Predictive CFD
Past, Present and Future

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KAUST PCCFD
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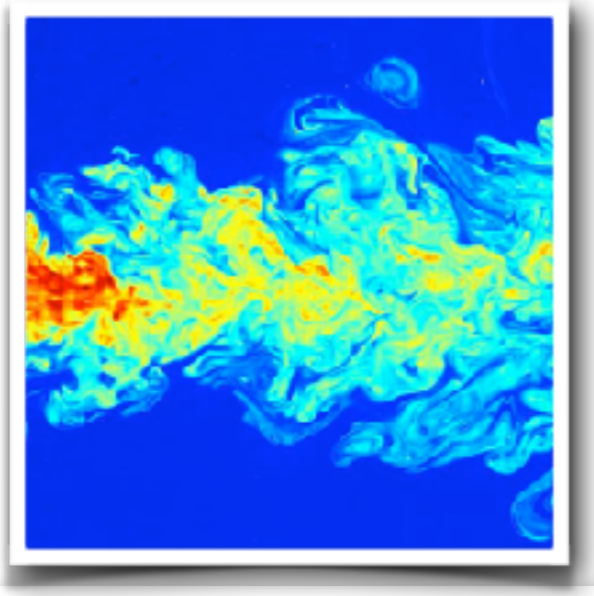
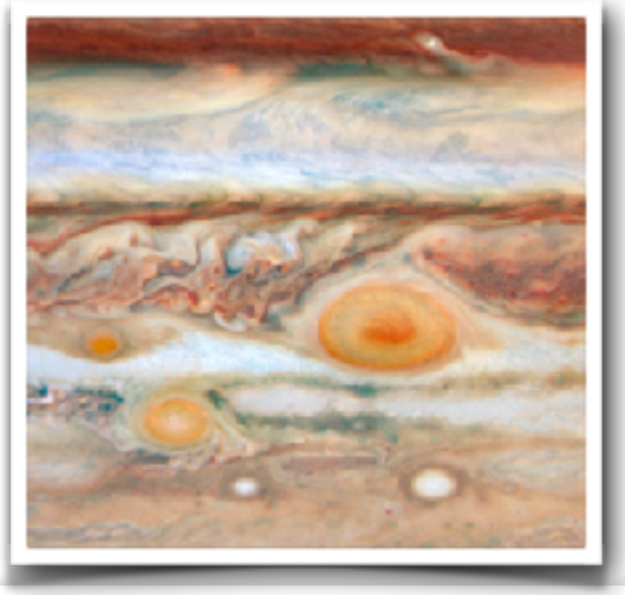
Outline

1. **Context**
2. History
3. CFD code development
4. Industrial use of CFD
5. Current status of CFD
6. Overview of numerical methods
7. Flux Reconstruction
8. Modern hardware and PyFR
9. LES computations
10. Summary and conclusions

Context

"When I die and go to Heaven there are two matters on which I hope enlightenment. One is quantum electrodynamics and the other is turbulence. About the former, I am really rather optimistic."





Sources: Wikipedia.org; NASA.gov; Hubblesite.org; *et al.*; H. Lamb (1932)

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History of CFD in Van Leer's View

Top level: Jay Boris, Vladimir Kolgan, Bram van Leer, Antony Jameson
Ground level: Richard Courant, Kurt Friedrichs, Hans Lewy, Robert MacCormack, Philip Roe, John von Neumann, Stanley Osher, Amiram Harten, Peter Lax, Sergei Godunov

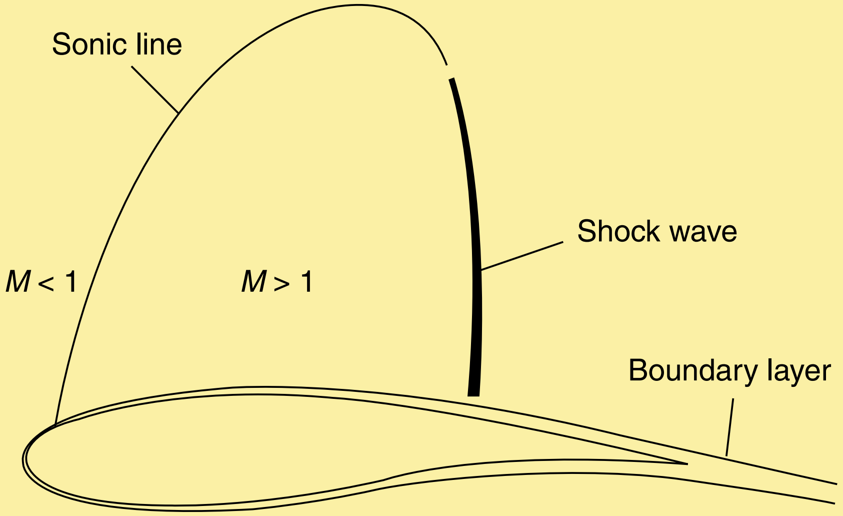
Emergence of CFD

- In 1960 the underlying principles of fluid dynamics and the formulation of the governing equations (potential flow, Euler, RANS) were well established
- The new element was the emergence of powerful enough computers to make numerical solution possible – to carry this out required new algorithms
- The emergence of CFD in the 1965–2005 period depended on a combination of advances in computer power and algorithms.

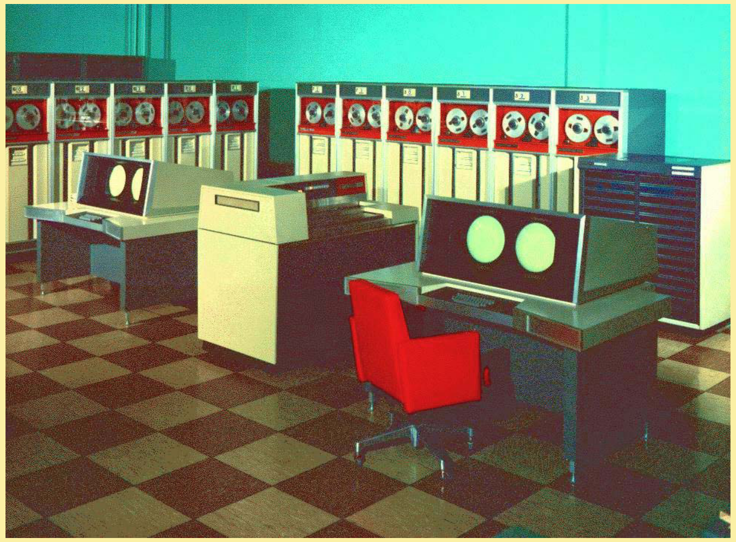
<u>Some significant developments in the ‘60s:</u>

- birth of commercial jet transport – B707 & DC-8
- intense interest in transonic drag rise phenomena
- lack of analytical treatment of transonic aerodynamics
- birth of supercomputers – CDC6600

DC-8



Transonic Flow



CDC6600

Why Transonic Flow?

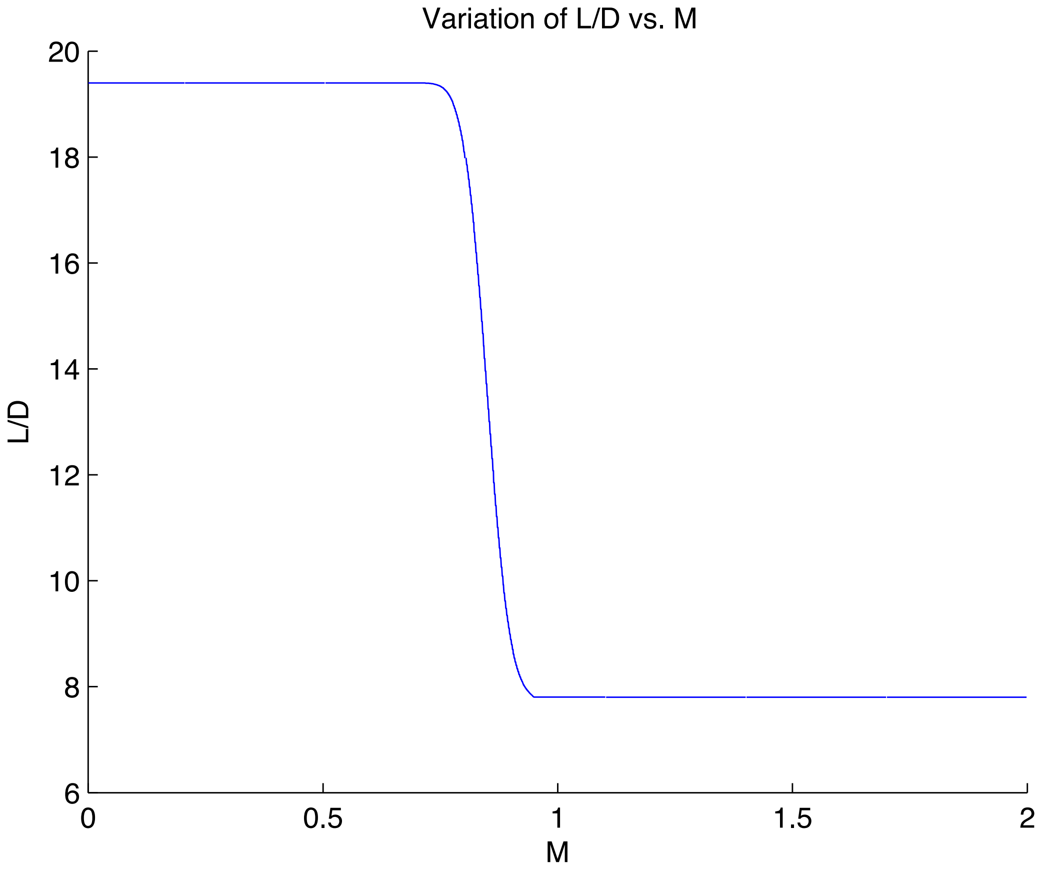
A good first estimate of performance is provided by the Breguet range equation:

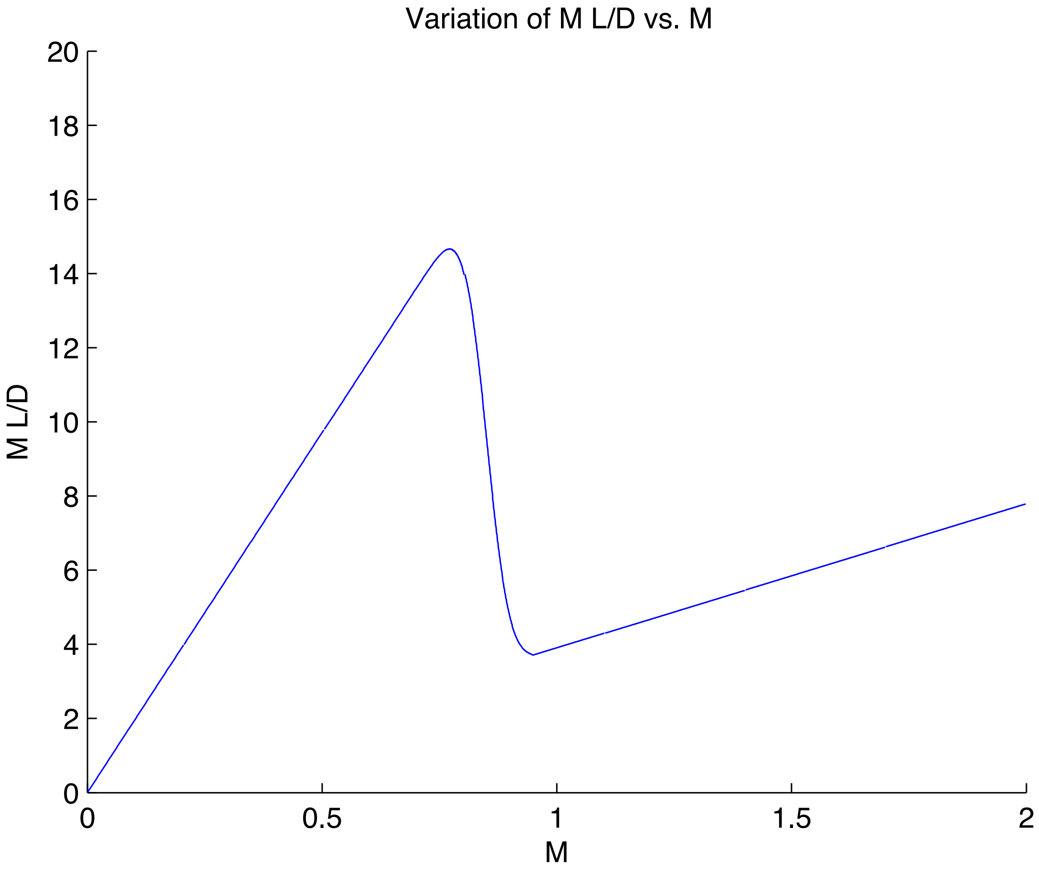
$$\text{Range} = \frac{VL}{D}\frac{1}{SFC}\log\frac{W_0 + W_f}{W_0}. \tag{1}$$

Here V is the speed, L/D is the lift to drag ratio, SFC is the specific fuel consumption of the engines, W_0 is the loading weight (empty weight + payload + fuel resourced), and W_f is the weight of fuel burnt.
Equation (1) displays the multidisciplinary nature of design.

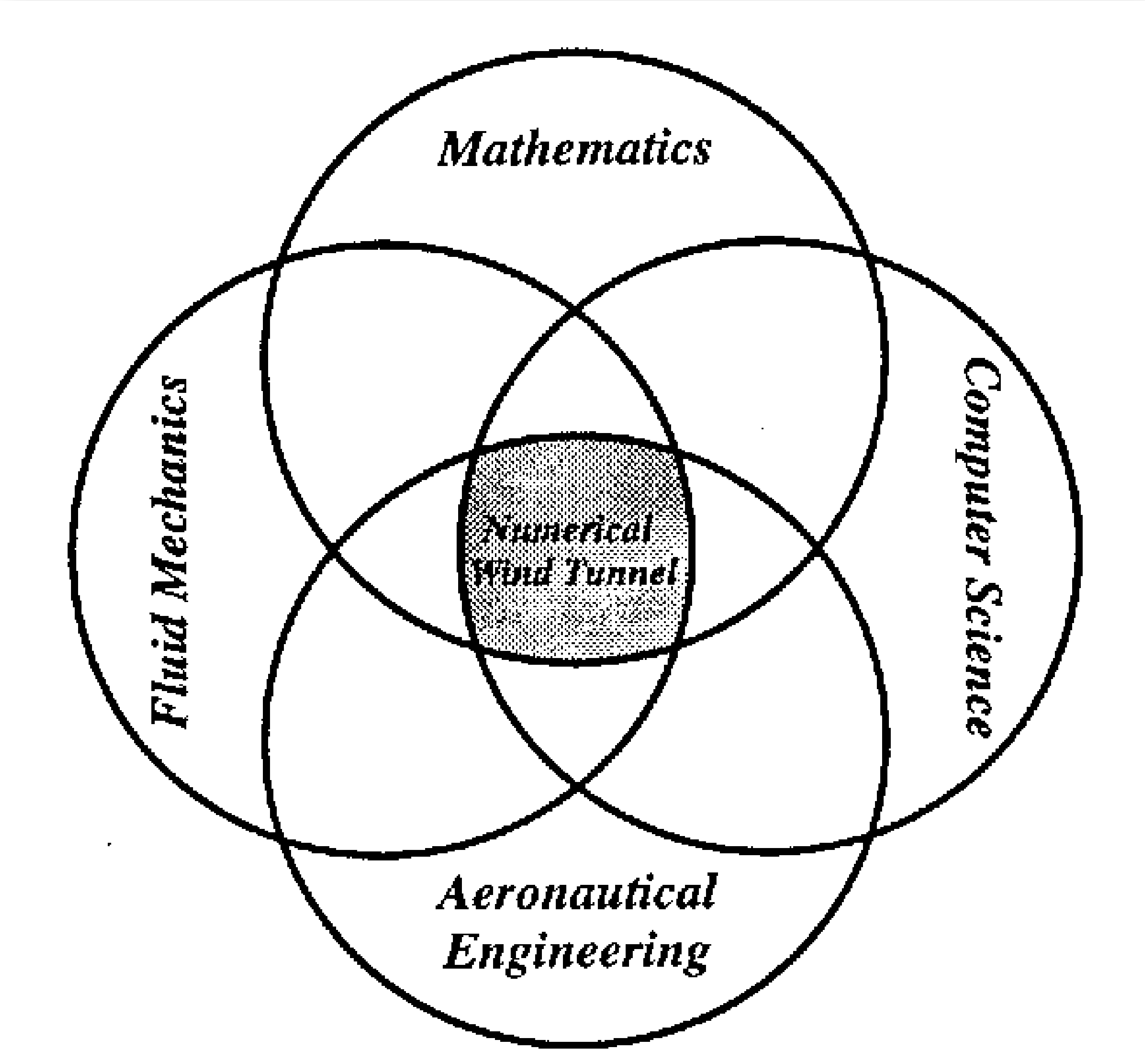
A light structure is needed to reduce W_0. SFC is the province of the engine manufacturers. The aerodynamic designer should try to maximize $\frac{VL}{D}$. This means the cruising speed V should be increased until the onset of drag rise at a Mach Number $M = \frac{V}{C} \sim .85$. But the designer must also consider the impact of shape modifications in structure weight.

Why Transonic Flow?

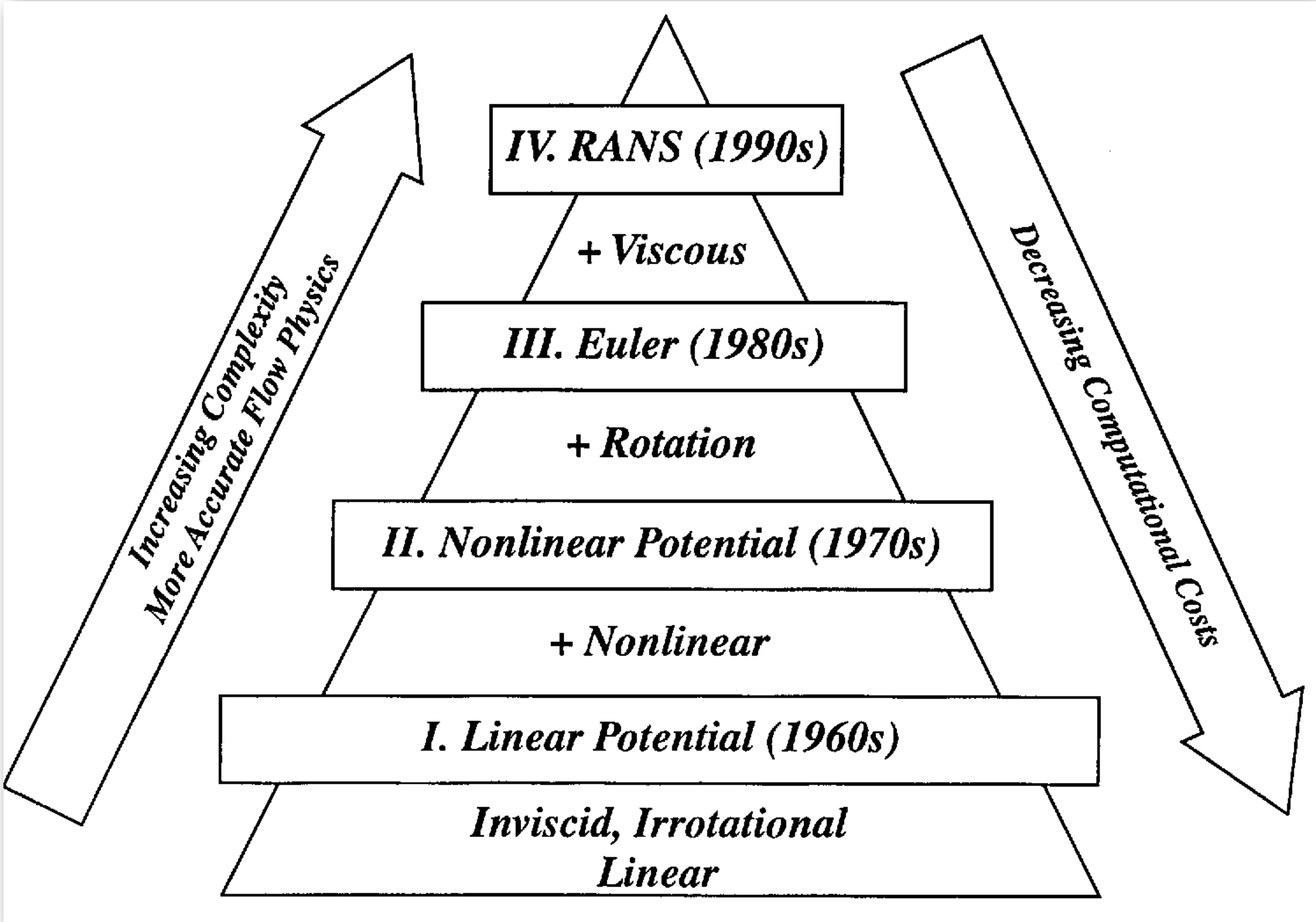




Multi-Disciplinary Nature of CFD



Hierarchy of Governing Equations



IV. RANS (1990s)

+ Viscous

III. Euler (1980s)

+ Rotation

II. Nonlinear Potential (1970s)

+ Nonlinear

I. Linear Potential (1960s)

Inviscid, Irrotational
Linear

Increasing Complexity
More Accurate Flow Physics

Decreasing Computational Costs

50 Years of CFD

- 1960–1970: **Early Developments**
  Riemann-based schemes for gas dynamics (Godunov), 2nd-order dissipative schemes for hyperbolic equations (Lax-Wendroff), efficient explicit methods for Navier-Stokes (MacCormack), panel method (Hess-Smith)
- 1970–1980: **Potential Flow Equations**
  type-dependent differencing (Murman-Cole), complex characteristics (Garabedian), rotated difference (Jameson), multigrids (Brandt), complete airplane solution (Glowinsky)
- 1980–1990: **Euler and Navier-Stokes Equations**
  oscillation control via limiters (Boris-Book), high-order Godunov scheme (van Leer), flux splitting (Steger-Warming), shock capturing via controlled diffusion (Jameson-Schmit-Turkel), approximate Riemann solver (Roe), total variation diminishing (Harten), multigrids (Jameson, Ni), solution of complete airplane (Jameson-Baker-Weatherill)
- 1990–2000: **Aerodynamic Shape Optimization**
  adjoint based control theory
- 2000–2010: **Discontinuous Finite Element Methods**
  Discontinuous Galerkin, Spectral Difference, Flux Reconstruction, *etc.*

Advances in Computer Power

1970	CDC6600	1 Megaflops	**10^6**
1980	Cray 1 Vector Computer	100 Megaflops	**10^8**
1994	IBM SP2 Parallel Computer	10 Gigaflops	**10^{10}**
2007	Linux Clusters	100 Teraflops	**10^{14}**
2009	HP Pavilion Quadcore Notebook $1,099	1 Gigaflops	**10^9**
2011	MacBook Pro Quadcore Laptop $2,099	2.5 Gigaflops	**2.5×10^9**
2012	Titan supercomputer @ ORNL 18,688 × NVIDIA K20 GPUs	20 Petaflops	**2×10^{16}**

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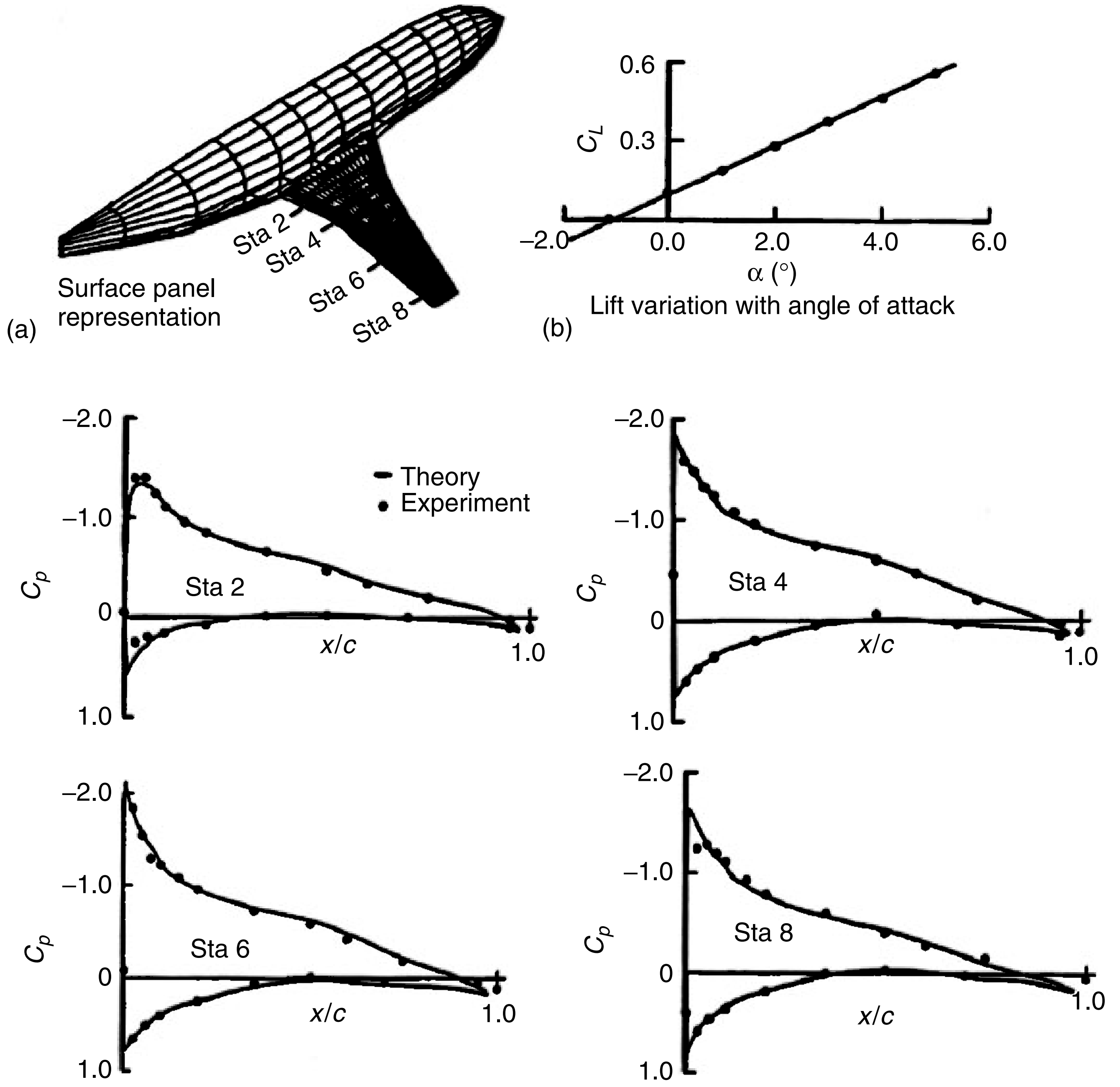
CFD Code Development

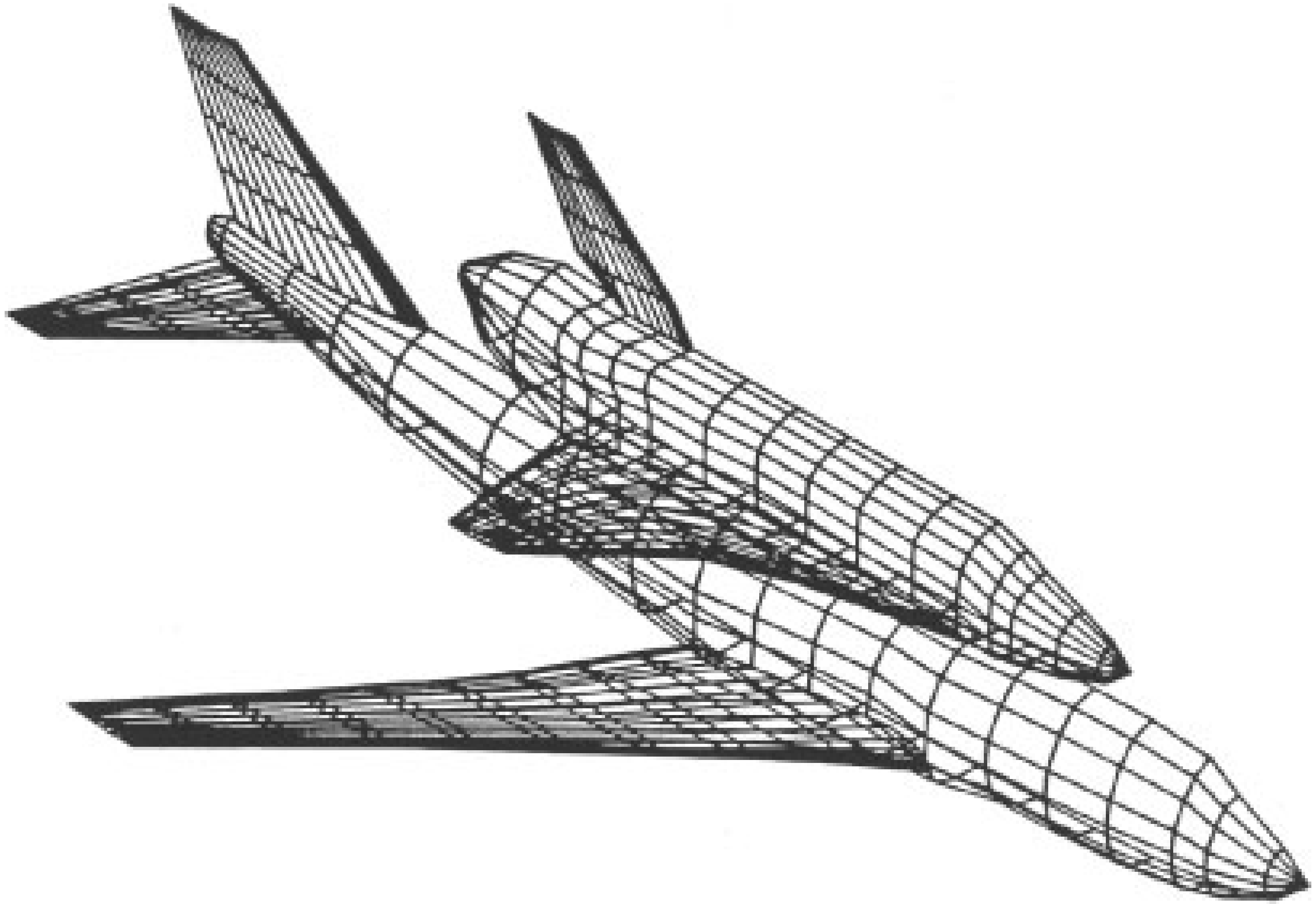
- 1970–1980: **Potential Flows**
  solution of inverse problem by conformal mapping (SYN1), solution of 2D potential flow by conformal mapping (FLO1), 2D transonic potential flow using rotated difference scheme (FLO6), first transonic potential flow solution for a swept wing (FLO22), 3D potential flow in general grid with trilinear isoparametric elements (FLO27), multigrid solution of 2D transonic potential flow (FLO36)
- 1980–1990: **Euler & Navier-Stokes Equations**
  solution of 3D Euler (FLO57), multigrid solution of 3D Euler (FLO67), multigrid solution of 2D Euler (FLO82), first solution of Euler equations for a complete aircraf with tetrahedral meshes (FLOPLANE), cell-vertex and cell-centered schemes for 3D Navier-Stokes (FLO107)
- 1990–2000: **Aerodynamic Shape Optimization**
  airfoil design via control theory using 2D Euler (SYN83), wing design using 3D Euler (SYN88), airfoil design using 2D Navier-Stokes (SYN103), wing design using 3D Navier-Stokes (SYN107), aerodynamic design of complete aircraft with tetrahedral mesh (SYNPLANE), viscous flow solution on arbitrary polyhedral meshes (FLO3XX)
- 2000–2010: **High-order Methods for Navier-Stokes Equations**
  high-order discontinuous finite element methods for unsteady compressible Navier-Stokes equations on unstructured meshes (Spectral Difference Method, Energy Stable Flux Reconstruction Method)

Panel Codes for Potential Flow



Panel method applied to Boeing 747. (Supplied by Paul Rubbert, the Boeing Company.)

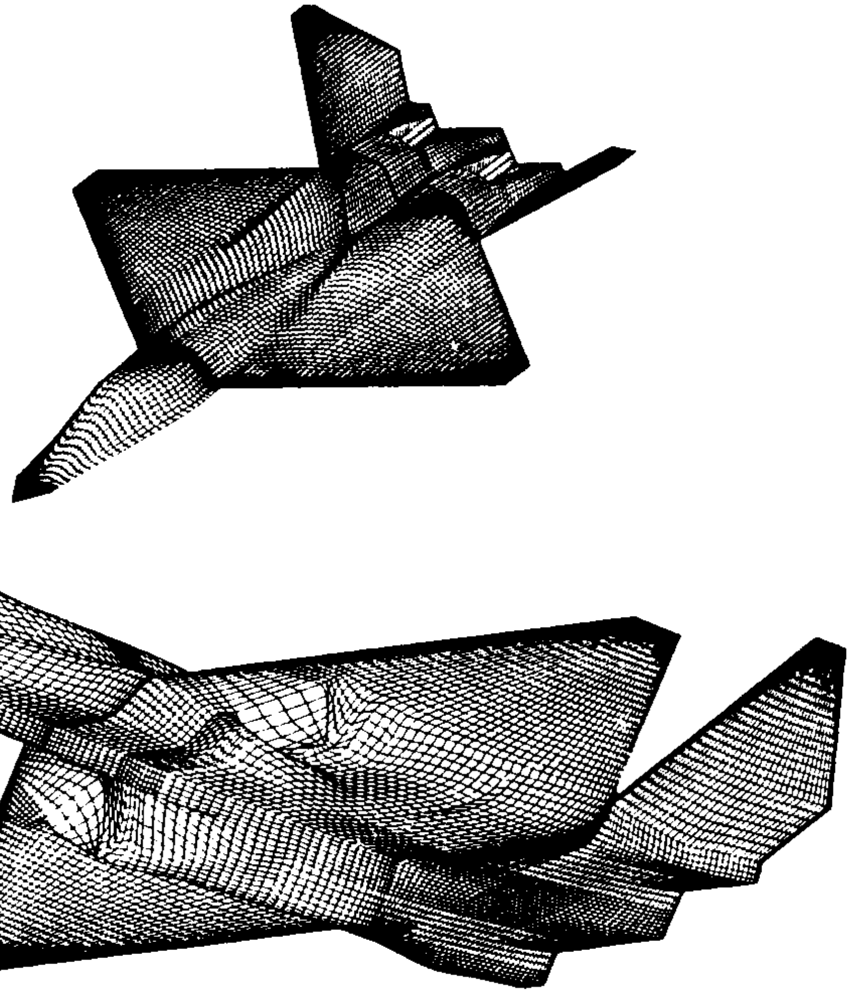
Panel Codes for Potential Flow

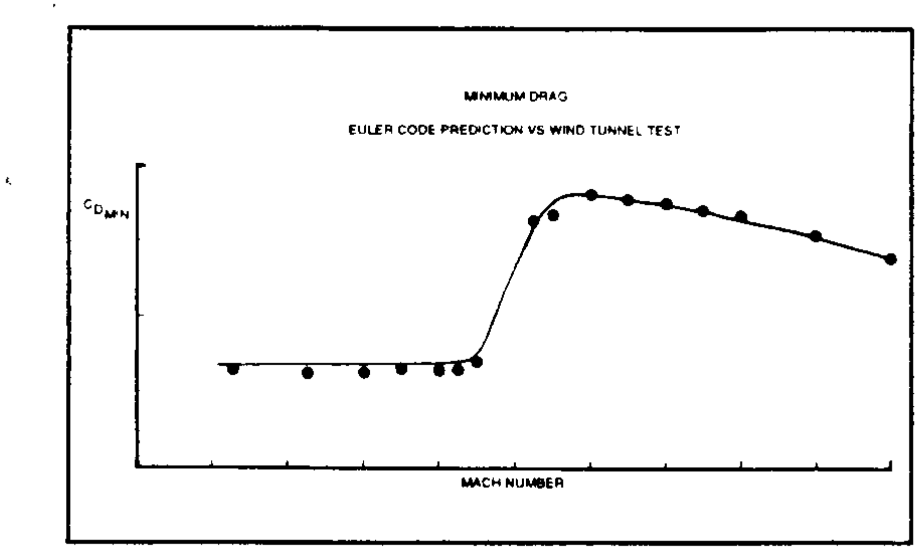


Panel method applied to flow around Boeing 747 and space shuttle.
Supplied by Allen Chen, the Boeing Company.

