Introduction of STFC and the computational engineering group

Scientific Computing Department, STFC Daresbury Laboratory, UKRI

UK high-speed aerodynamics SIG meeting 2022
10th June, STFC Daresbury Laboratory, Keckwick Lane,
Daresbury, WA4 4AD

Science and Technology Facilities Council (STFC)

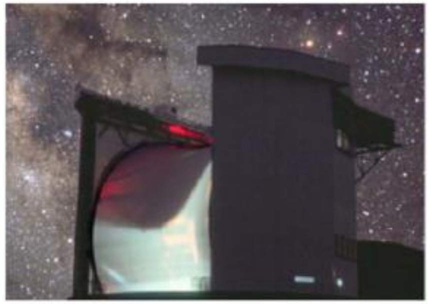
ATC Edinburgh

Daresbury Laboratory

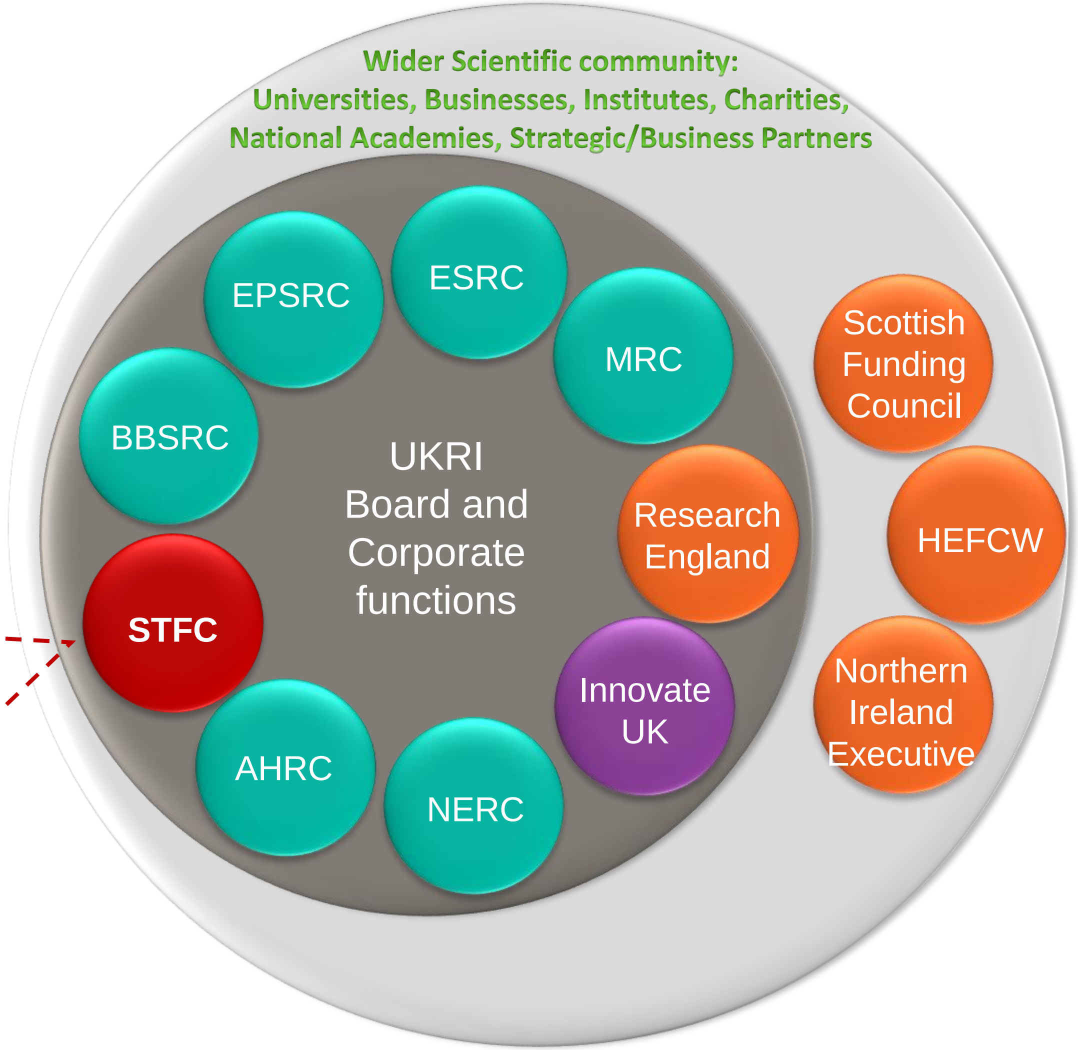
4.2m William Herschel Telescope, La Palma

Rutherford-Appleton Laboratory

Chilbolton Observatory



15m James Clerk Maxwell Submillimetre Telescope, Hawaii

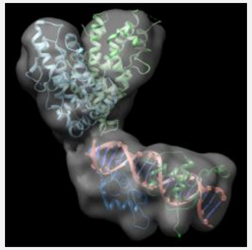


STFC Scientific Computing Department - SCD

Computational Science

We develop computational science methods and software packages to solve problems in the physical and biological sciences.

- structural biology, molecular simulation and bioinformatics
- electronic structure of the solid state and surfaces, atomic and molecular physics
- Computational fluid dynamics (CFD), heat, turbulent flows - molecular dynamics, quantum chemistry and QM/MM techniques, and mesoscale methods



Large Scale Systems

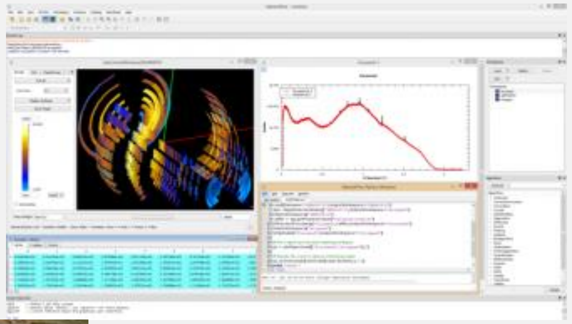
SCD designs, builds and operates large scale computing systems to support UKRI science

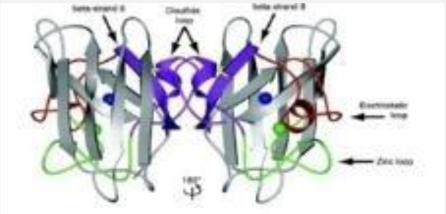
- JASMIN
  - Superdata cluster for environmental science
- IRIS - STFC Research Cloud
  - High performance CPU, GPU, IPU, FPGA and storage for UKRI science
- High-throughput computing
  - UK's Grid for LHC computing
- Very large data storage
  - 100Pb+ disk, 400Pb tape

Digital Infrastructures

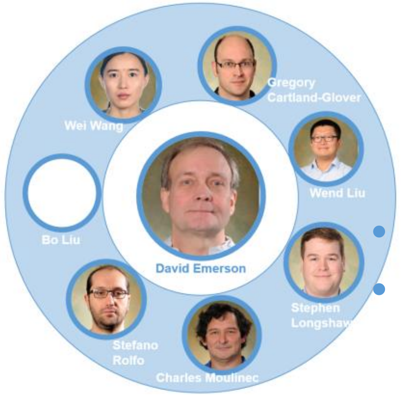
Through our **Ada Lovelace Centre** initiative, SCD develops and operates digital research infrastructure to support the national facilities

- Cloud enabled data analysis platforms
- Data catalogues
- FAIR data and open research





CFD for Low Carbon Energy



- General thermal hydraulics
- CFD in Gen IV nuclear reactors: SCWR, MSR
- CFD Gen II & III nuclear reactors: AGR, PWR
- General thermal FSI
- Multi-scale and multi-physics simulations
- Code-coupling
- Renewable energy (off-shore wind turbines)
- Numerical methods
- High Performance Computing (HPC)

Science and Technology Facilities Council

CFD for Space

Space-related research topics:

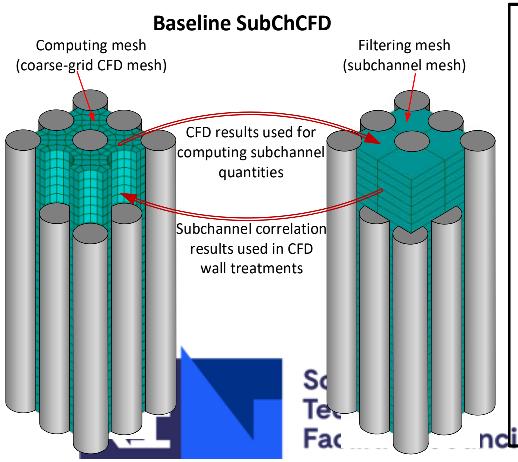
- Hypersonic aero-thermodynamics
- Shock-Boundary layer Interactions
- Rarefied Gas dynamics
- Satellite aerodynamics and Thruster propulsion modelling
- Multi-Scale & Multi-Physics Simulations
- High Performance Computing (HPC)

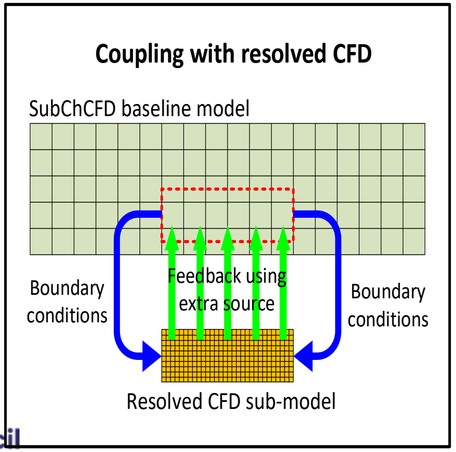
Key Software and capabilities:

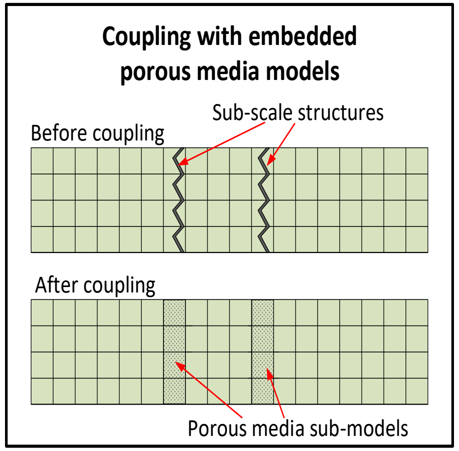
- CFD – ASTR, FLASH, Code_Saturne
- DSMC – SPARTA, dsmcFOAM+
- PIC – PICLas
- Code coupling – MUI
- All codes highly scalable, typically over 100,000 cores

Development of Subchannel CFD for Nuclear Thermal Hydraulics (B. Liu)

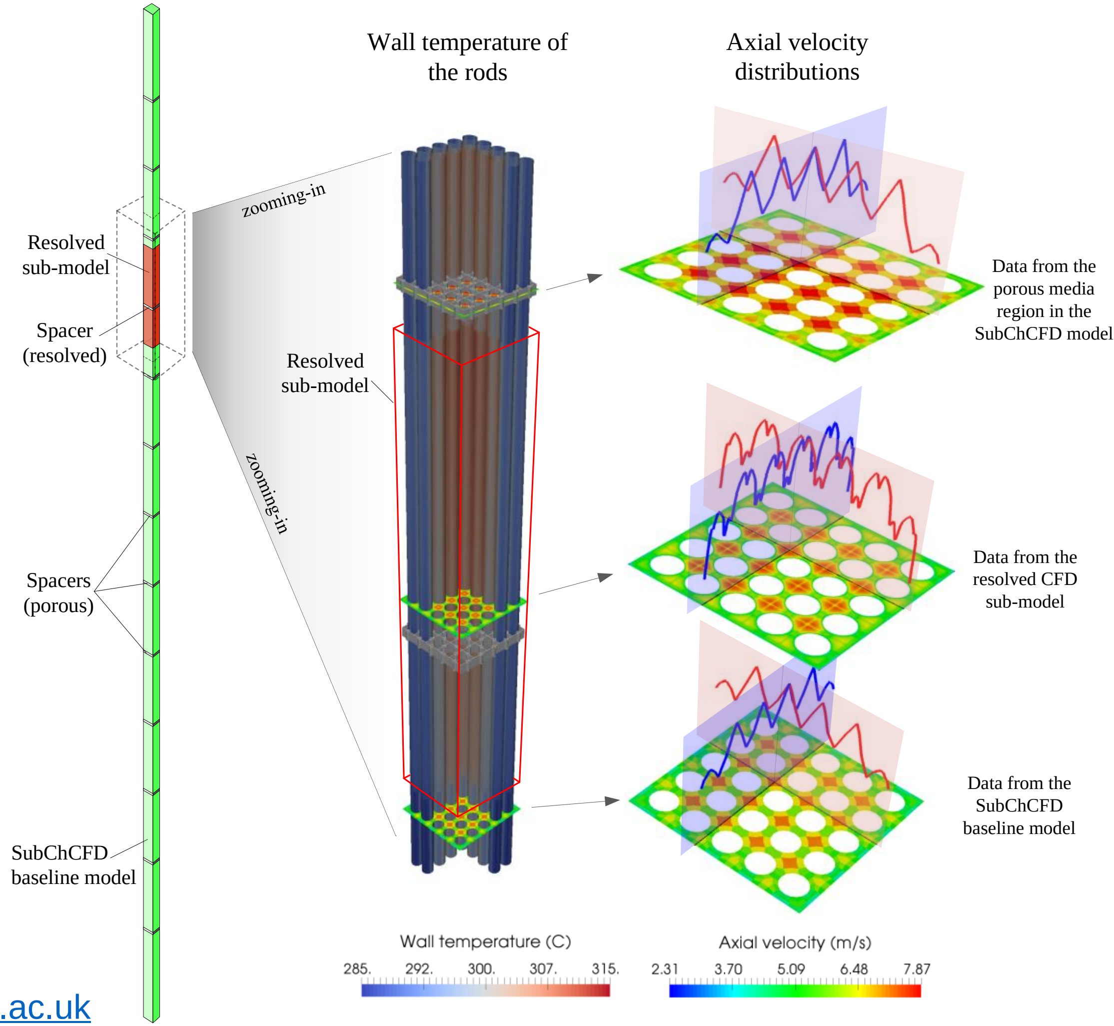
- **What is Subchannel CFD?**
  - A coarse-grid CFD-based subchannel framework for nuclear reactor thermal hydraulic analyses, combining features of modern CFD and traditional subchannel code
- **Key features**
  - Dual mesh system (coarse-grid computing + subchannel mesh)
  - Sub-channel correlations used to replace CFD wall functions
  - Models can be calibrated for specific reactor designs to reduce calculation uncertainties
  - Can naturally be coupled with conventional resolved CFD for flexible local refinement of simulations
  - Can also be coupled with porous media CFD for handling of subscale complex reactor structures







- **A demonstration case**
  - A 5x5 rod bundle with spacers: i) coarse-grid for the entire heated length with porous media for the spacers, ii) detailed CFD for one span with spacer resolved explicitly

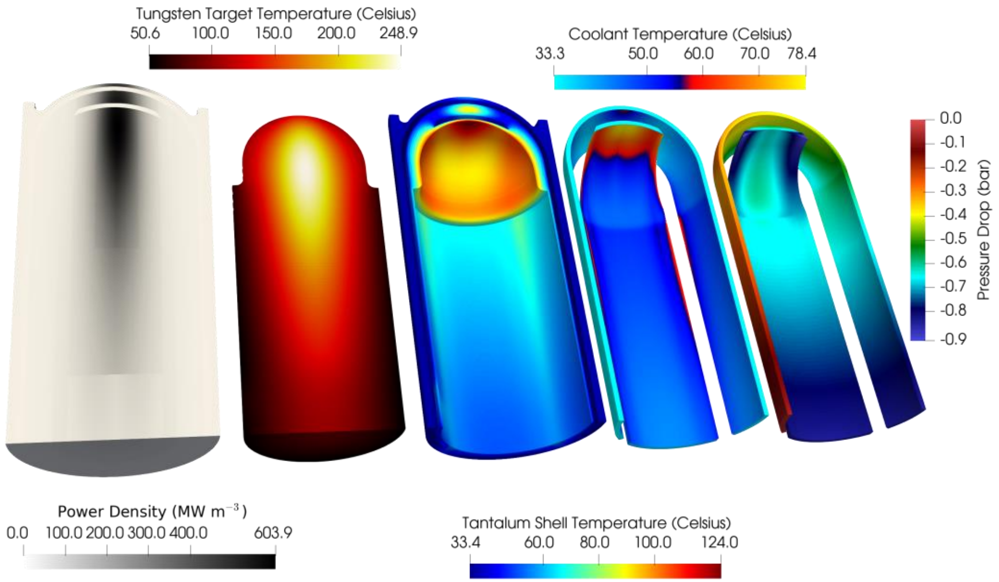


†Dr Bo Liu, Computational scientist, STFC Daresbury Laboratory, UK. Email: bo.liu@stfc.ac.uk

