On the order of accuracy of spatial discretizations in numerical simulation of turbulent flows

Parviz Moin

In celebration of Paolo Orlandi's vortical and turbulent life

Roma, Italy, September 19th, 2014

My fond memories of Paolo

- 1978 – Visiting professor at Stanford (I was a student)
- 1987 – Summer Visitor, Center for Turbulence Research

1987 CTR Summer Program

Paolo and me

- Paolo frequently visited CTR
- Paolo wrote the first staggered FD code for general geometry at CTR
- EDQNM, polymers, MHD, contrails, mixing layers, helicity fluctuations, vortex rings, immersed boundary, curved BLs, buoyant flows, …

Paolo's positions

Selected quotes from his book *"Fluid Flow Phenomena: A Numerical Toolkit"*

- "Finite-differences are simple to understand/use and produce satisfactory results comparable to the more elaborate pseuospectral methods."
- "… staggered second order finite differences produce results as good as those by pseuospectral methods" for isotropic turbulence (1998 study at CTR)
- "… boundary conditions and geometry make extension of pseudospectral methods very difficult" in practical flows; this is an "easy task" for FD
- "… immersed boundaries [are] simple, versatile & have satisfactory accuracy;" "I shall put all my efforts to insert body forces into codes that at the base solve Navier-Stokes in Cartesian/cylindrical coordinates."
- "… generation of turbulent fields is a very easy task; good scholars produce ideas from these data to improve our knowledge & way of life."

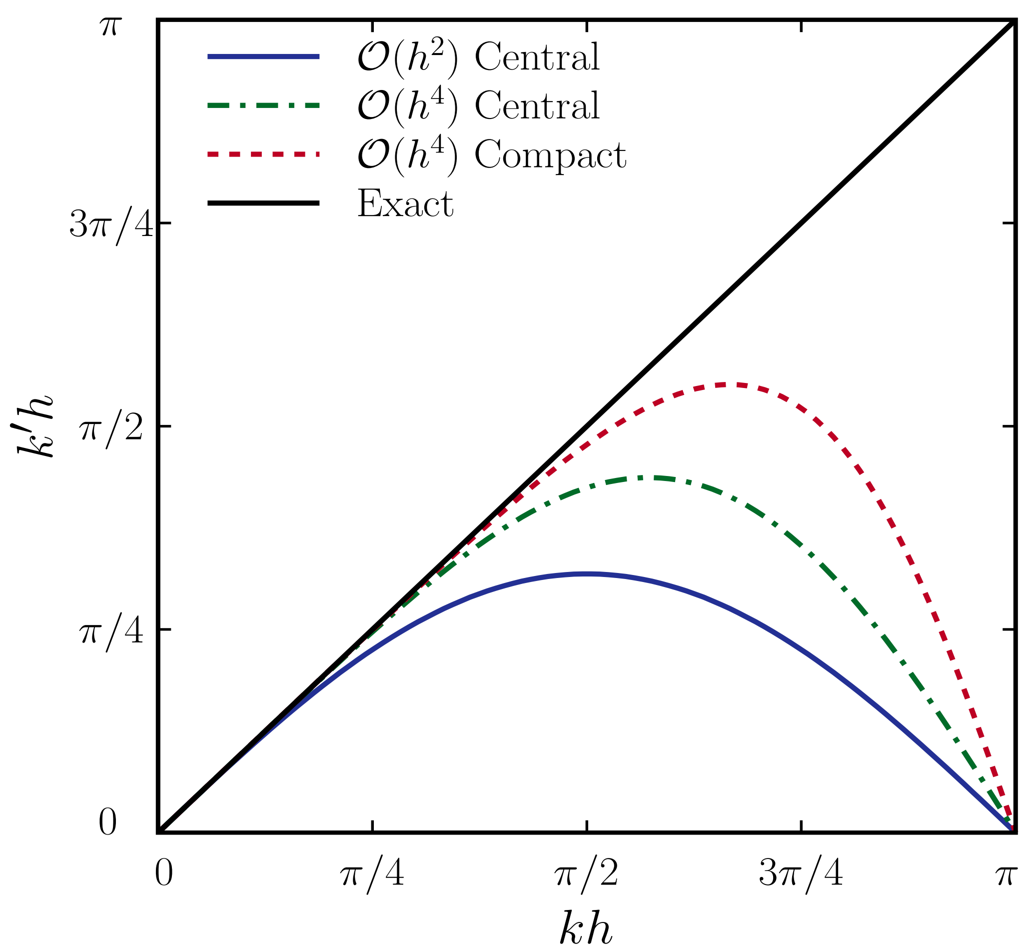
Outline of talk

- Will focus on low vs. high order discretizations

- Advantages of high-order
  - Fewer grid points for same error, asymptotically
  - Less data movement, more work per grid point
    - Memory slow, flops cheap on today's computers
    - Fewer memory loads/stores; more flops between them
- Advantages of low-order
  - Simple to understand, use & extend to new problems
  - Modeling errors often greater than numerical errors
    - Order of accuracy limited by the weakest link in practice, e.g. geometry definition, LES SGS models, chemistry, aliasing, etc.
- 2nd-order schemes adopted in recent CTR work

What do you get with higher-order?

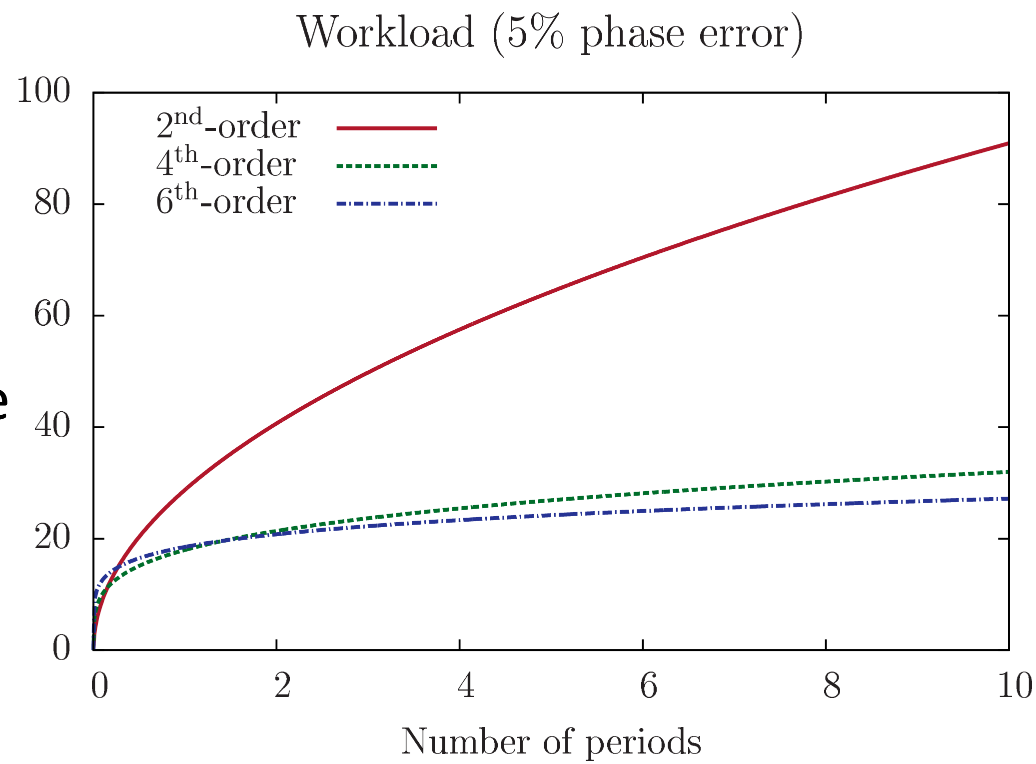
- Turbulence is multi-scale
  - On grid of size h, the "modified wavenumber" quantifies the numerical differentiation error
- Turbulence is non-linear
  - Sub-grid λ<2h eddies interact with flow near the grid cut-off λ=2h
  - Aliasing error is largest at the smallest scales owing to discrete representation
- Higher-order methods allow more scales but introduce additional errors (e.g., aliasing)



High-order advantages: accuracy

- Tight link between fewer points with greater coupling
  - Reduces per-core memory bandwidth needs, but
  - Block dense (high-order) more difficult to solve than sparse (lower-order) linear systems; precondition with low-order

- Compute savings in 1D
  (Kreiss & Oliger, 1972)
  - 8x fewer points in 3D
    (5% phase error, 4th-order)
  - 4th-order more attractive for high-accuracy & very long-time integration
  - $u_t + cu_x = 0;\ u(x,0)=e^{i2\pi kx}$



2D Example

Hyperbolic PDE with Periodic Boundary Condition

$$\frac{\partial u(x,y,t)}{\partial t} - y\frac{\partial u(x,y,t)}{\partial x} + x\frac{\partial u(x,y,t)}{\partial y} = 0$$

Periodic B.C: $u(x \pm 2\pi, y \pm 2\pi, t) = u(x,y,t)$

The solution is constant along the characteristics: $x + iy = (x_0 + iy_0)e^{it}$

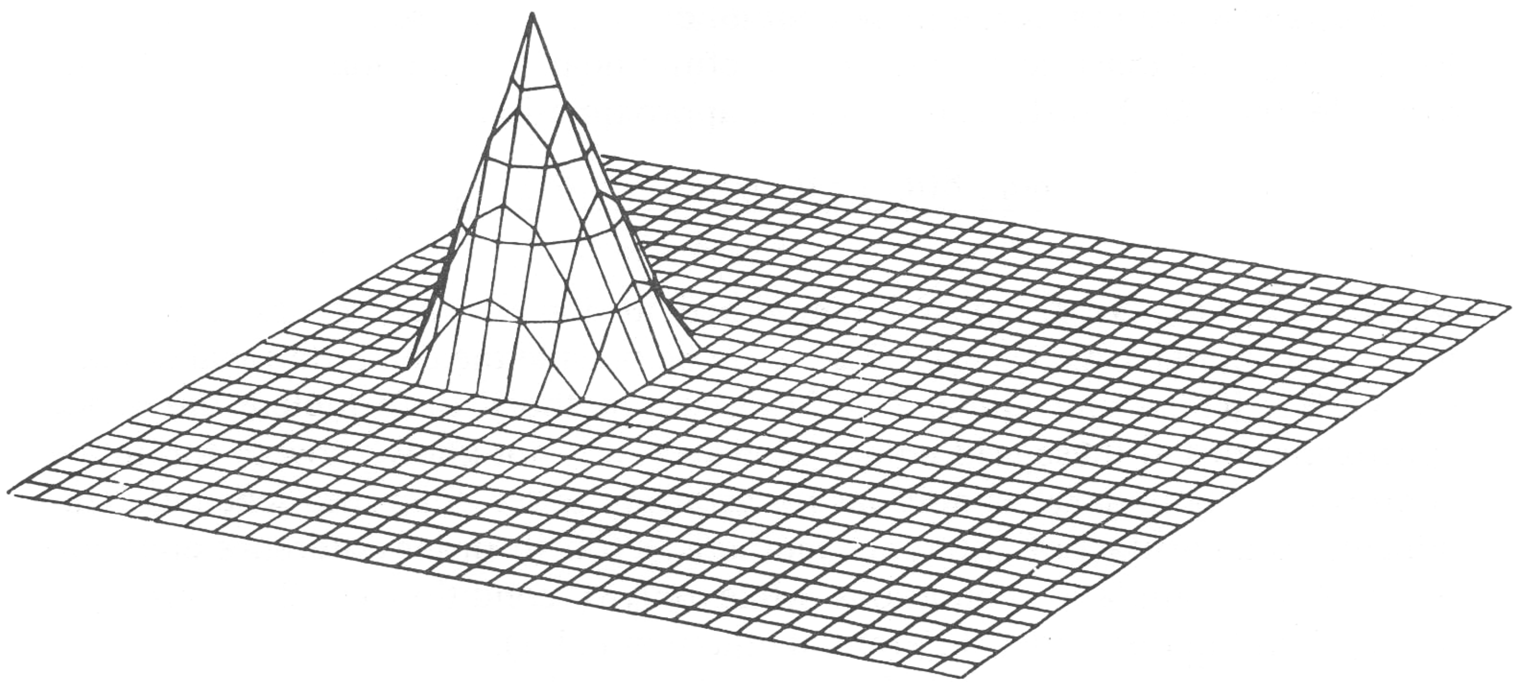
$$u(x,y,2\pi) = u(x,y,0)$$

1. 2nd order central difference with a 32x32 grid
2. 4th order central difference with a 32x32 grid
3. Fourier-spectral method with 32x32 nodes

From numerical analysis of spectral methods: theory and applications by Gottlieb and Orszag