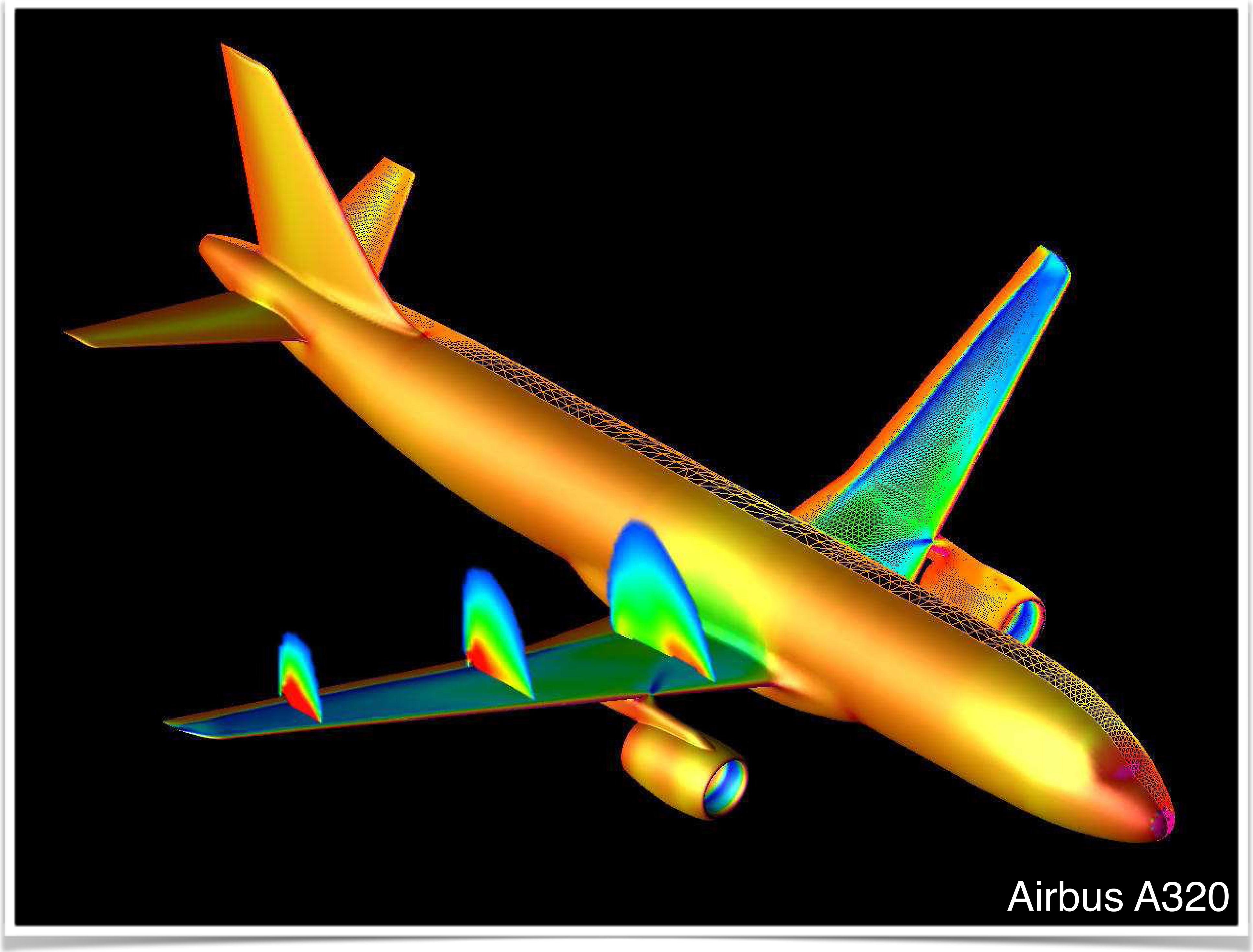
CFD Code Development

Northrop YF-23
Extended version of FLO57
by Richard Busch, Jr.

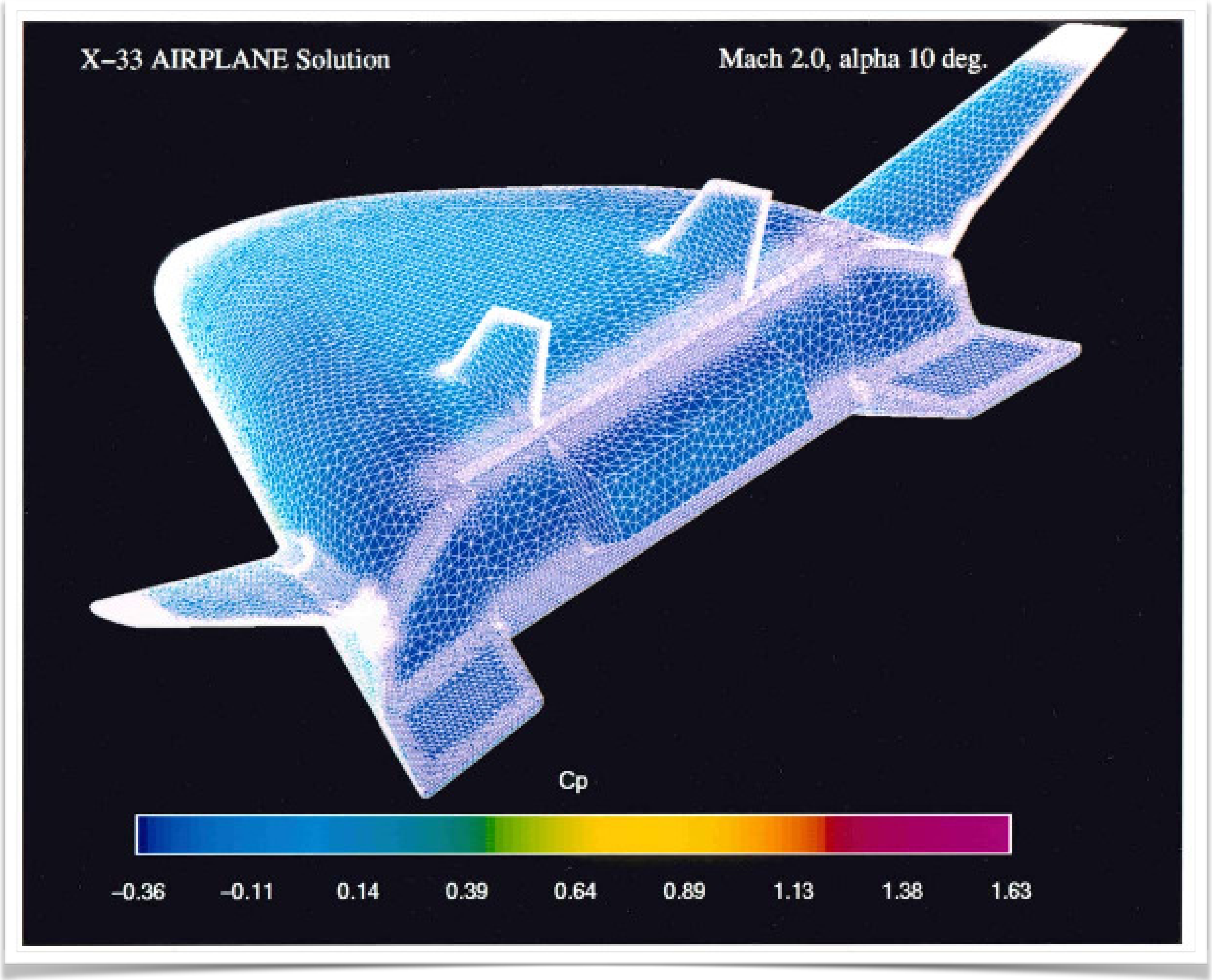




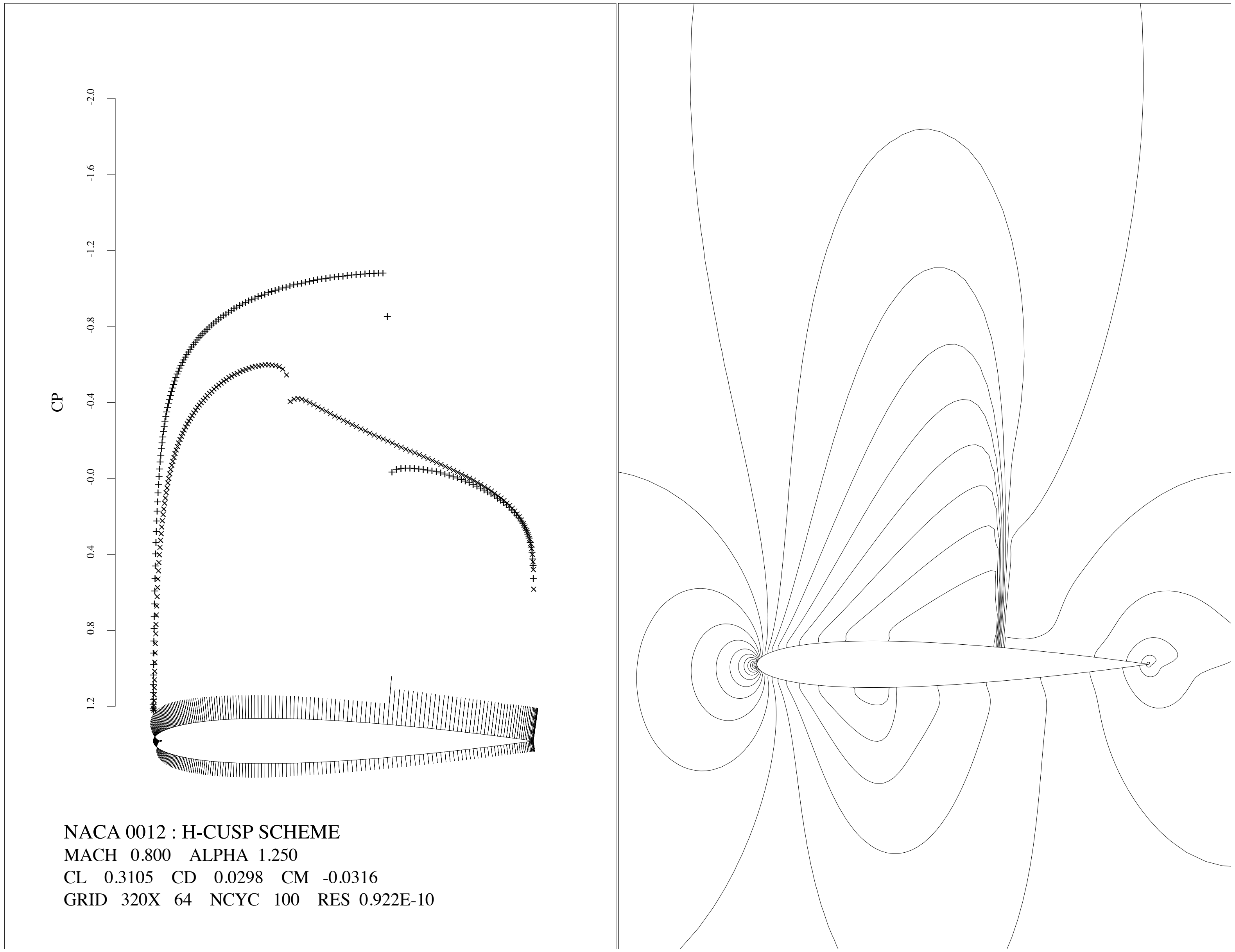
CFD Code Development


Airbus A320

CFD Code Development

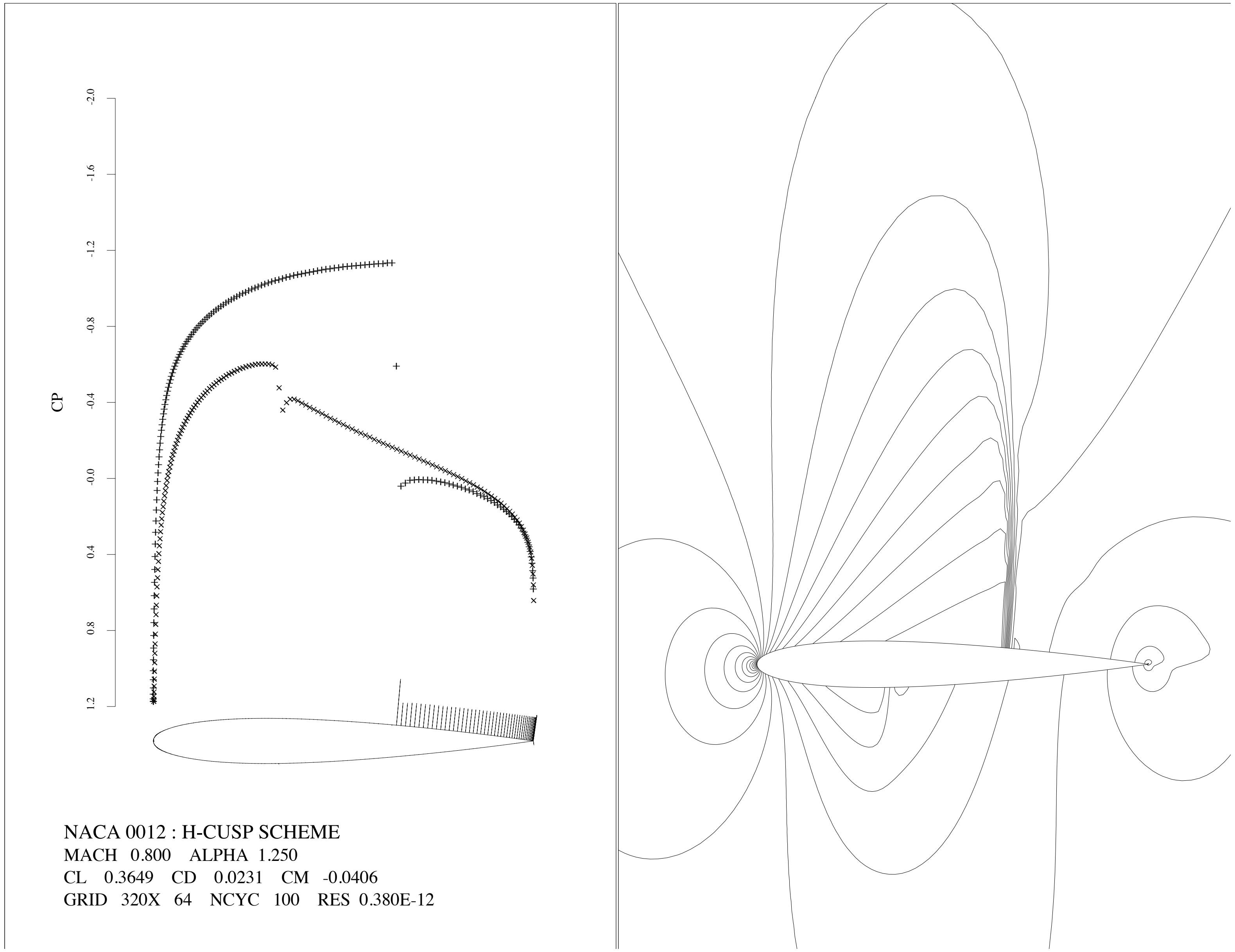


First and Second Order Accuracy



First order accurate (320 by 64 grid)

First and Second Order Accuracy

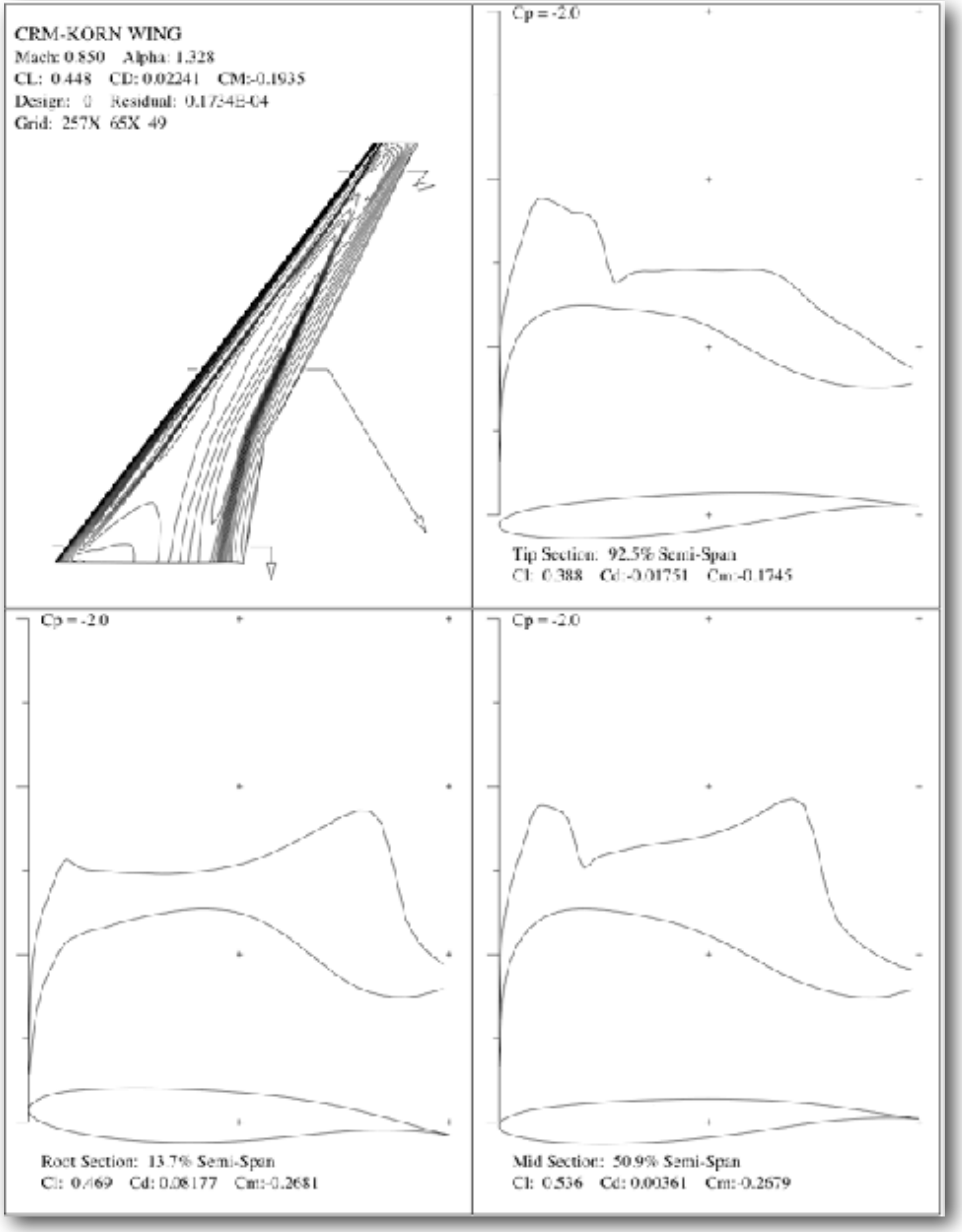


```
NACA 0012 : H-CUSP SCHEME
MACH  0.800    ALPHA  1.250
CL   0.3649   CD    0.0231   CM   -0.0406
GRID   320X   64    NCYC   100    RES  0.380E-12
```

Second order accurate (320 by 64 grid)

Wing Optimization Using SYN107

State of the Art Wing Design Process in 2 Stages, starting from Garabedian-Korn Airfoil and NASA Common Research Model



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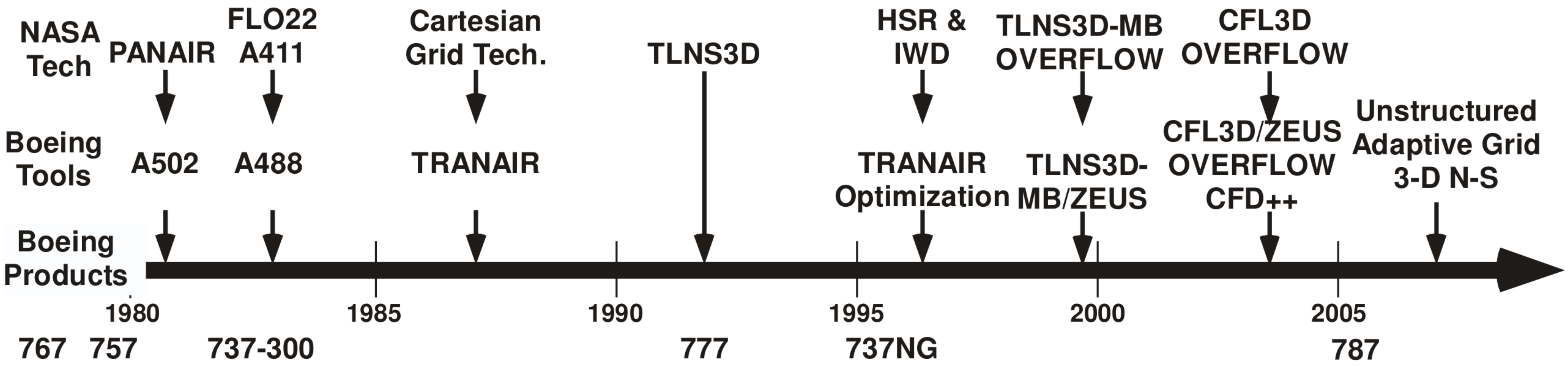
Impact of CFD on Configuration Lines & Wind Tunnel Testing



NASA Tech: PANAIR, FLO22 A411, Cartesian Grid Tech., TLNS3D, HSR & IWD, TLNS3D-MB OVERFLOW, CFL3D OVERFLOW

Boeing Tools: A502, A488, TRANAIR, TRANAIR Optimization, TLNS3D-MB/ZEUS, CFL3D/ZEUS OVERFLOW CFD++, Unstructured Adaptive Grid 3-D N-S

Boeing Products: 1980, 1985, 1990, 1995, 2000, 2005

767 757 737-300 777 737NG 787

1980 state of the art

Modern close coupled nacelle installation, 0.02 Mach faster than 737-200

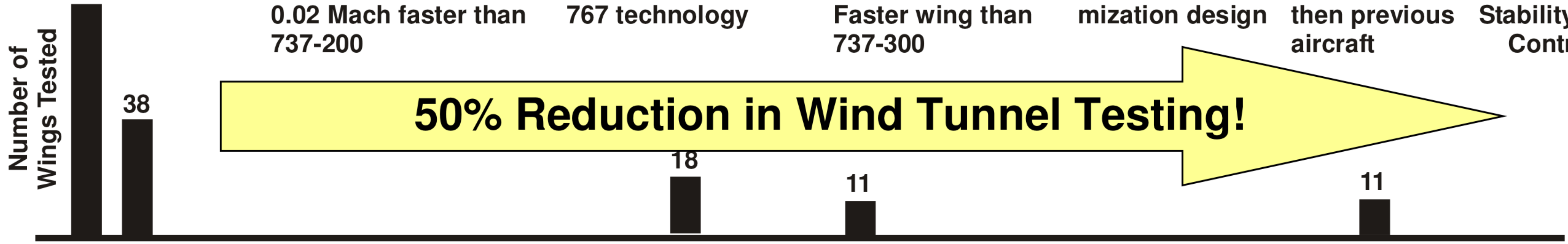
21% thicker faster wing than 757, 767 technology

Highly constrained wing design Faster wing than 737-300

Successful multipoint optimization design

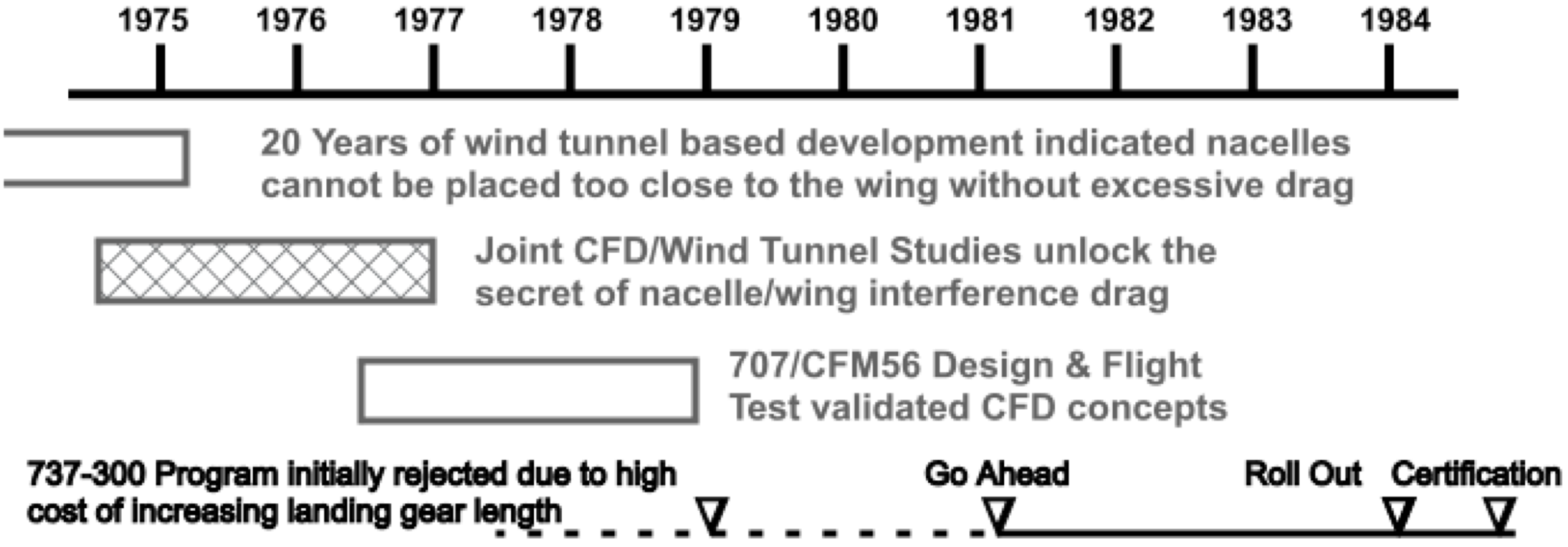
Faster and more efficient then previous aircraft

CFD for Loads and Stability and Control



50% Reduction in Wind Tunnel Testing!

Impact of CFD on B737-300 Program



20 Years of wind tunnel based development indicated nacelles cannot be placed too close to the wing without excessive drag

Joint CFD/Wind Tunnel Studies unlock the secret of nacelle/wing interference drag

707/CFM56 Design & Flight Test validated CFD concepts

737-300 Program initially rejected due to high cost of increasing landing gear length

Go Ahead

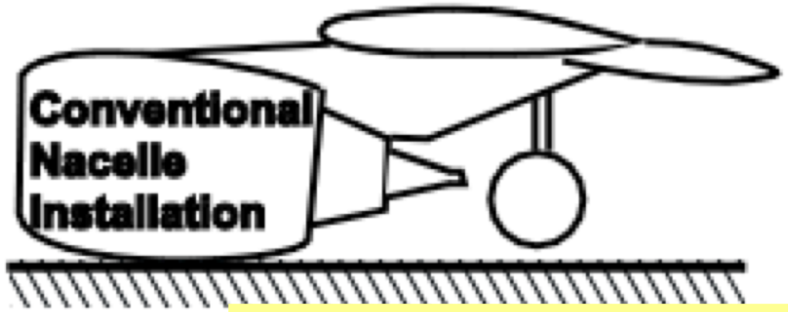
Roll Out

Certification

Initial Studies

737-300 Program

McDonnell-Douglas MD-80 Go Ahead



Without the understanding gained from CFD there would not have been a 737-300 Program!

Walt Gillette

Manager, 737 Aerodynamics - then

Vice President, 787 Engineering – retired

5000+ Additional Sales!

Computational Methods at Boeing

TRANAIR:

- Full Potential with directly coupled Boundary Layer
- Cartesian solution adaptive grid
- Drela lag-dissipation turbulence model
- Multi-point design/optimization

Navier-Stokes Codes:

- CFL3D – Structured Multiblock Grid
- TLNS3D – Structured Multiblock Grid, Thin Layer
- OVERFLOW – Overset Grid

N-S Turbulence Models:

- S-A Spalart-Allmaras
- Menter's k-ω SST

CFD Contributions to B787

Wind-Tunnel Corrections

Vertical Tail and Aft Body Design

Planform Design

Wing-Tip Design

Wing Controls

Reynolds-Number Corrections

High-Speed Wing Design

Flutter

Cab Design

Aeroelastics

Vortex Generators

Interior Air Quality

High-Lift Wing Design

Icing

APU Inlet And Ducting

Control-Surface Failure Analysis

ECS Inlet Design

Wing-Body Fairing Design

Air-Data System Location

APU and Propulsion Fire Suppression

Avionics Cooling

Exhaust-System Design

Cabin Noise

Inlet Design

Buffet Boundary

Engine/Airframe Integration

Inlet Certification

Design For Stability & Control

Thrust-Reverser Design

Engine-Bay Thermal Analysis

Design for FOD Prevention

Community Noise

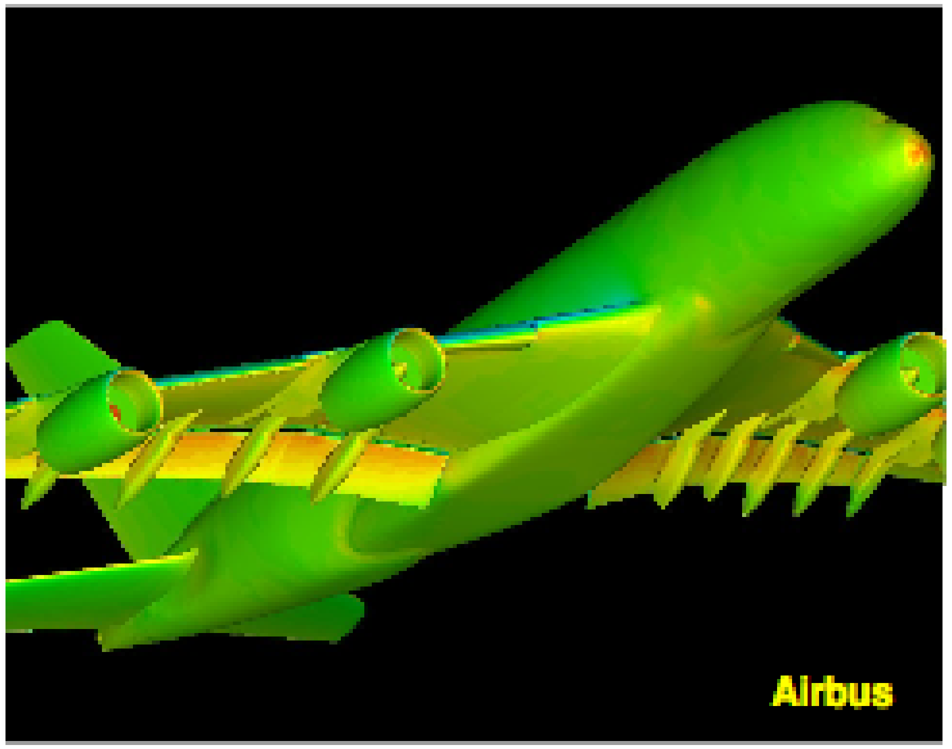
Nacelle Design

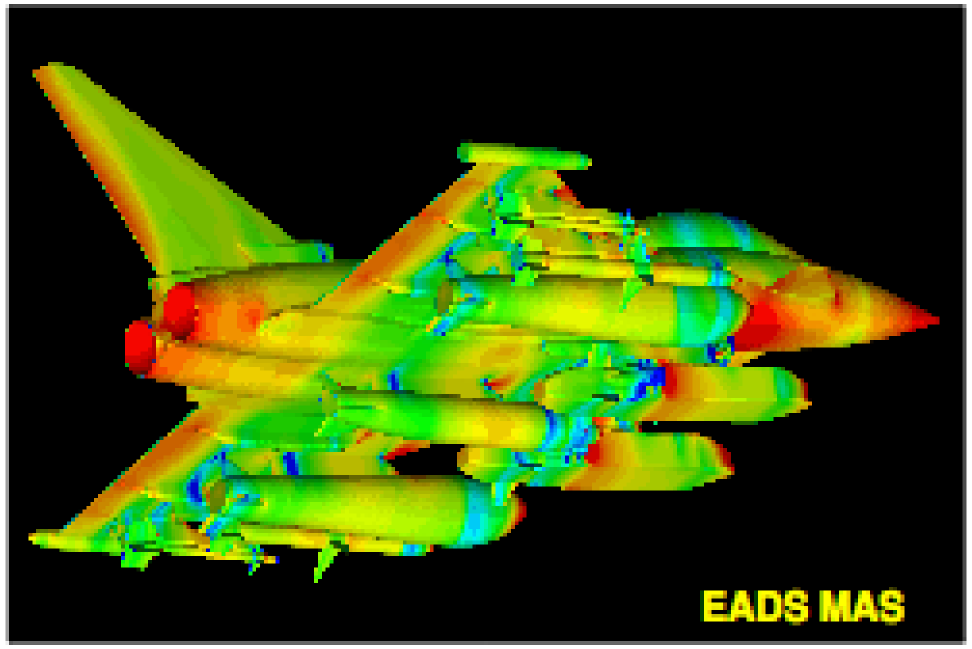
CFD Development for Aircraft Design

MEGAFLOW / MEGADESIGN
- National CFD Initiative (since 1995)

Development & validation of a national CFD software for complete aircraft applications which

- allows computational aerodynamic analysis for 3D complex configurations at cruise, high-lift & off-design conditions
- builds the basis for shape optimization and multidisciplinary simulation
- establishes numerical flow simulation as a routinely used tool at DLR and in German aircraft industry
- serves as a development platform for universities

