Lessons learnt in developing compressible flow solvers

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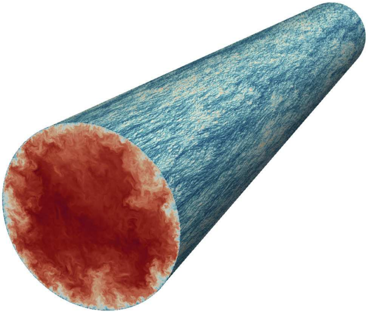
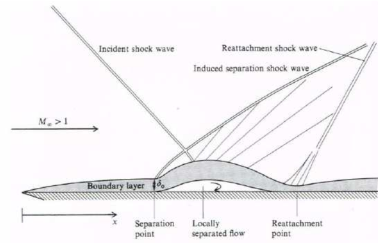
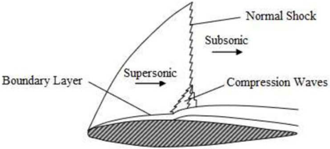
Our interests

- Turbulence



- High-speed flows



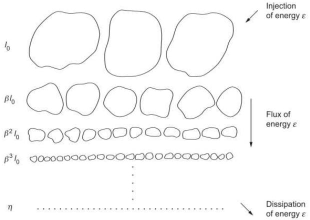


Fluid turbulence

- Fluid turbulence: 'cahotic' behavior of Navier-Stokes equations at 'high' Reynolds number
- Reynolds number : inertial / viscous forces

$$Re = \frac{U\ell_0}{\nu}$$

- Richardson cascade



- Kolmogorov length scale

$$\eta = (\nu^3/\varepsilon)^{1/4}$$

Direct numerical simulation (DNS)

- Ratio of integral-to-dissipative scale

$$\frac{\ell_0}{\eta} \sim \mathit{Re}^{3/4}$$

- By definition, DNS should resolve all energetically relevant flow scales
- Mesh spacings in proportion to Kolmogorov length scale
- Estimated number of grid points (in 3D!)

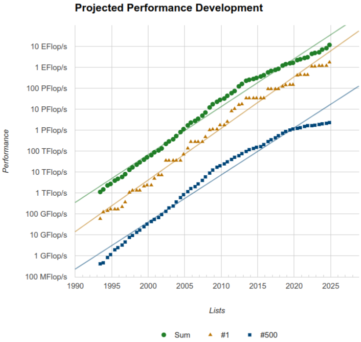
$$N \sim \mathit{Re}^{9/4}$$

- Flows of engineering interest have $\mathit{Re} = 10^3 - 10^{10}$
- Estimated computational effort

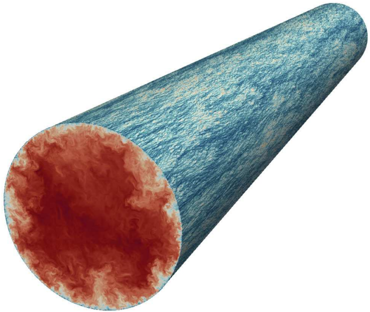
$$\mathrm{FLOPS} \sim \mathit{Re}^{12/4}$$

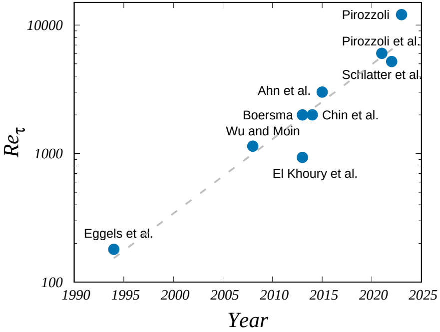
DNS and supercomputers

- Huge amount of memory and floating-point operations
- Pace set by computer power growth



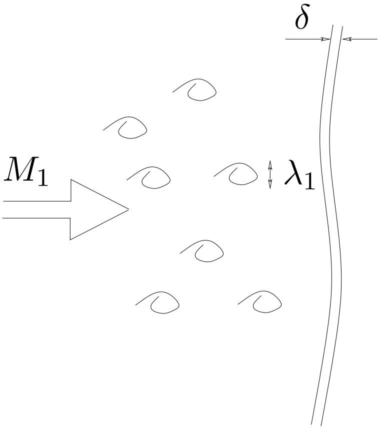
Timeline - DNS of turbulent pipe flow





- Exponential progress in time
- Expecting to reach $Re_\tau \approx 30,000$ before 2030

Turbulence and shock waves



- Estimate of shock thickness (Mahesh et al. 96)

$$\frac{\delta}{\lambda_1} \approx \frac{5.1}{Re_\lambda} \frac{M_t}{M_1 - 1}$$

$$R_\lambda >> 1$$

$$M_t = u_{rms}/c_1 << 1$$

$$\frac{\delta}{\lambda_1} << 1$$

Conclusion: shocks cannot be resolved!

Our requirements

Numerical schemes for DNS of compressible flow must be

- Efficient (billions of grid points)
- Accurate (turbulence does not forgive numerical errors)
- Robust (shocks are not resolved -> Gibbs phenomenon)
- Handle "complex" geometries (aircraft is the benchmark)

Early work (late 90s)

- Interest was rising on STI and SBLI
- CAA was in its early days
- Study prototype problems: shock/vortex, shock/sound, shock/entropy interactions
- FV schemes were used in the compressible flow community

Theoret. Comput. Fluid Dynamics (2000) 13: 421–456

Theoretical and Computational Fluid Dynamics

Shock-Wave–Vortex Interactions: Shock and Vortex Deformations, and Sound Production⋆

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optimized to achieve maximum time accuracy. The two-dimensional Euler equations of compressible gas dynamics are written as

$$\boldsymbol{w}_t + \boldsymbol{f}(\boldsymbol{w})_x + \boldsymbol{g}(\boldsymbol{w})_y = 0, \qquad (1)$$

where

$$\begin{aligned} \boldsymbol{w} &= (\rho, \rho u, \rho v, \rho E), \\ \boldsymbol{f} &= \left(\rho u, \rho u^2 + p, \rho u v, \rho u\left(E + \frac{p}{\rho}\right)\right), \\ \boldsymbol{g} &= \left(\rho v, \rho u v, \rho v^2 + p, \rho v\left(E + \frac{p}{\rho}\right)\right), \end{aligned}$$

and $p = \rho(\gamma - 1)(E - (u^2 + v^2)/2)$. The system (1) is integrated on a cartesian grid of rectangular cells,

$$S_{i,j} \equiv [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}], \qquad 1 \le i \le N_x, \quad 1 \le j \le N_y,$$

