PyFR: Next-Generation High-Order Computational Fluid Dynamics on Many-Core Hardware

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24th June 2015

Our Motivation

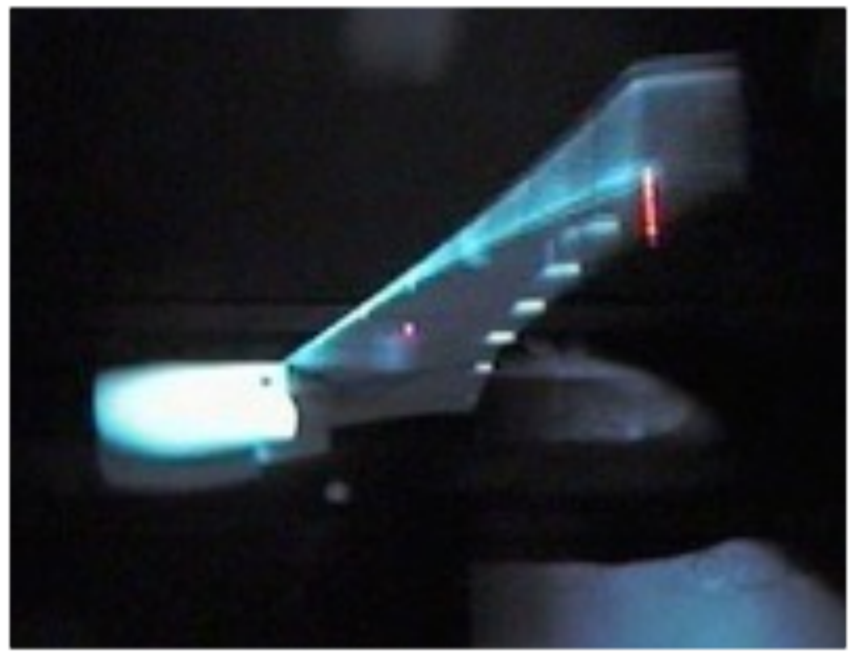
Our Motivation

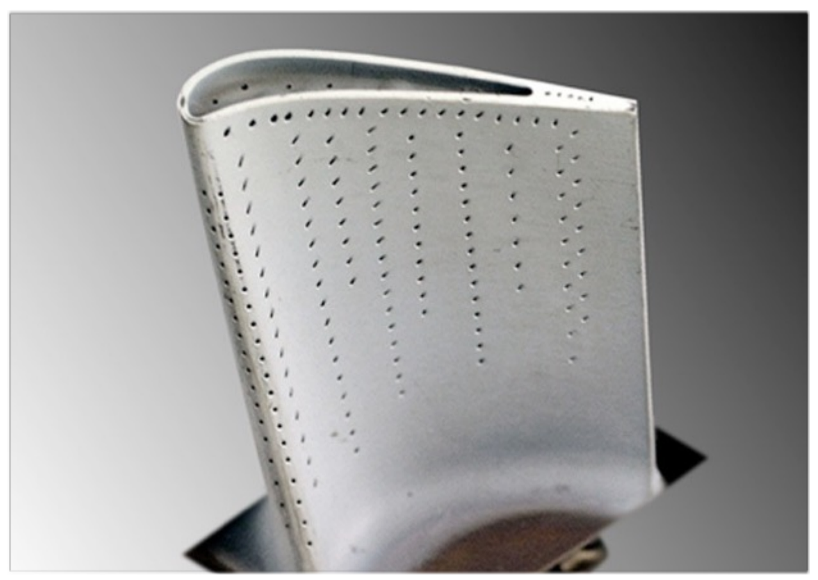
Current industry standard CFD tools have limited capabilities

Our Motivation

Technology is decades old and designed for solving steady flow problems (using RANS approach)

Our Motivation





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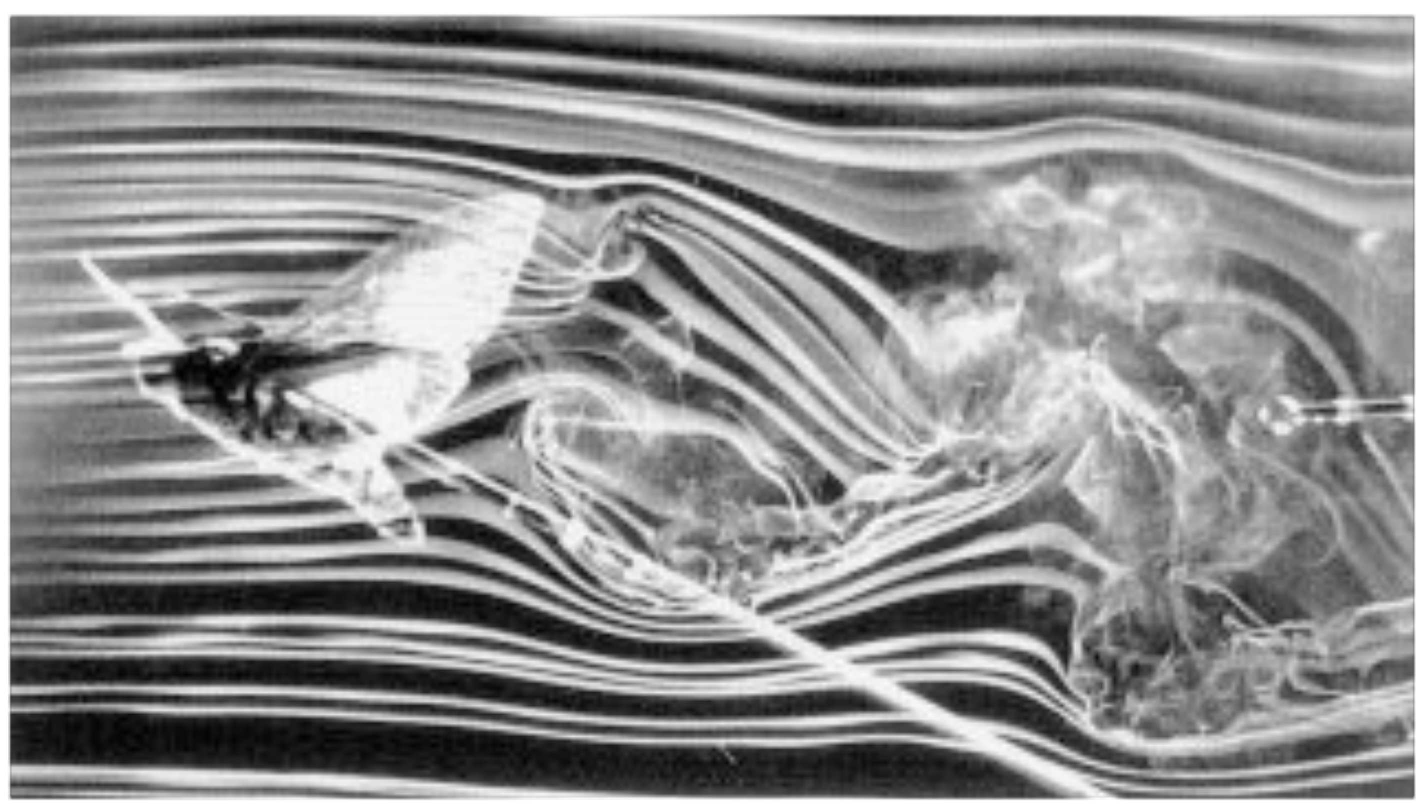
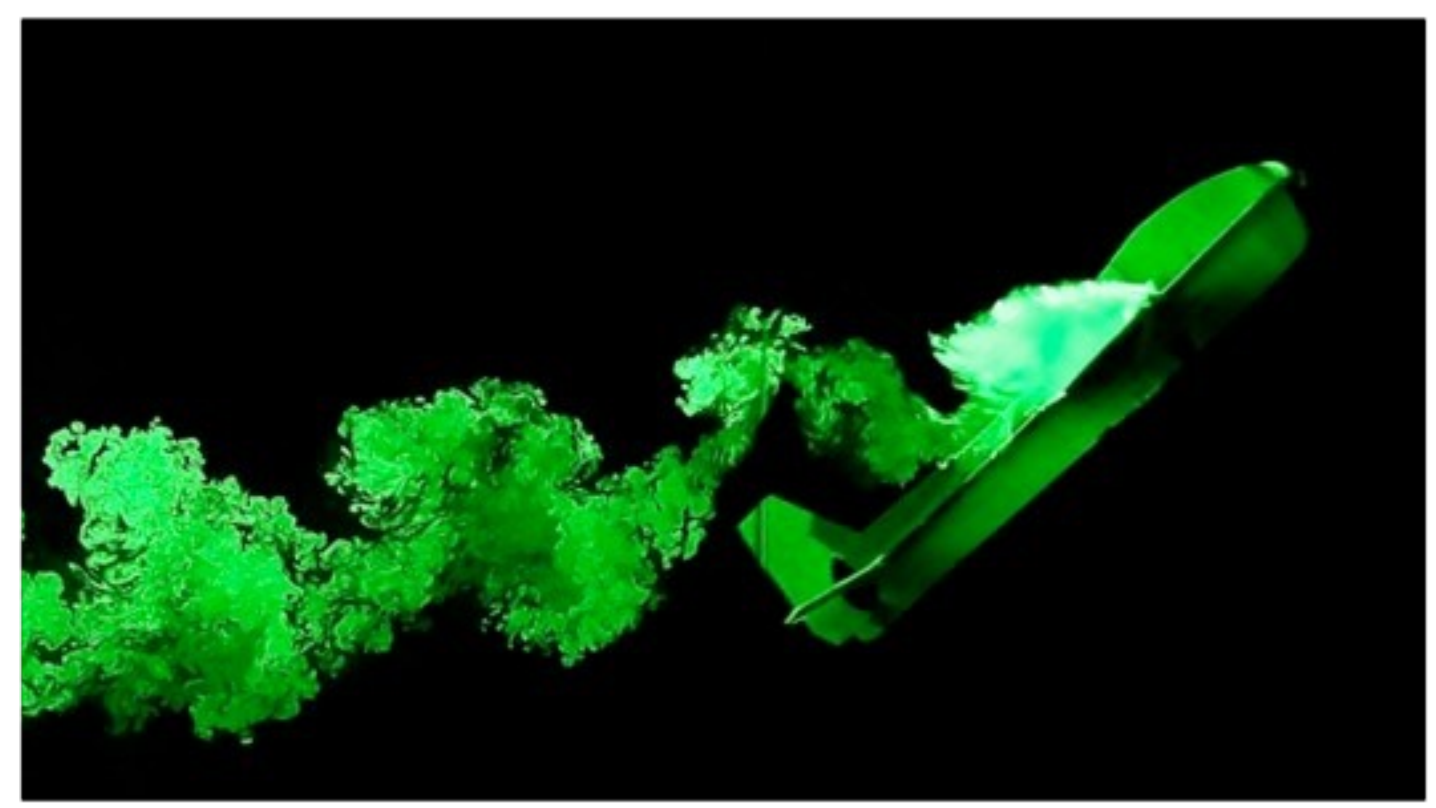
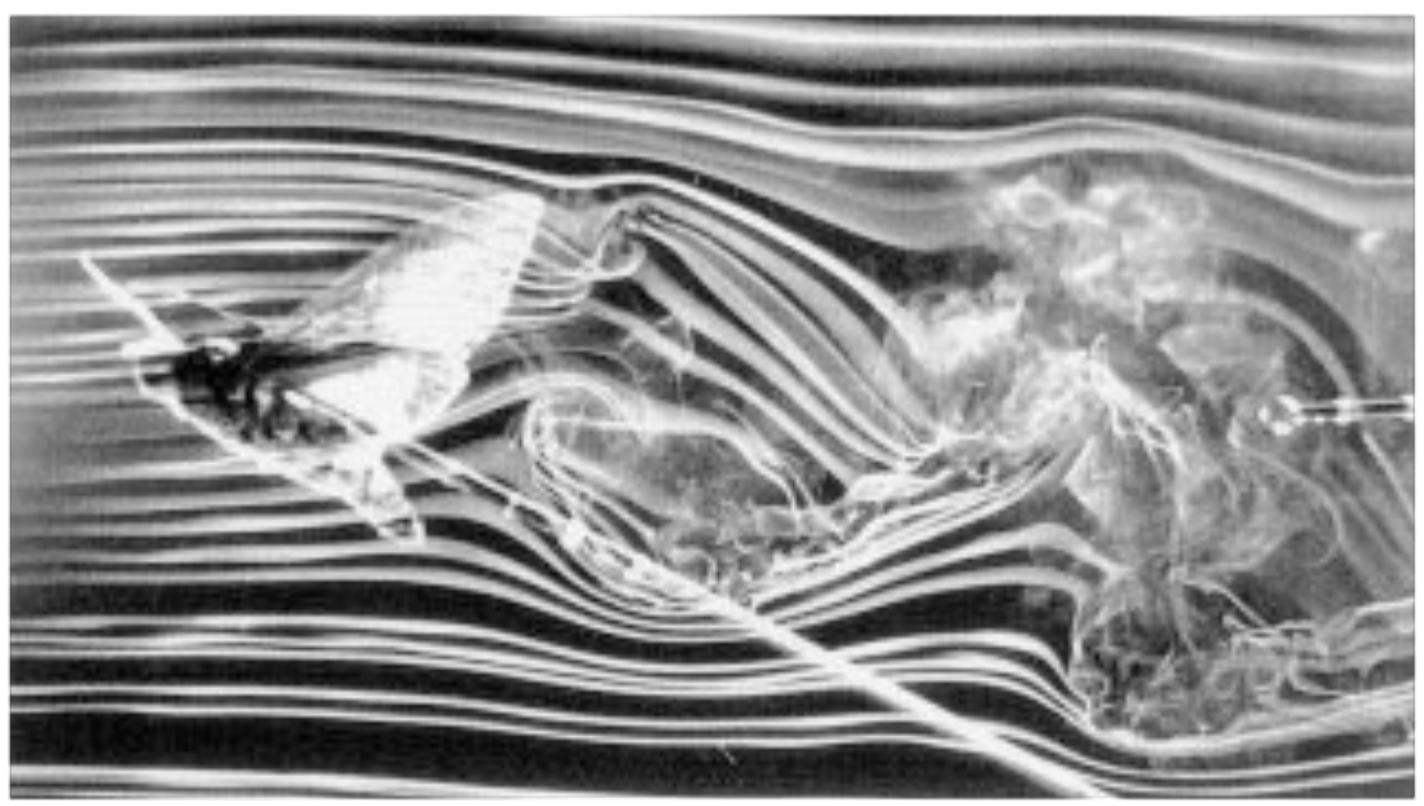
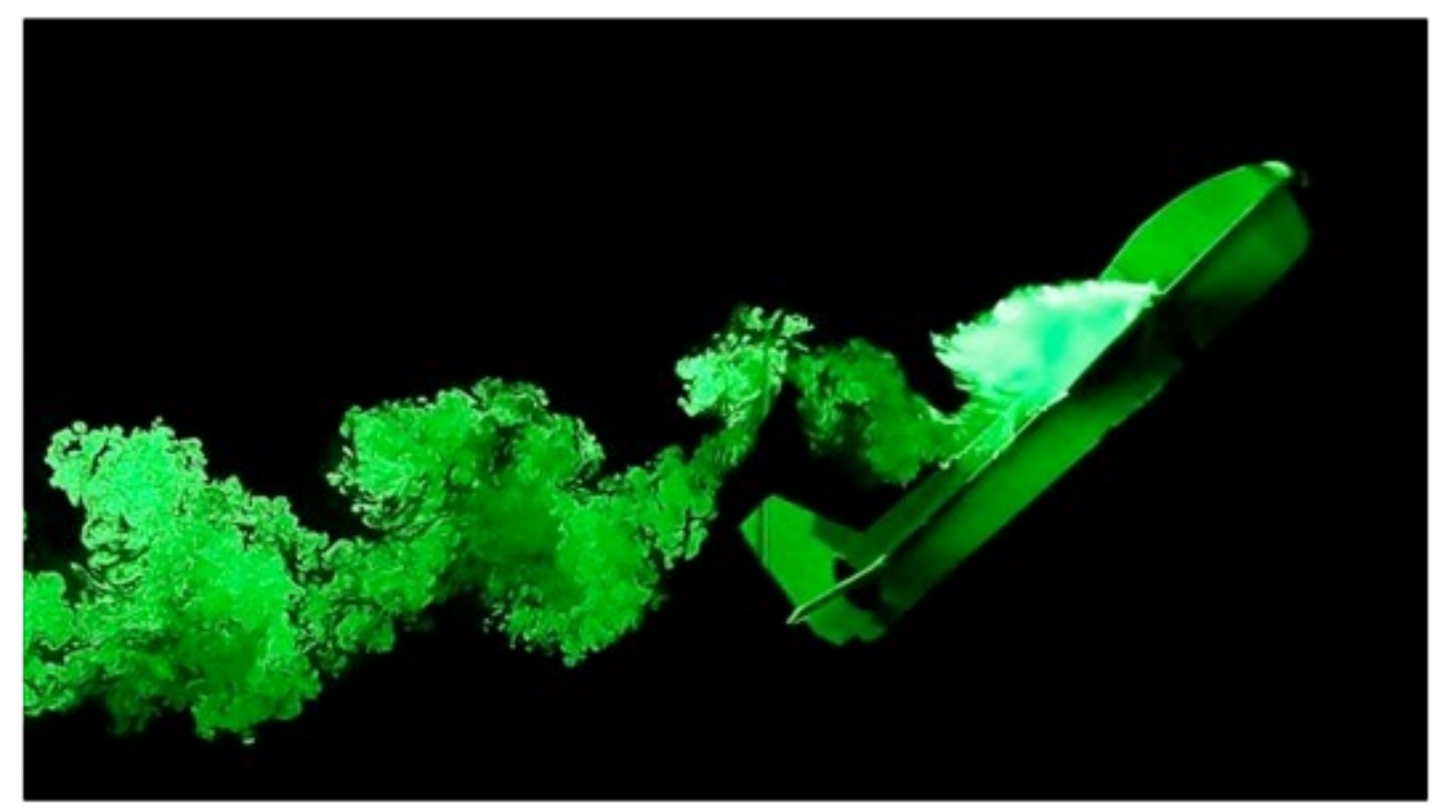