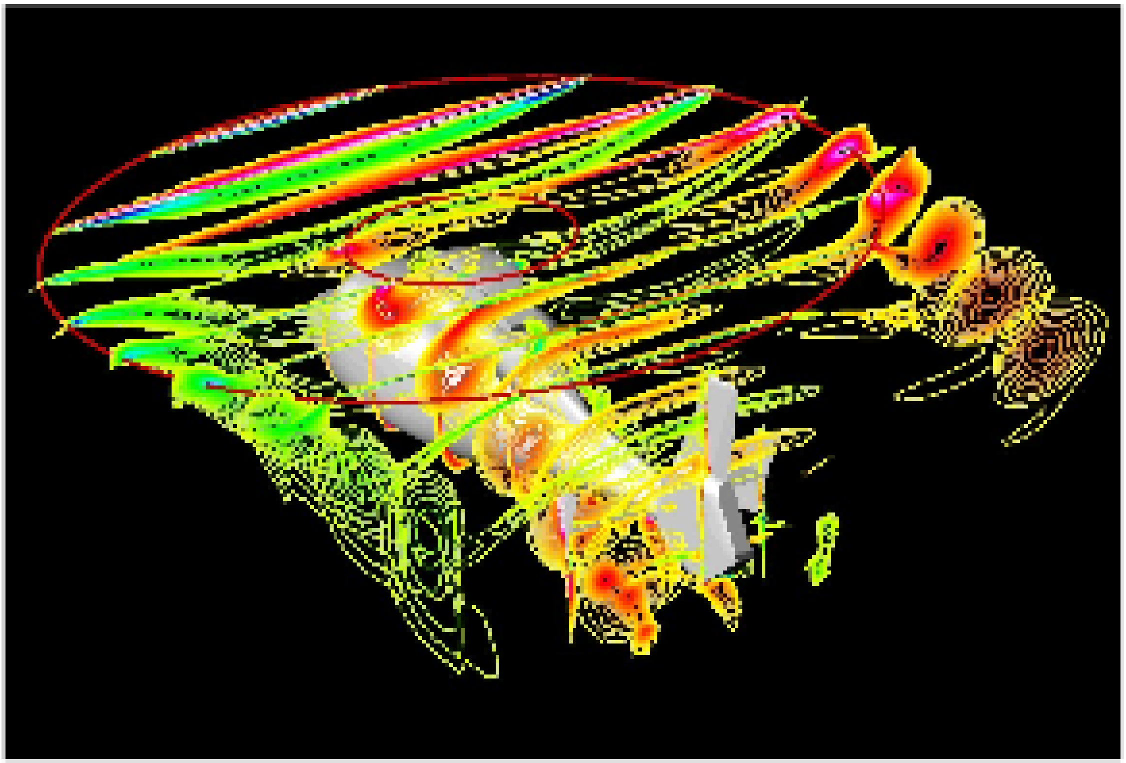


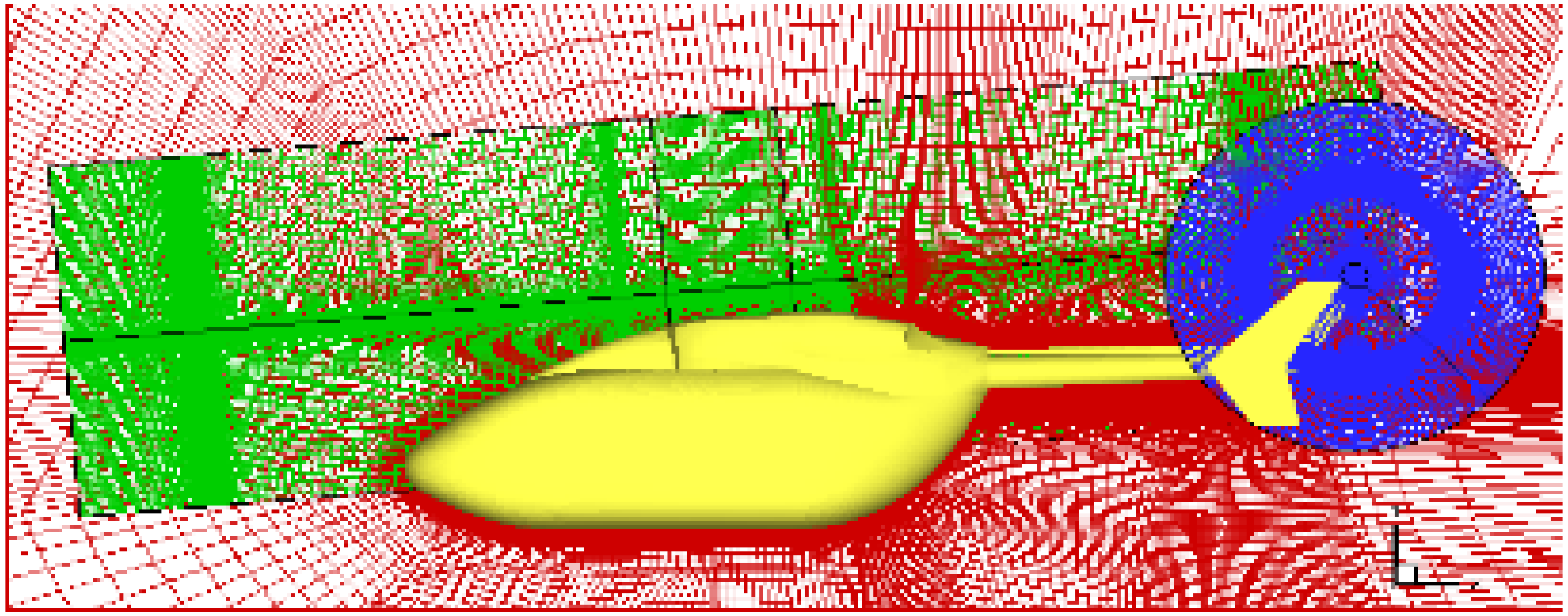


Block-Structured RANS Capability: FLOWer

Efficient simulation tool for configurations of moderate complexity

- advanced turbulence and transition models (RSM, DES)
- state-of-the-art algorithms
  - baseline: JST scheme, multigrid
  - robust integration of RSM (DDADI)
- chimera technique for moving bodies
- fluid / structure coupling
- design option (inverse design, adjoint)





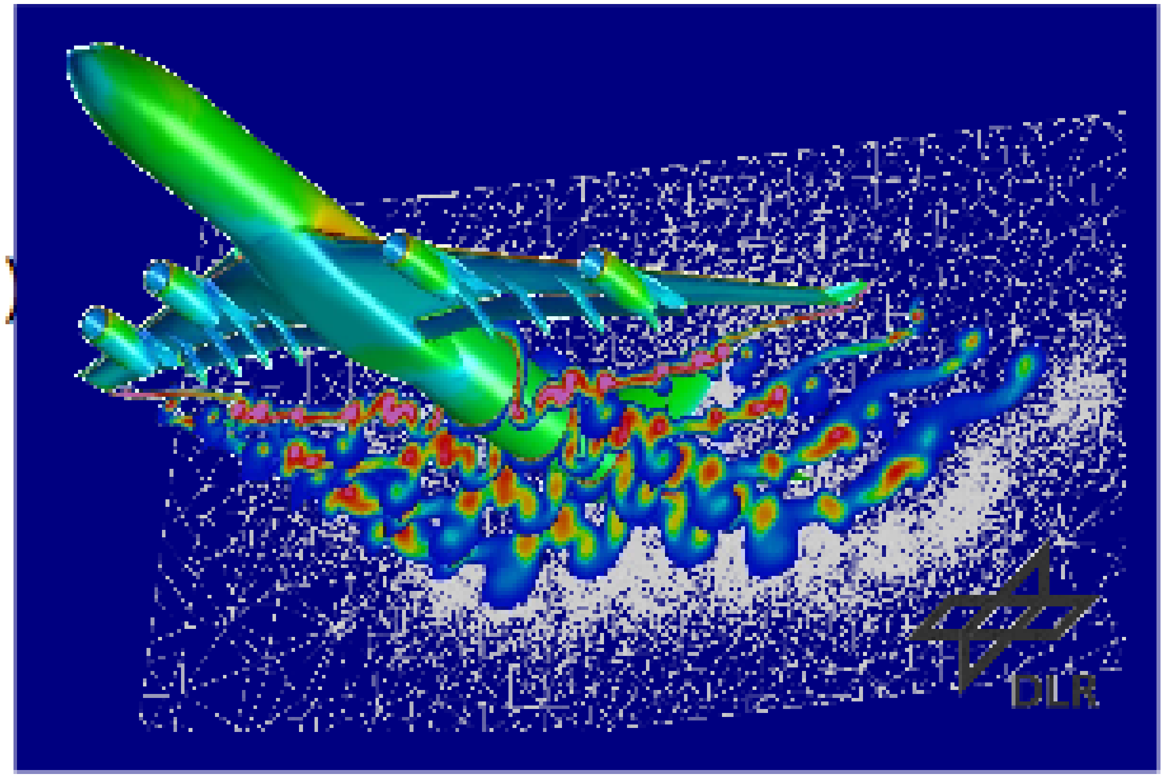
FLOWer-Code

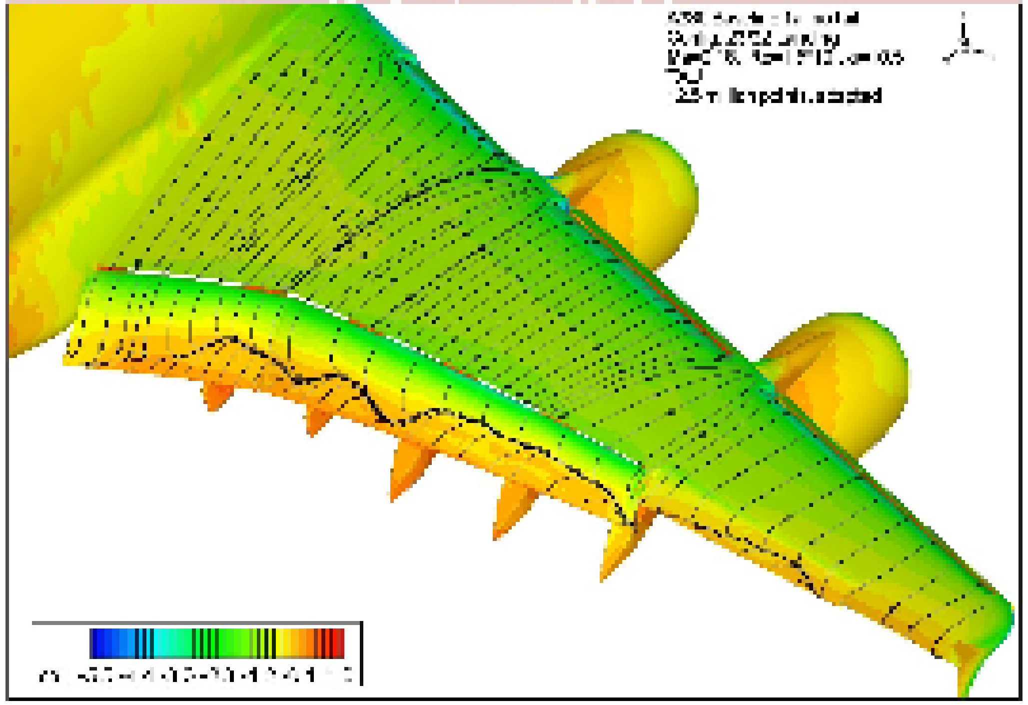
- Fortran
- portable code
- parallelization based on MPI

Unstructured RANS Capability: TAU

Tool for complex configurations

- hybrid meshes, cell vertex / cell centered
- high-level turbulence & transition models (RSM, DES, linear stability methods)
- state-of-the-art algorithms (JST, multigrid, …)
- local mesh adaptation
- chimera technique
- fluid / structure coupling
- continuous/discrete adjoint
- extensions to hypersonic flows



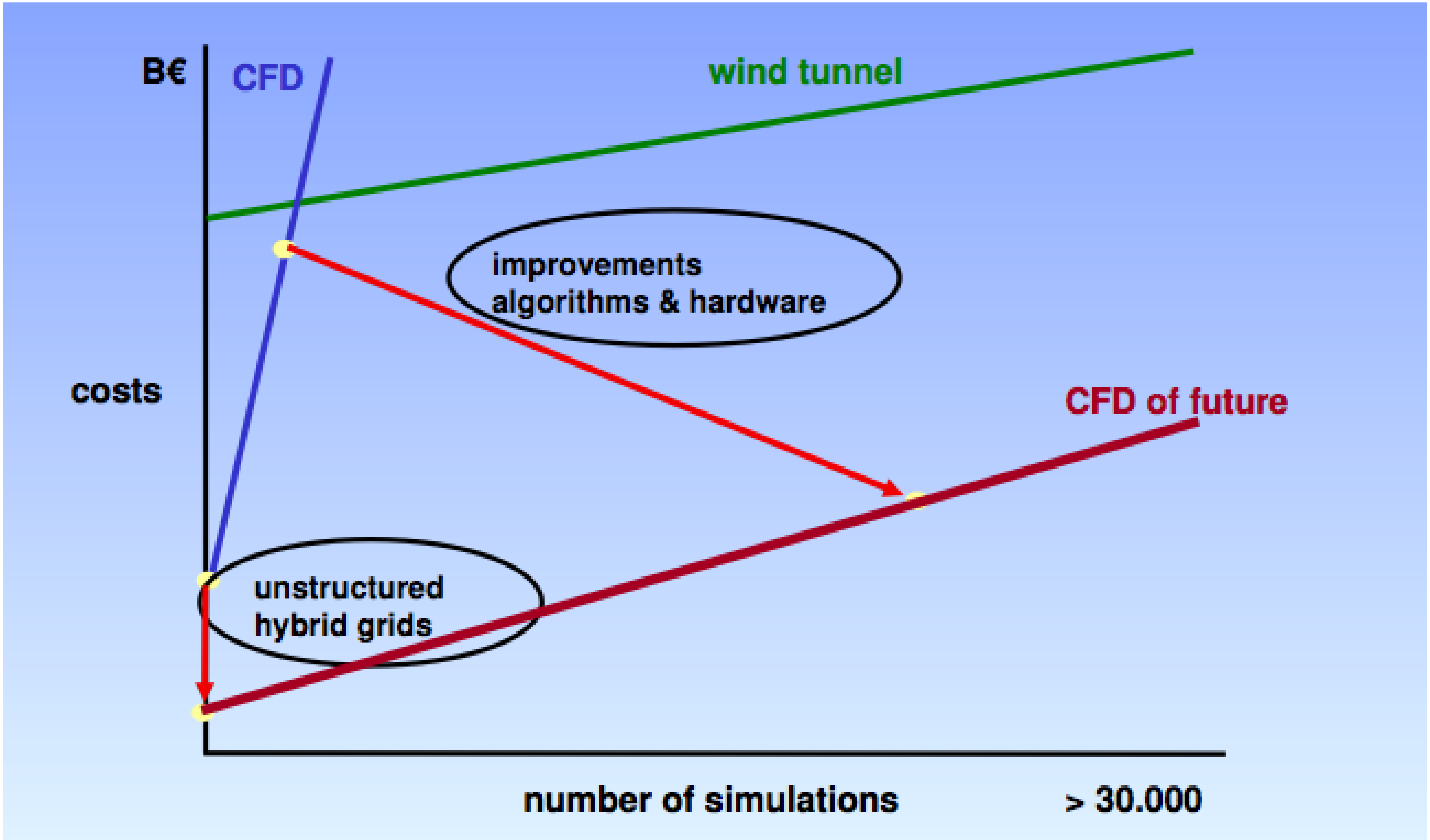


TAU-Code

- unstructured database
- C-code, Python
- portable code, optimized for cache hardware
- high performance on parallel computer

Numerical Flow Simulation

Relation CFD / wind tunnel



✈ CFD cost effective alternative

CFD Contribution to A380

- Frequent use
- Moderate use
- Growing use

Flutter Prediction

Sting Corrections

Performance Prediction

High Speed Wing Design

Ice Prediction

Flow Control Devices (VG/Strakes)

Cabin Ventilation

Cockpit/Avionics Ventilation

Cabin Noise

Fuselage Design

Low Speed Wing Design

Spoiler/ Control Surfaces

Tails Design

Powerplant Integration

Nacelle Design

Fuel System Design

ECS Inlet/Outlet Design

Belly Fairing Design

Nozzle Design

Inlet Design

APU Inlet/Outlet Design

Ground Effect

Pack Bay Thermal Analysis

Engine Core Compartment

Wing Tip Design

External Noise Sources

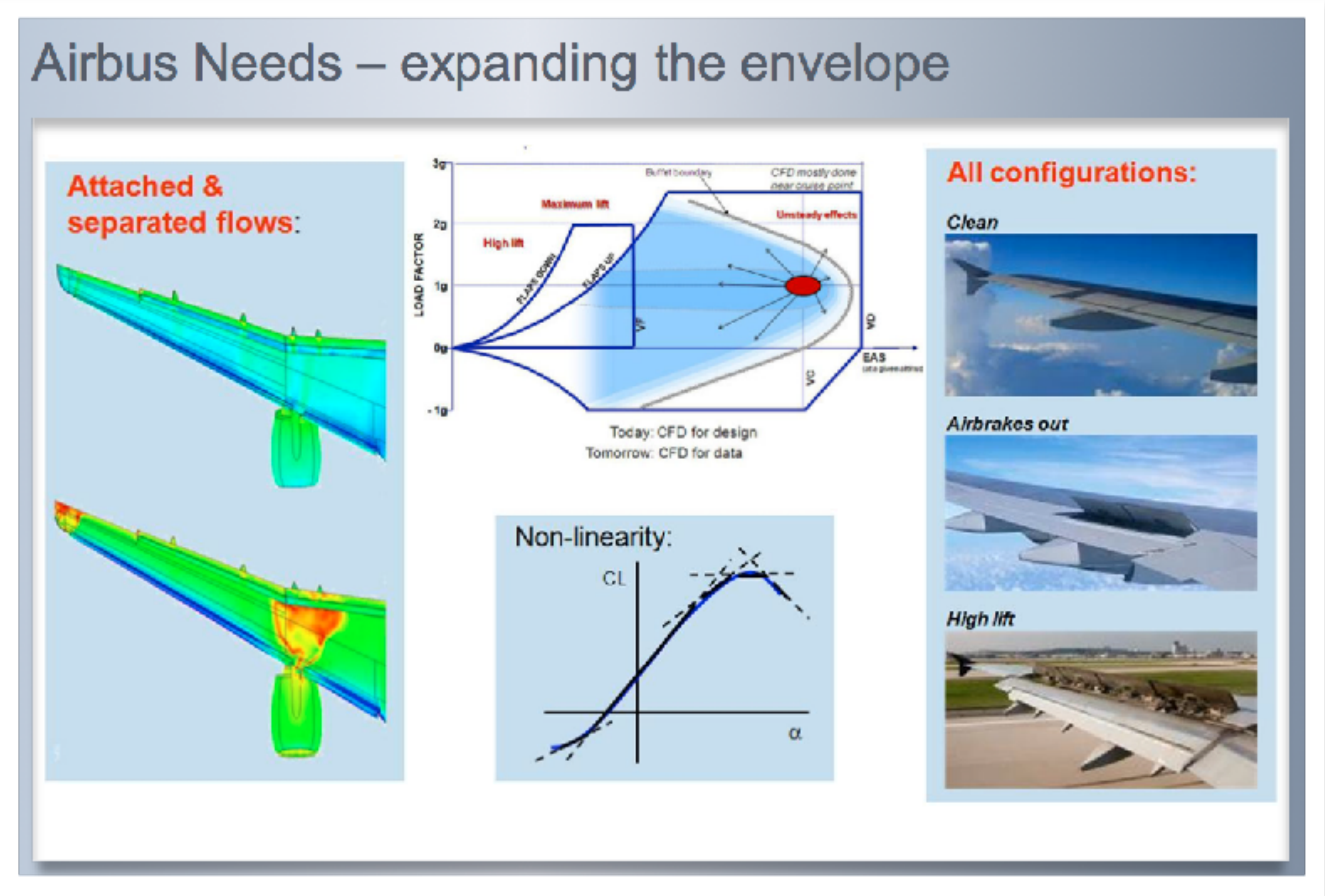
Handling Quality Data

Static Deformation

Aero Loads Data

Thrust Reverser Design

The Future of CFD (?)



Airbus Needs – expanding the envelope

Attached & separated flows:

Today: CFD for design
Tomorrow: CFD for data

Non-linearity:

All configurations:

Clean

Airbrakes out

High lift

Murray Cross, Airbus, Technology Product Leader - Future Simulations (2012)

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The Current Status of CFD

- Worldwide commercial and government codes are based on algorithms developed in the ‘80s and ‘90s
- These codes can handle complex geometry but are generally limited to 2nd order accuracy
- They cannot handle turbulence without modeling
- Unsteady simulations are very expensive, and questions over accuracy remain

The Future of CFD (?)

CFD has been on a plateau for the past 15 years

- Representations of current state of the art:
    - Formula 1 cars
    - Complete aircraft
- The majority of current CFD methods are not adequate for vortex dominated and transitional flows:
    - Rotorcraft
    - High-lift systems
    - Formation flying

Large-Eddy Simulation

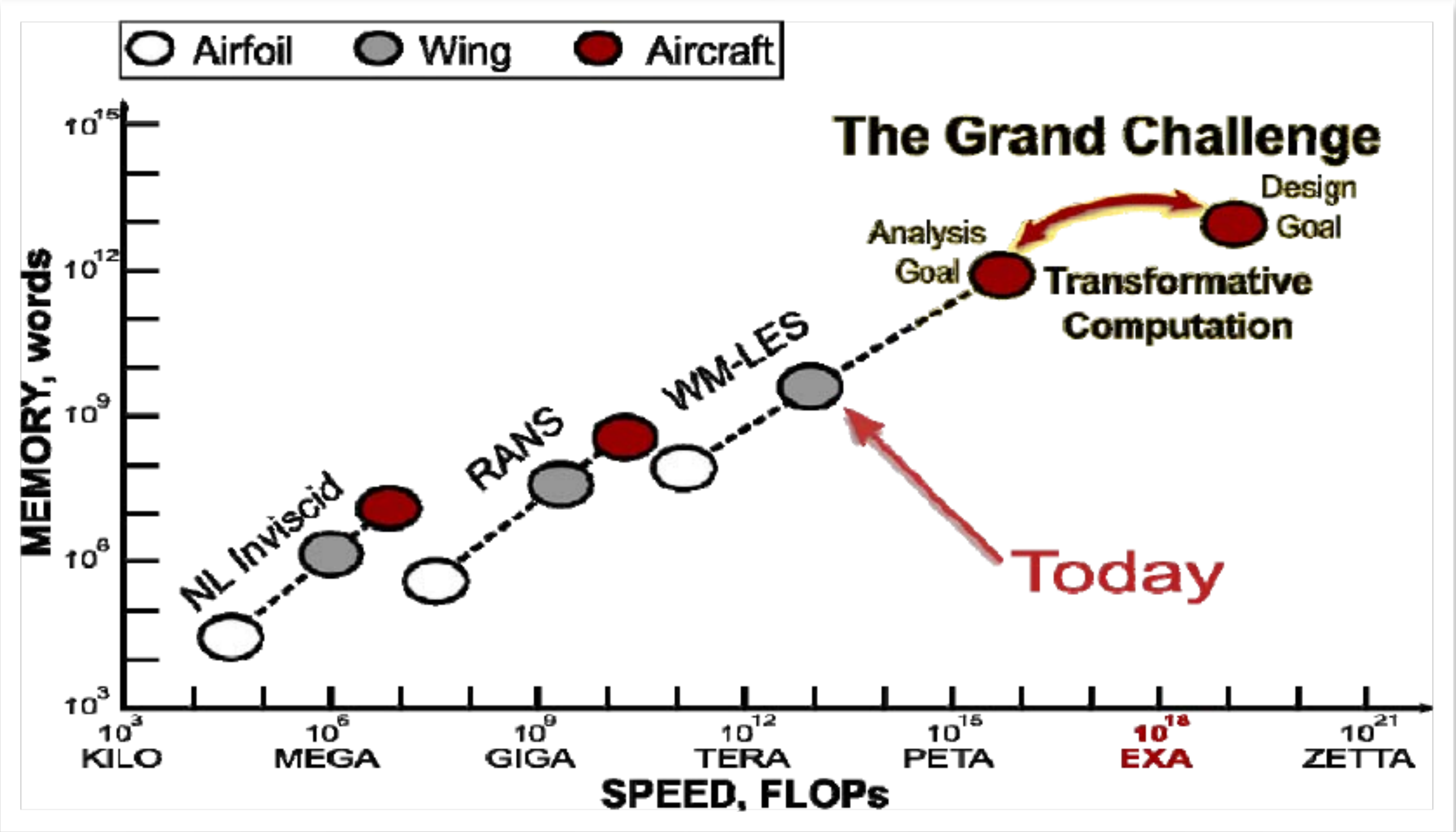
The number of DoF for an LES of turbulent flow over an airfoil scales as **$Re_c^{1.8}$ (resp. $Re_c^{0.4}$) if the inner layer is resolved (resp. modeled)**

Rapid advances in computer hardware should make LES feasible within the foreseeable future for industrial problems at high Reynolds numbers. To realize this goal requires

- high-order algorithms for unstructured meshes (complex geometries)
- Sub-Grid Scale models applicable to wall bounded flows
- massively parallel implementation

Chapman (1979), AIAA J. 17(12)

Large-Eddy Simulation



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Typical Requirements of CFD

Traditional numerical schemes for engineering problems are too dissipative and do not provide sufficient accuracy for LES and DNS

Accuracy:	solution must be right
Small numerical dissipation:	unsteady flow features
Unstructured grids:	complex geometries
Numerical flux:	wave propagation problems
High resolution capabilities:	transitional and turbulent flows
Efficiency:	code parallelism
...	

A Review of the Literature

Past Research on DG Schemes:

- Modern development of DG schemes for hyperbolic conservation laws stems from the work of Cockburn & Shu [1989a,1989b,1990,1998,2001]

Recent Research:

Attempts to reduce complexity and avoid quadrature:

- Spectral Difference (SD) scheme by Kopriva & Kolias [1996], Liu, Vinokur & Wang [2006]
- Nodal Discontinuous Galerkin (NDG) scheme by Atkins & Shu [1998], Hesthaven & Warburton [2007]
- Flux Reconstruction (FR) scheme by Huynh [2007,2009]
- Lifting Collocation Penalty (LCP) schemes by Wang et al. [2009]
- Energy Stable FR (ESFR) schemes by Vincent et al. [2011]

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Summary of FR

- Map each element onto a reference element using a Jacobian J.
- Represent solution and discontinuous flux inside each element as

$$u_h = \sum_{j=0}^{p} u_j \ell_j(\xi) \quad f_h = \sum_{j=0}^{p} f_j \ell_j(\xi)$$

- Compute common interface fluxes f^*_L and f^*_R.
- Extrapolate discontinuous flux to the boundary to give f_L and f_R.
- Introduce a pair of correction functions g_L and g_R.
- Update solution as

$$J\frac{\partial u_h}{\partial t} + \frac{\partial f_h}{\partial \xi} + (f_L^\star - f_L)g_L' + (f_R^\star - f_R)g_R' = 0$$

Linear Energy Stability

- **There exists a family of Flux Reconstruction schemes that are guaranteed to be linearly stable [Vincent et al., J. Sci. Comput, 2011]**
  - Parameterized with a constant *c* which changes the scheme
  - Recover NDG, SD, plus other previously-found energy-stable FR schemes

$$g_R = \frac{1}{2}\left[L_p + \frac{\eta_p L_{p-1} + L_{p+1}}{1+\eta_p}\right] \qquad \eta_p = \frac{c(2p+1)(a_p p!\,)^2}{2} \qquad a_p = \frac{(2p)!}{2^p(p!\,)^2}$$

- **Energy stable in the norm**

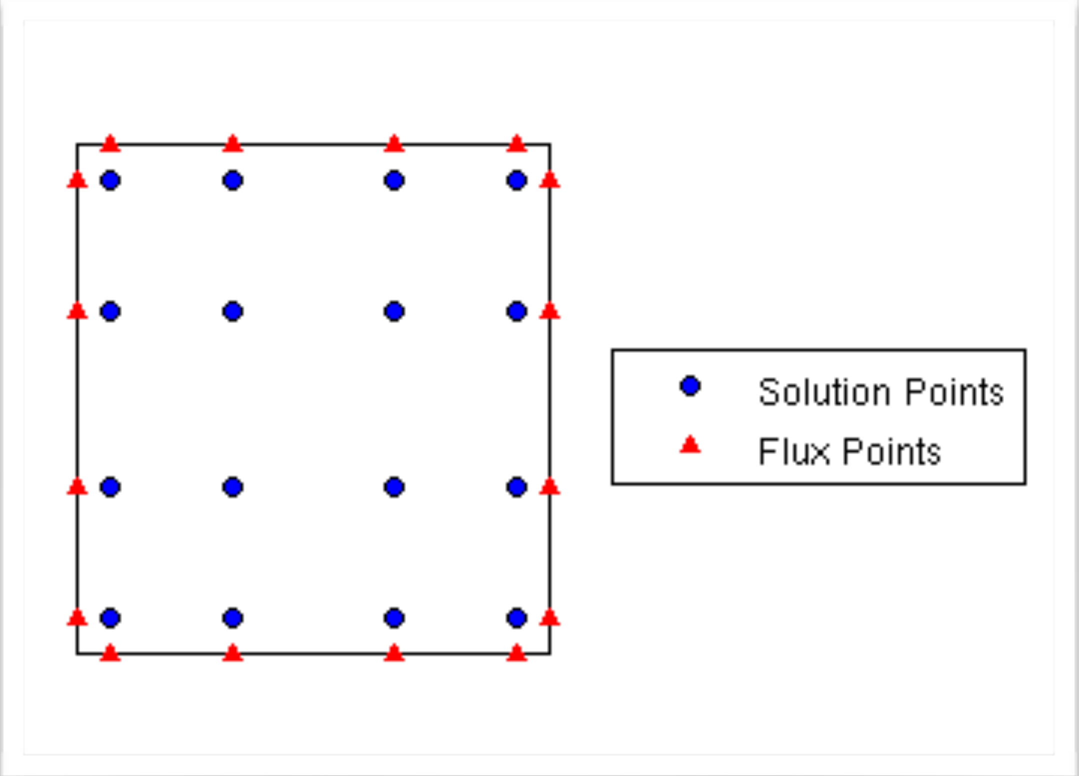
$$\sum \frac{1}{J}\int u_h^2 + \frac{c}{2}\left(\frac{\partial^p u_h}{\partial \xi^p} J^p\right)^2 \mathrm{d}x$$

Linear Energy Stability

- Key results for ESFR schemes
  - ESFR on triangles, Castonguay et al. JSC 2012
  - ESFR for advection diffusion, Castonguay et al. CMAME 2013
  - ESFR for advection diffusion on triangles, Williams et al. JCP 2013.
  - Stability of tensor product ESFR schemes, Sheshadri and Jameson, JSC 2015.
  - Extended range of ESFR schemes, Vincent et al. CMAME 2015.
  - Direct flux reconstruction, Romero et al. JSC 2015.

Stability of ESFR in Quadrilaterals

- Consider a simple tensor product extension of 1D ESFR to quadrilaterals.



However, stability when $c \neq 0$ is unclear

Stability of ESFR in Quadrilaterals

Theorem 1. *If the FR scheme for a 2D conservation law with periodic boundary conditions is used in conjunction with the Lax-Friedrichs formulation for the common interface flux with* $0 \leq \lambda \leq 1$, *then it can be shown that for a linear advective flux and any Cartesian mesh, the following holds:*

$$\frac{d}{dt}\|u^D\|^2 = \Theta_{adv} + c\Theta_{extra} \leq 0 \quad if \quad c \geq 0$$

$$\|u^D\|^2_{W^{2p,2}_\delta} = \sum_{k=1}^{N}\left(\int_{\Omega_k}\left[(u_k^D)^2+\frac{c}{2}\left(\left(\frac{\partial^p u_k^D}{\partial\xi^p}\right)^2+\left(\frac{\partial^p u_k^D}{\partial\eta^p}\right)^2\right)+\frac{c^2}{4}\left(\frac{\partial^{2p}u_k^D}{\partial\xi^p\partial\eta^p}\right)^2\right]d\Omega_k\right)$$

Sheshadri et al. (2015). J. Sci Comput.

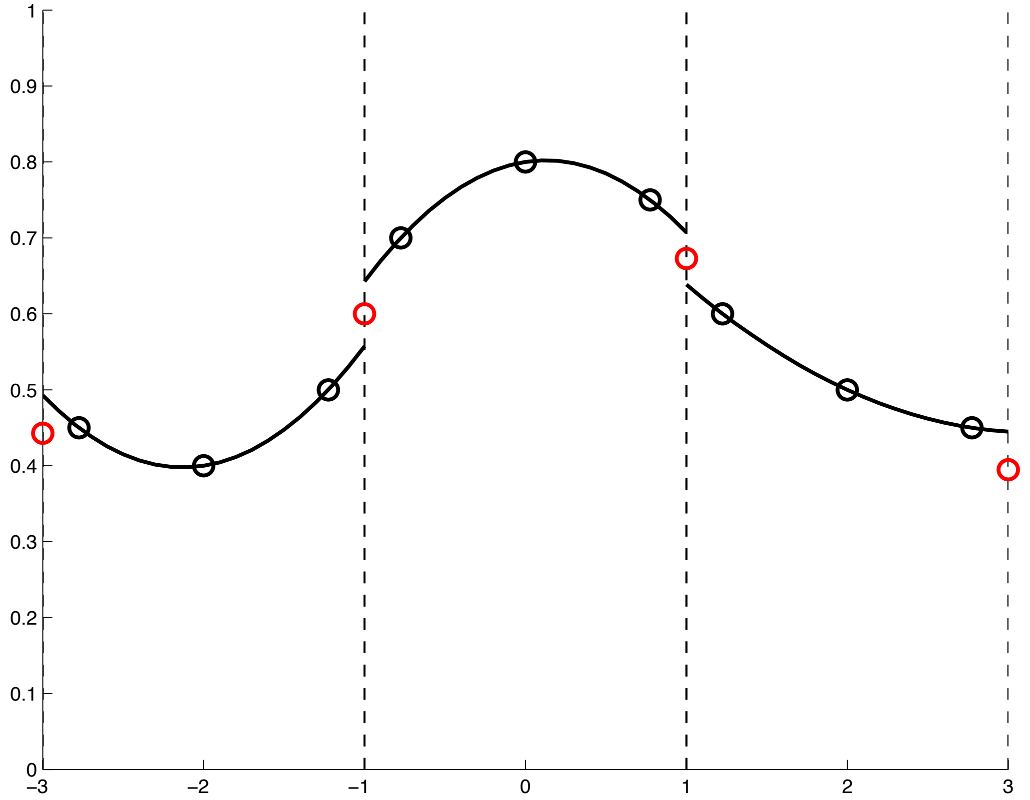
Direct Flux Reconstruction (DFR)

- In existing FR method, reconstruction process involves several distinct computational steps, all aimed at applying correction polynomials to construct the continuous flux.
- Correction polynomials introduced by Huynh to generate continuous flux of order $P+1$ so that terms in conservation law are of consistent order P.