yielding

$$\frac{\mathrm{d}\overline{\overline{\boldsymbol{w}}}_{i,j}}{\mathrm{d}t} = -\frac{1}{\Delta x_i}(\hat{\boldsymbol{f}}_{i+1/2,j} - \hat{\boldsymbol{f}}_{i-1/2,j}) - \frac{1}{\Delta y_j}(\hat{\boldsymbol{g}}_{i,j+1/2} - \hat{\boldsymbol{g}}_{i,j-1/2}),$$

where $\overline{\overline{(\cdot)}}$ is the cell average

$$\overline{\overline{\boldsymbol{w}}}_{i,j} \equiv \frac{1}{\Delta x_i \Delta y_j} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \boldsymbol{w}(\xi, \eta, t)\, \mathrm{d}\xi\, \mathrm{d}\eta,$$

and the numerical fluxes $\hat{\boldsymbol{f}}_{i+1/2,j}$ and $\hat{\boldsymbol{g}}_{i,j+1/2}$ are defined at two gaussian points (per cell face) to achieve fourth-order accuracy. For example, $\hat{\boldsymbol{f}}_{i+1/2,j}$ is

$$\hat{\boldsymbol{f}}_{i+1/2,j} = \sum_{\alpha=1,2} \gamma_\alpha \boldsymbol{h}(\boldsymbol{w}^-(x_{i+1/2}, y_j + \beta_\alpha \Delta y_j), \boldsymbol{w}^+(x_{i+1/2}, y_j + \beta_\alpha \Delta y_j)), \qquad (2)$$

where $\gamma_1 = \gamma_2 = 1/2$ and $\beta_1 = -\beta_2 = -\sqrt{3}/6$. The numerical flux function $\boldsymbol{h}$ has been obtained by performing a local characteristic projection in the direction normal to the cell face, and using, for each characteristic field, Roe's approximate Riemann solver. For example, the left and right state for the vector unknown $\boldsymbol{w}^\pm(x_{i+1/2}, y_j + \beta_\alpha \Delta y_j)$ are determined by performing two successive one-dimensional WENO reconstructions of the cell averages $\overline{\overline{\boldsymbol{w}}}_{i,j}$ first in the y- and then in the x-direction. For more details see Shu (1997), Hu and Shu (1998), and Grasso and Pirozzoli (1999b).

Early work (late 90s)

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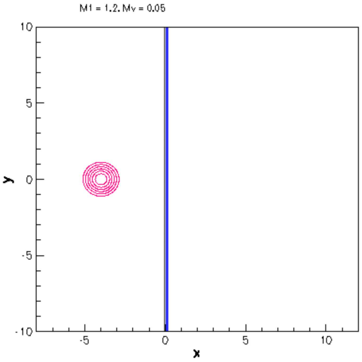

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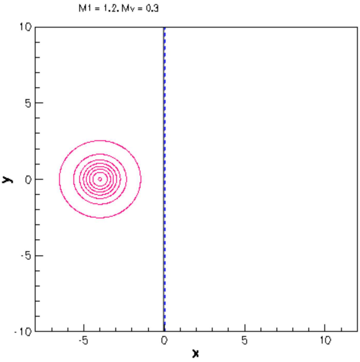

WENO schemes

- ENO schemes became popular in the 90's
- Paper by Jiang & Shu (1996) came in
- High-order was the keyword

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ARTICLE NO. 0130

Efficient Implementation of Weighted ENO Schemes*

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Received August 14, 1995; revised January 3, 1996

In this paper, we further analyze, test, modify, and improve the high order WENO (weighted essentially non-oscillatory) finite difference schemes of Liu, Osher, and Chan. It was shown by Liu *et al.* that WENO schemes constructed from the rth order (in L^1 norm) ENO schemes are $(r + 1)$th order accurate. We propose a new way of measuring the smoothness of a numerical solution, emulating the idea of minimizing the total variation of the approximation, which results in a fifth-order WENO scheme for the case $r = 3$, instead of the fourth-order with the original smoothness measurement by Liu *et al.* This fifth-order WENO scheme is as fast as the fourth-order WENO scheme of Liu *et al.* and both schemes are about twice as fast as the fourth-order ENO schemes on vector supercomputers and as fast on serial and parallel computers. For Euler systems of gas dynamics, we suggest computing the weights from pressure and entropy instead of the characteristic values to simplify the costly characteristic procedure. The resulting WENO schemes are about twice as fast as the WENO schemes using the characteristic decompositions to compute weights and work well for problems which do not contain strong shocks or strong reflected waves. We also prove that, for conservation laws with smooth solutions, all WENO schemes are convergent. Many numerical tests, including the 1D steady state nozzle flow problem and 2D shock entropy wave interaction problem, are presented to demonstrate the remarkable capability of the WENO schemes, especially the WENO scheme using the new smoothness measurement in resolving complicated shock and flow structures. We have also applied Yang's artificial compression method to the WENO schemes to sharpen contact discontinuities.

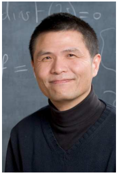
or perhaps with a forcing term $\mathbf{g}(\mathbf{u}, \mathbf{x}, t)$ on the right-hand side. Here $\mathbf{u} = (u_1, ..., u_m)$, $\mathbf{f} = (\mathbf{f}_1, ..., \mathbf{f}_d)$, $\mathbf{x} = (x_1, ..., x_d)$ and $t > 0$.

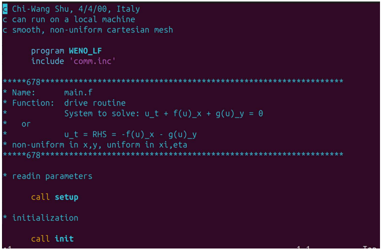
WENO schemes are based on ENO (essentially non-oscillatory) schemes, which were first introduced by Harten, Osher, Engquist, and Chakravarthy [5] in the form of cell averages. The key idea of ENO schemes is to use the "smoothest" stencil among several candidates to approximate the fluxes at cell boundaries to a high order accuracy and at the same time to avoid spurious oscillations near shocks. The cell-averaged version of ENO schemes involves a procedure of reconstructing point values from cell averages and could become complicated and costly for multi-dimensional problems. Later, Shu and Osher [14, 15] developed the flux version of ENO schemes which do not require such a reconstruction procedure. We will formulate the WENO schemes based on this flux version of ENO schemes. The WENO schemes of Liu *et al.* [9] are based on the cell-averaged version of ENO schemes.

