PyFR: An Open Source Python Framework for High-Order CFD on Heterogeneous Platforms

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Our Motivation

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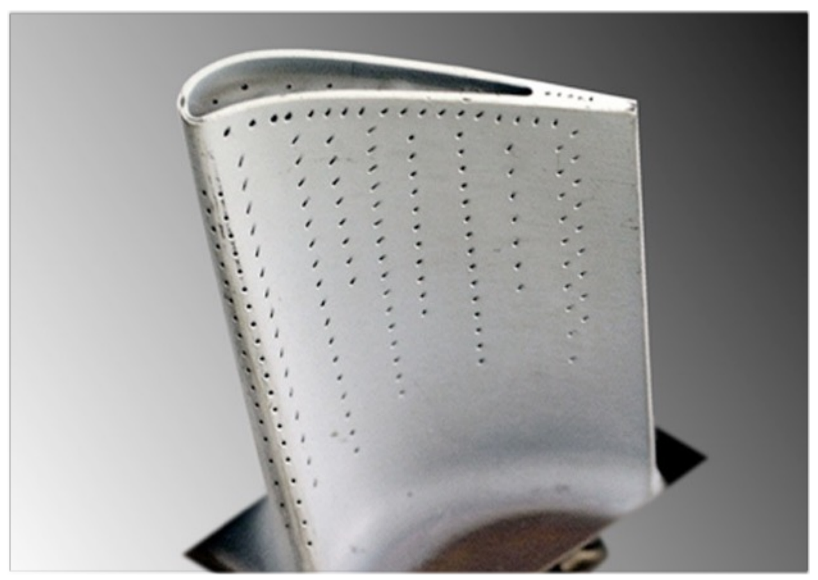
Current industry standard CFD tools have limited capabilities

Our Motivation

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

Our Motivation



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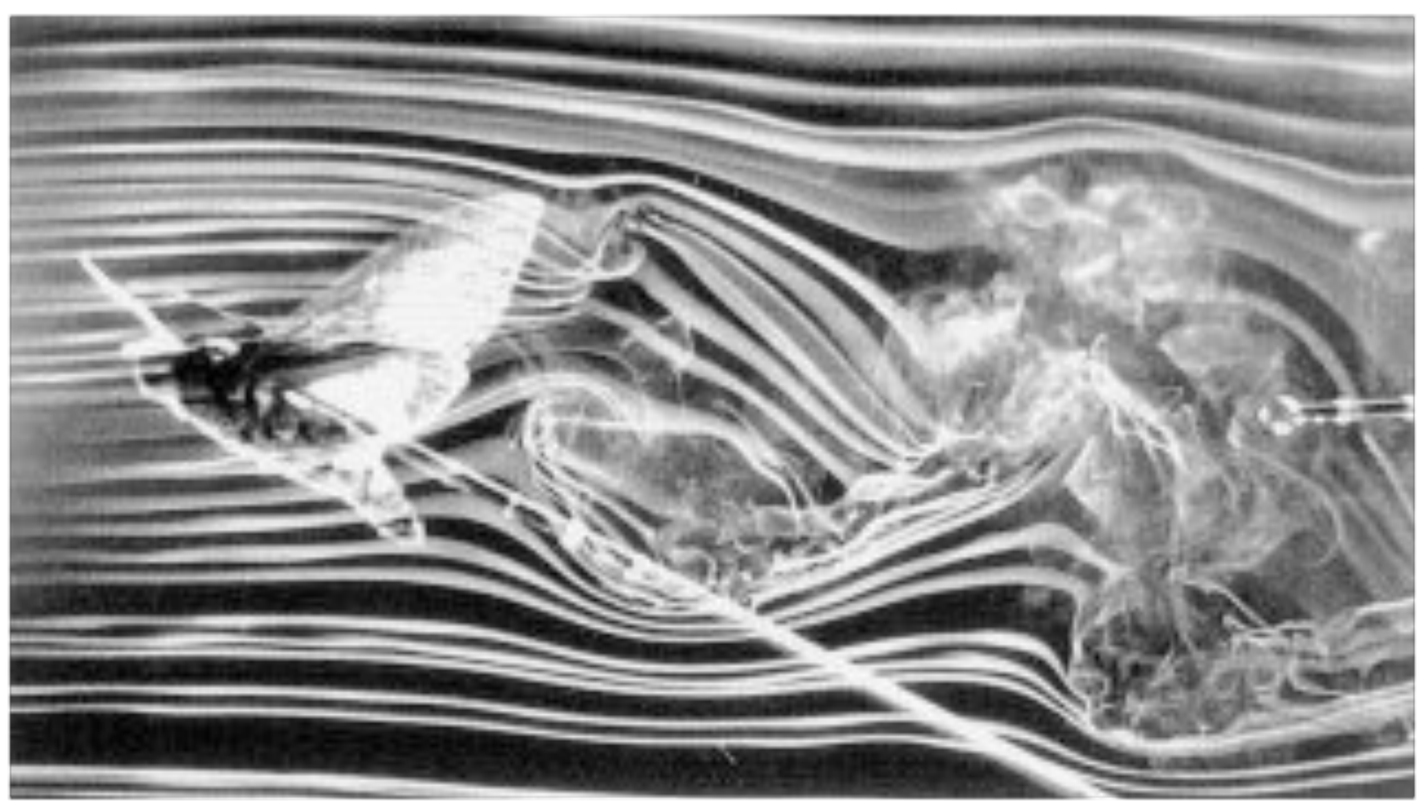
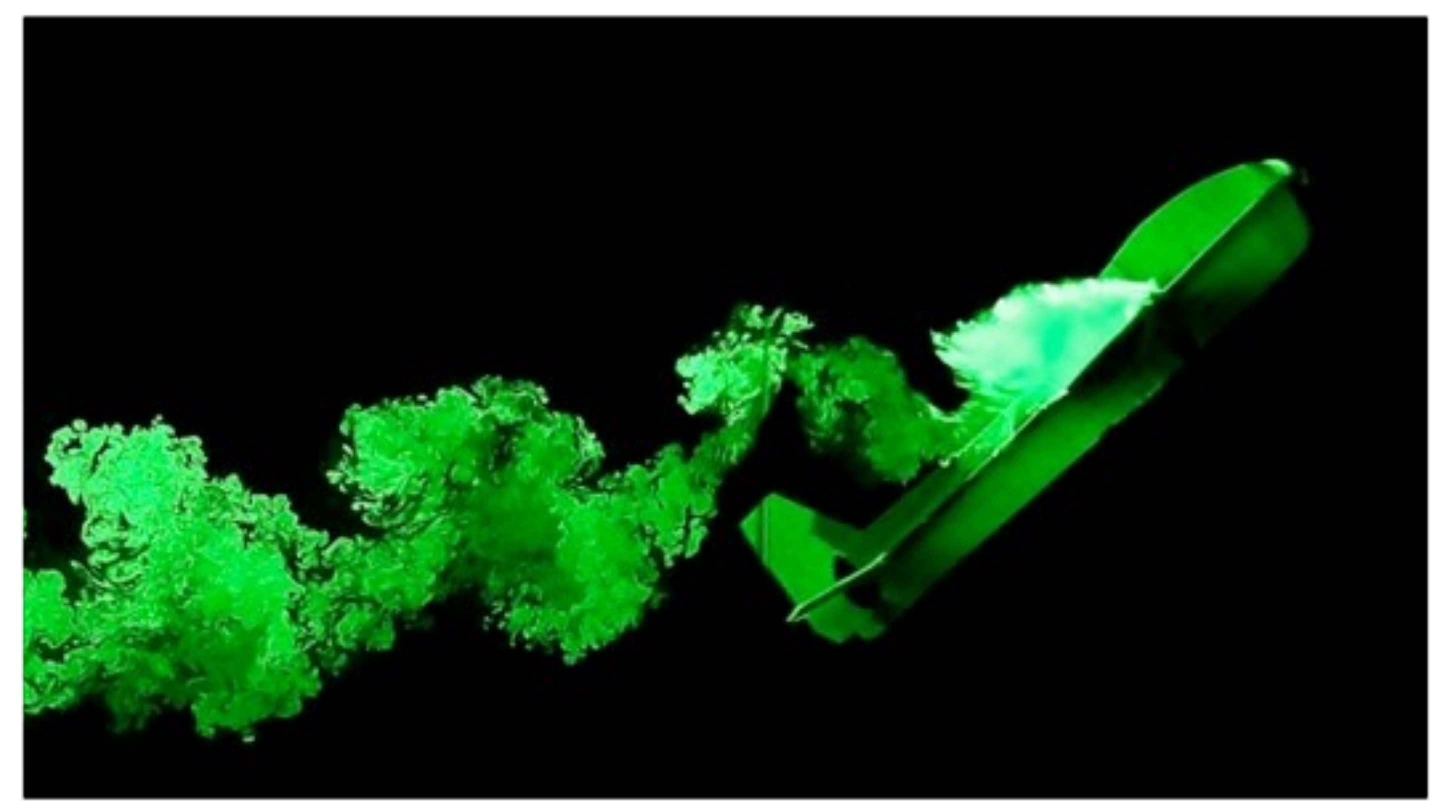
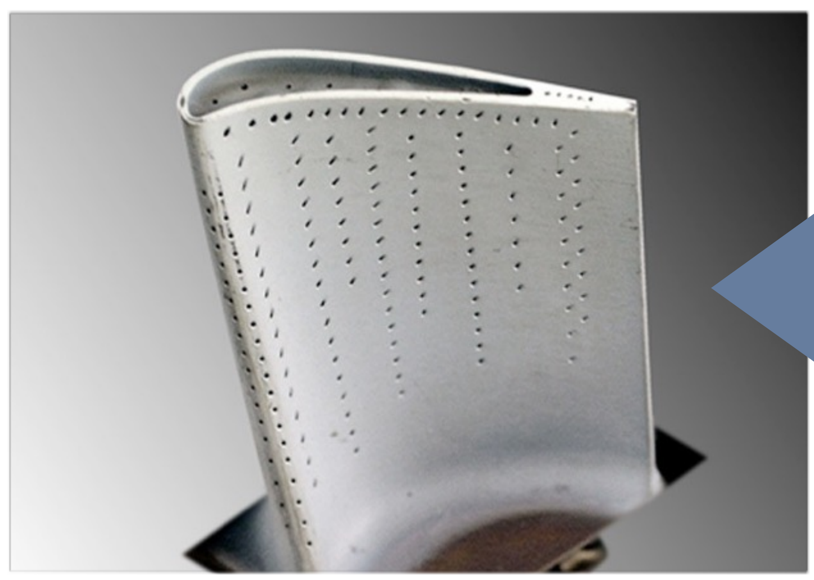
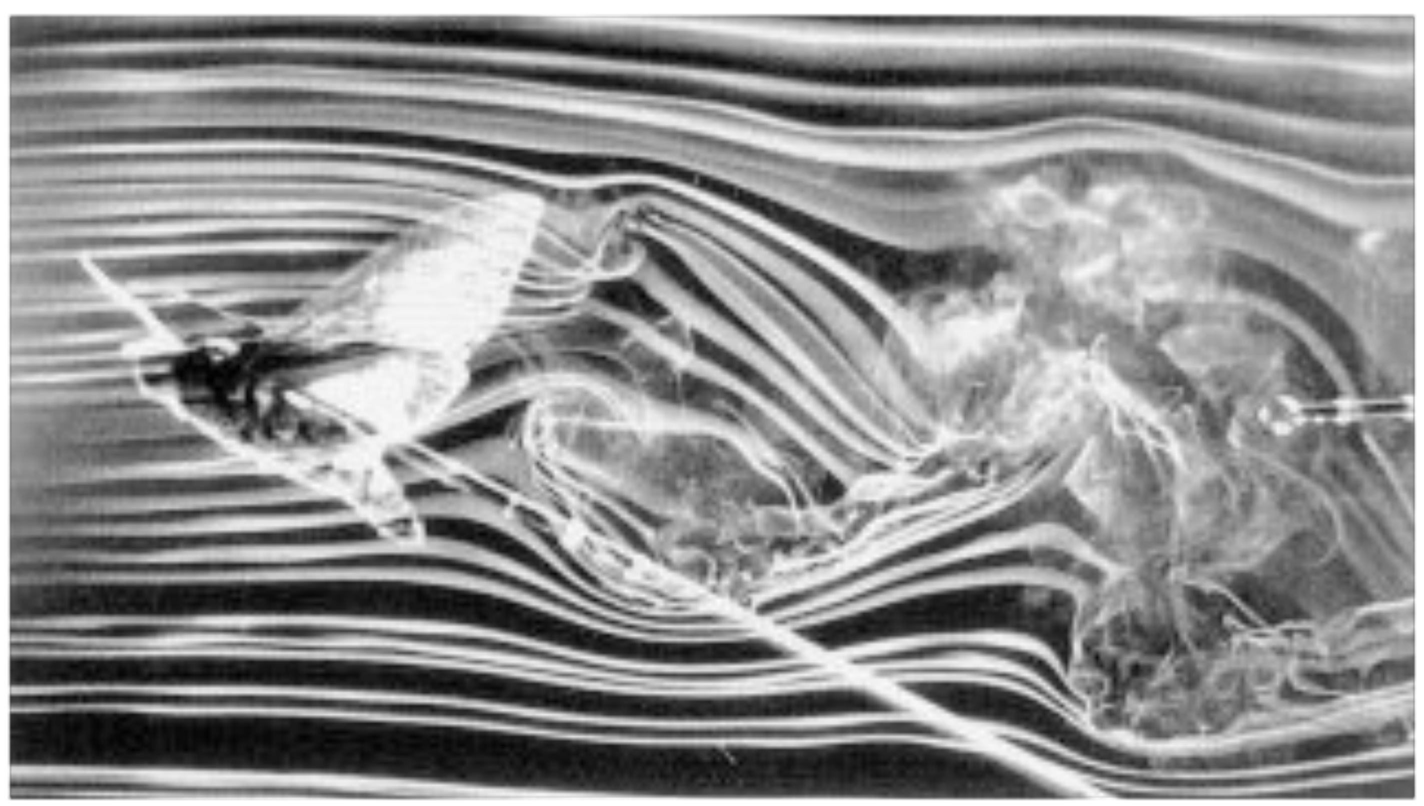