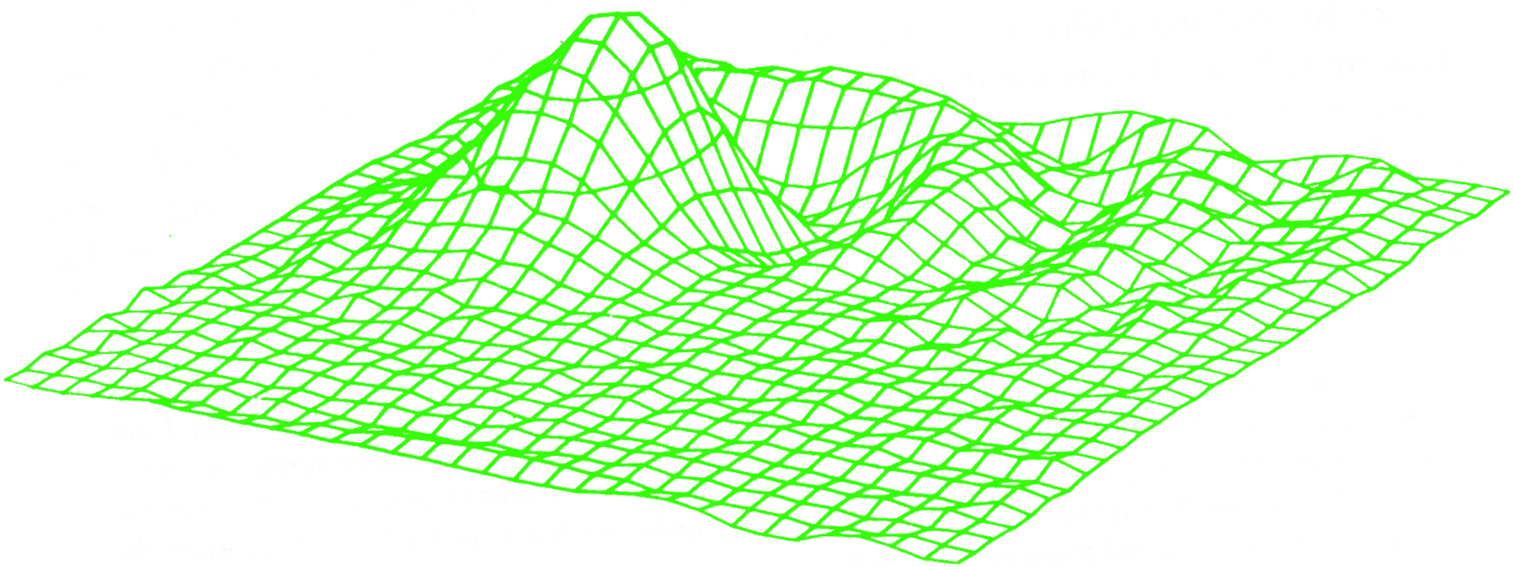
The Initial Condition

Initial condition: $u(x, y, t = 0)$



2nd order Central Difference

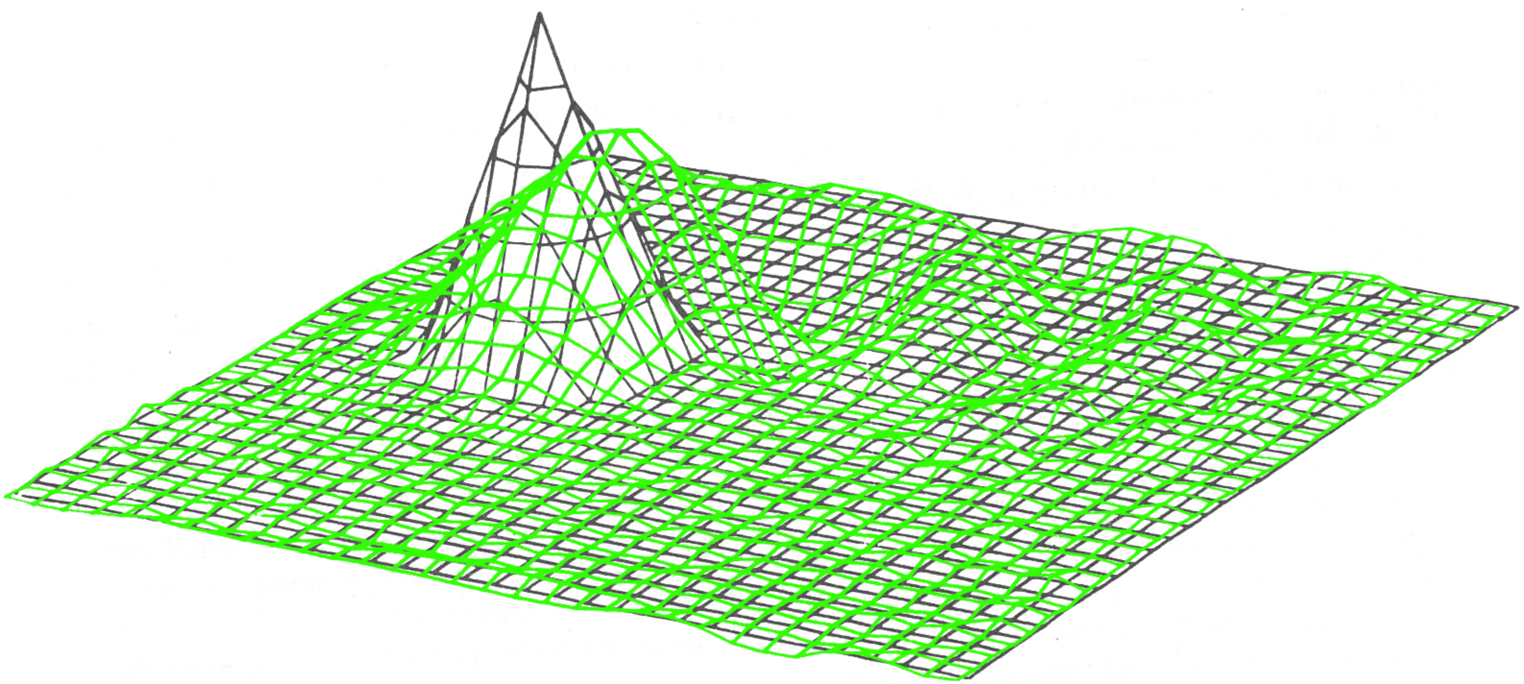
After one revolution: $u(x,y,t=2\pi)$



2^{nd} order Central Difference

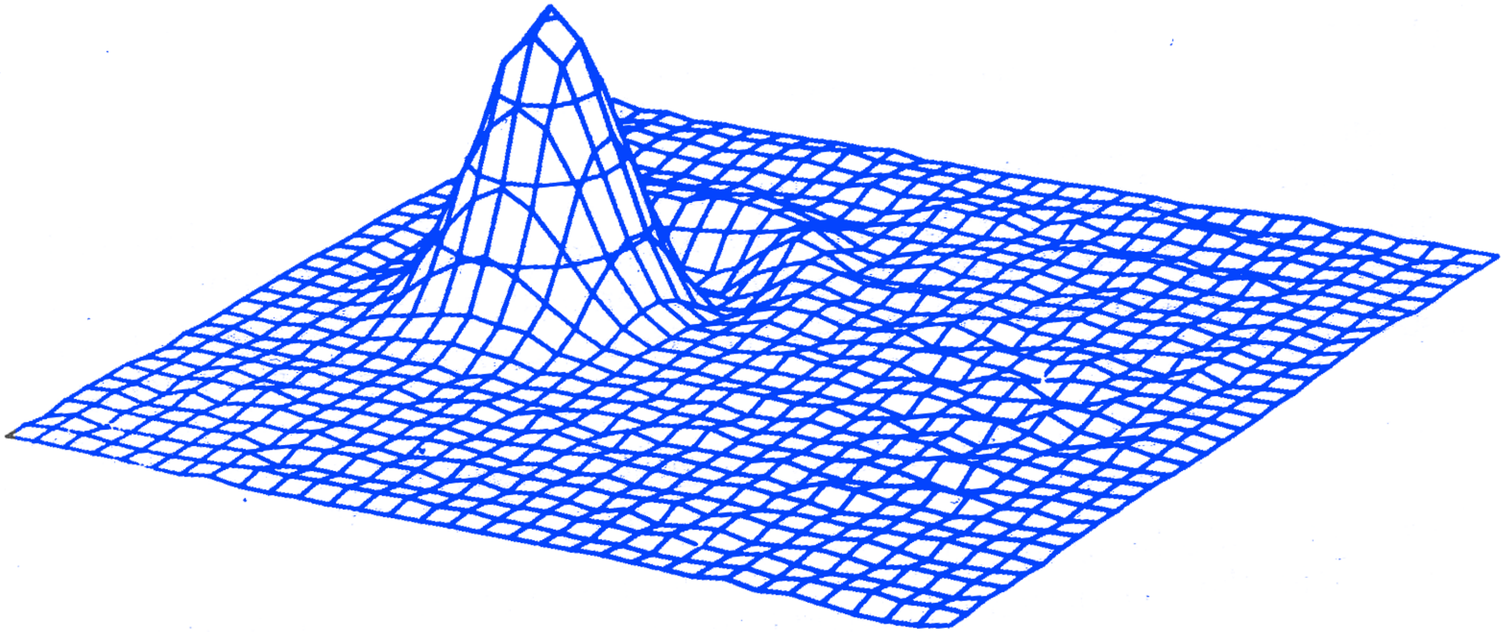
Initial condition: $u(x,y,t=0)$

After one revolution: $u(x,y,t=2\pi)$



4^{th} order Central Difference

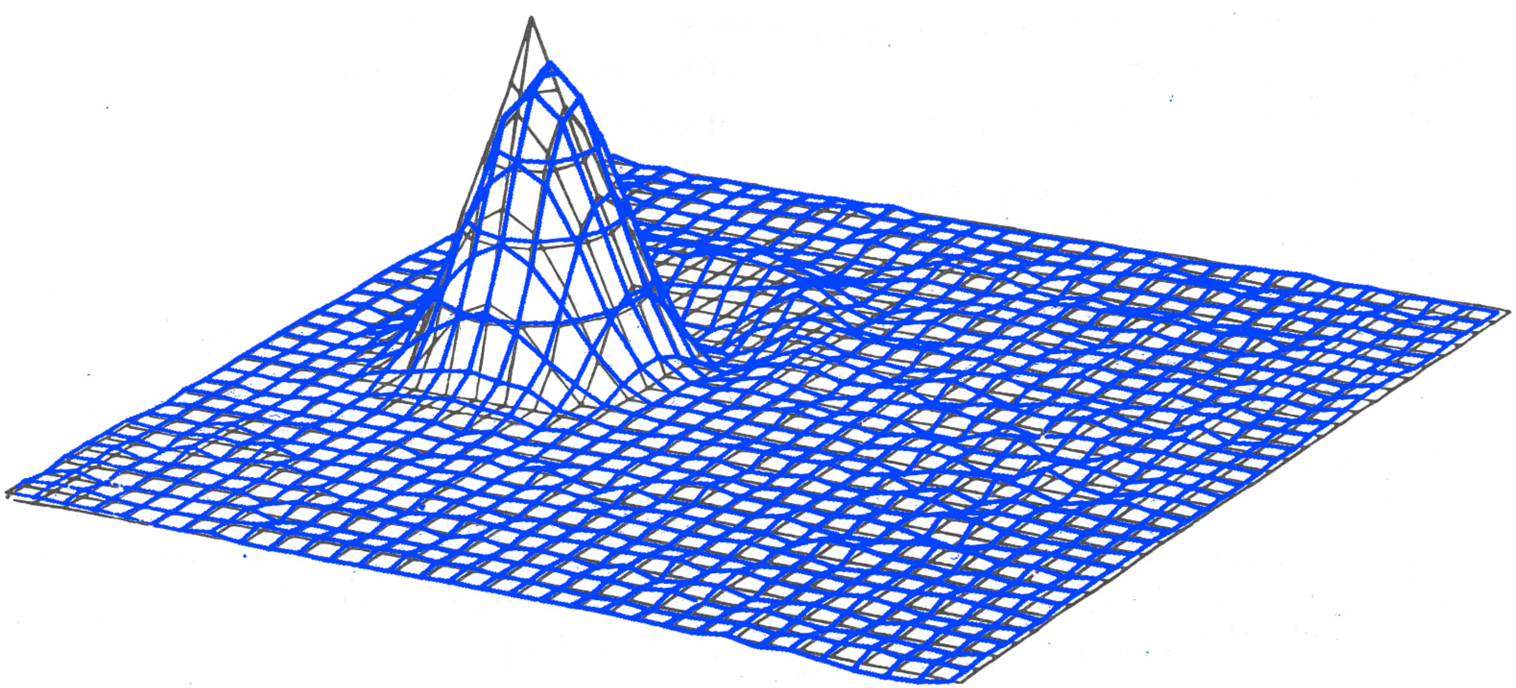
——— After one revolution: $u(x,y,t=2\pi)$