For applications involving shocks, second-order schemes are usually adequate if only relatively simple structures are present in the smooth part of the solution (e.g., the shock tube problem). However, if a problem contains rich structures as well as shocks (e.g., the shock entropy wave interaction problem in *Example 4*, Section 8.3), high order

WENO schemes

- ENO schemes became popular in the 90's
- Paper by Jiang & Shu (1996) came in
- High-order was the keyword
- Chi-Wang Shu in Rome: better move to FD





```
c Chi-Wang Shu, 4/4/00, Italy
c can run on a local machine
c smooth, non-uniform cartesian mesh

      program WENO_LF
      include 'comm.inc'

*****678*********************************************************************
* Name:      main.f
* Function:  drive routine
*            System to solve: u_t + f(u)_x + g(u)_y = 0
*   or
*            u_t = RHS = -f(u)_x - g(u)_y
* non-uniform in x,y, uniform in xi,eta
*****678*********************************************************************

* readin parameters

      call setup

* initialization

      call init
```

Early DNS

- DNS limited to incompressible flow
- Isotropic turbulence (Blaisdell *et al.*, 1996)
- Some early attempts based on temporal approach (Guarini *et al.*, 2000)
- Developed my own DNS (WENO-based) solver

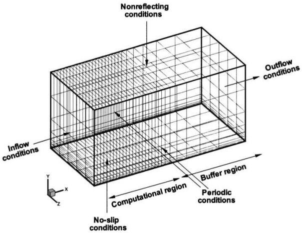
Direct numerical simulation and analysis of a spatially evolving supersonic turbulent boundary layer at $M=2.25$

S. Pirozzoli and F. Grasso
Dipartimento di Meccanica ed Aeronautica, Università di Roma "La Sapienza," via Eudossiana 18, 00184 Roma, Italy

T. B. Gatski
Computational Modeling & Simulation Branch, NASA Langley Research Center, Hampton, Virginia 23681

(Received 4 November 2002; accepted 15 October 2003; published online 13 January 2004)

A spatially developing supersonic adiabatic flat plate boundary layer flow (at $M_\infty=2.25$ and $Re_\theta \approx 4000$) is analyzed by means of direct numerical simulation. The numerical algorithm is based on a mixed weighted essentially nonoscillatory compact-difference method for the three-dimensional Navier–Stokes equations. The main objectives are to assess the validity of Morkovin's hypothesis and Reynolds analogies, and to analyze the controlling mechanisms for turbulence production, dissipation, and transport. The results show that the essential dynamics of the investigated turbulent supersonic boundary layer flow closely resembles the incompressible pattern. The Van Driest transformed mean velocity obeys the incompressible law-of-the-wall, and the mean static temperature field exhibits a quadratic dependency upon the mean velocity, as predicted by the Crocco–Busemann relation. The total temperature has been found not to be precisely uniform, and total temperature fluctuations are found to be non-negligible. Consistently, the turbulent Prandtl number is not unity, and it varies between 0.7 and 0.8 in the outer part of the boundary layer. Nonetheless, a modified strong Reynolds analogy is still verified. In agreement with the low Mach number results, the streamwise velocity component and the temperature are only weakly anti-correlated. The turbulent kinetic energy budget also shows similarities with the incompressible case provided all terms of the equation are properly scaled; indeed, the leading compressibility contributions are negligible throughout the boundary layer.
[DOI: 10.1063/1.1637604]



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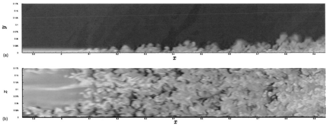

FIG. 8. Numerical flow visualization: density field in the transition region: (a) $x-y$ plane; (b) $x-z$ plane at $y^+=100$.

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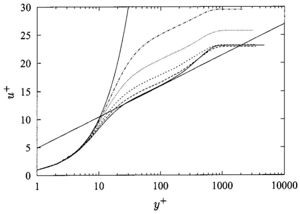

FIG. 2. Grid sensitivity study: distribution of mean streamwise velocity normalized by shear velocity at $x = 8.8$, $Re_\theta = 4263$) in inner scaling. (—), A (seventh order); (– – –) A (fifth order); (---) B; (···) C; (-··-) D.

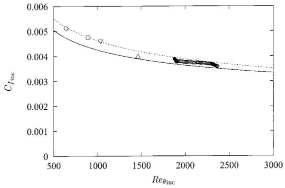

FIG. 11. Skin friction distribution as a function of Reynolds number based on momentum thickness. (○) Present DNS; (□) Guarini *et al.*; (△) Maeder *et al.* ($M = 3$); (▽) Maeder *et al.* ($M = 4.5$); (◇) Maeder *et al.* ($M = 6$).

DNS of SBLI

- DNS with shocks
- SBLI prototype problem
- First DNS of SBLI
- VERY slow!

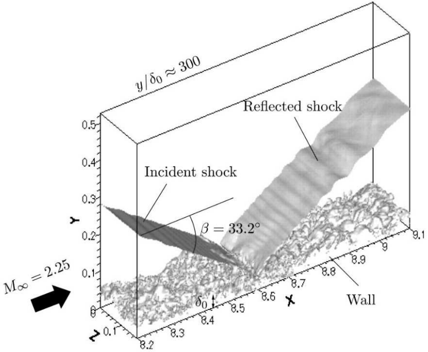

FIG. 1. Zoom of the computational domain in the proximity of the interaction zone. δ_0—boundary layer thickness in the absence of interacting shock; β—shock angle.

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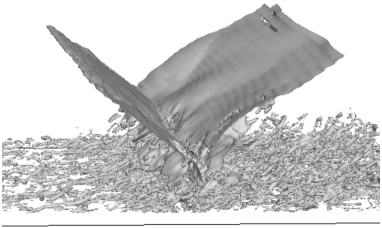

Can we do better?

- Problems with LES
- Start searching "old" papers

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Numerical Methods for High-Speed Flows

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Keywords

shock waves, shock-capturing schemes, energy conservation, numerical dissipation

Abstract

We review numerical methods for direct numerical simulation (DNS) and large-eddy simulation (LES) of turbulent compressible flow in the presence of shock waves. Ideal numerical methods should be accurate and free from numerical dissipation in smooth parts of the flow, and at the same time they must robustly capture shock waves without significant Gibbs ringing, which may lead to nonlinear instability. Adapting to these conflicting goals leads to the design of strongly nonlinear numerical schemes that depend on the geometrical properties of the solution. For low-dissipation methods for smooth flows, numerical stability can be based on physical conservation principles for kinetic energy and/or entropy. Shock-capturing requires the addition of artificial dissipation, in more or less explicit form, as a surrogate for physical viscosity, to obtain nonoscillatory transitions. Methods suitable for both smooth and shocked flows are discussed, and the potential for hybridization is highlighted. Examples of the application of advanced algorithms to DNS/LES of turbulent, compressible flows are presented.