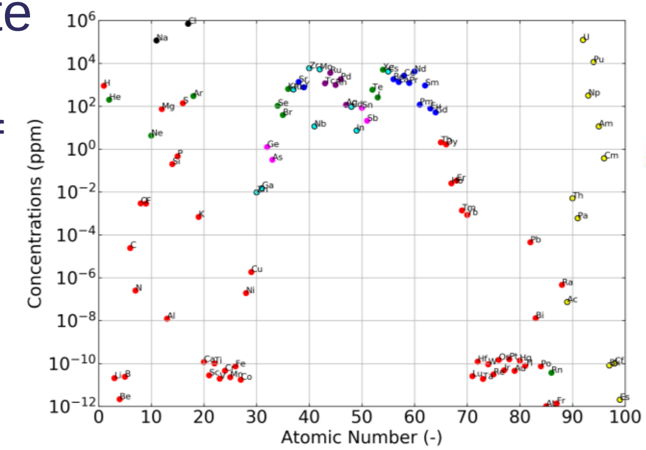
Neutron Source & Molten Salt Reactor (G. Cartland-Glover)

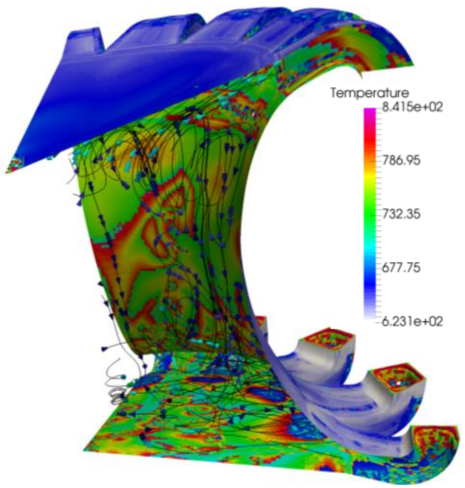
- ISIS Muon and Neutron Source: Conjugate heat transfer and interphase mass transfer in Target Station 2
  - To try to understand the potential impact of radiolysis and thermal striping on target operational lifetime

- Molten salt fast reactors - Depositio MSFR with University of Liverpool and Computational and Theoretical Physics:
  - Depletion of nuclear fuel salts and conjugate heat transfer modelling
  - To try to understand the impact of plating of noble metals on CHT



ISIS Target Station 2



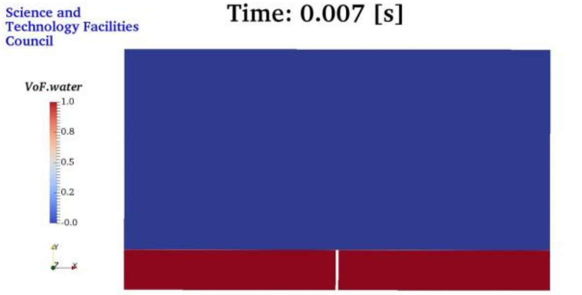


EVOL-Optimised MSFR code_saturne

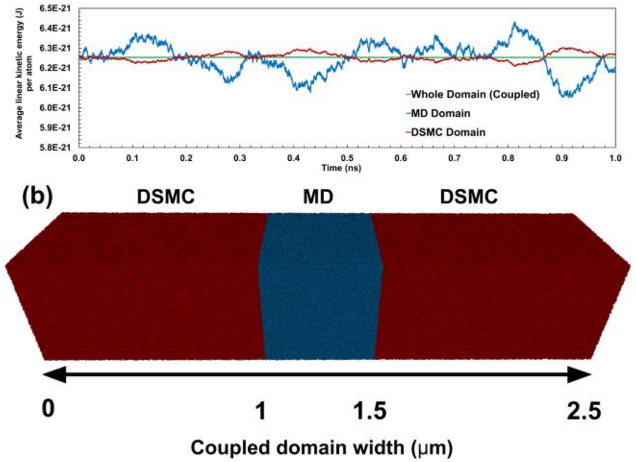
Frozen salt film at the wall

Science and Technology Facilities Council

Flow-Structure Interaction (W. Liu & S. Longshaw)

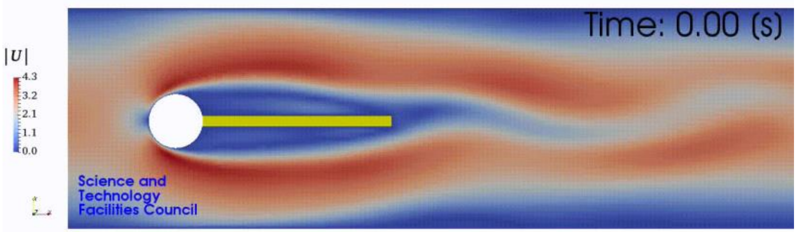


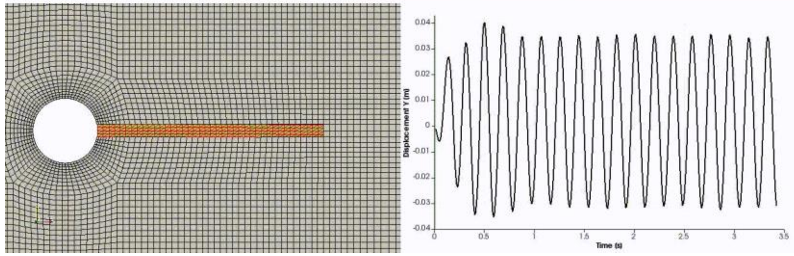
2-D roll tank with flexible beam



Multiscale Universal Interface Coupling Library

https://github.com/MxUI





2-D Flow Pass Elastic Plate Behind a Rigid Cylinder

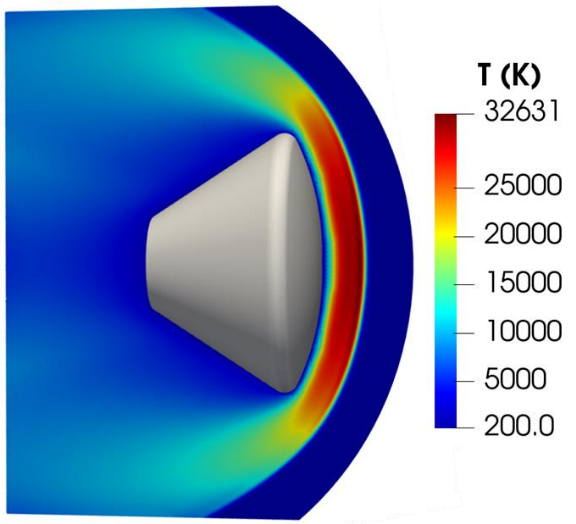
Hypersonics – DSMC (B. John)

- Hypersonics is a key feature of the UK's involvement in future **satellite deployment**, **sub-orbital flights** and for partnering in **space exploration** programmes.

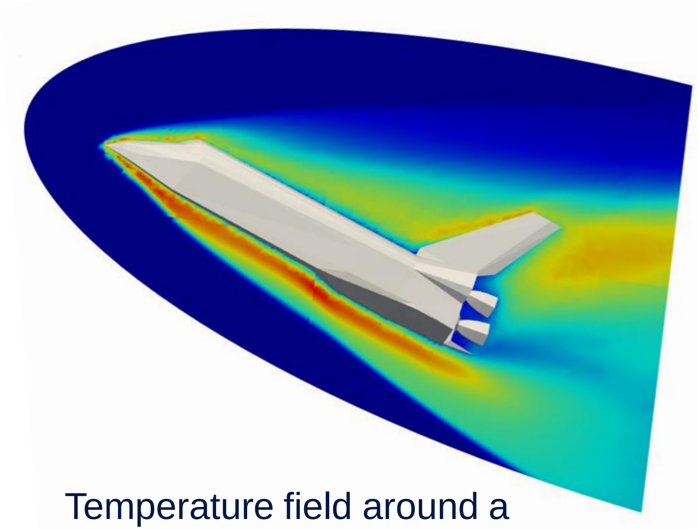
- Hypersonic simulations (**Mach>5**) require a multi-model approach. Gas-phase chemical reactions, ionization, radiation etc. need to be considered as gas temperature increases with Mach number, e.g. in designing materials for **thermal protection systems (TPS)**.

- SCD has capabilities in computational fluid dynamics (**CFD**) and molecular level methods (**DSMC**) for modelling a range of high-Mach flight conditions ranging from **low-altitude supersonic** to **high-altitude hypersonic** flight.

- A key example is aerothermodynamics of **re-entry** of capsules, probes, UAV etc. to planetary atmosphere. The images on the right are our simulation results from the open-source DSMC code, SPARTA.



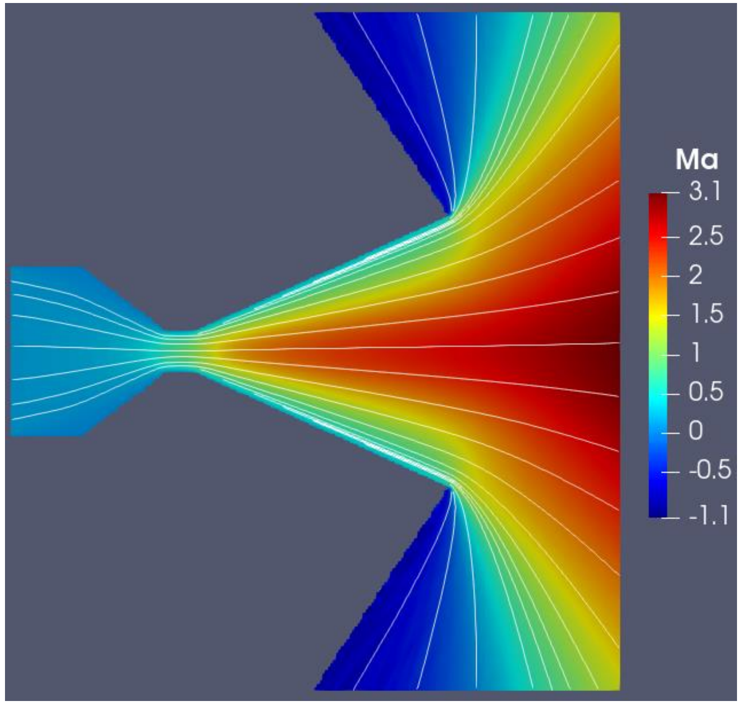
Orion capsule re-entry simulation at Mach 25 (Temperature field)



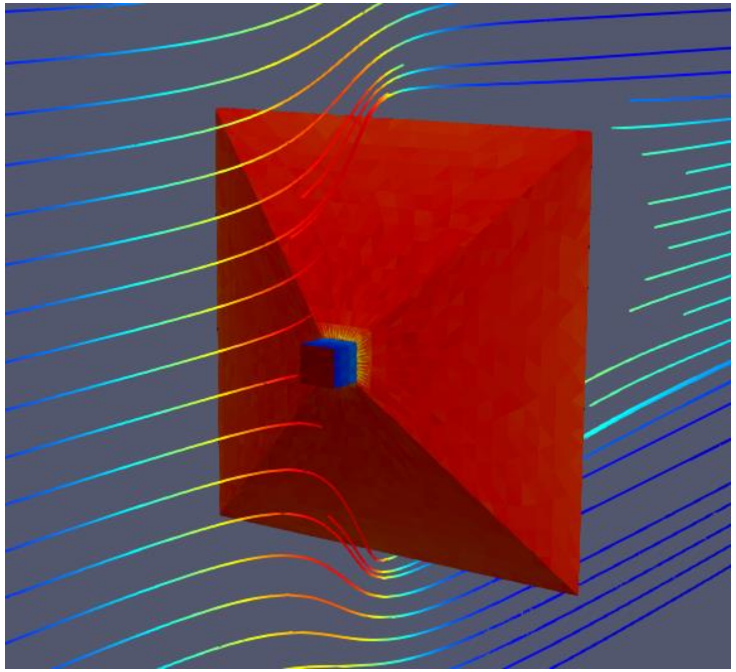
Temperature field around a NASA **Space Shuttle** (Mach 25)

Science and Technology Facilities Council

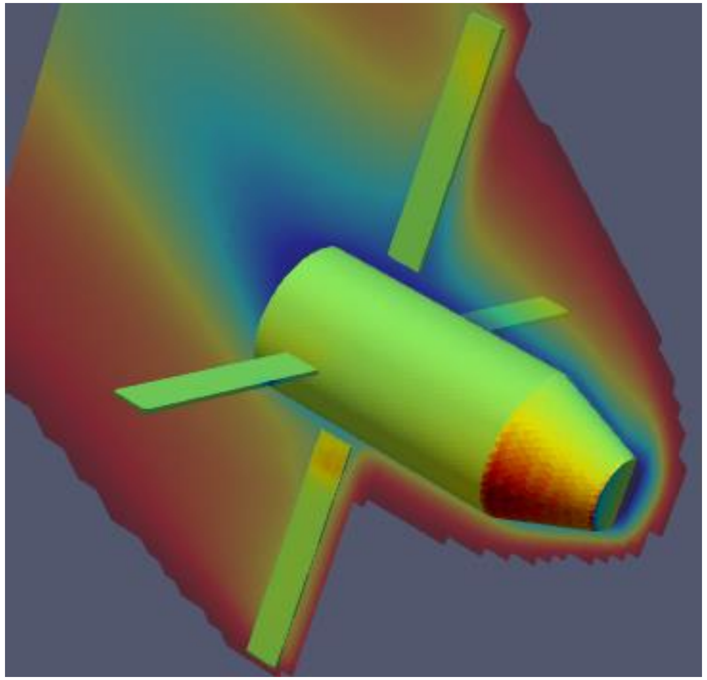
Modelling and Simulation for Satellite Applications - Thruster Propulsion and Satellite Aerodynamics



Representative simulation result showing Thruster propulsion and Nozzle plume expansion



Flow-field & thermal load on a **CubeSat De-orbit Sail** satellite (at H=125 km)



Flow-field & forces on a descending satellite (**ESA satellite debris** test case)

Science and Technology Facilities Council

Science and Technology Facilities Council

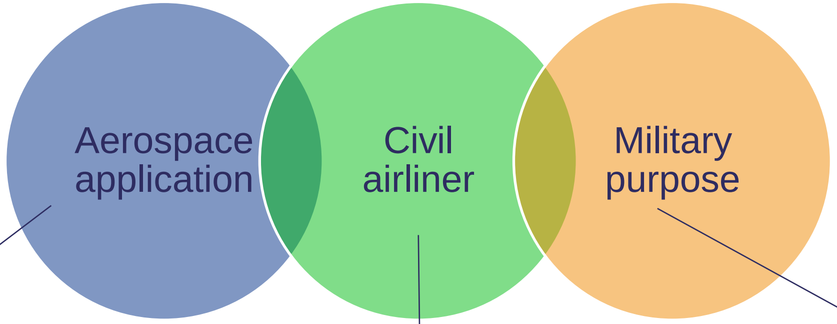
Research on Shock-Wave/Boundary Layer Interaction

Jian Fang
Scientific Computing Department, STFC Daresbury Laboratory, UKRI

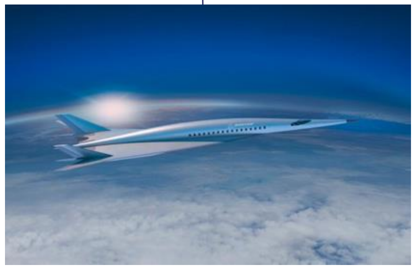
May 30, 2022, Visit to Prof. Sergio Pirozzoli at Università di Roma Italy

