Direct Numerical Simulation (DNS) of High-Speed Flows using Graphics Processing Units (GPUs)

CfH Seminar

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  - Objectives
  - Flow solver (Spatz)
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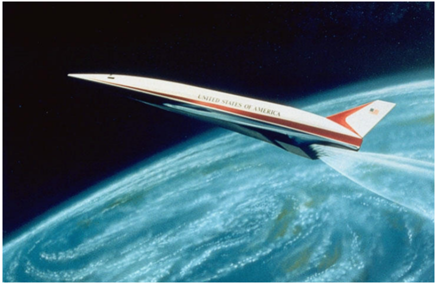
- Flat plate investigations

Motivation



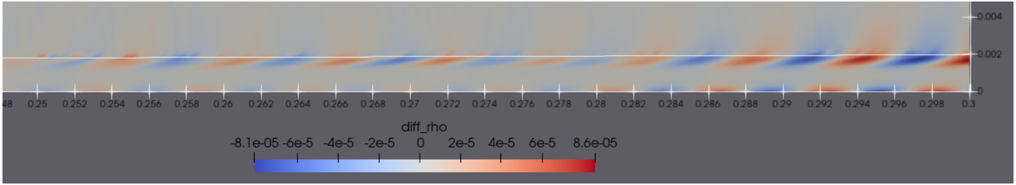
Source: *https://thehighfrontier.blog/2016/01/02/reagans-impossible-dream-the-x-30-national-aerospace-plane/*

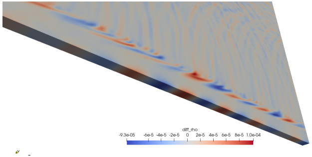
- Predicting transition on hypersonic vehicles one of key challenges in their design
- Transition prediction directly influences estimate of aerodynamic heating and drag
- For National Aerospace Plane (NASP) payload-to-gross-weight ratio nearly doubled depending on how optimistic or conservative predictions of transition were made

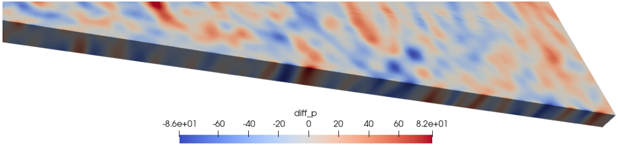
Motivation

- Compared to Reynolds-averaged Navier-Stokes (RANS) and Large Eddy Simulations (LES), direct numerical simulation (DNS) most computationally expensive turbulence simulation technique, but gives highest physical fidelity
- Approach to manage large computational cost of DNS is to improve computational efficiency
  - algorithm enhancement
  - hardware advancement
- Find and develop fluid algorithms best suited to new hardware accelerators
- Graphics Processing Units (GPUs) as hardware accelerators
- Current Literature on DNS on GPUs shows promising speed-ups for certain problem sizes and suitable algorithms
- GPUs dominant choice amongst high performance compute systems across the world

Transition investigation on a flat plate







Flow solver development - Proof-of-concept

Is there a performance benefit for GPUs compared to CPUs for compressible flow simulations?

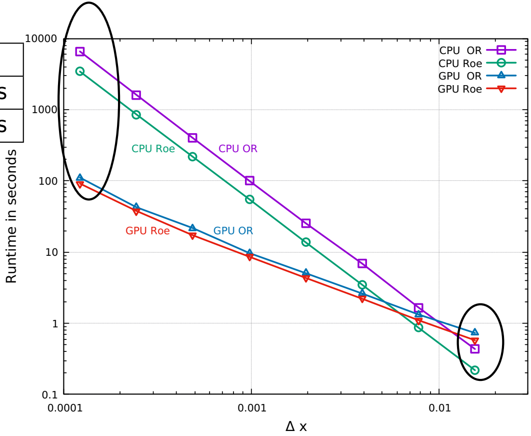
Strategy: Build 1D flow solver and test with two flux calculators on both architectures

8192 cells:

	GPU	CPU
OR	111.01s	6558.33s
Roe	91.33s	3424.68s

Speed-up: 59.1 OR

Speed-up: 37.5 Roe



64 cells:

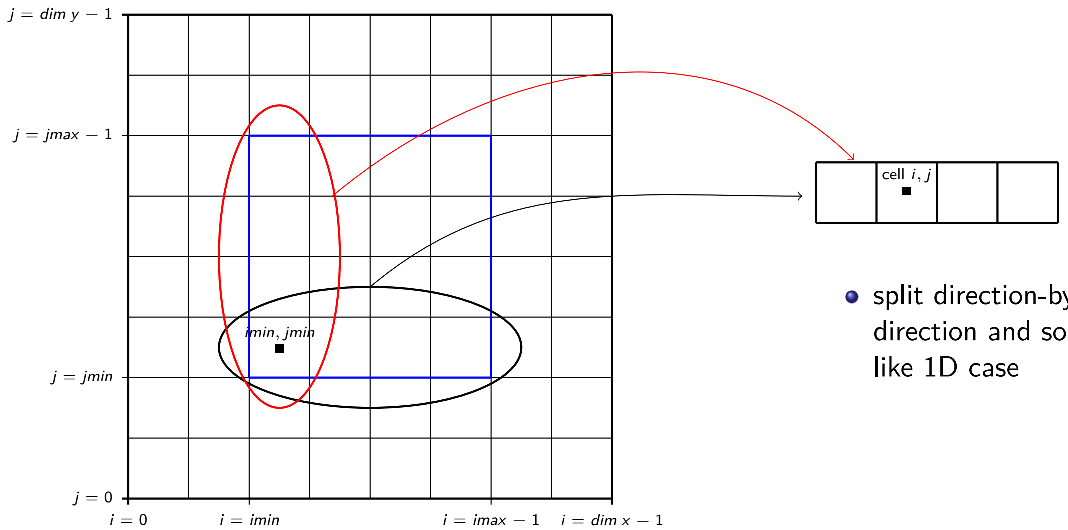
	GPU	CPU
OR	0.73s	0.43s
Roe	0.58s	0.22s

Flow solver development - Objectives

Goals

- Speed-up DNS with GPUs
  - Extend 1D code to 2D/3D on CPU and GPU
  - Test and verify 2D solver
  - Test and verify 3D solver
- Investigate flow physics underlying hypersonic transition
  - Apply GPU solver on heat flux case study

2D / 3D extension from 1D flow solver

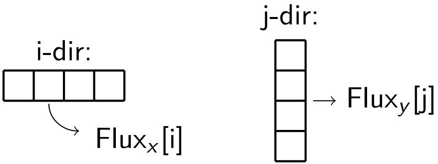


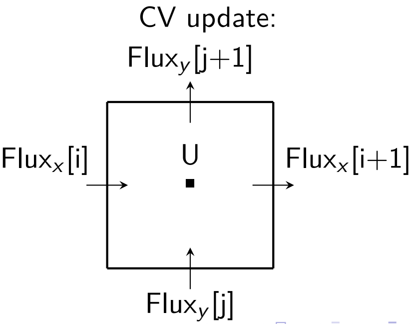
- split direction-by-direction and solve like 1D case

Algorithm

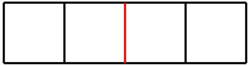
CPU Code

- Initialisation (Flow states in cells)
- Start time loop
  - i-dir:
    - Flux calculation
  - j-dir:
    - Transform to local frame
    - Flux calculation
    - Transform to global frame
  - Conserved quantities update
  - Cell average flow properties update
    - Output
- End time loop



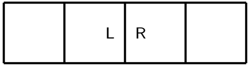


Flux calculators in Spatz



Reconstruction - Evolution:

- Approximate Osher-type Riemann (OR) solver
- Roe flux solver



Flux-Solver(L,R) $\rightarrow$ Flux over Face

Flux - Reconstruction:

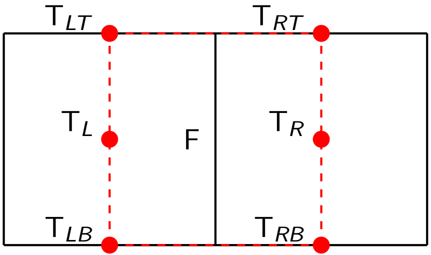
- Summation-by-parts Alpha-Splitting-Flux (SBP-ASF)

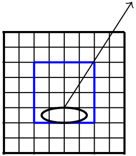
(*Direct numerical simulations of instabilities in the entropy layer of a hypersonic blunted slender cone*, Whyborn, L., 2023)

Flux-Solver(□□□□) $\rightarrow$ Flux over Face

Viscous Flow

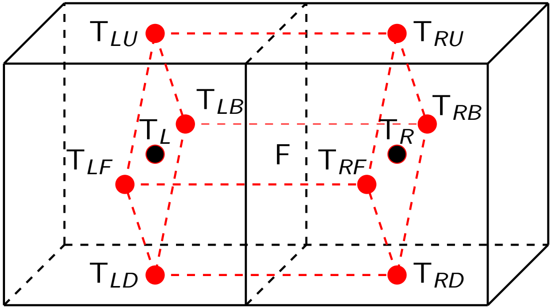
2D viscous flux stencil in x-direction:





$$\frac{\partial T}{\partial x} = \frac{T_{R-av} - T_{L-av}}{dx}$$

3D viscous flux stencil in x-direction:



$$\frac{\partial T}{\partial x} = \frac{T_{R-av} - T_{L-av}}{dx}$$

Divergence theorem: $\int_C F \hat{n} \mathrm{d}S = \iint_R divF \mathrm{d}A$

Adjustments for GPU implementation

CPU Code (Host)