4^{th} order Central Difference

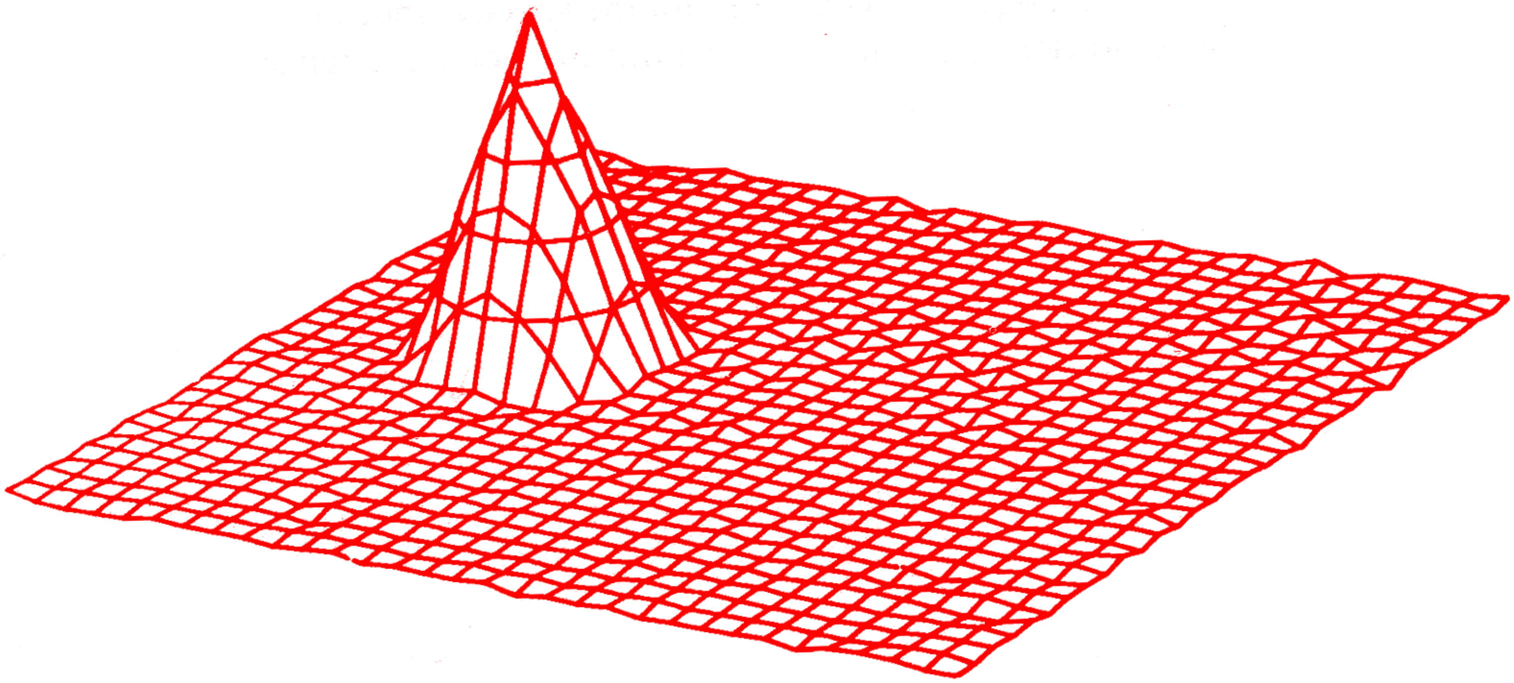
Initial condition: $u(x, y, t = 0)$

After one revolution: $u(x, y, t = 2\pi)$



Fourier-Spectral Method

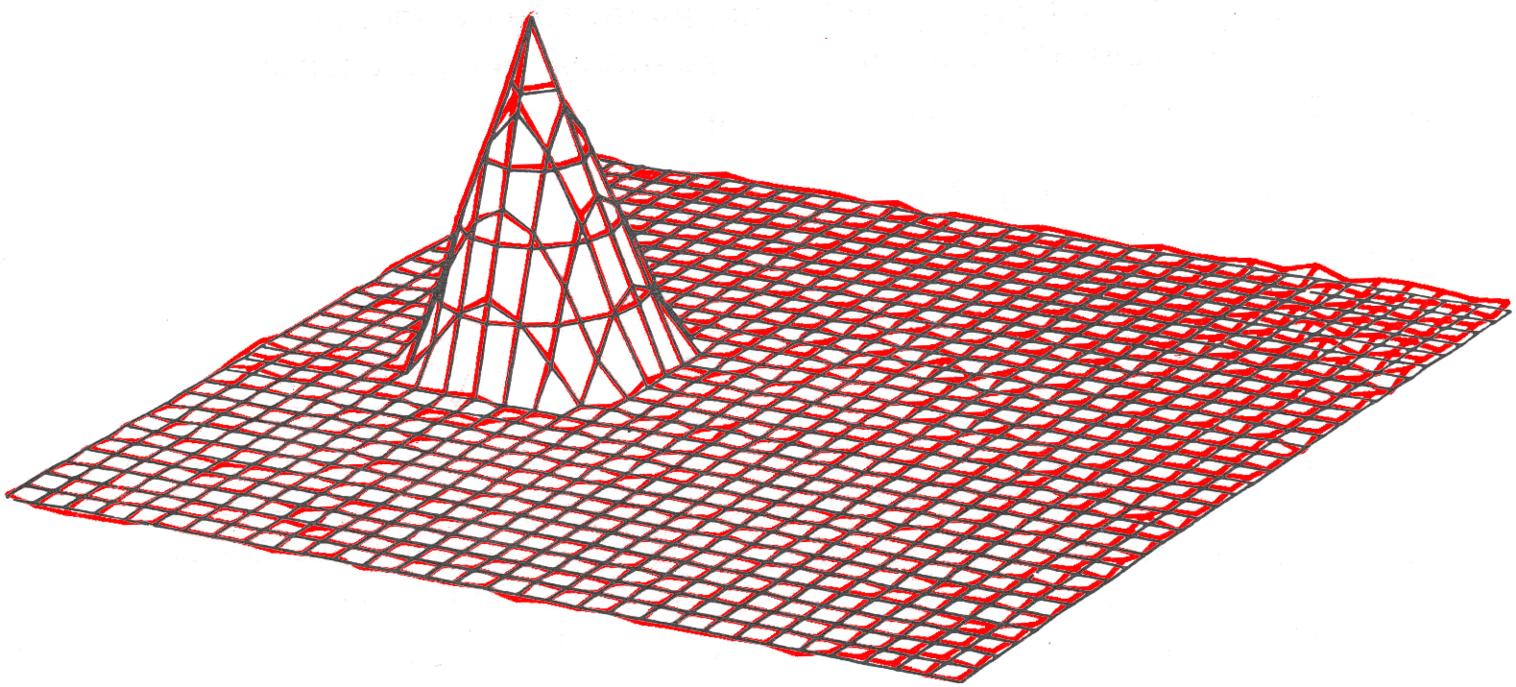
After one revolution: $u(x,y,t=2\pi)$



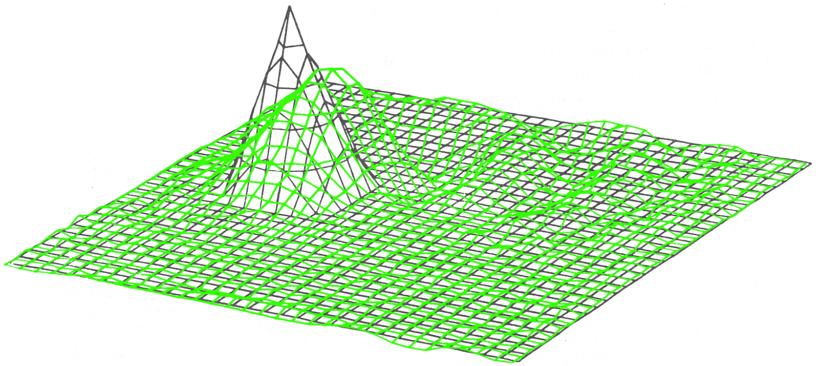
Fourier-Spectral Method

Initial condition: $u(x,y,t=0)$

After one revolution: $u(x,y,t=2\pi)$

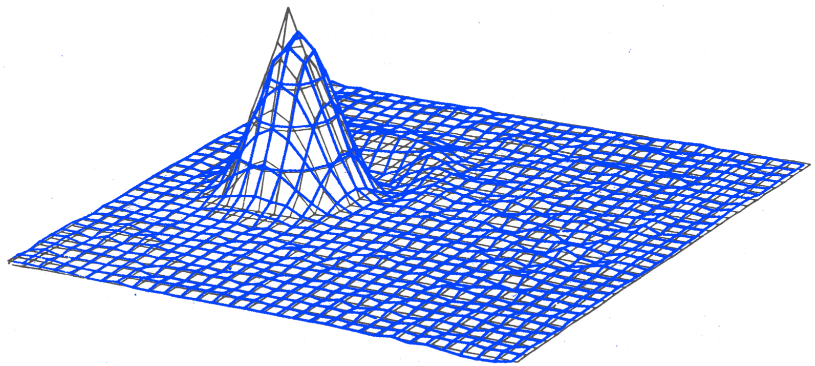


Comparison



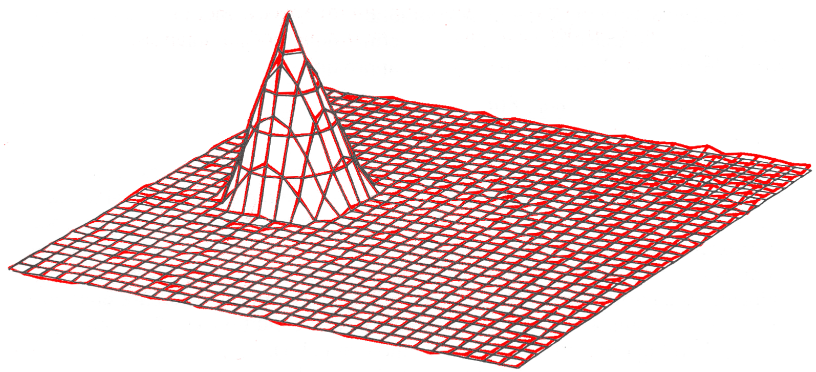
2nd order Central Difference

32x32 grid



4th order Central Difference

32x32 grid



Fourier-Spectral Method

32x32 nodes

Waves do very little mixing

- Why track waves over long distances with high-order FD when mixing is essential to all turbulent flows?

High-order advantages: modeling

- For high-order LES, ignoring Leonard term piles-up energy at small scales; no other mechanism to remove it (Kwak, Reynolds & Ferziger, 1975, TF-5)

$$\tau_{ij}^{\mathrm{R}} = \cancel{L_{ij}} + C_{ij} + R_{ij}$$
$$= \cancel{\overline{\overline{u}_i\overline{u}_j} - \overline{u}_i\overline{u}_j} + C_{ij} + R_{ij}$$

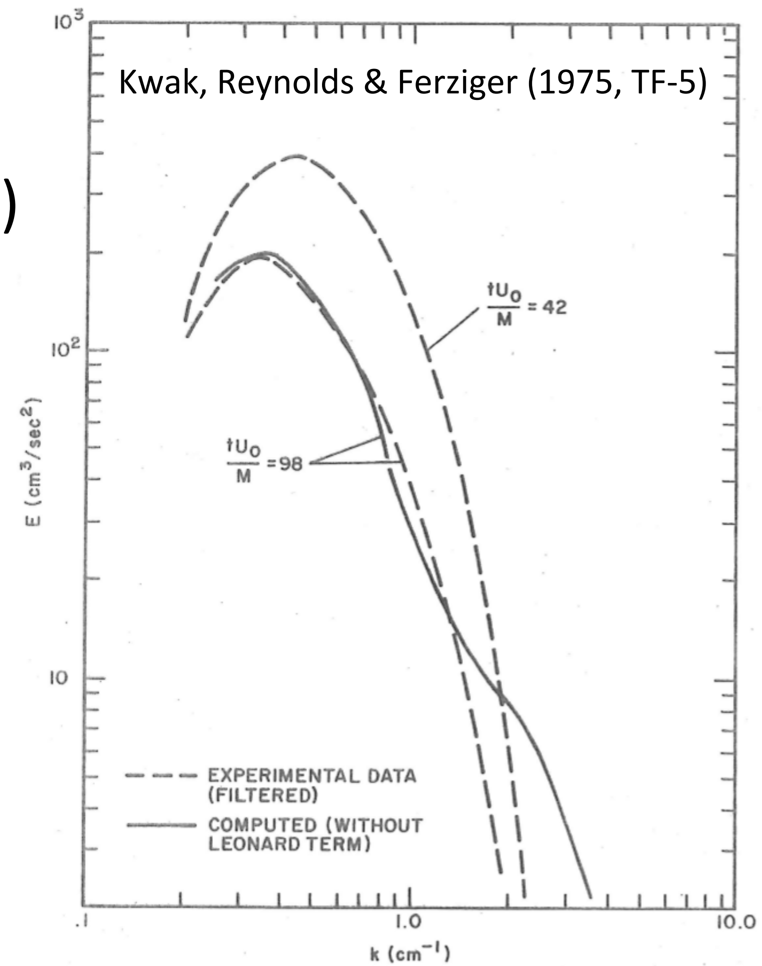


Fig. 4.7. Filtered Energy Spectra-Effect of Leonard Term 16x16x16 Mesh: Vorticity Model:

$\Delta_A = 2\Delta$; $\Delta = 1.5$ cm

High-order advantages: modeling

- For LES, in limit of small filter width Δ_A,

$$L_{ij} = \overline{\overline{u}_i \overline{u}_j} - \overline{u}_i \overline{u}_j$$
$$= \frac{\Delta_A^2}{24} \frac{\partial^2 \overline{u}_i \overline{u}_j}{\partial x_k \partial x_k} + \mathcal{O}(\Delta_A^4)$$

- Separates modeling from some discretization errors
  - No new modeling ideas since the dynamic procedure (CTR, 1990)
  - Explicit filtering a better approach to separate errors (Bose & Moin, 2010)