Science and Technology Facilities Council

Hypersonic vehicles



SSTO



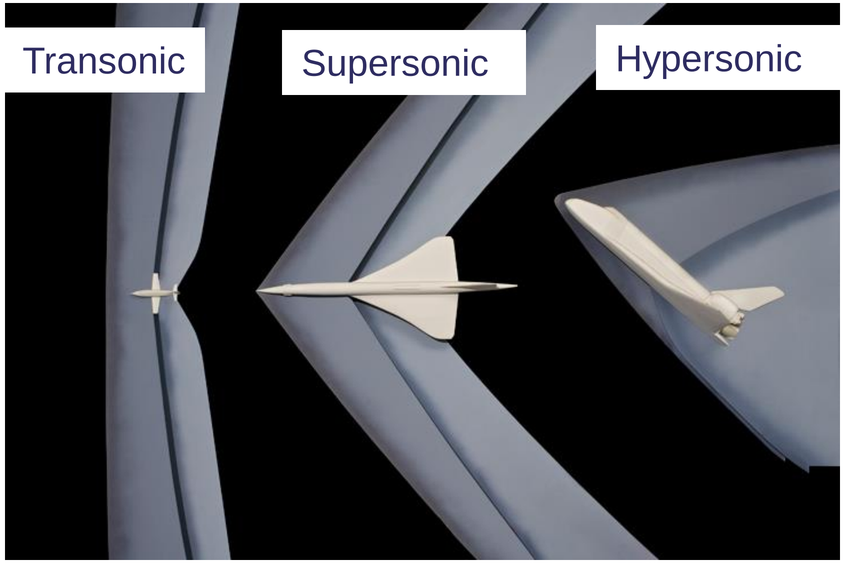
Boeing's Hypersonic Passenger Plane

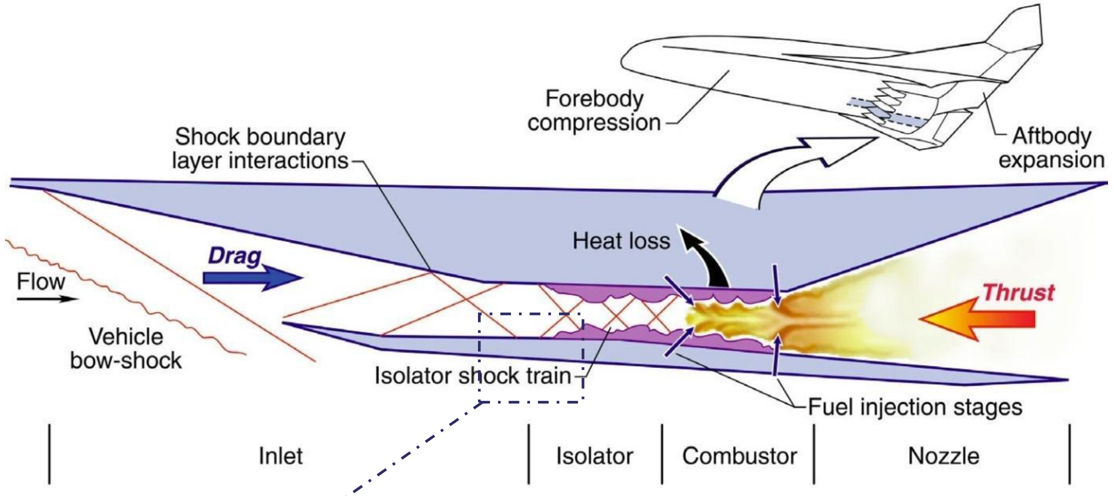
SR-72

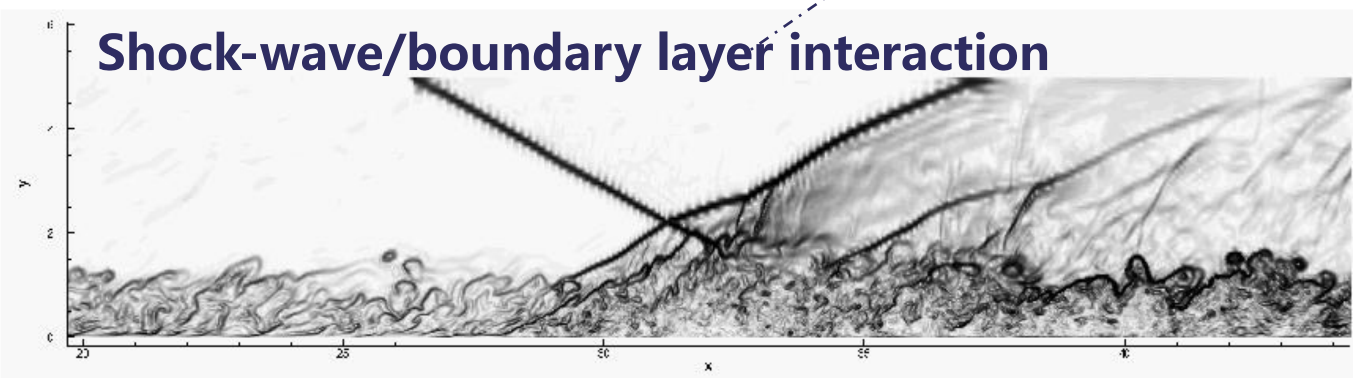
Hypersonic vehicles proposed around the world
via Naval News Instagram Page

Science and Technology Facilities Council

Shock-wave







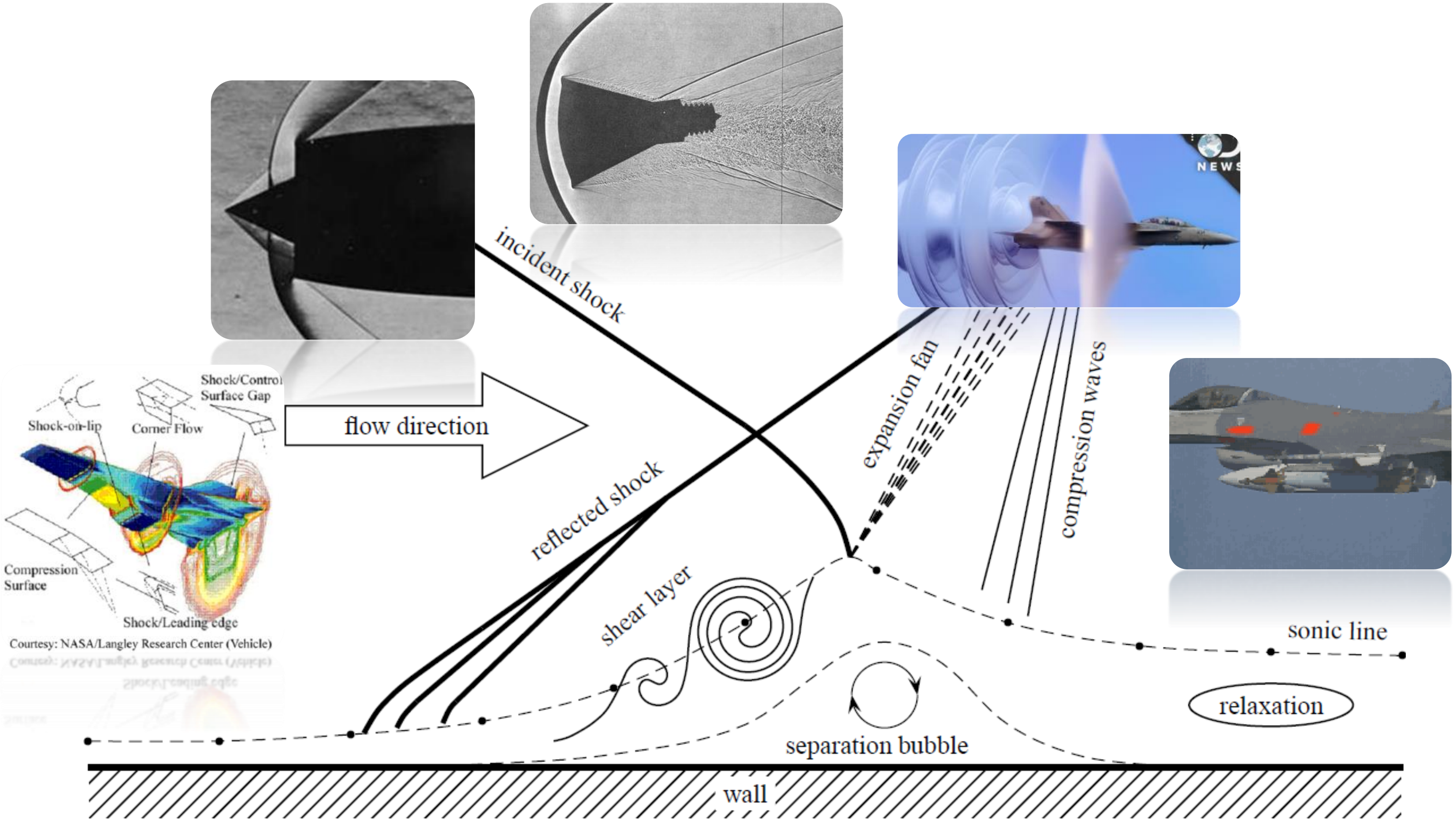
Science and Technology Facilities Council

Introduction

SWTBLI connects to

- **Intake unstart**
- **Low-cycle fatigue**
- **Wing vibration**
- **Control efficiency**
- **Heat flux**
- **Noise…**

The lack of understandings of SWBLI and the uncertainty in engineering CFD are the two significant bottlenecks of developing hypersonic



Science and Technology Facilities Council

Computational fluid dynamics (CFD)

Direct-numerical Simulation
- Resolve all spatial-temporal flow structures
- Accurate
- Very expensive and mainly used in academics
- Not ready for industry

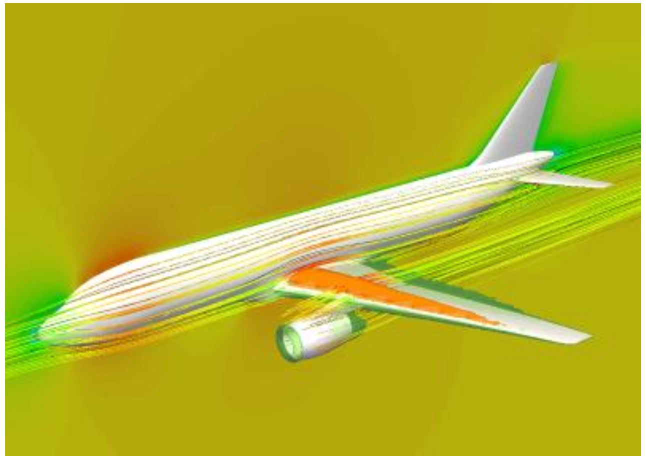

Source: KTH Mechanics

CFD

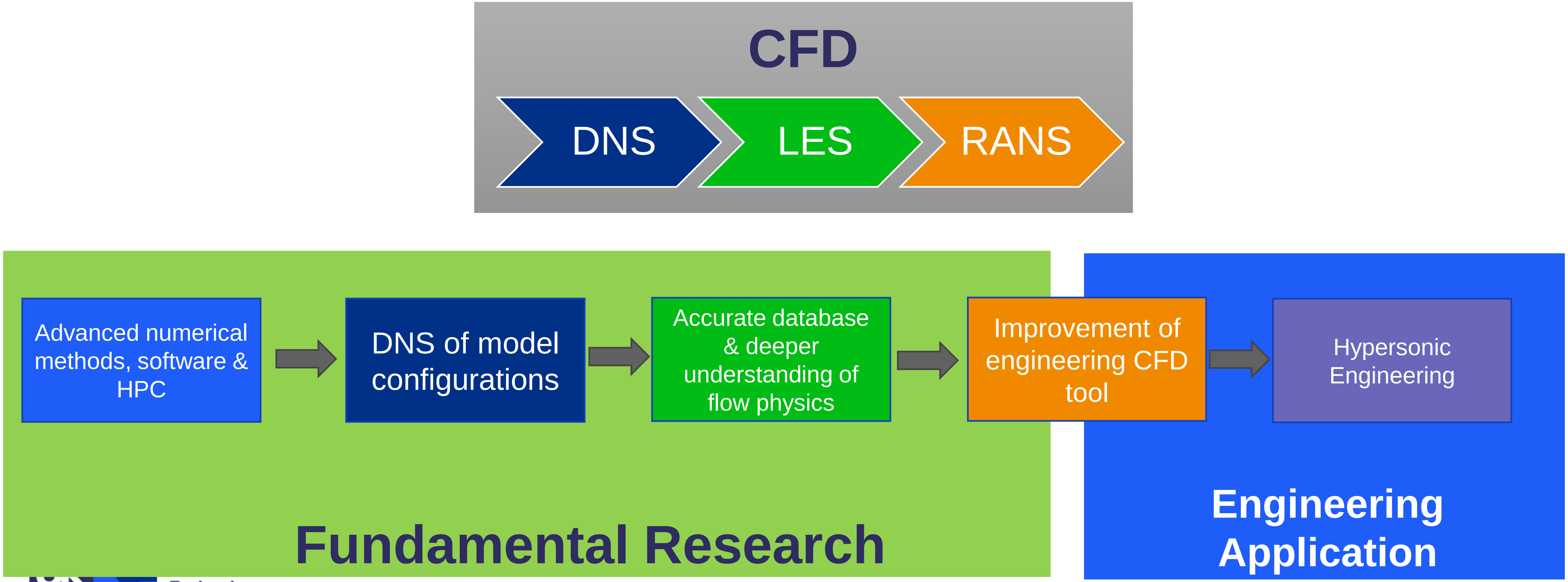
DNS → LES → RANS

- Affordable and much faster
- Detailed flow field data
- Extensively applied in engineering design and academic research

Reynolds-averaged Navier–Stokes
- Resolve only mean flow, and model turbulence
- Affordable for engineering design
- Uncertainty is from the turbulence model


https://www.simscale.com/projects/Ali_Arafat/compressible_aerodynamics_of_commercial_aircraft/

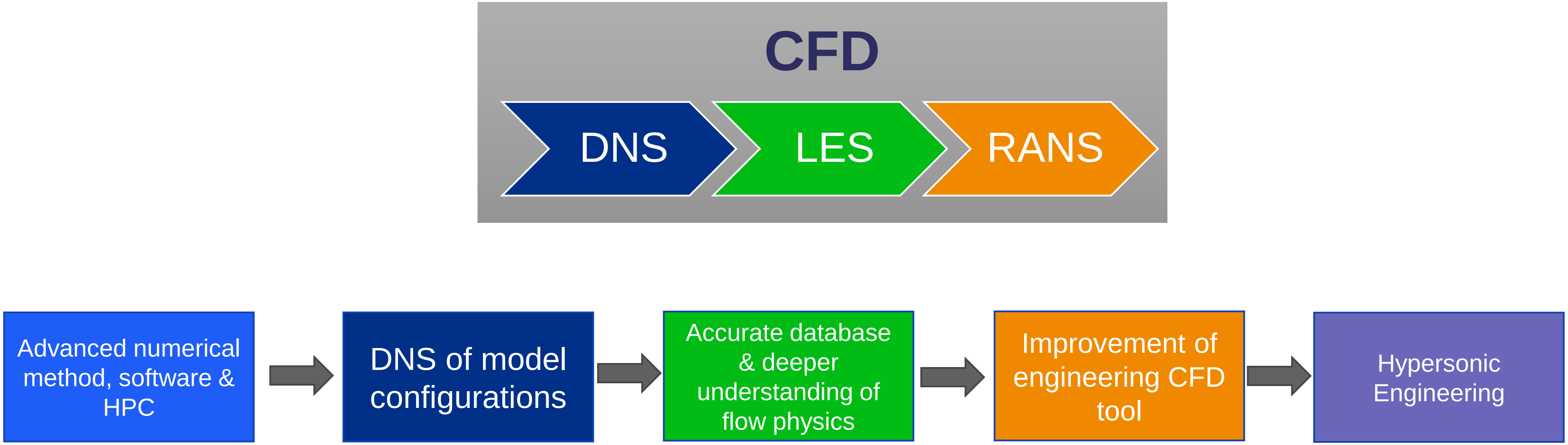
Computational fluid dynamics (CFD)



Technology Facilities Council

Computational fluid dynamics (CFD)

What have we done

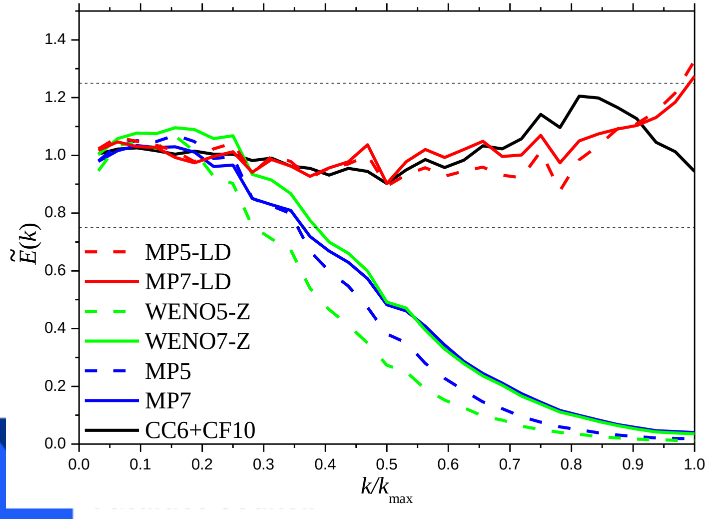


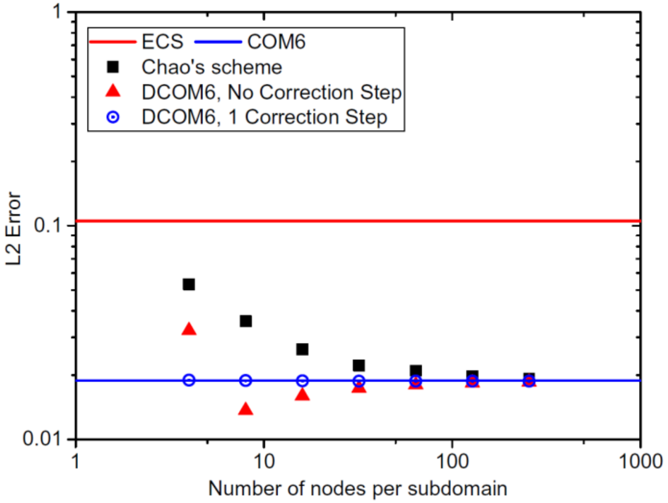
Science and Technology Facilities Council