- Initialisation (Flow states in cells)
- Memory allocation on GPU
- Data transfer to GPU
- Start time loop
    - Data transfer from GPU
    - Output
- End time loop
- Free GPU memory

GPU Code (Device)

- Boundary condition
- Flux calculation
- Conserved quantities update
- Cell average flow properties update

Verification cases

2D

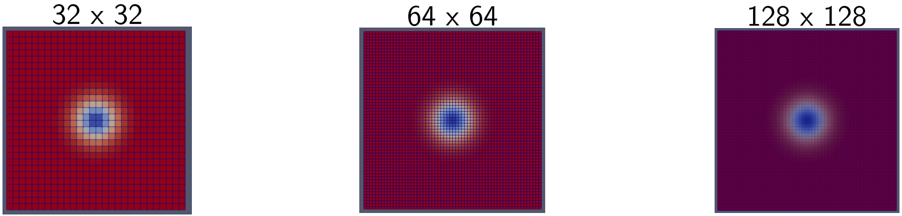
- Isentropic Vortex
- Method of Manufactured solutions (MMS)
  - inviscid
  - viscous
- Self-similar laminar boundary-layer

3D

- Method of Manufactured solutions (MMS)
  - inviscid
  - viscous

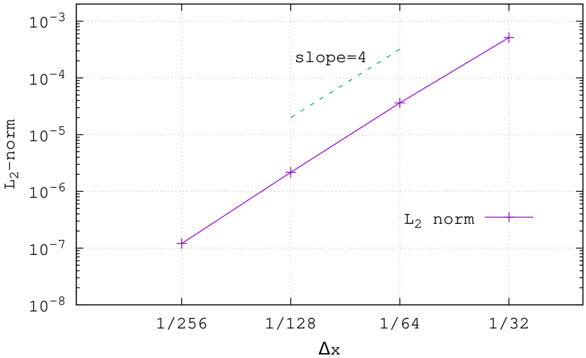
Verification - Isentropic Vortex

Simulation of one period



- Simulation of 1 period

Isentropic Vortex - L_2 Norm and Accuracy



$$L_2 = \sqrt{\frac{\sum_{i=0}^{N}[exact(i) - solver(i)]^2}{N}}$$

$$p = LOG(L_{k+1}/L_k)/log(r)$$

Figure: L_2-norm density and orders of accuracy p

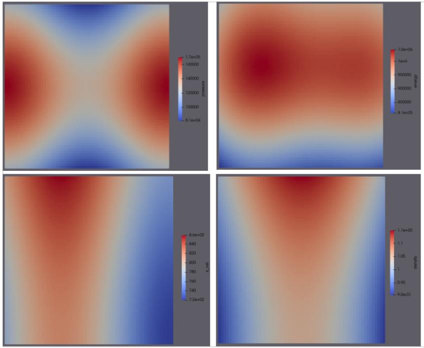
Verification - Method of Manufactured solutions (MMS)

Process

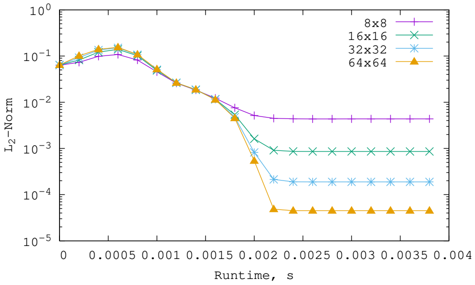
- define analytic solution
- generate source terms using governing equations
- boundary conditions: manufactured solution
- perform simulations with varying grid sizes and compare to exact solution

2D Method of Manufactured solutions (MMS) - inviscid

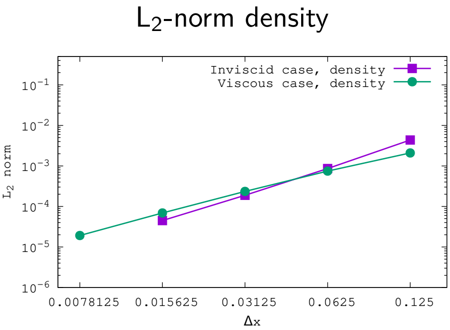
Simulation results

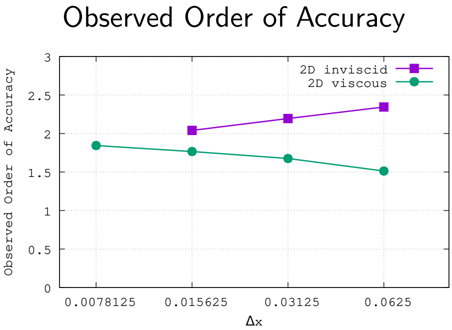


Convergence history - density



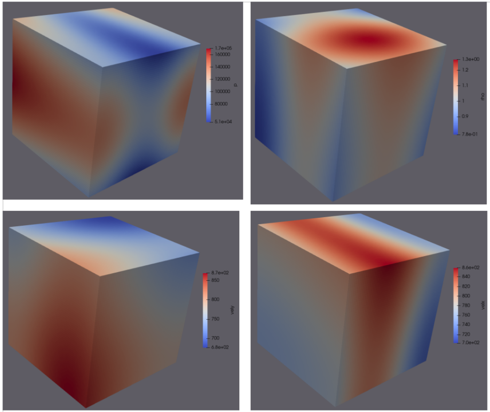
2D Method of Manufactured solutions (MMS) - results