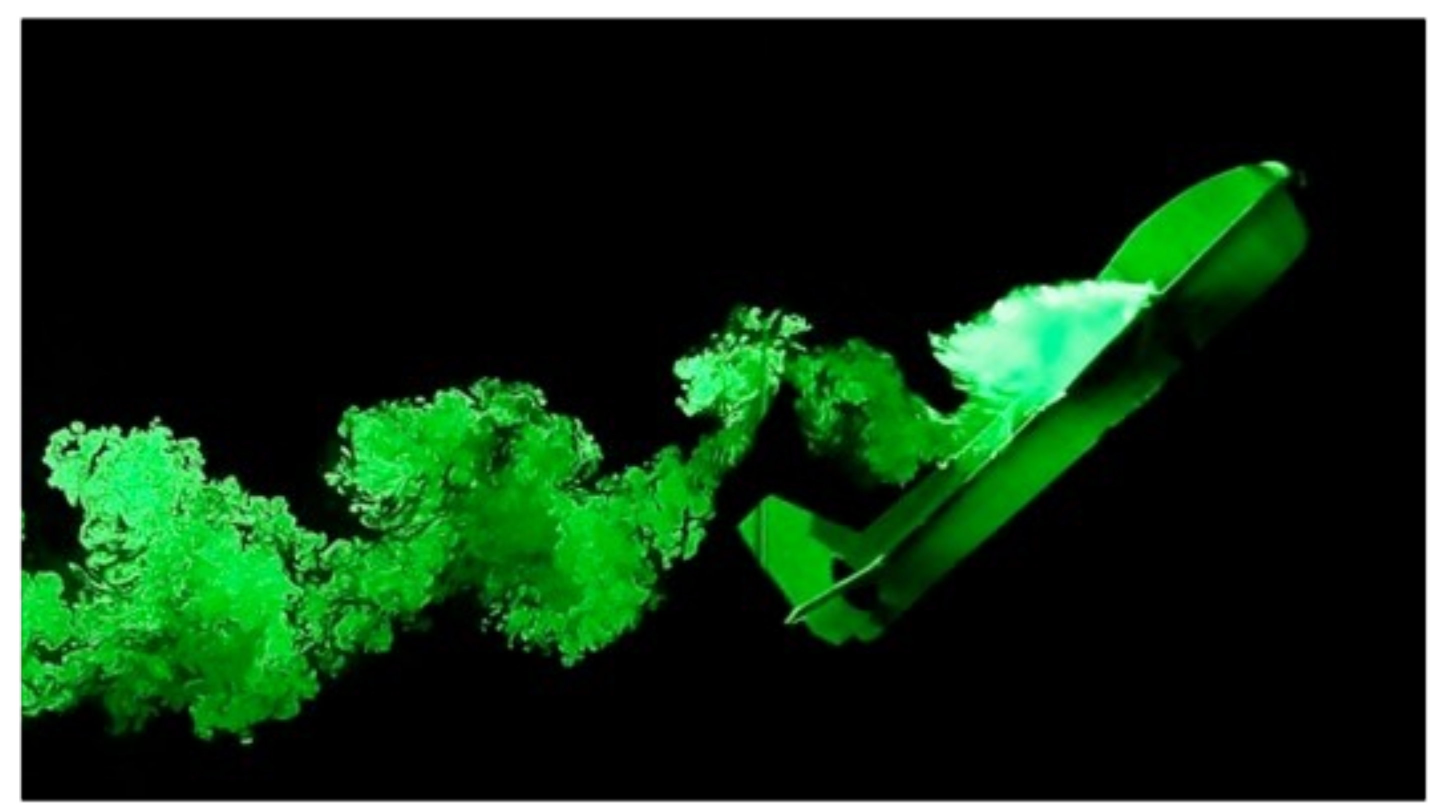


Our Motivation

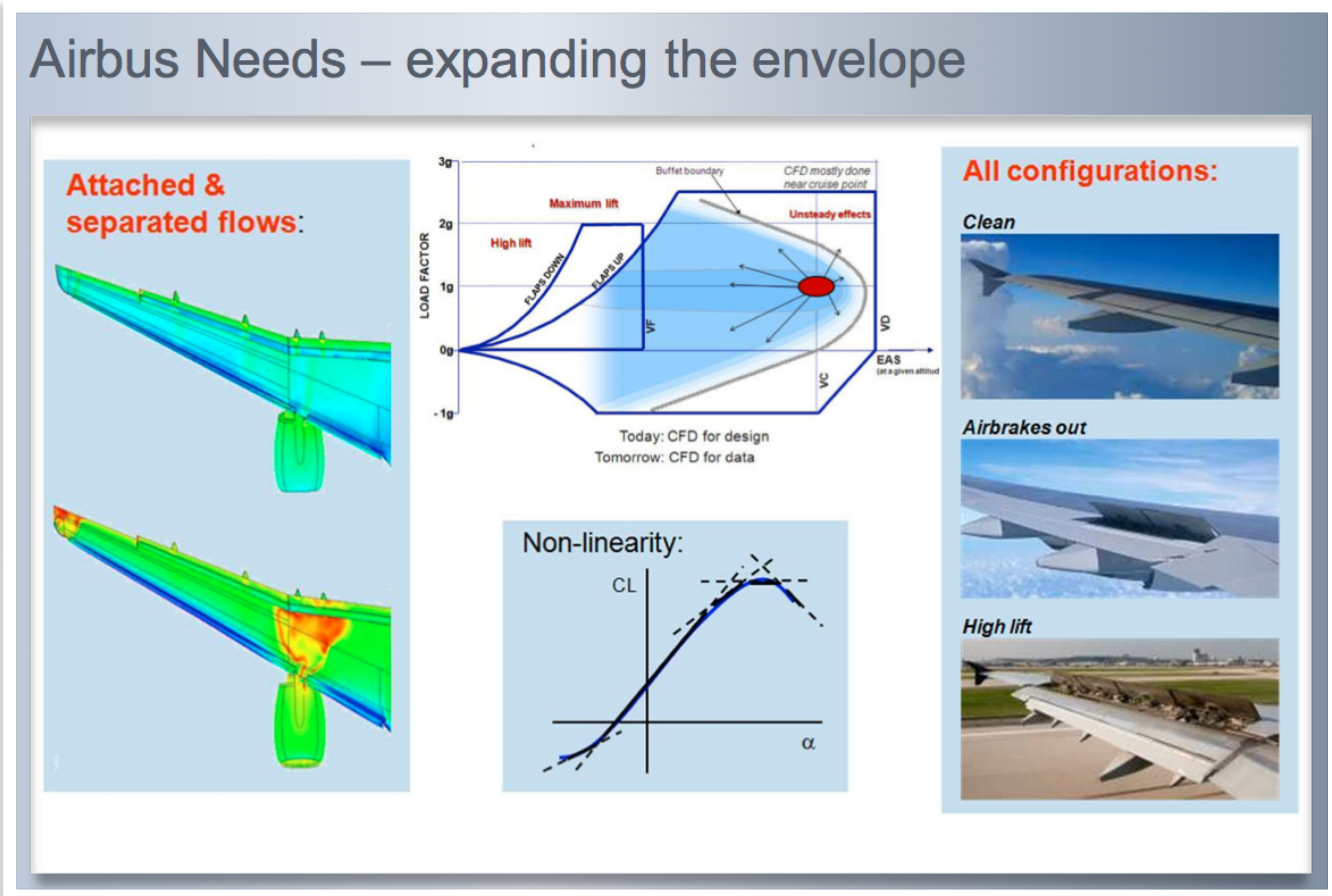


Need to expand the 'industrial CFD envelope'





Our Motivation



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

Our Motivation

- “reliable use of CFD has remained confined to a small but important region of the operating design space due to the inability of current methods to reliably predict turbulent separated flows” [2]

[2] J. Slotnick et al. Vision 2030 Study: A Path to Revolutionary Computational Aerosciences, NASA Langley Research Center Report, 2013

Our Motivation

- Objective of our research is to advance industrial CFD capabilities from their current 'RANS plateau'

Our Motivation

- Plan to achieve this by leveraging benefits of (and synergies between) high-order Flux Reconstruction (FR) methods for unstructured grids and massively-parallel modern hardware platforms

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

Flux Reconstruction

- Consider 1D scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0$$

- Divide 1D domain into elements

$$\Omega = \bigcup_{n=0}^{N-1} \Omega_n \qquad \bigcap_{n=0}^{N-1} \Omega_n = \emptyset \qquad \Omega_n = \{x | x_n < x < x_{n+1}\}$$

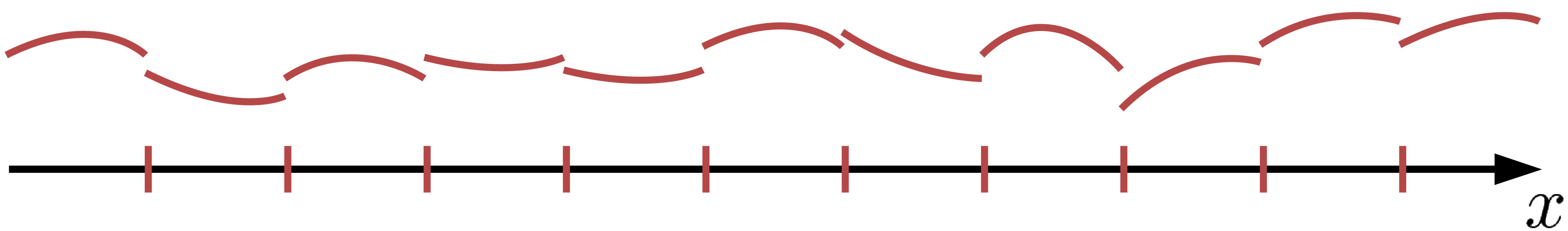
Flux Reconstruction

- Consider 1D scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0$$

- Represent solution by order k piecewise discontinuous polynomials in each element

$$u^\delta = \bigoplus_{n=0}^{N-1} u_n^\delta \approx u$$



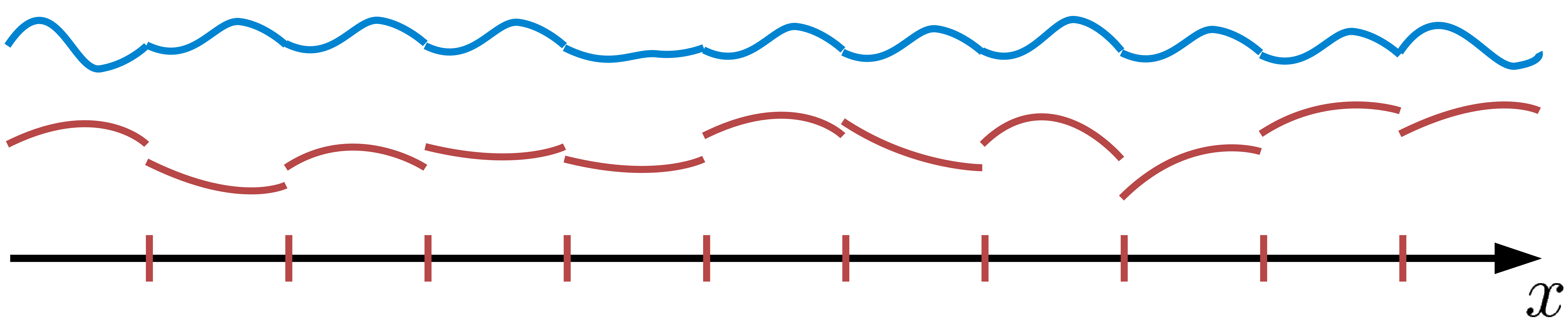
Flux Reconstruction

- Consider 1D scalar conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0$$

- Represent flux by order k+1 piecewise continuous polynomials within each element