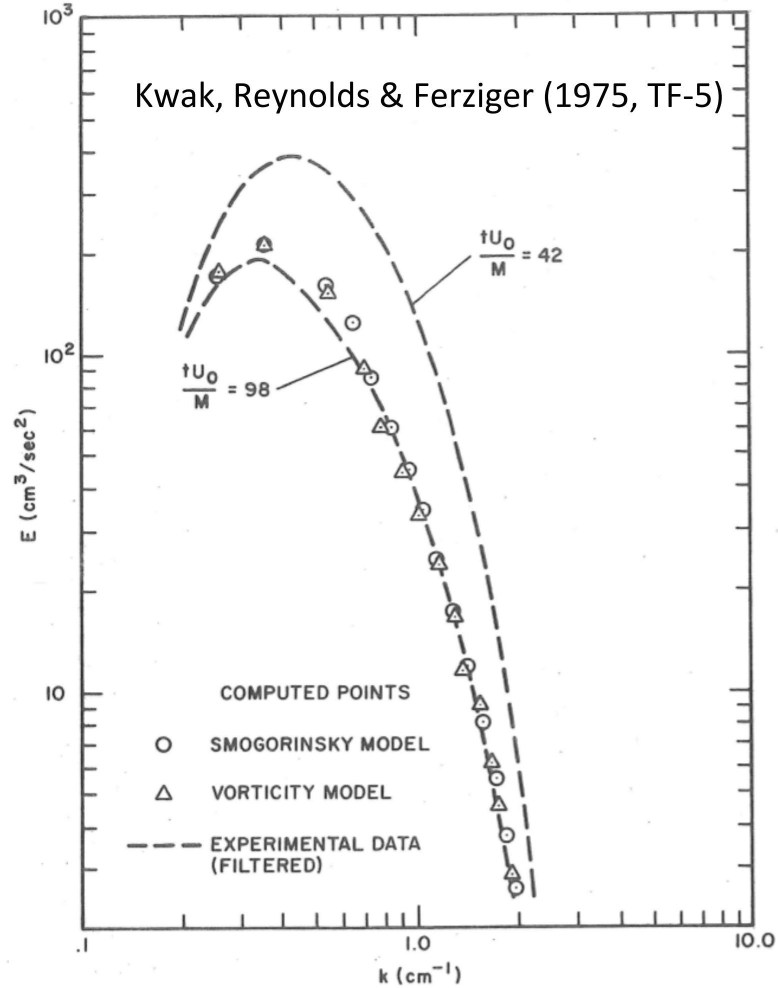
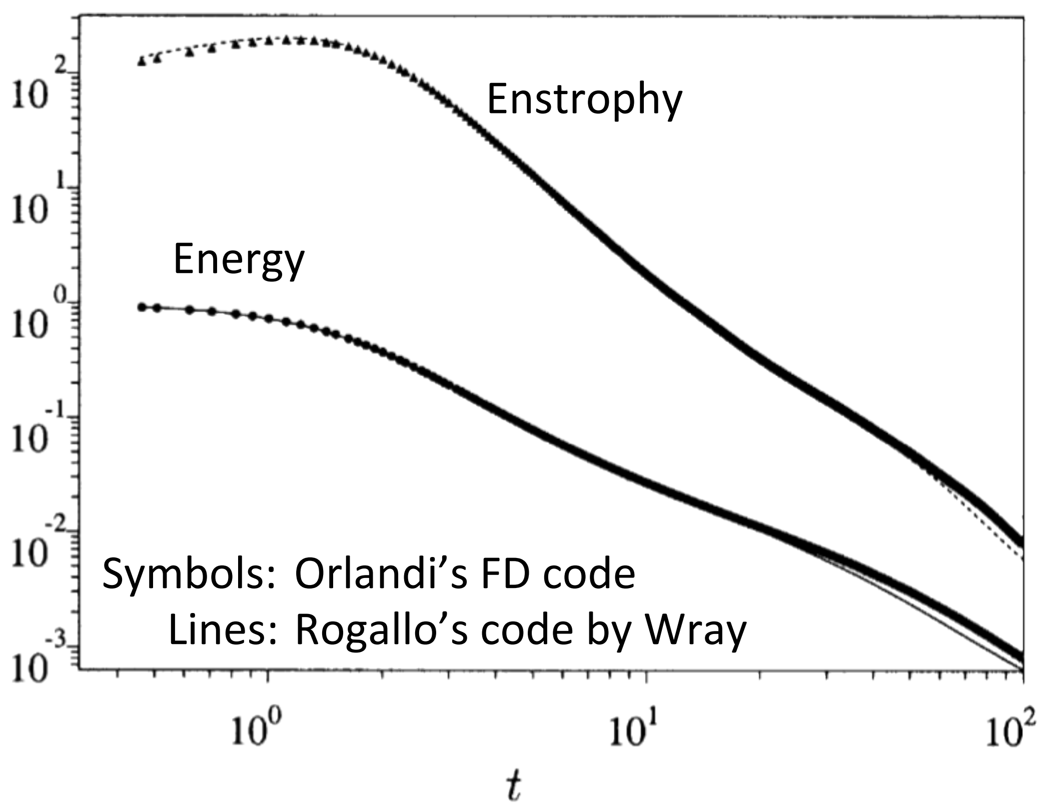
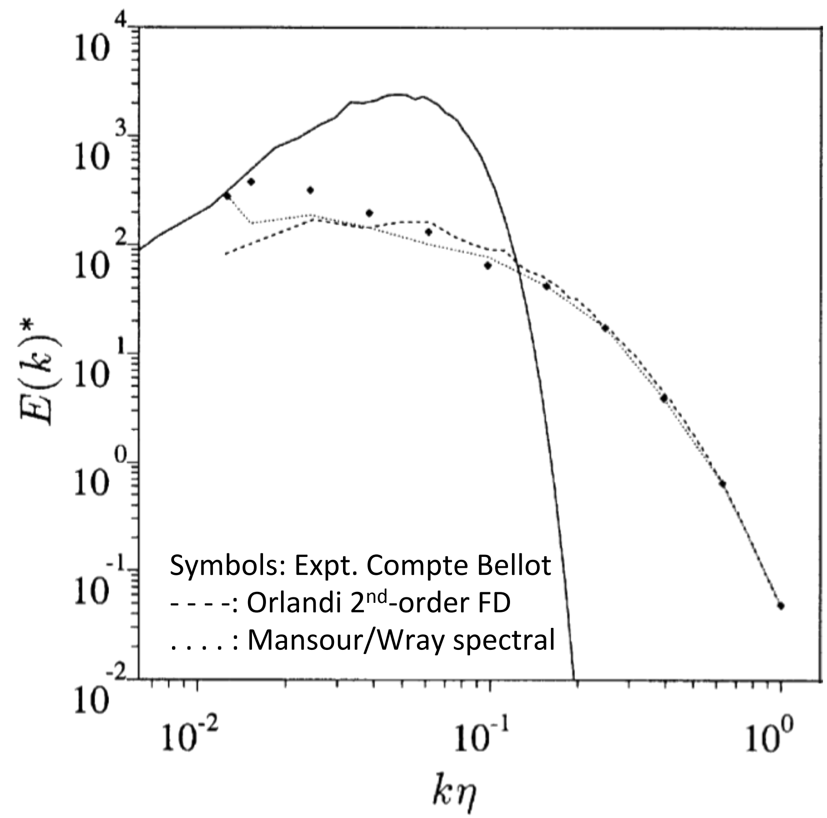


Fig. 4.6. Filtered Energy Spectra -- A Comparison of Smagorinsky and Vorticity Model
16x16x16 Mesh: $\Delta_A = 2\Delta$; $\Delta = 1.5$ cm

Low-order advantages: accuracy

- 2^{nd}-order, staggered FD as good as pseudospectral
  - FD reproduces both large and small scales
  - Same initial condition (t=0.46), 128^3 grid
  - Paolo showed this for the first time (Summer 1998 @ CTR)





From fluid flow phenomena: a numerical toolkit by Orlandi §8.11, p. 159-165

Low-order advantages: modeling

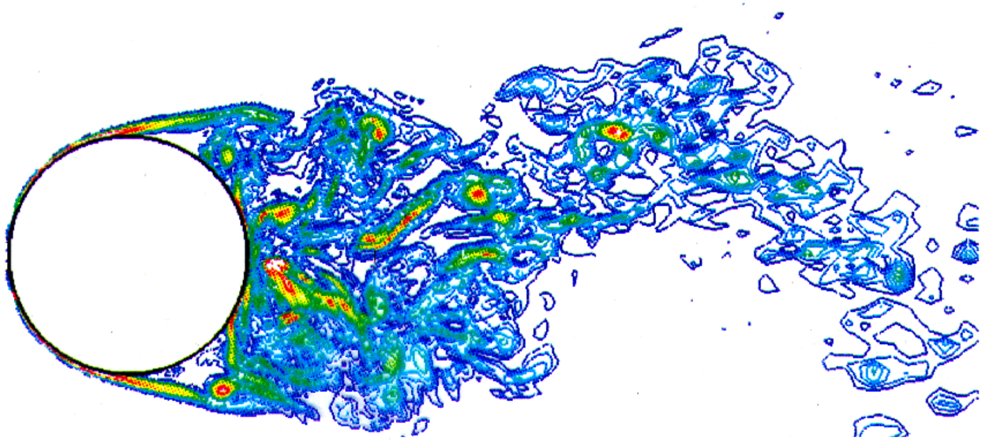
- 2^{nd}-order discretization error decays faster than LES model errors (Lilly, 1967, CTR 1988)

$$\tau_{ij}^{\mathrm{R}} \sim \mathcal{O}[(\varepsilon\Delta_A)^{2/3}]$$

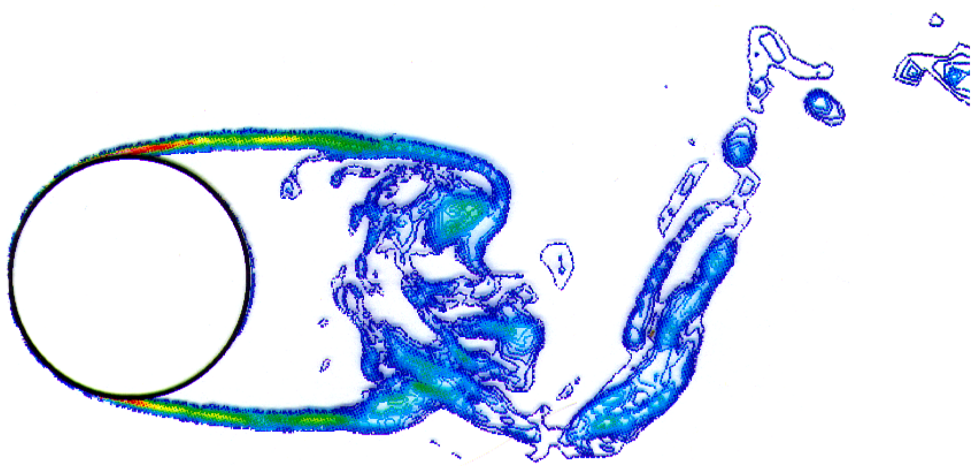
- Why use higher-order when modeled terms exceed 2^{nd}-order truncation error?

Which turbulence simulation is (more) correct?

1.

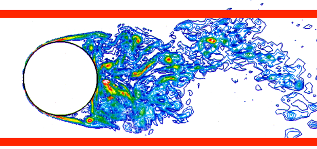


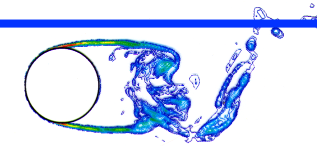
2.

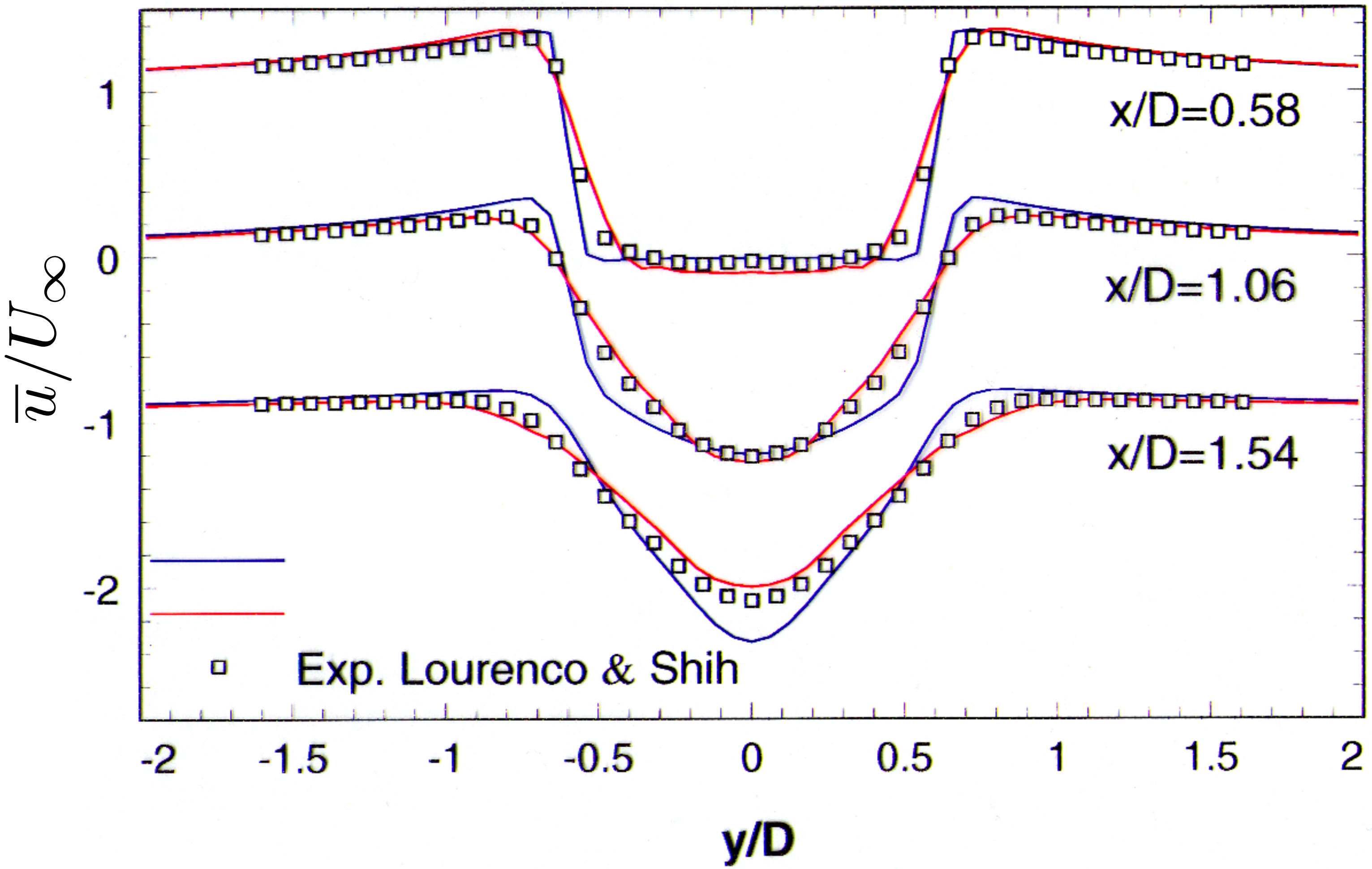


Cylinder, Re = 3900, Contours of instantaneous vorticity magnitude

Quiz: Continued...

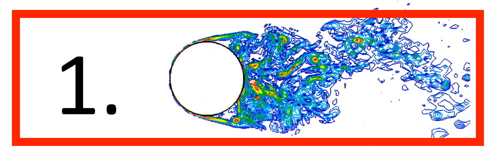
1. 