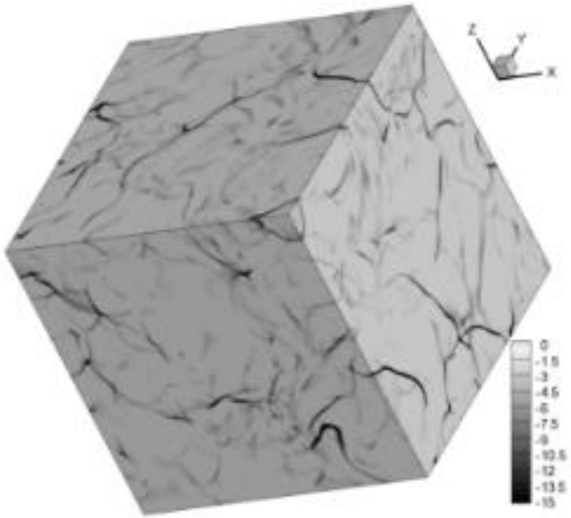
What have we done

Advanced numerical method, software & HPC

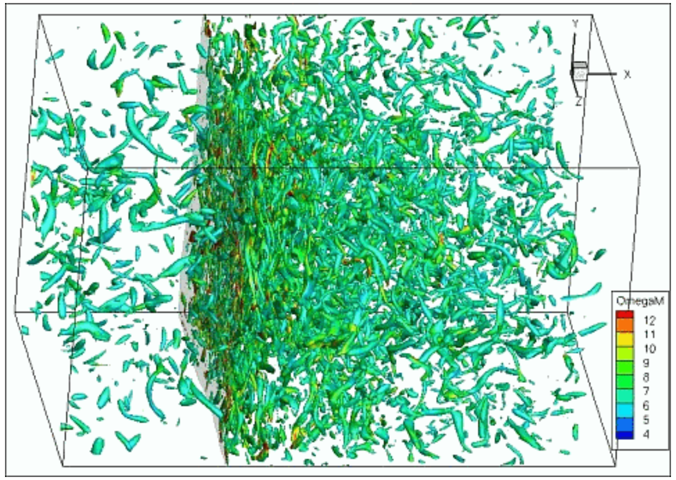
- *Development of high-order shock-capturing schemes*
- *Improvement of the parallel performance of compact scheme*







Shocklets in strongly compressible turbulence



Direct interaction between shock and turbulence

What have we done

Advanced numerical method, software & HPC

J Sci Comput
https://doi.org/10.1007/s10915-018-0717-7

CrossMark

Hybrid Optimized Low-Dissipation and Adaptive MUSCL Reconstruction Technique for Hyperbolic Conservation Laws

Jie Wu[1,2] · Yuan-yuan He[2] · Guo-hao Ding[2] · Yi-yu Han[2]

ENGINEERING APPLICATIONS OF COMPUTATIONAL FLUID MECHANICS, 2017
https://doi.org/10.1080/19942060.2017.1348991

Taylor & Francis
Taylor & Francis Group

OPEN ACCESS Check for updates

Assessment of the IDDES method acting as wall-modeled LES in the simulation of spatially developing supersonic flat plate boundary layers

Yiyu Han[a], Guohao Ding[a], Yuanyuan He[a], Jie Wu[a,b] and Jialing Le[a]

[a]Science and Technology on Scramjet Laboratory, China Aerodynamics Research and Development Center (CARDC), Mianyang, China; [b]School of Power and Energy, Northwestern Polytechnical University, Xi'an, China

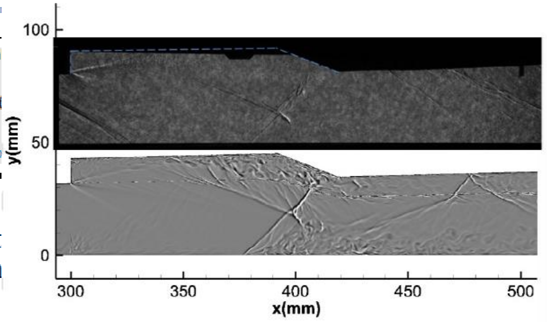
Aerospace Science and Techn

Contents lists availa

Aerospace Scienc

ELSEVIER

www.elsevier.co



Assessment of a hybrid RANS/LES simulat method in depicting the unsteady motion scramjet combustor

Yiyu Han *, Yuanyuan He, Ye Tian, Fuyu Zhong, Jialing Le

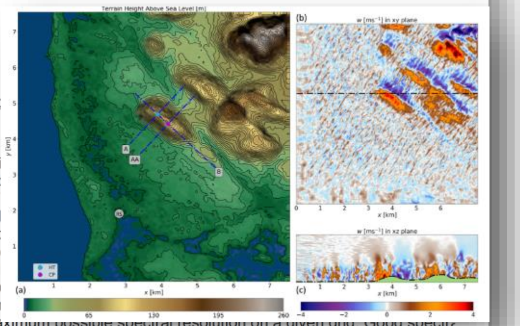
Science and Technology on Scramjet Laboratory of Hypervelocity Aerodynamics Institute, CARDC, China

3B.5 Improving Spectral Resolution of Finite Difference Scheme for Multiscale Modeling Applications Using Numerical Weather Prediction Model

Monday, 20 June 2016: 2:30 PM
Bryce (Sheraton Salt Lake City Hotel)

Branko Kosovic, NCAR, Boulder, CO;

Recorded Presentation



Advances in high performance computi resolving large synoptic scales and turb bridge numerical weather prediction (N simulations represent a number of chal physical processes, numerical effects c schemes vs. spectral resolution, etc. H numerical schemes for multiscale simu simulations of canonical, horizontally h with periodic lateral boundary condition Pseudospectra simulations achieve maximum possible spectral resolution on a given grid. Good spectral resolution can also be achieved with high even order finite difference schemes. However, in the presenc of strong gradients such schemes can result in spurious high frequency oscillations. Such numerical artifacts can be avoided if upwind differencing is utilized. Upwind schemes are numerically dissipative and result in inferior spectral resolution. We therefore propose a hybrid scheme developed by Fang et a (2013) that combines high order upwind and centered schemes. We implemented the hybrid scheme in the Weather Research and Forecasting model and HIGRAD model. We then carried out a series of LES of convective boundary layers characterized by different stability parameters zi/L. The results of these LES were compared to pseudospectral LES. The results show that the hybrid scheme provides optimal performance with enhanced spectral resolution compared to upwind schemes and no undesired numerical artifacts associated with centered schemes of similar order.

- Indicates paper has been withdrawn from meeting
- Indicates an Award Winner

See more of: Theoretical and Practical Issues Associated with Multi-Scale Simulations
See more of: 22nd Symposium on Boundary Layers and Turbulence

AIAA JOURNAL

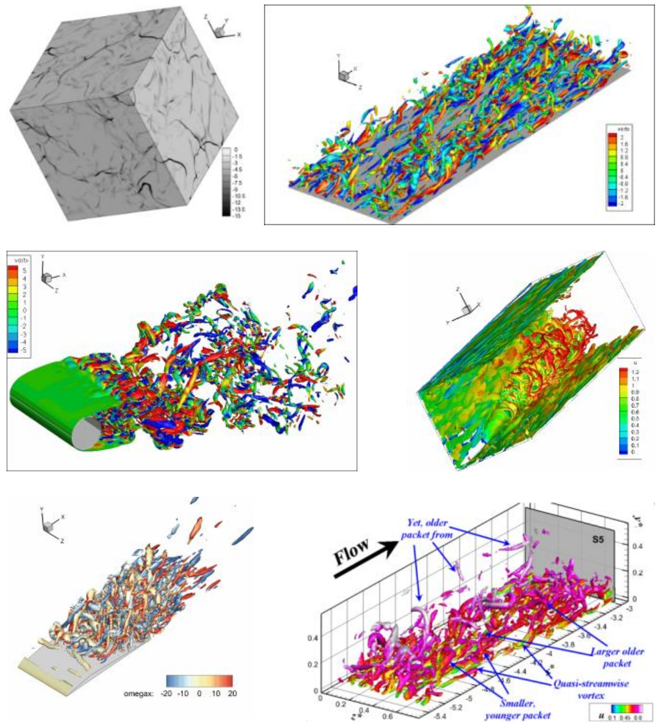
Modification to Improved Delayed Detached-Eddy Simulation Regarding the Log-Layer Mismatch

Yiyu Han,* Yuanyuan He,† and Jialing Le‡
China Aerodynamics Research and Development Center, 621000 Mianyang, People's Republic of China

Science and Technology Facilities Council

What have we done

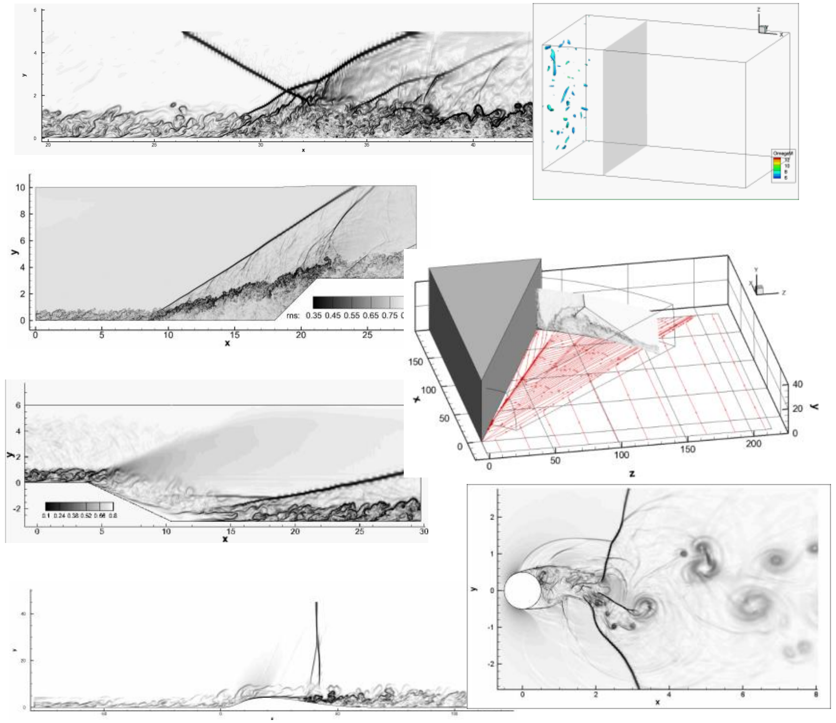
Advanced numerical method, software & HPC



Turbulence Study

ASTR code

- A high-order FDM solver for compressible Navier-Stokes equations on a generalised coordinate system.
- Modern FORTRAN language and MPI parallelisation.
- Different types of high-order schemes:
  - 6th-order compact schemes
  - 5th/7th-order upwind-biased shock-capturing schemes
  - Several Riemann solvers: Steger-Warming, AUSMPW+
- Installed and tested on many HPC systems
  - HECToR, ARCHER, ARCHER2, HAWK
- Linear acceleration up to 100k cores

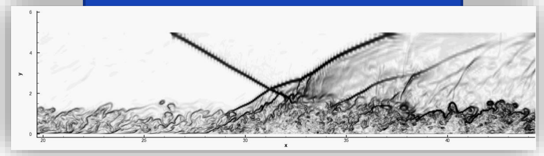


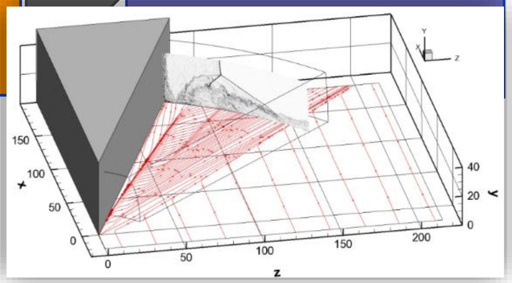
SWBLI Flows

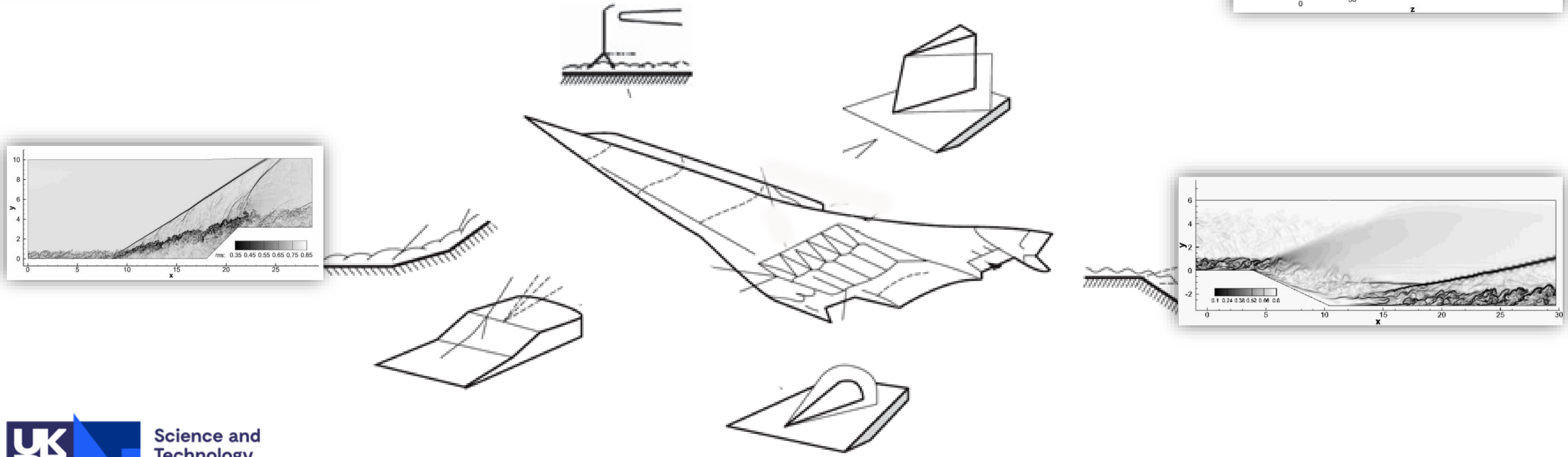
Technology Facilities Council

What have we done

Advanced numerical method, software & HPC → DNS of model configurations → Accurate database & deeper understanding of flow physics → Improvement of engineering CFD tool → Hypersonic





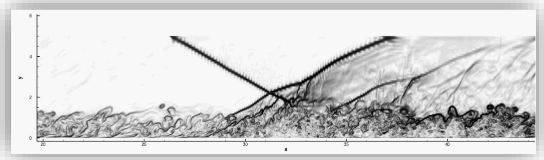


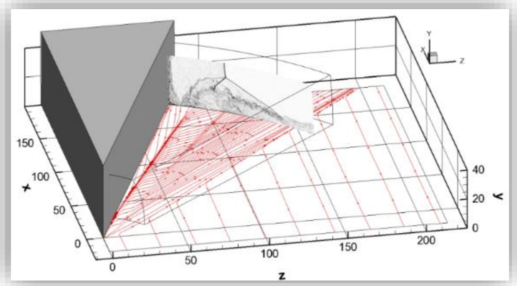
Key flow configurations for hypersonic vehicles by proposed Zheltovodov (2006)

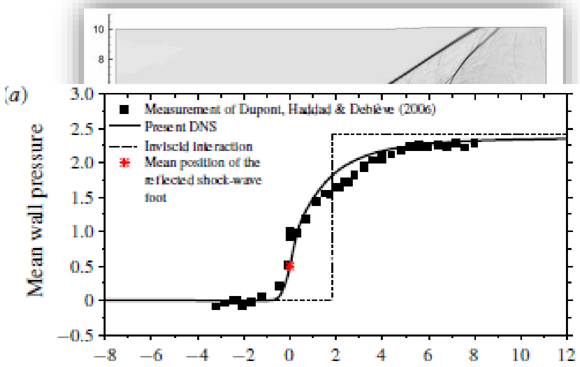
Science and Technology Facilities Council

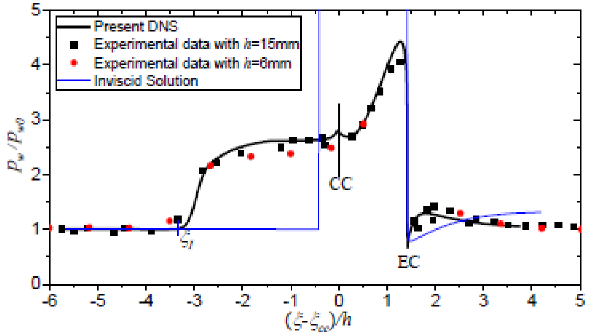
What have we done

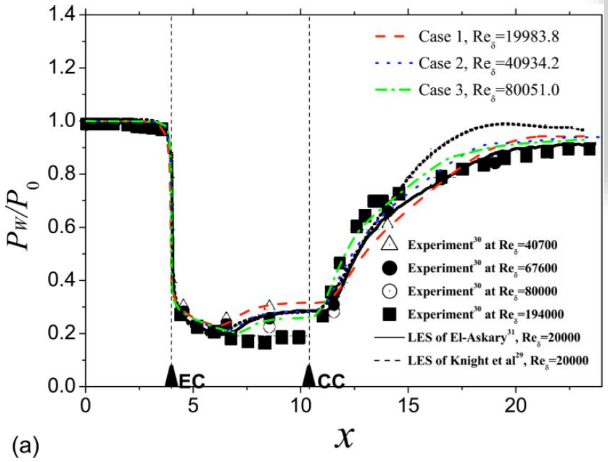
DNS of model configurations

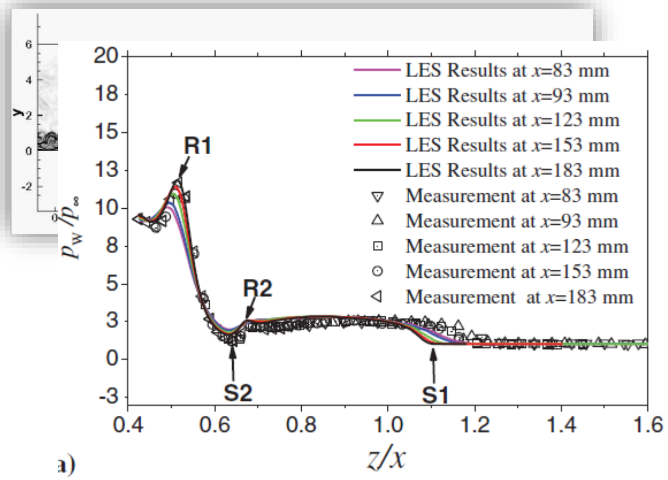








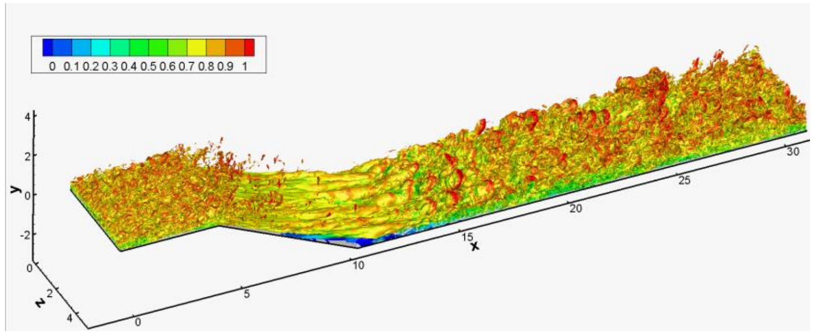




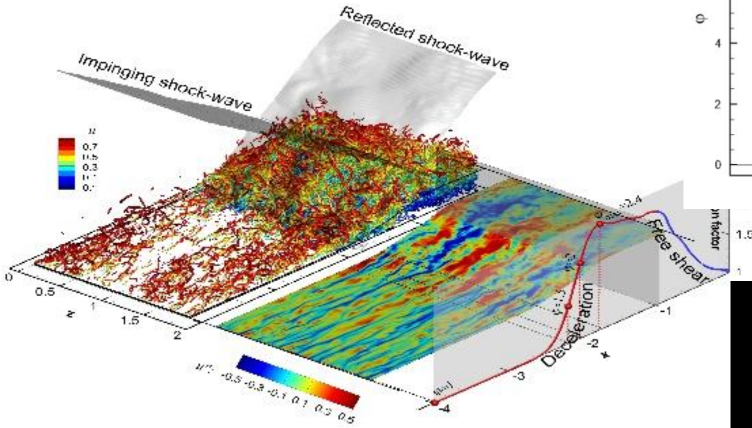
Science and Technology Facilities Council