$$f^{\delta} = \bigoplus_{n=0}^{N-1} f_n^{\delta} \approx f$$



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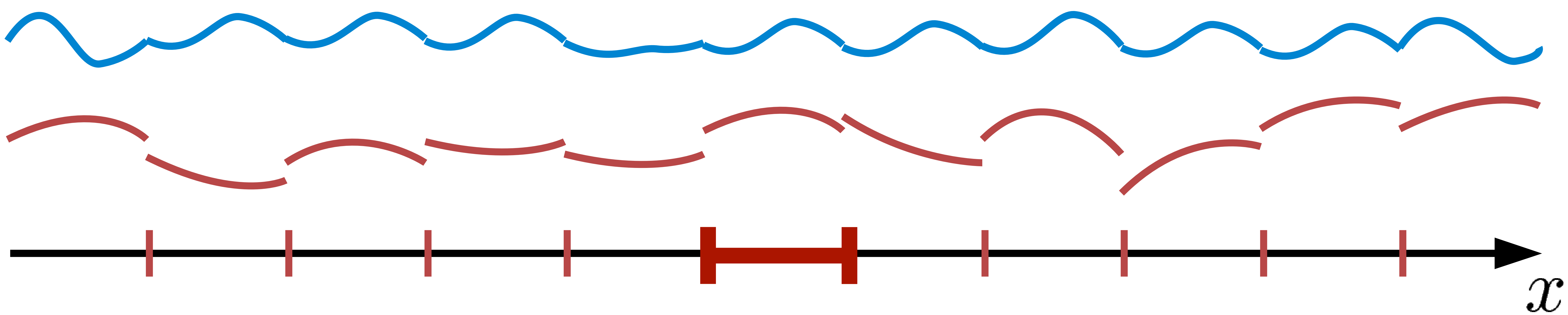
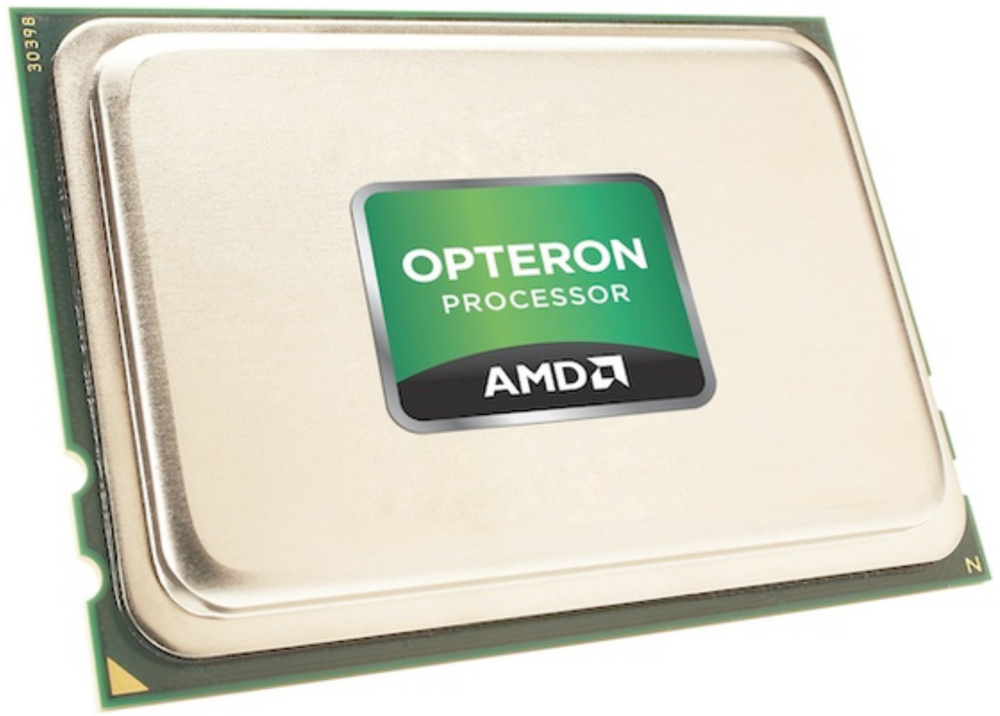


Flux Reconstruction

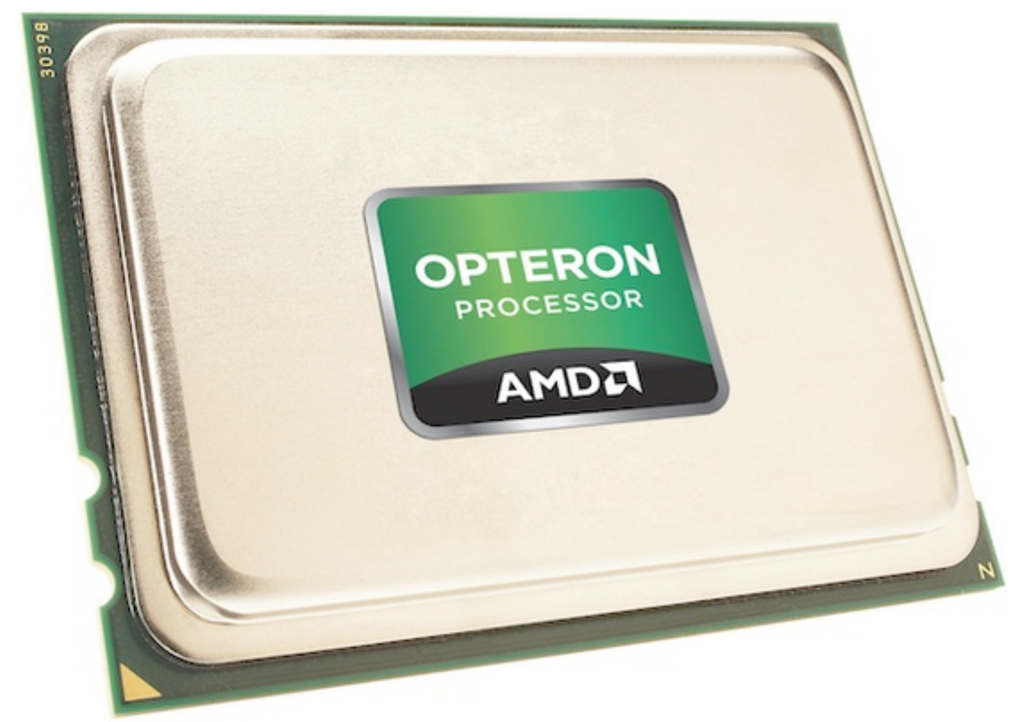
- Nature of FR scheme depends on location of solution points, interface flux, correction function
- Can recover a wide range of schemes via judicious choice of correction function [5]
- A family of provably stable FR schemes have been identified [6]

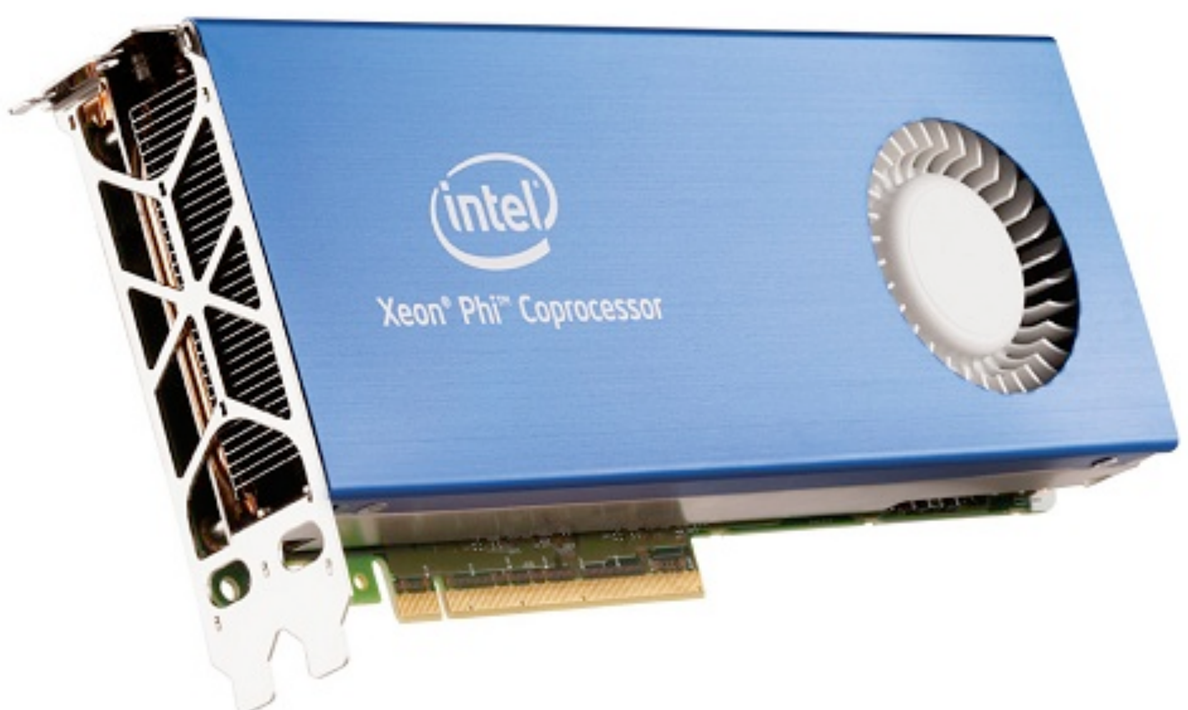
[5] H.T. Huynh. A flux Reconstruction Approach to High-Order Schemes Including Discontinuous Galerkin Methods. AIAA Paper 2007-4079. 2007
[6] P. E. Vincent, et al. An Extended Range of Stable-Symmetric-Conservative Flux Reconstruction Correction Functions. Computer Methods in Applied Mechanics and Engineering. 2015

Modern Hardware



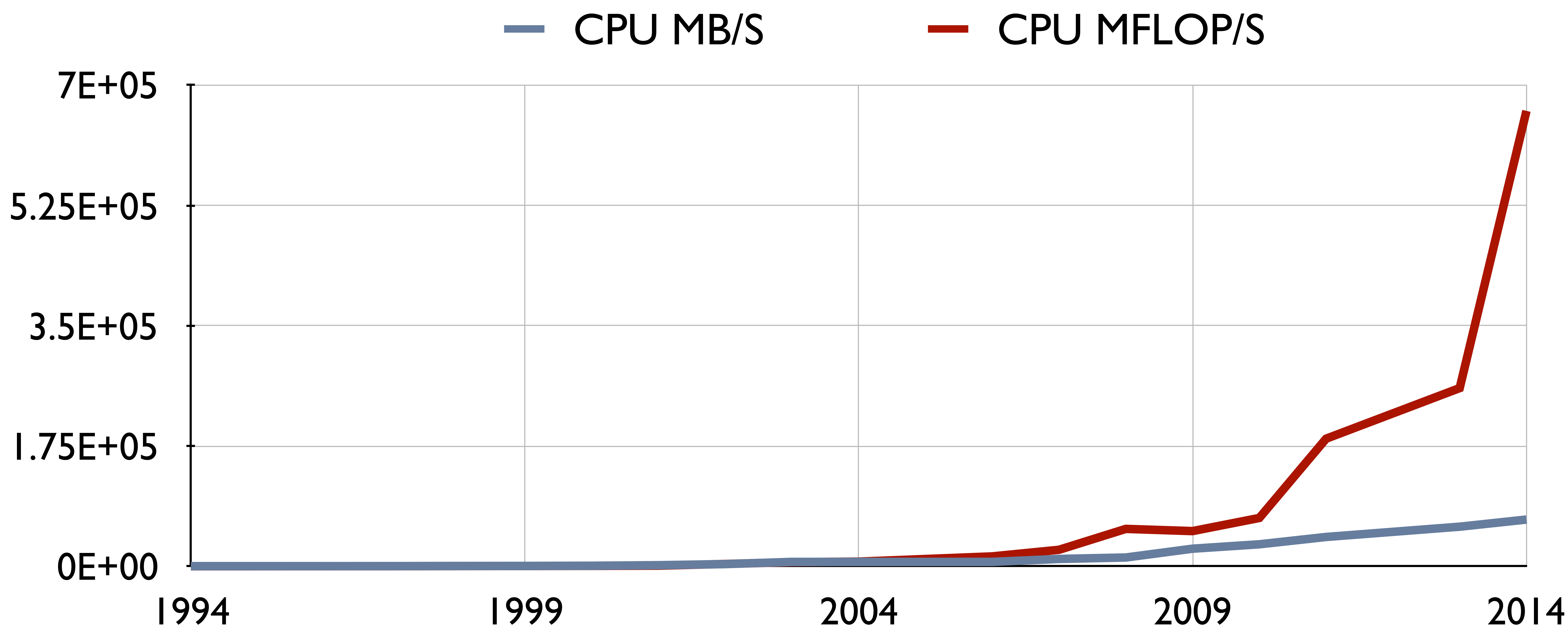
Modern Hardware





Modern Hardware

- FLOPS increasing faster than memory bandwidth [7]