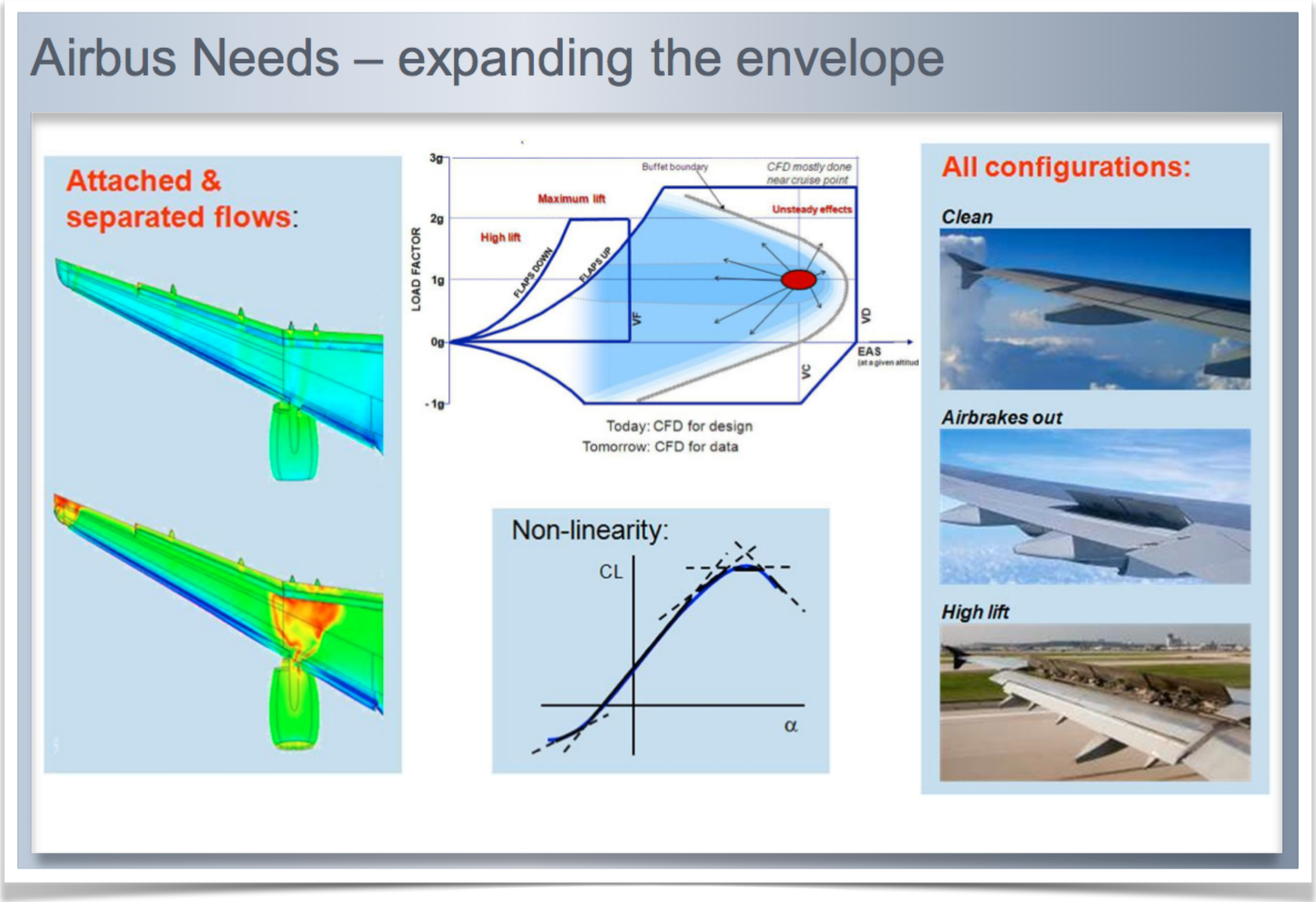
Our Motivation

Need to expand the 'industrial CFD envelope'





Our Motivation



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

Our Motivation

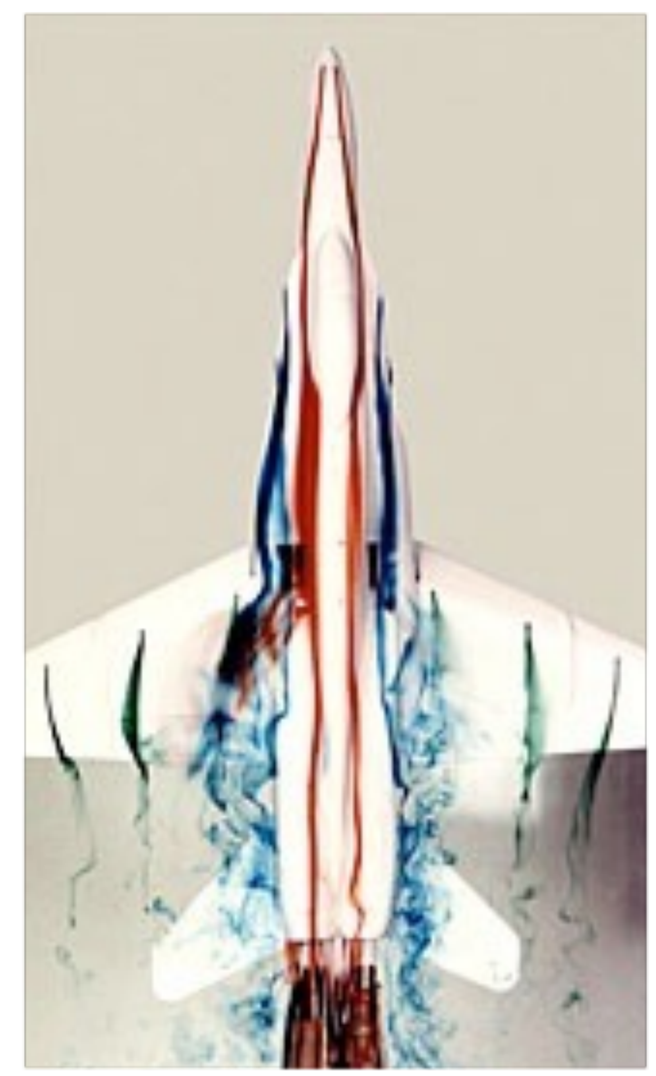
Flux Reconstruction

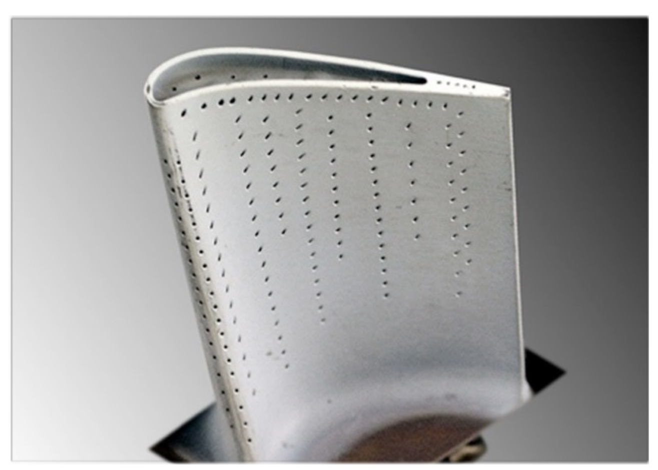
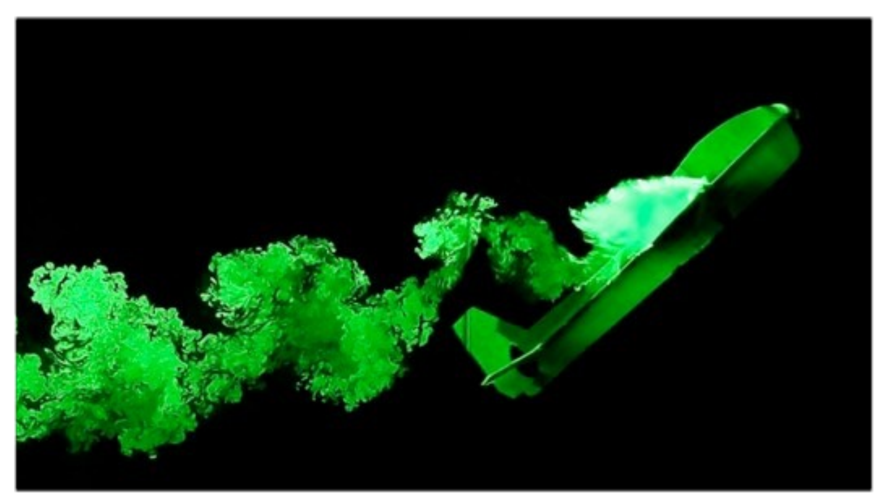
+

Modern Hardware







Flux Reconstruction

- Flux Reconstruction (FR) approach to high-order methods was first proposed by Huynh in 2007 [3]
- High-order accurate in space
- Works on unstructured grids

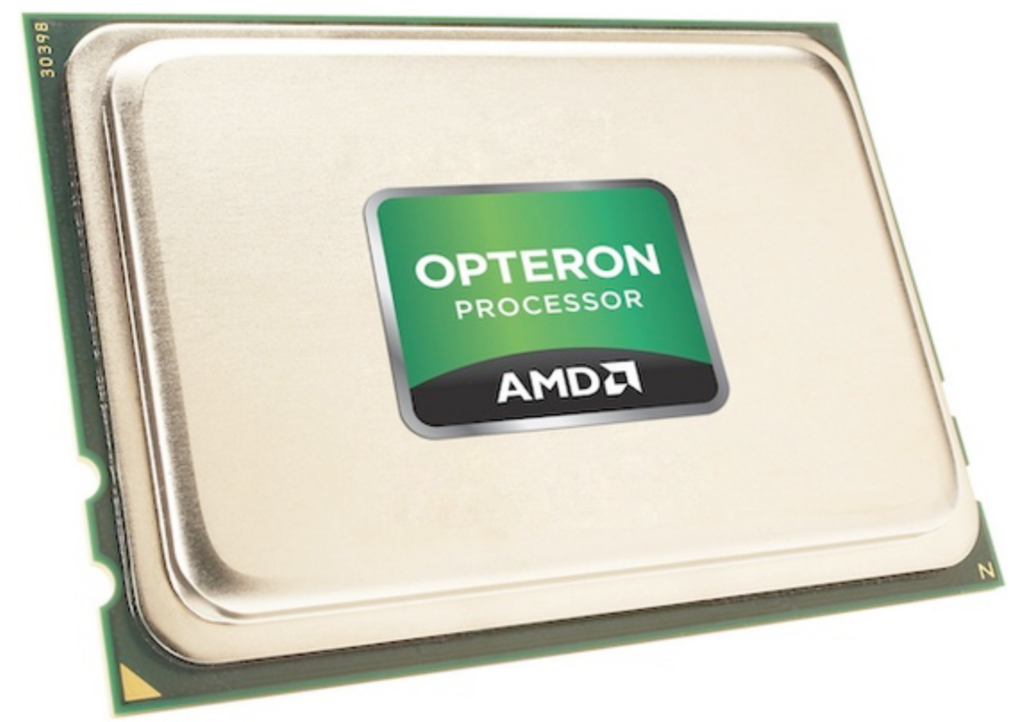
[3] H.T. Huynh. A Flux Reconstruction Approach to High-Order Schemes Including Discontinuous Galerkin Methods. AIAA Paper 2007-4079. 2007

Flux Reconstruction

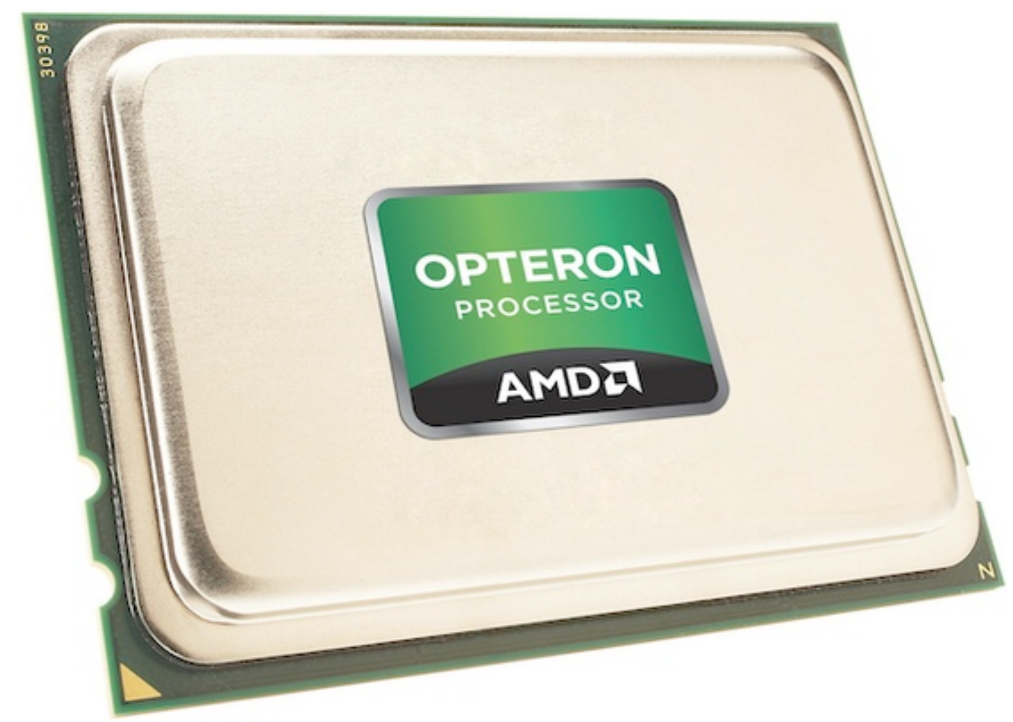
- So ...

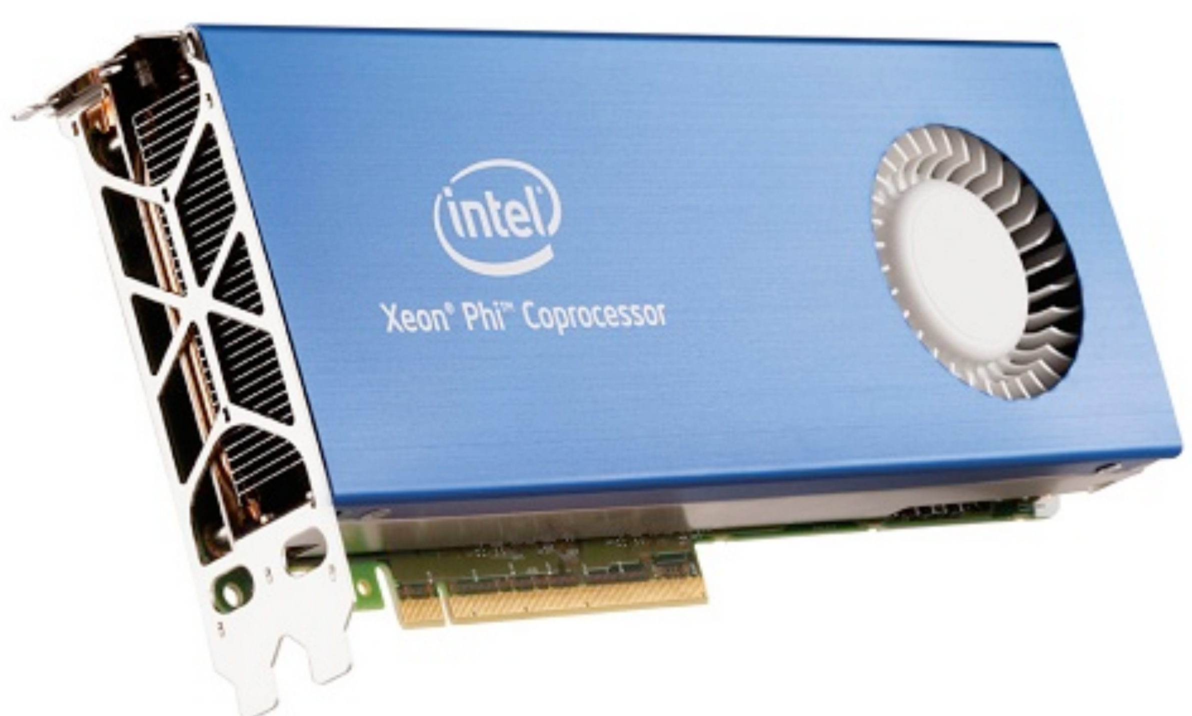
High Accuracy + Complex Geometry

Modern Hardware



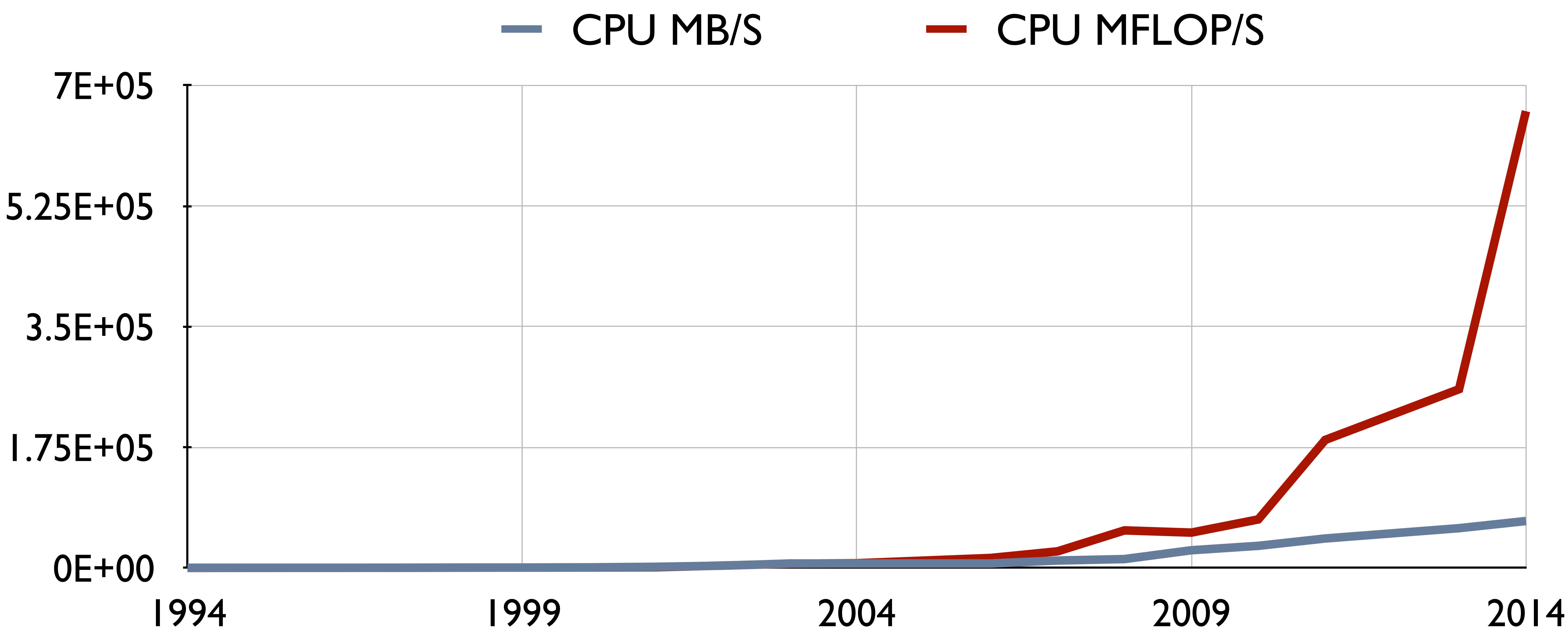
Modern Hardware





Modern Hardware

- FLOPS increasing faster than memory bandwidth [7]



[7] F. D. Witherden, A. M. Farrington, P. E. Vincent. PyFR: An Open Source Framework for Solving Advection-Diffusion Type Problems on Streaming Architectures using the Flux Reconstruction Approach. Computer Physics Communications. 2014. Data courtesy of Jan Treibig.