Direct Flux Reconstruction (DFR)

If this consistency constraint is abandoned, entire reconstruction process can be consolidated into a single Lagrange interpolation through the combined set of interior solution points and interface flux points.

$$f^C = f_L^I \tilde{l}_0 + \sum_{n=1}^{P+1} f_n \tilde{l}_n + f_R^I \tilde{l}_{P+2}$$



Degree P

Direct Flux Reconstruction (DFR)

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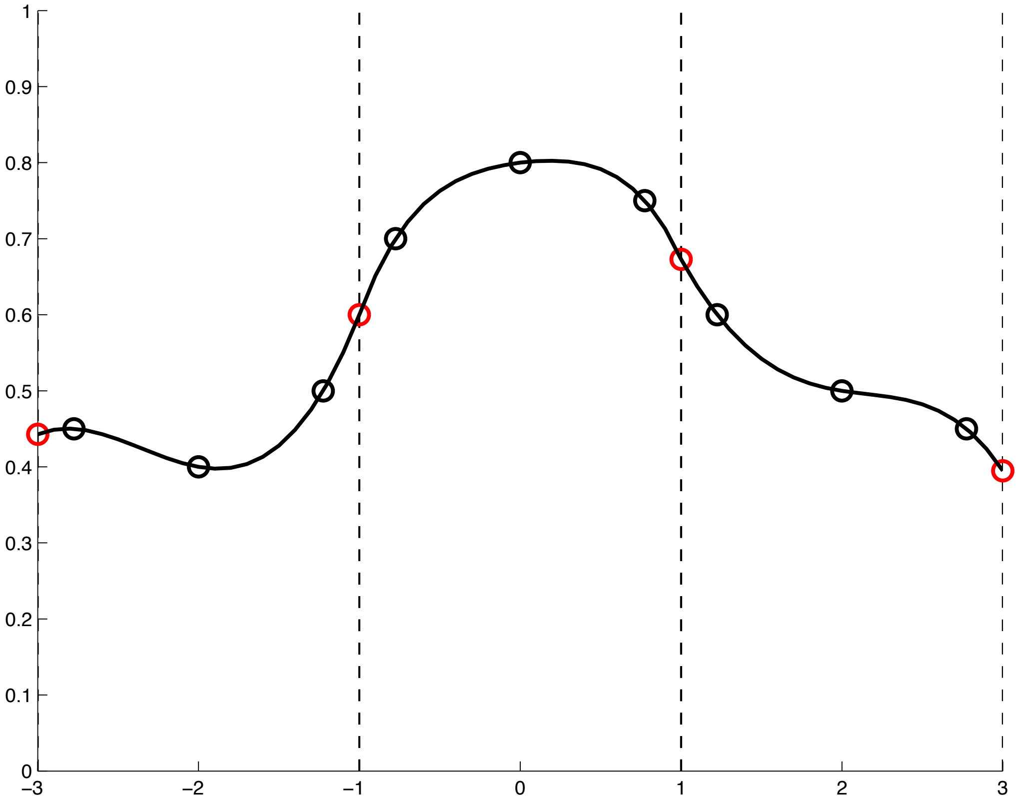
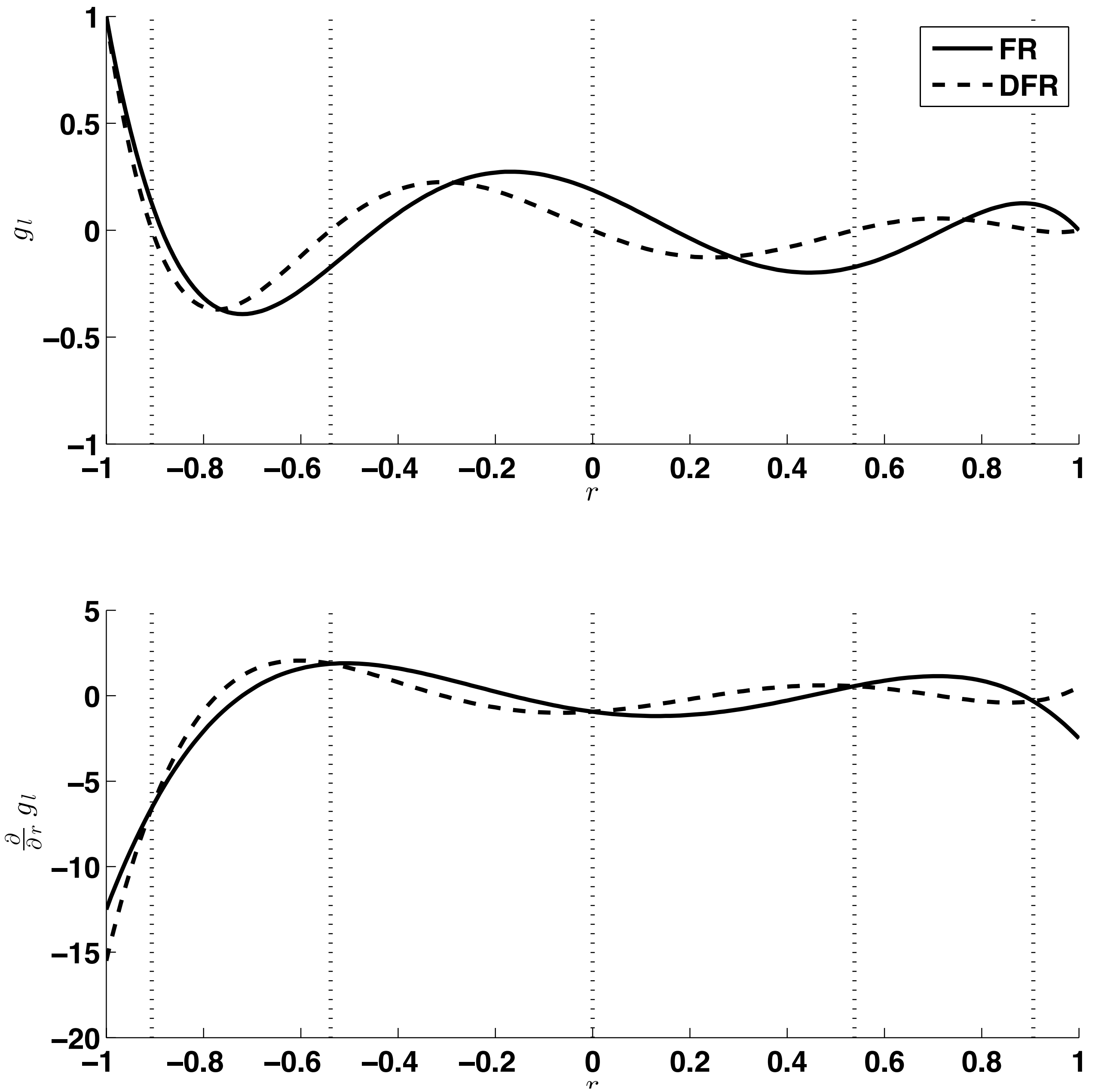


Degree $P+2$

Direct Flux Reconstruction (DFR)



Shock Capturing

Method	Advantages	Disadvantages
Limiting	• Eliminates oscillations • Robust	• Smeared over elements • Expensive
Artificial Viscosity	• Sub-cell shock capturing • Smoothly varying viscosity	• High-order derivatives • Time-step restrictions • Too many parameters
Filtering	• Sub-cell shock capturing • Very Inexpensive	• Varying dissipation not easy • Needs a good sensor

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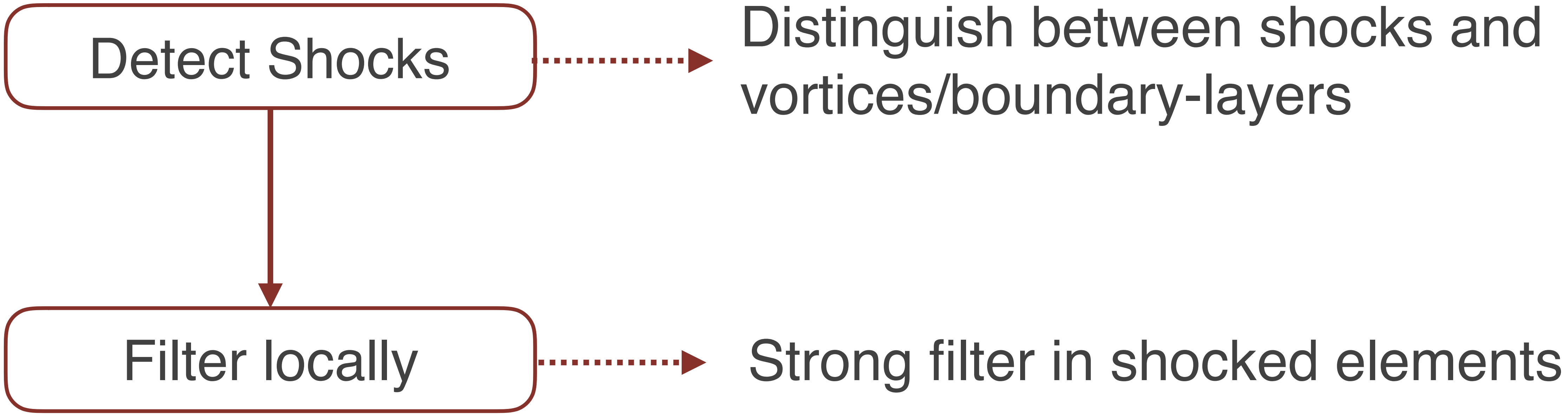
For explicit FR on GPUs filtering is attractive…but requires a good sensor.

Shock Capturing: Our Approach

Two-step approach

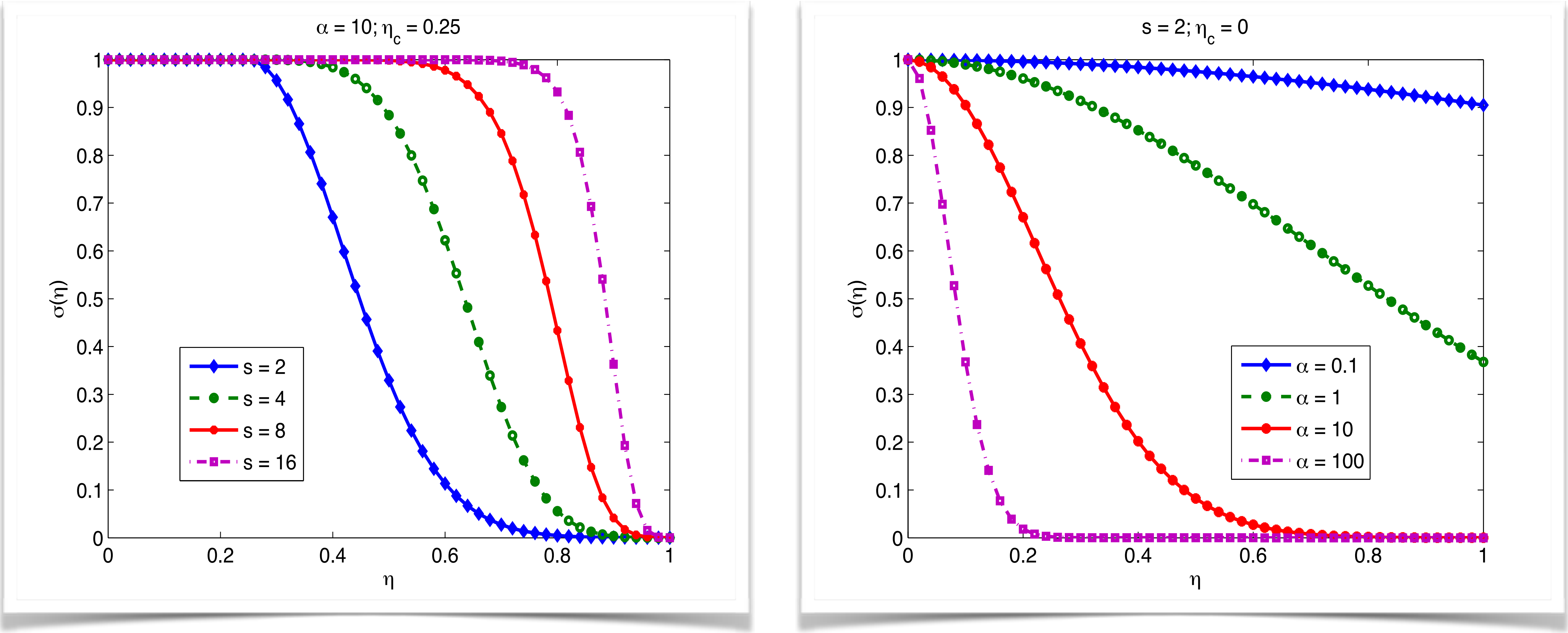


Detect Shocks → Distinguish between shocks and vortices/boundary-layers

Filter locally → Strong filter in shocked elements

Minimize parameter fine-tuning

Shock Capturing: Exponential Modal Filtering



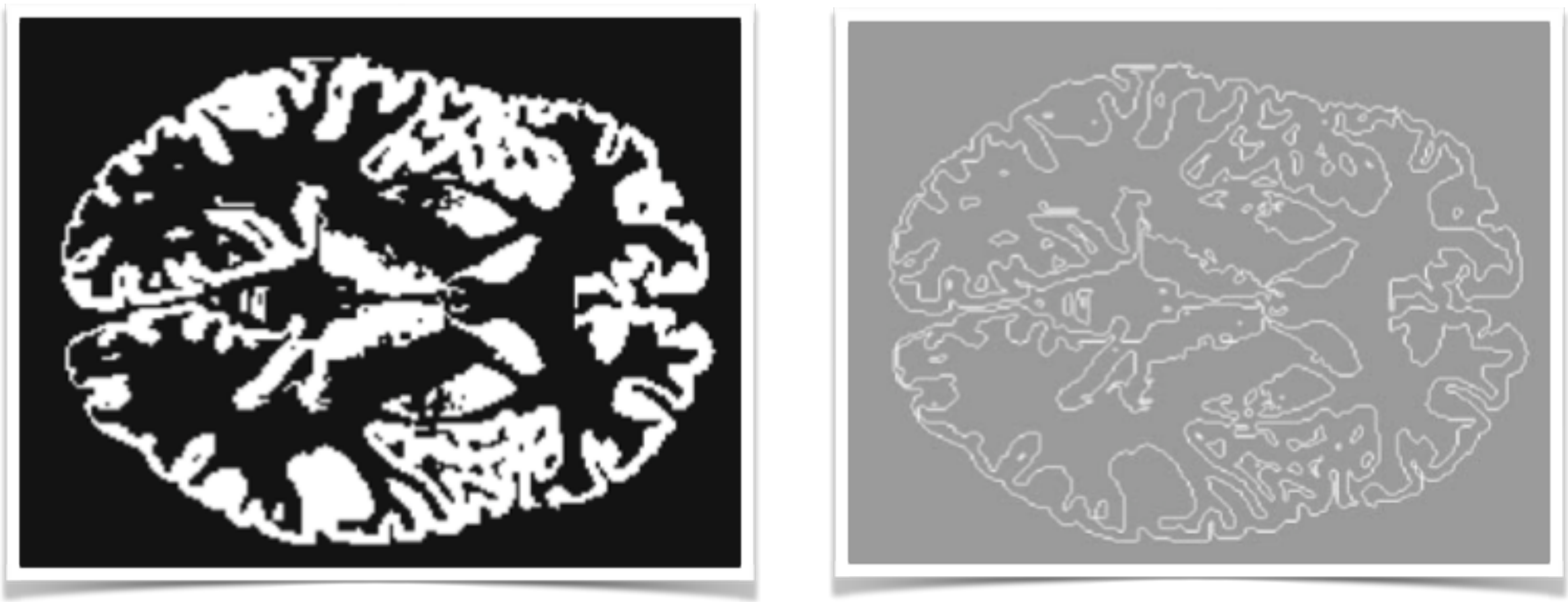
$$\sigma(\eta) = \begin{cases} 1, & 0 \leq \eta \leq \eta_c = \frac{N_c}{P} \\ \exp\left(-\alpha\left(\frac{\eta-\eta_c}{1-\eta_c}\right)^s\right), & \eta_c \leq \eta \leq 1 \end{cases}$$

Shock Capturing: Current Sensors

- **Physics based**
    - Specific to problem or type of discontinuity
    - Need derivatives: expensive
    - Hard to extend to unstructured grids

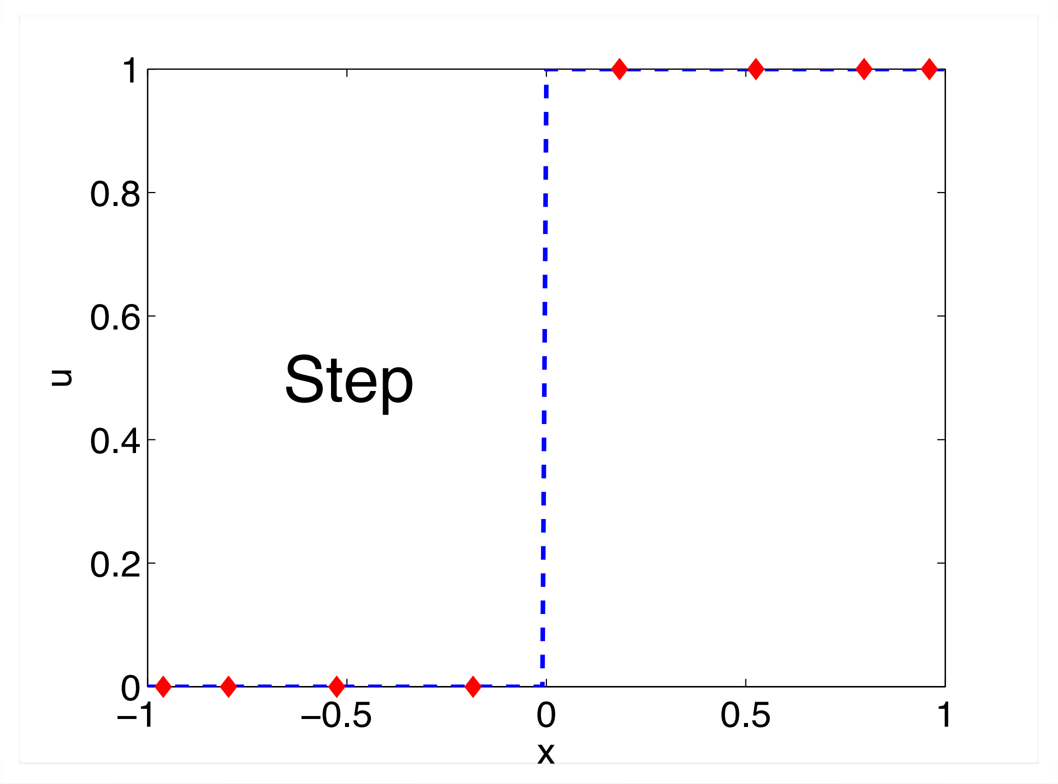
- **Smoothness based**
    - Used successfully in low-order schemes
    - Persson and Peraire — high order unstructured methods

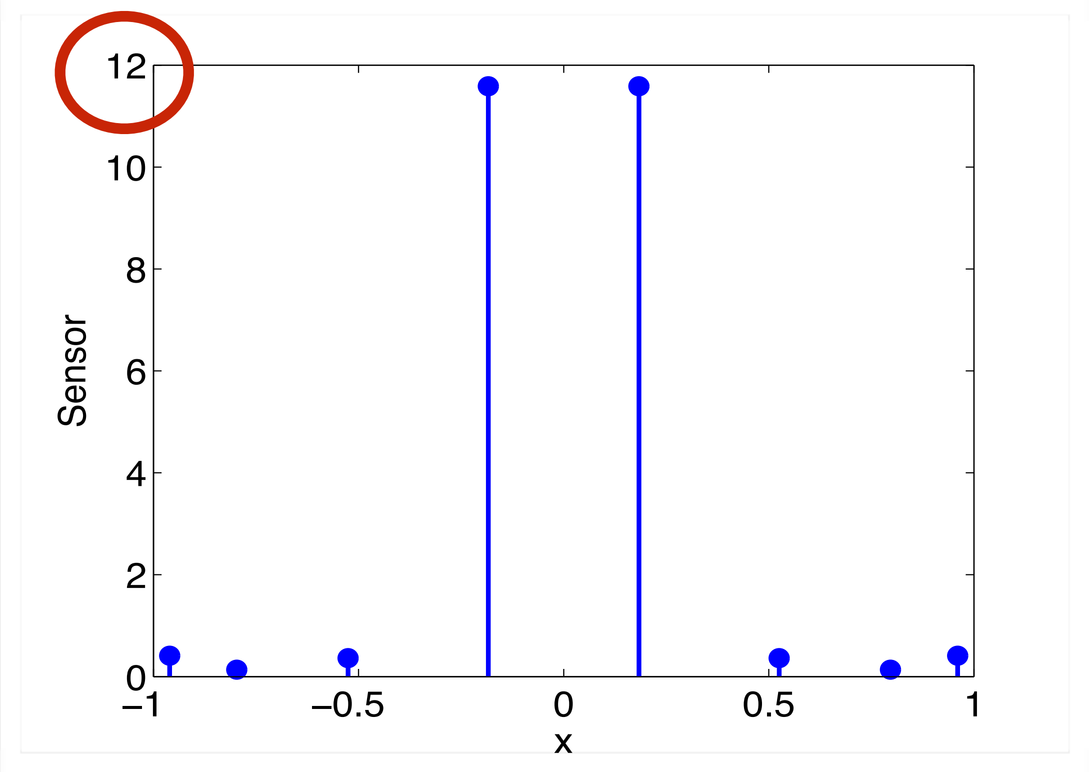
Shock Capturing: Concentration Method

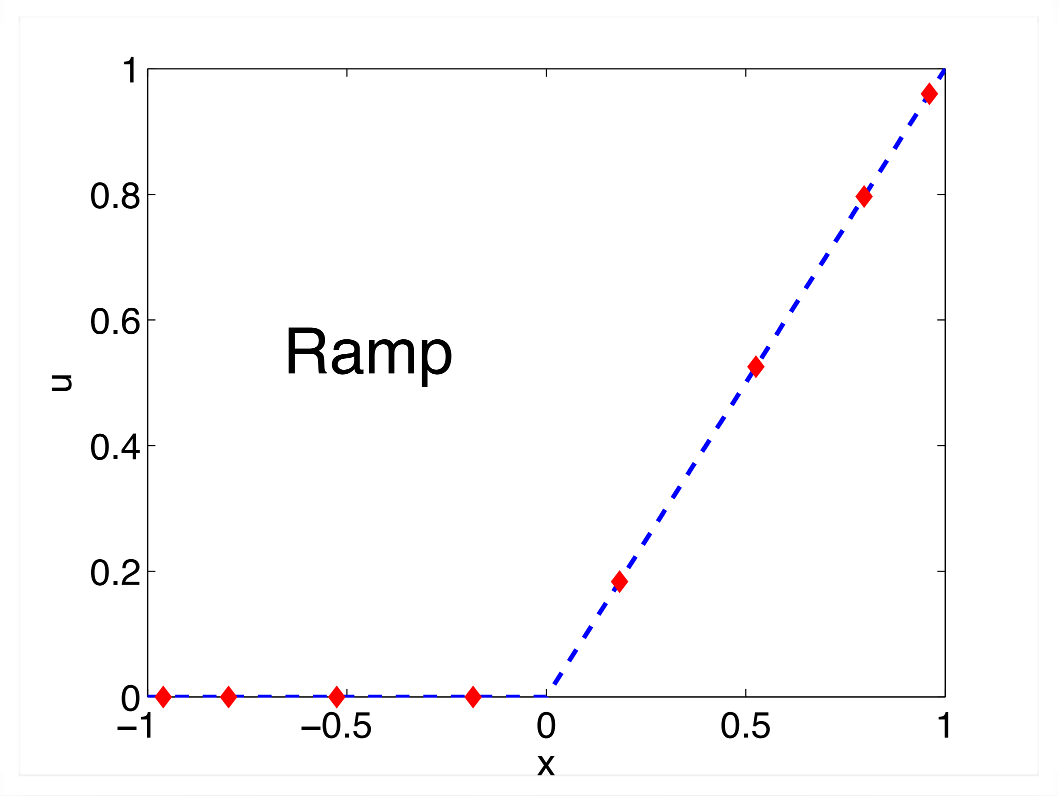


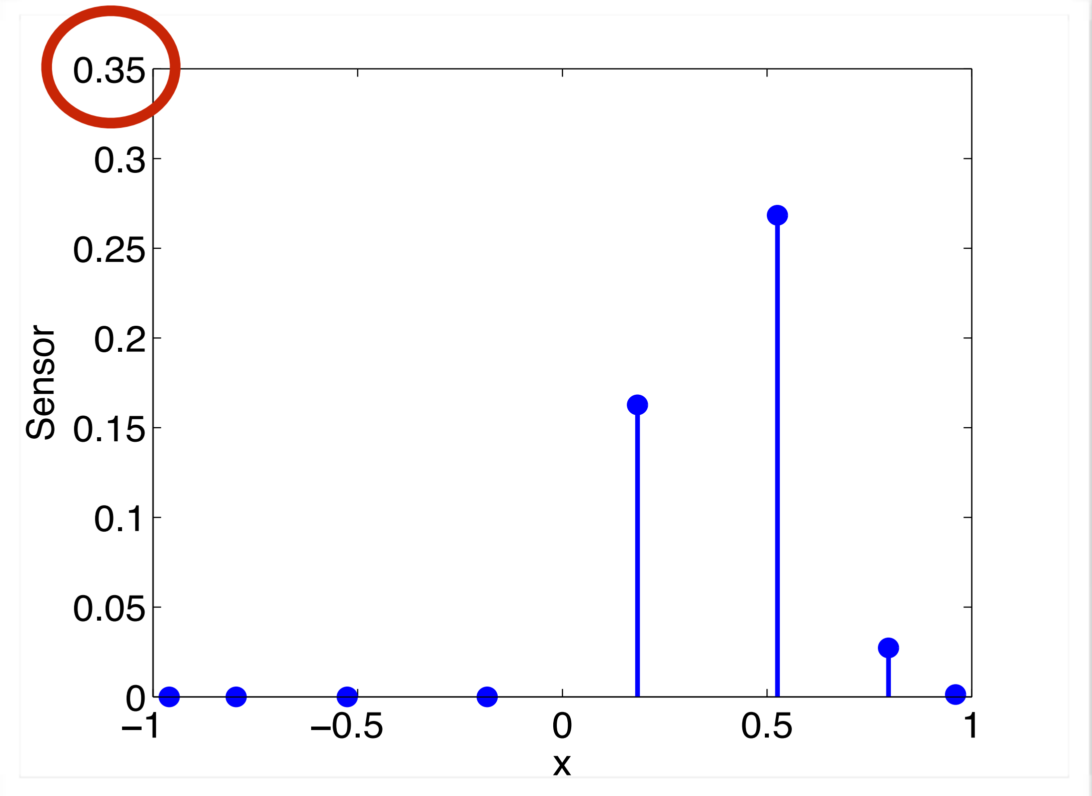
- Used for image/MRI edge detection
- Works directly on Fourier spectral information