[7] F. D. Witherden et al. 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 …

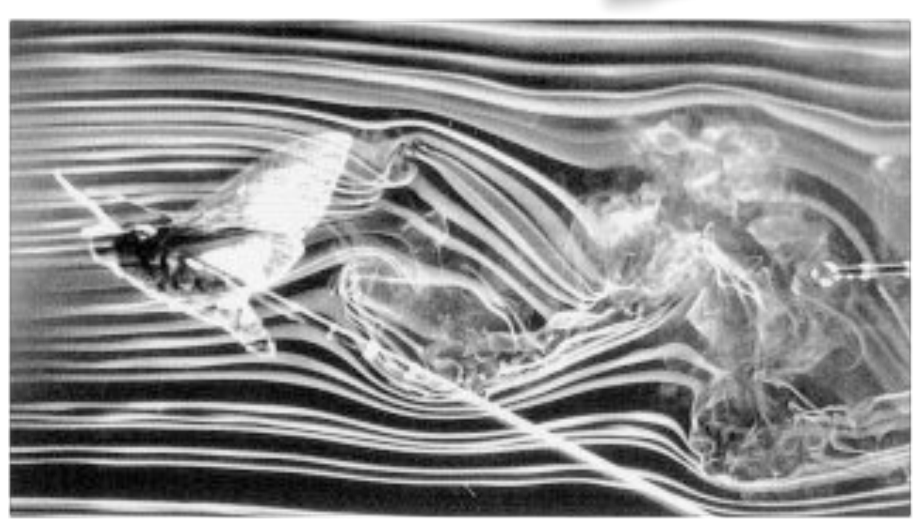
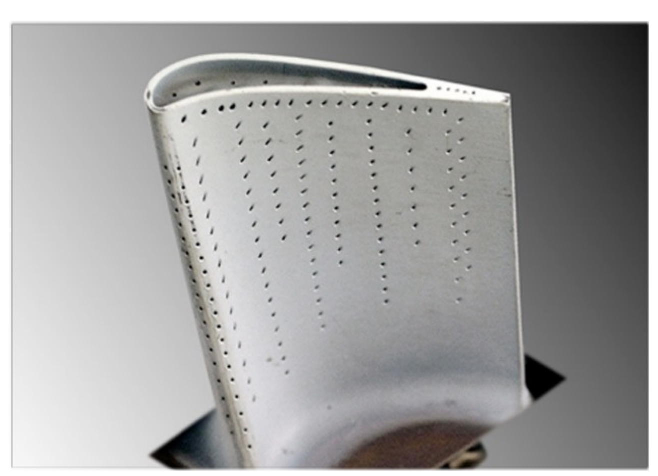
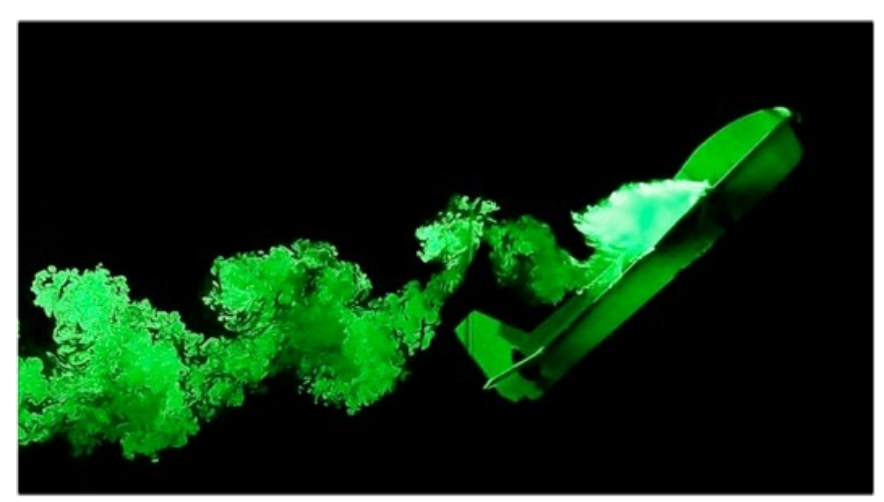
2.91TFLOPS
(Double Precision)

PyFR

Flux Reconstruction
PyFR
Modern Hardware





PyFR

- Features (v1.4.0 - released tomorrow)

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) Xeon Phi Clusters (PyMIC-MPI)
Precision	Single Double
Input	Gmsh, CGNS
Output	Paraview

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PyFR

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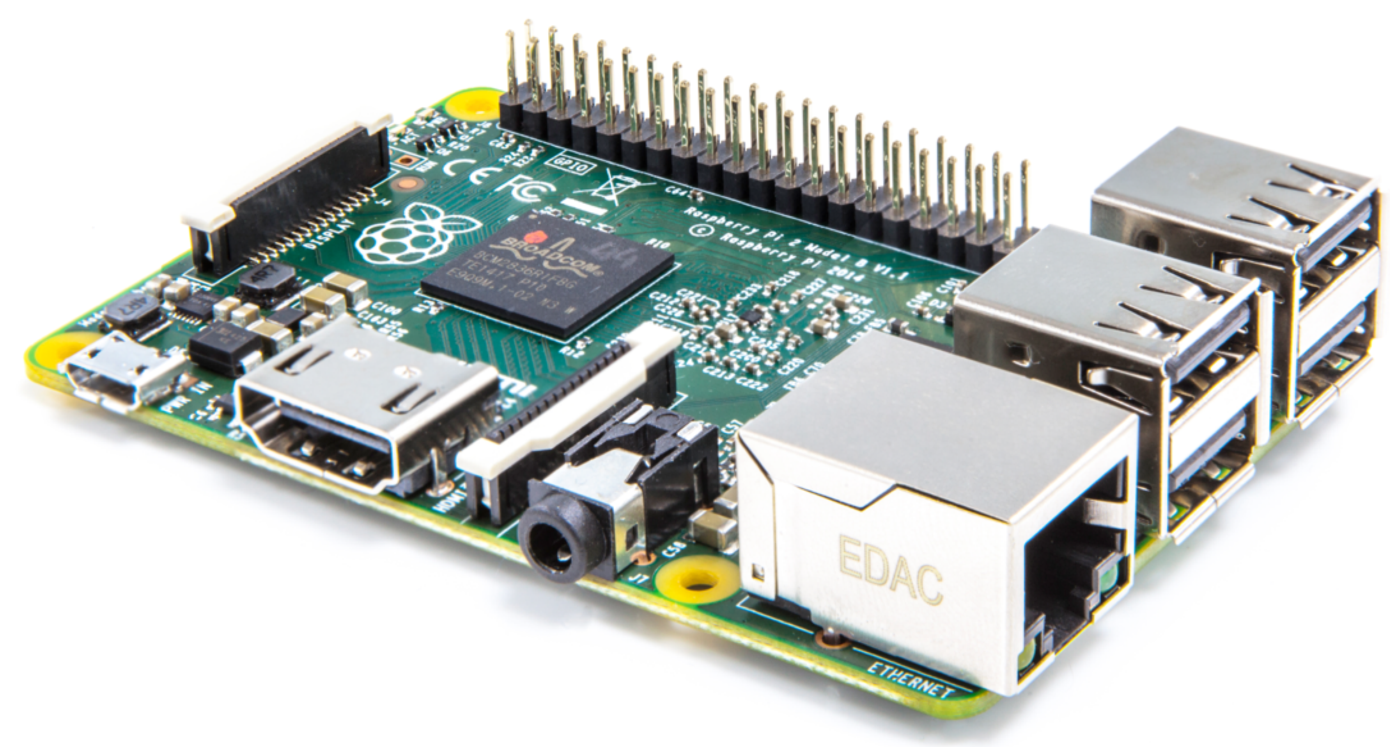

Raspberry Pi

PyFR

PyFR →

Macbook Pro

PyFR

PyFR

Heterogeneous Workstation

PyFR

Wilkes (UK)

PyFR

PyFR

Piz Daint
(Switzerland)

PyFR

PyFR →

Titan (USA)

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)

- Setup
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Matrix Multiply Kernels

- Data interpolation/ extrapolation etc.

Point-Wise Nonlinear Kernels

- Flux functions, Riemann solvers etc.

PyFR

- For matrix multiply kernels it is pretty easy …

Python Outer Layer
(Hardware Independent)

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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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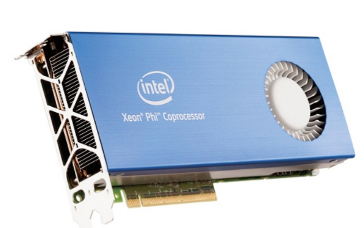
C/OpenMP Hardware Specific Kernels

CUDA Hardware Specific Kernels

PyMIC Hardware Specific Kernels



OpenCL Hardware Specific Kernels

PyFR

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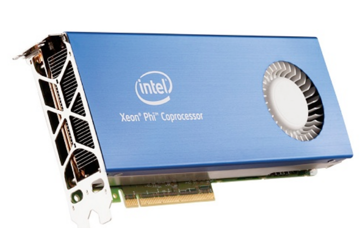
PyMIC
Hardware Specific Kernels



OpenCL
Hardware Specific Kernels

Use DGEMM from vendor supplied BLAS

Pass Mako derived kernel templates through Mako derived templating engine

PyFR

- ~8.0k lines of code

PyFR

- Open source '3 Clause New Style BSD License'

open source initiative®

PyFR

PyFR

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

[8] F. D. Witherden et al. PyFR: An Open Source Framework for Solving Advection-Diffusion Type Problems on Streaming Architectures using the Flux Reconstruction Approach. Computer Physics Communications. 2014