Modern Hardware

- Also FLOPS come in parallel …

Modern Hardware

- And, different programming languages for different devices …

Modern Hardware

- So a challenging environment ...

Modern Hardware

- But significant FLOPS now available if they can be harnessed …

2.91TFLOPS
(Double Precision)

PyFR

Flux Reconstruction

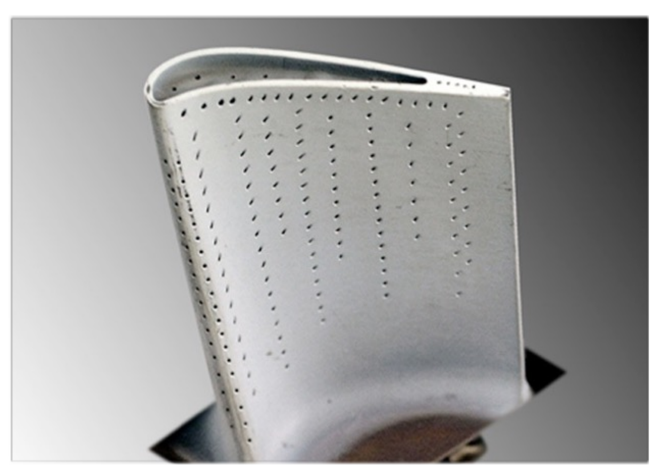
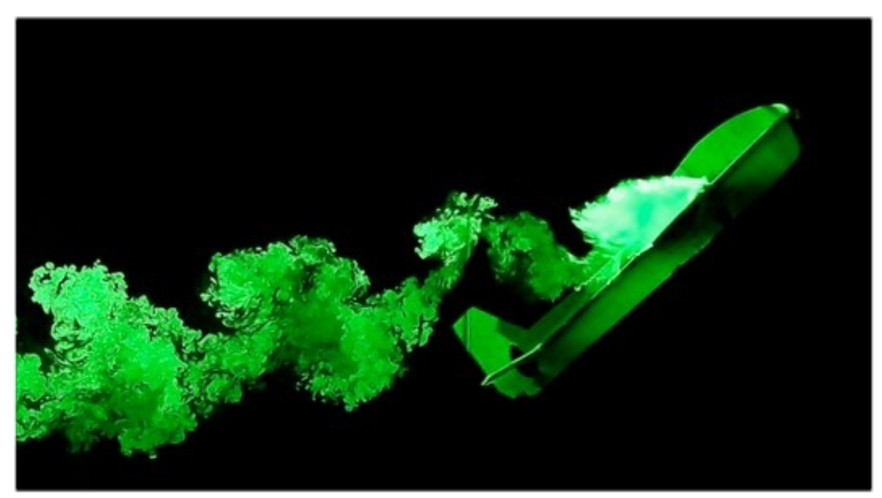
+

Modern Hardware







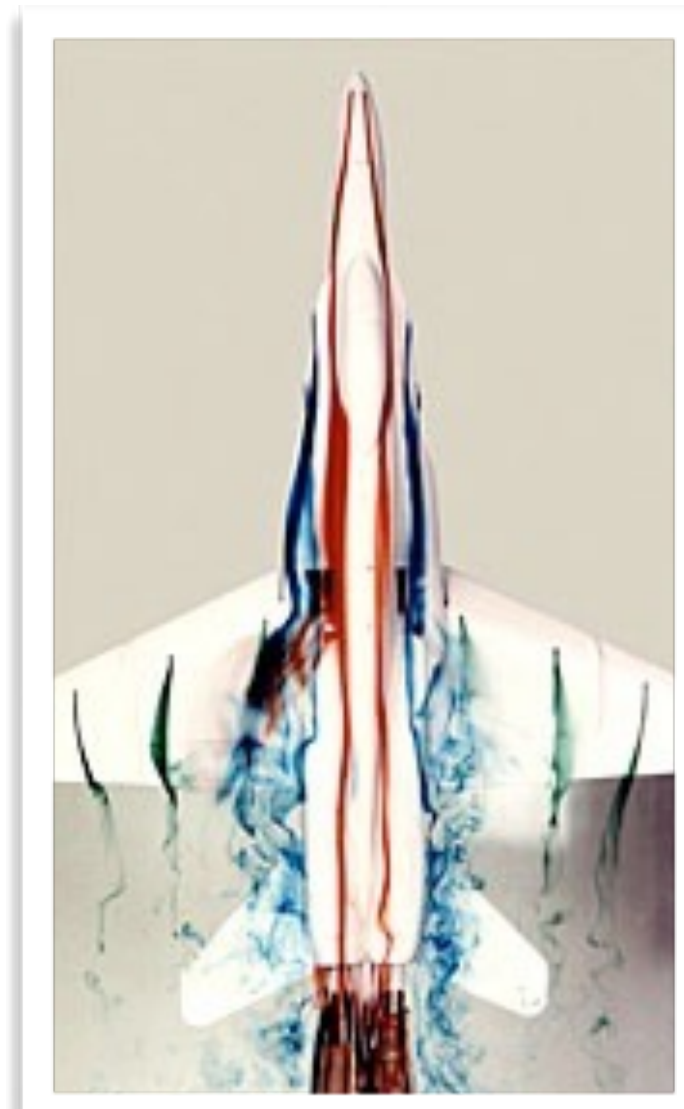
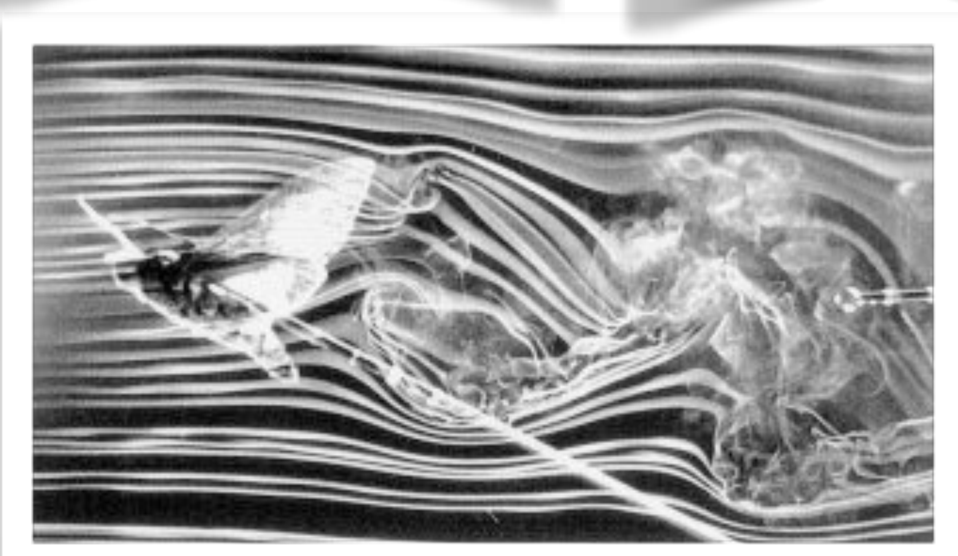
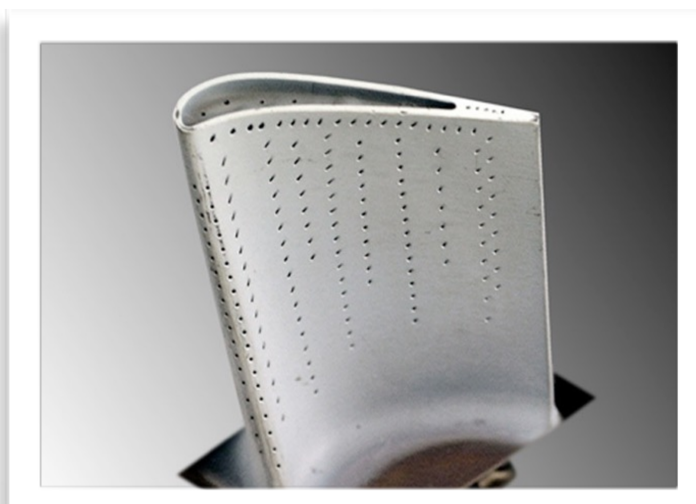
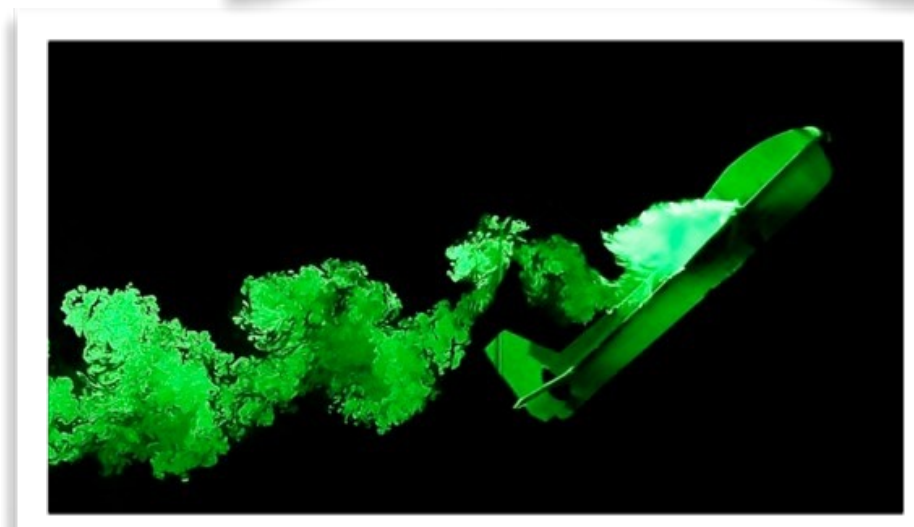



PyFR

PyFR





PyFR

- Features

Governing Equations	Compressible Euler Compressible Navier Stokes
Spatial Discretisation	Arbitrary order FR on mixed unstructured grids (tris, quads, hexes, tets, prisms, pyraminds)
Temporal Discretisation	Range of explicit Runge-Kutta schemes
Platforms	CPU clusters (C-OpenMP-MPI) Nvidia GPU clusters (CUDA-MPI) AMD GPU clusters (OpenCL-MPI)
Precision	Single Double
Input	Gmsh
Output	Paraview

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PyFR

- Python Outer Layer (Hardware Independent)

Python Outer Layer
(Hardware Independent)

- Setup
- Distributed memory parallelism
- Outer 'for' loop and calls to Hardware Specific Kernels

PyFR

- Need to generate the Hardware Specific Kernels

Python Outer Layer
(Hardware Independent)

- Setup
- Distributed memory parallelism
- Outer 'for' loop and calls to Hardware Specific Kernels

PyFR

- Two types of kernel are required …

Python Outer Layer (Hardware Independent)	Matrix Multiply Kernels	Point-Wise Nonlinear Kernels
• Setup • Distributed memory parallelism • Outer ‘for’ loop and calls to Hardware Specific Kernels	• Data interpolation/ extrapolation etc.	• Flux functions, Riemann solvers etc.

PyFR

- For matrix multiply kernels it is pretty easy …

Python Outer Layer (Hardware Independent)

- Setup
- Distributed memory parallelism
- Outer 'for' loop and calls to Hardware Specific Kernels

Matrix Multiply Kernels

- Data interpolation/ extrapolation etc.

Use DGEMM from vendor supplied BLAS

Point-Wise Nonlinear Kernels

- Flux functions, Riemann solvers etc.

PyFR

- Harder for point-wise nonlinear kernels …

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Pass Mako derived kernel templates through Mako derived templating engine

PyFR

- These can now be called

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C/OpenMP
Hardware Specific Kernels

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PyFR

PyFR

- Website: www.pyfr.org
- Twitter: @PyFR_Solver
- Paper: Computer Physics Communications [8]

[8] F. D. Witherden, A. M. Farrington, P. E. Vincent. PyFR: An Open Source Framework for Solving Advection-Diffusion Type Problems on Streaming Architectures using the Flux Reconstruction Approach. Computer Physics Communications. 2014

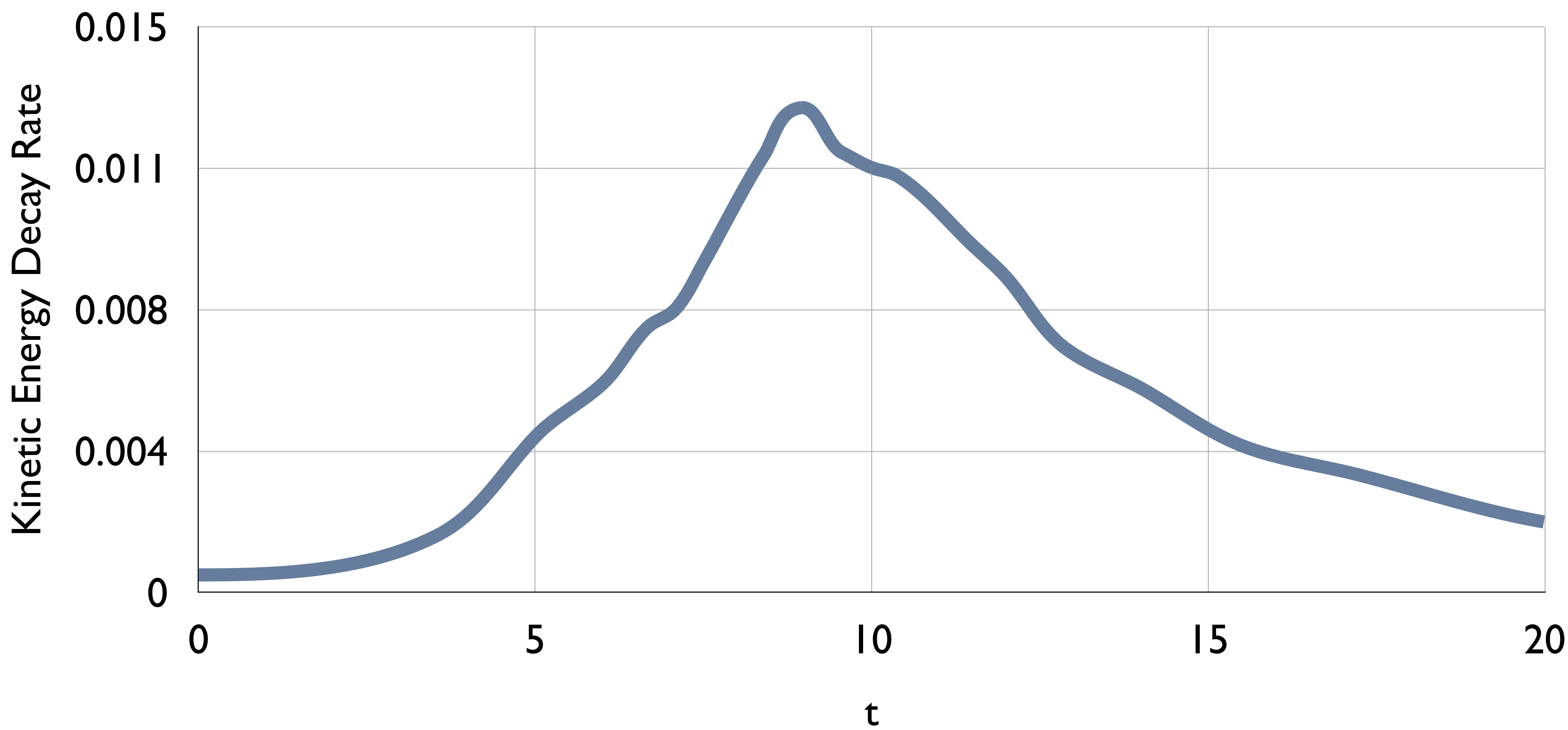
Results

- 3D Taylor-Green vortex breakdown
- Compare with spectral DNS results of van Rees et al. [9]

[9] W. M. van Rees, A. Leonard, D.I. Pullin, and P. Koumoutsakos. A Comparison of Vortex and Pseudo-Spectral Methods for the Simulation of Periodic Vortical Flows at High Reynolds Numbers. Journal of Computational Physics, 2011