Shock Capturing: Our Sensor

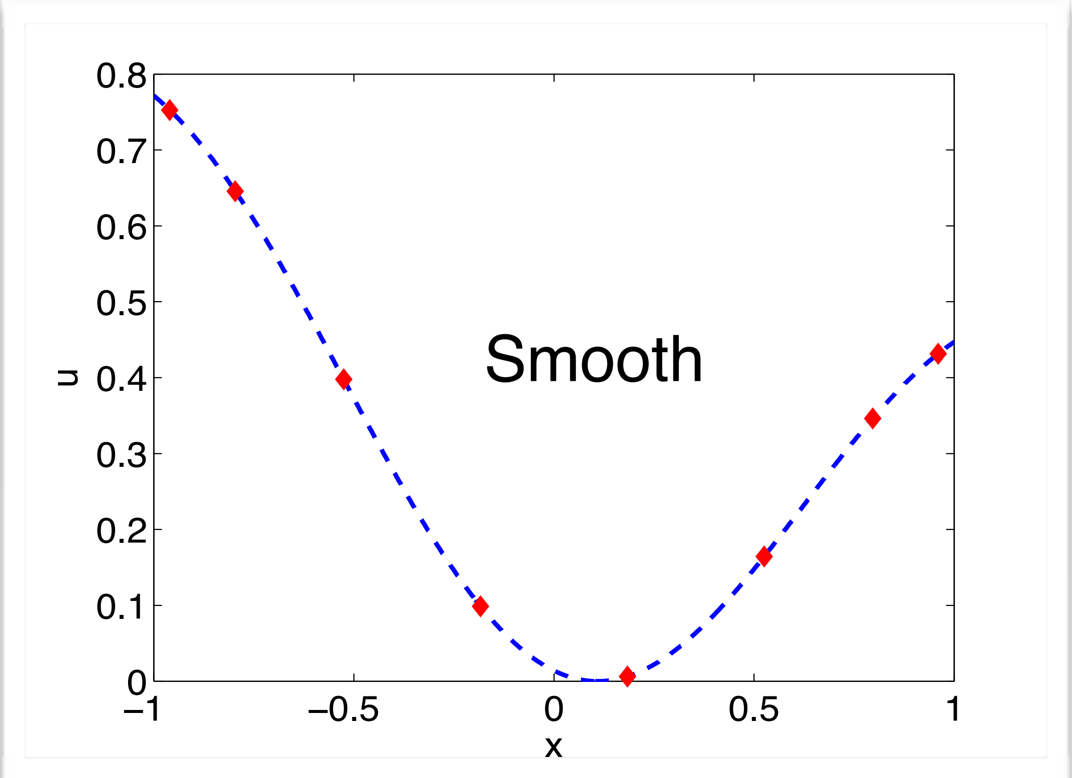


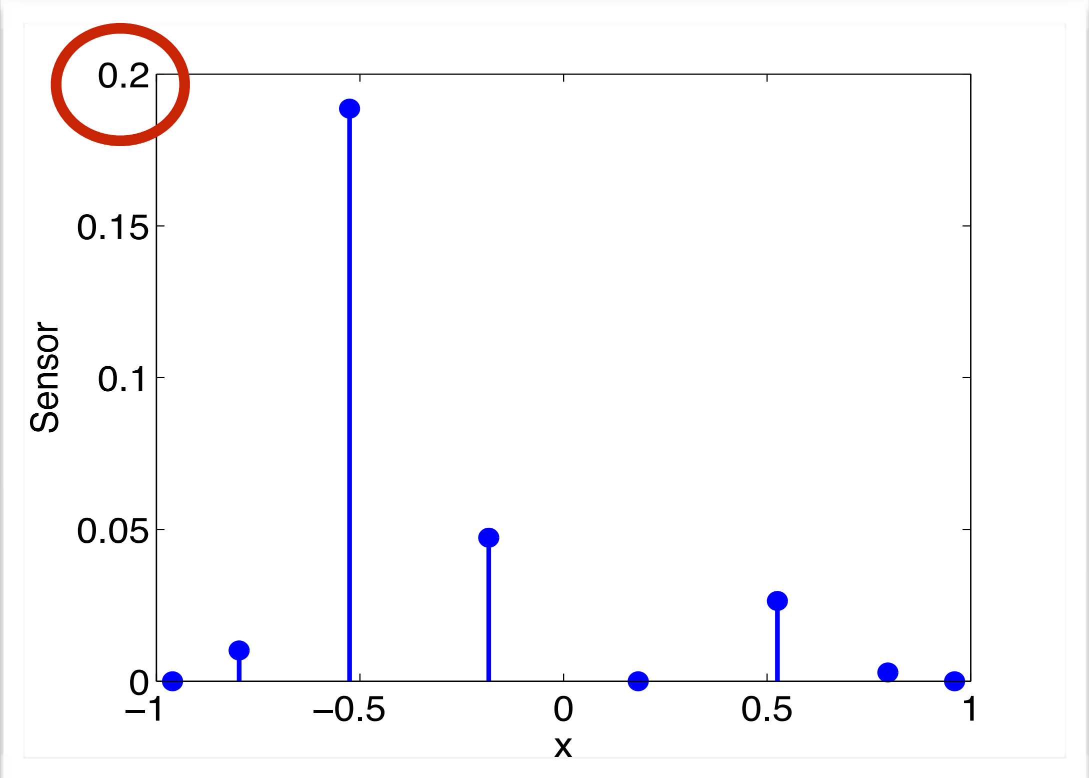


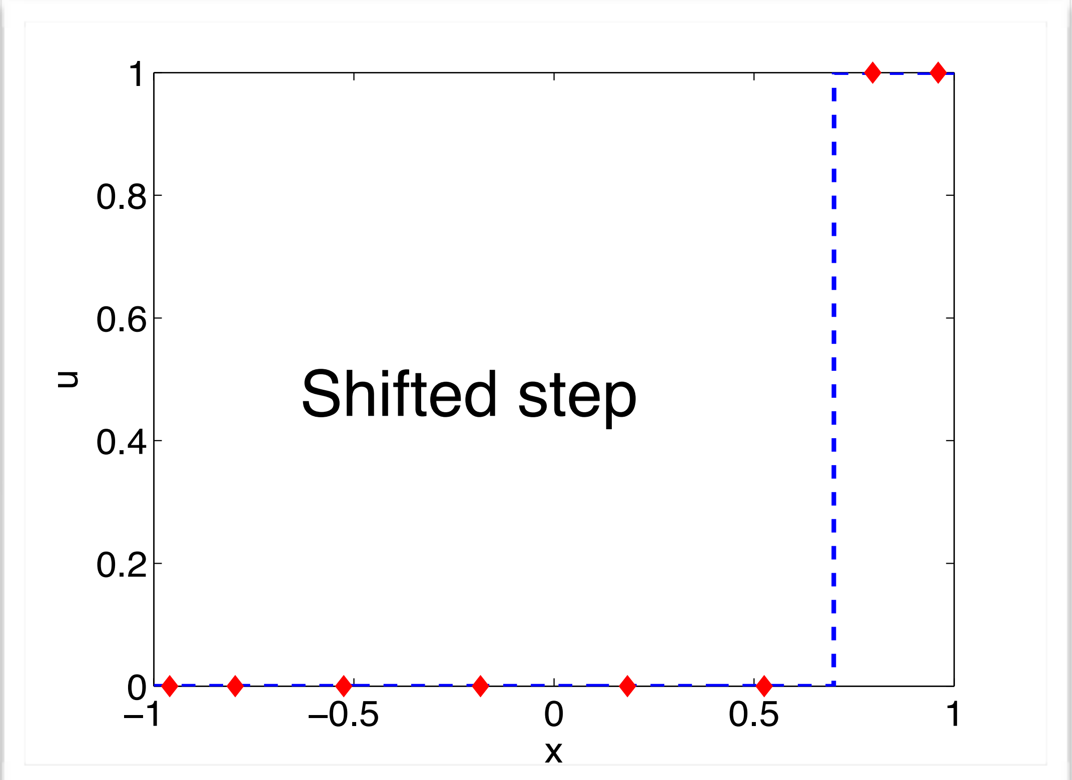


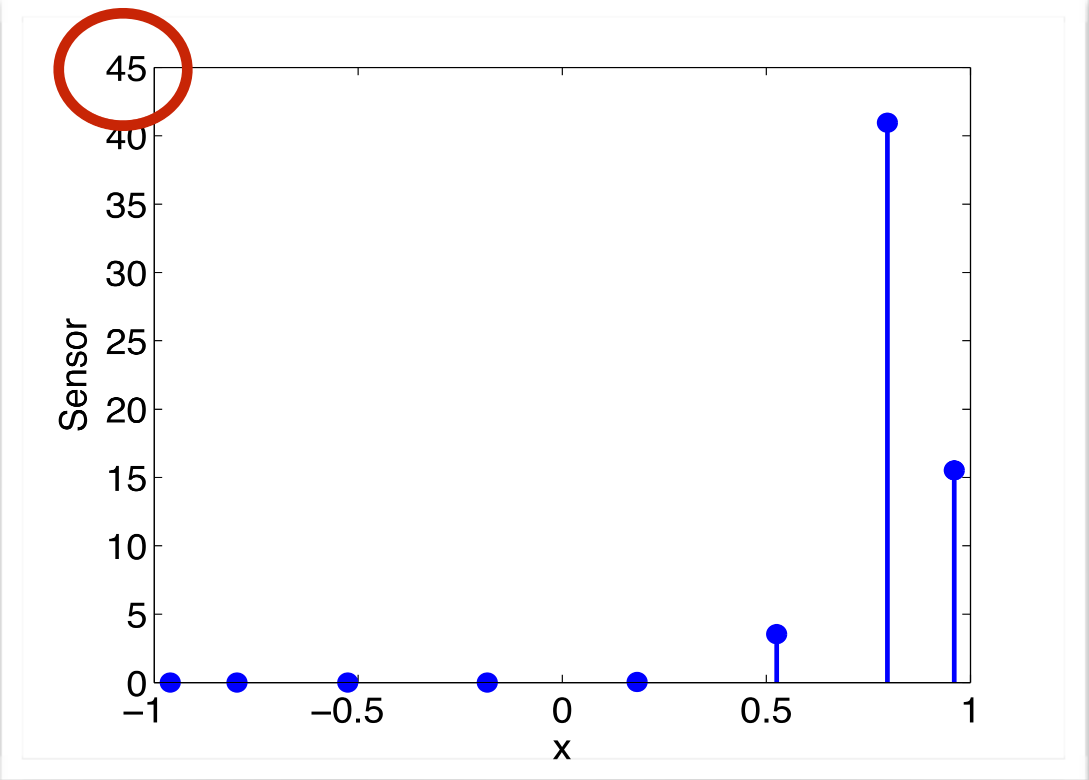


Shock Capturing: Our Sensor

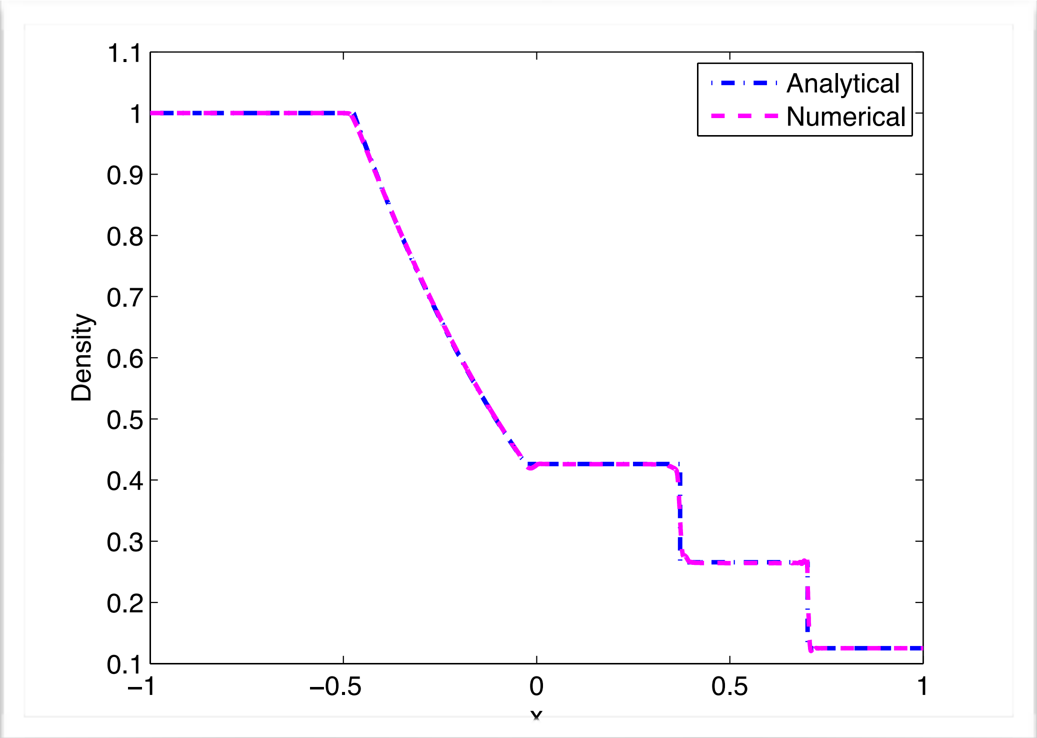


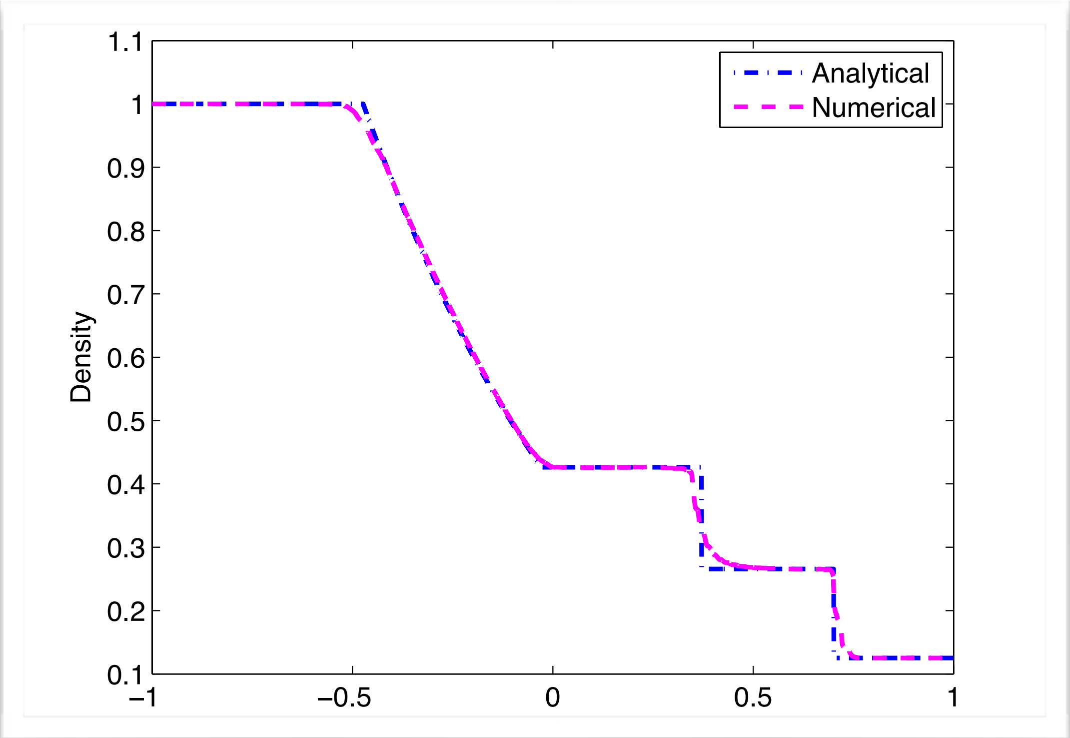


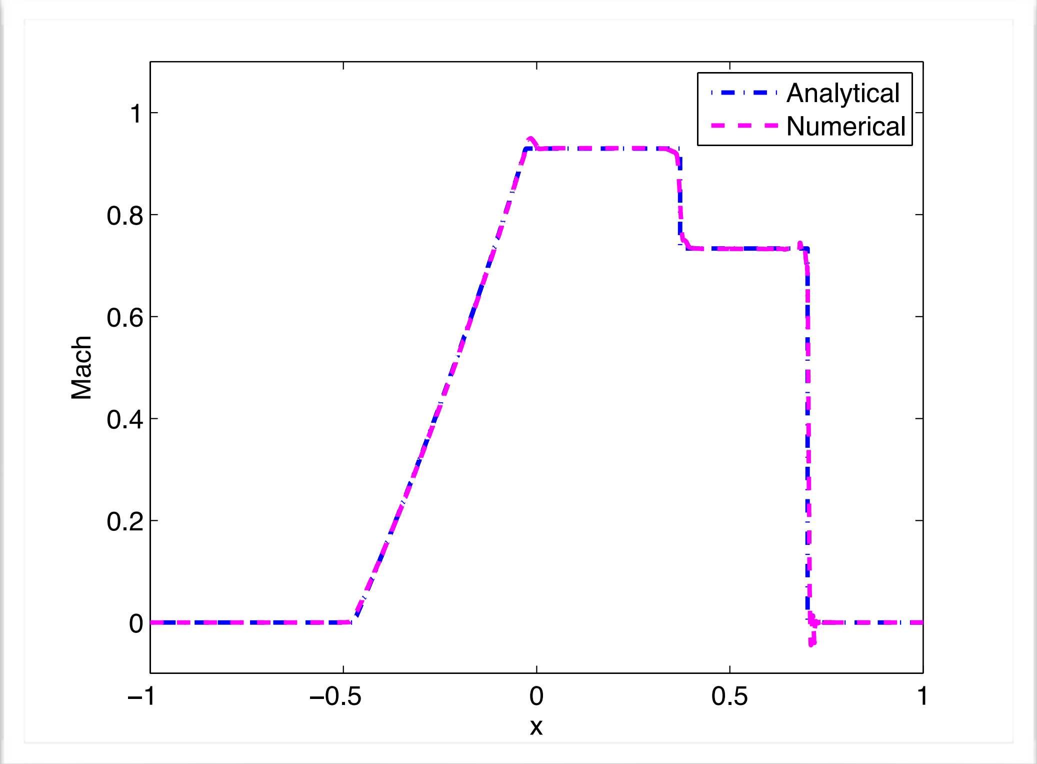


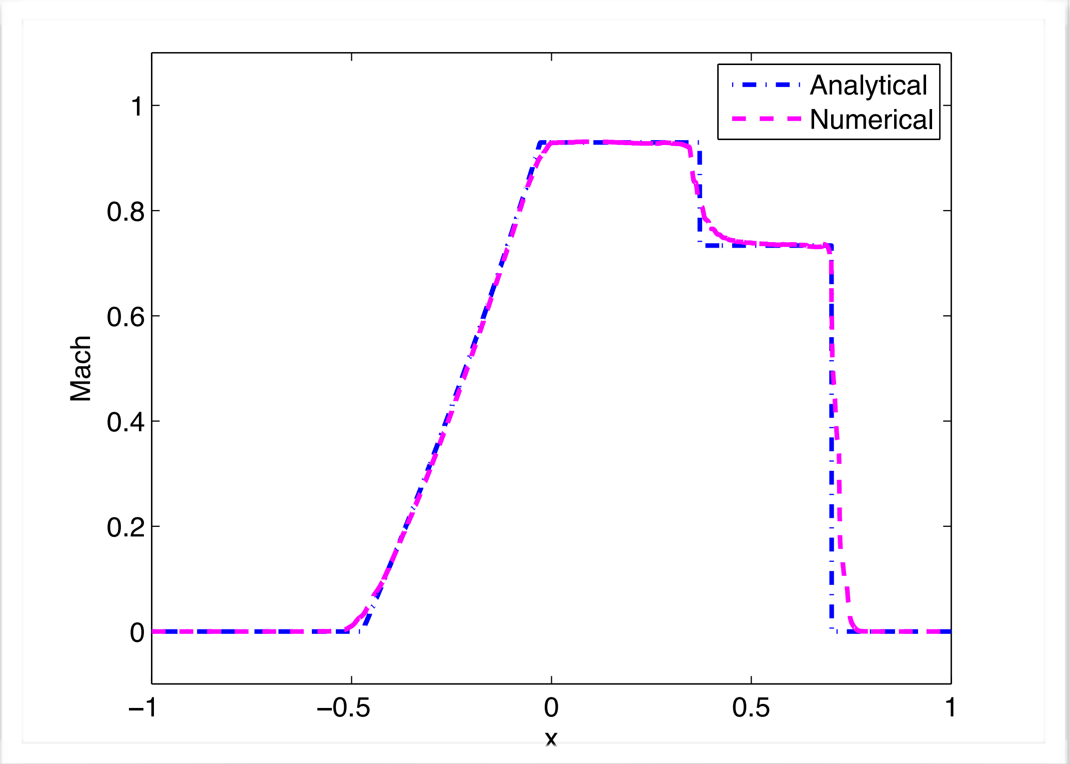


Shock Capturing: 1D Shock Tube

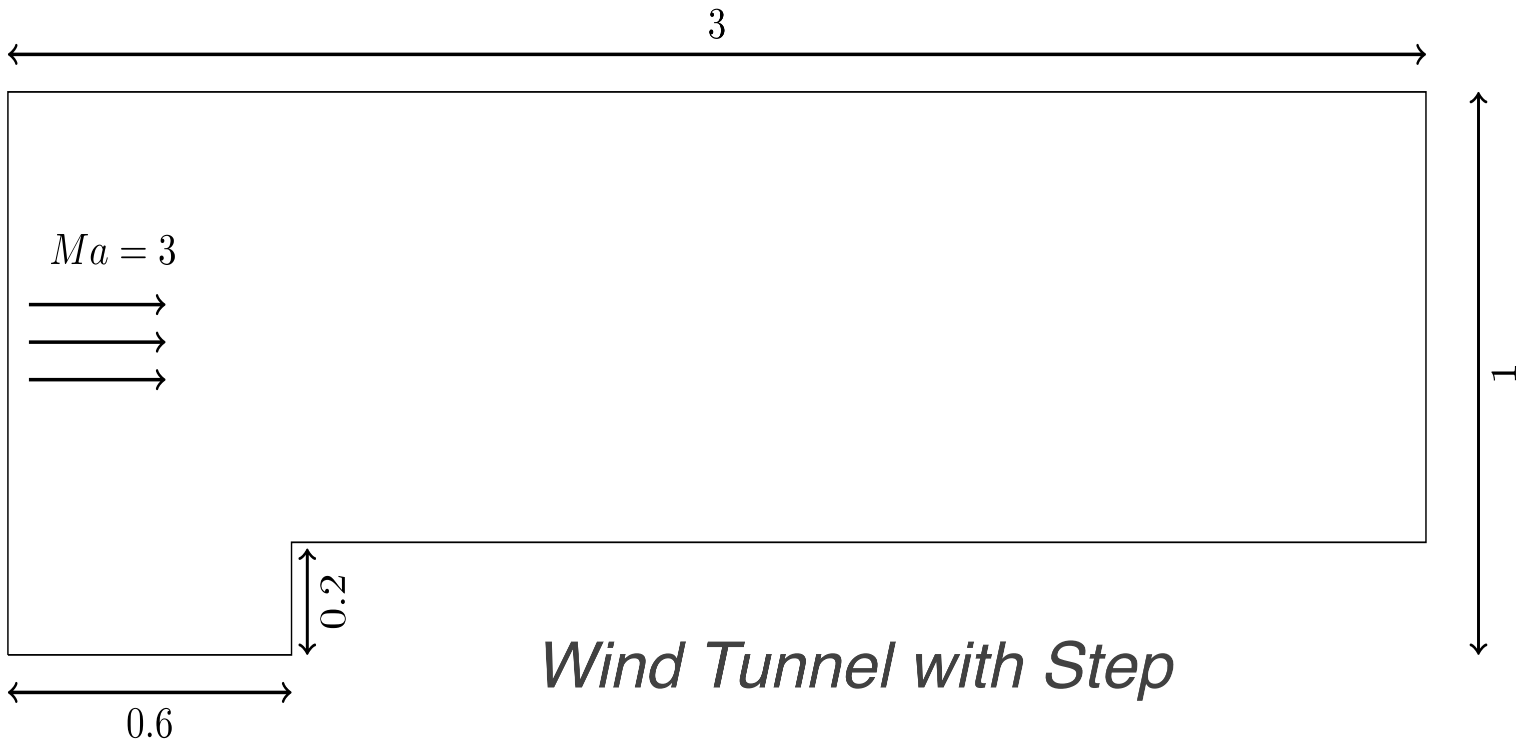








Shock Capturing: Flow Over a Step

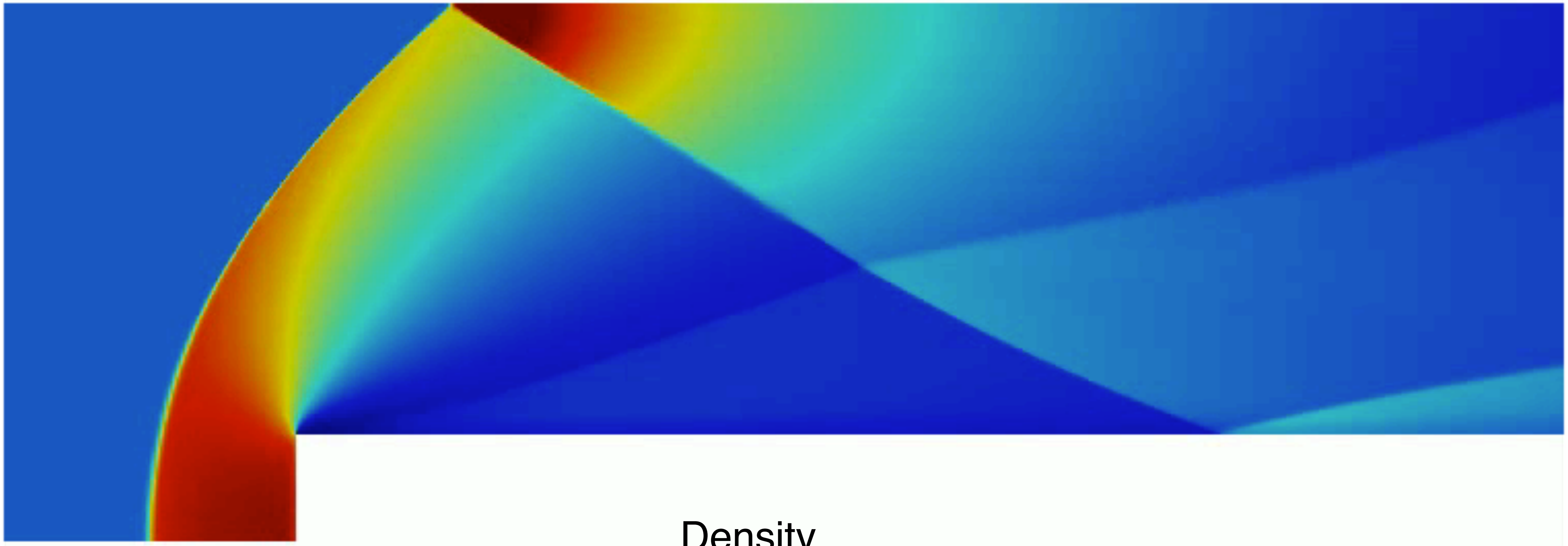


Wind Tunnel with Step

- Euler Equations
- Structured Quad Mesh
- Sensor at ramp
- Positivity Limiter

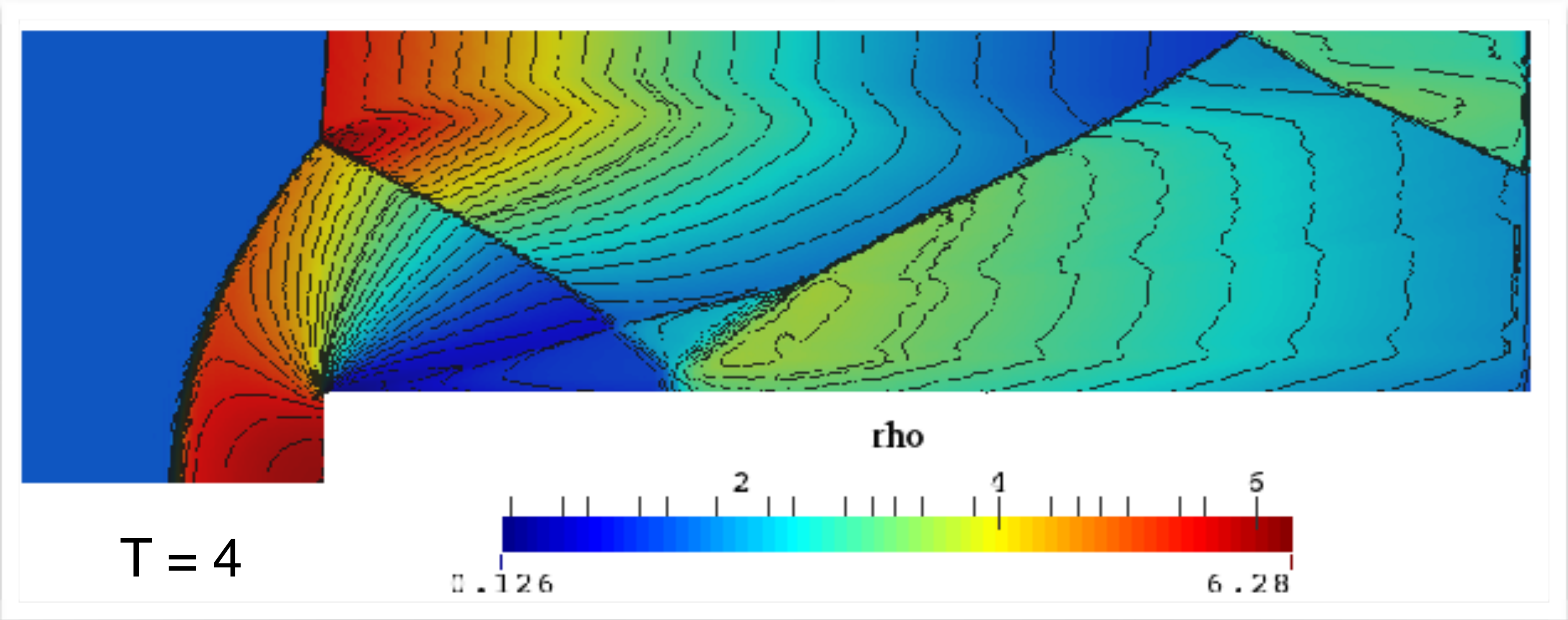
Mach	Flow Angle	Num Elem	Order	Filter Order	Filter Strength
3.0	0°	63,004	3	2	5

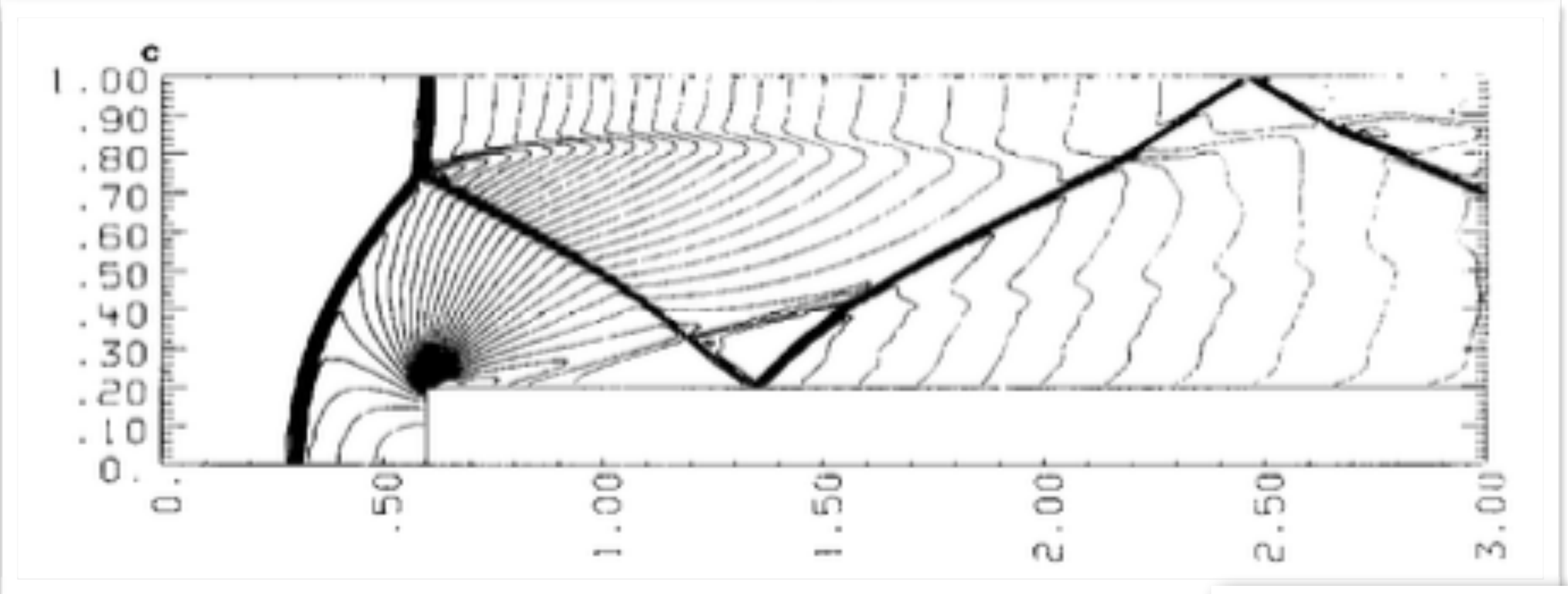
Shock Capturing: Flow Over a Step



Density

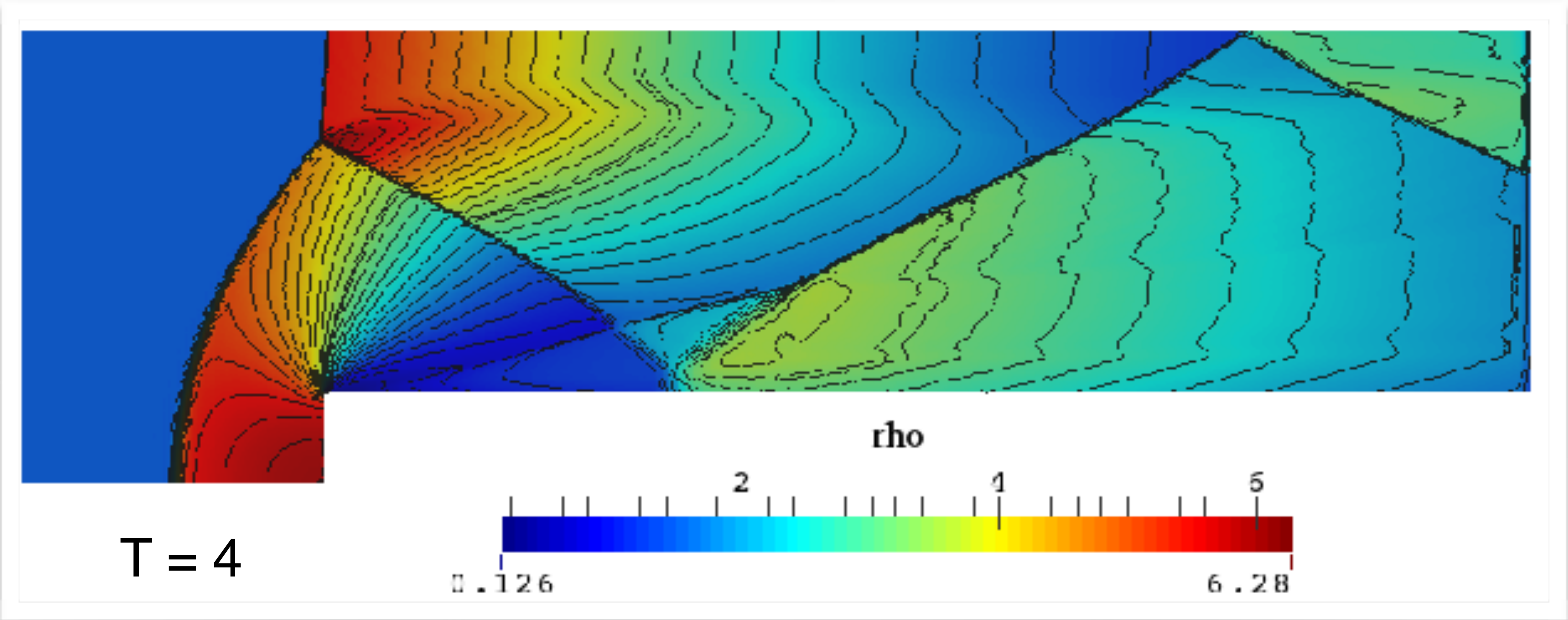
Shock Capturing: Flow Over a Step

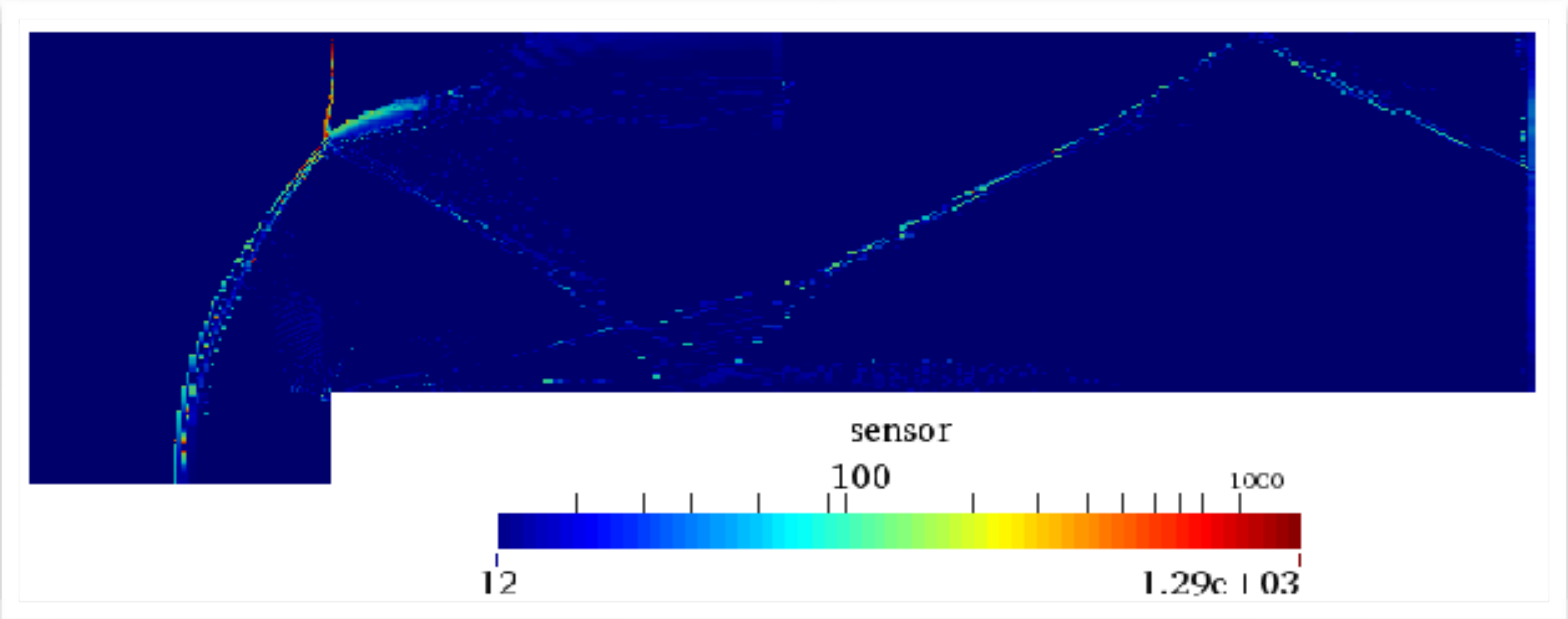




Reference: Woodward and Colella

Shock Capturing: Flow Over a Step





Convergence Acceleration

Recent work has focused on convergence acceleration.

Convergence Acceleration: BDF1

- Fully discrete equation

$$\frac{\Delta \boldsymbol{u}_{\mathrm{ele}}}{\Delta t} = \frac{(\boldsymbol{u}_{\mathrm{ele}}^{n+1} - \boldsymbol{u}_{\mathrm{ele}}^{n})}{\Delta t} = \boldsymbol{R}(\boldsymbol{u}_{\mathrm{ele}}^{n+1}, \boldsymbol{u}_{\mathrm{eleN}}^{n+1})$$

- Linearize to obtain global linear system

$$\left(\frac{I}{\Delta t} + \frac{\partial \boldsymbol{R}_{\mathrm{ele}}^{n}}{\partial \boldsymbol{u}_{\mathrm{ele}}}\right) \Delta \boldsymbol{u}_{\mathrm{ele}} - \sum_{\mathrm{eleN}} \frac{\partial \boldsymbol{R}_{\mathrm{ele}}^{n}}{\partial \boldsymbol{u}_{\mathrm{eleN}}} \Delta \boldsymbol{u}_{\mathrm{eleN}} = \boldsymbol{R}(\boldsymbol{u}_{\mathrm{ele}}^{n}, \boldsymbol{u}_{\mathrm{eleN}}^{n})$$

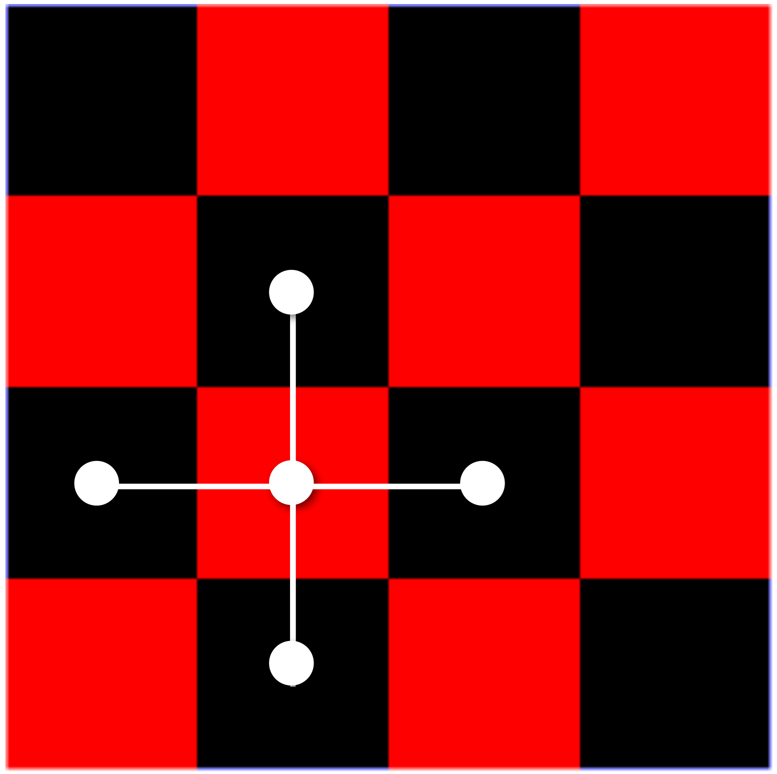
Element local Jacobian   Element neighbor Jacobian

Convergence Acceleration: BDF1

- Solve using multicolored Gauss-Seidel.
- For example with red/black coloring:

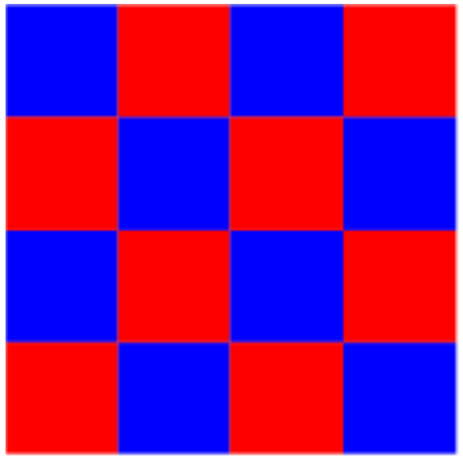
$$\begin{pmatrix} D_R & C_B \\ C_R & D_B \end{pmatrix} \begin{pmatrix} x_R \\ x_B \end{pmatrix} = \begin{pmatrix} b_R \\ b_B \end{pmatrix}$$

$$x_R^{n+1} = D_R^{-1}\left(b_R - C_B x_B^n\right)$$
$$x_B^{n+1} = D_B^{-1}\left(b_B - C_R x_R^n\right)$$

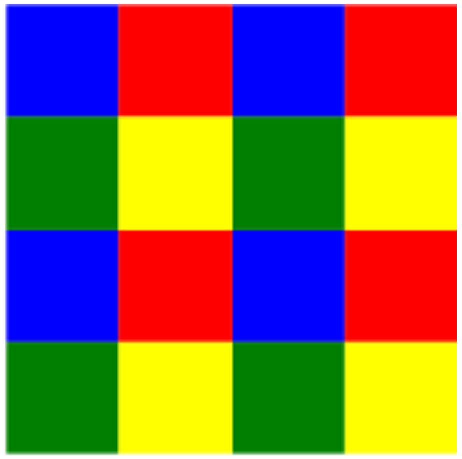


Convergence Acceleration: Mesh Coloring

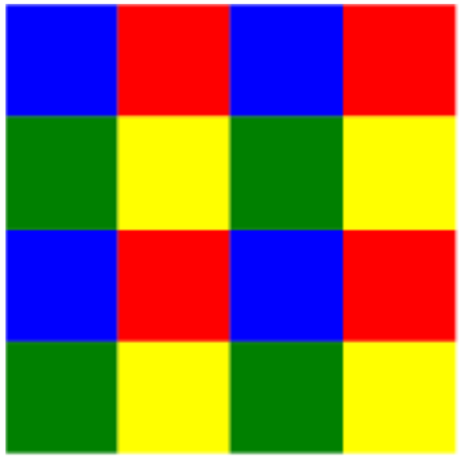
- **Requirements**
  - Minimise number of colours
  - Distribute work evenly