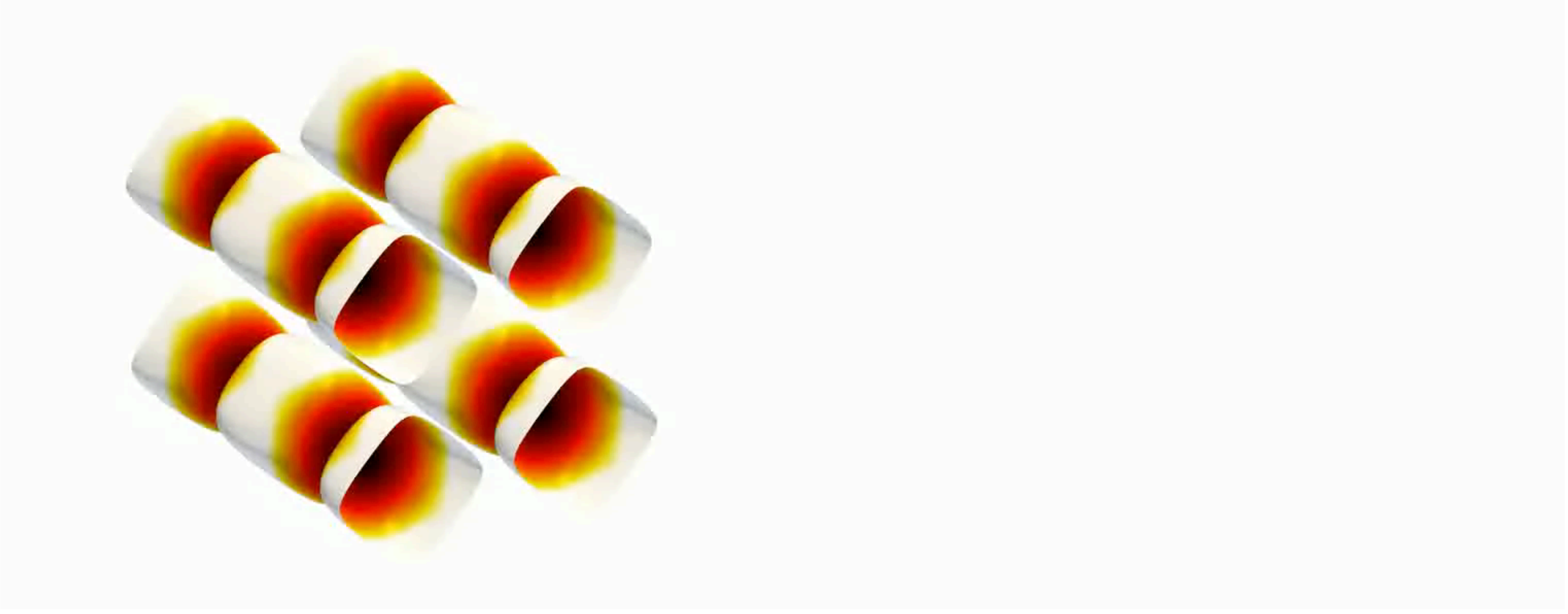
Results

- 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

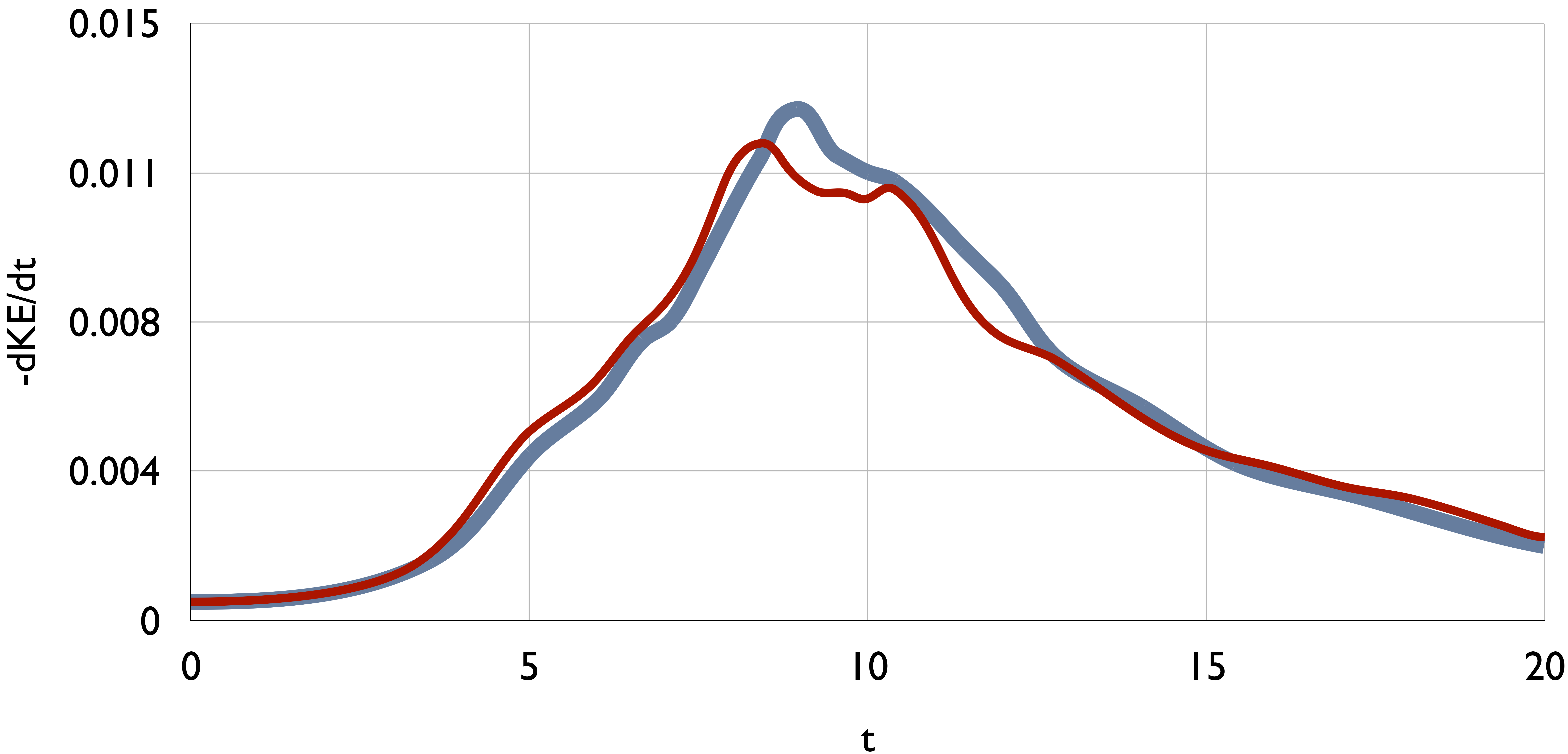
Results

- A movie ...



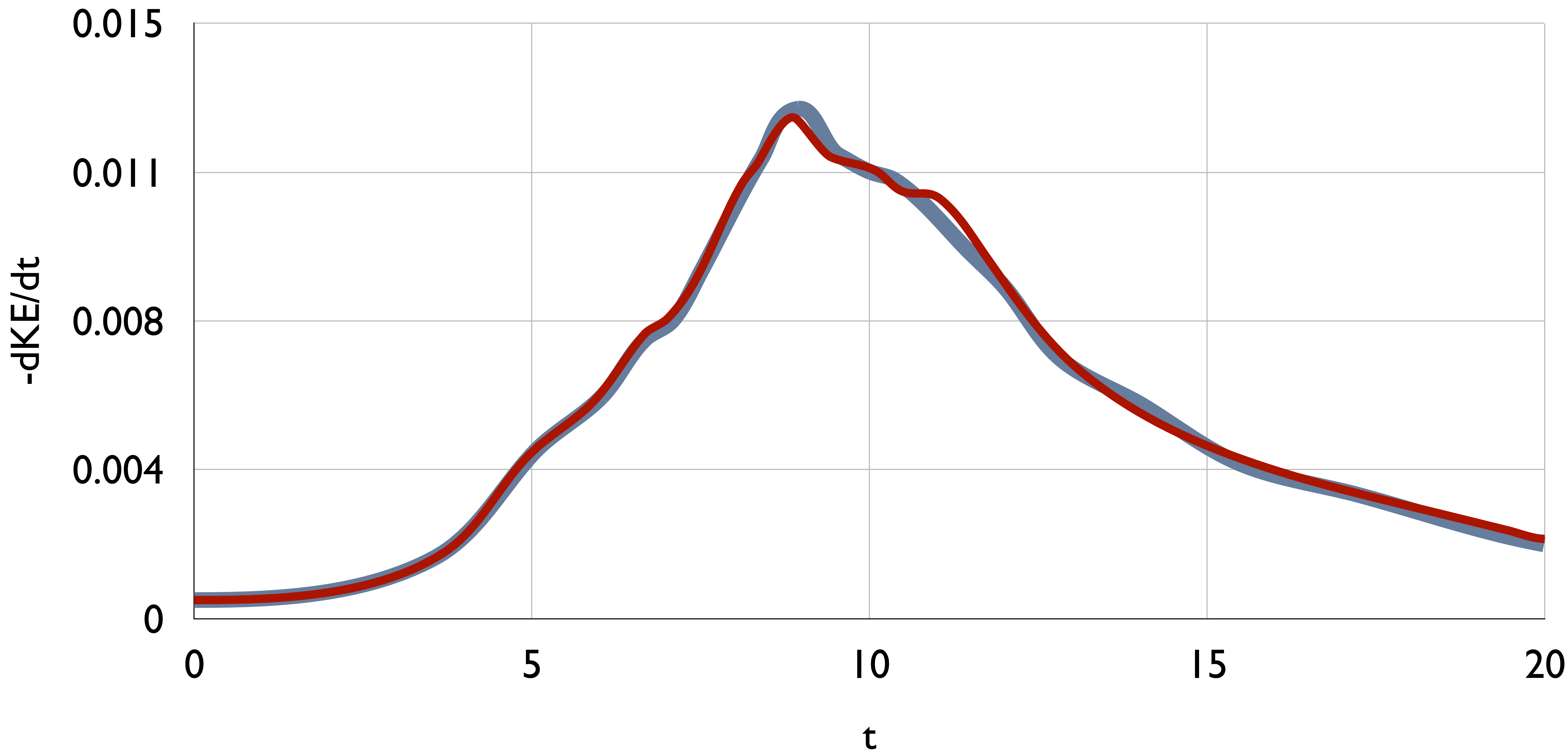
Results

- van Rees et al. spectral DNS + PyFR (2nd order hex)



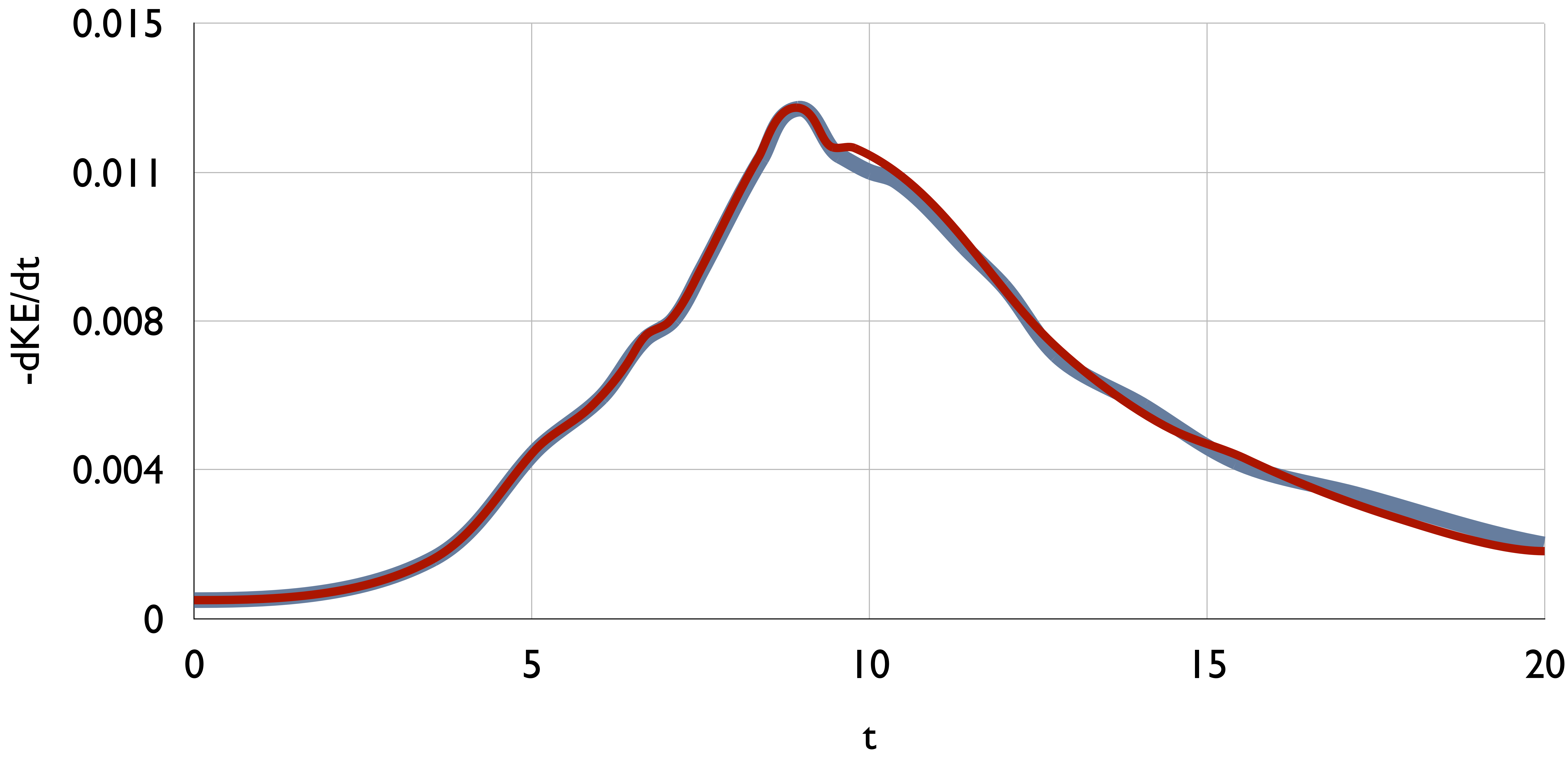
Results

- van Rees et al. spectral DNS + PyFR (3rd order hex)