What have we done

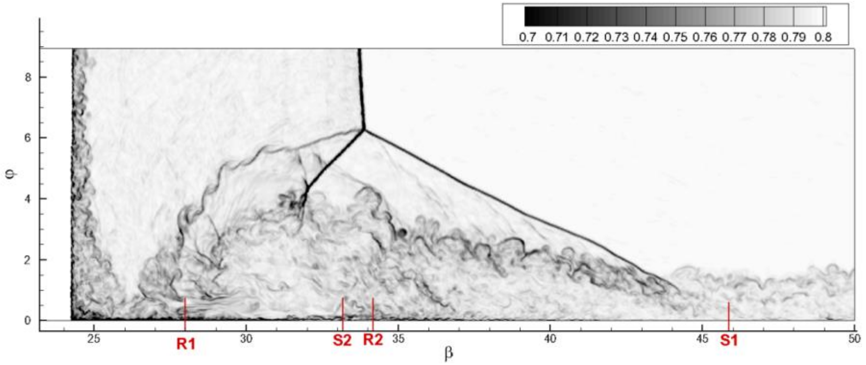
Advanced numerical method and software → DNS of model configurations → Accurate database & deeper understanding of flow physics → Improvement of engineering CFD tool → Hypersonic Engineering



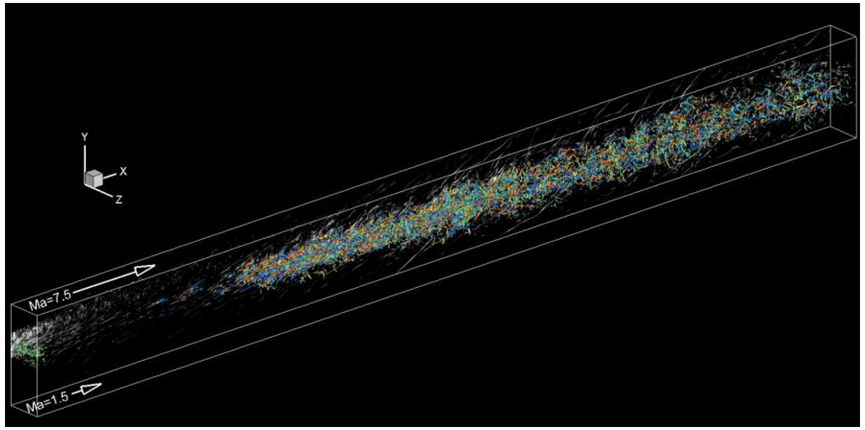
Görtler-like vortices for the supersonic backward facing step flow



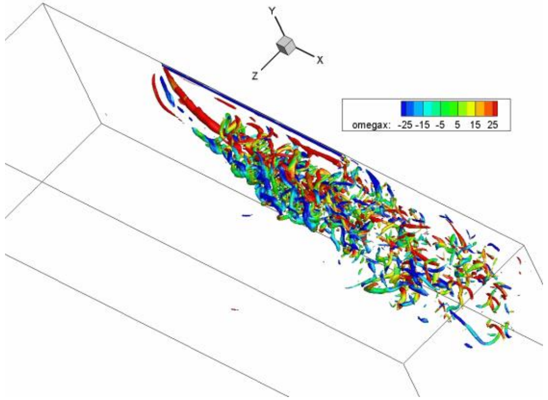
Amplification of turbulence in SWBLI



Flow structures in 3-D SWBLI



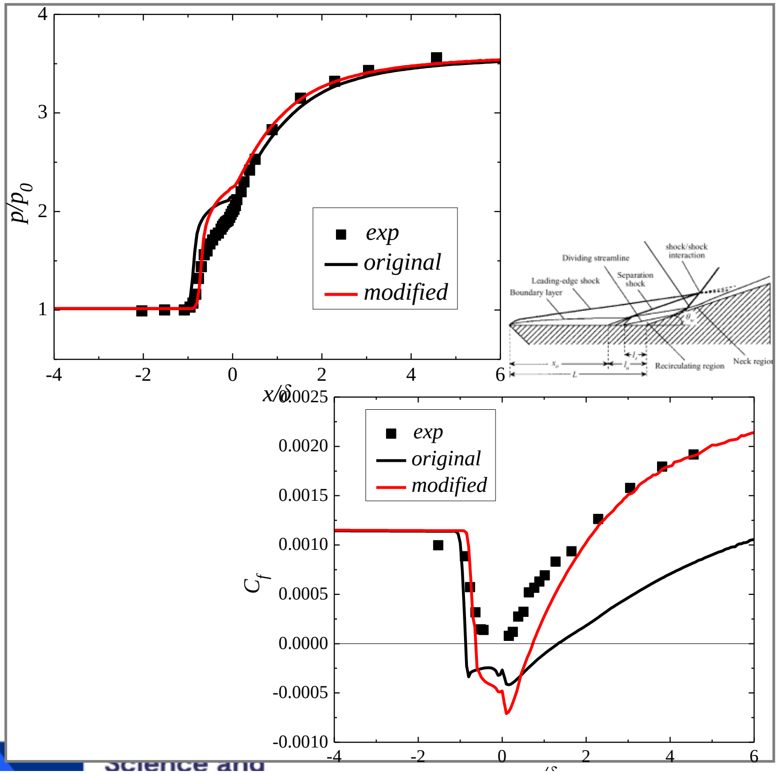
Turbulence structures in supersonic mixing layer



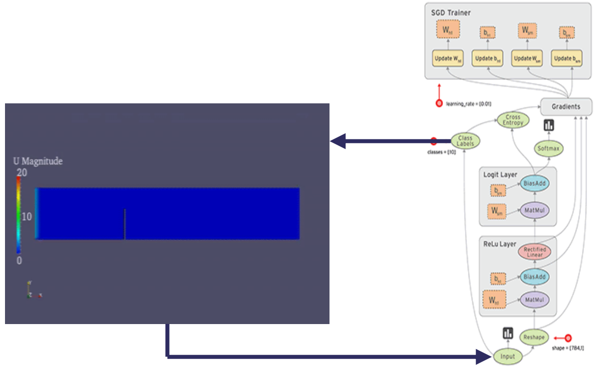
Wall jet

What have we done

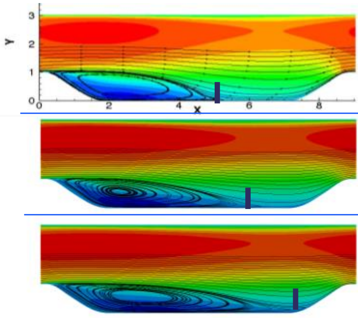
Advanced numerical method and software → DNS of model configurations → Accurate database & deeper understanding of flow physics → Improvement of engineering CFD tool → Hypersonic Engineering

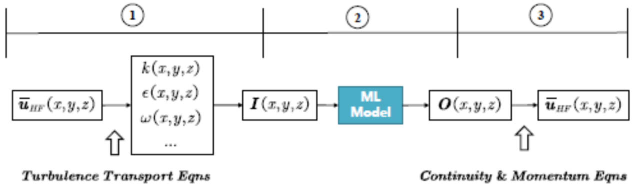


Improvement of the S-A turbulence model



The development of the TensorFlow-OpenFOAM Interface



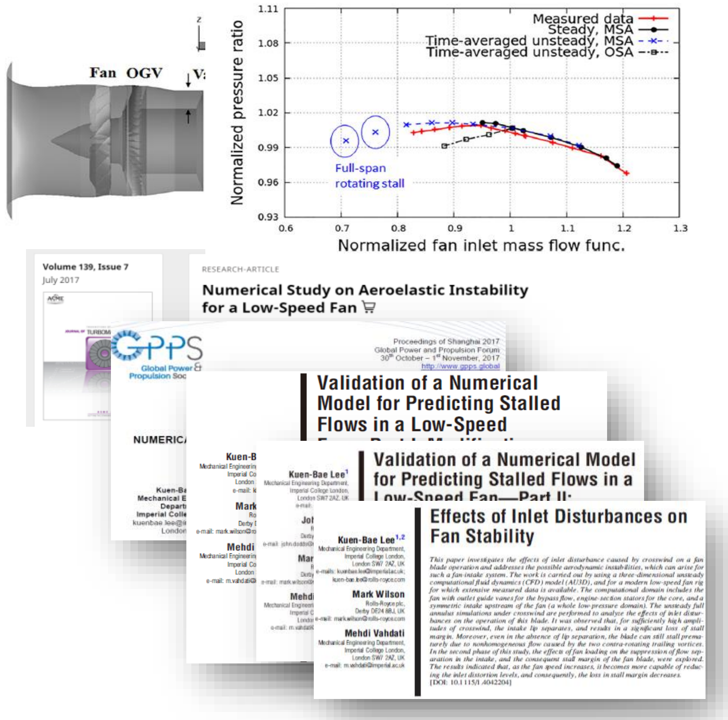


Combination of transport equations with ANN

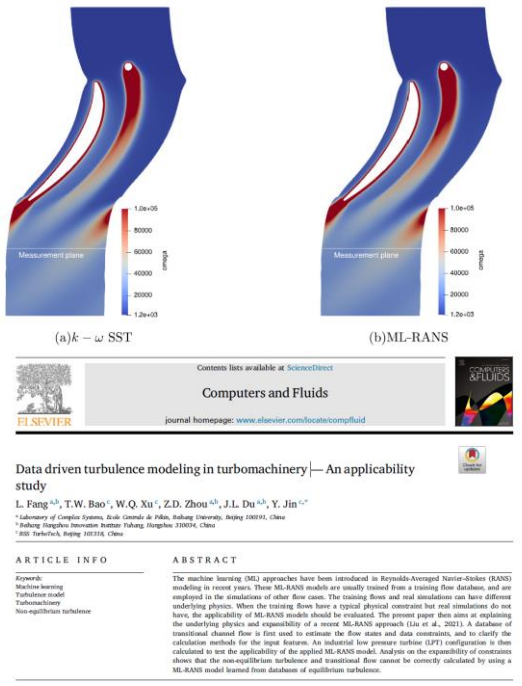
Data driven turbulence modeling

What have we done

Improvement of engineering CFD tool



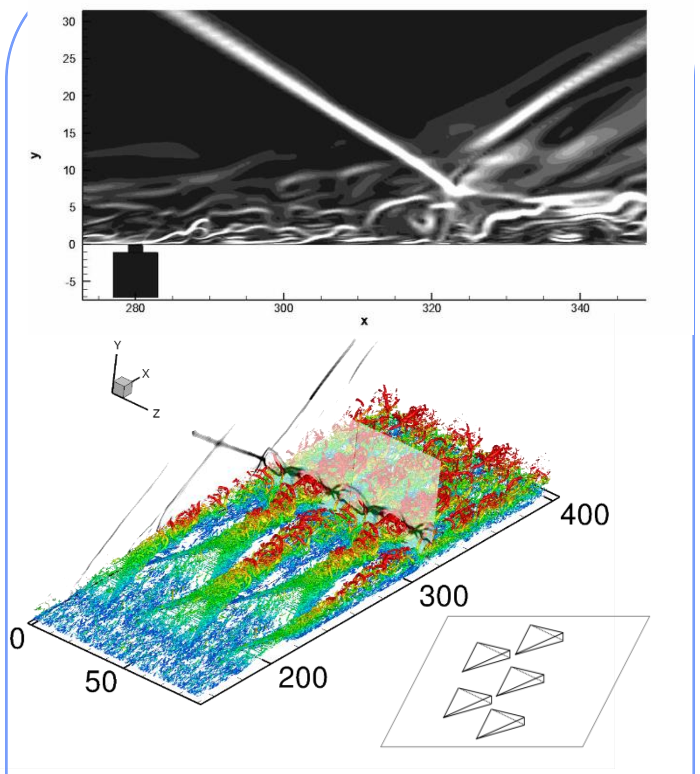
The model has been applied by R&R company in aeroengine



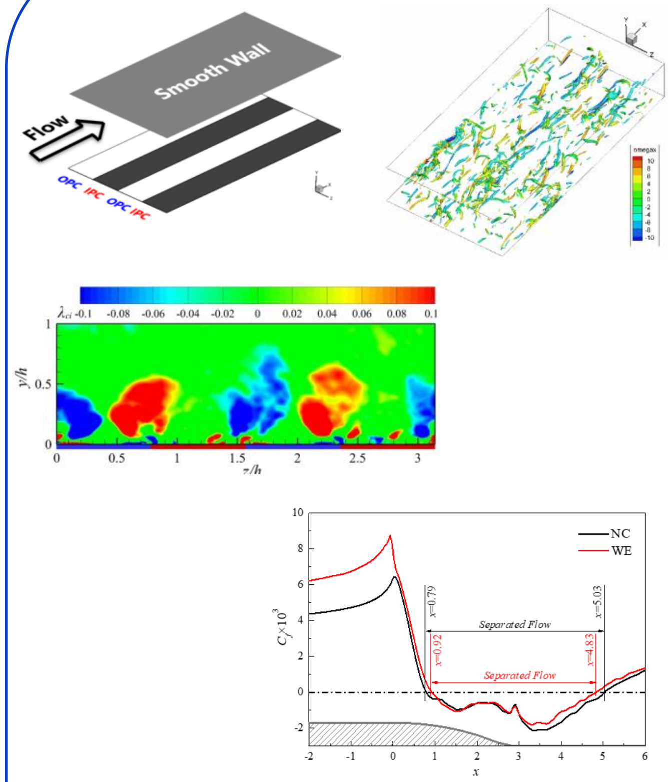
The machine-learning model has been used by southern Snecma company to study flow in turbine