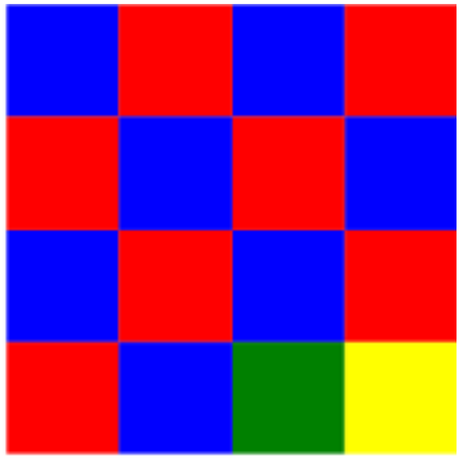
Good



Bad

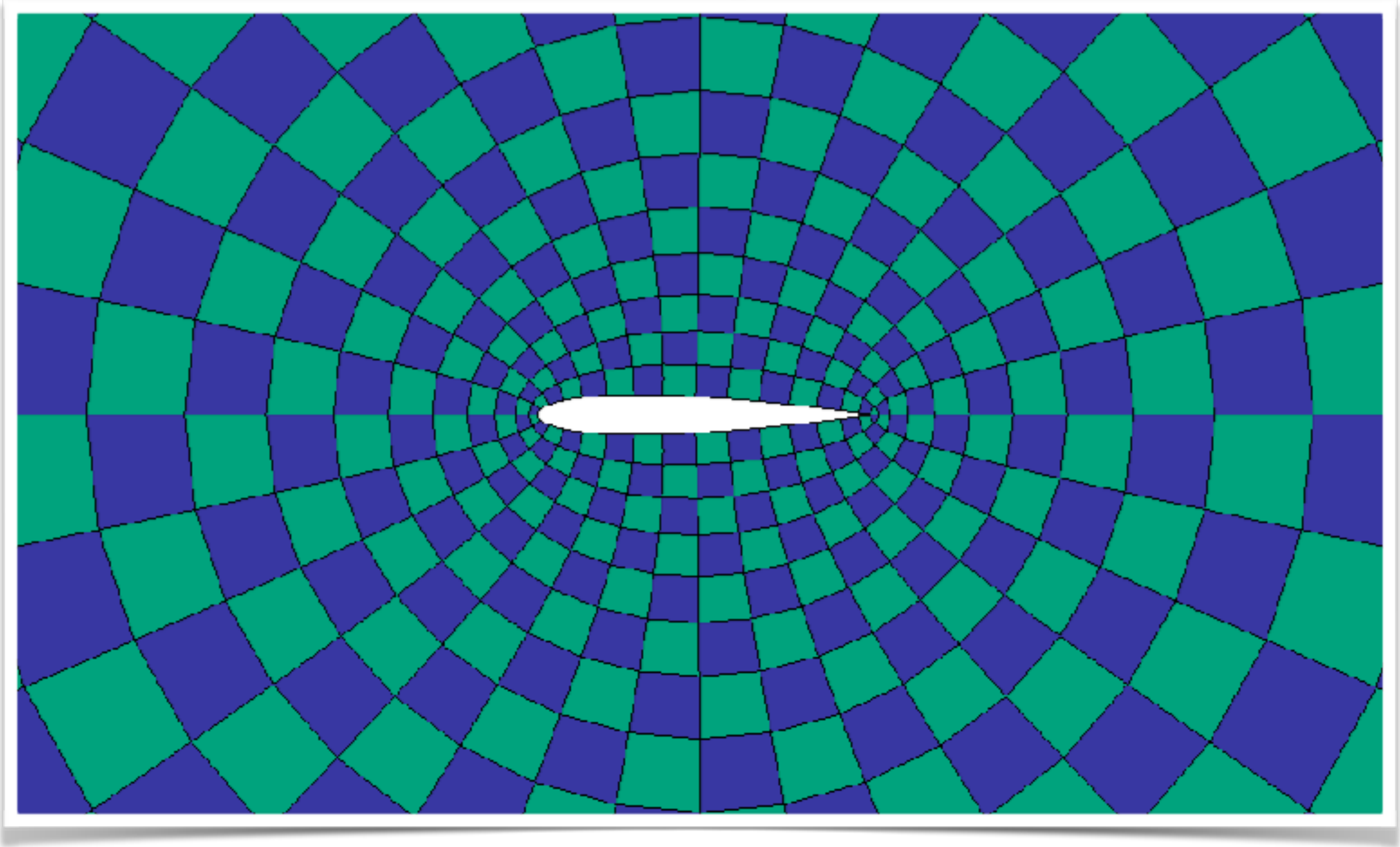


Good



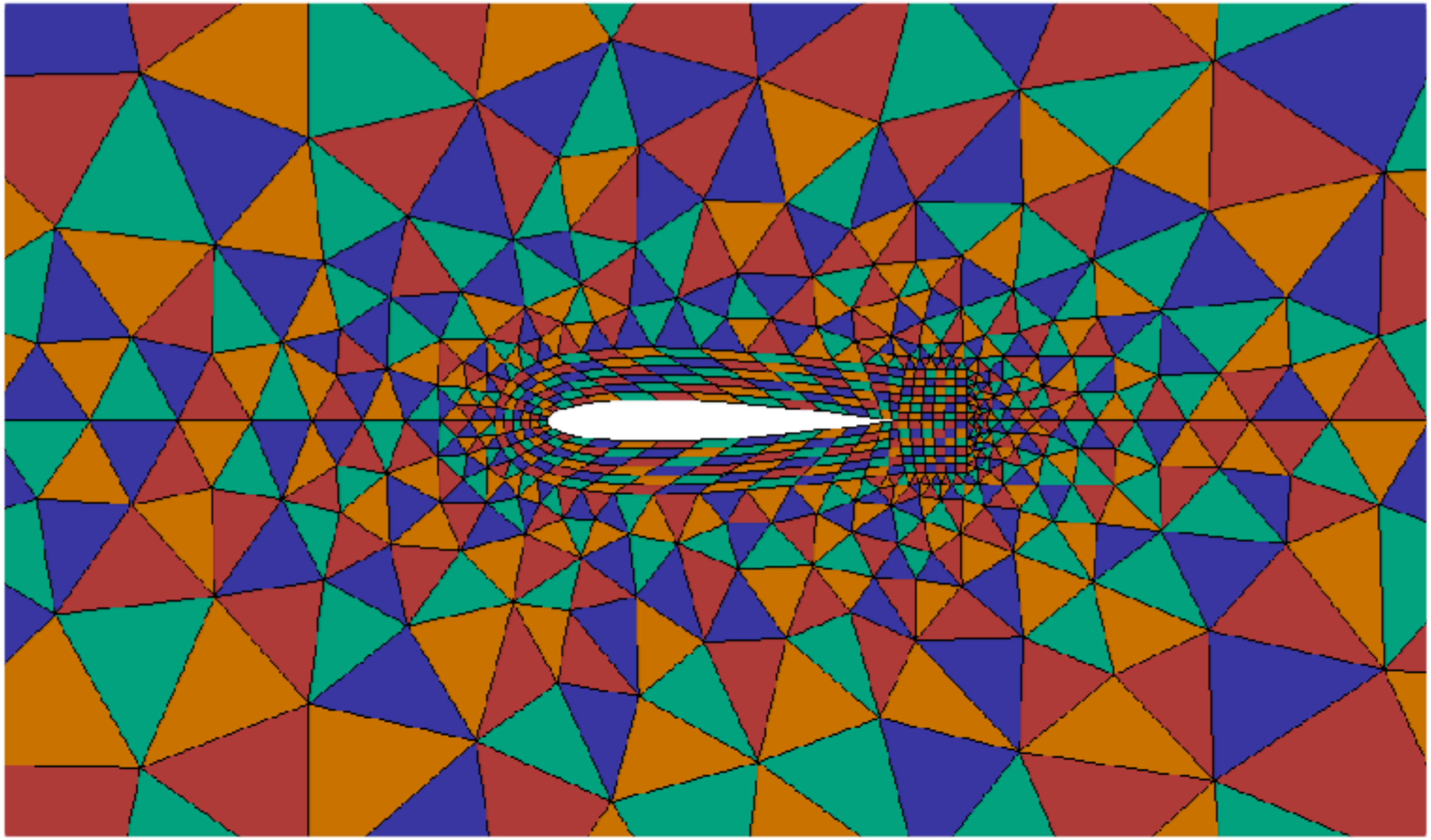
Bad

Convergence Acceleration: Mesh Coloring



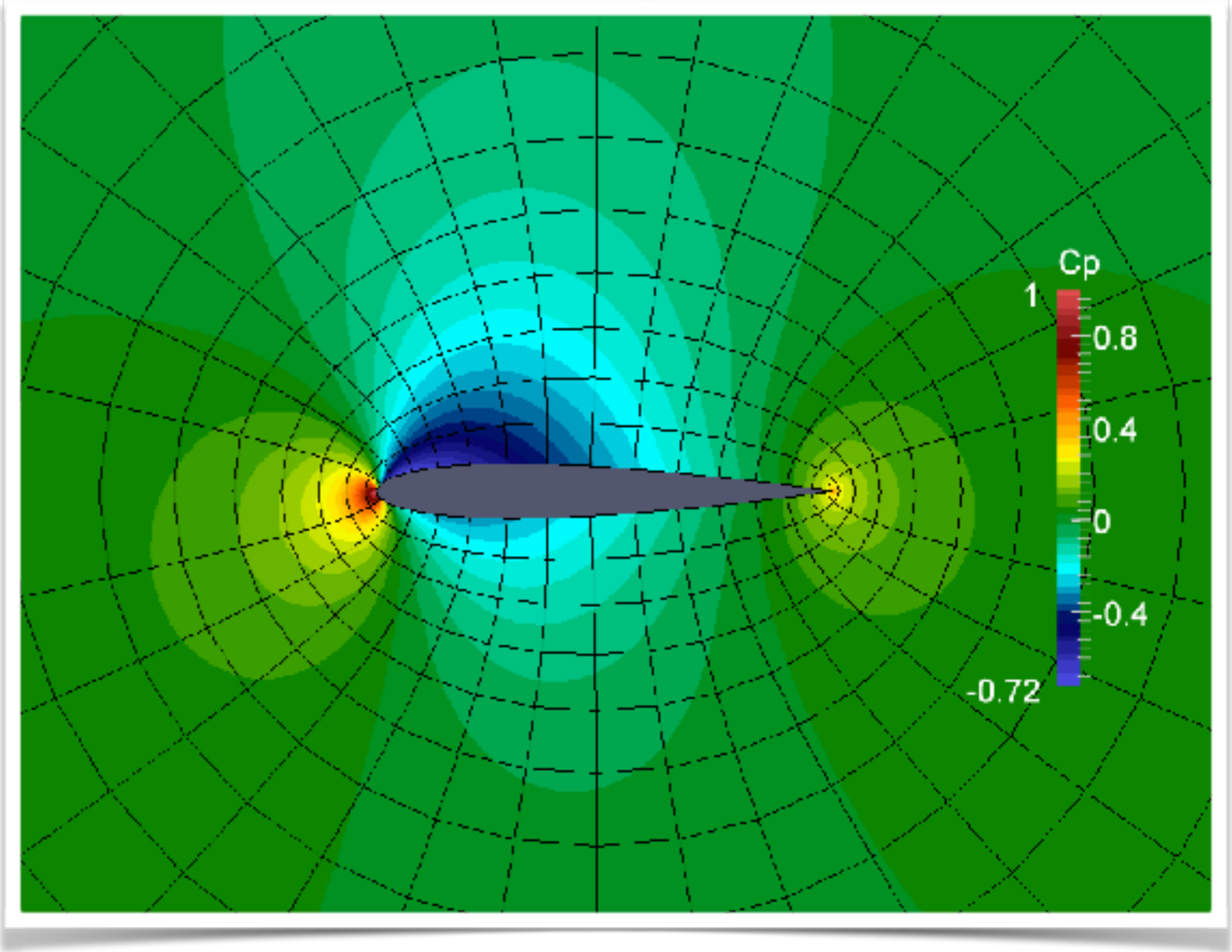
Structured NACA 0012

Convergence Acceleration: Mesh Coloring



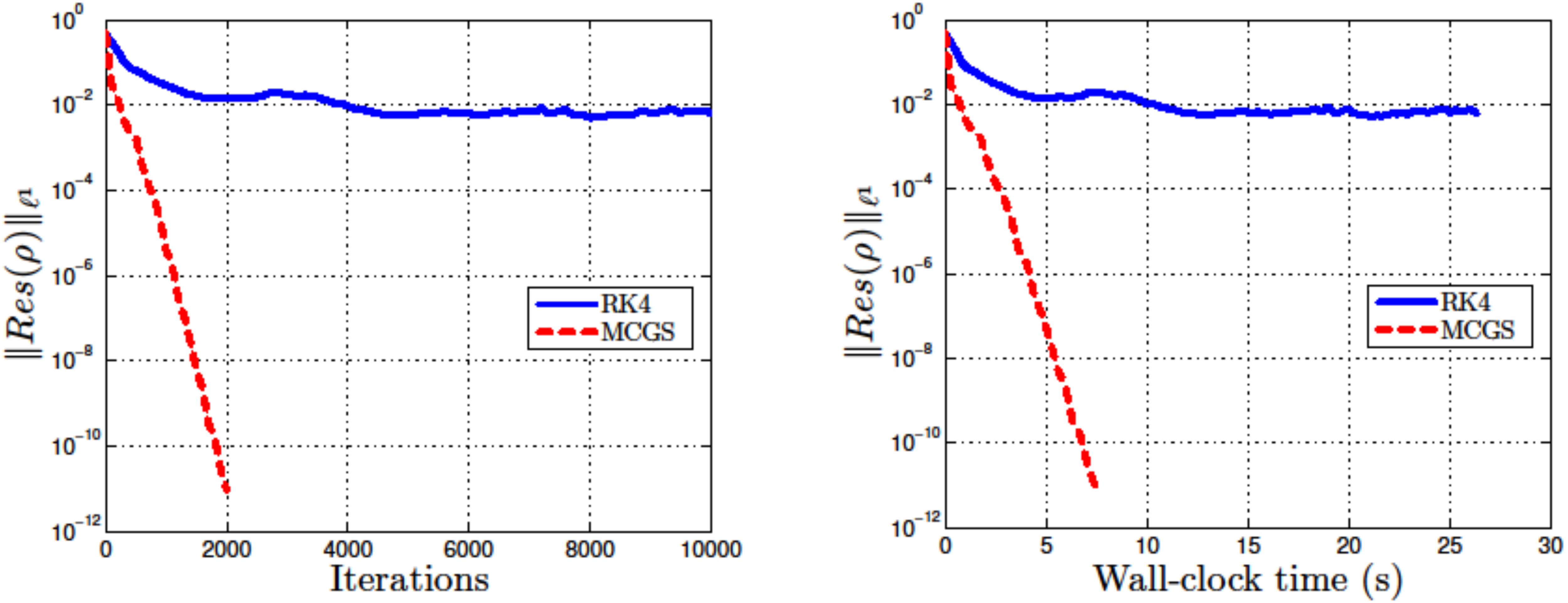
Unstructured NACA 0012

Convergence Acceleration: NACA 0012



Euler eq, NACA 0012, 32 by 32 grid, P = 4, Ma = 0.5, α = 1.25°

Convergence Acceleration: NACA 0012



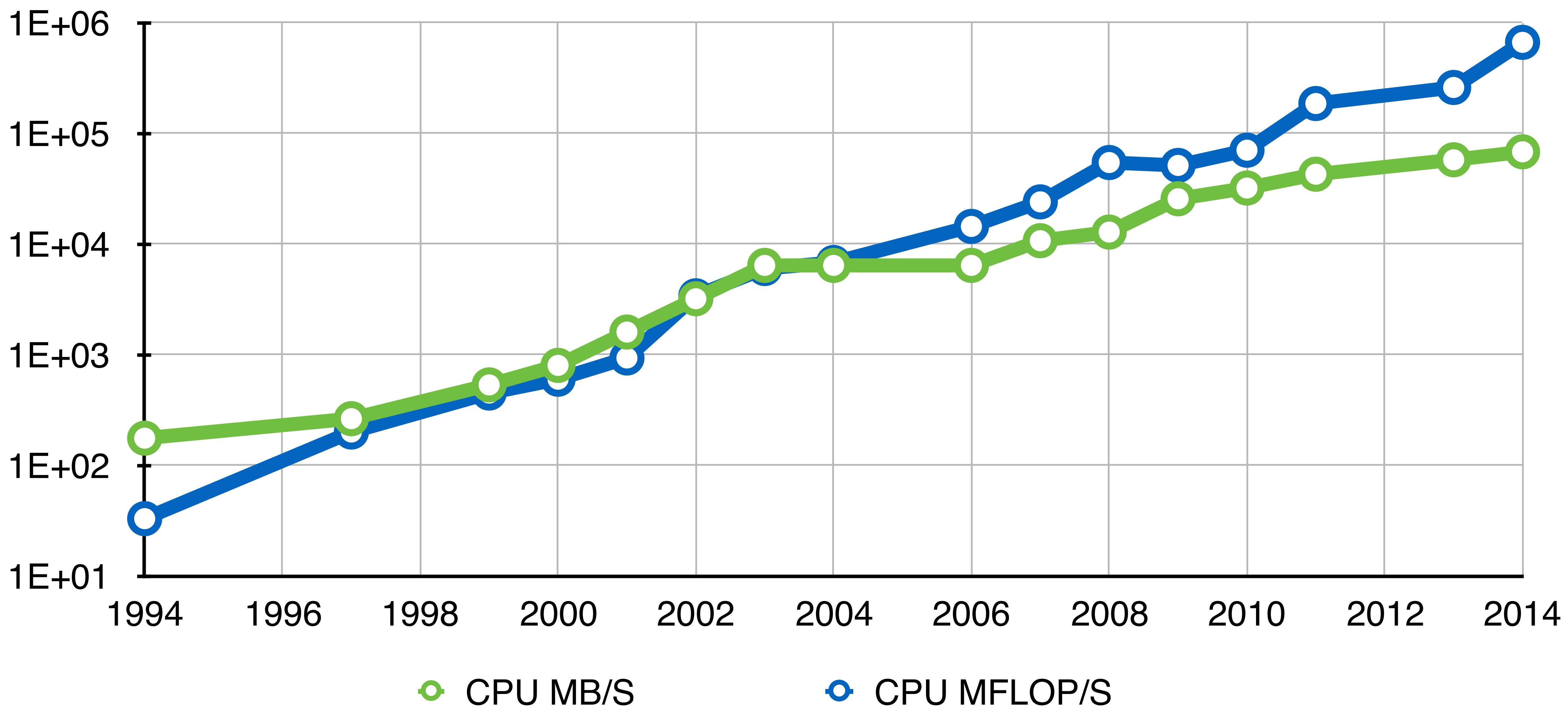
Rapid improvement compared with explicit RK4.

Outline

1. Context
2. History
3. CFD code development
4. Industrial use of CFD
5. Current status of CFD
6. Overview of numerical methods
7. Flux Reconstruction
8. **Modern hardware and PyFR**
9. LES computations
10. Summary and conclusions

Modern hardware and FR

- As we have seen performing LES requires a lot of FLOP/s.
- But the FLOP rate of massively parallel machines is also increasing exponentially.
- However, this is not the whole story.



Modern hardware and FR

- Drilling down.

	1994	2014	Ratio
MFLOP/s	33	604,000	18,303
MB/s	176	68,000	386

Modern hardware and FR

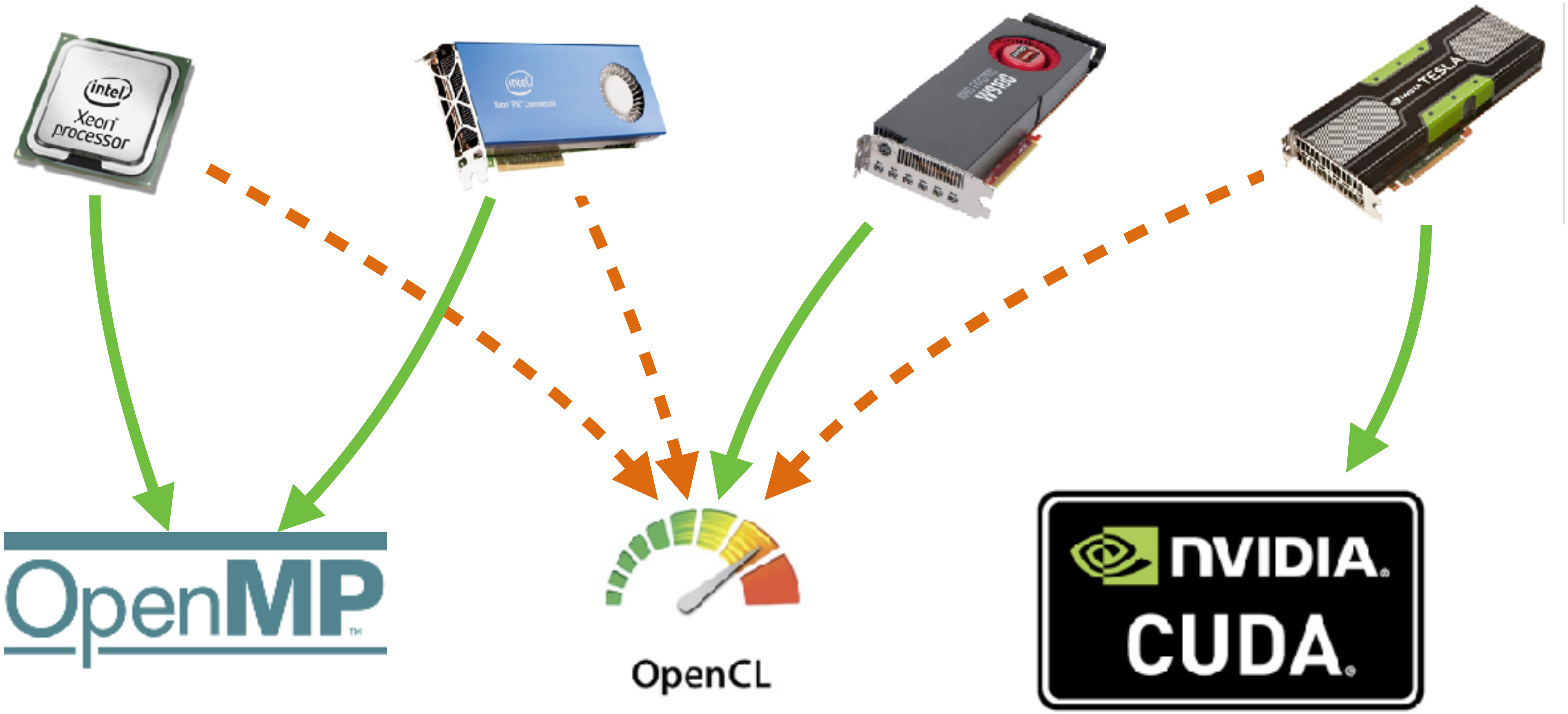
- Worse, everything has started coming in **parallel**.
- Intel
  - Multiple cores each with a wide vector unit.
  - Parallelism exposed via *MIMD + SMT + SIMD + ILP*.

- NVIDIA
  - Streaming Multi-Processors each with CUDA cores.
  - Parallelism exposed via *SIMT*.

- AMD
  - Compute Units each with Stream Processors.
  - Parallelism exposed via *SIMT*.

Modern hardware and FR

- It is also a challenging programming environment.
- Fortran + MPI just won’t cut it!

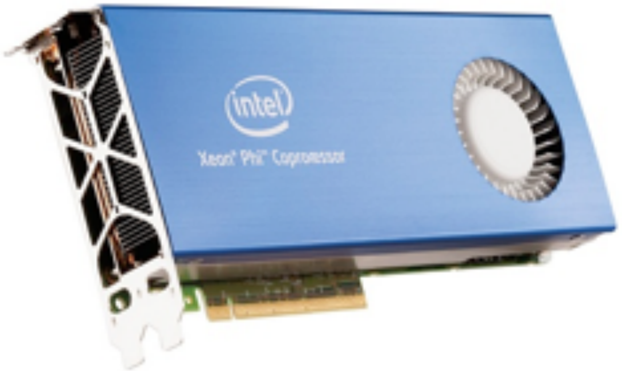


Modern hardware and FR

- The environment is also becoming heterogeneous.
- Consider *Stampede* at *TACC* ranked at #10 on the top 500.

Intel Xeon

2.2 PFLOP/s



Intel Xeon Phi

7.4 PFLOP/s

Modern hardware and FR

- To be of utility for large-scale simulations in 2016 and beyond algorithms must
  - be highly parallel;
  - conserve memory bandwidth;
  - avoid indirection and mask latency.

Flux reconstruction schemes are a very good fit.

PyFR

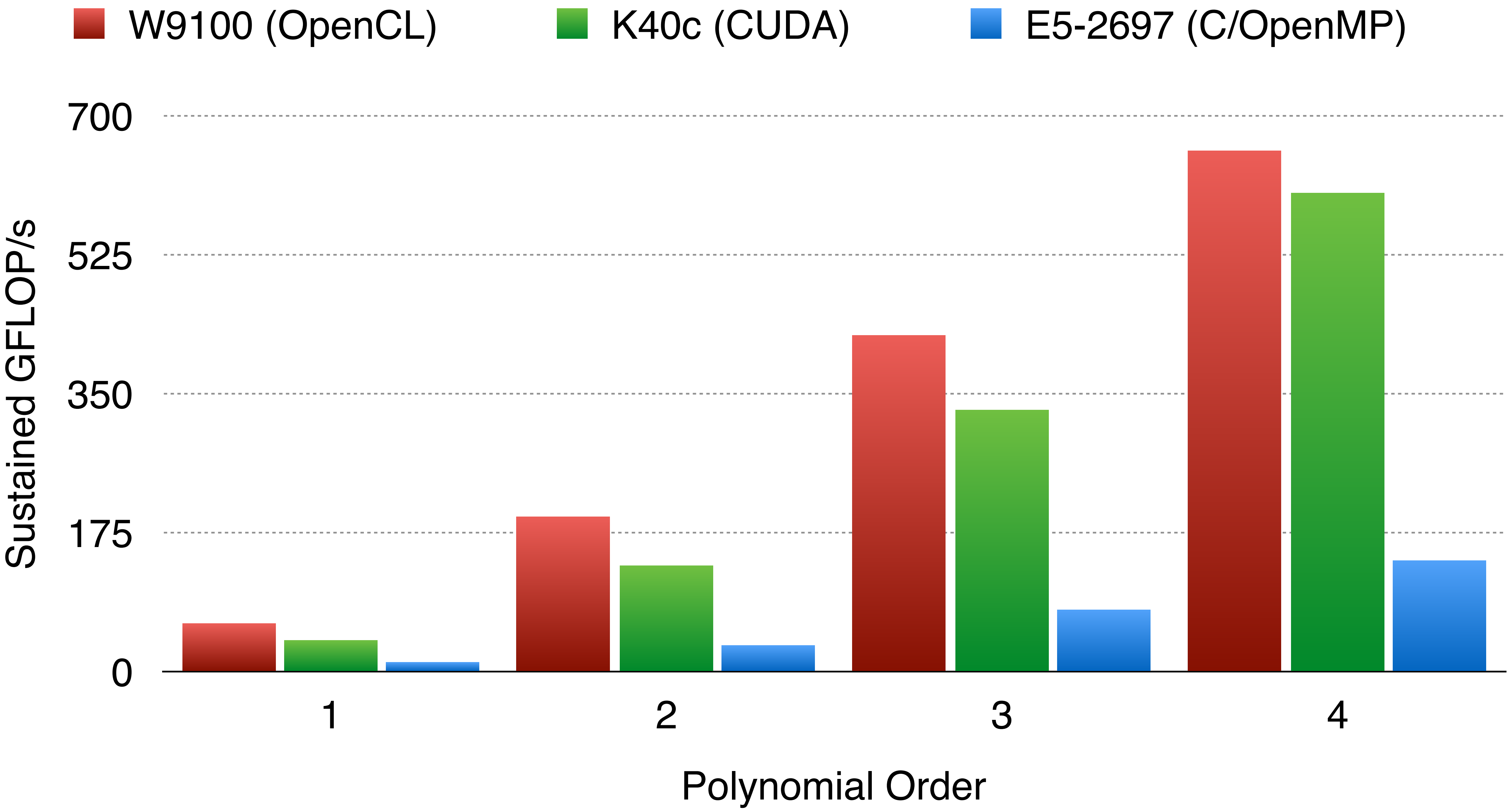
- Open source implementation of FR for modern hardware.
- Started at Imperial College London
    - PI: Peter Vincent.
    - Lead developer: Freddie Witherden
    - Many other contributors!

PyFR

Governing Equations	Compressible Euler/Navier-Stokes (Incompressible Euler/Navier-Stokes)
Spatial Discretisation	Arbitrary order FR on mixed unstructured grids
Temporal Discretisation	Range of explicit Runge-Kutta schemes
Backends	CPUs, NVIDIA GPUs, AMD GPUs, (Intel MIC).
Precision	Single, Double
Input	Gmsh, (CGNS)
Output	VTK, (In situ)

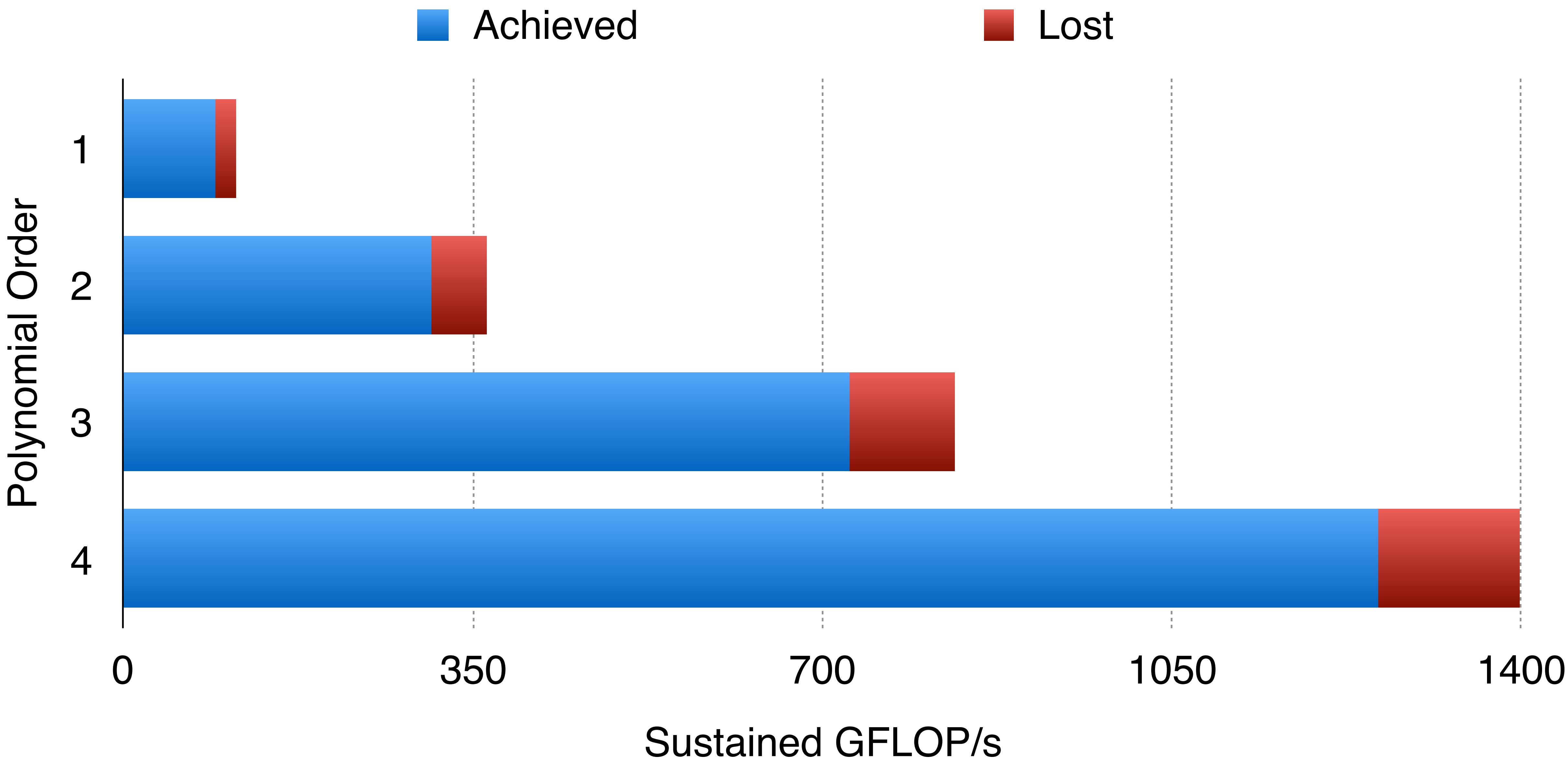
PyFR

- Single node performance on a mixed prism/tet grid.



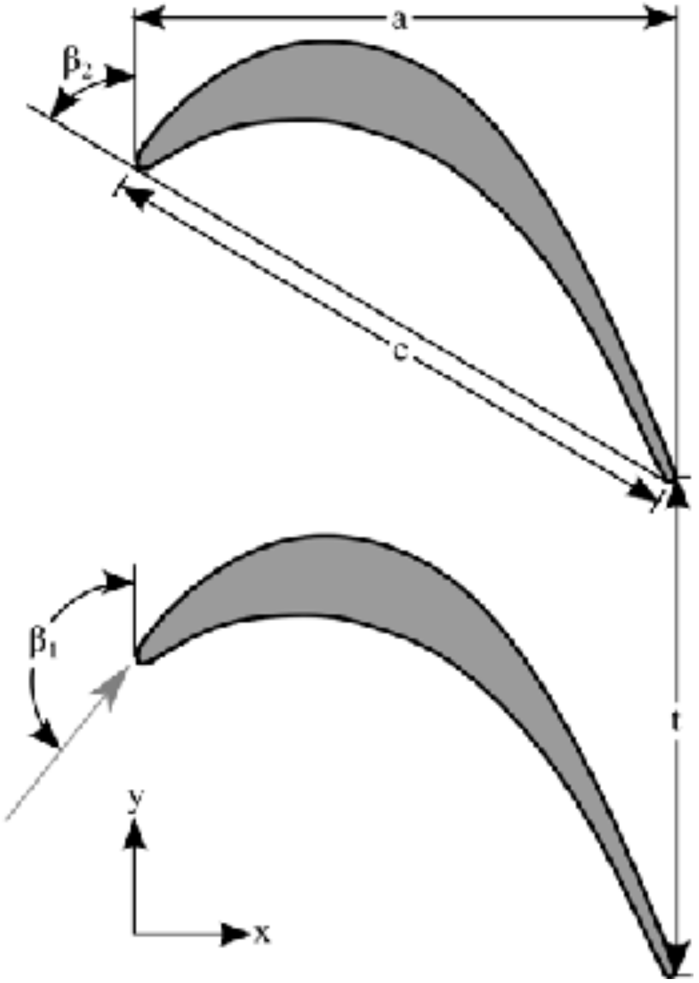
PyFR

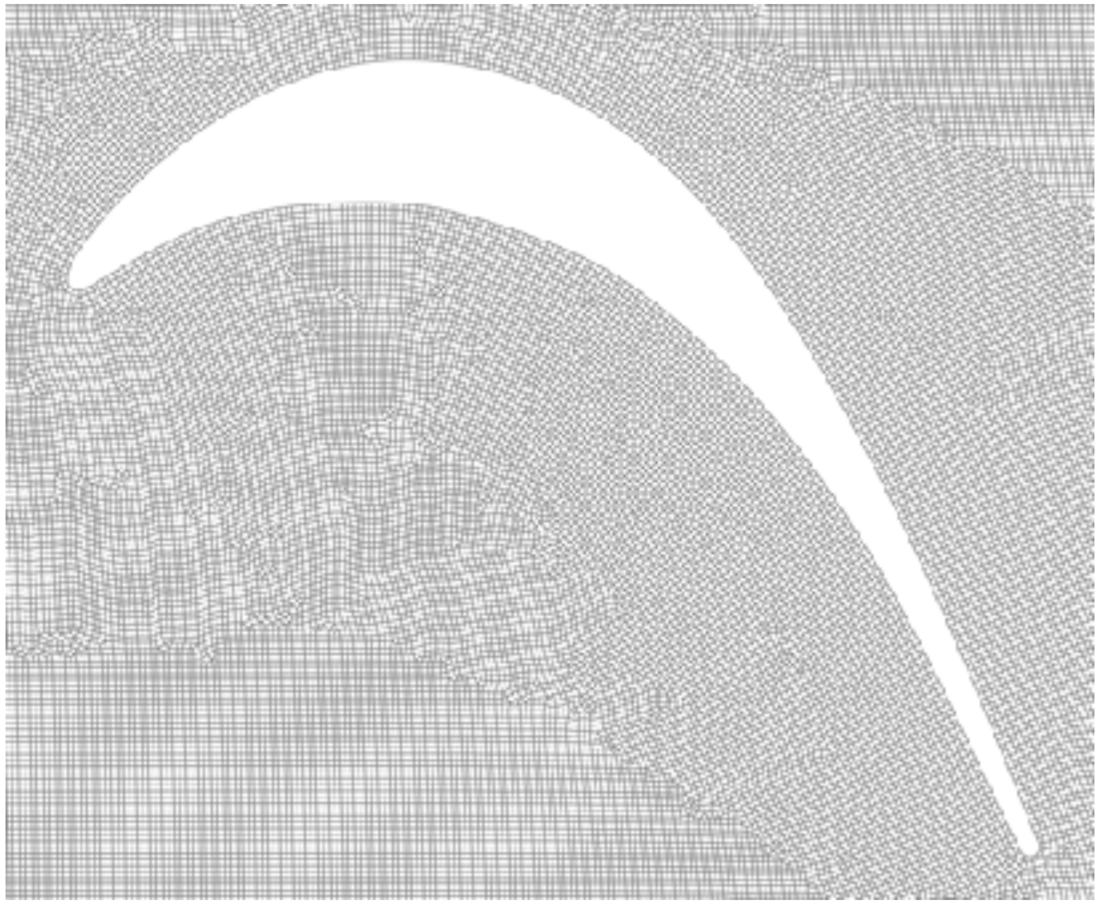
- Multi node heterogeneous performance on the same grid.