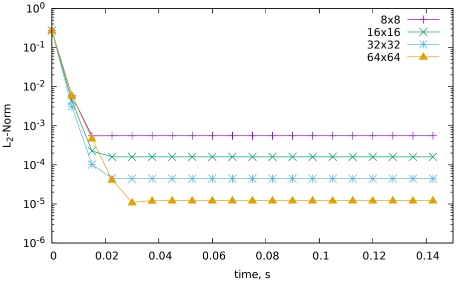


3D Method of Manufactured solutions (MMS) - viscous

Simulation results (viscous)

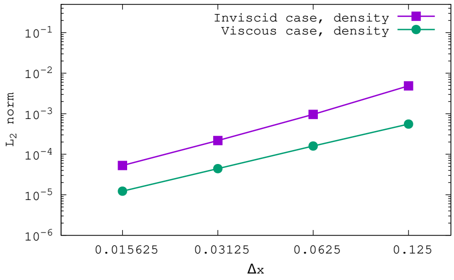


Convergence history - density

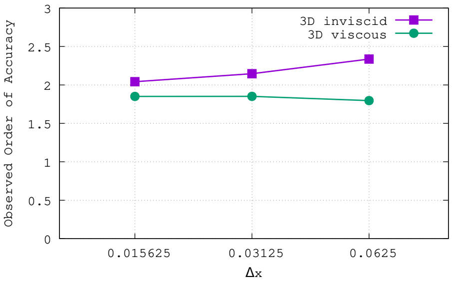


3D Method of Manufactured solutions (MMS) - results

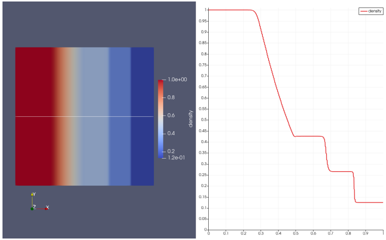
L$_2$-norm density

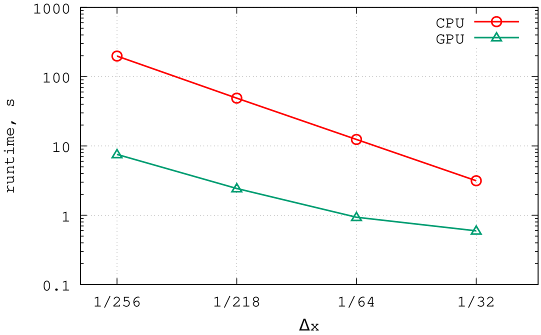


Observed Order of Accuracy



2D Sod's shock tube on CPU (Intel Core i7-4790) and GPU (NVIDIA GeForce GTX 1070)

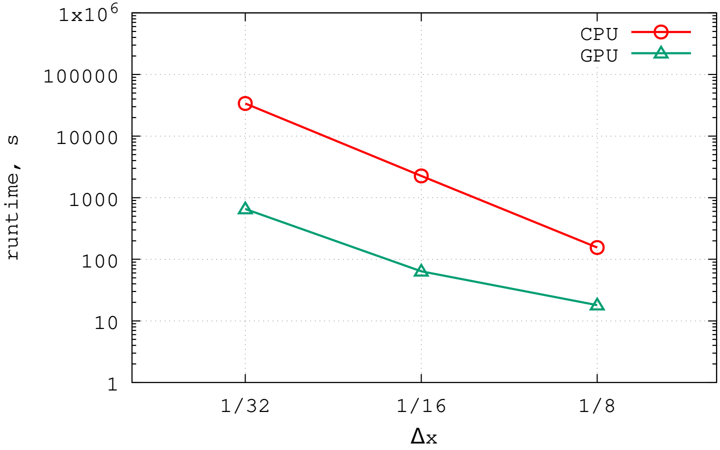




GPU speed up: 26.3

Performance: 3D run-time comparison viscous flow

3D viscous MMS on CPU (Intel Core i7-4790) and GPU (NVIDIA GeForce GTX 1070)