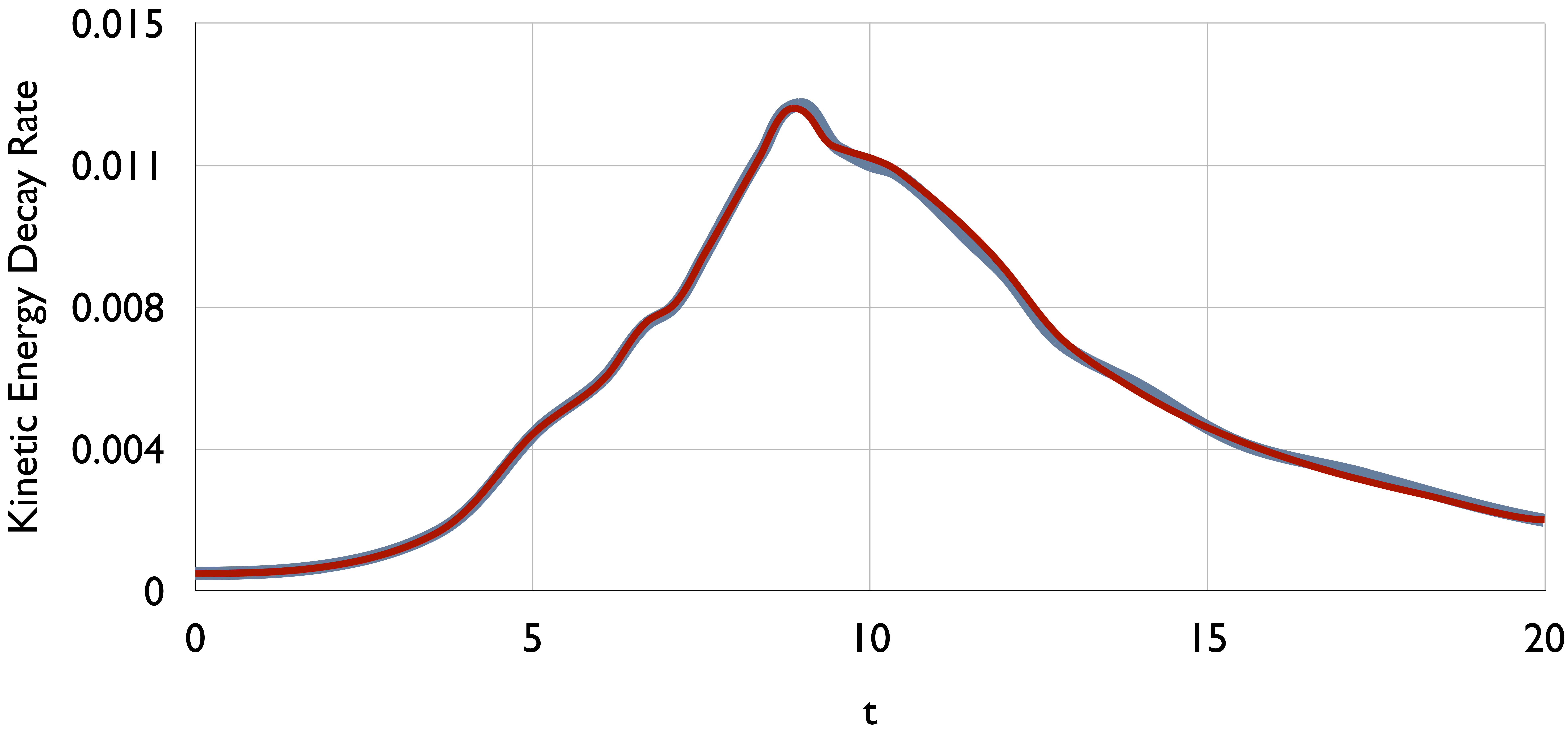
Results

- van Rees et al. spectral DNS



Results

- van Rees et al. spectral DNS + PyFR 6th order



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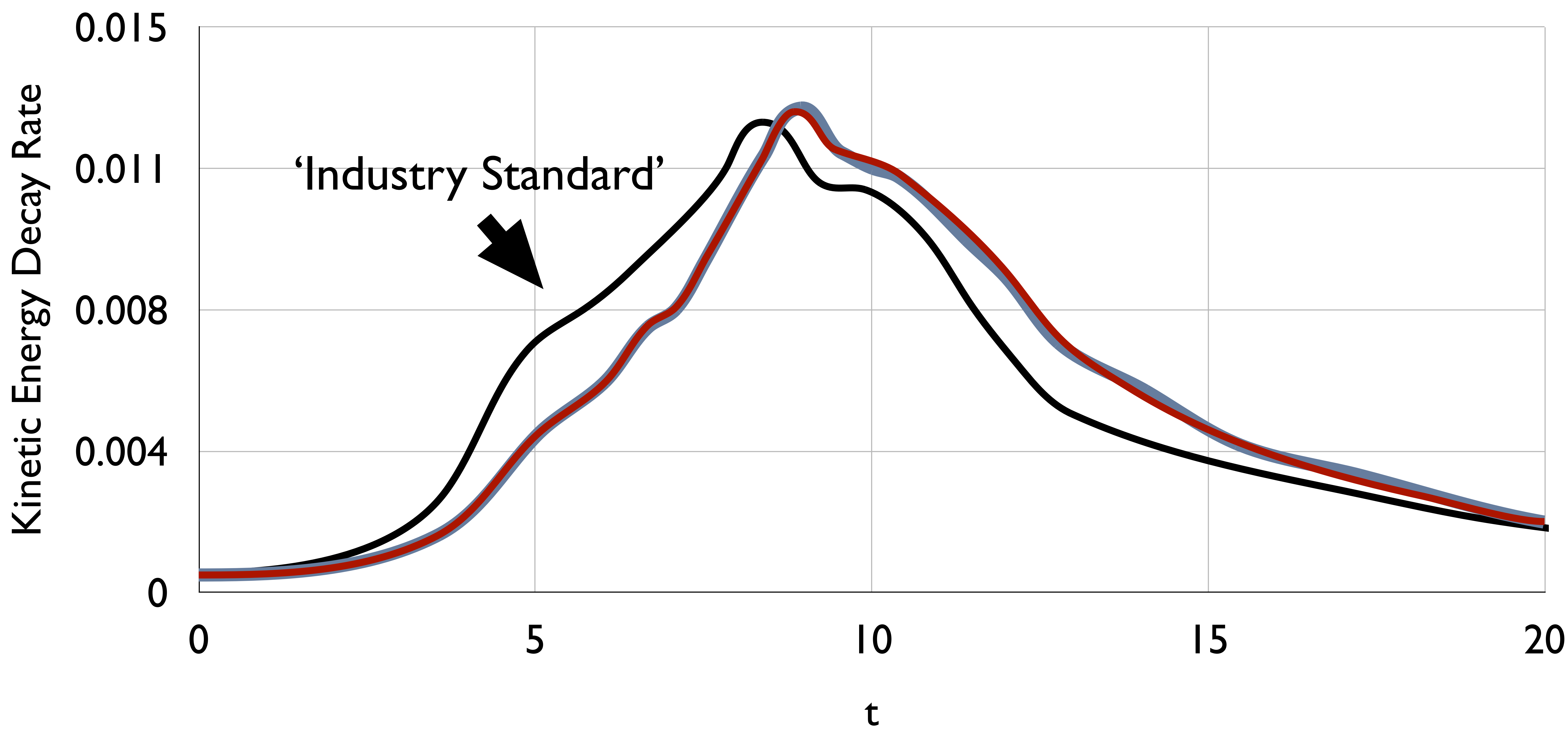

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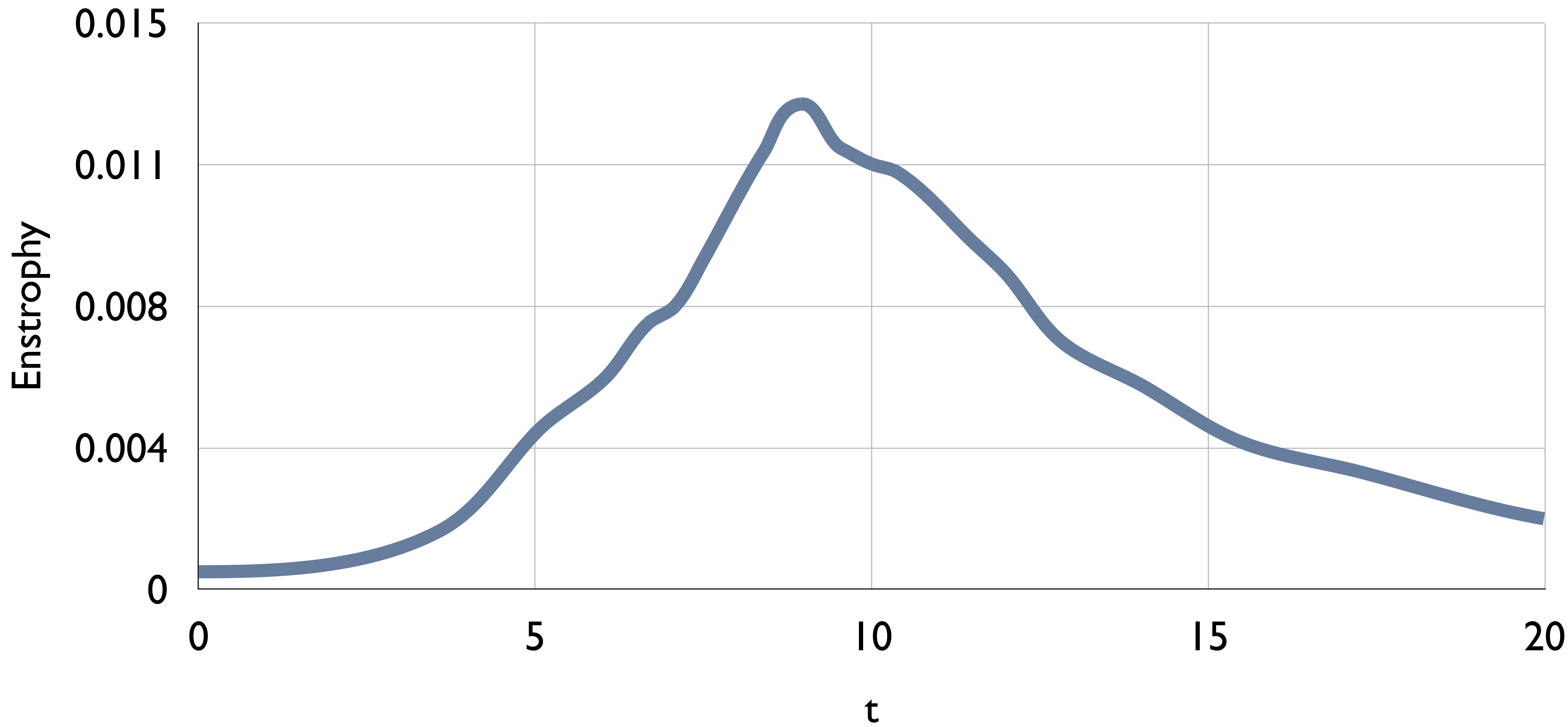

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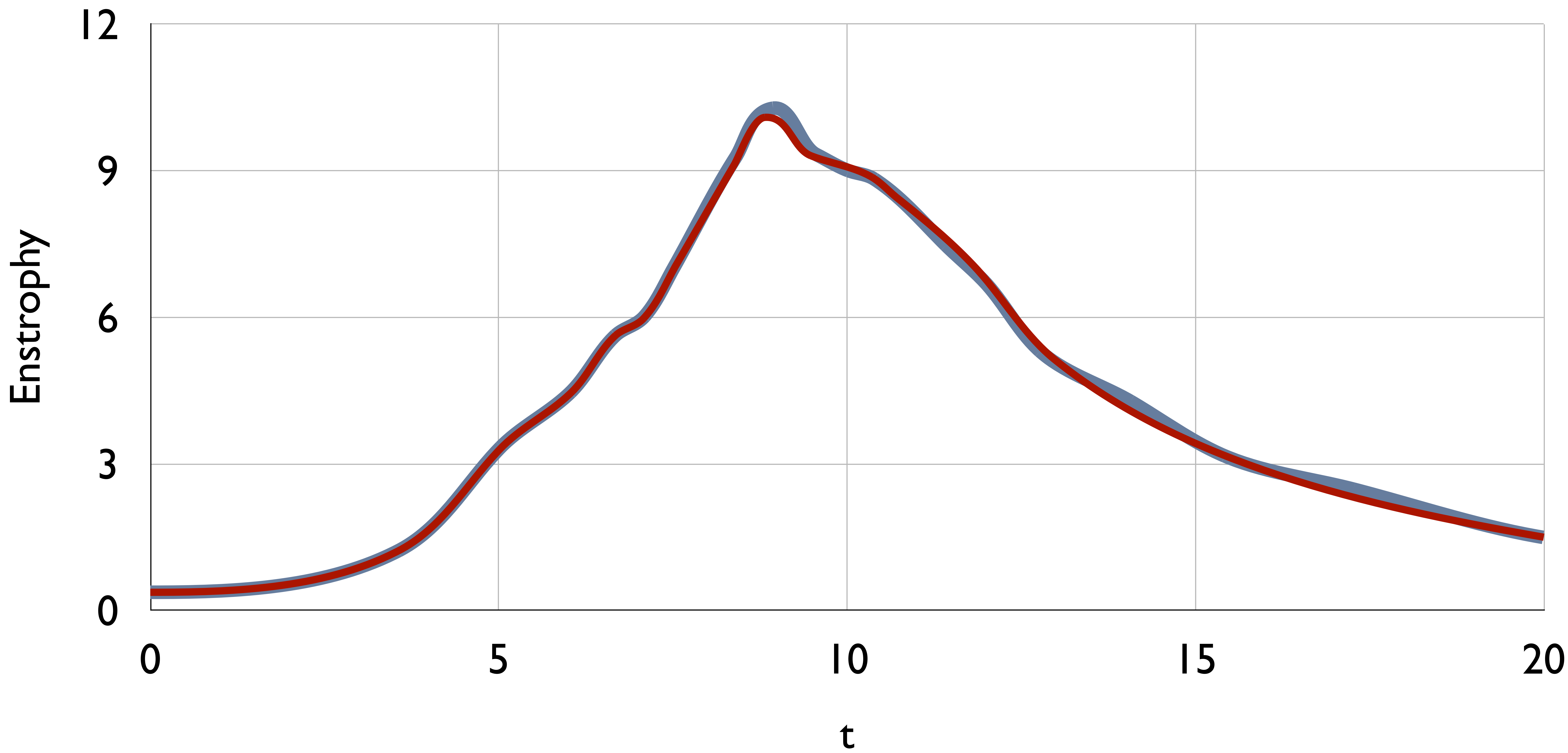

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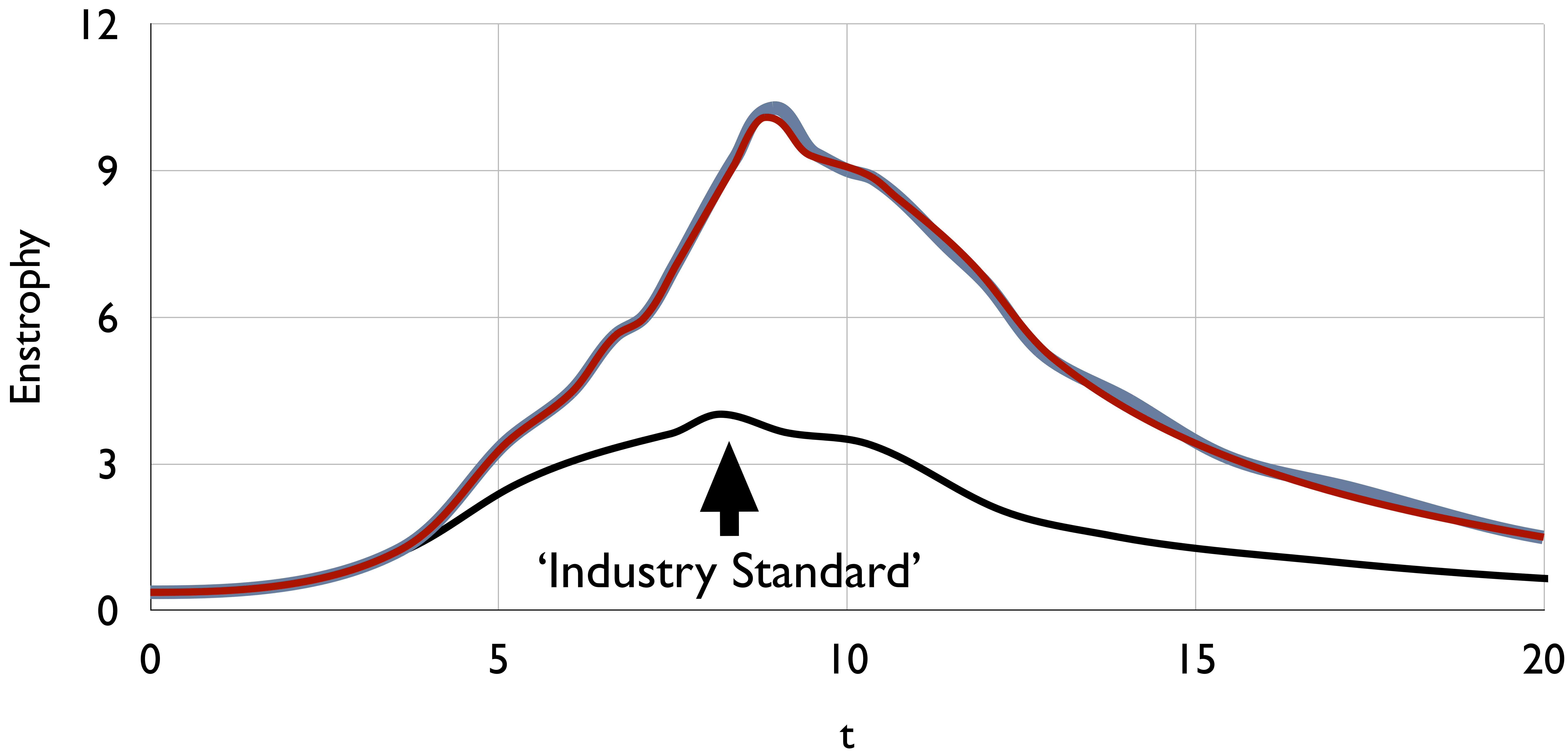
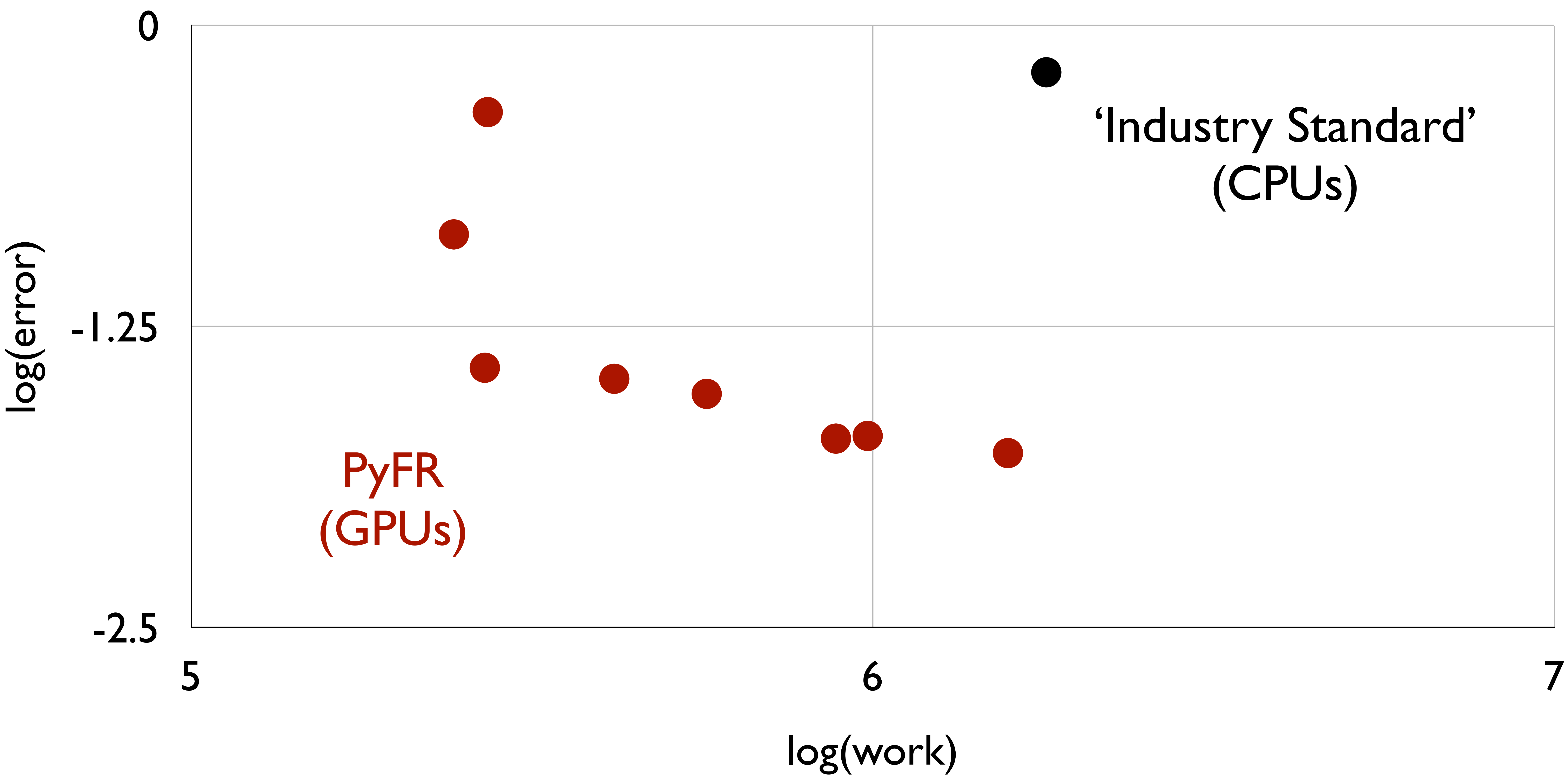