Can we do better?

- Problems with LES
- Start searching "old" papers
- Feiereisen *et al.* (1981)

NUMERICAL SIMULATION OF A COMPRESSIBLE, HOMOGENEOUS, TURBULENT SHEAR FLOW

NASA-CR-164953
19820003523

by
W. J. Feiereisen,
W. C. Reynolds,
and
J. H. Ferziger

Artificial production or dissipation by means of finite-difference approximations to the convective terms is still possible and must be eliminated for a valid simulation. We shall again rewrite the convective terms in the momentum equations in a different but equivalent form that not only prevents artificial kinetic energy production but regains the total energy conservation that we lost earlier.

We must ensure that the numerical method that we shall use is incapable of artificially creating kinetic energy. To show this, we shall write the kinetic energy equation and integrate it over the periodic domain.

$$\frac{\partial}{\partial x_j} \rho u_i u_j = \frac{1}{2} \frac{\partial}{\partial x_j} \rho u_i u_j + u_i \frac{\partial}{\partial x_j} \rho u_j + \rho u_j \frac{\partial}{\partial x_j} u_i \quad (2.2.5)$$

Can we do better?

- Problems with LES
- Start searching "old" papers
- Feiereisen *et al.* (1981)
- Blaisdell *et al.* (1996)

ELSEVIER Applied Numerical Mathematics 21 (1996) 207–219 APPLIED NUMERICAL MATHEMATICS

The effect of the formulation of nonlinear terms on aliasing errors in spectral methods

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The convective terms in the momentum and internal energy equation were written in the general form

$$\alpha \frac{\partial}{\partial x_j}\left(f_i g_j\right) + (1-\alpha)\left(f_i \frac{\partial g_j}{\partial x_j} + \frac{\partial f_i}{\partial x_j} g_j\right), \qquad (4.1)$$

where in the momentum equation $f_i = \rho u_i$ and $g_j = u_j$, while in the energy equation $f_i = \rho C_v T$ and $g_j = u_j$. (Note that the internal energy equation is solved in LES of compressible turbulence, rather

Can we do better?

- Problems with LES
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- Feiereisen *et al.* (1981)
- Blaisdell *et al.* (1996)
- Kennedy & Gruber (2008)

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Reduced aliasing formulations of the convective terms within the Navier–Stokes equations for a compressible fluid

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Extending these ideas to quarticly or quinticly nonlinear operators by example of the cubically nonlinear operator, (33), is rewritten as

$$\nabla(fgh) = \alpha\nabla(fgh) + \beta[f\nabla(gh) + g\nabla(fh) + h\nabla(fg)] + \gamma[gh\nabla f + fh\nabla g + fg\nabla h] \quad (46)$$

Energy consistency

- FD discretization of mass and momentum equations

$$\frac{\mathrm{d}\rho_j}{\mathrm{d}t} + D_S\left(\rho u\right)_j = 0$$

$$\frac{\mathrm{d}(\rho u)_j}{\mathrm{d}t} + D_S\left(\rho u^2\right)_j + Dp_j = 0$$

D_S denotes suitable approximation of the convective derivatives

- Convective derivatives can be expressed as

$$\frac{\partial \rho u \varphi}{\partial x}$$

where $\varphi = 1$ for continuity and $\varphi = u$ for momentum

- Discrete energy consistency can be achieved by expanding the convective derivative

$$\frac{\partial \rho u \varphi}{\partial x} = \frac{1}{2}\frac{\partial \rho u \varphi}{\partial x} + \frac{1}{2}\varphi\frac{\partial \rho u}{\partial x} + \frac{1}{2}\rho u\frac{\partial \varphi}{\partial x}$$

- ... and applying a SBP discretization to each term

$$D_S(\rho u \varphi)_j = \frac{1}{2}D\left(\rho u \varphi\right)_j + \frac{1}{2}\varphi_j D\left(\rho u\right)_j + \frac{1}{2}\rho_j u_j D\varphi_j$$

SBP operators

- Integration by parts

$$\int_a^b \left(v\frac{\partial w}{\partial x} + w\frac{\partial v}{\partial x} \right) \mathrm{d}x = - \left[vw \right]_a^b$$

- Summation-by-parts (SBP)

$$h \sum_1^N \left(V_j D W_j + W_j D V_j \right) = - \left(V_N W_N - V_1 W_1 \right)$$

- Any Cn operator is SBP in periodic domains
- More cumbersome to build SBP operators in finite domains

- Discrete total kinetic energy

$$K = \frac{h}{2}\sum_{j=1}^{N} \rho_j u_j^2 = \frac{h}{2}\sum_{j=1}^{N} \frac{(\rho u)_j^2}{\rho_j}$$

- Combine mass and momentum equations

$$\frac{\mathrm{d}K}{\mathrm{d}t} = \frac{h}{2}\sum_{j=1}^{N}\left(-2u_j D_S(\rho u^2)_j - 2u_j D p_j + u_j^2 D_S(\rho u)_j\right)$$

- Use expanded form of convective derivative

$$\frac{\mathrm{d}K}{\mathrm{d}t} = \frac{h}{2}\sum_{j=1}^{N}\left[-u_j\left(D(\rho u^2)_j + u_j D(\rho u)_j + \rho_j u_j D u_j\right) + u_j^2 D(\rho u)_j - 2u_j D p_j\right] =$$

$$\frac{h}{2}\sum_{j=1}^{N}\left[-u_j D(\rho u^2)_j - \rho_j u_j^2 D u_j - 2u_j D p_j\right]$$

- Assume $D \in SBP$

$$\frac{\mathrm{d}K}{\mathrm{d}t} = -(\rho_N u_N^3/2 + p_N u_N) + (\rho_1 u_1^3/2 + p_1 u_1) + h\sum_{j=1} p_j D u_j$$

which proves discrete conservation of K.