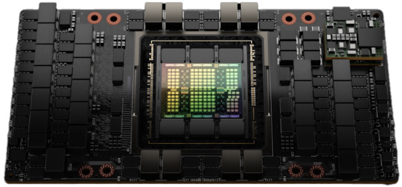


GPU speed up: 51.7

Case study - Hardware

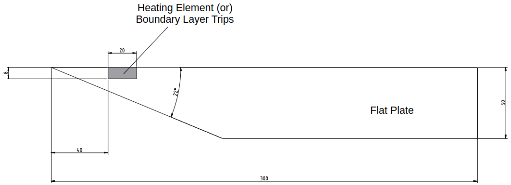
Bunya - HPC at UQ

- NVIDIA H100 GPU
- 7 H100 nodes with 3 H100 cards each
- each H100 has 80GB of GPU RAM
- nodes have 2TB of CPU RAM



NVIDIA H100 GPU
Source: *https://resources.nvidia.com/en-us-tensor-core/gtc22-whitepaper-hopper?ncid=no-ncid*

Case study - Flat plate hypersonic transition



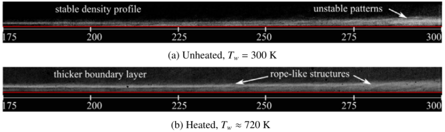


Fig. 18. Flat plate schlieren - Mach 7 enthalpy, $Re_u = 5.06 \times 10^6$ 1/m.

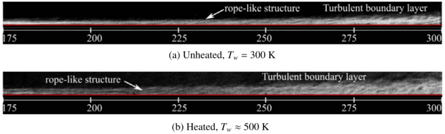


Fig. 19. Flat plate schlieren - Mach 5.5 enthalpy, $Re_u = 9.58 \times 10^6$ 1/m.

Source: *Electrically-heated flat plate testing in a free-piston driven shock tunnel* Chang, E.W.K., Chan, W.Y.K., Hopkins, K.J., McIntyre, T.J. and Veeraragavan, A. (2020)

Case study - Flow properties

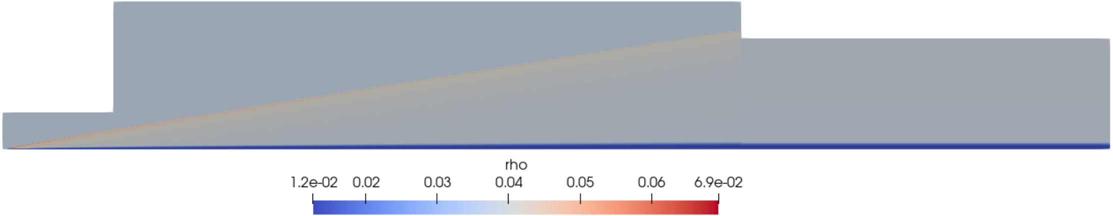
Flow properties according to T4 experiments by Eric Chang

Flow parameter	**M 7 enthalpy**	**M 5.5 enthalpy**
Pressure	2624	2649
Velocity	2221	1857
Temperature	250	162
Mach	7	7.3
Re_{unit}(/m)	5.06e+06	9.58e+06

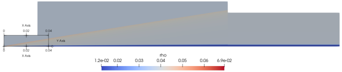
Source: *Electrically-heated flat plate testing in a free-piston driven shock tunnel* Chang, E.W.K., Chan, W.Y.K., Hopkins, K.J., McIntyre, T.J. and Veeraragavan, A. (2020)

Case study - Flow field

Flat plate simulation - stages



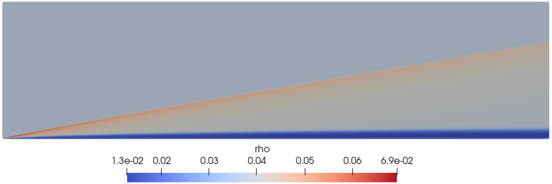
- Stage 0: x: 0-40mm, y: 10mm
- Stage 1: x: 30-200mm, y: 40mm
- Stage 2: x: 175-300mm, y: 30mm



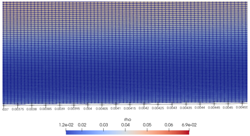
Boundaries

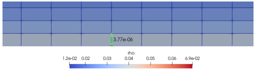
Outflow: linear extrapolation

Inflow: Free stream conditions



Outflow: linear extrapolation

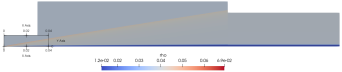




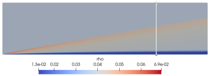
No-slip wall with fixed temperature

Number of cells in simulation: 2000 x 400

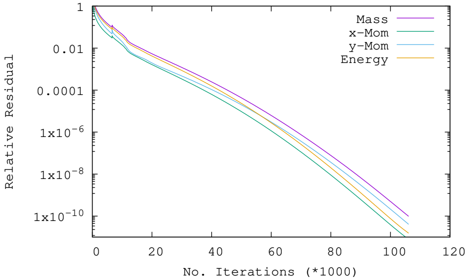
Case study - Stage 0 results

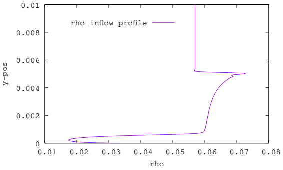


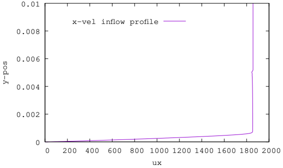
Obtained inflow profile at position x = 0.03m