Results

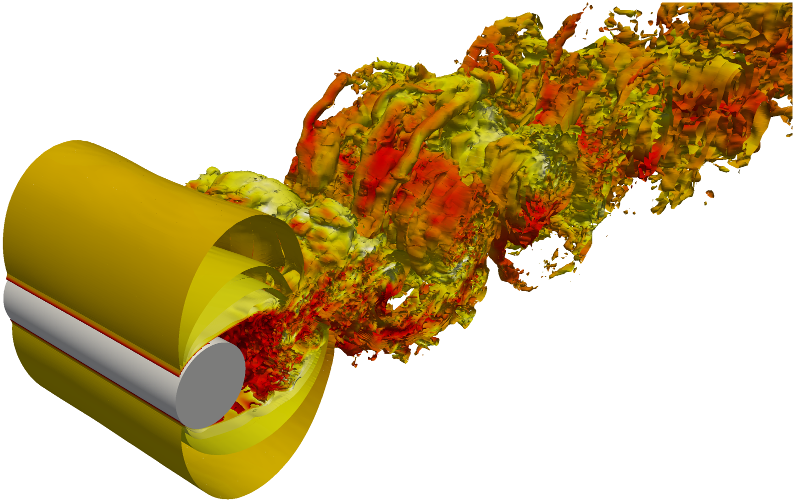
- L_∞ error in enstrophy



Results

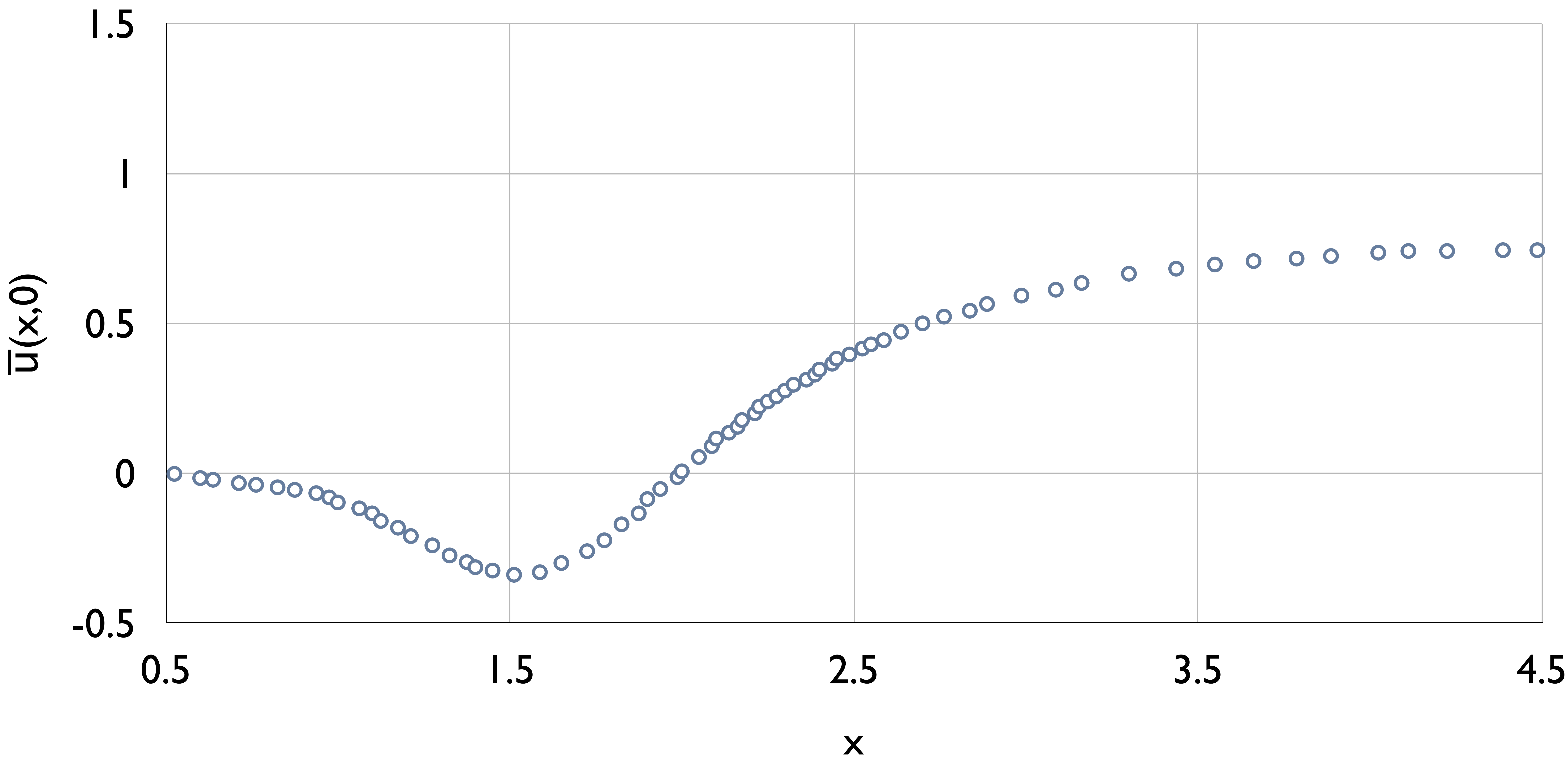
- Flow over a circular cylinder
- Re = 3900
- Ma = 0.2
- Compare with Parnaudeau et al. [10]

[10] P. Parnaudeau, J. Carlier, D. Heitz, E. Lamballais. Experimental and Numerical Studies of the Flow Over a Circular Cylinder at Reynolds Number 3900. Physics of Fluids. 2008



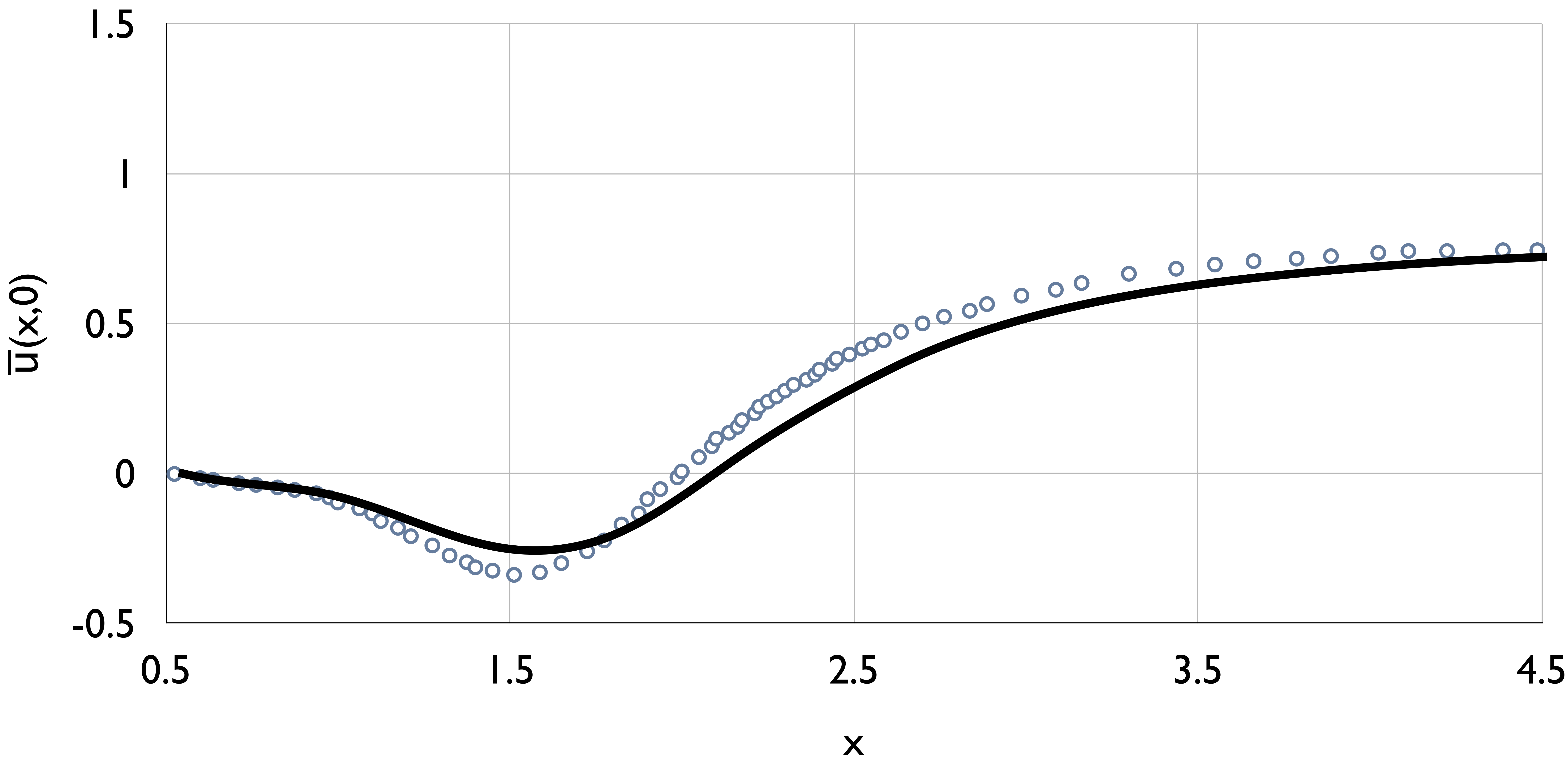
Results

- Parnaudeau et al. experiment



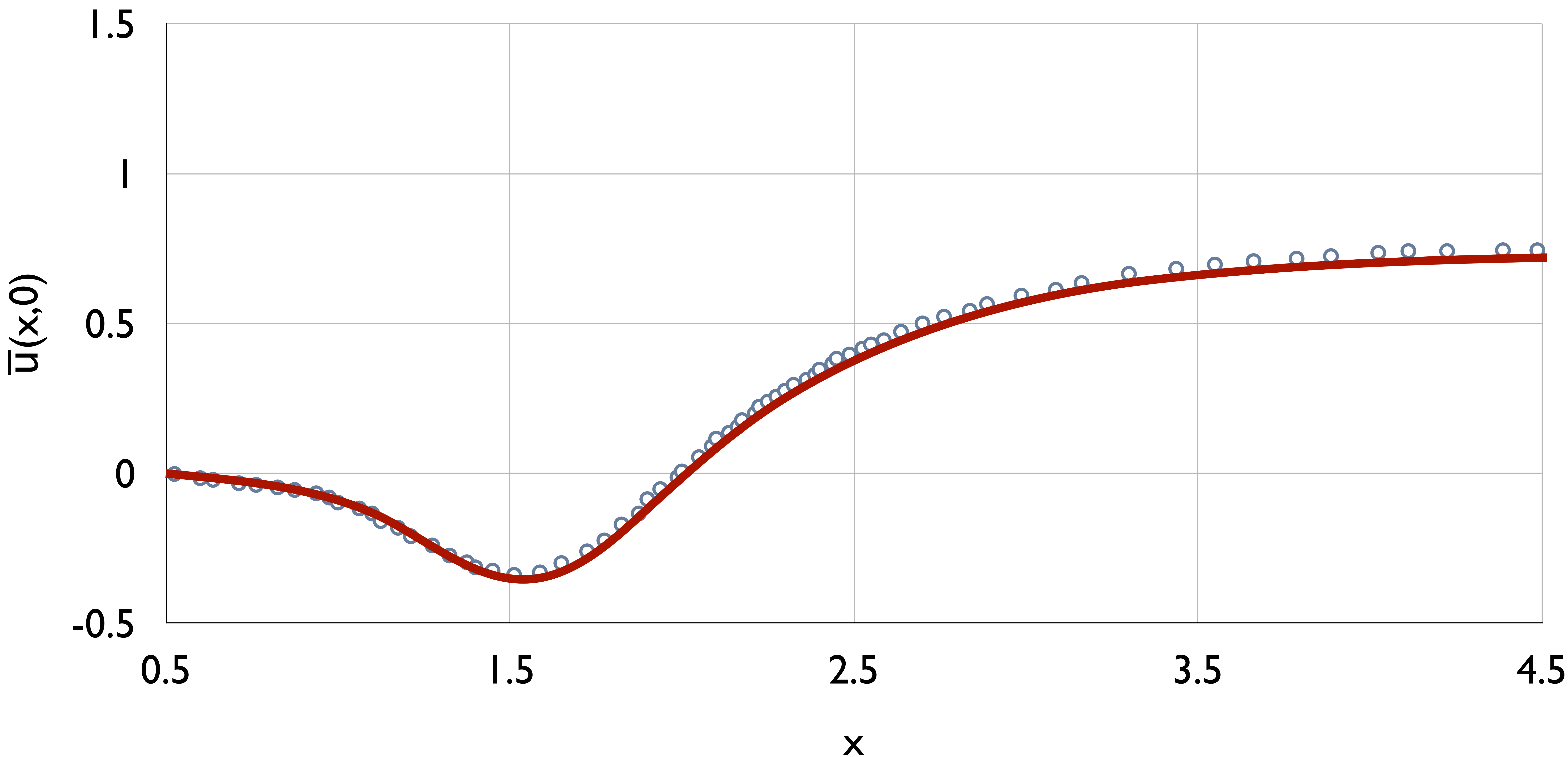
Results

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



Results

- Parnaudeau et al. experiment + PyFR 5th order



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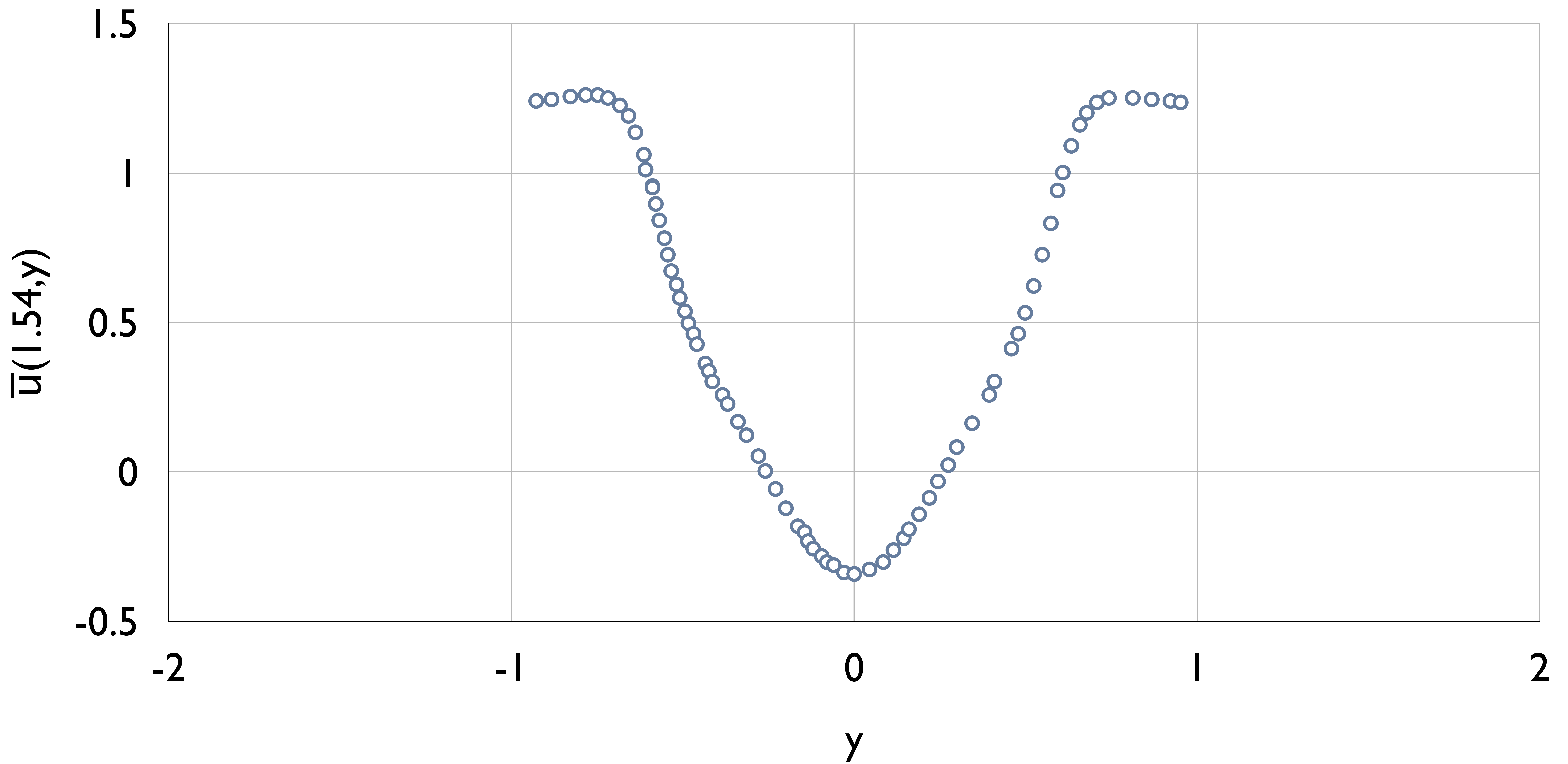