Science and Technology Facilities Council

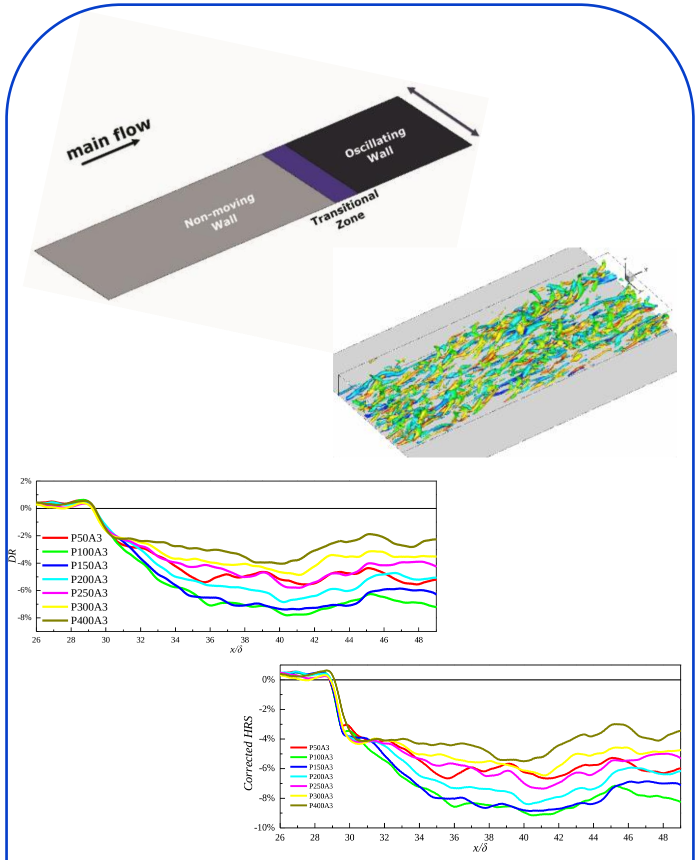
Research of BL control



SWBLI controls



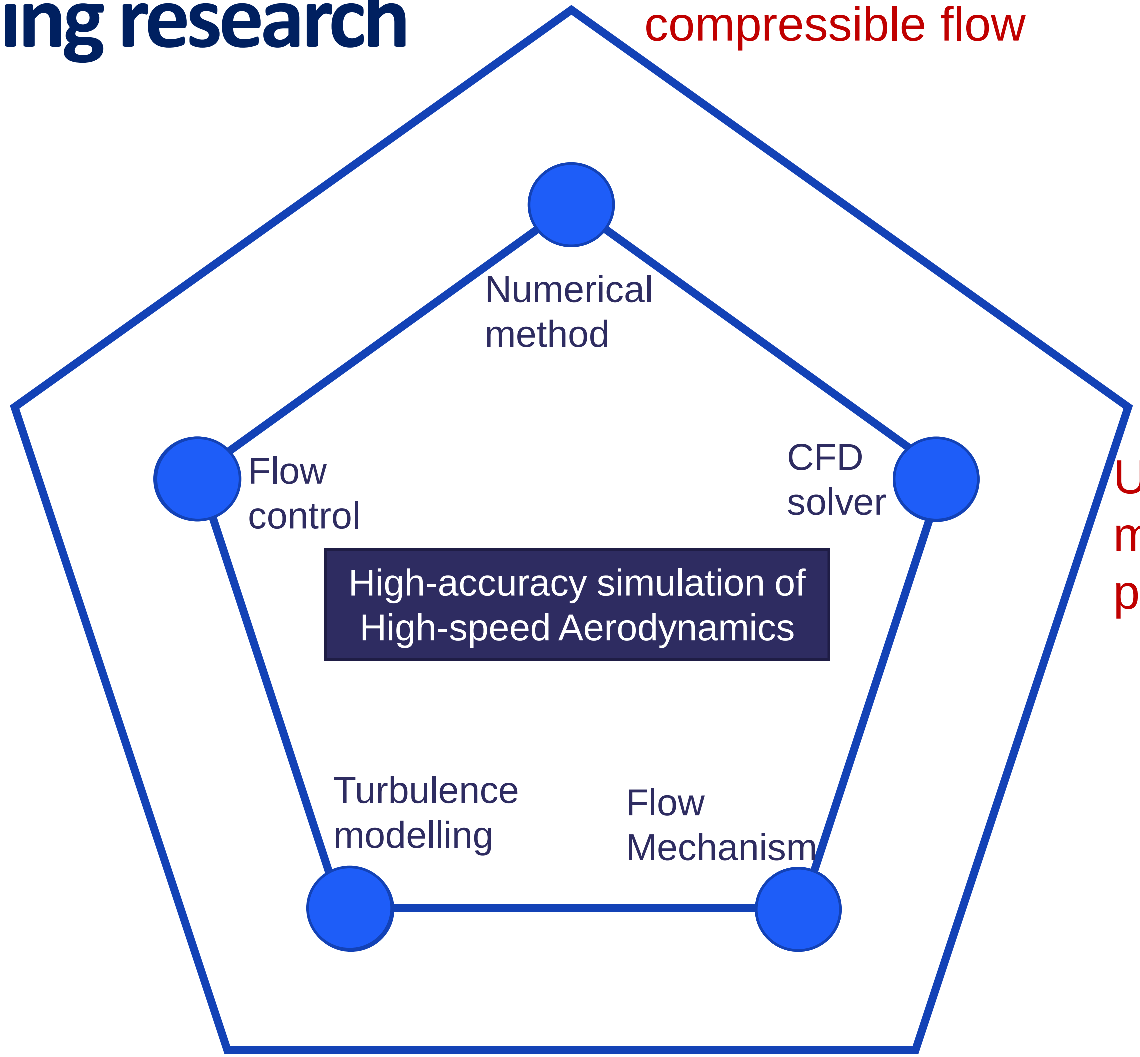
Boundary layer control



Wall heat flux control

Summary & On-going research

Better scheme for compressible flow



Novel SWBLI control scheme

Upgrade ASTR code for more complex multi-physics problems

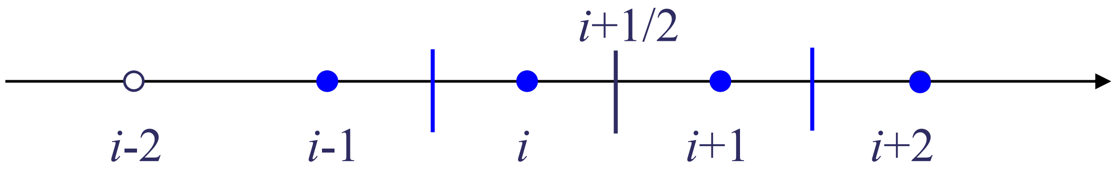
ML model for engineering applications

Hypersonic aerodynamics

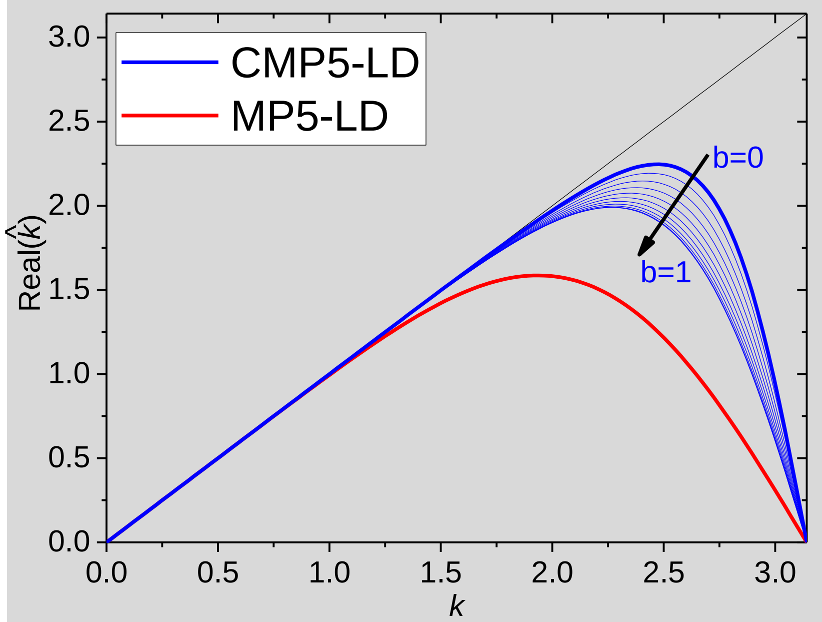
UKRI Science and Technology Facilities Council

High-order compact MP scheme

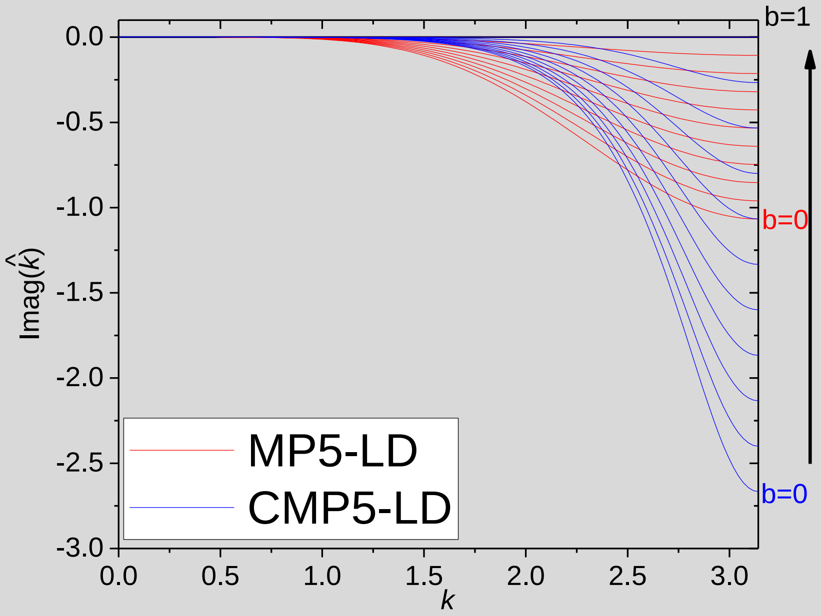
CMP5-LD: $\alpha_{-1}F^L_{i-1/2} + F^L_{i+1/2} + \alpha_1 F^L_{i+3/2} = a_{-1}F_{i-1} + a_0F_i + a_1F_{i+1} + \frac{b}{36}F_{i+2}$



$$\begin{pmatrix} a_{-1} \\ a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} \frac{1}{18} - \frac{b}{36} \\ \frac{19}{18} - \frac{b}{4} \\ \frac{5}{9} + \frac{b}{40} \end{pmatrix}; \begin{pmatrix} \alpha_{-1} \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} - \frac{b}{6} \\ \frac{1}{6} + \frac{b}{6} \end{pmatrix}$$



Bandwidth resolution

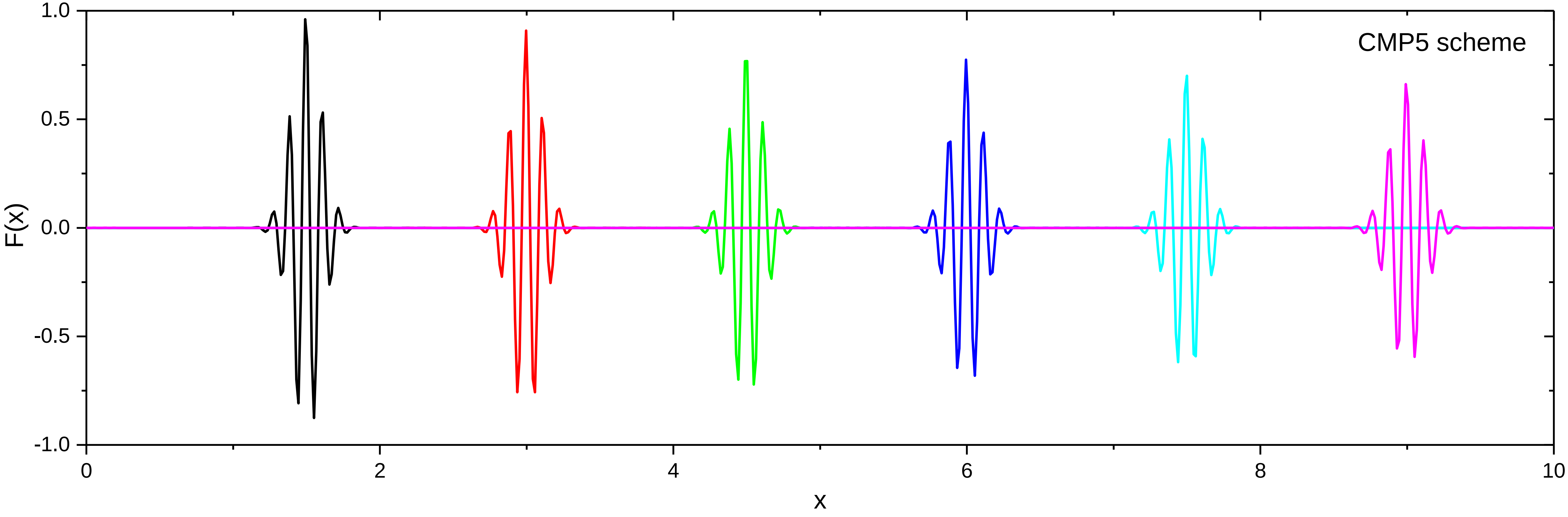


Bandwidth dissipation

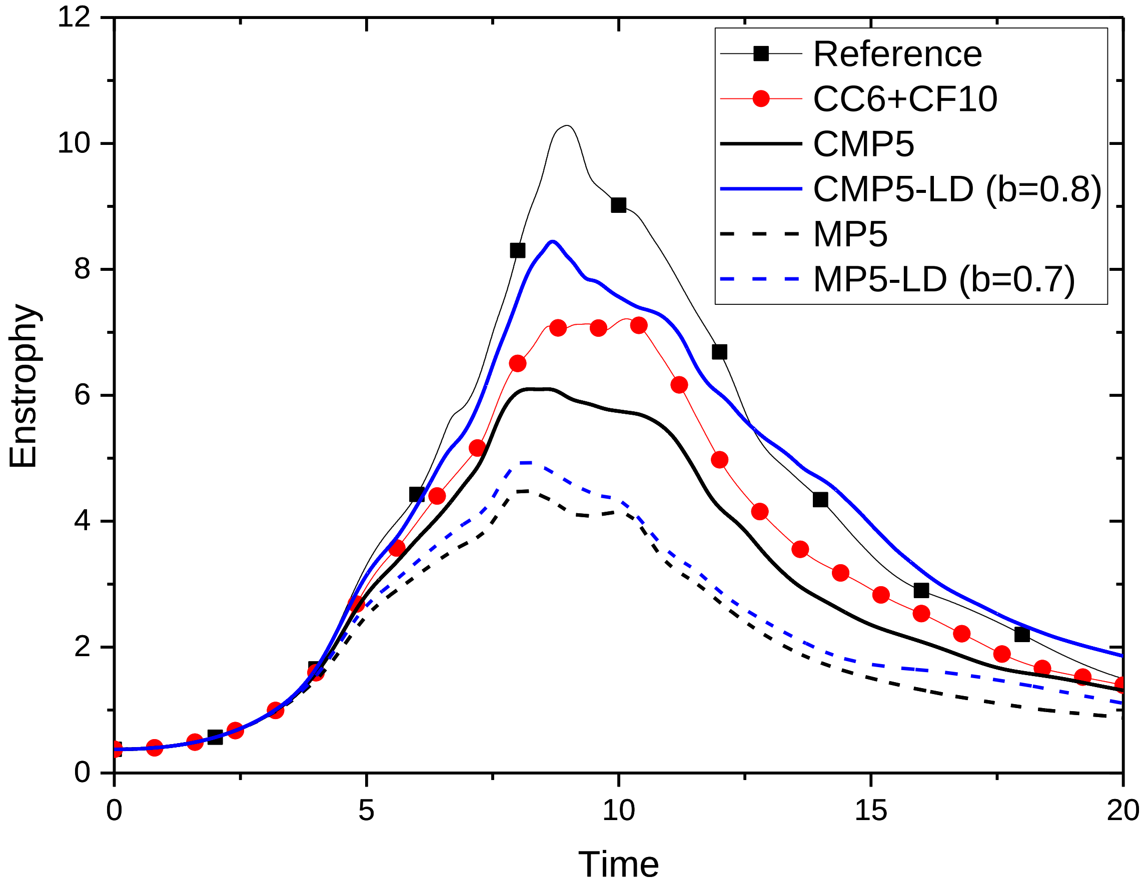
High-order compact MP scheme

$$\frac{\partial F(x,t)}{\partial t} + c\frac{\partial F(x,t)}{\partial x} = 0, x \in [0,10) \quad F(x,0) = e^{-A(x-x_0^2)} sin(\omega_0 x)$$

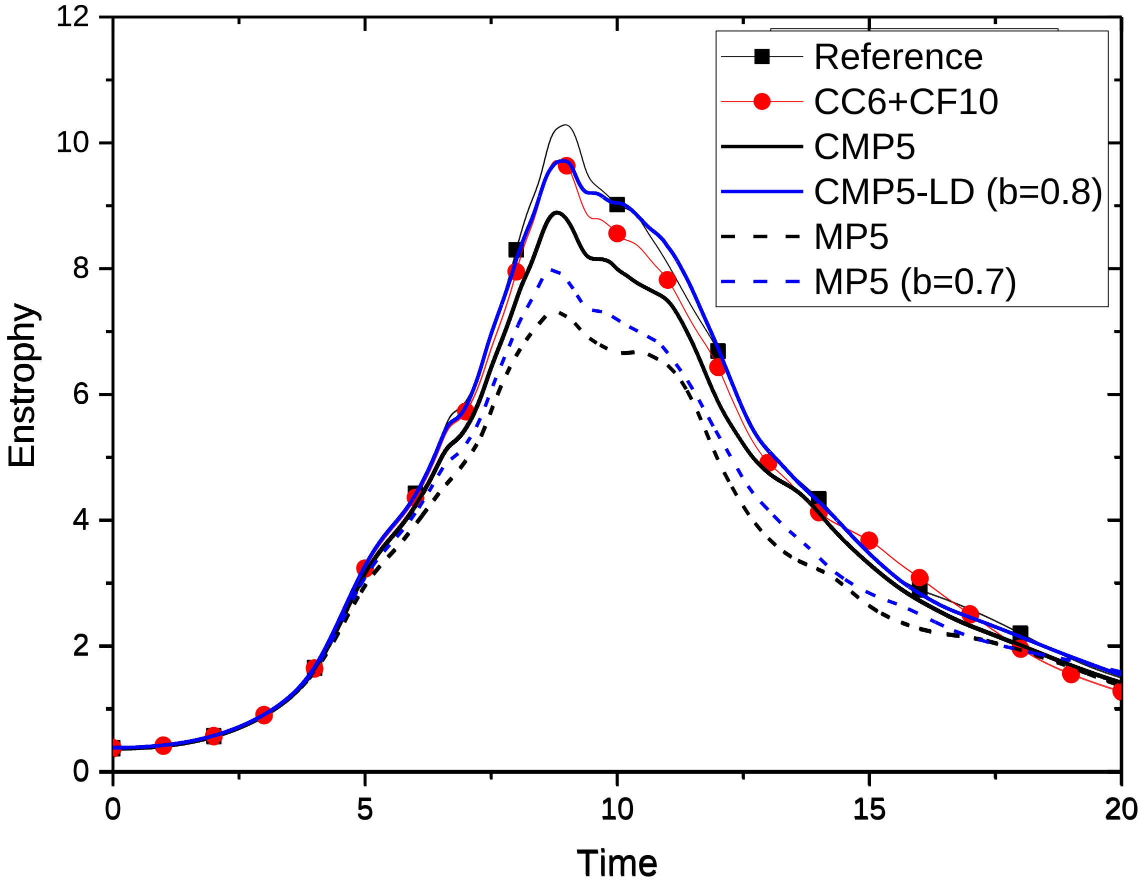
c	A	ω_0	x_0
0.5	50	$0.838242/\Delta x$	1.5