A new splitting

- Splitting of convective terms ($\varphi = 1, u_i, H$)

Feiereisen *et al.* (1981)

$$\frac{\partial \rho u_j \varphi}{\partial x_j} = \frac{1}{2}\,\frac{\partial \rho u_j \varphi}{\partial x_j} + \frac{1}{2}\,\varphi\,\frac{\partial \rho u_j}{\partial x_j} + \frac{1}{2}\,\rho u_j\,\frac{\partial \varphi}{\partial x_j}$$

Blaisdell *et al.* (1996)

$$\frac{\partial \rho u_j \varphi}{\partial x_j} = \frac{1}{2}\,\frac{\partial \rho u_j \varphi}{\partial x_j} + \frac{1}{2}\,u_j\,\frac{\partial \rho \varphi}{\partial x_j} + \frac{1}{2}\,\rho \varphi\,\frac{\partial u_j}{\partial x_j}$$

Pirozzoli (2010)

$$\frac{\partial \rho u_j \varphi}{\partial x_j} = \frac{1}{4}\,\frac{\partial \rho u_j \varphi}{\partial x_j} + \frac{1}{4}\left(u_j\,\frac{\partial \rho \varphi}{\partial x_j} + \rho\,\frac{\partial u_j \varphi}{\partial x_j} + \varphi\,\frac{\partial \rho u_j}{\partial x_j}\right) + \frac{1}{4}\left(\rho u_j\,\frac{\partial \varphi}{\partial x_j} + \rho \varphi\,\frac{\partial u_j}{\partial x_j} + u_j \varphi\,\frac{\partial \rho}{\partial x_j}\right)$$

- Replace $\partial/\partial x_j$ with $D \in \mathrm{SBP}$ yields discrete kinetic energy preservation, if applied to both mass and momemtum eqn

Locally conservative formulation

- Look for numerical conservative flux $\hat{f}_{j+1/2}$

$$\left.\frac{\partial \rho u \varphi}{\partial x}\right|_{x=x_j} \approx \frac{1}{h}(\hat{f}_{j+1/2} - \hat{f}_{j-1/2})$$

- Assume general Cn operator ($n = 2L$)
- Arrive (...) to (Pirozzoli, JCP 2010)

$$\hat{f}_{j+1/2} = 2\sum_{\ell=1}^{L} a_\ell \sum_{m=0}^{\ell-1} (\widetilde{\rho, u, \varphi})_{j-m,\ell}, \;\; (\widetilde{\rho, u, \varphi})_{j,\ell} = \frac{1}{8}(\rho_j + \rho_{j+\ell})(u_j + u_{j+\ell})(\varphi_j + \varphi_{j+\ell})$$

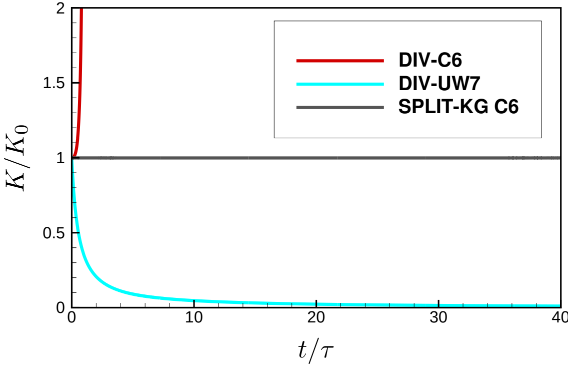
- For $n = 2$

$$\hat{f}_{j+1/2} = \frac{(\rho_j + \rho_{j+1})}{2}\frac{(u_j + u_{j+1})}{2}\frac{(\varphi_j + \varphi_{j+1})}{2}$$

- Primary conservation properties automatically follow
- Easy hybridization with shock-capturing schemes

Euler turbulence, $M_t = 0.07$

- Under-resolved simulations on 32^3 grid at $\nu = 0$
- Divergence form with C6 and UW7
- Energy-consistent form with C6



Time reversibility test

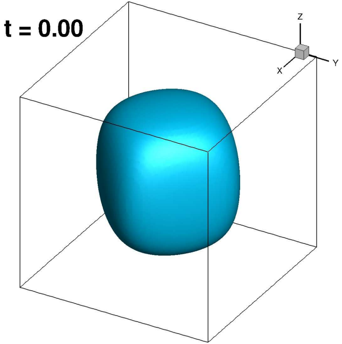
- Taylor-Green flow

$$u = u_0 \sin(k_0 x) \cos(k_0 y) \cos(k_0 z)$$
$$v = -u_0 \cos(k_0 x) \sin(k_0 y) \cos(k_0 z)$$
$$w = 0$$

- Velocity vectors reversed at $t = 8.0$

$$\mathbf{u}(t, \mathbf{x}) \Rightarrow -\mathbf{u}(-t, \mathbf{x})$$

- Energy-consistent discretization



Time reversibility test

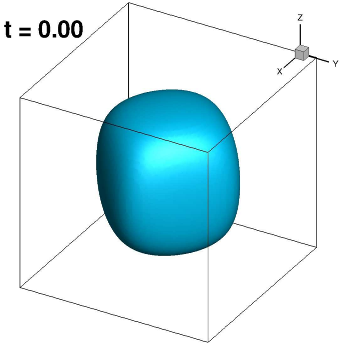
- Taylor-Green flow

$$
\begin{aligned}
u &= u_0 \, \sin\left(k_0\, x\right)\, \cos\left(k_0\, y\right)\, \cos\left(k_0\, z\right) \\
v &= -u_0 \, \cos\left(k_0\, x\right)\, \sin\left(k_0\, y\right)\, \cos\left(k_0\, z\right) \\
w &= 0
\end{aligned}
$$

- Velocity vectors reversed at $t = 8.0$

$$\mathbf{u}(t, \mathbf{x}) \Rightarrow -\mathbf{u}(-t, \mathbf{x})$$

- Non-conservative discretization (DNSFoam)



Boundary layers

- Much greater efficiency
- Start of PRACE HPC initiative
- Could use for first time billions of grid points
- Reach $Re_\tau \approx 4000$

J. Fluid Mech. (2011), *vol.* 688, *pp.* 120–168. © Cambridge University Press 2011 120
doi:10.1017/jfm.2011.368

Turbulence in supersonic boundary layers at moderate Reynolds number

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PHYSICS OF FLUIDS **25**, 021704 (2013)

Probing high-Reynolds-number effects in numerical boundary layers

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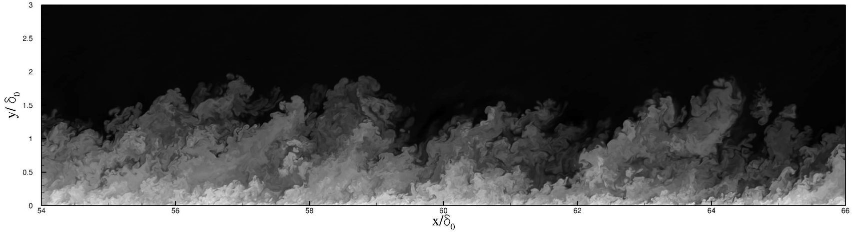
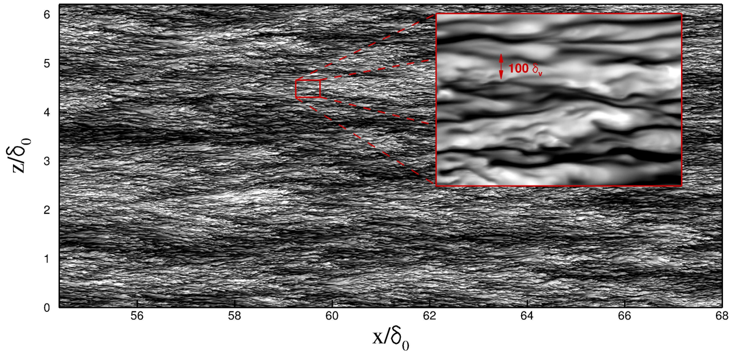
We study the high-Reynolds-number behavior of a turbulent boundary layer in the low supersonic regime through very-large-scale direct numerical simulation (DNS).