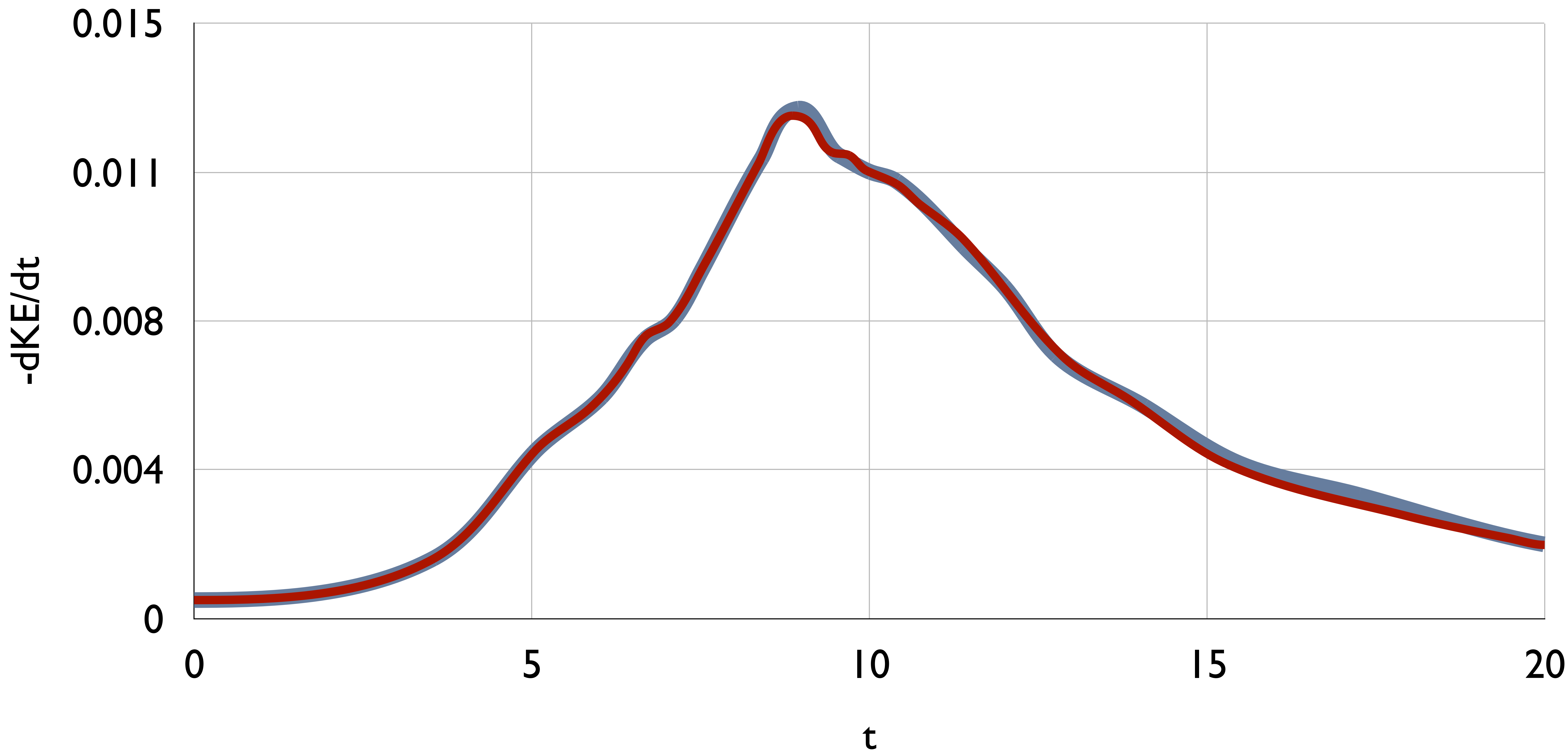
Results

- van Rees et al. spectral DNS + PyFR (4th order hex)



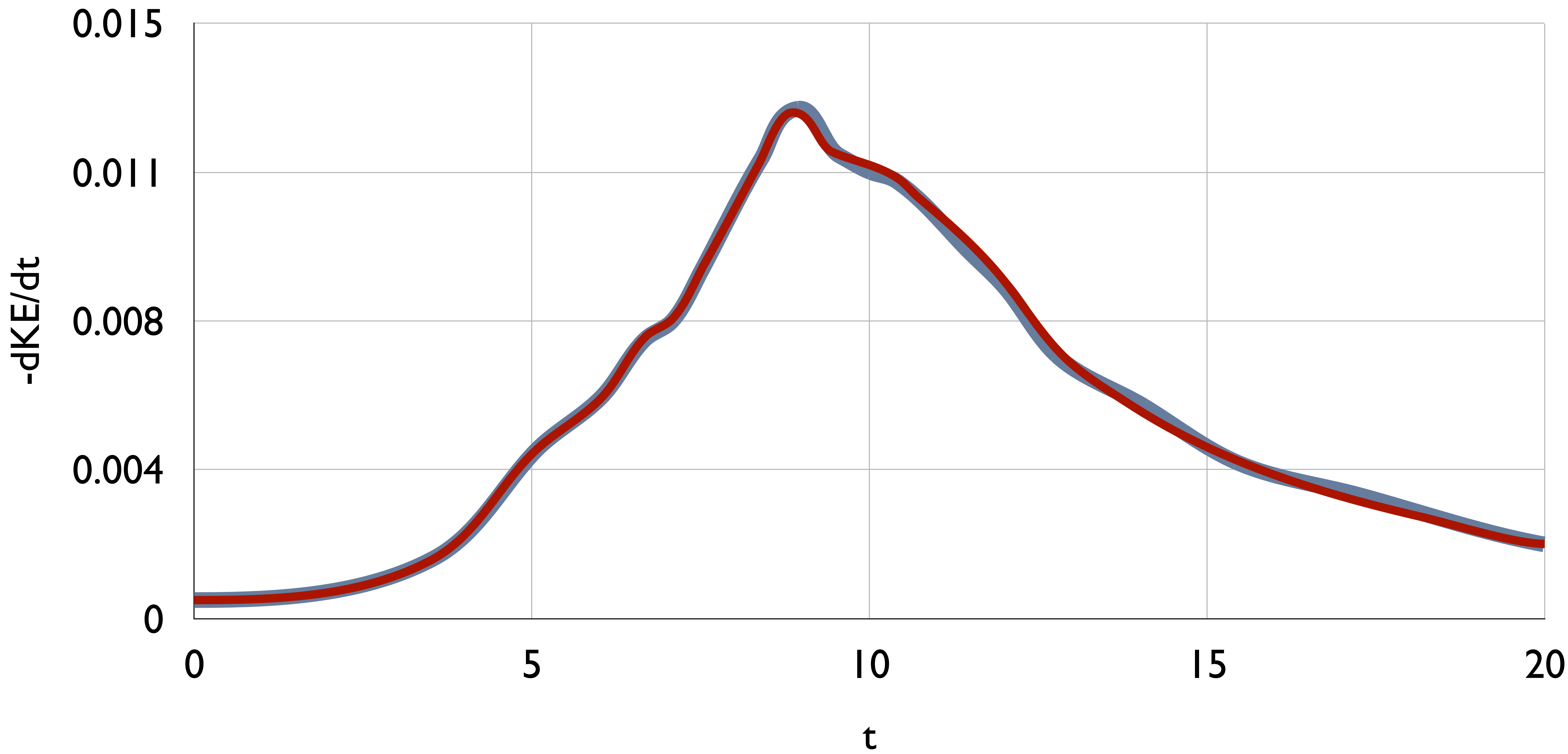
Results

- van Rees et al. spectral DNS + PyFR (5th order hex)