PyFR

- Scaling evaluated on the *Tian* cluster at *ORNL*.
- Test case is a T106D low pressure turbine cascade.
- Forth order solution polynomials on a hexahedral grid with anti-aliasing.





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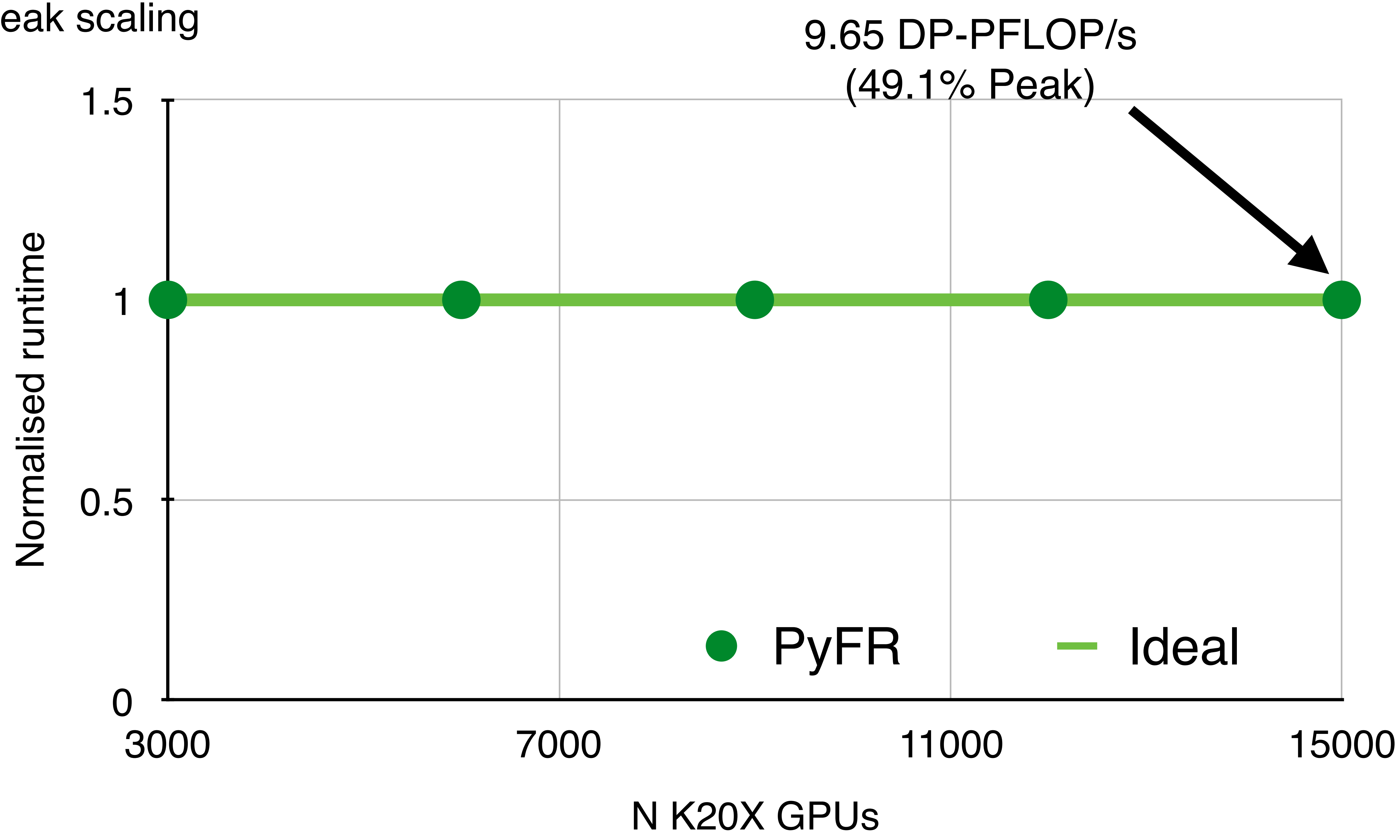
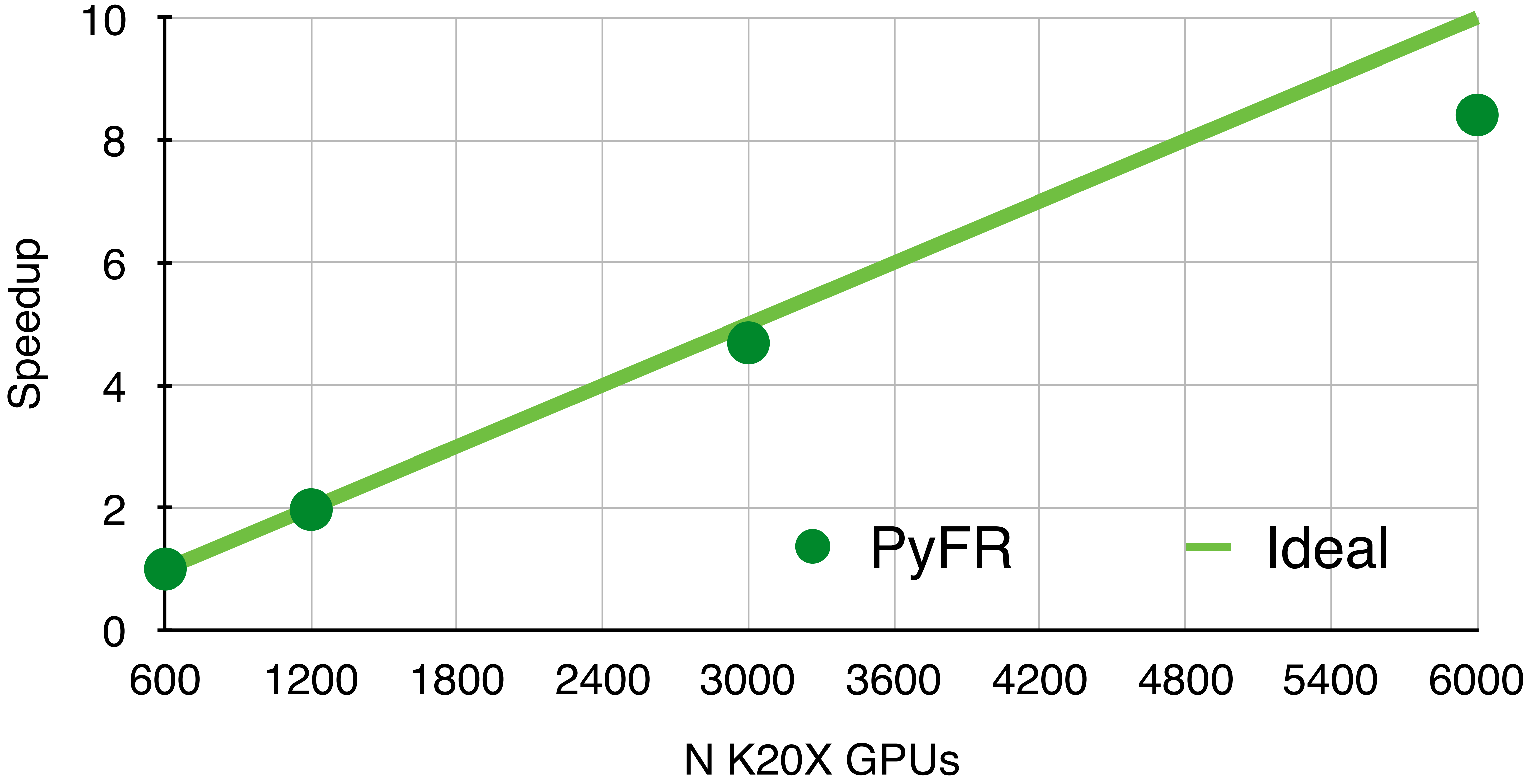
PyFR

- Weak scaling



PyFR

- Strong scaling



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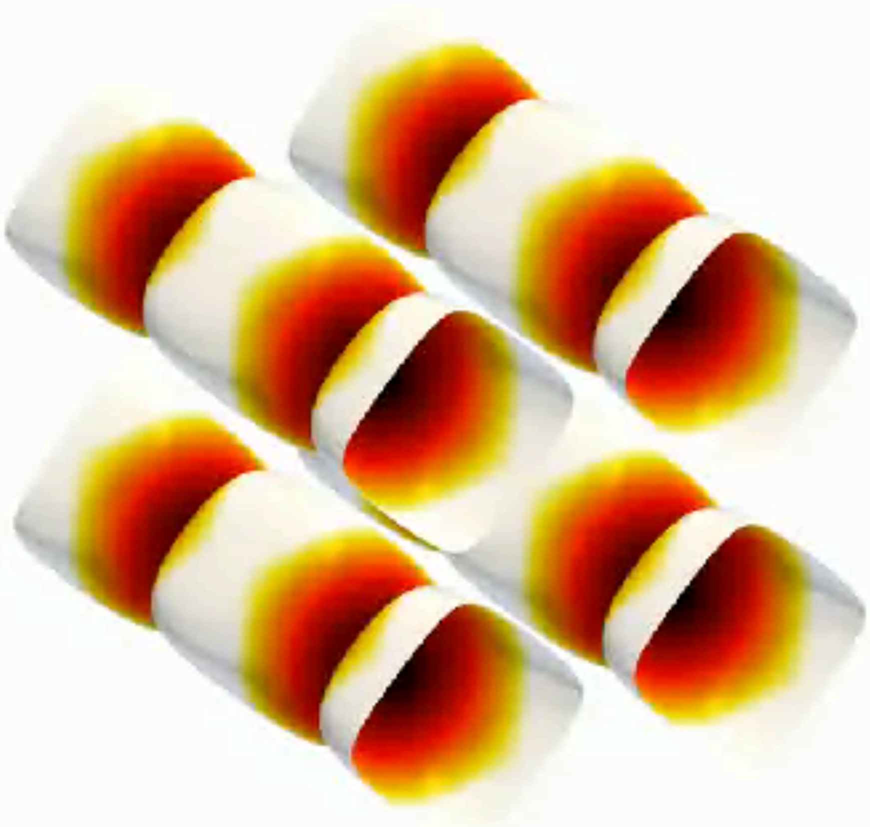
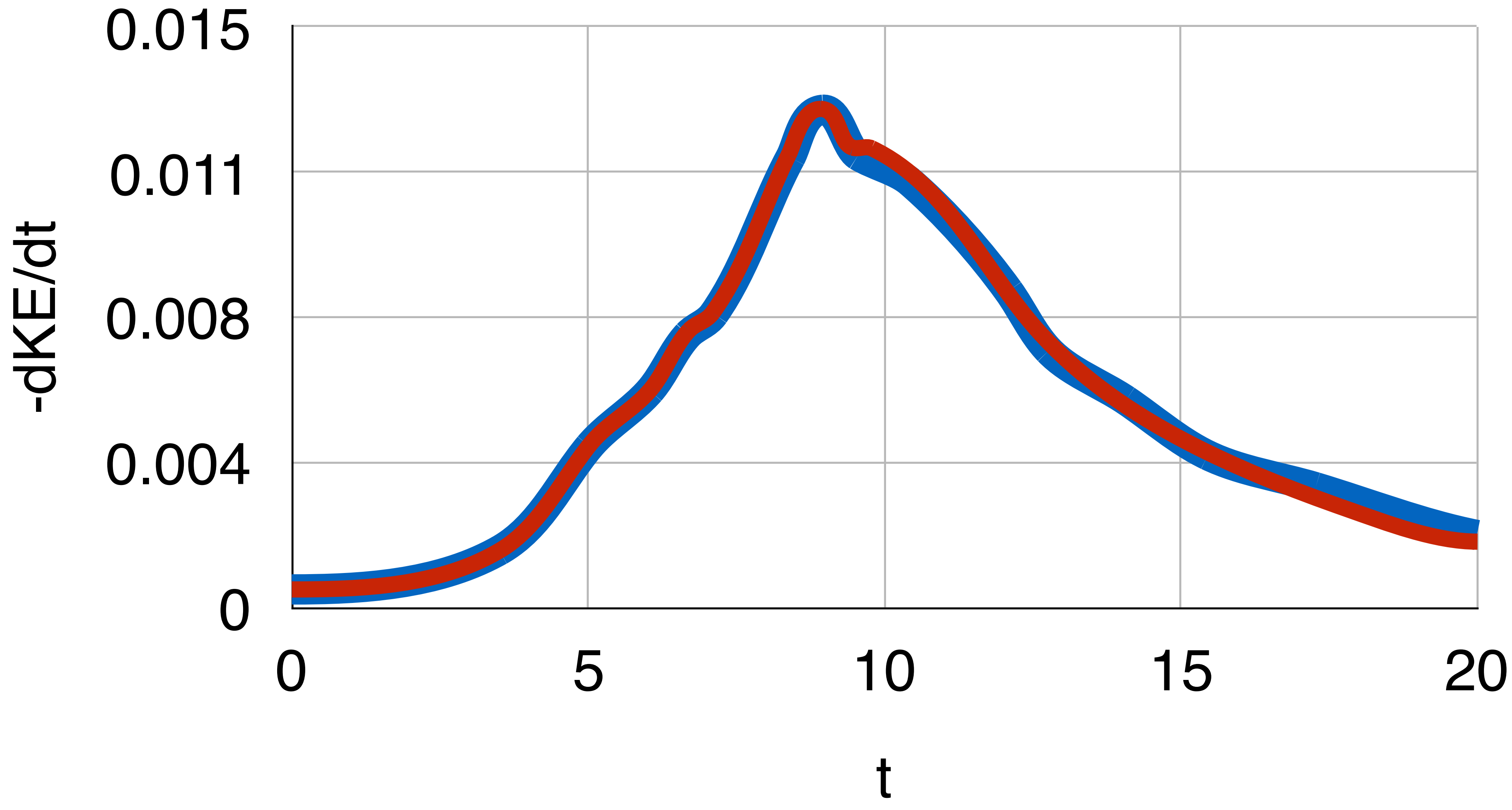
Taylor Green Vortex

- Standard test case for high-order codes.
- Iso-surfaces of Q coloured by velocity magnitude.

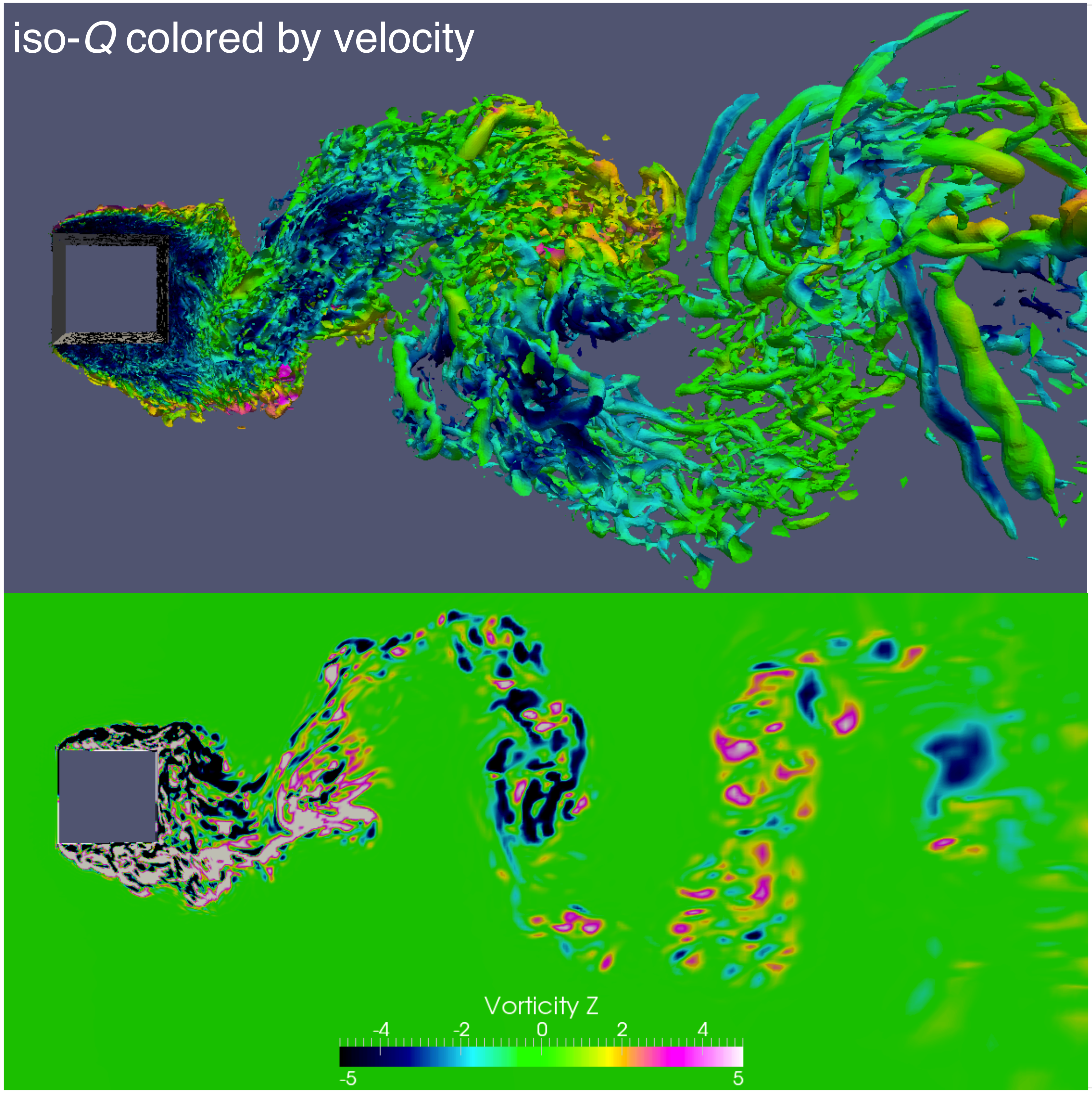


Taylor Green Vortex

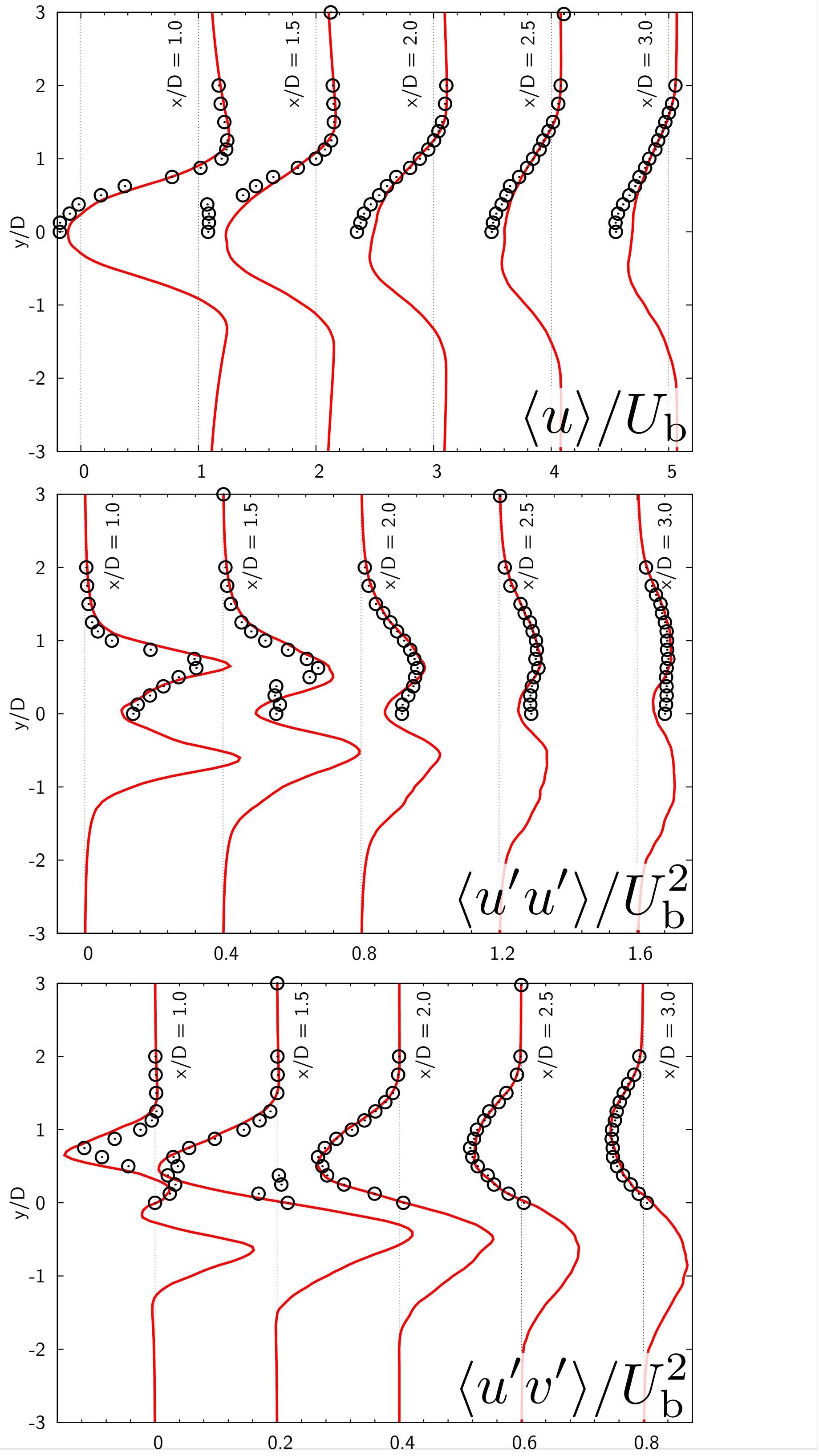
- Kinetic energy decay rate for a structure grid with ~256^3 DOFs and forth order solution polynomials compared with the spectral DNS of Van Rees et al.



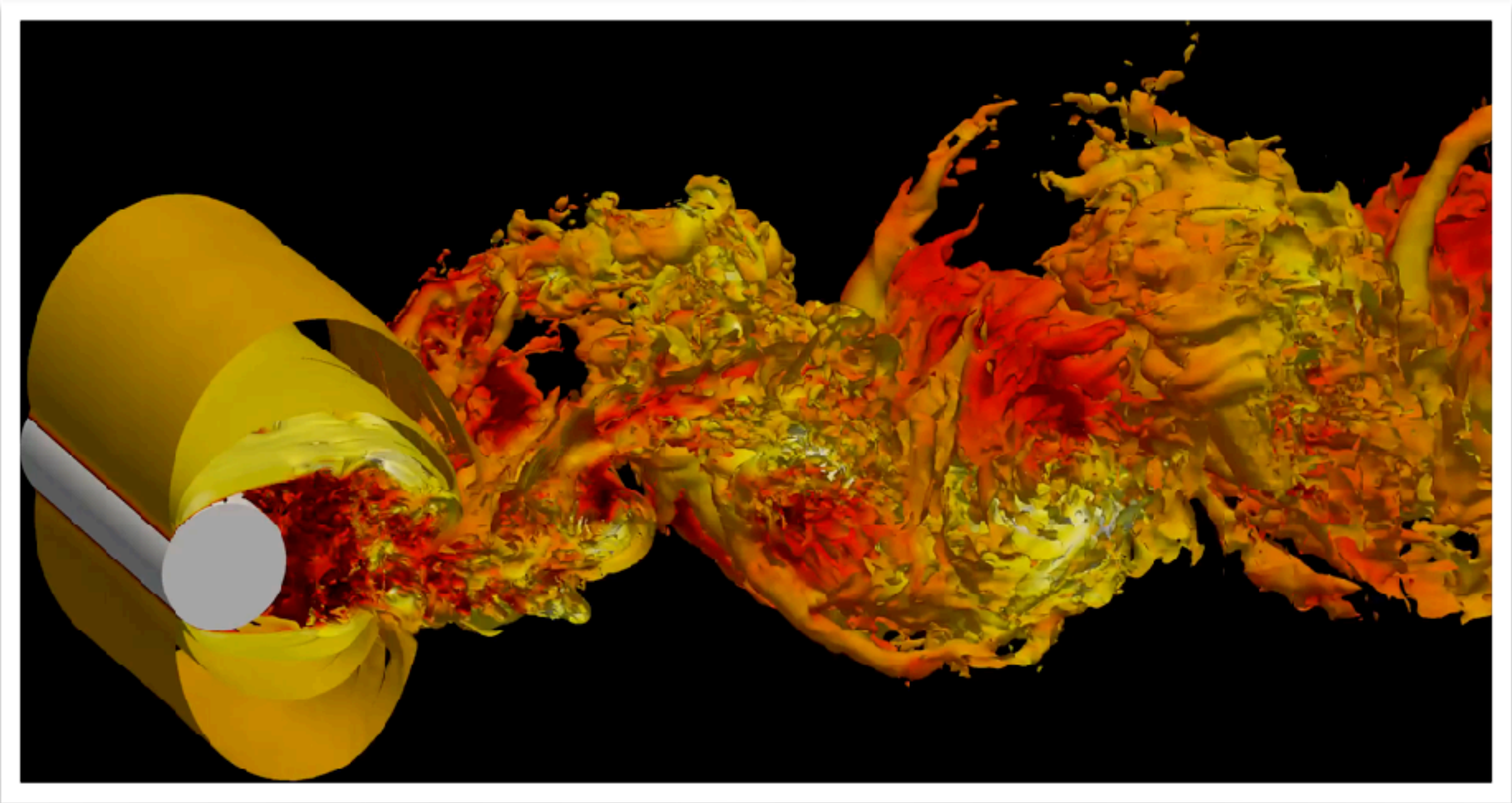
Flow past a Square Cylinder: $Re_D = 21400$



iso-Q colored by velocity

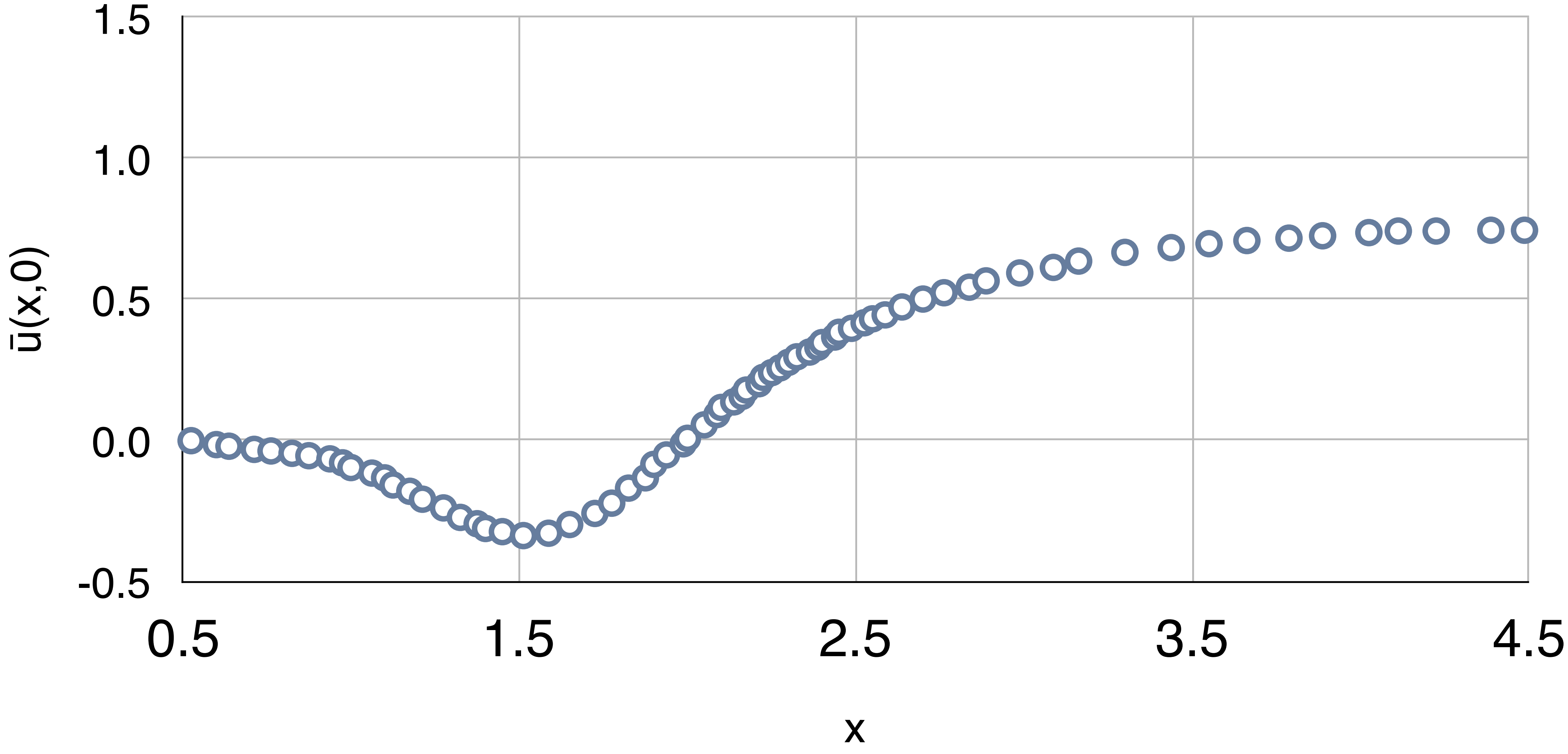


Flow past a Circular Cylinder: $Re_D = 3600$



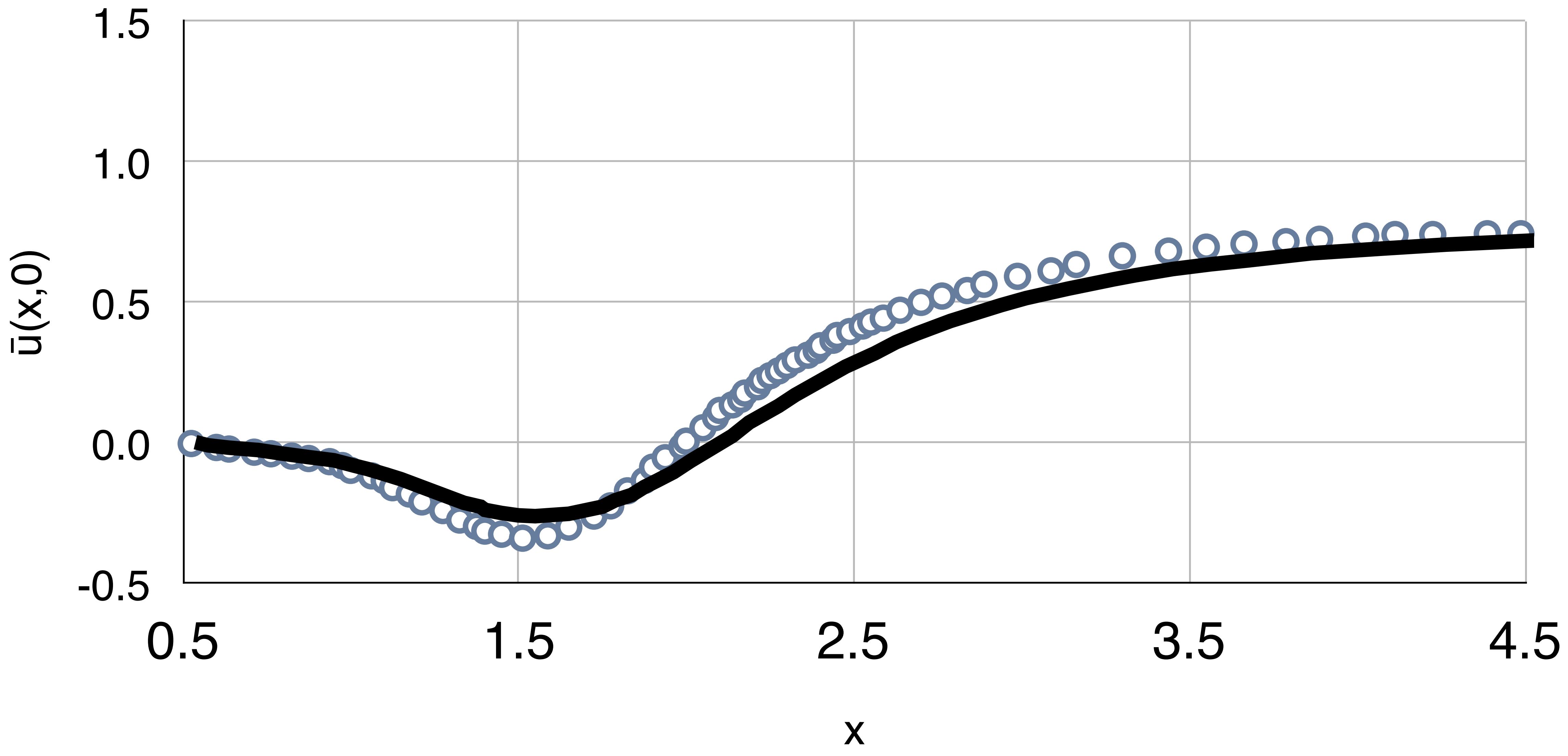
Flow past a Circular Cylinder: $Re_D = 3600$

- Parnaudeau et al. experiment.



