcal{B} - Q, \quad \mathcal{B} = \text{diag}(-1, 0, \ldots, 0, 1)
\]
Nonlinearly Stable Wall BCs

- 3-D square cylinder with nonuniform grid
- Re = 200, M = 0.1
- Scheme retains accuracy on boundary

**No-slip BC**

**Entropy Flow**