Results

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

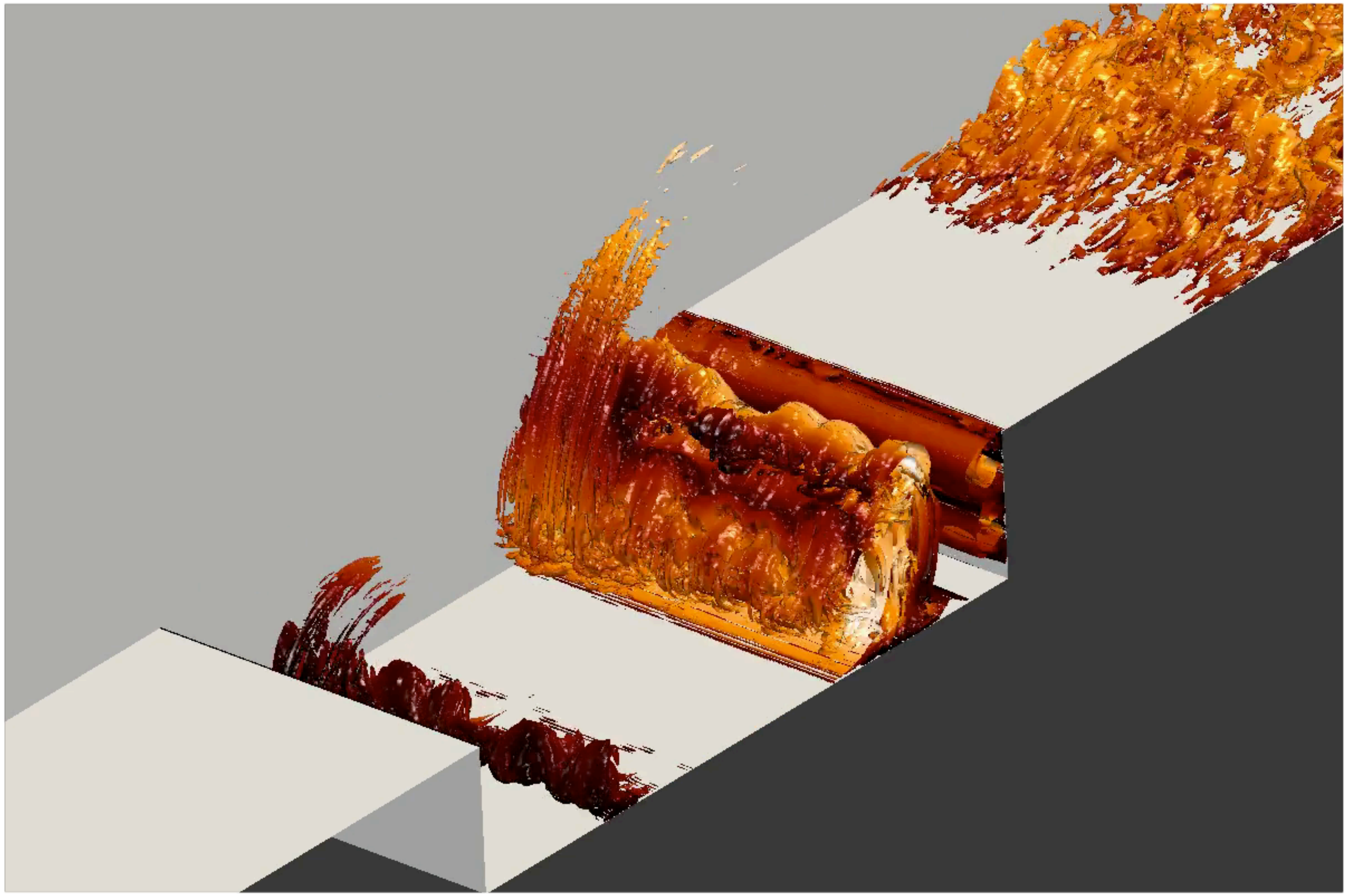


Results

- Flow over a cavity
- Re ~ 30,000
- Ma ~ 0.8

Results

- A movie …



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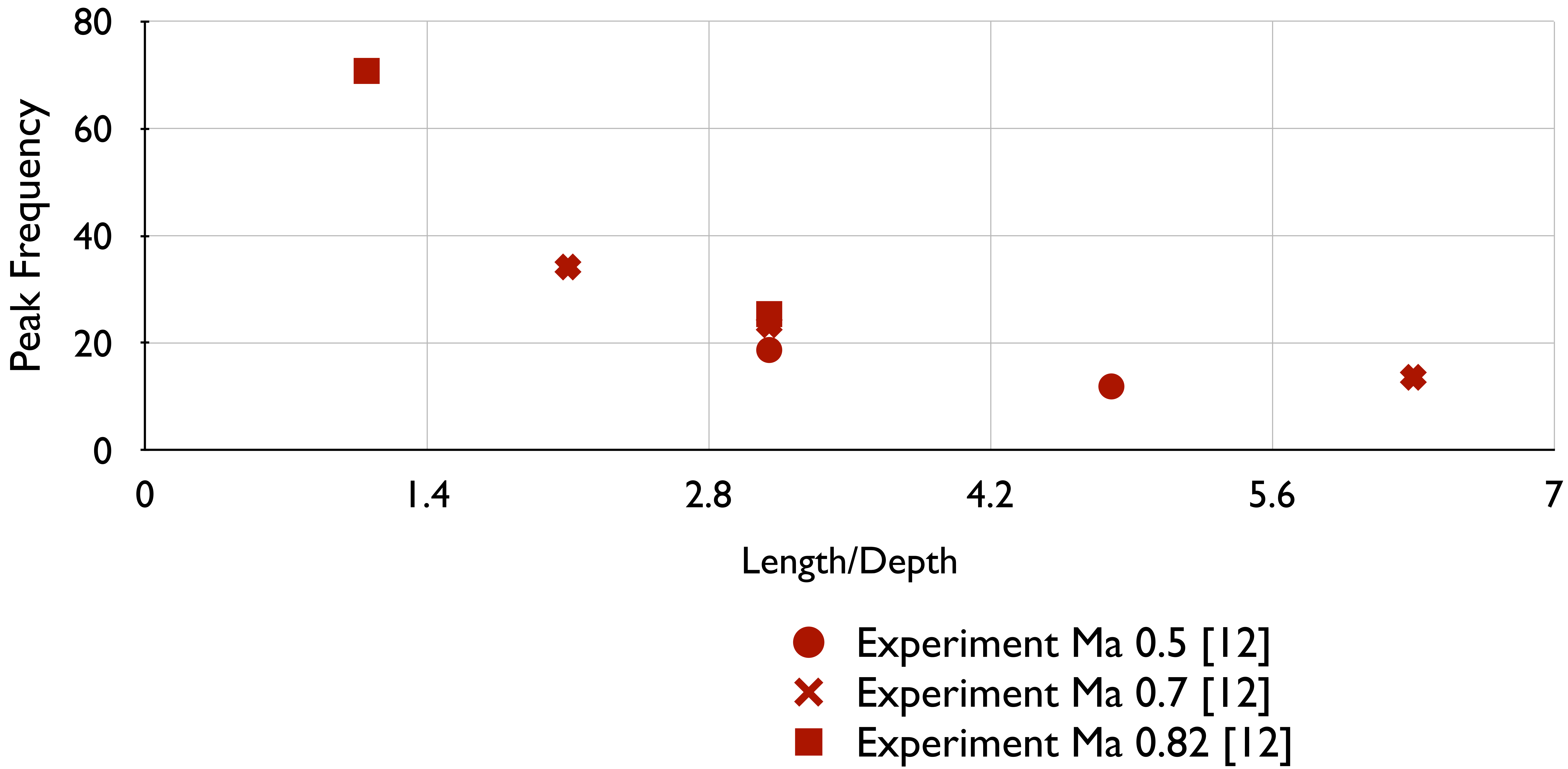
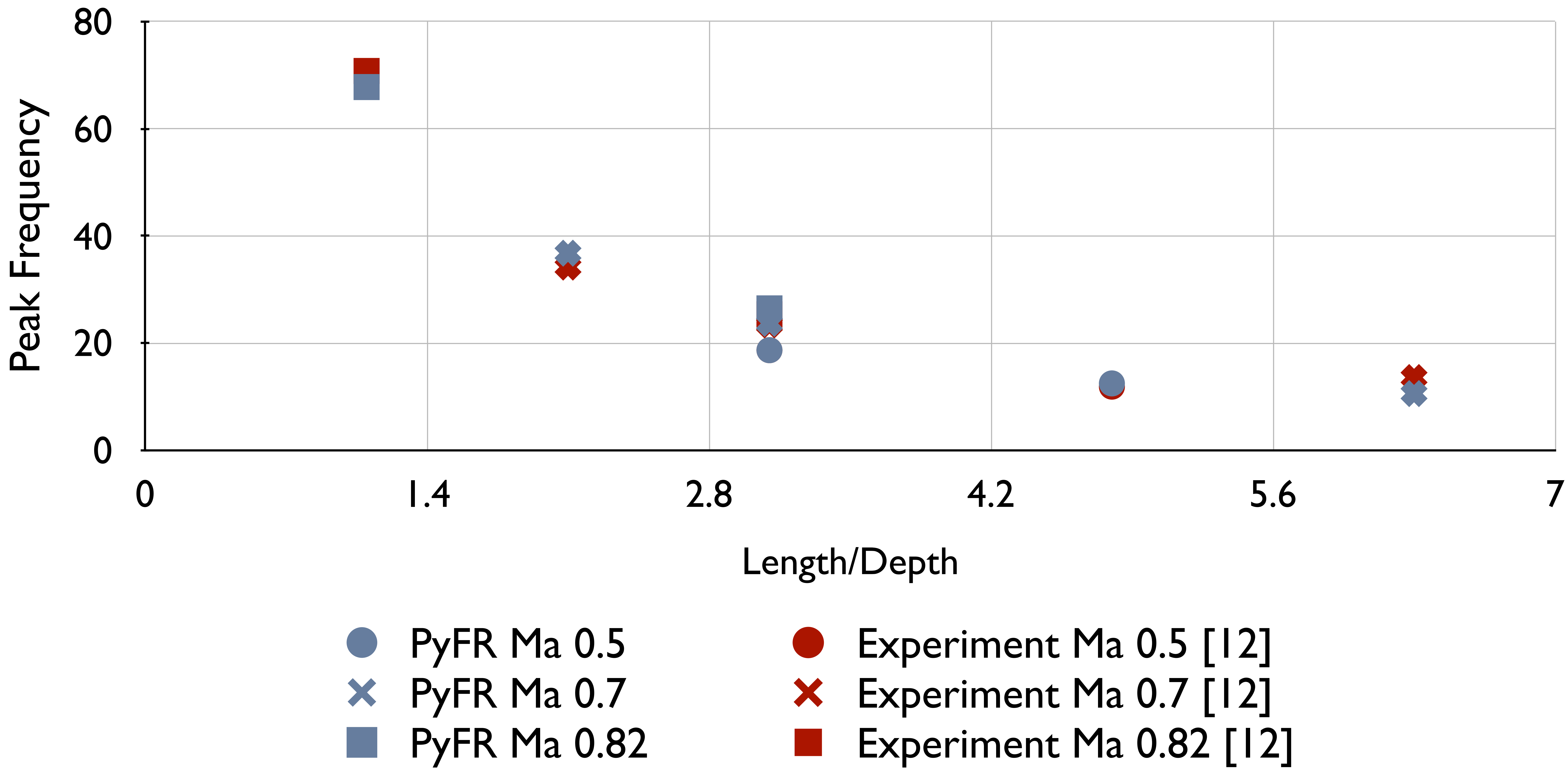


[10] K. Krishnamurty. Acoustic radiation from two-dimensional rectangular cutouts in aerodynamic surfaces. National Advisory Comittee for Aeronautics (NACA) TN3487. 1955

Results



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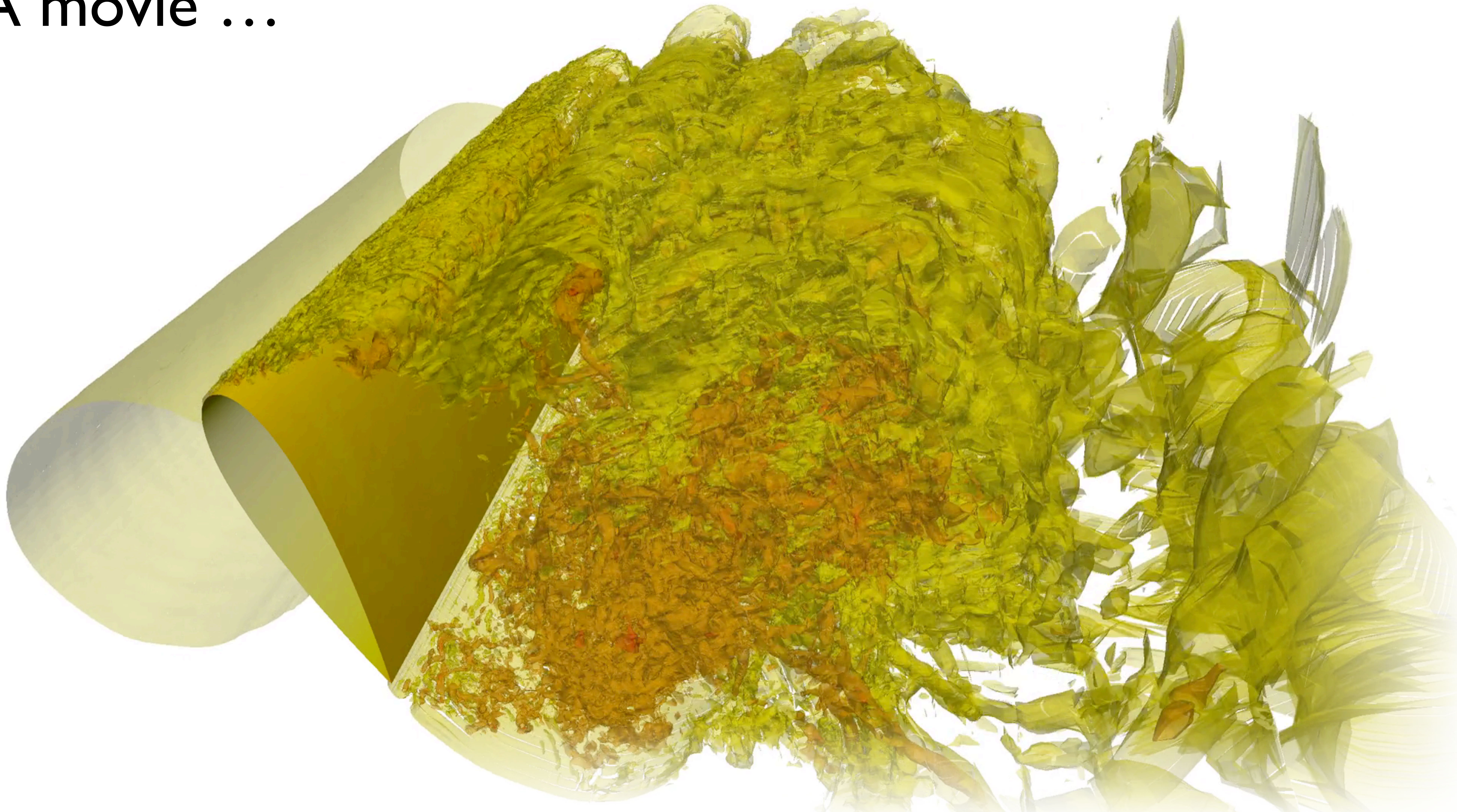
Results

- Flow over a NACA 0021 at 60 degree AoA
- Re = 270,000
- Ma = 0.1
- 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

- A movie …



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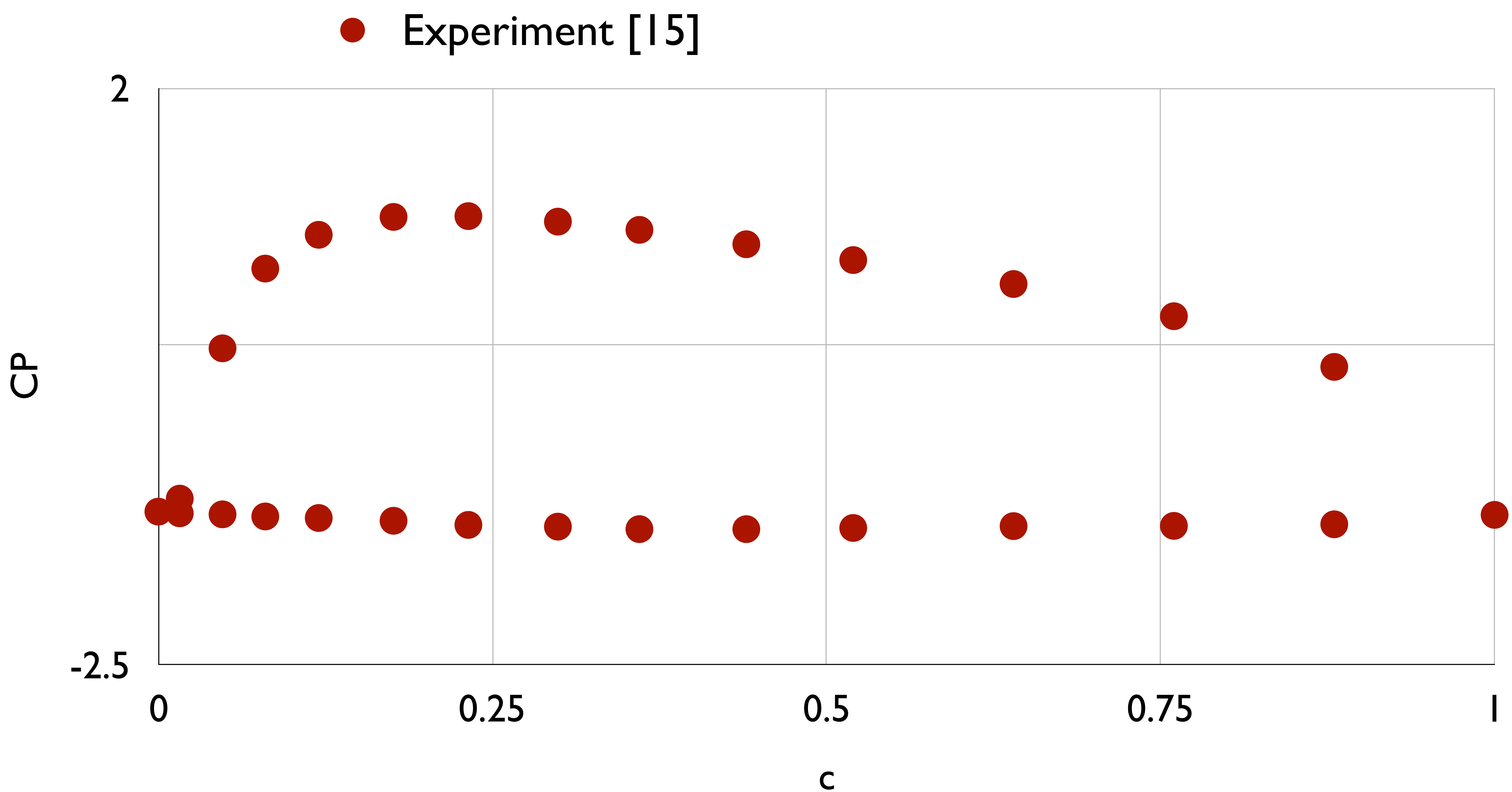

[15] K. Swalwell. The Effect of Turbulence on Stall of Horizontal Axis Wind Turbines. PhD Thesis. 2005.