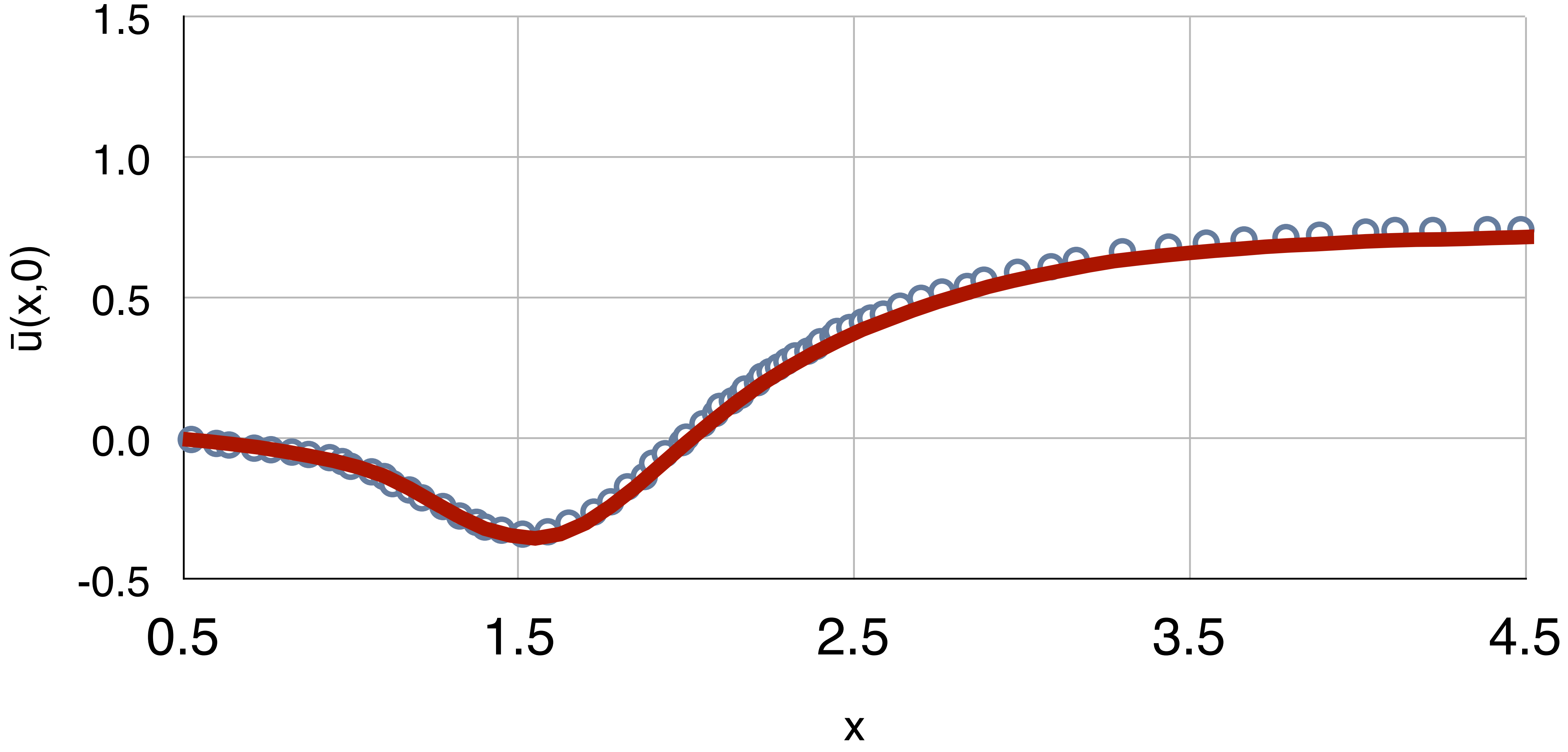
Flow past a Circular Cylinder: $Re_D = 3600$

- Parnaudeau et al. experiment + Parnaudeau et al. LES.



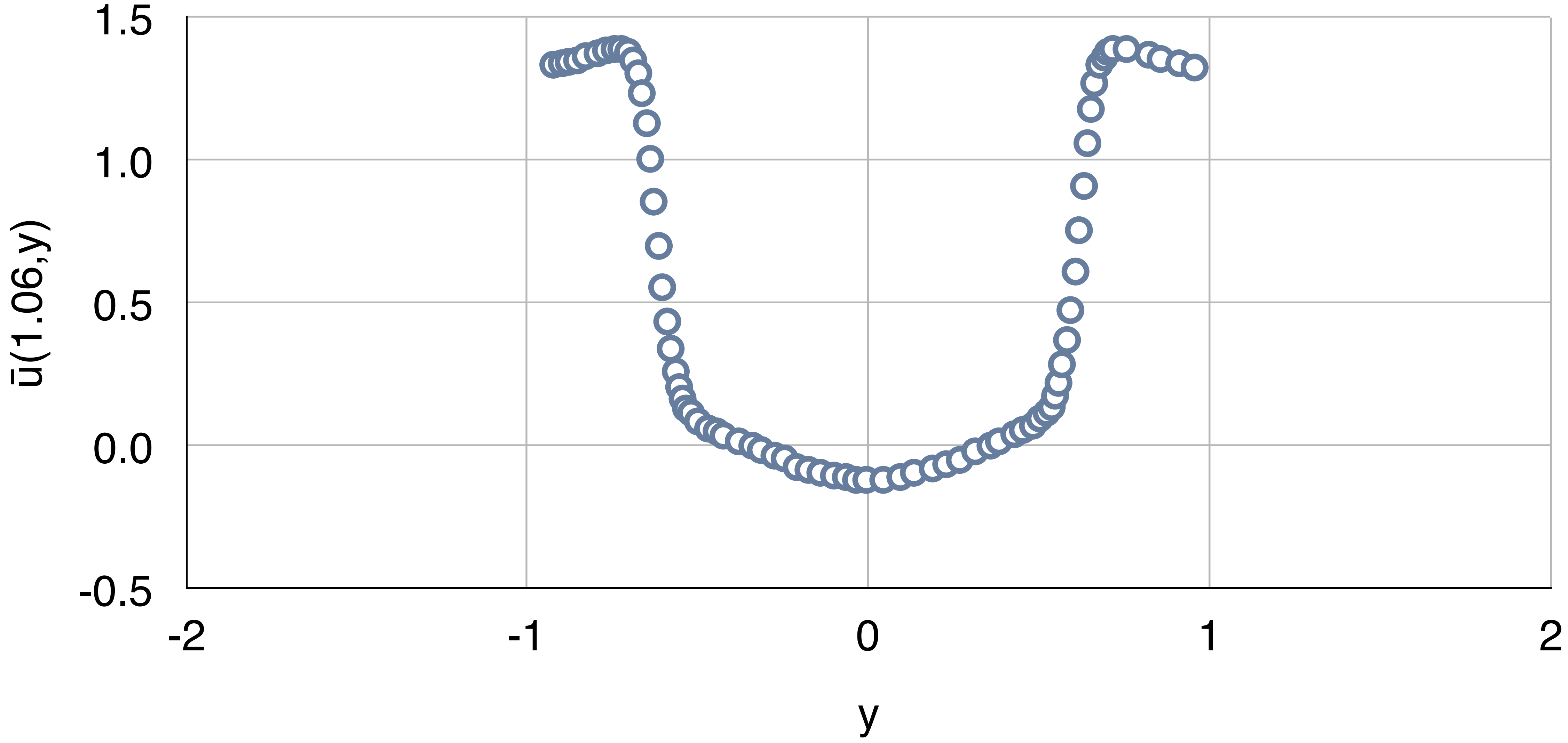
Flow past a Circular Cylinder: $Re_D = 3600$

- Parnaudeau et al. experiment + PyFR (5th order hex) ILES.



Flow past a Circular Cylinder: $Re_D = 3600$

- Parnaudeau et al. experiment.



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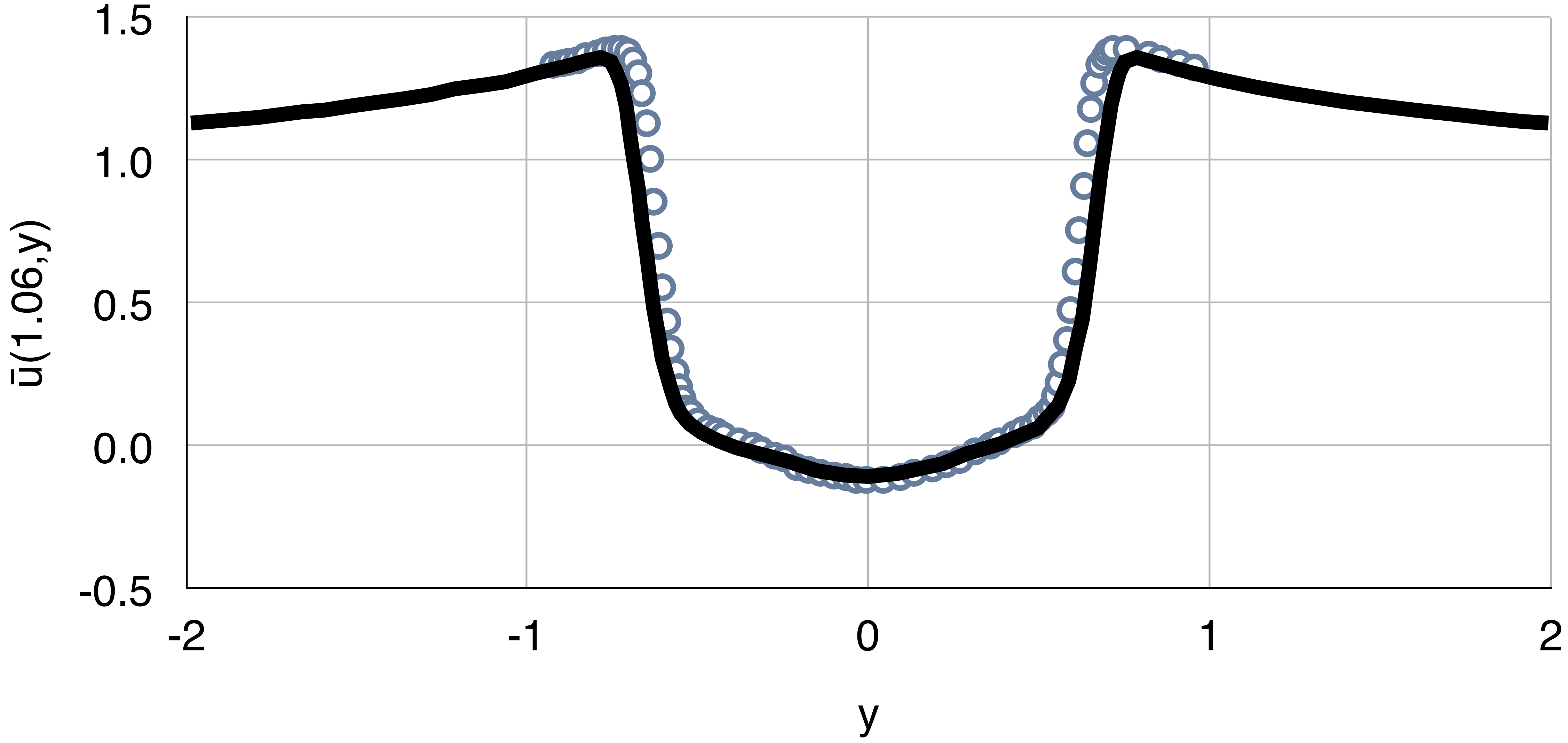
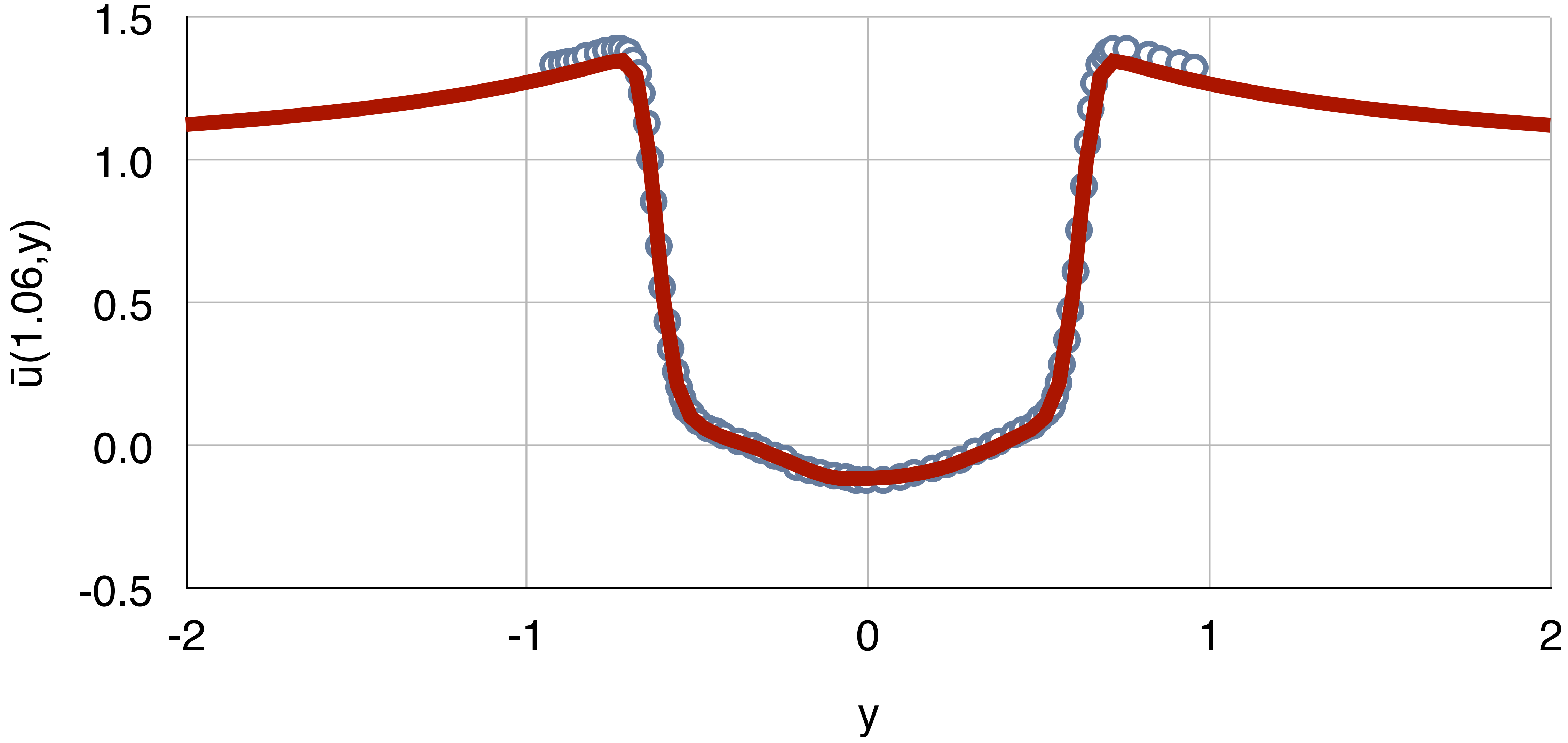
- Parnaudeau et al. experiment + Parnaudeau et al. LES.



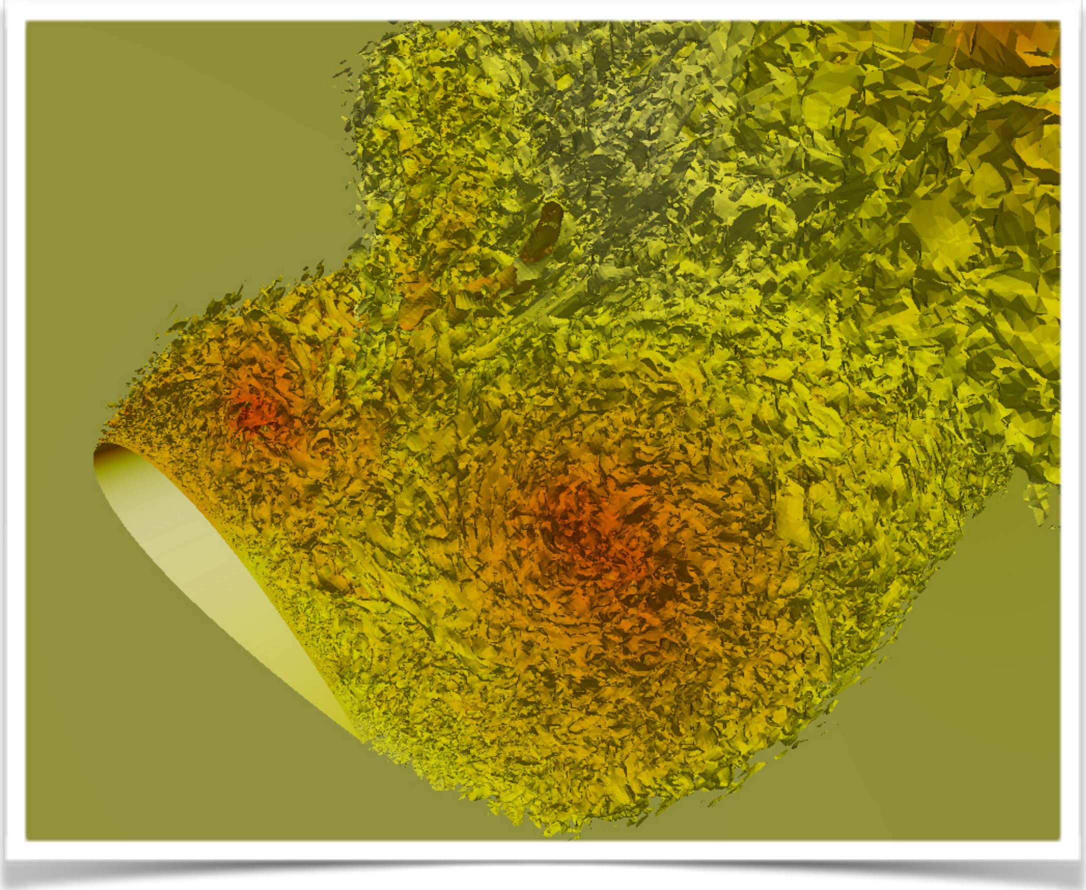
Flow past a Circular Cylinder: $Re_D = 3600$

- Parnaudeau et al. experiment + PyFR (5th order hex) ILES.



Flow past a NACA 0021 in Deep Stall

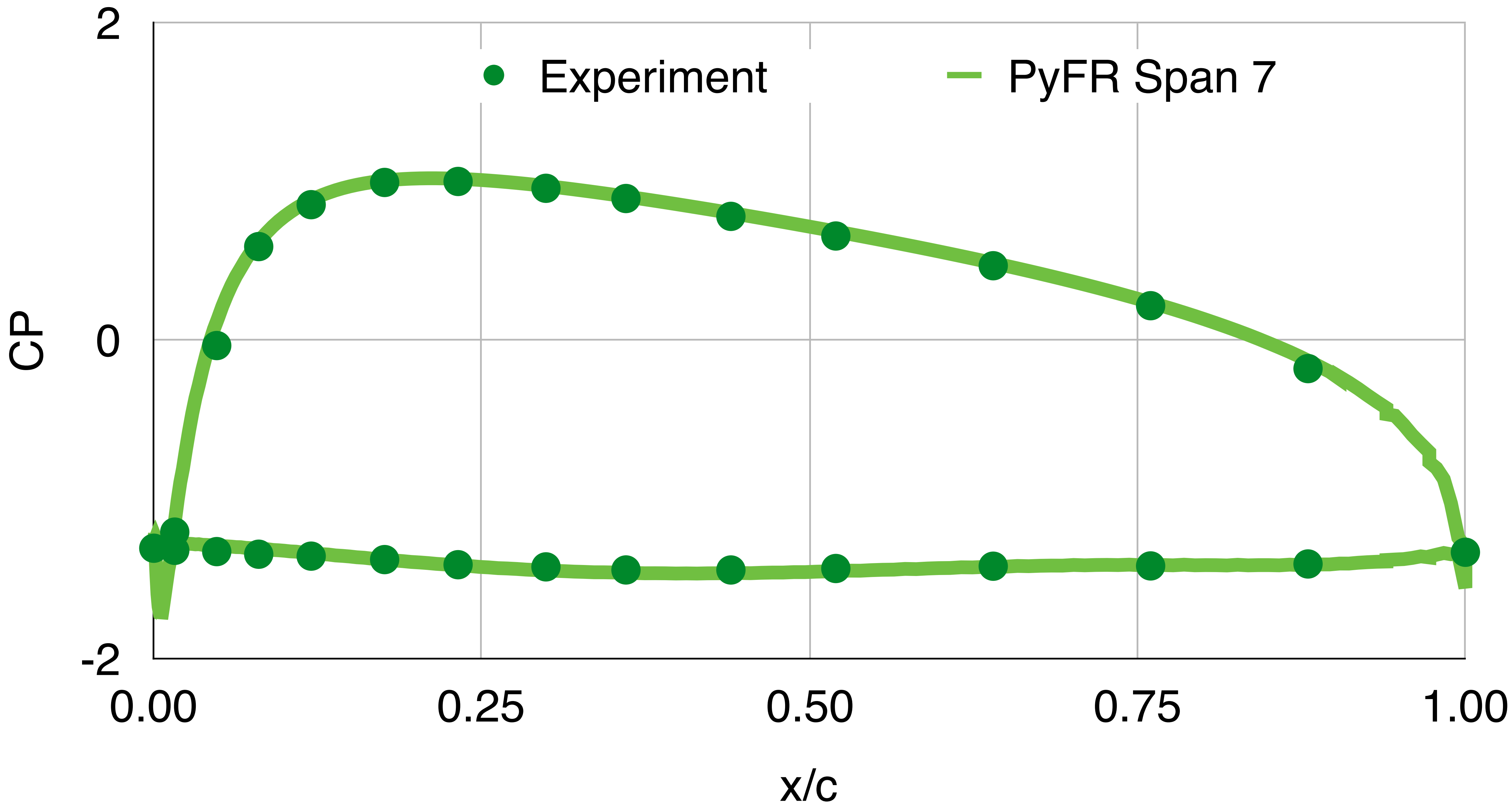
- Flow over a NACA 0021 at 60 degree AoA
- Re = 270,000 and Ma = 0.1
- Compare with Swalwell and DESider
- Use fourth order solution polynomials on a quadratically curved hexahedral grid with 361,424 elements.



Refs: K. Swalwell. PhD Thesis, Monash University. 2005.
W. Haase et al. Springer. 2009.

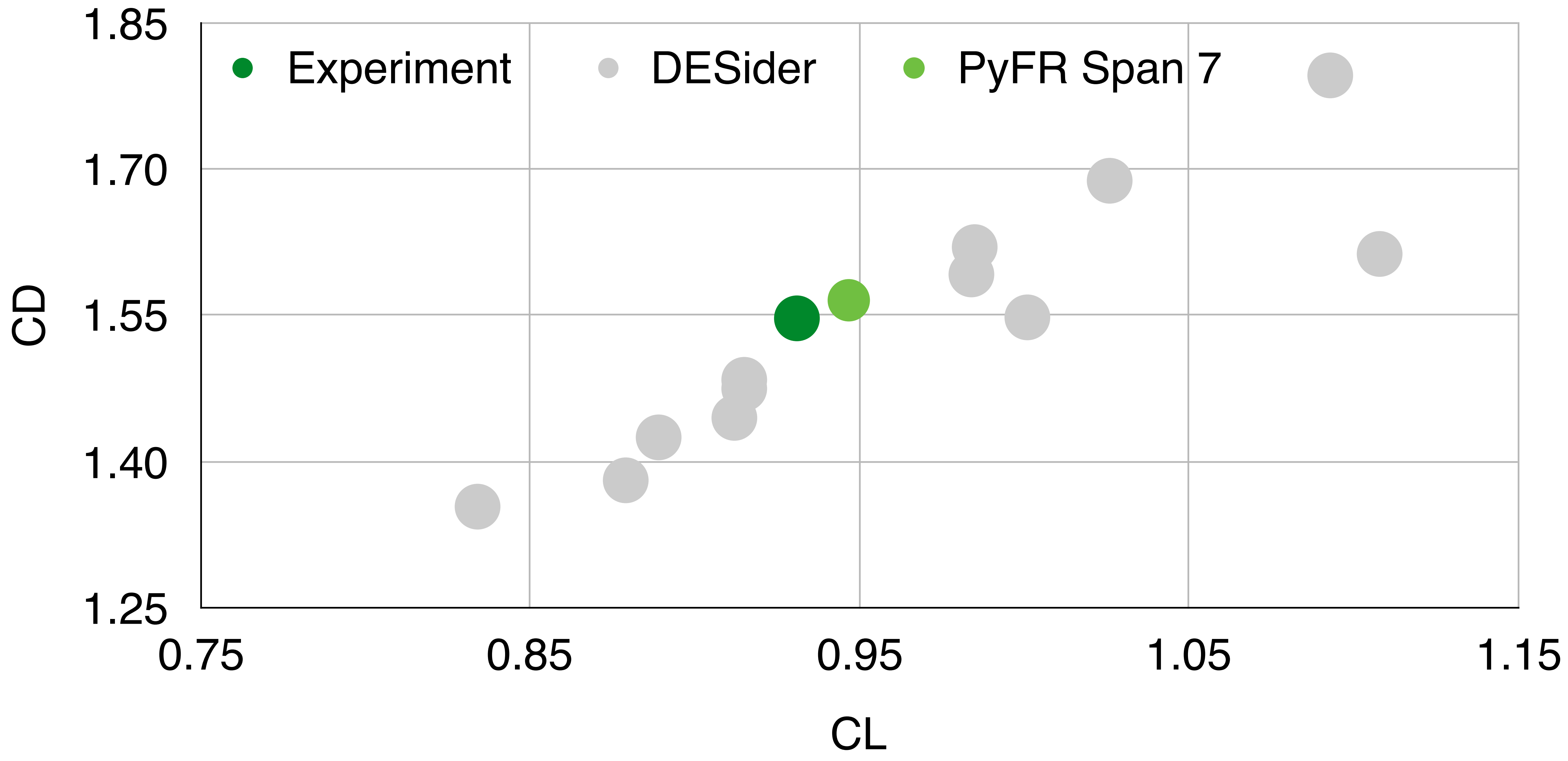
Flow past a NACA 0021 in Deep Stall

- Time-span averaged pressure distribution over the surface of the airfoil.



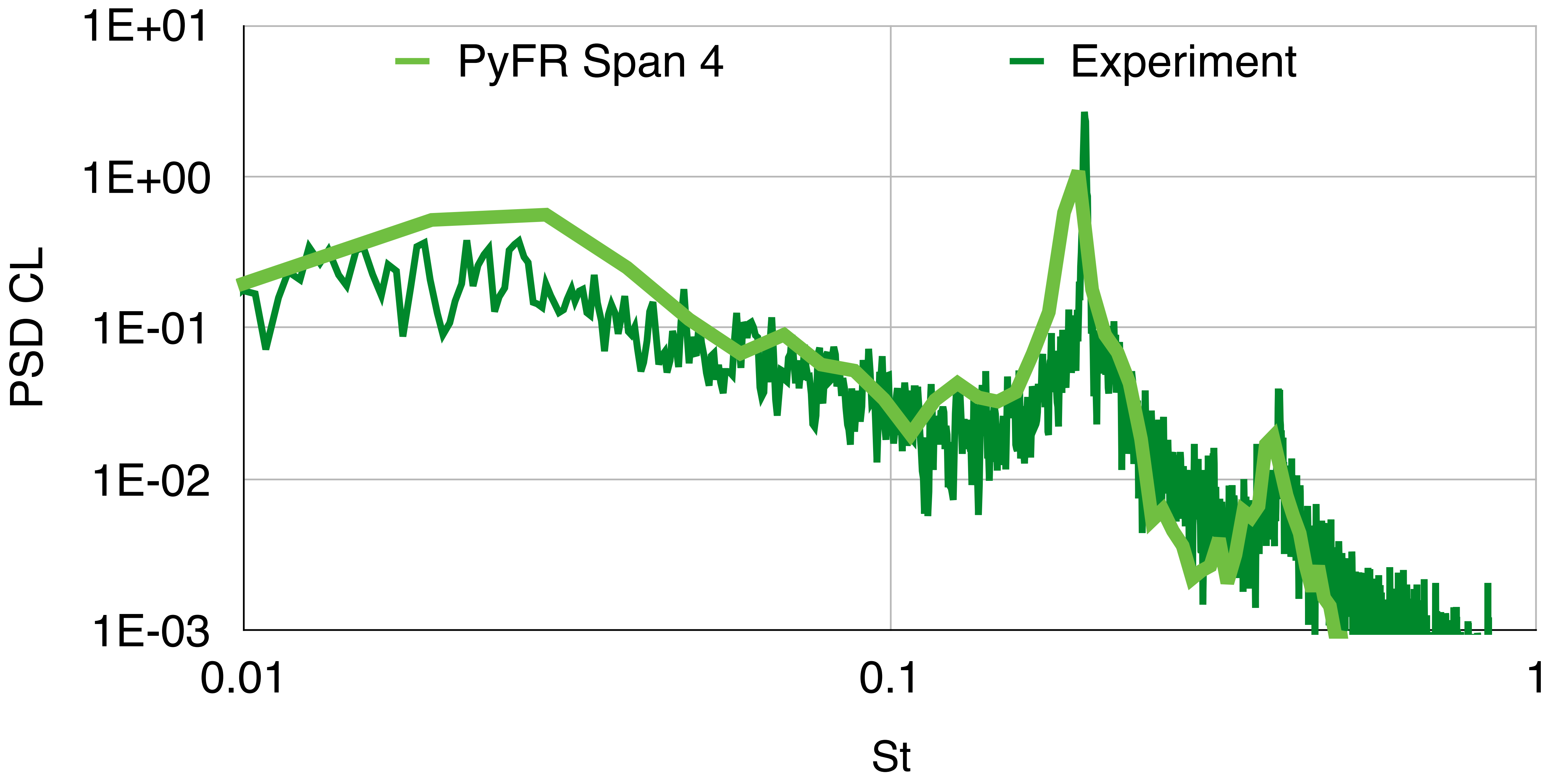
Flow past a NACA 0021 in Deep Stall

- Time averaged lift and drag coefficients.



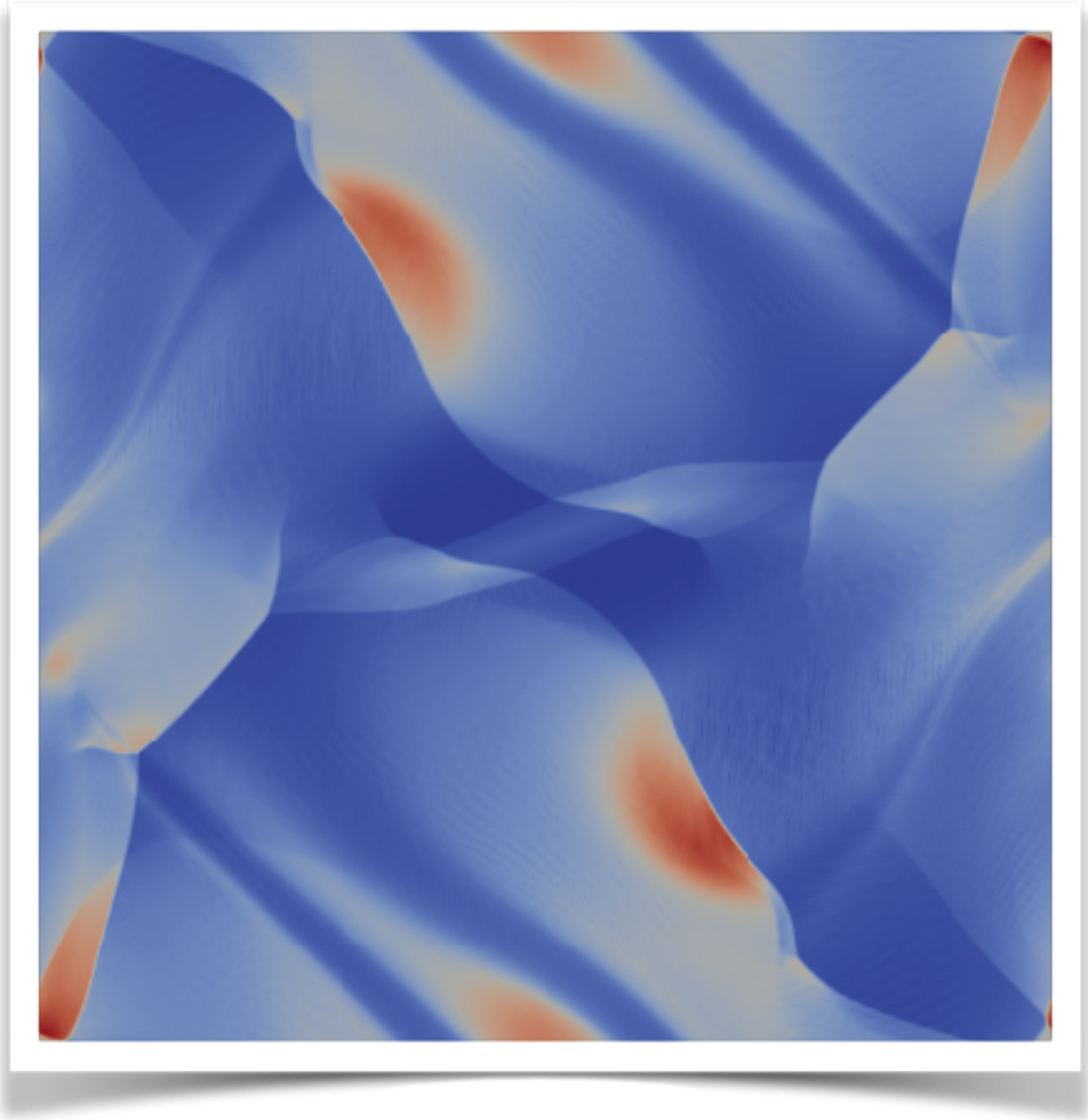
Flow past a NACA 0021 in Deep Stall

- Power spectrum density of the lift coefficient against the Strohoul number.



Ideal MHD

- Also working towards an FR based ideal MHD solver.
- Uses *Powell's method*.
- Right: snapshot of pressure for a 2D Orszag-Tang vortex test-case.



Outline

1. Context
2. History
3. CFD code development
4. Industrial use of CFD
5. Current status of CFD
6. Overview of numerical methods
7. Flux Reconstruction
8. Modern hardware and PyFR
9. LES computations
10. **Summary and conclusions**

Summary and Conclusions

Predicting the future is generally ill advised.
However, the following are the author’s opinions:

- The early development of CFD in the Aerospace Industry was primarily driven by the need to calculate steady transonic flows: ***this problem is quite well solved***
- CFD has been on a plateau for the last 15 years with 2nd-order accurate FV methods for the RANS equations almost universally used in both commercial and government codes which can treat complex configurations. These methods cannot reliably predict complex separated, unsteady and vortex dominated flows
- Ongoing advances in both numerical algorithms and computer hardware and software should enable an advance to LES for industrial applications within the foreseeable future
- Research should focus on high-order methods with minimal numerical dissipation for unstructured meshes to enable the treatment of complex configurations

Summary and Conclusions

Current obstacles to the wider adoption of high-order methods which call for further research include:

- slow convergence for steady state problems - this might be alleviated by a better design of a multi-hp convergence acceleration scheme
- the need for a more efficient implicit time stepping scheme for unsteady problems
- more robust high-order schemes for nonlinear problems such as are encountered in high speed gas dynamics
- more efficient and user friendly mesh generation techniques

Summary and Conclusions

Current issues in LES include:

- the need for wall models to enable simulations of wall bounded flows at affordable computational costs
- the need for further research on subgrid filtering techniques on unstructured meshes
- the need for continuing research on subgrid models, including approximate deconvolution and exact SGS models, and a careful evaluation of implicit LES methods

Automatic shape design methods based on control theory or other optimization methods will be increasingly used in aerospace design

Design problems in unsteady flow, such as turbomachinery, rotorcraft, or unsteady separated flows are particularly challenging

Summary and Conclusions

Eventually DNS may become feasible for high Reynolds number flows

hopefully with a smaller power requirement than a wind tunnel

Acknowledgement

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Questions & Anwers

Thank you for listening