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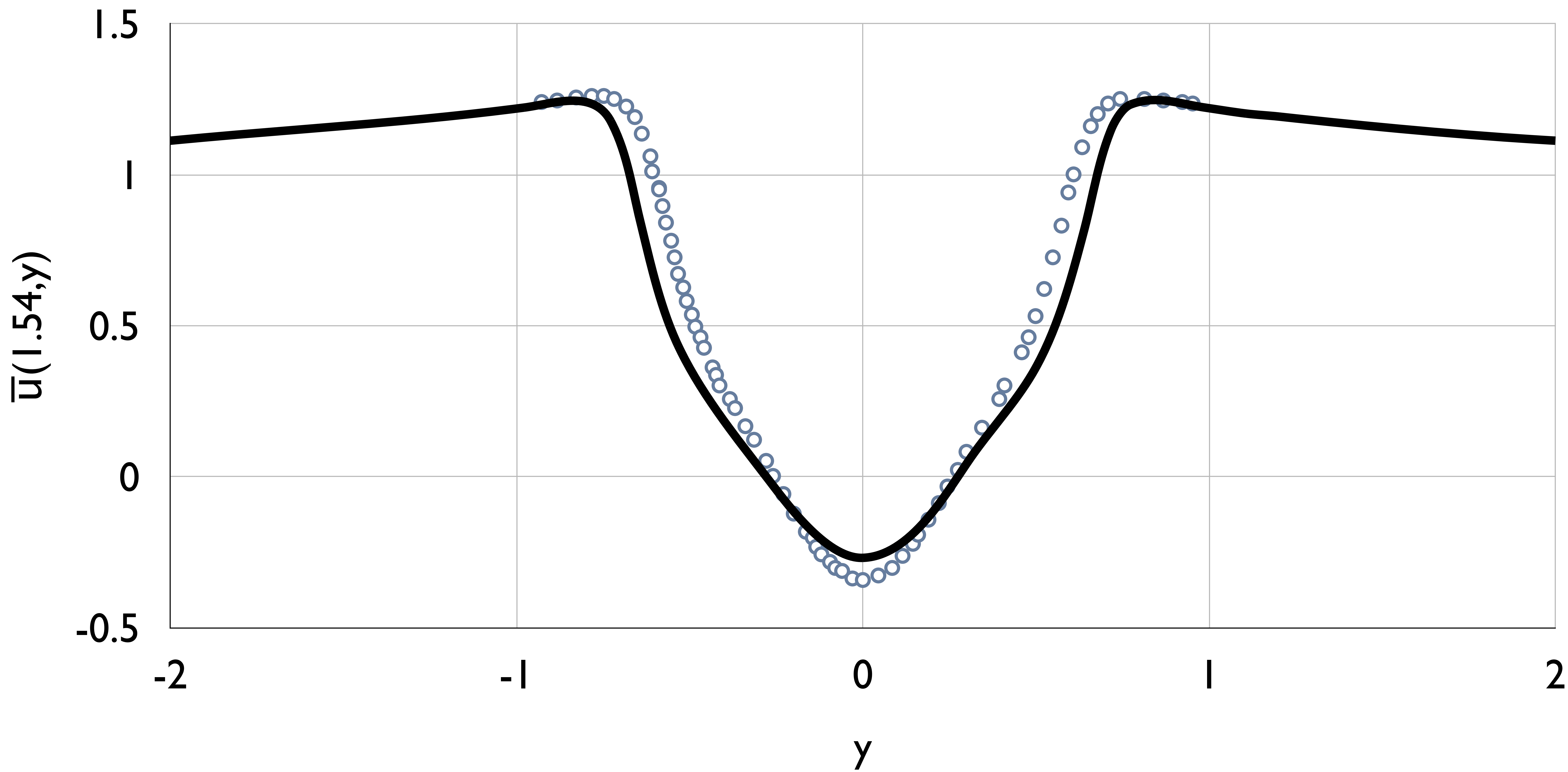

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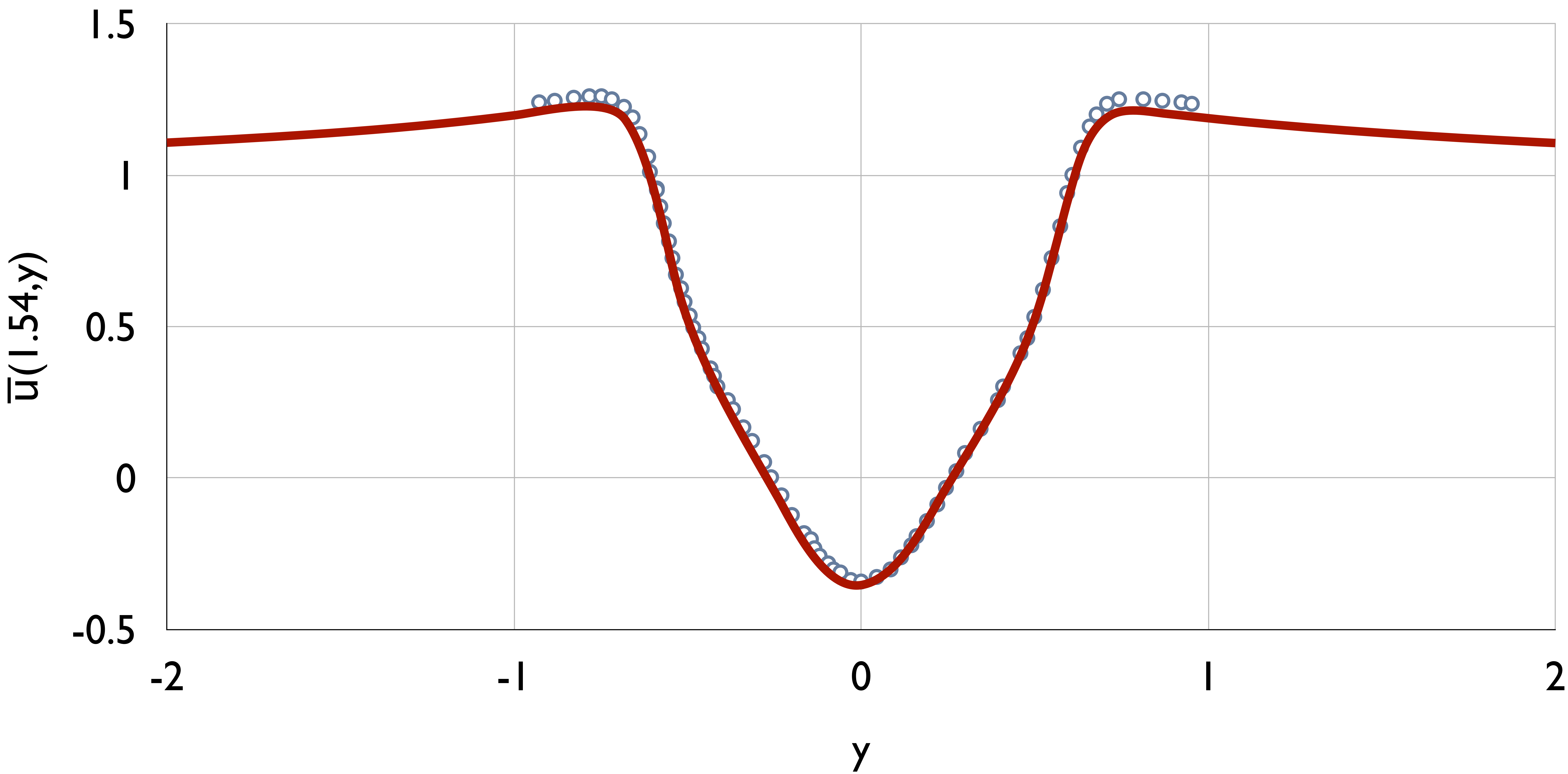
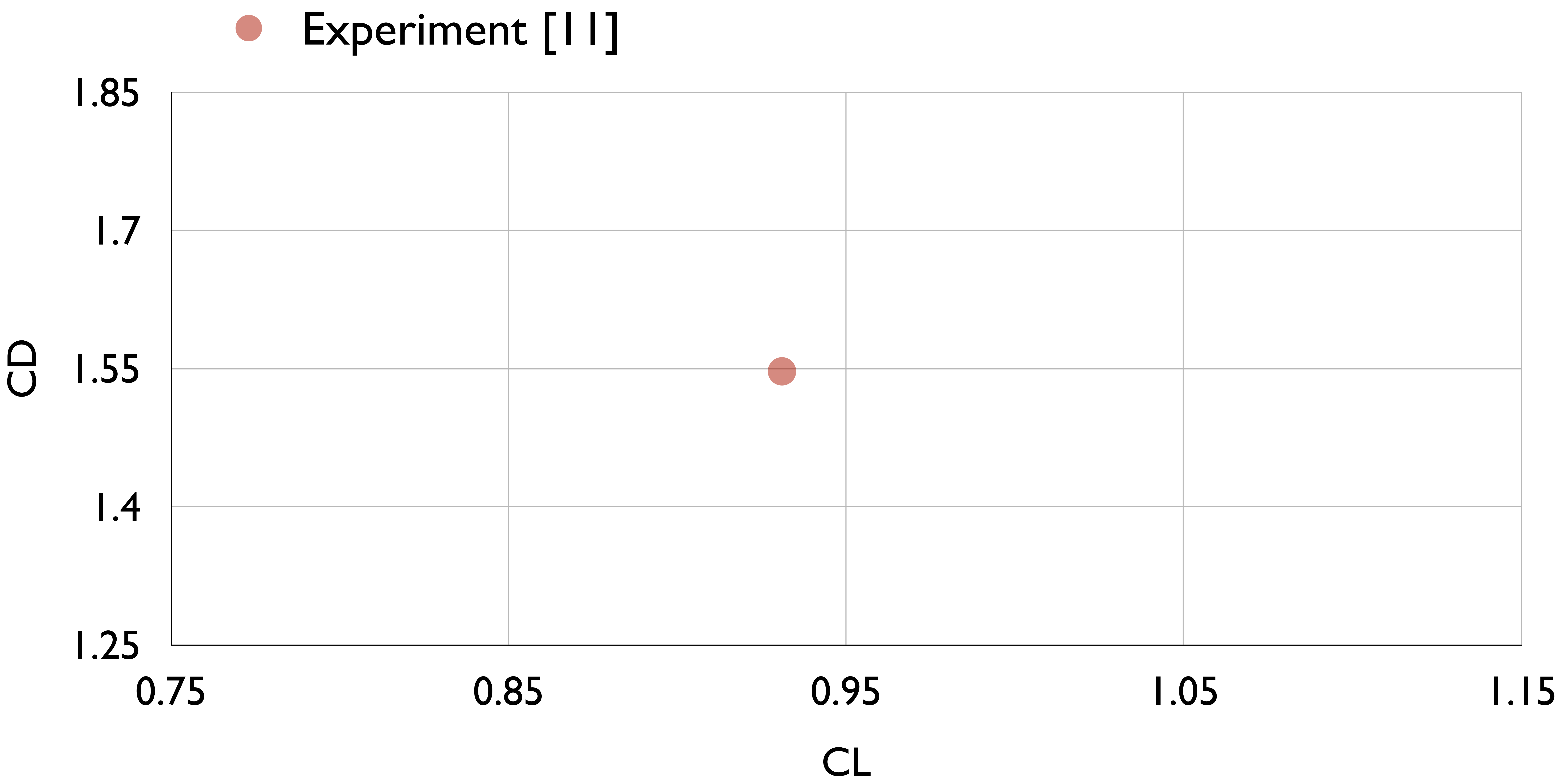


Results

- Flow over a NACA 0021 at 60 degree AoA
- Re = 270,000
- Ma = 0.2
- Compare with Swalwell and DESider [11][12]

[11] K. Swalwell. The Effect of Turbulence on Stall of Horizontal Axis Wind Turbines. PhD Thesis. 2005.
[12] W. Haase, M. Braza, A. Revell. DESider A European Effort on Hybrid RANS-LES Modelling. 2009.

Results



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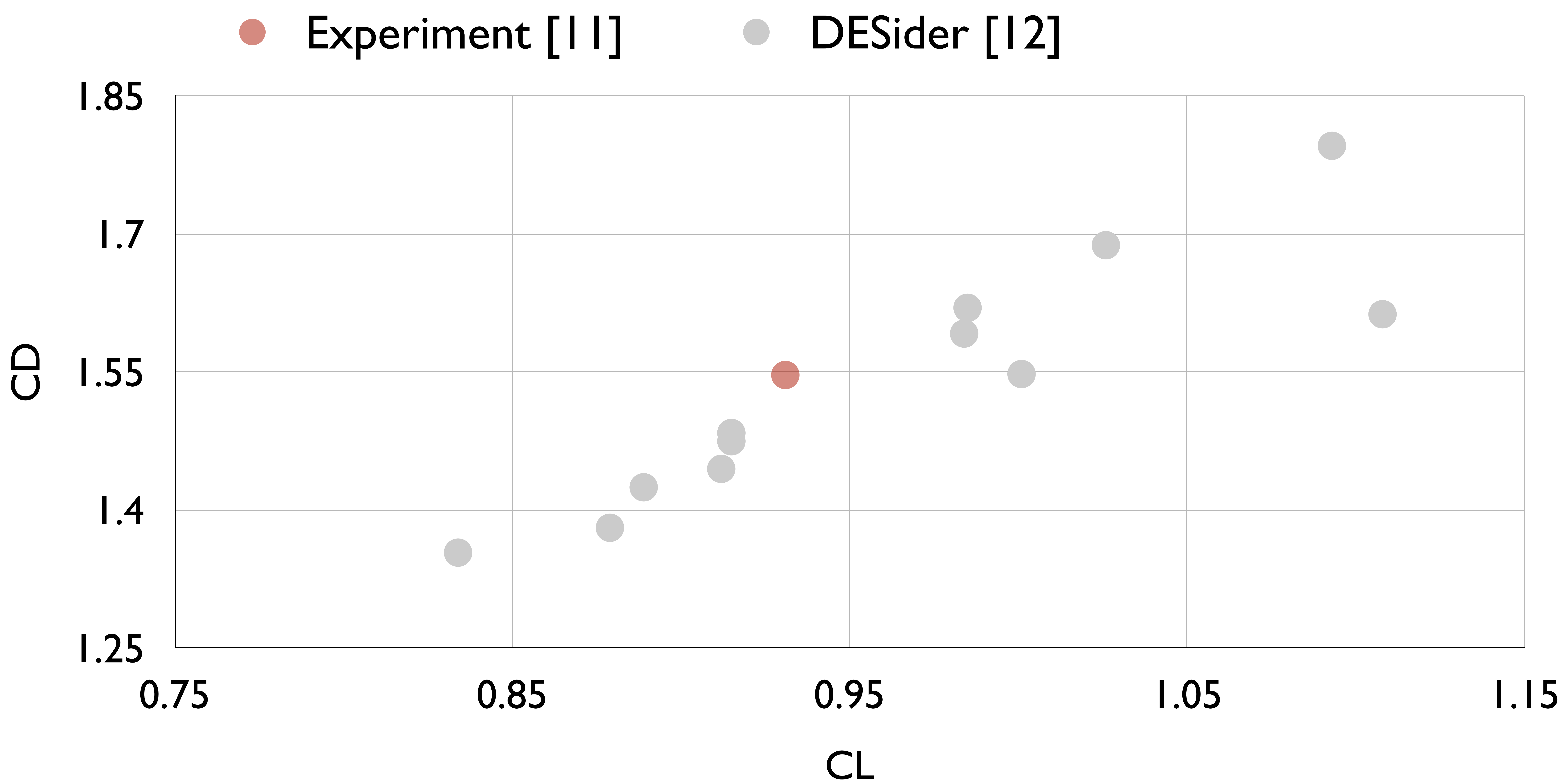