2. 

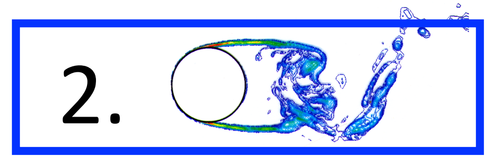


Quiz: Continued…

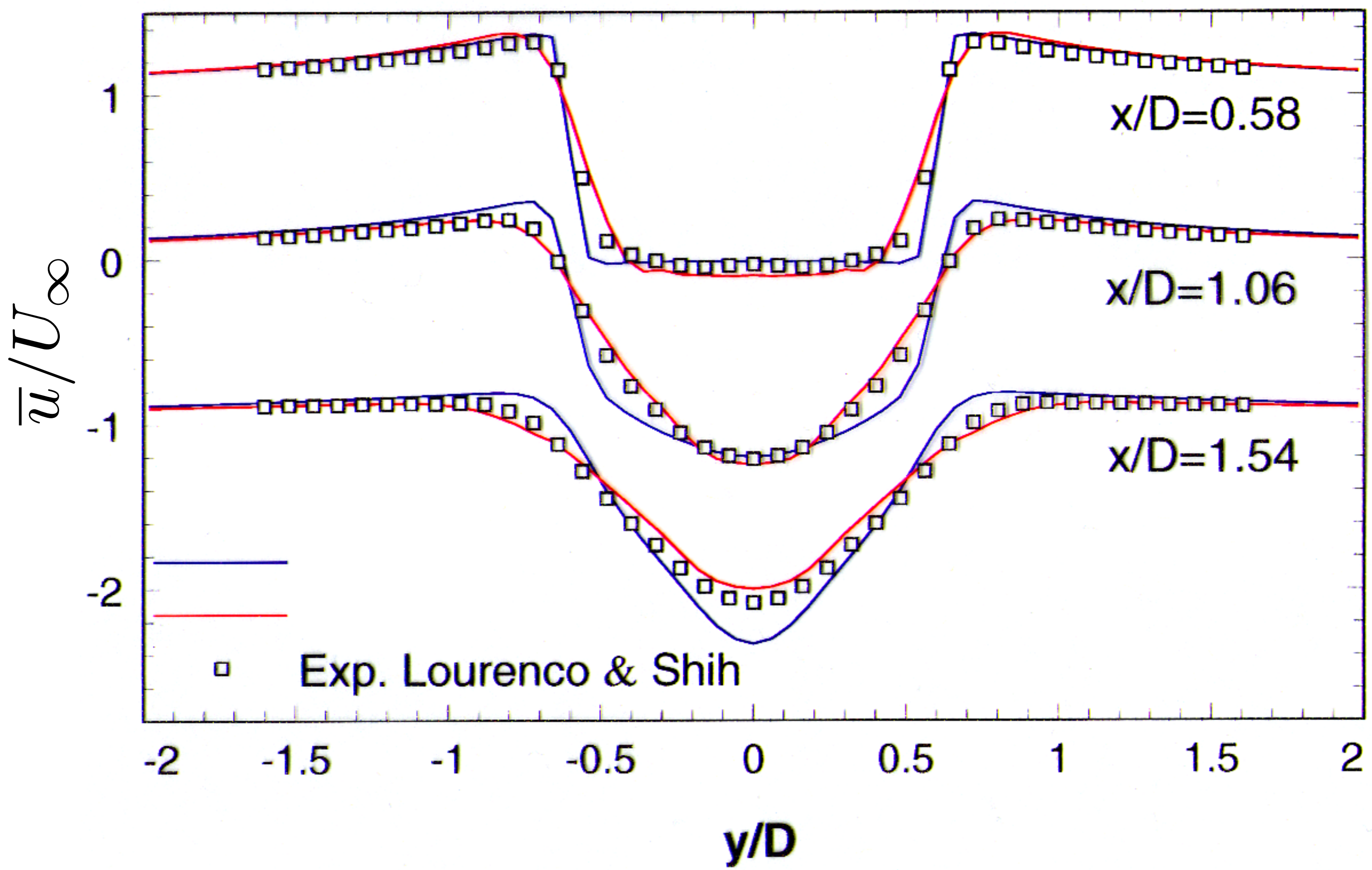
Comparison of mean streamwise velocity to experiments:



N_z=4

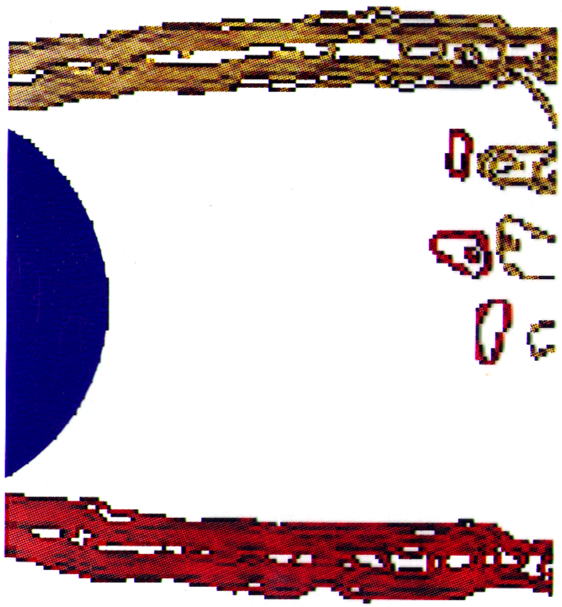


N_z=48

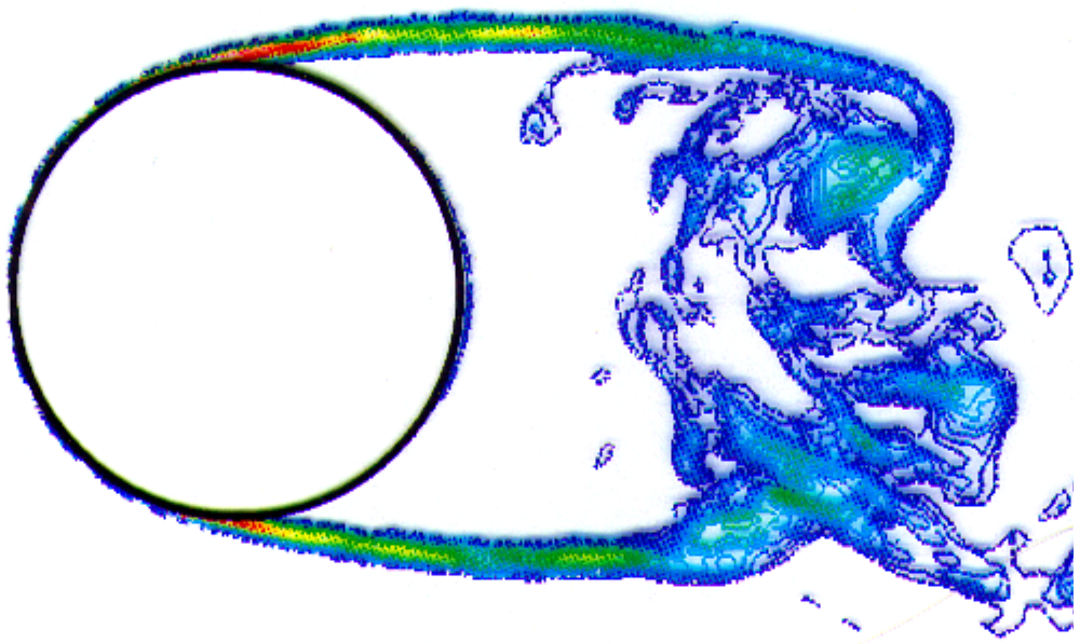


Answer: Number 2!

- Early transition was occurring in both experiment (due to vibration) and the coarse high-order simulation.
- Other experiments confirm the finer simulations.



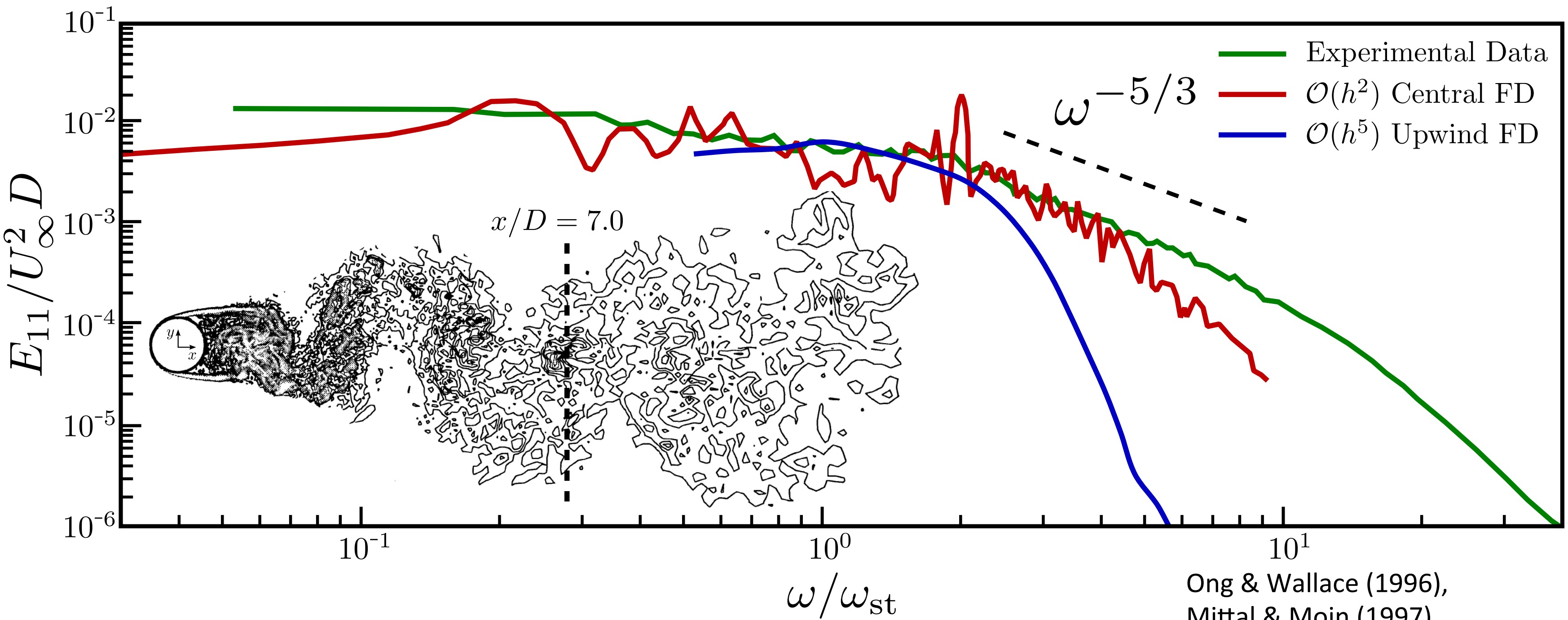
PIV Experiment of
Chyu and Rockwell (1996)



Numerical simulations with Nz = 48
Kravchenko and Moin (2000)

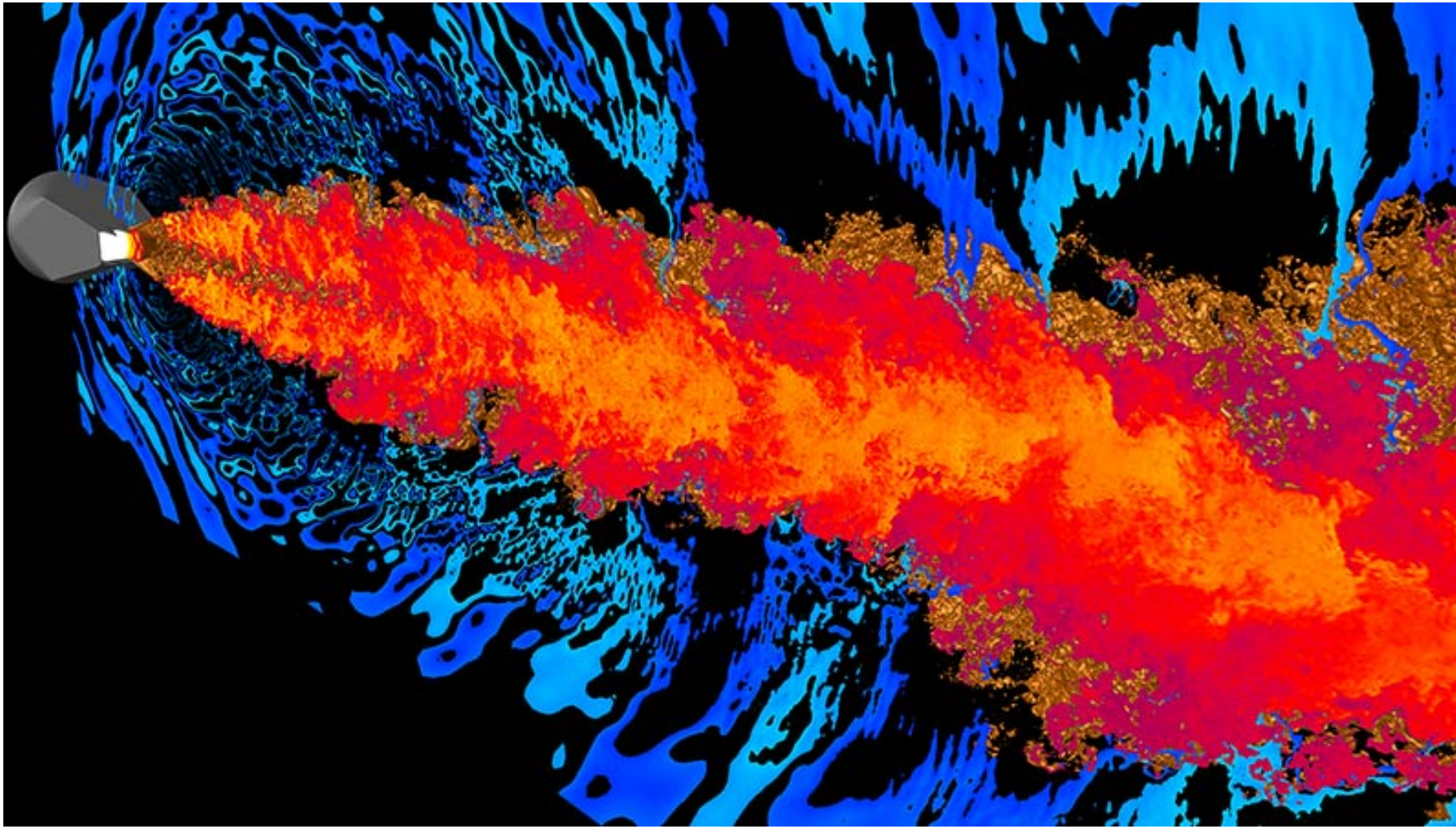
Higher-order does not mean higher-accuracy