TBL at $M = 2$, $Re_\tau = 4000$ - side view



TBL at $M = 2$, $Re_\tau = 4000$ - wall-parallel plane



Shock-boundary layer interactions

- Hybridization with WENO schemes

$$\Theta = \frac{(\nabla \cdot u)^2}{(\nabla \cdot u)^2 + (\nabla \times u)^2 + (u_\infty/\delta_{\text{in}})^2}, \qquad 0 \le \Theta \le 1$$

- Retain computational efficiency of baseline solver

- Could use billions of grid points for very long time integration (low-frequency dynamics)

J. Fluid Mech. (2010), *vol.* 657, *pp.* 361–393. © Cambridge University Press 2010 361
doi:10.1017/S0022112010001710

Direct numerical simulation of transonic shock/boundary layer interaction under conditions of incipient separation

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Technical Notes

Direct Numerical Simulation Database for Impinging Shock Wave/Turbulent Boundary-Layer Interaction

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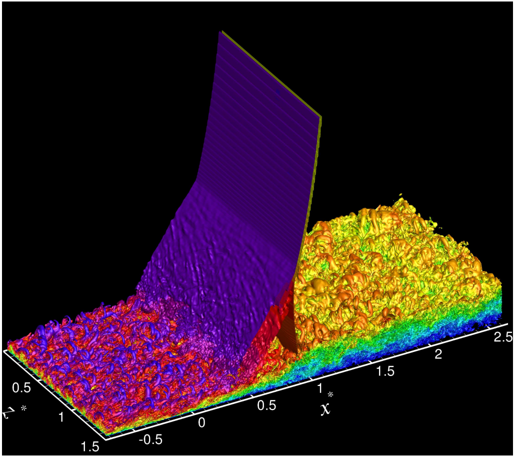
DOI: 10.2514/1.J050901

Normal shock/boundary layer interaction $M = 1.3$



Numerical boundary conditions

- Behavior of non-dissipative solvers strongly dependent on quality of numerical boundary conditions (NBC)
- Soft NBC enforcement fundamental to avoid appearance of saw-tooth waves
- Stimulate incoming disturbances with good fidelity and no spurious ‘noise’
- Characteristic decomposition -> LODI approach (Poinsot & Lele JCP 1992)

One-dimensional characteristic projection

- Project in normal-to-boundary direction (say x)

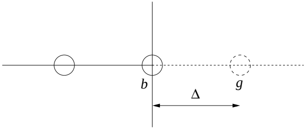
$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = \frac{\partial \mathbf{u}}{\partial t} + \mathbf{R}_x \boldsymbol{\mathcal{L}} = \mathbf{C}, \quad \boldsymbol{\mathcal{L}} = \boldsymbol{\Lambda}_x \mathbf{L}_x \frac{\partial \mathbf{u}}{\partial x}$$

- Wave decomposition: **i**ncoming + **o**utgoing

$$\boldsymbol{\mathcal{L}} = \boldsymbol{\mathcal{L}}^{\mathrm{o}} + \boldsymbol{\mathcal{L}}^{\mathrm{i}} = \boldsymbol{\Lambda}_x^{\mathrm{o}} \mathbf{L}_x \frac{\partial \mathbf{u}}{\partial x} + \boldsymbol{\Lambda}_x^{\mathrm{i}} \mathbf{L}_x \frac{\partial \mathbf{u}}{\partial x}$$

- Discretization

$$\boldsymbol{\mathcal{L}} \approx \boldsymbol{\Lambda}_x^{\mathrm{o}} \mathbf{L}_x \, D_u \mathbf{u}_b + n_x \boldsymbol{\Lambda}_x^{\mathrm{i}} \mathbf{L}_x \mathbf{P} \, \frac{\mathbf{v}_g - \mathbf{v}_b}{\Delta}$$



Semidiscrete ODE system

- Return to conservative variables

$$\frac{\mathrm{d}\mathbf{u}_b}{\mathrm{d}t} = -\mathbf{R}_x \mathbf{\Lambda}_x^{\mathrm{o}} \mathbf{L}_x \, D_u \mathbf{u}_b + n_x \mathbf{R}_x \mathbf{\Lambda}_x^{\mathrm{i}} \mathbf{L}_x \mathbf{P} \, \frac{(\mathbf{v}_b - \mathbf{v}_g)}{\Delta} + \mathbf{C}_b$$

- In terms of characteristic variables

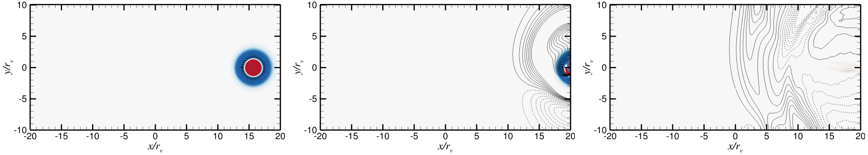
$$\frac{\mathrm{d}\mathbf{w}_b}{\mathrm{d}t} = -\mathbf{\Lambda}_x^{\mathrm{o}} \, D_u \mathbf{w}_b + n_x \mathbf{\Lambda}_x^{\mathrm{i}} \, \frac{(\mathbf{w}_b - \mathbf{w}_g)}{\Delta} + \mathbf{L}_{xb} \mathbf{C}_b$$

- Akin to addition of a relaxation term
- Reminds of previous, primitive-based relaxation techniques (e.g. Rudy & Strikwerda JCP 1980, Yoo et al. CTM 05, SBP-SAT)
- Characteristic-based relaxation yields substantial improvement in terms of reflection and response to incoming disturbances (Pirozzoli & Colonius, JCP 2013)