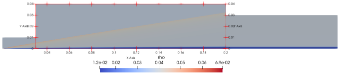
Convergence stage 0







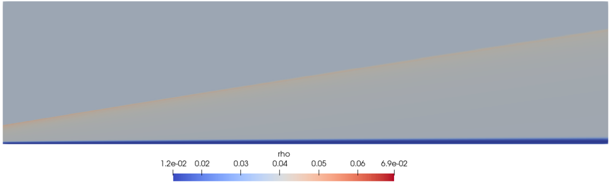
Wall-clock time: 00:47:43



Boundaries

Outflow: linear extrapolation

Inflow: Profile from stage 0

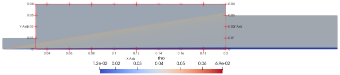


Outflow: linear extrapolation

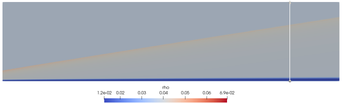
No-slip wall with fixed temperature

Number of cells in simulation: 2800 x 480

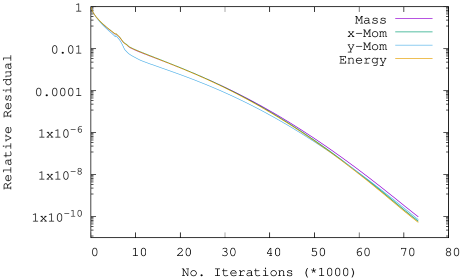
Case study - Stage 1 results

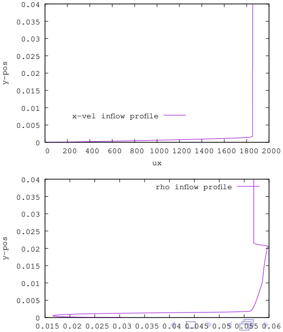


Obtained inflow profile at position $x = 0.175m$



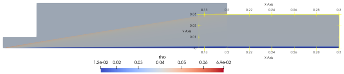
Convergence stage 1





Wall-clock time: 00:17:57

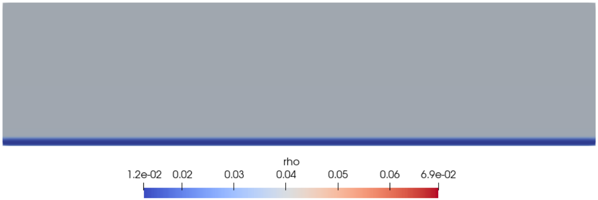
Case study - Stage 2 setup



Boundaries

Outflow: linear extrapolation

Inflow: Profile from stage 1



Outflow: linear extrapolation

No-slip wall with fixed temperature

Number of cells in simulation: 1800 x 540

Case study - Pressure disturbance

Pressure disturbance according to Johnston and Candler 2022: *Modal analysis of instabilities in the bolt-2 flowfield*:

$$p' = A(2R - 1)$$

$$\rho' = p' \frac{1}{\bar{a}_\infty^2}$$

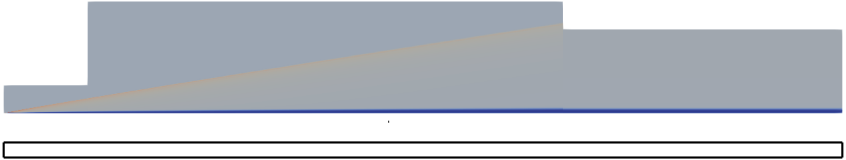
$$u_i' = p'$$

$$T' = p' \frac{(\gamma - 1)\bar{T}}{\bar{\rho}\bar{a}_\infty^2}$$

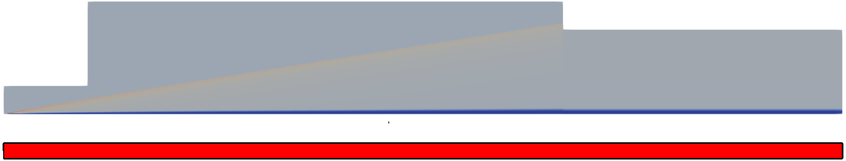
R: random number between 0 and 1, A: magnitude of white noise disturbance
In this case study (according to T4 white noise measured in experiments):
A = 0.7% of free stream pressure