- Assumes resolution is in the asymptotic limit
- For practical simulations of turbulent flows in complex geometry, this limit is not reached



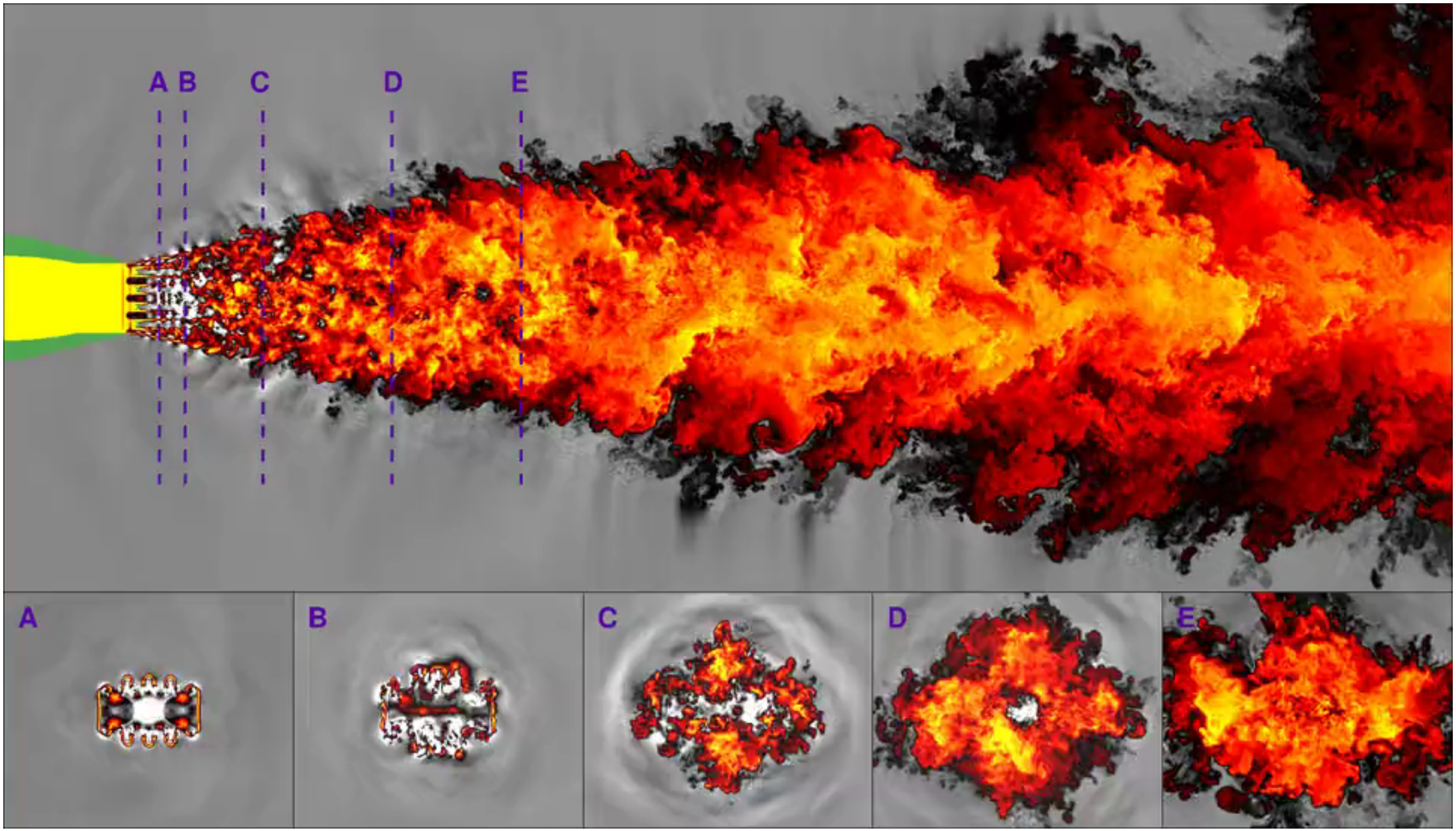
Ong & Wallace (1996),
Mittal & Moin (1997),
Beaudan & Moin (1994, TF-62)

Complex geometry with 2nd-order



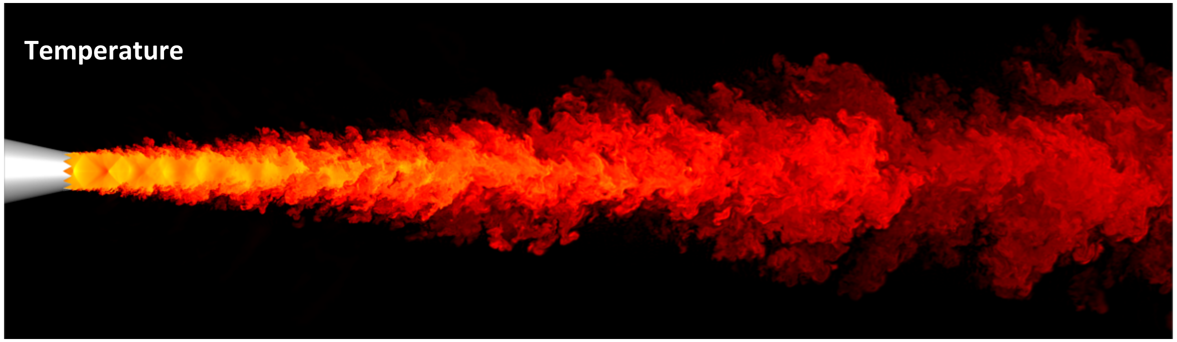
1 million core calculation of supersonic jet noise from a nozzle with chevrons - J. Nichols

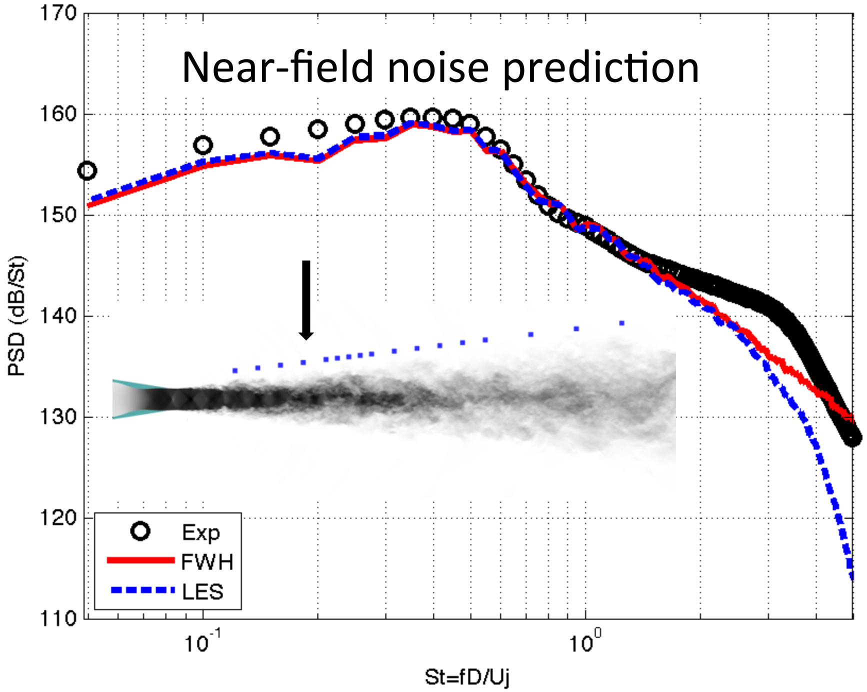
Complex geometry with 2nd-order

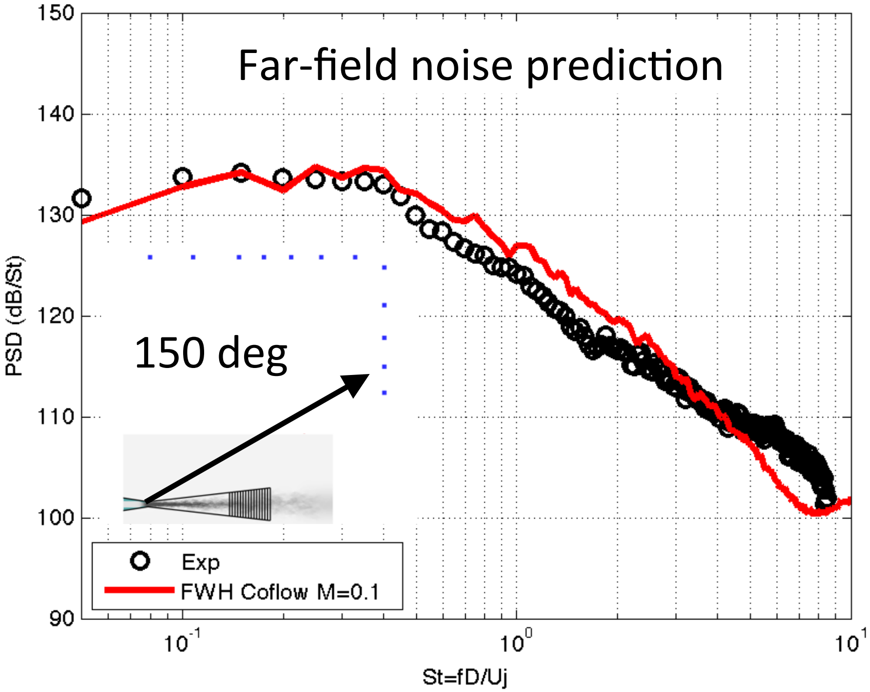


Hot Supersonic Over-Expanded Jet (Chevron Nozzle) Noise Predictions (1 Million cores)