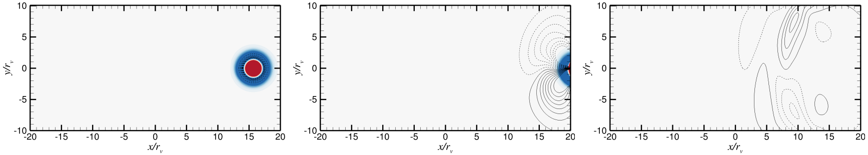
Advection of cylindrical vortex

$M_0 = 0.3$, $M_v = 0.4$

Pressure-based relaxation



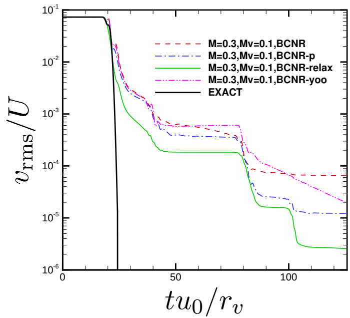
Characteristic-based relaxation



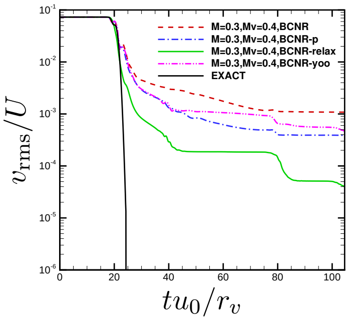
Advection of cylindrical vortex

r.m.s. vertical velocity

$M_0 = 0.3,\ M_v = 0.1$

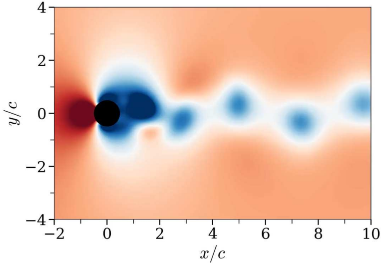


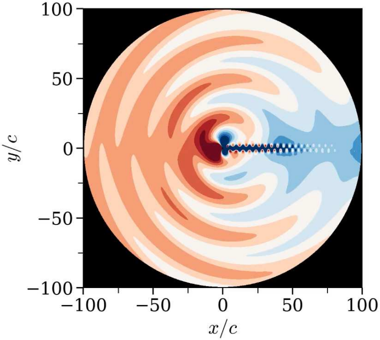
$M_0 = 0.3,\ M_v = 0.4$



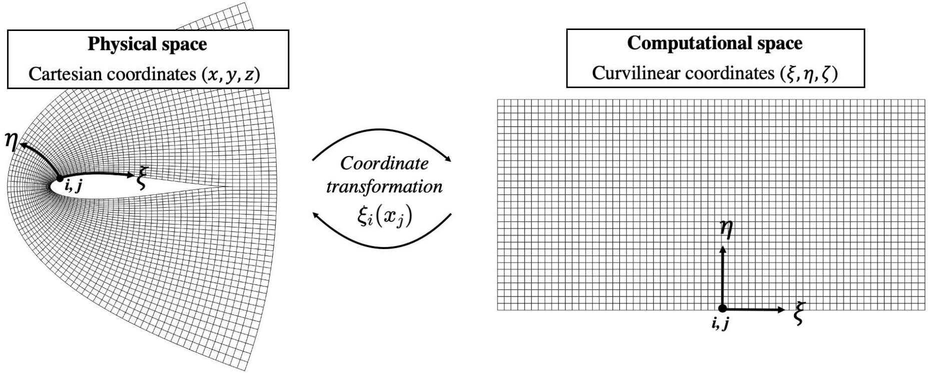
Numerical tests

Sound generation from a cylinder





Curvilinear coordinates



Strong conservation form (Vinokur, 1974)

$$\frac{1}{J}\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial \xi_j}\left(\frac{\mathbf{f}_j}{J}\right) = 0, \; \mathbf{u} = \begin{bmatrix} \rho \\ \rho u_i \\ \rho E \end{bmatrix}, \; \mathbf{f}_j = \begin{bmatrix} \rho \tilde{u}_j \\ \rho u_i \tilde{u}_j + p J_{ji} \\ \rho \tilde{u}_j H \end{bmatrix}, \; i = 1, \ldots, d$$

- $\tilde{u}_j = J_{jk}\, u_k$ contravariant velocity
- $J_{jk} = \partial \xi_j / \partial x_k$ Jacobian matrix
- $J = \det(J_{jk})$

Energy preservation (Pirozzoli, 2011)

- Split convective terms in generic transport equation ($\varphi = 1, u_i, H$)

$$\frac{\partial}{\partial \xi_j}\left(\frac{\rho \tilde{u}_j \varphi}{J}\right) = \frac{1}{4}\frac{\partial \rho \hat{u}_j \varphi}{\partial \xi_j} + \frac{1}{4}\left(\rho \frac{\partial \hat{u}_j \varphi}{\partial \xi_j} + \hat{u}_j \frac{\partial \rho \varphi}{\partial \xi_j} + \varphi \frac{\partial \rho \hat{u}_j}{\partial \xi_j}\right)$$

$$+\frac{1}{4}\left(\rho \hat{u}_j \frac{\partial \varphi}{\partial \xi_j} + \rho \varphi \frac{\partial \hat{u}_j}{\partial \xi_j} + \hat{u}_j \varphi \frac{\partial \rho}{\partial \xi_j}\right)$$

with $\hat{u}_j = \tilde{u}_j / J$

- Apply to each equation and discretize

$$\frac{d\mathbf{u}_{\mathcal{N}}}{dt} = -\frac{J_{\mathcal{N}}}{4}\begin{bmatrix} 2D_j(\rho\hat{u}_j) + 2\rho D_j(\hat{u}_j) + 2\hat{u}_j D_j(\rho) \\ D_j(\rho u_i \hat{u}_j) + \hat{u}_j D_j(\rho u_i) + \rho D_j(u_i \hat{u}_j) + u_i D_j(\rho \hat{u}_j) + \rho u_i D_j(\hat{u}_j) + u_i \hat{u}_j D_j(\rho) + \rho \hat{u}_j D_j(u_i) + \\ +2D_j(pJ_{ji}) + 2pD_j(J_{ji}) + 2J_{ji}D_j(p) \\ D_j(\rho\hat{u}_j H) + \rho D_j(\hat{u}_j H) + \hat{u}_j D_j(\rho H) + HD_j(\rho \hat{u}_j) + \hat{u}_j H D_j(\rho) + \rho H D_j(\hat{u}_j) + \rho \hat{u}_j D_j(H) \end{bmatrix}_{\mathcal{N}}.$$

- Total kinetic energy is preserved

$$\hat{K} = \frac{1}{2}\sum_{\mathcal{N}} \frac{1}{J_{\mathcal{N}}}\left(\rho u_i u_i\right)_{\mathcal{N}}$$