High-order compact MP scheme



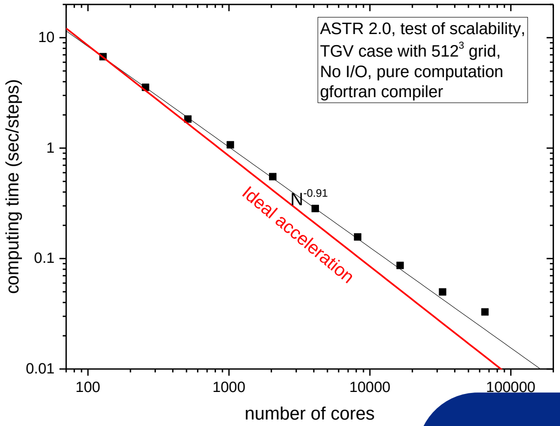
Evolution of enstrophy under 128^3 mesh

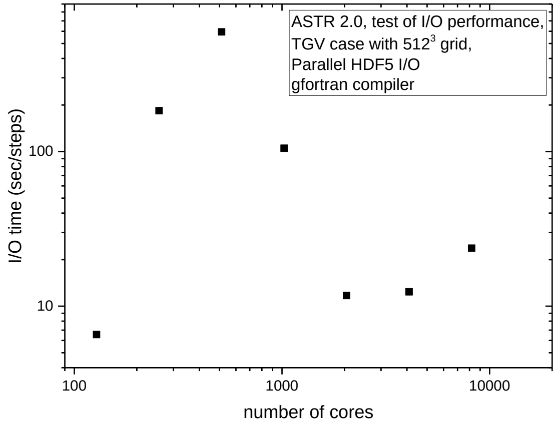


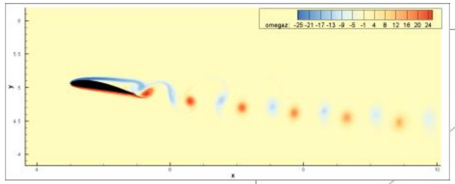
Evolution of enstrophy under 256^3 mesh

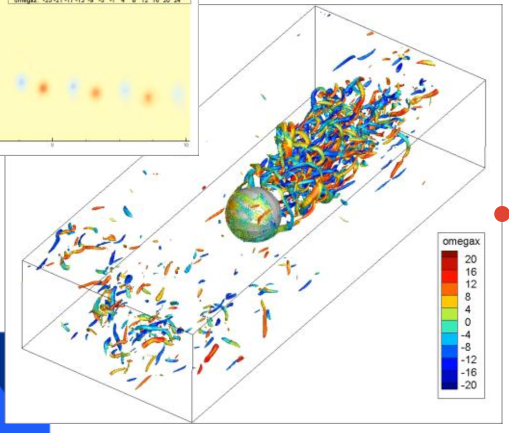
Science and Technology Facilities Council

ASTR 2





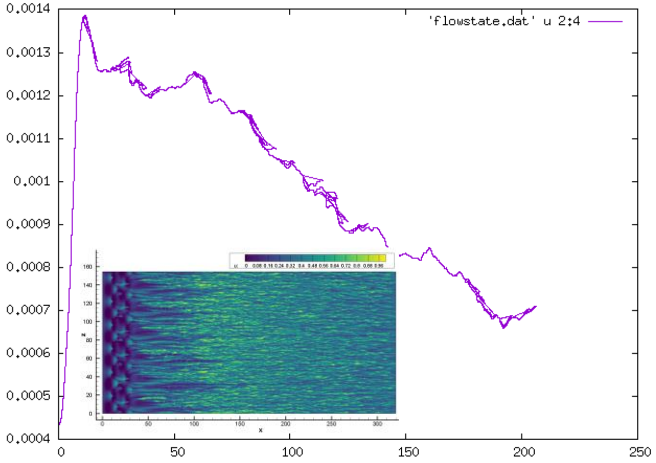


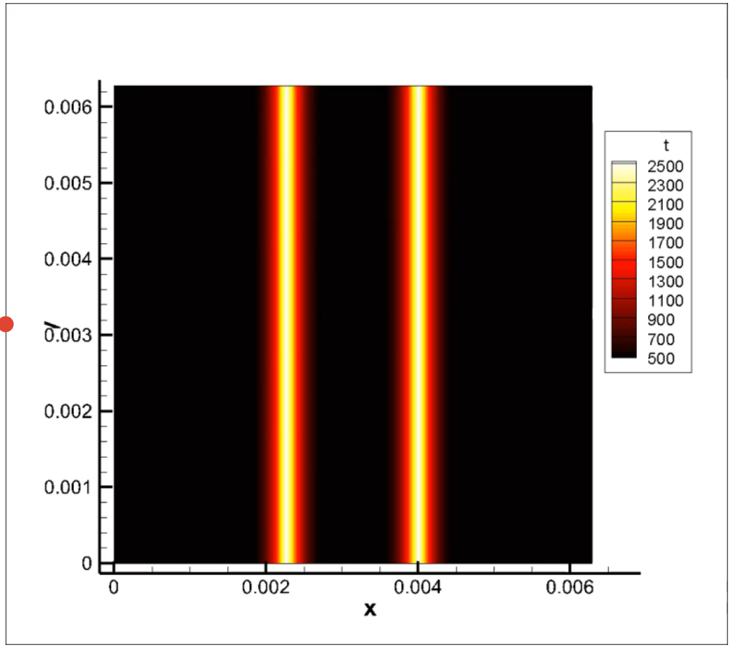


ASTR 2

- **High-speed, complex geometry, multi-physics problems**
- Compressible flow solver
- High-order FDM
- Structured mesh

✓ Object-oriented FORTRAN
✓ User-defined transport equations (5+x equations)
✓ Parallel HDF5 I/O
✓ Crash control
✓ Fully compact
❖ Immersed boundary
❖ Chemical reaction
❖ Machine-learning model
○ Method of Moment
○ Multi-block mesh
○ Adaptive mesh refinement

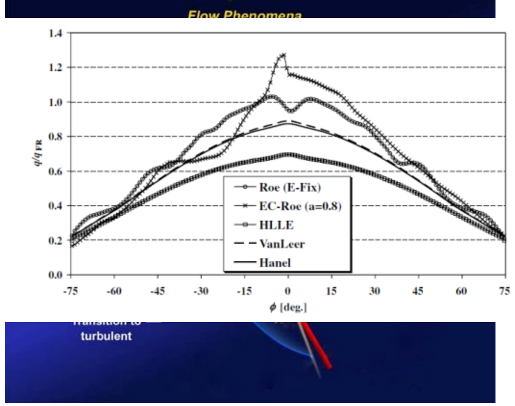


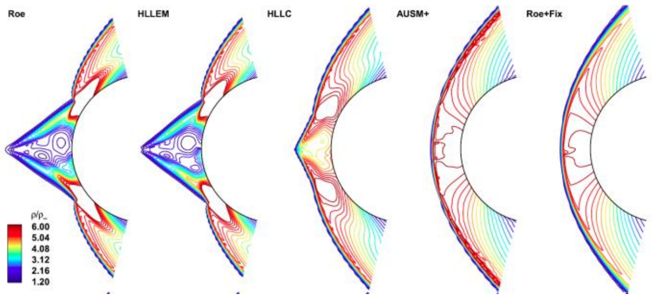


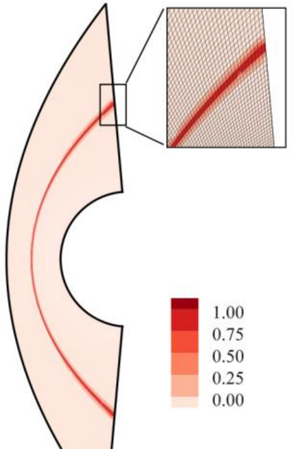
✓ Fully implemented & tested
❖ Partly Implemented
○ Plan to do