Flat plate heating setups

unheated

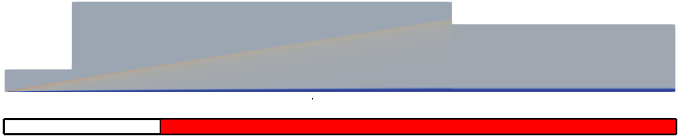


heated

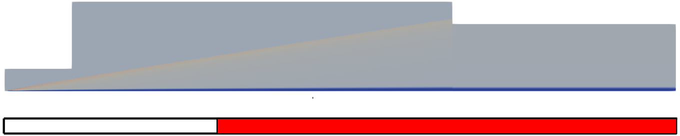


Flat plate heating setups

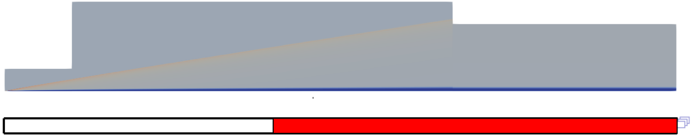
heated at 70mm



heated at 95mm

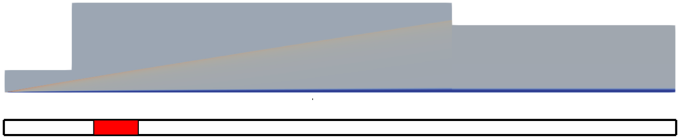


heated at 120mm

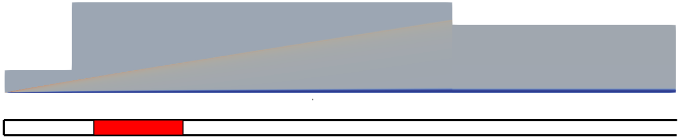


Flat plate heating setups

heated strip - 20mm wide at 40mm



heated strip - 40mm wide at 40mm



Schlieren results for Mach 7.3 case

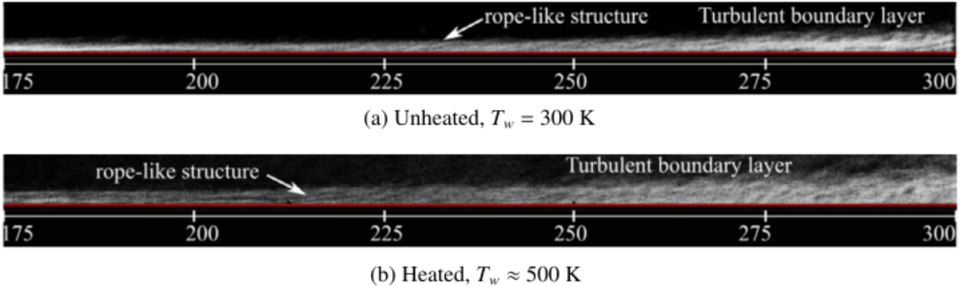
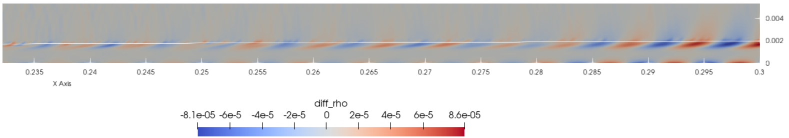


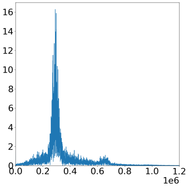
Fig. 19. Flat plate schlieren - Mach 5.5 enthalpy, $Re_u = 9.58 \times 10^6$ 1/m.

Source: *Electrically-heated flat plate testing in a free-piston driven shock tunnel* Chang, E.W.K., Chan, W.Y.K., Hopkins, K.J., McIntyre, T.J. and Veeraragavan, A. (2020)

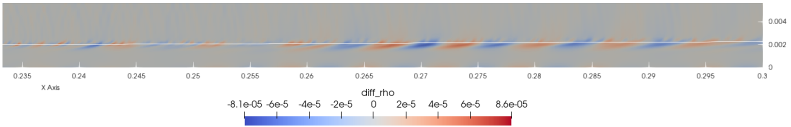
DNS results Mach 7.3 - unheated vs fully heated (500K)

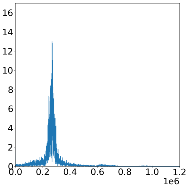
Simulation results for Mach 7.3 case





(a) Unheated flat plate ($T_w = 300$K)





(b) Heated flat plate ($T_w = 500$K)