$M_j = 1.35$
$M_a = 1.84$
$T_j = 1.85$
$Re_j = 130{,}000$
mesh: 55M cells



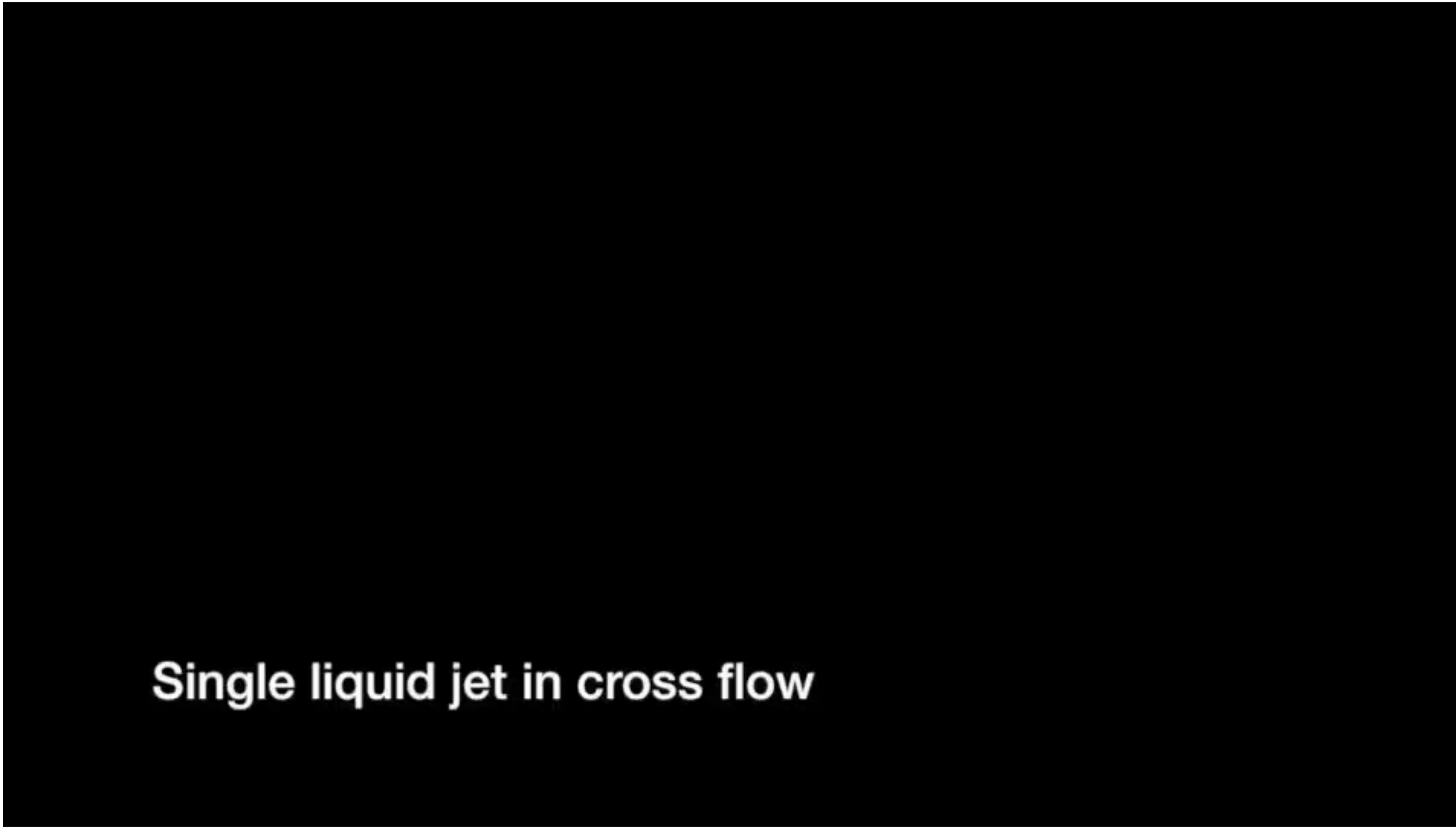




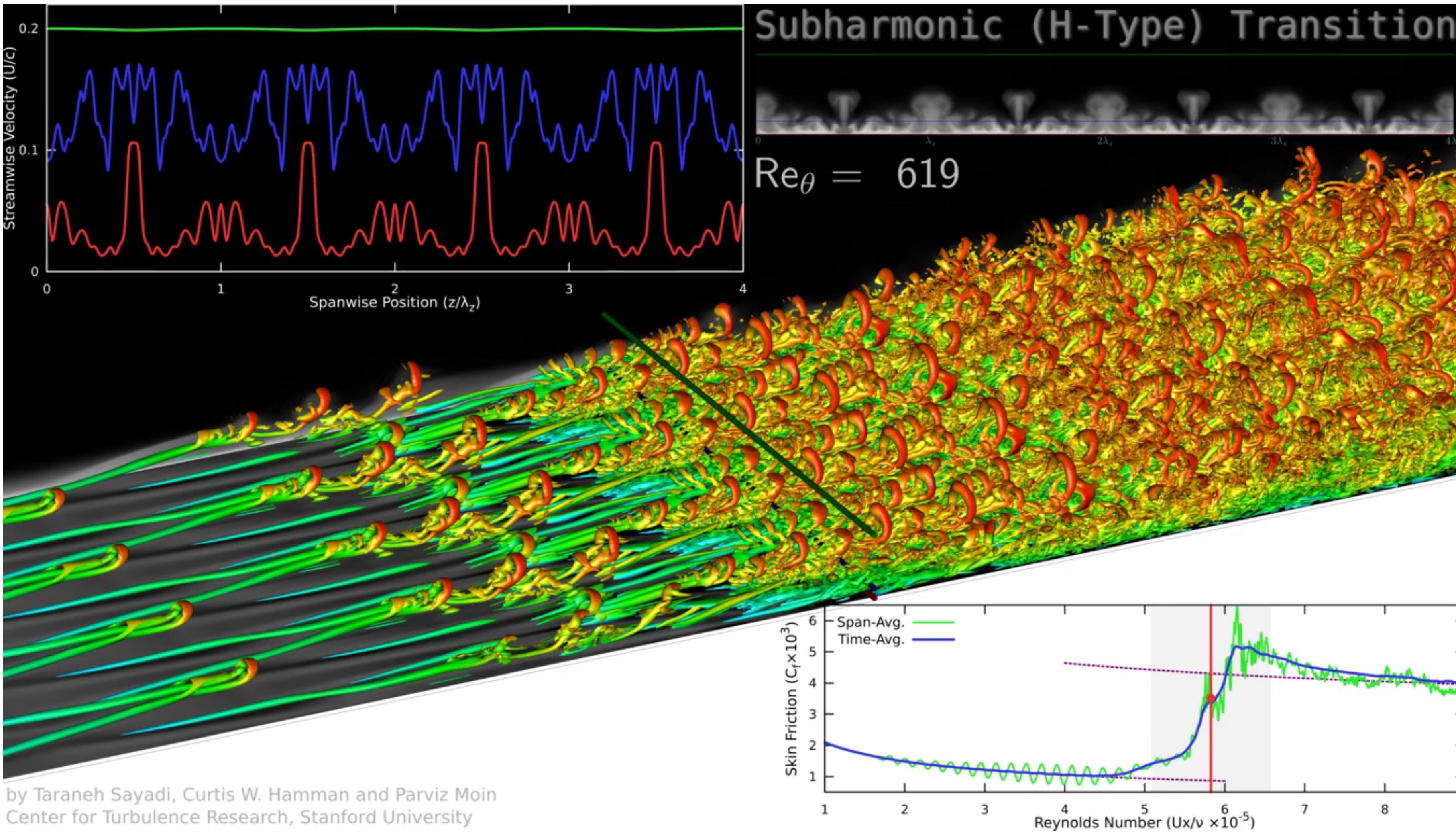
Blind comparison with UTRC experiment

CASCADE TECHNOLOGIES

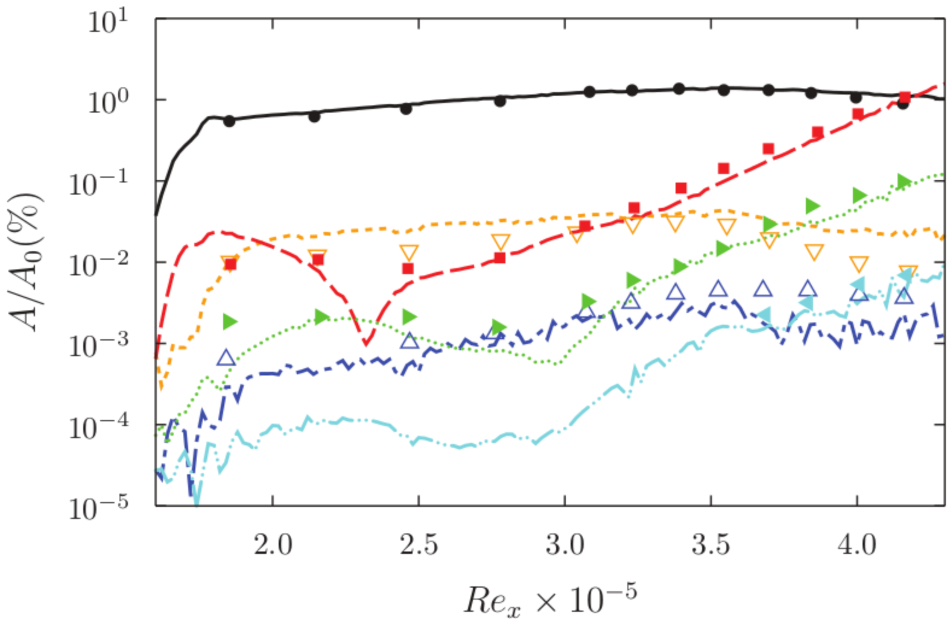
Two-phase flows with 2nd-order

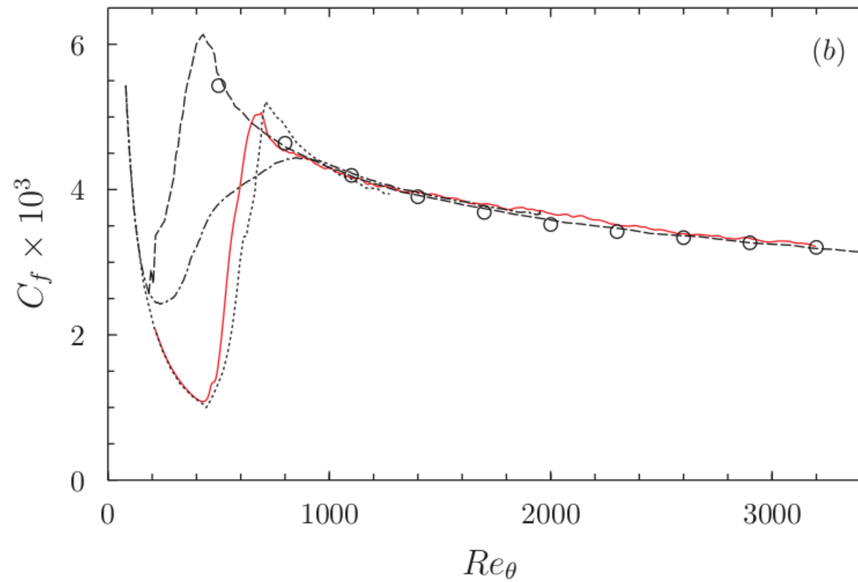


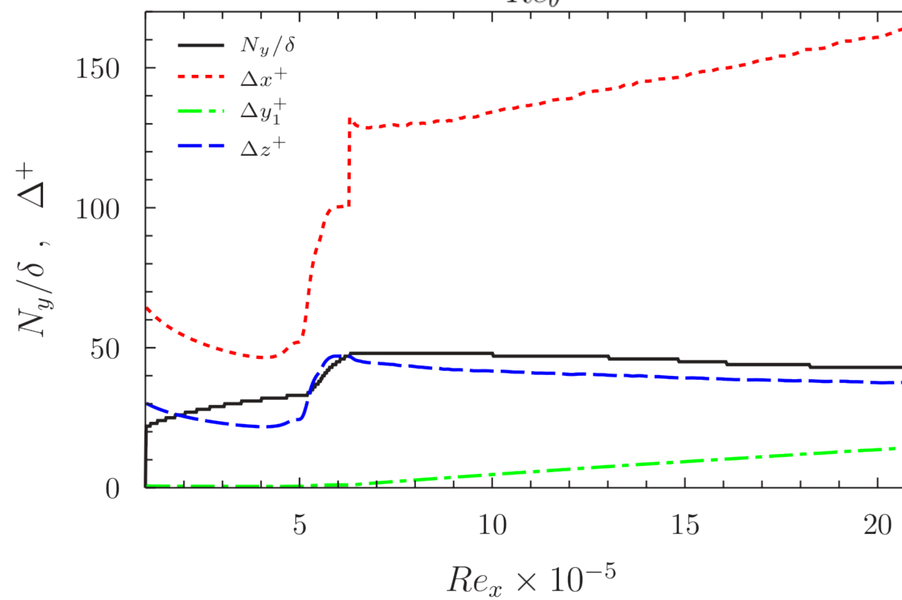
Boundary layer transition (4th-order)



2^{nd}-order predicts flow transition



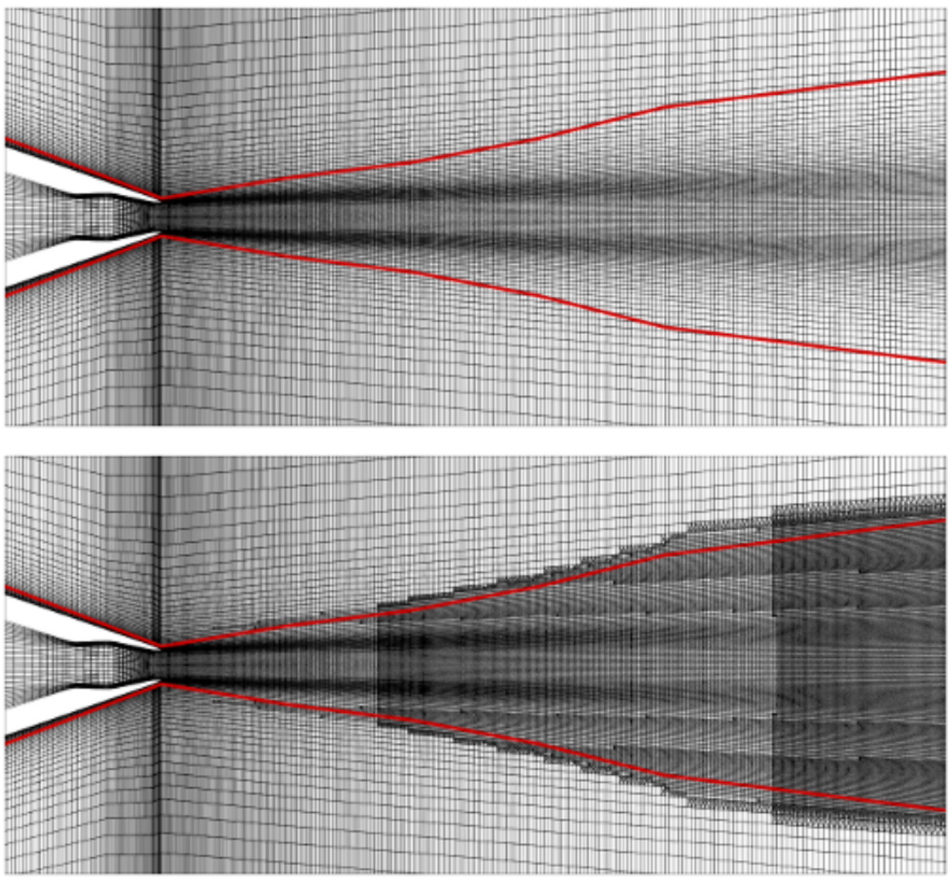




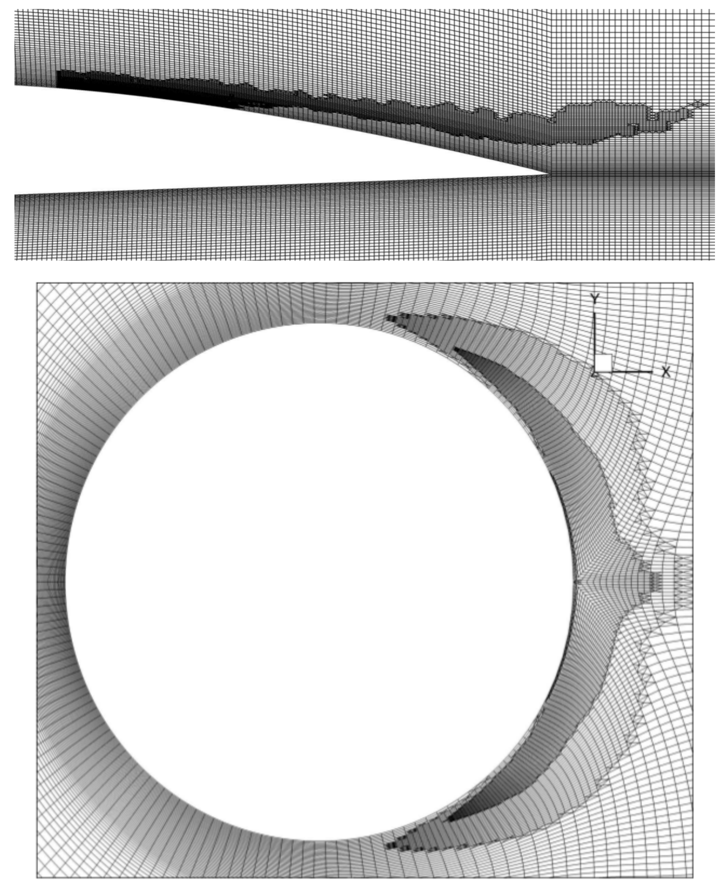
- CharLES 2^{nd}-order unstructured LES code (Park & Moin, 2014) predicted instability waves over long distance on **coarse** grid.
- Spectral elements filter near skin-friction peak to avoid blow-up due to aliasing errors (Ohlsson, Schlatter, Fischer, Henningson, 2011)