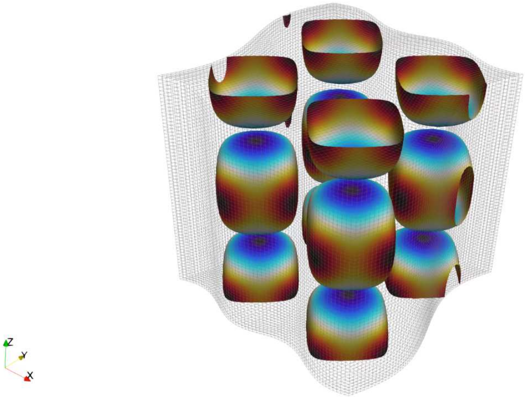
Locally conservative form

$$\frac{\mathrm{d}\mathbf{u}_{\mathcal{N}}}{\mathrm{d}t} = -J_{\mathcal{N}} \sum_{j=1}^{d} \left(\hat{\mathbf{f}}_{j;1/2} - \hat{\mathbf{f}}_{j;-1/2}\right)_{\mathcal{N}}$$

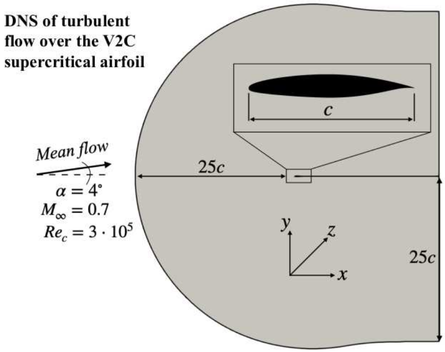
$$\left(\hat{\mathbf{f}}_{j;1/2}\right)_{\mathcal{N}} = 2\sum_{\ell=1}^{L} a_\ell \sum_{m=0}^{\ell-1} \begin{bmatrix} \left(\rho, \widetilde{\hat{u}_j, 1}\right)_{j;-m,\ell} \\ \left(\rho, \widetilde{\hat{u}_j, u_i}\right)_{j;-m,\ell} + \left(p, \widetilde{J_{ji}, 1}\right)_{j;-m,\ell} \\ \left(\rho, \widetilde{\hat{u}_j, H}\right)_{j;-m,\ell} \end{bmatrix}_{\mathcal{N}}, \quad i = 1, \ldots, d$$

Numerical test

Taylor-Green vortex on distorted mesh



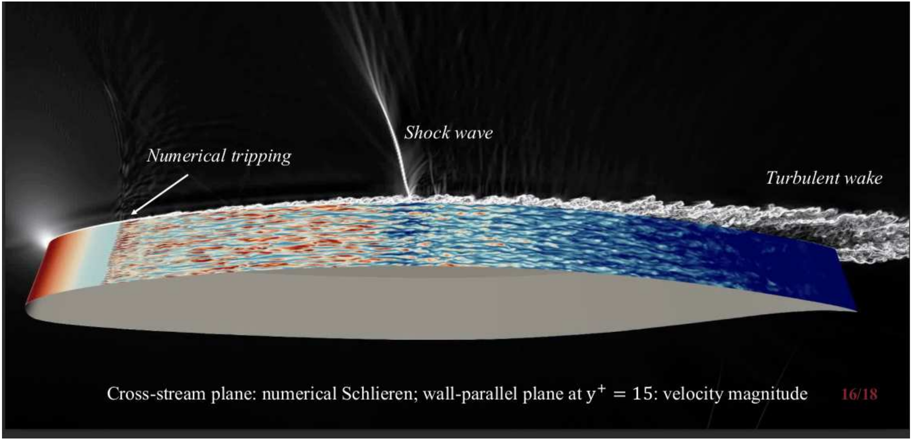
Flow over transonic airfoil



Numerical setup

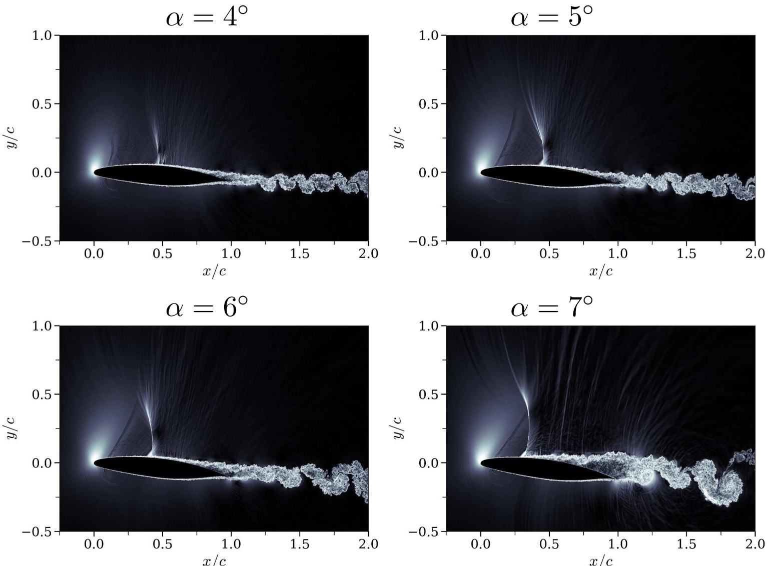
- Mach number $M_0 = 0.7$
- Incidence angle $\alpha = 4° - 7°$
- Reynolds number $Re_c = 3 \cdot 10^5$
- Grid ponts $4096 \times 512 \times 256$

Flow over transonic airfoil

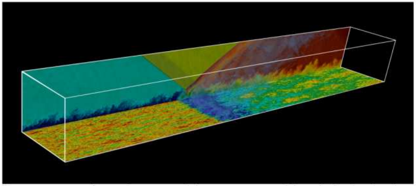


Cross-stream plane: numerical Schlieren; wall-parallel plane at $y^+ = 15$: velocity magnitude

Flow over transonic airfoil



The STREAmS solver



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streamsdns

Documentation: https://streams-cfd.github.io/STREAmS-2/

Github: https://github.com/STREAmS-CFD/STREAmS-2

Main features[a]:

- Open source GPL-3.0 license
- Direct numerical simulation of wall bounded flows
- Three different backends: CPU, NVIDIA, AMD, Intel GPU
- Object oriented framework, modern Fortran

[a] Bernardini *et al.* (2021). Comput. Phys. Commun., 263, 107906.

Conclusions

- Energy preservation principles leveraged to achieve numerical stability
- Shocks handled through hybridization with shock-capturing schemes
- Proper treatment of boundary conditions
- Can handle moderately complex geometries with use of curvlinear coordinates
- "Almost" unbeatable computational efficiency

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