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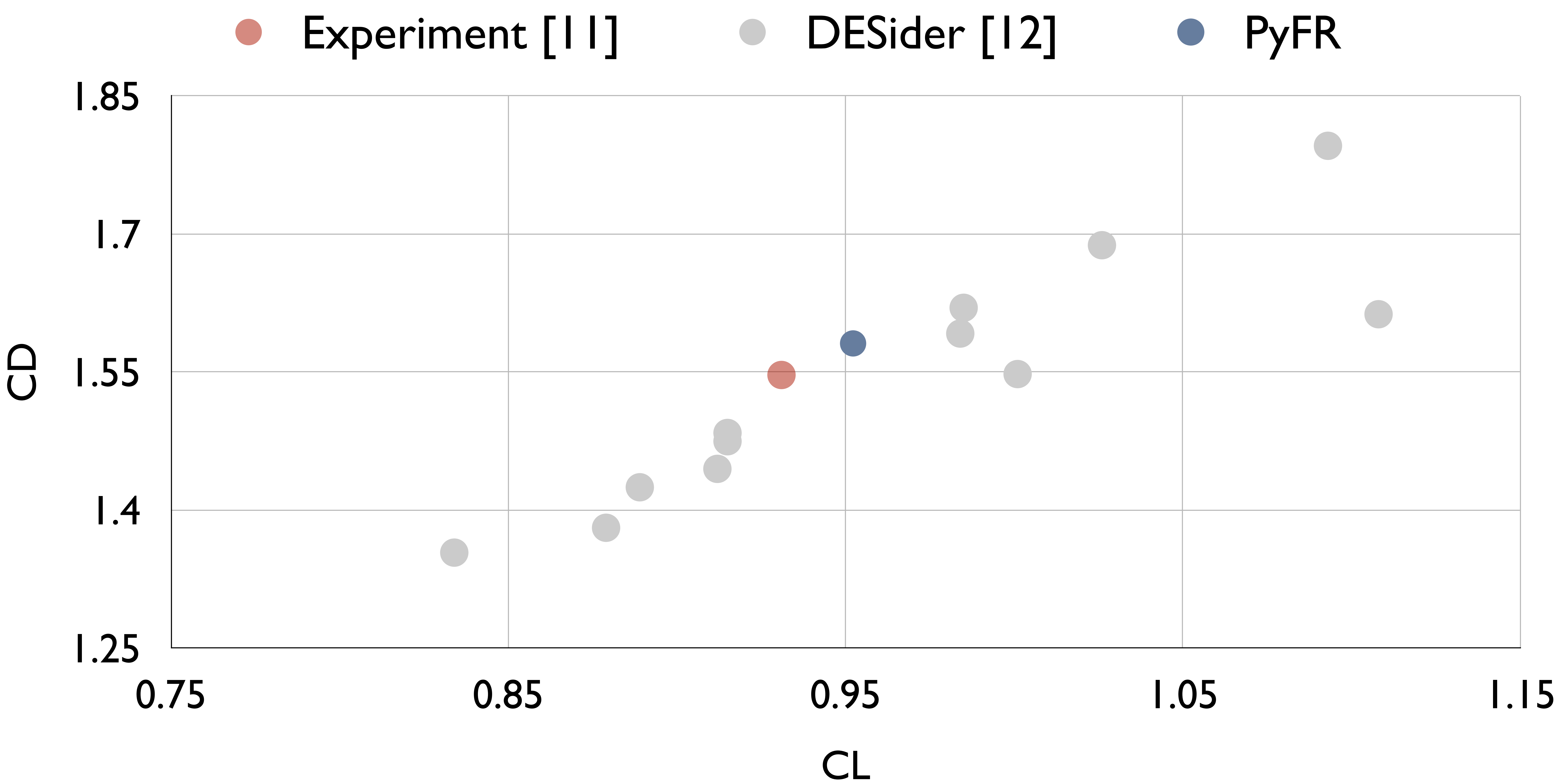

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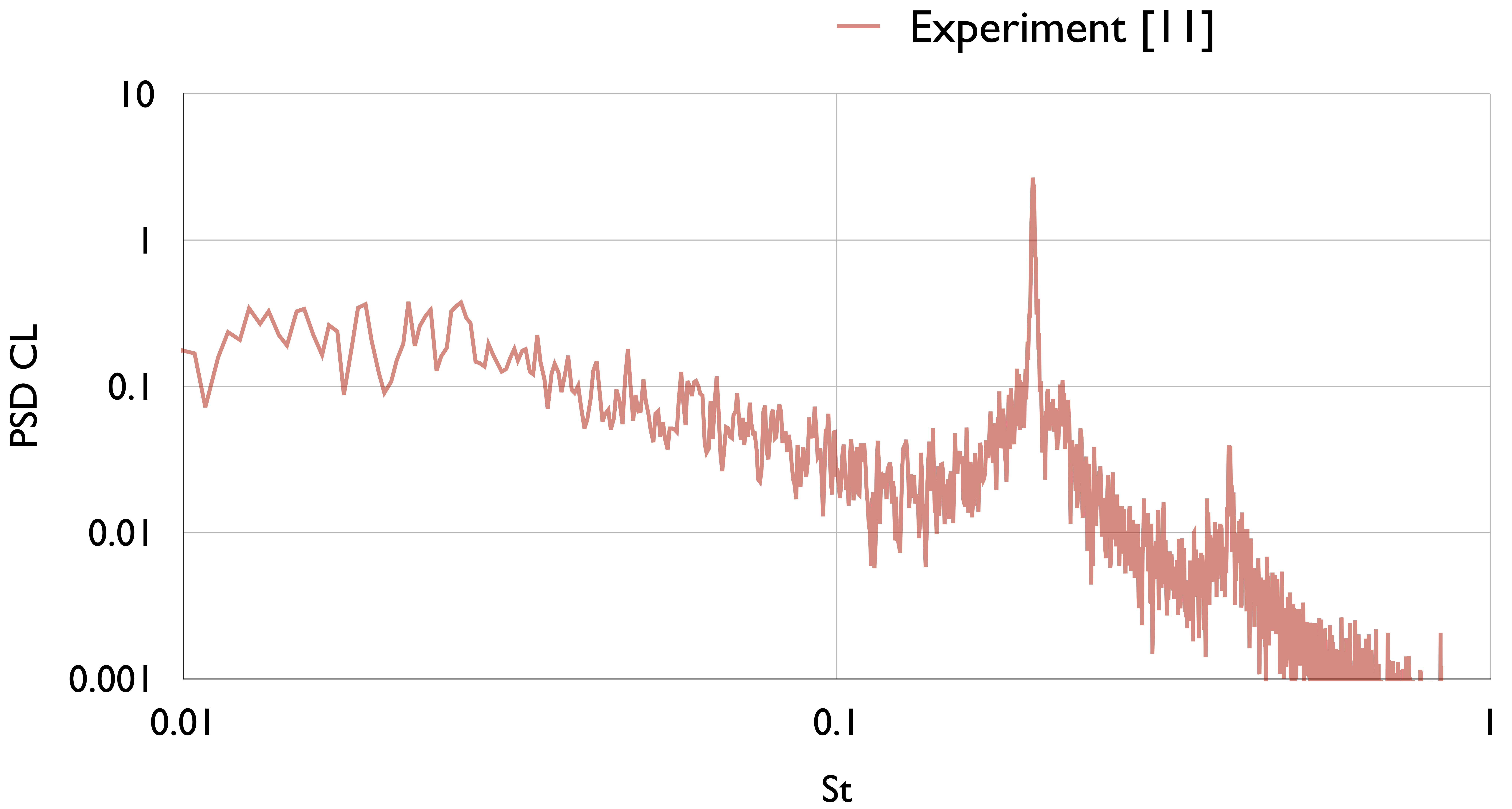

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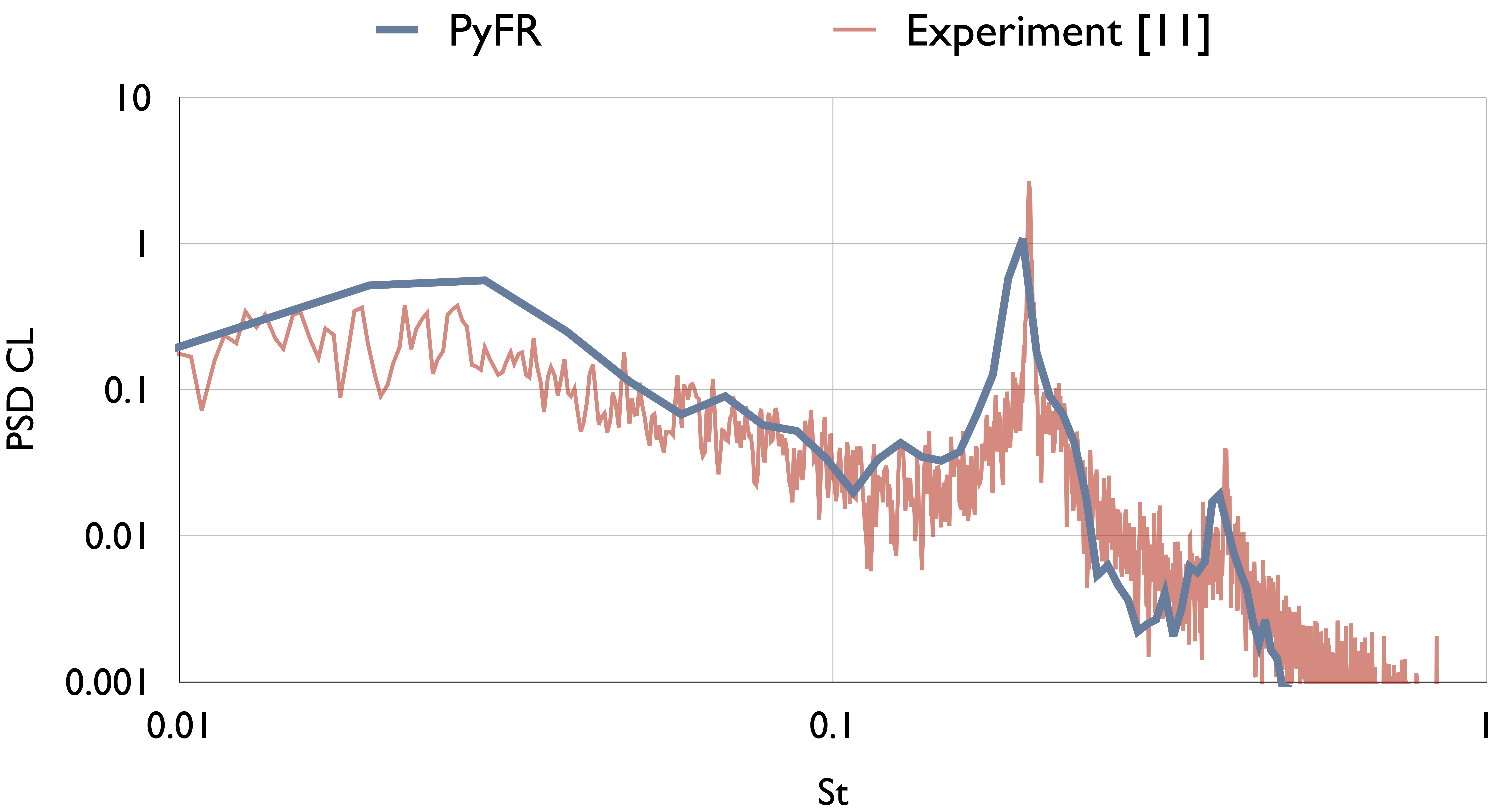


[11] K. Swalwell. The Effect of Turbulence on Stall of Horizontal Axis Wind Turbines. PhD Thesis. 2005.

Results

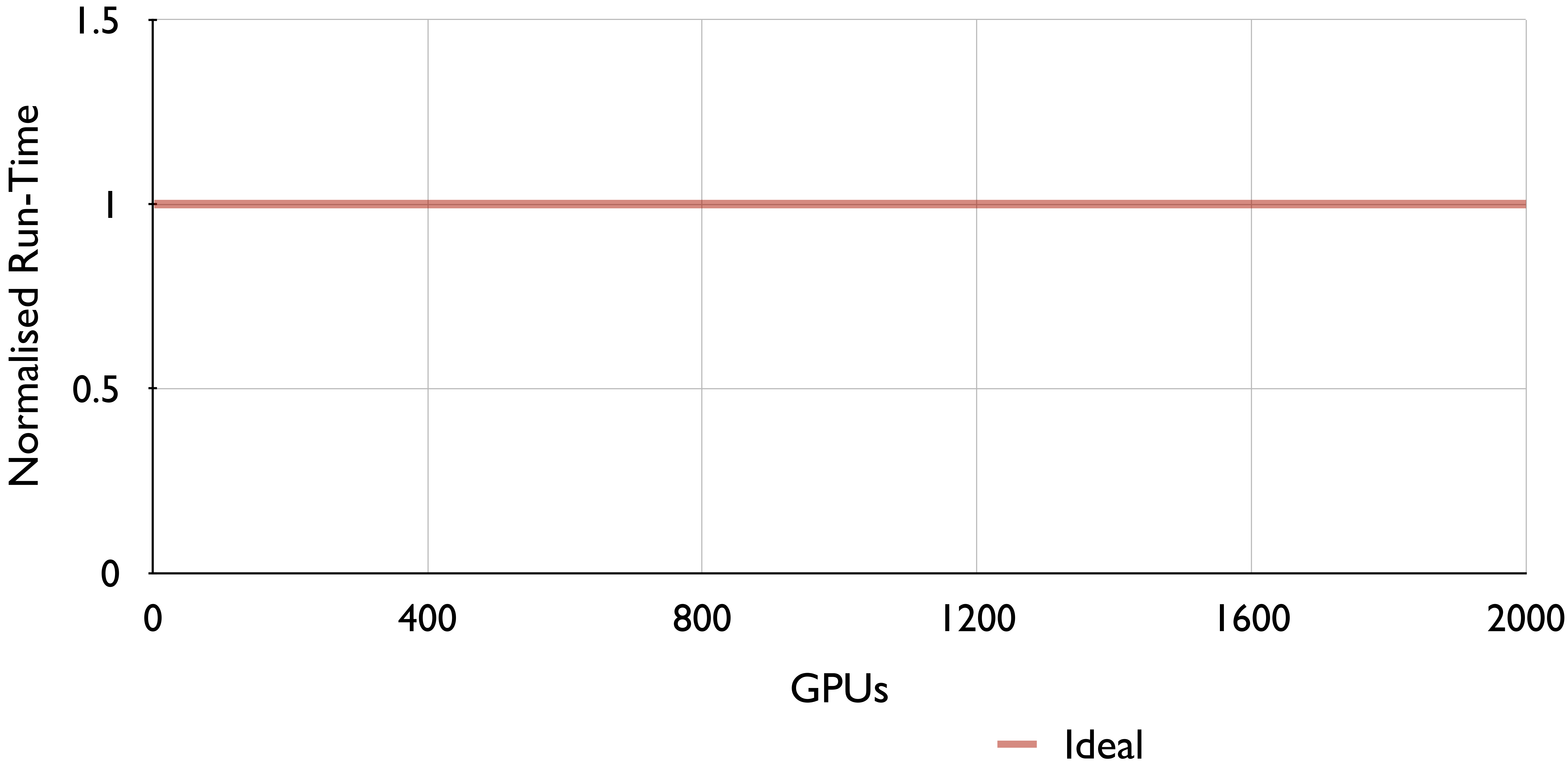
- Flow over a tandem cylinder and NACA 0012
- Re = 500,000
- Ma = 0.2

Results

- Flow over a wedge
- Ma = 1.34

Results

- 3D Navier-Stokes weak scaling on Piz Daint



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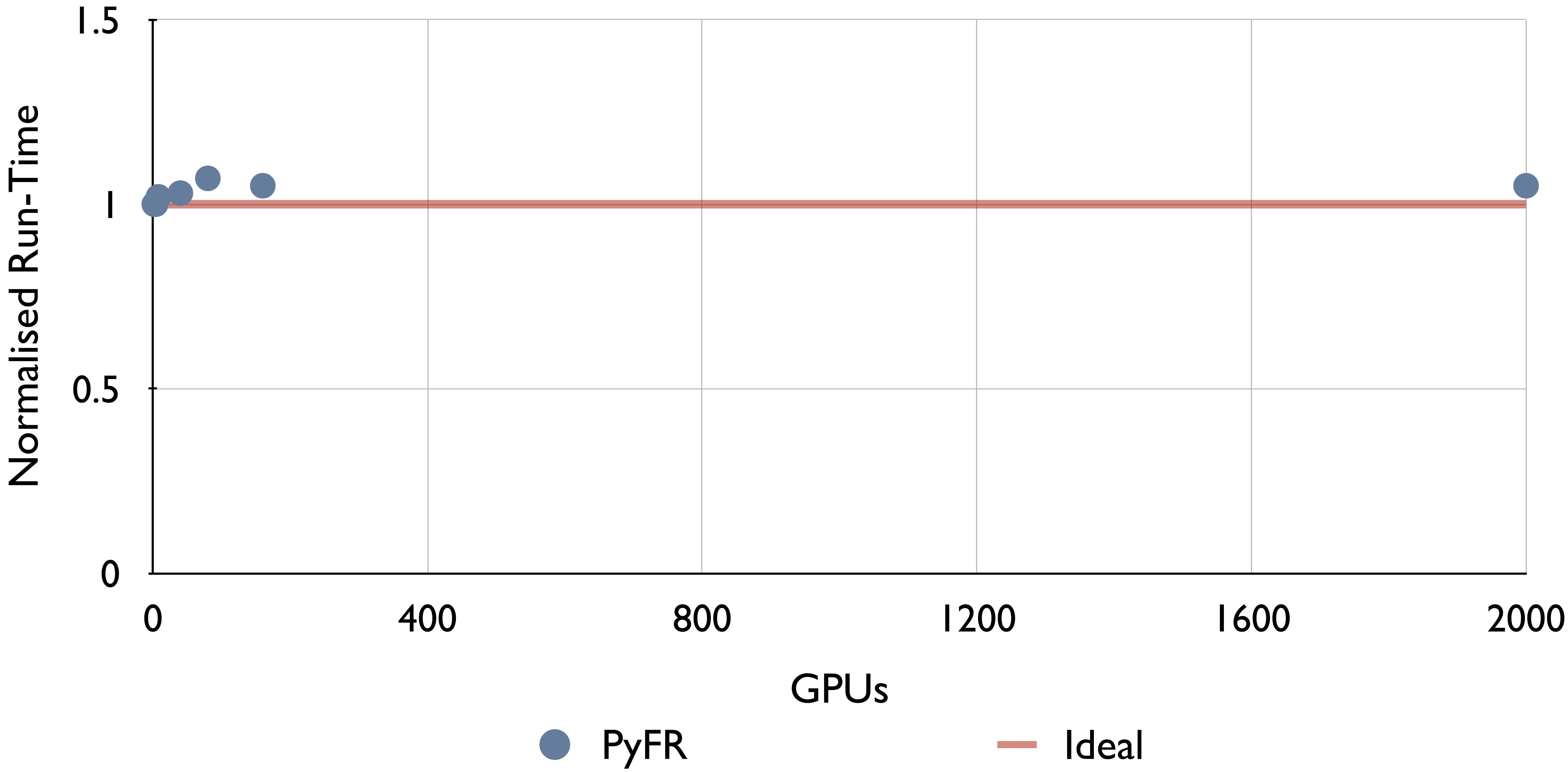