Schlieren results for Mach 7 case

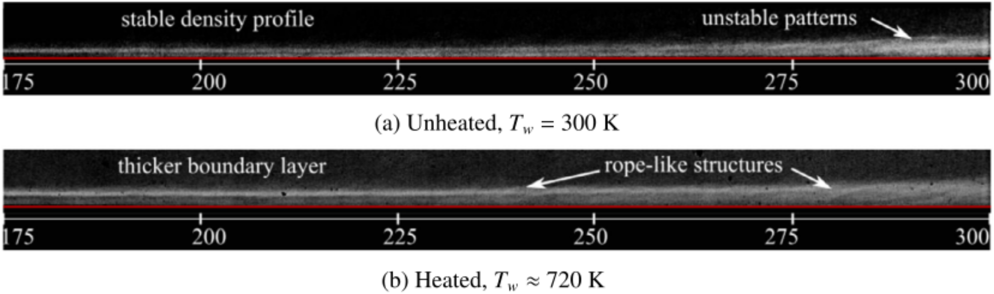
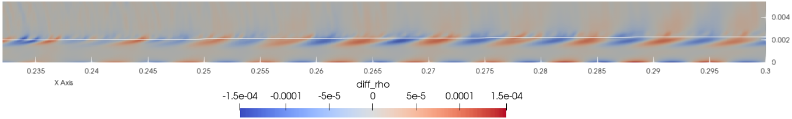


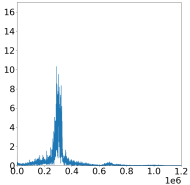
Fig. 18. Flat plate schlieren - Mach 7 enthalpy, $Re_u = 5.06 \times 10^6$ 1/m.

Source: *Electrically-heated flat plate testing in a free-piston driven shock tunnel* Chang, E.W.K., Chan, W.Y.K., Hopkins, K.J., McIntyre, T.J. and Veeraragavan, A. (2020)

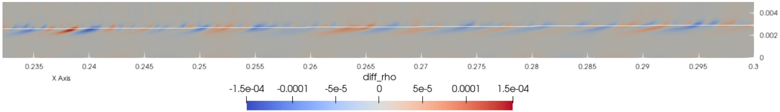
DNS results Mach 7 - unheated vs fully heated (825K)

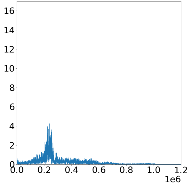
Simulation results for Mach 7 case





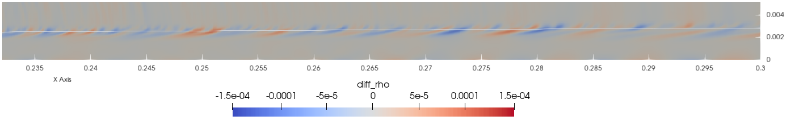
(a) Unheated flat plate ($T_w = 300$K)

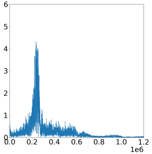




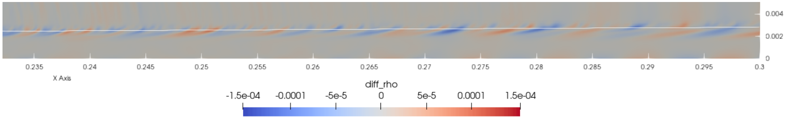
(b) Heated flat plate ($T_w = 825$K)

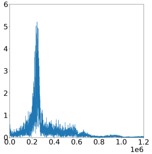
DNS results Mach 7 - partially heated (825K)



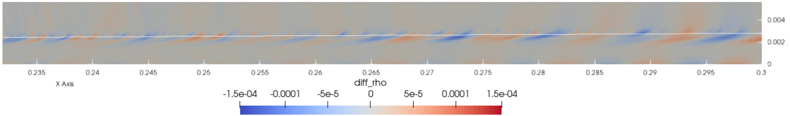


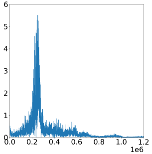
(a) Heated from 70 mm along flat plate



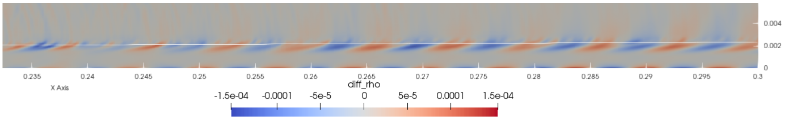


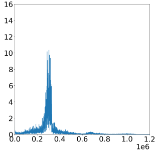
(b) Heated from 95 mm along flat plate



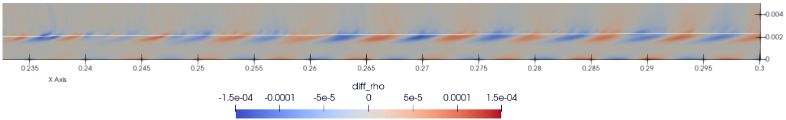


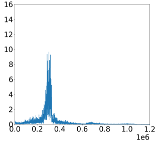
(b) Heated from 120 mm along flat plate





(a) Heated strip 20mm wide





(b) Heated strip 40mm wide

Summary

- GPU code developed
- Verification completed
- Single-GPU enough performance for transition investigation
- Application: unheated and heated flat plate