Hypersonic flow over blunt body

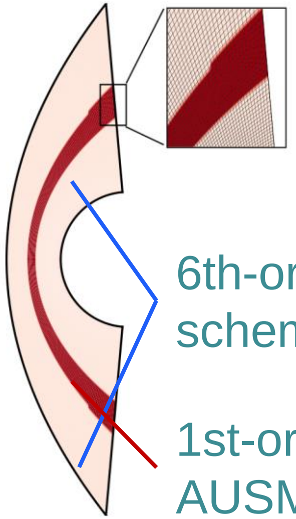
The carbuncle phenomenon





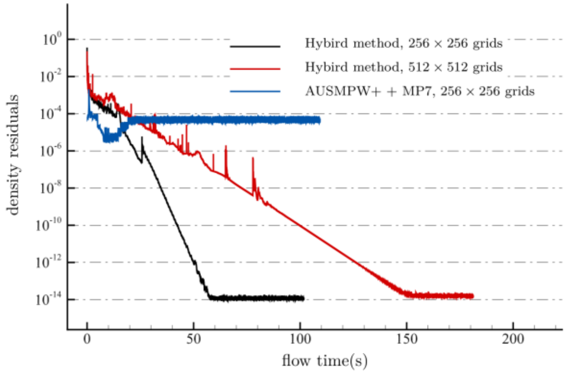


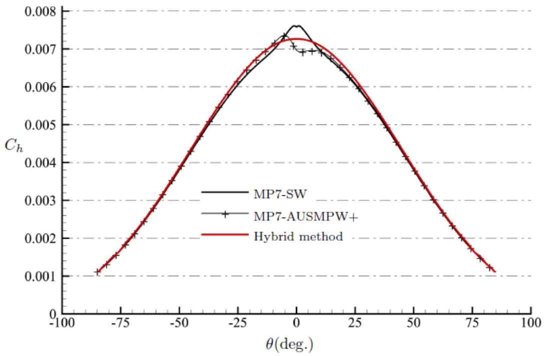
Shock sensor



6th-order central scheme

1st-order AUSMPW+ scheme

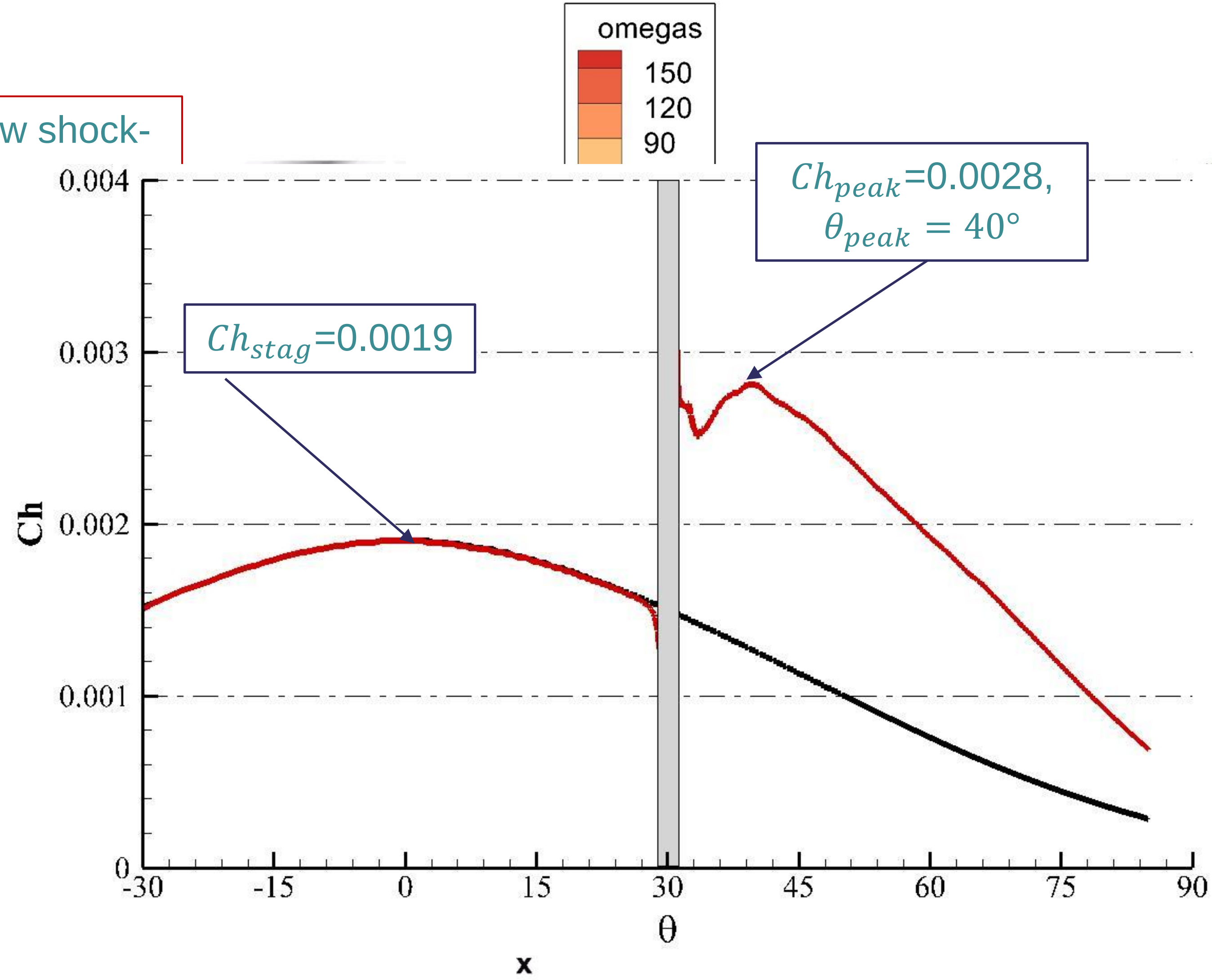


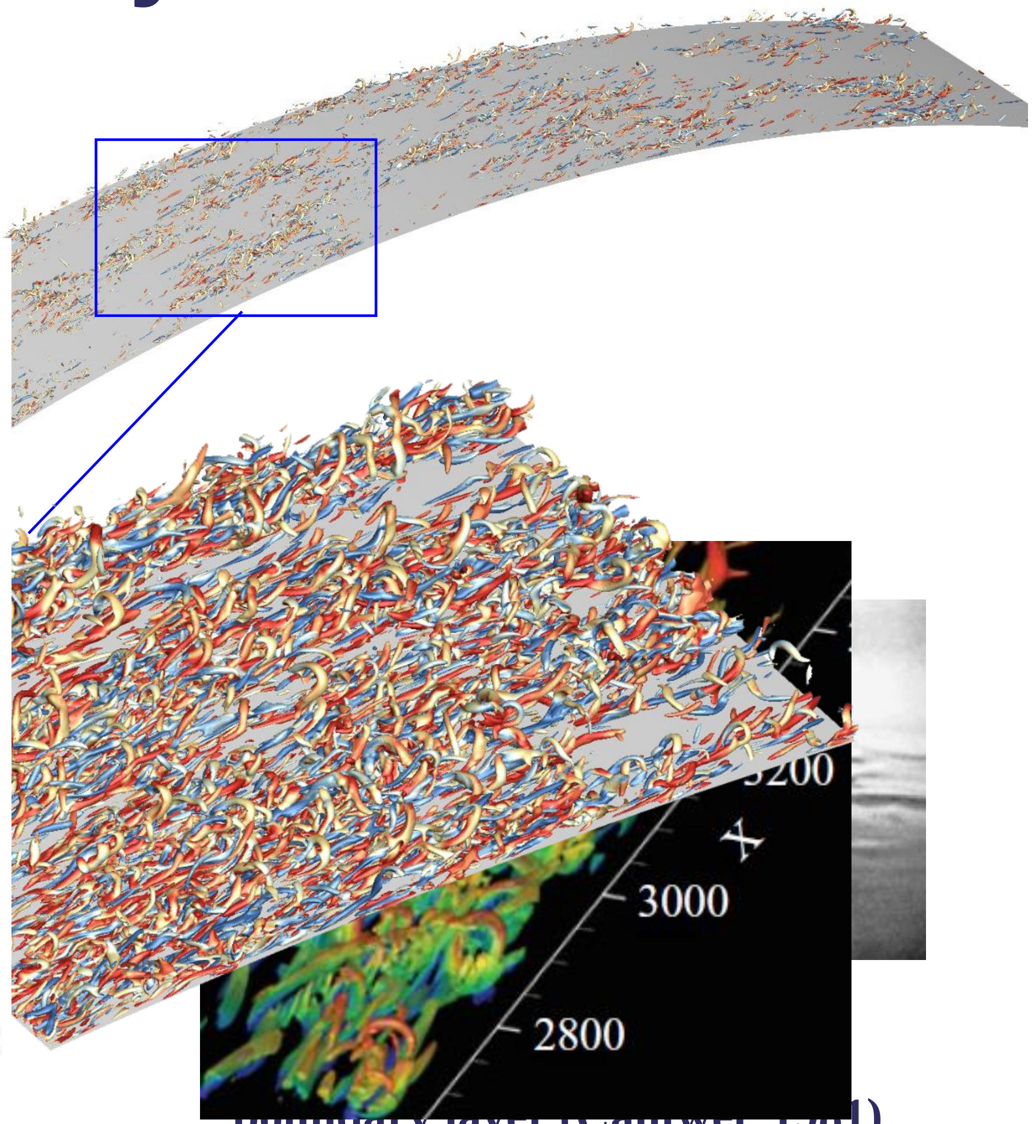


Science and Technology Facilities Council

Hypersonic flow over blunt body

Bow shock-

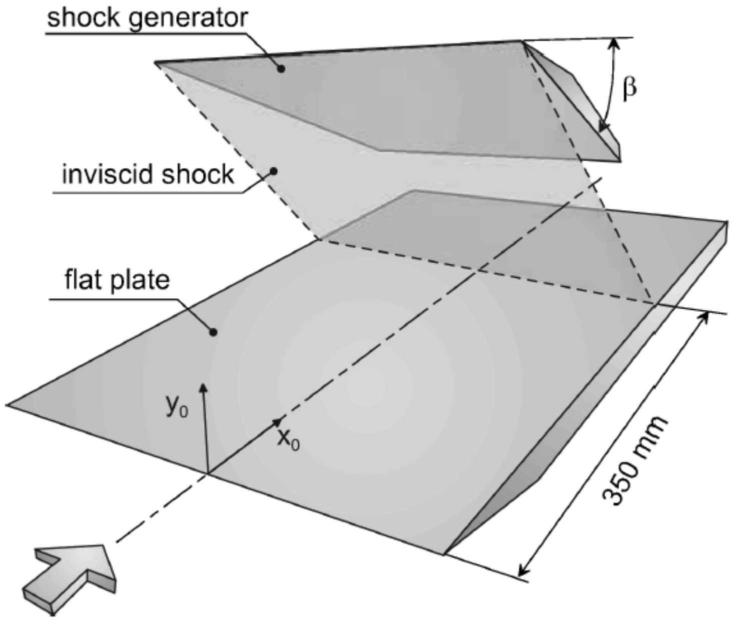


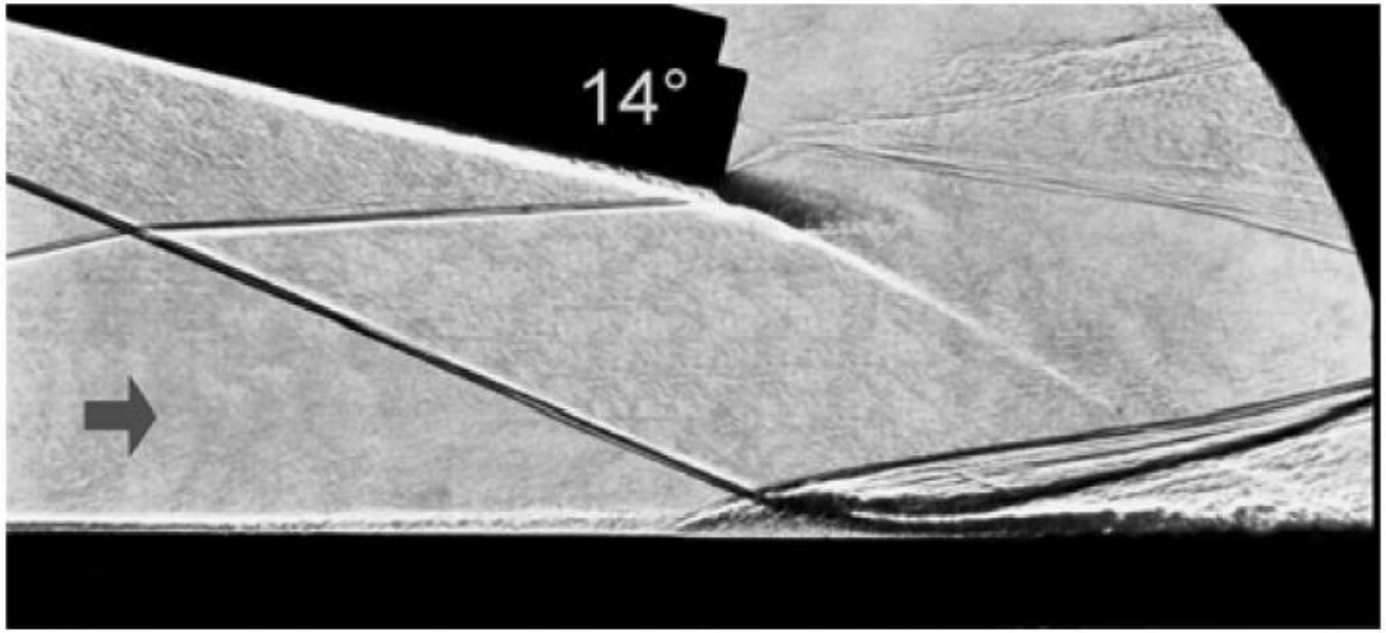


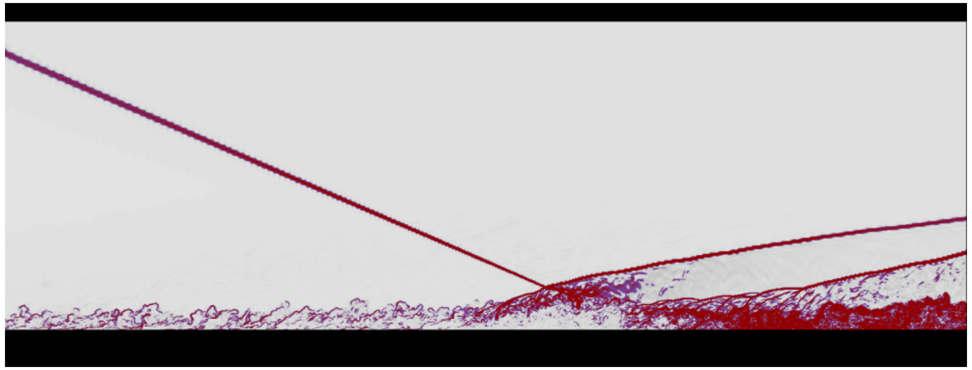
boundary layer (Cantwell, 1981).

Horseshoe vortex in a incompressible turbulent BL (Wu & Moin 2009)

Hypersonic SWTBLI

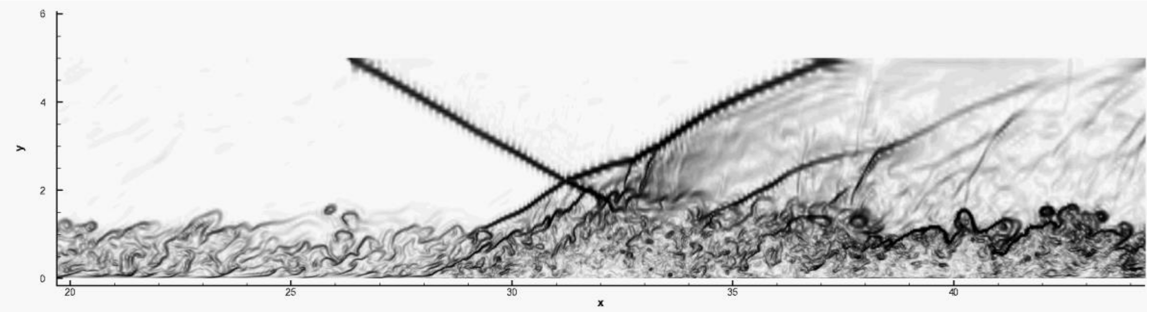




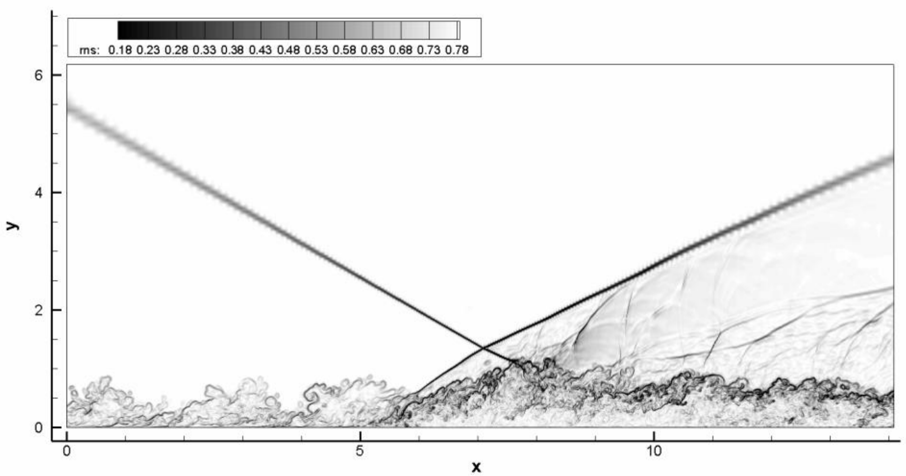


- Ma=5, Re_δ =71,566
- β =14°, α=23.3°, T_s=62.5k, T_w=5.24645T_s,
- Computational Domain size: 65δ×20δ×4δ
- Mesh: 1450×260×256
- CFD solver: ASTR 2, MP7-LD+CC6+RK3
- Experiment data from Schülein (2006)
  - Ma=5, Re_δ =173,900

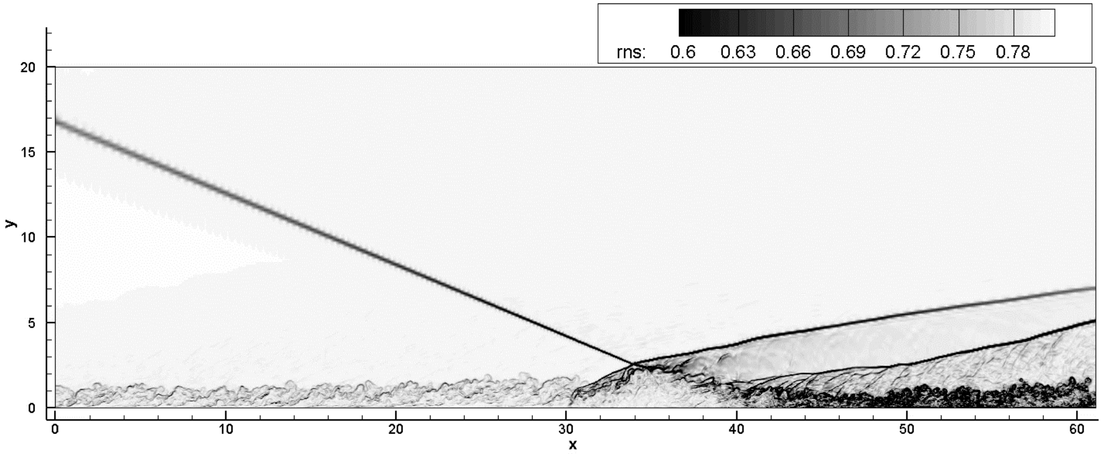
Hypersonic SWTBLI

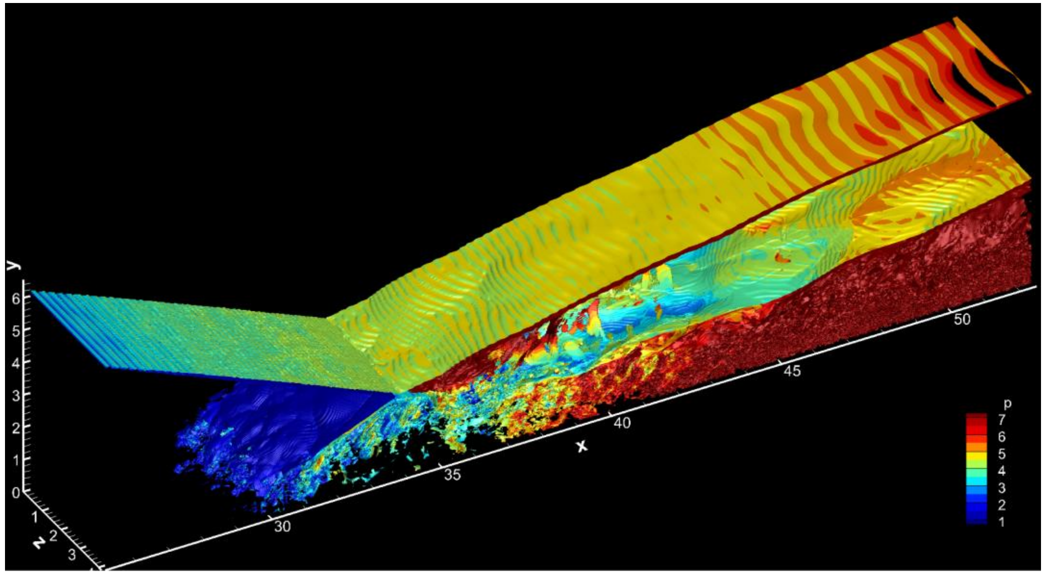


Ma=2.25, α=33.2°



Ma=3, α=33°

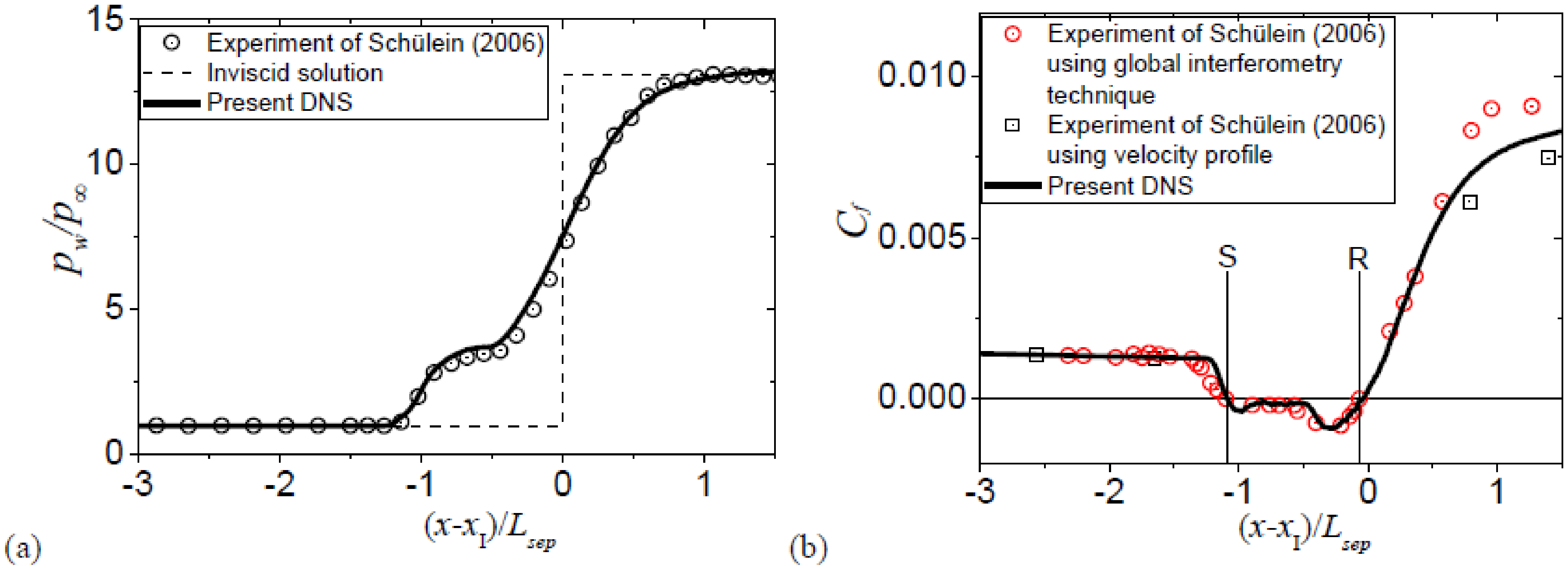




Facilities Council

Ma=5, α=23.3°

Hypersonic SWTBLI



Science and Technology Facilities Council

Summary

- We have conducted a systematic research focused on high-speed flows:
  - from the derivation of numerical scheme to the development of CFD code
  - from the study of fundamental fluid mechanics to the development of engineering models.
- The outcomes have shown some positive impacts to research communities and aerospace industries.

- There is a current clear push for hypersonic in the UK, as shown by the National Space strategy recently released by the government, and the opening of the new North West Space Cluster this May
  - there are a clear opportunities for us to develop further some of our activities

Science and Technology Facilities Council