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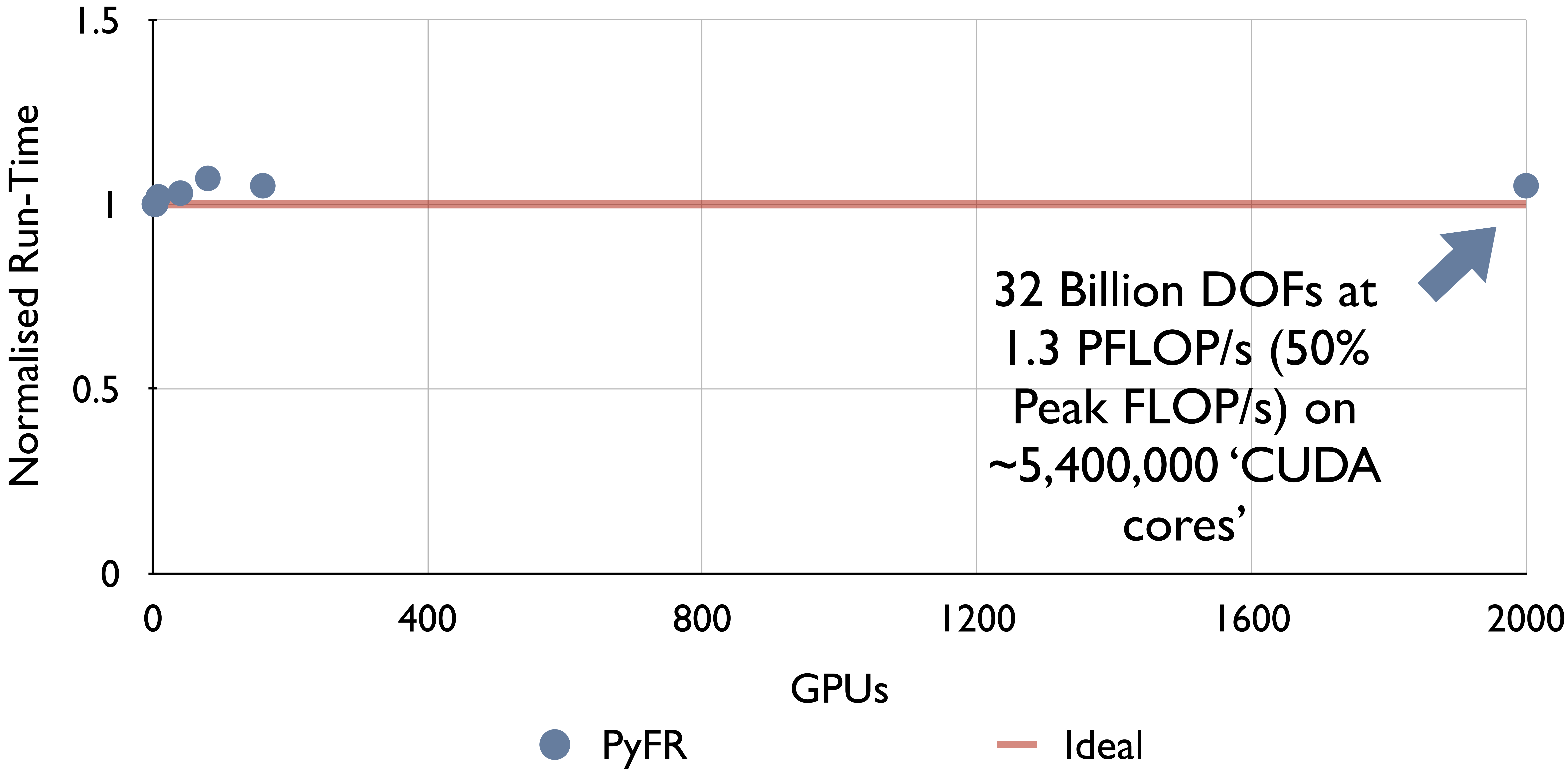

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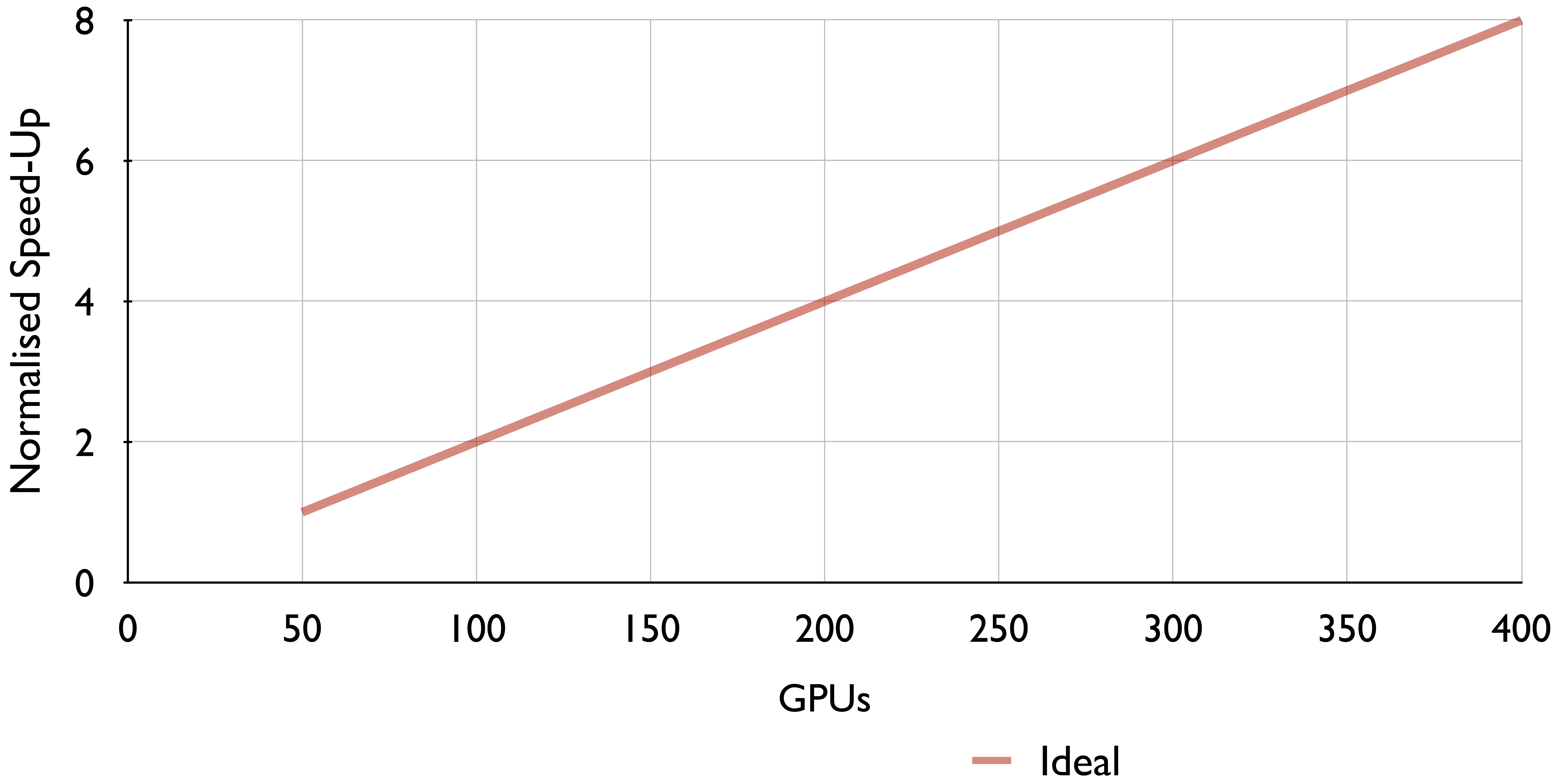

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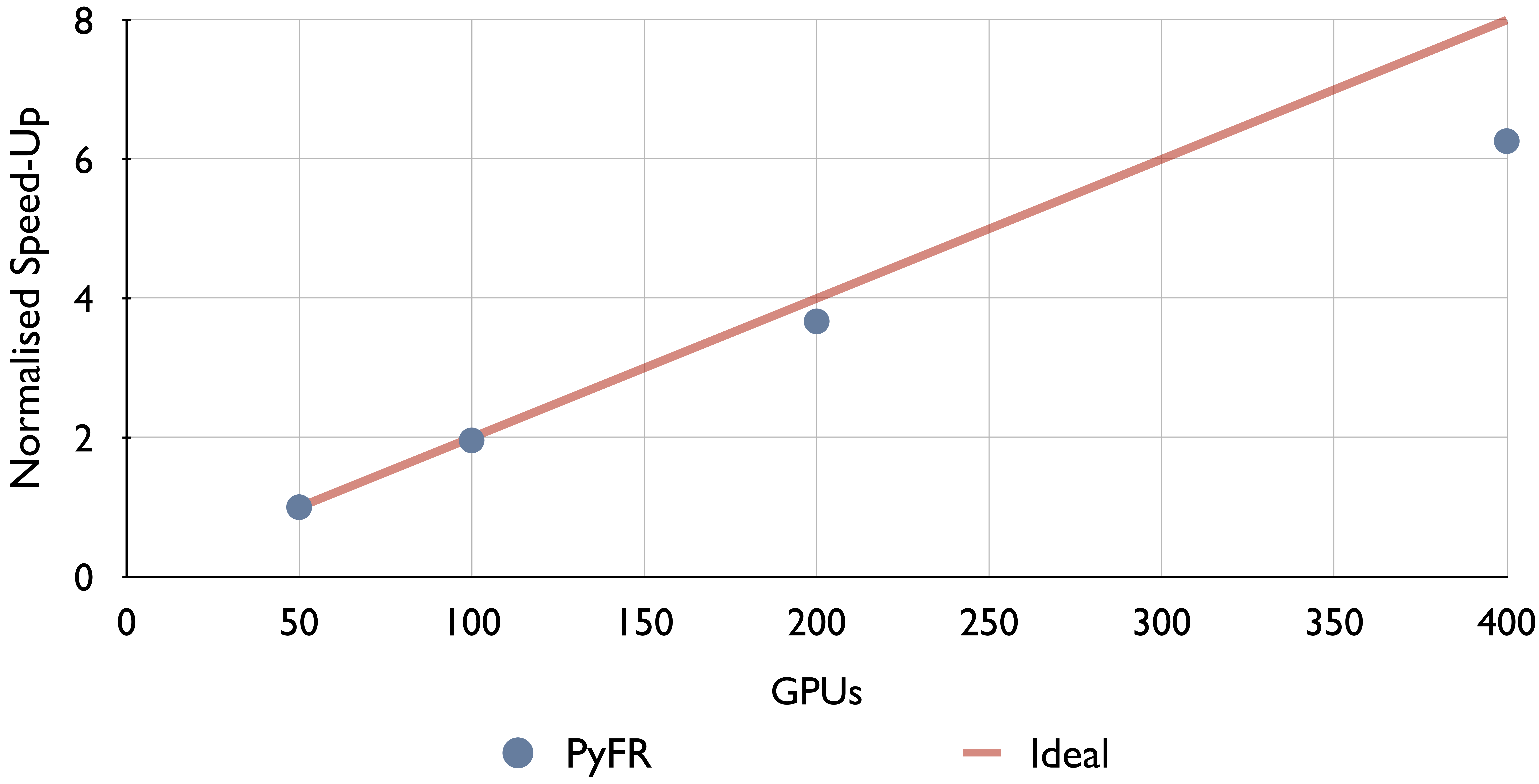

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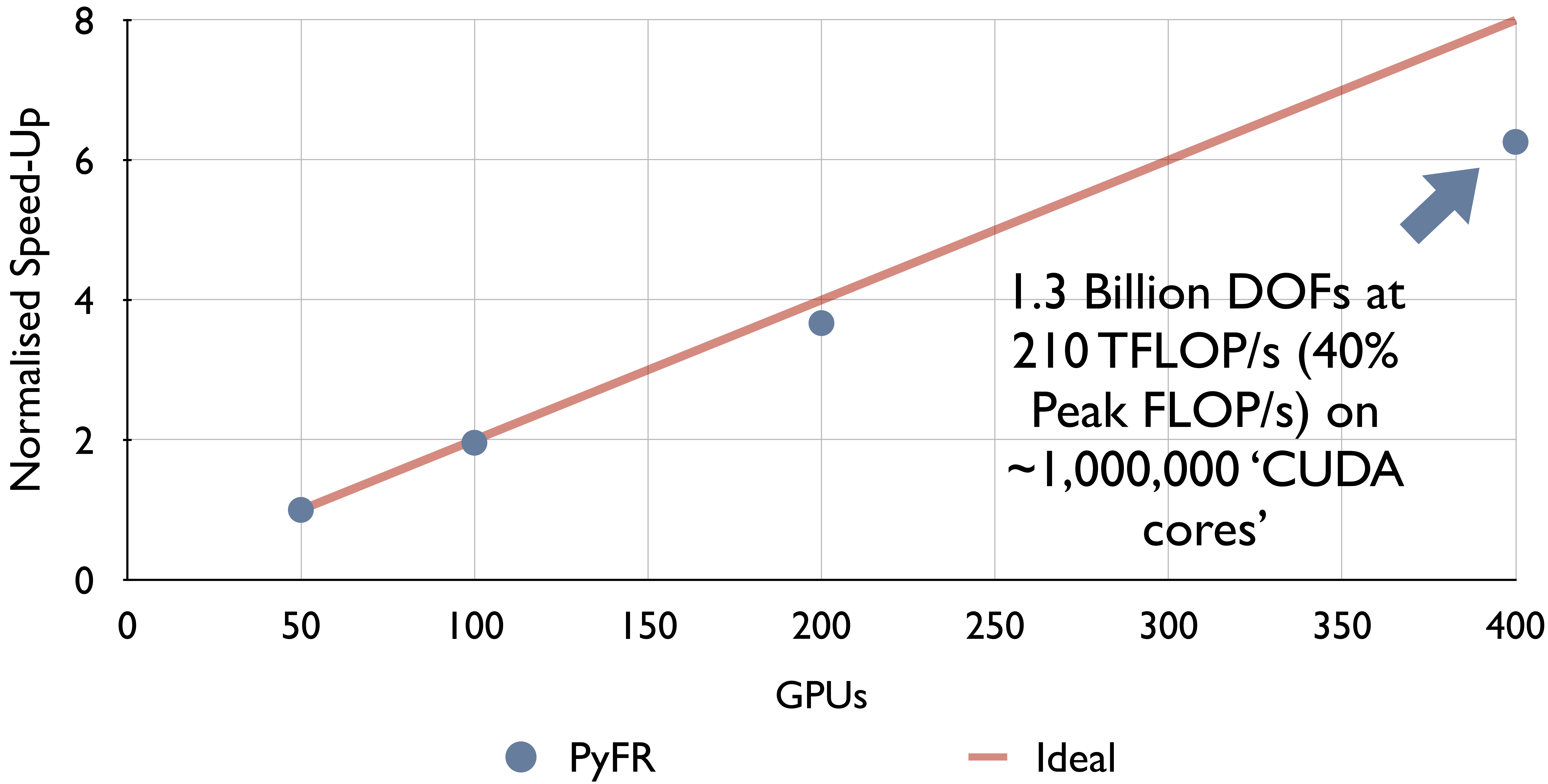

Team


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Francesco Iori


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Niki Loppi


Yaguang Liu

Funding

EPSRC
Pioneering research and skills

Innovate UK
Technology Strategy Board

European Commission

AIRBUS

BAE SYSTEMS

NVIDIA

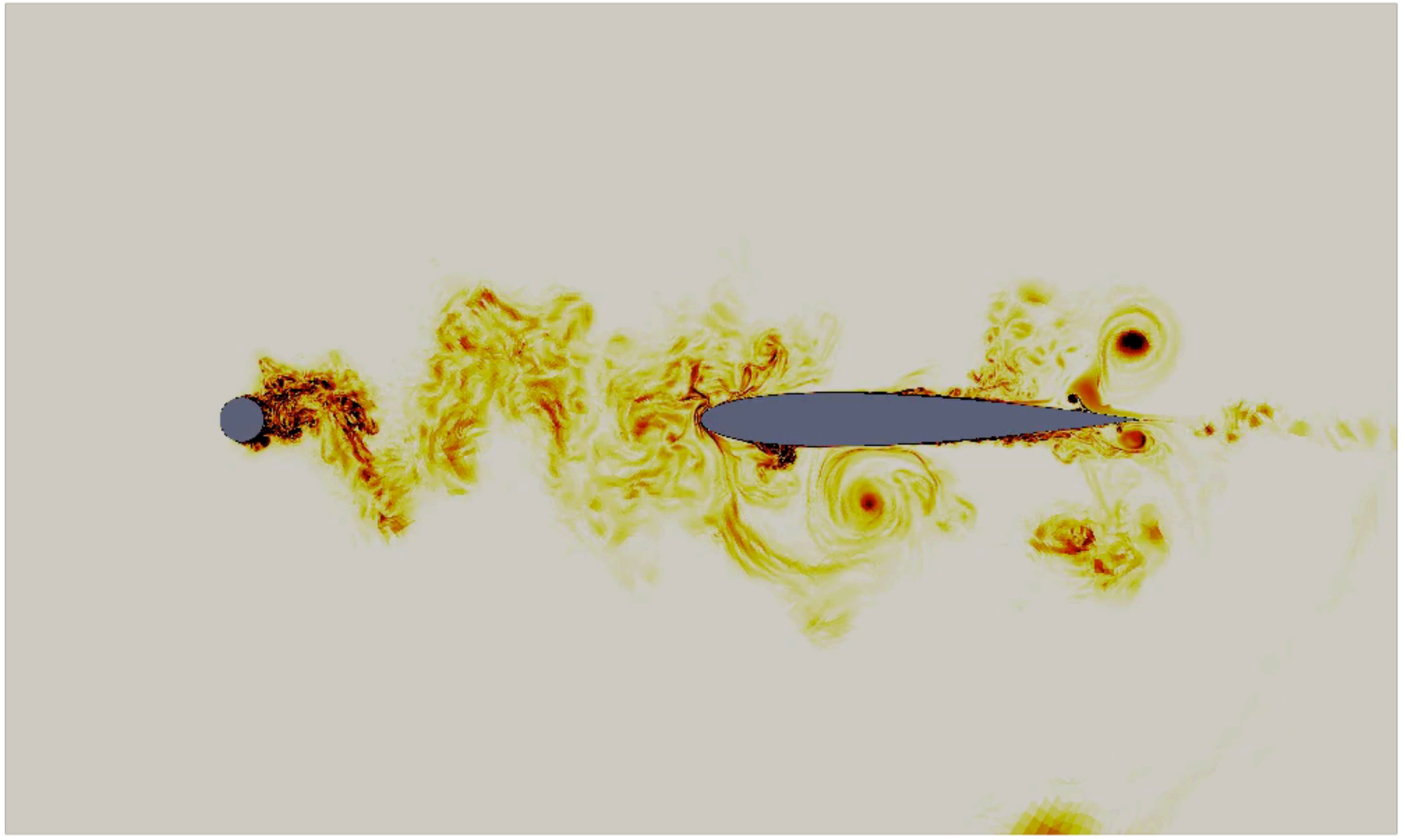
AMD
FIREPRO TECHNOLOGY

intel

Computers

- Emerald (CFI - UK)
- Wilkes (Cambridge University - UK)
- Piz Daint (CSCS - Switzerland)

Questions



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