Adaptive grid refinement

- 2^{nd}-order more suitable for grid refinement
- Must use non-dissipative operators for LES



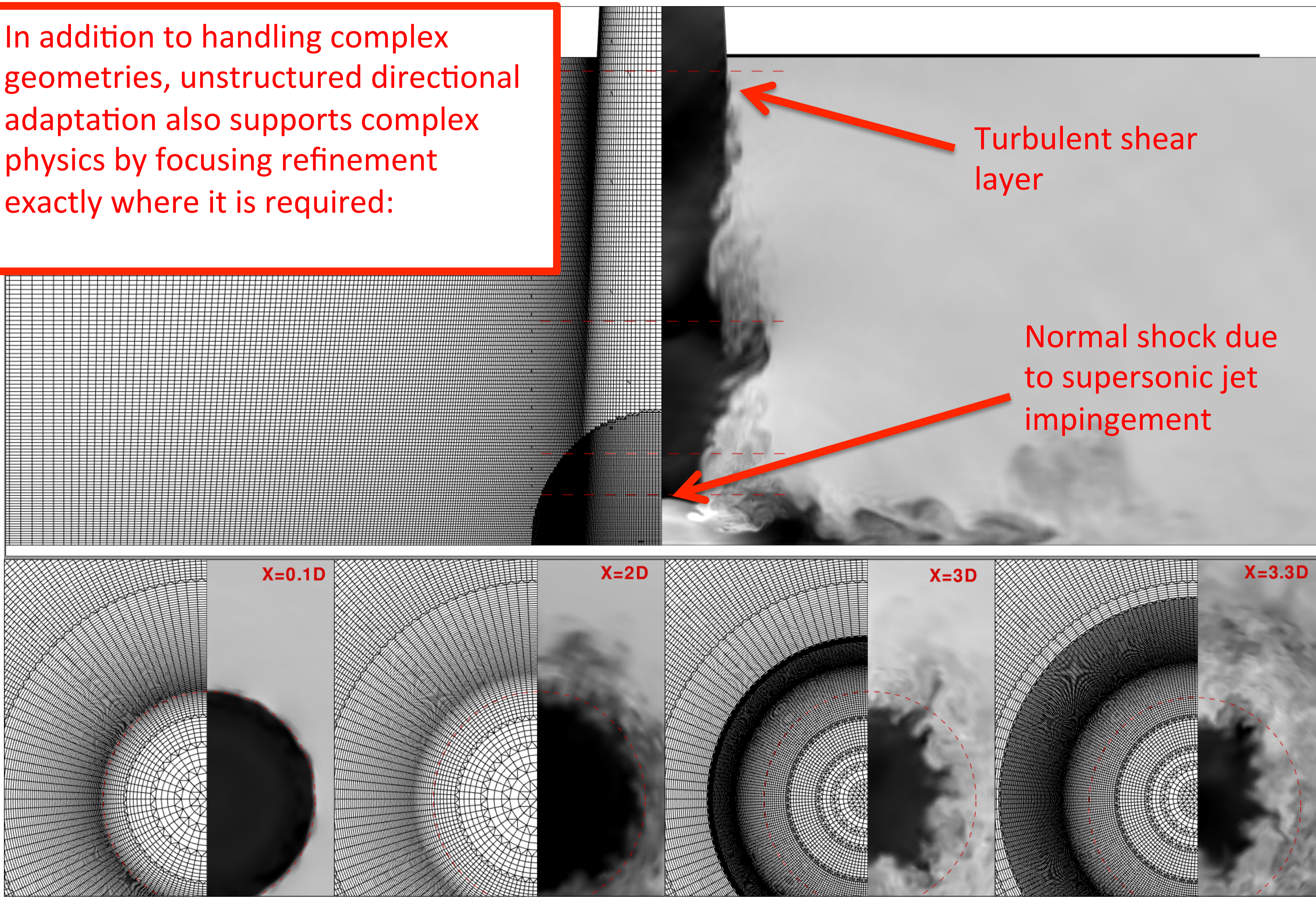
Jet noise (Nichols et al., 2012)



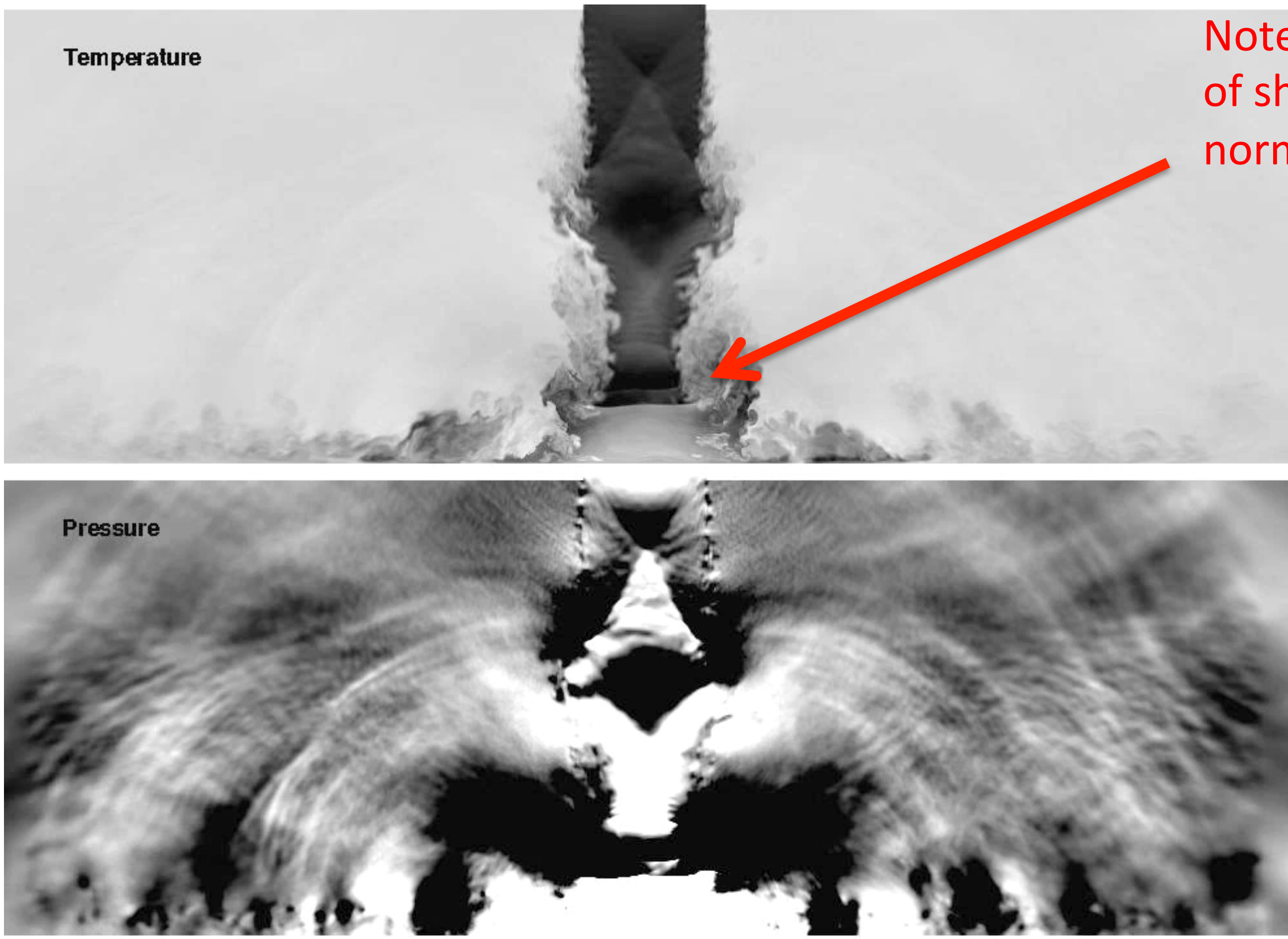
Complex geometry (Bose et al., 2012)

Directional-refinement capability in

In addition to handling complex geometries, unstructured directional adaptation also supports complex physics by focusing refinement exactly where it is required:

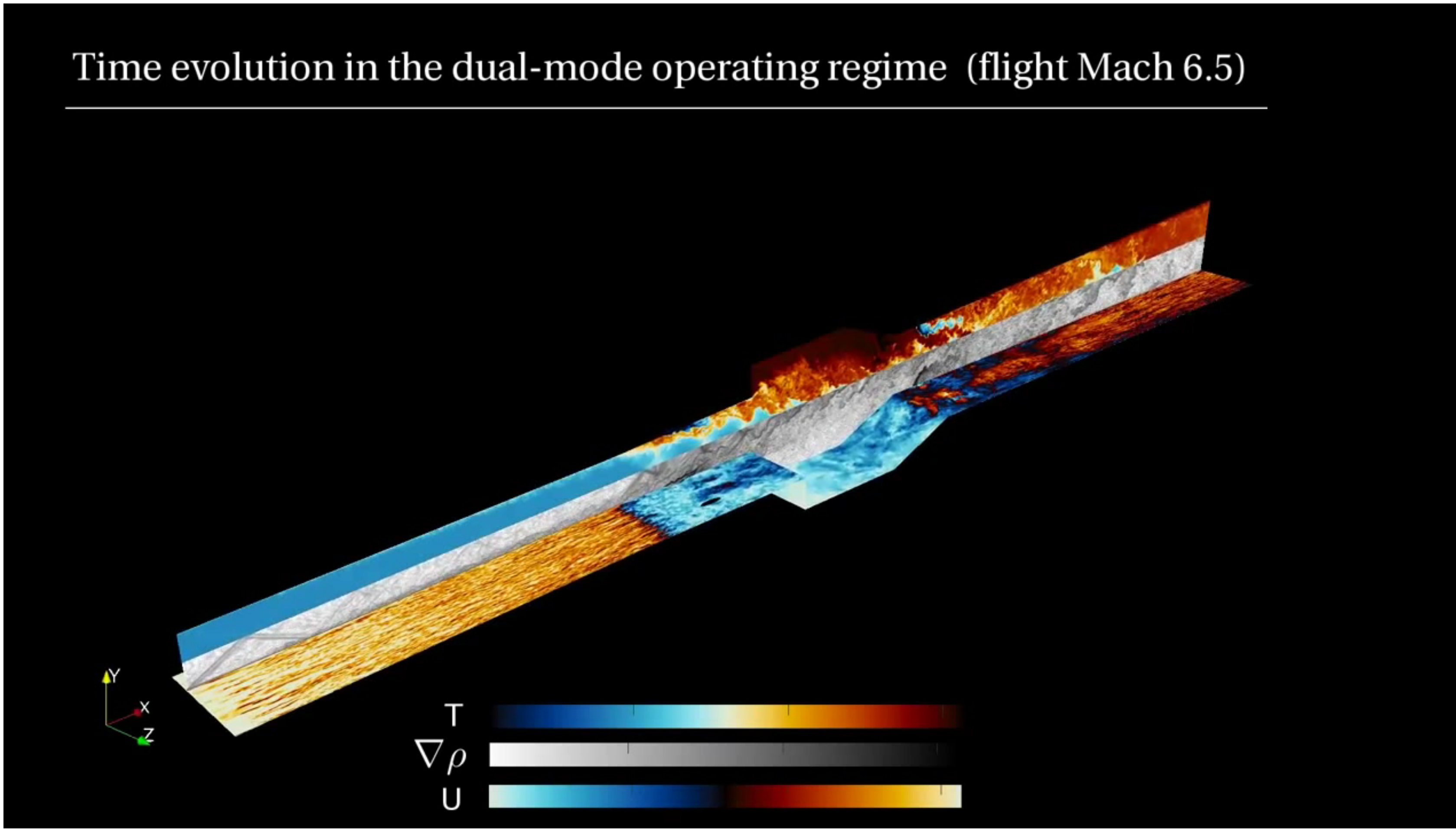


impingement (ideally-expanded)



Note interaction of shear layer and normal shock

Complex, multi-physics, reacting flows



Summary

- High-order has less dispersion error than 2nd-order
  - Helicopter tip vortices hitting the body, aeroacoustics
- Only for very long-time, linear advection equation
  - Easily lost for real geometry or non-smooth data
- Less need for high-order given other modeling errors
  - LES SGS models, aliasing, time-discretization, etc.
  - If you must filter? Why use higher order?
  - Not every step is high-order (meshing & geometry definition)
  - No clear advantage for real problems
- "High-order" calculations with insufficient resolution prone to mistaking numerical dynamics for fluid dynamics

Paolo at CTR summer programs

1990 CTR SP

Paolo and me (1987 CTR Summer Program)

1994 CTR SP

1992 CTR SP

1988 CTR SP

1998 CTR SP

2002 CTR SP

2000 CTR SP

1996 CTR SP

Anyone for a nice argument?!

Paolo and Javier (2002 CTR Summer Program)