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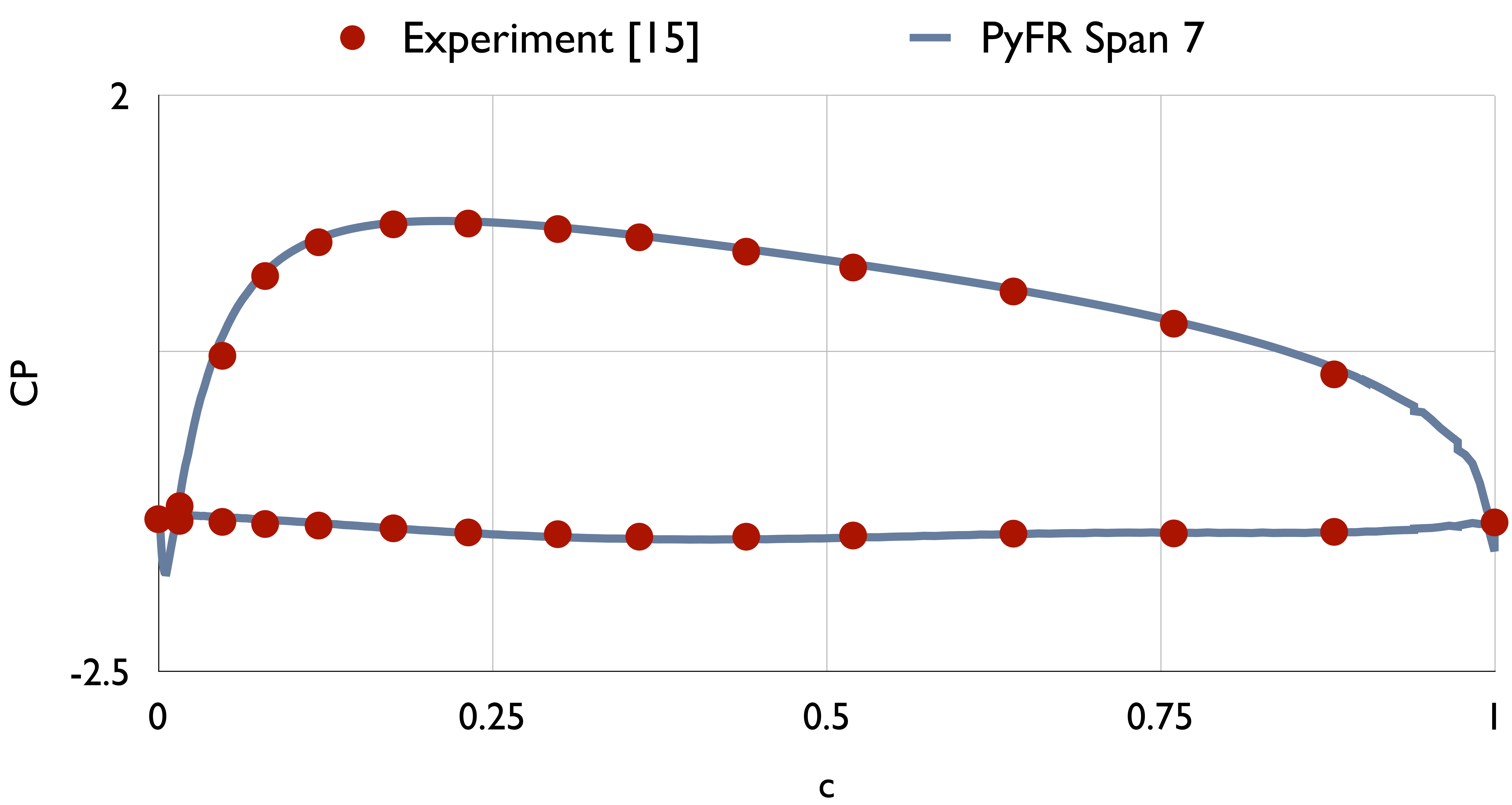

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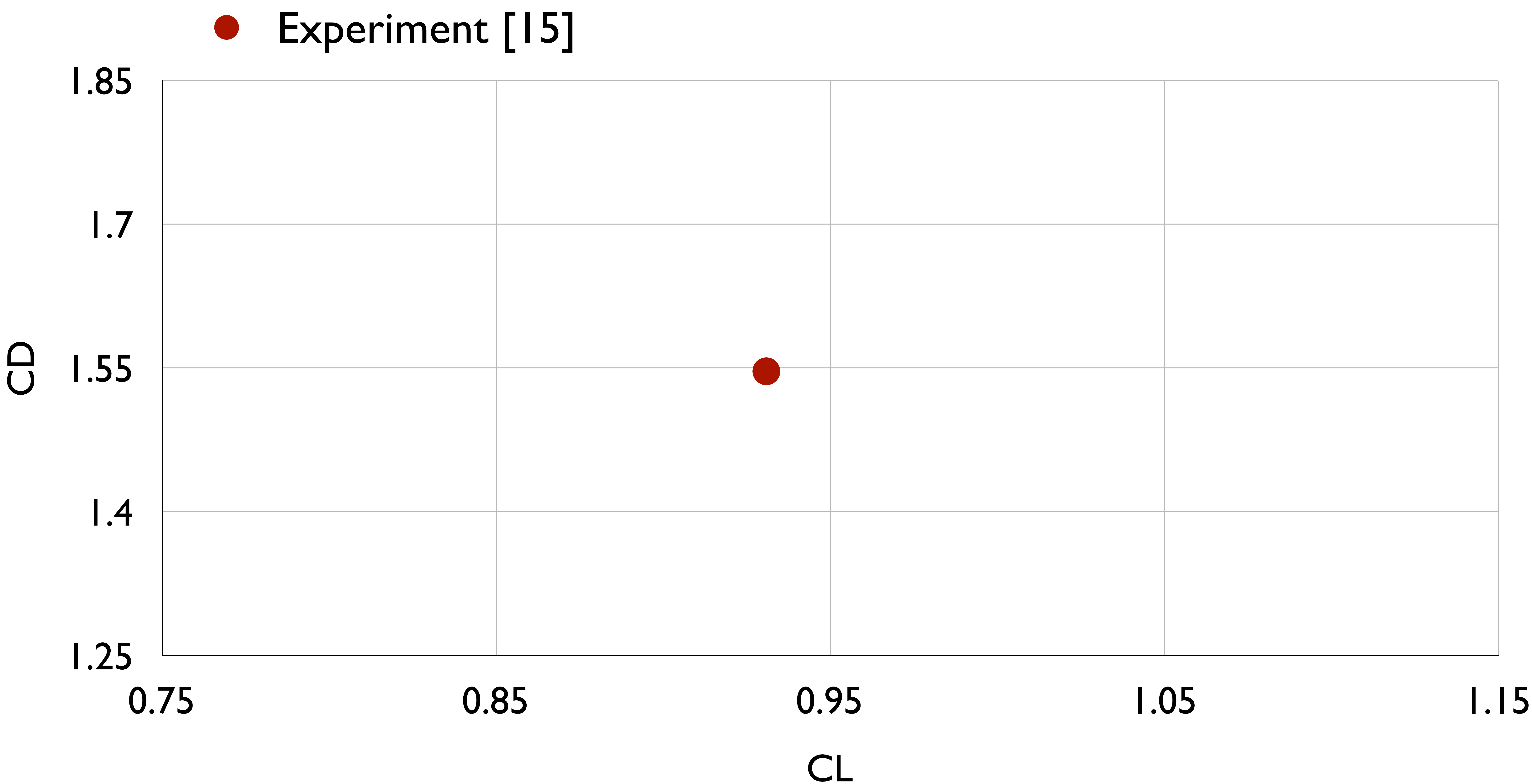

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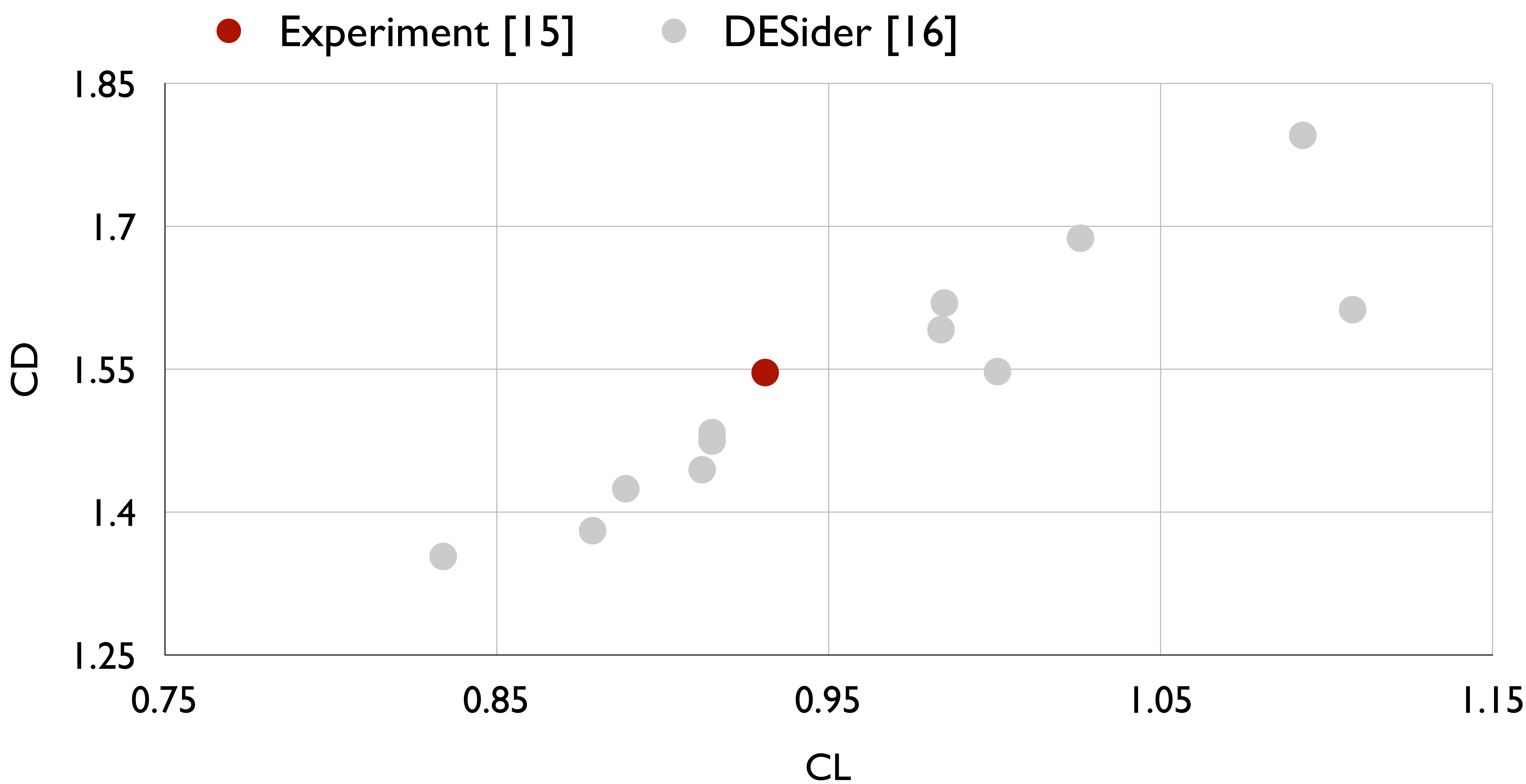

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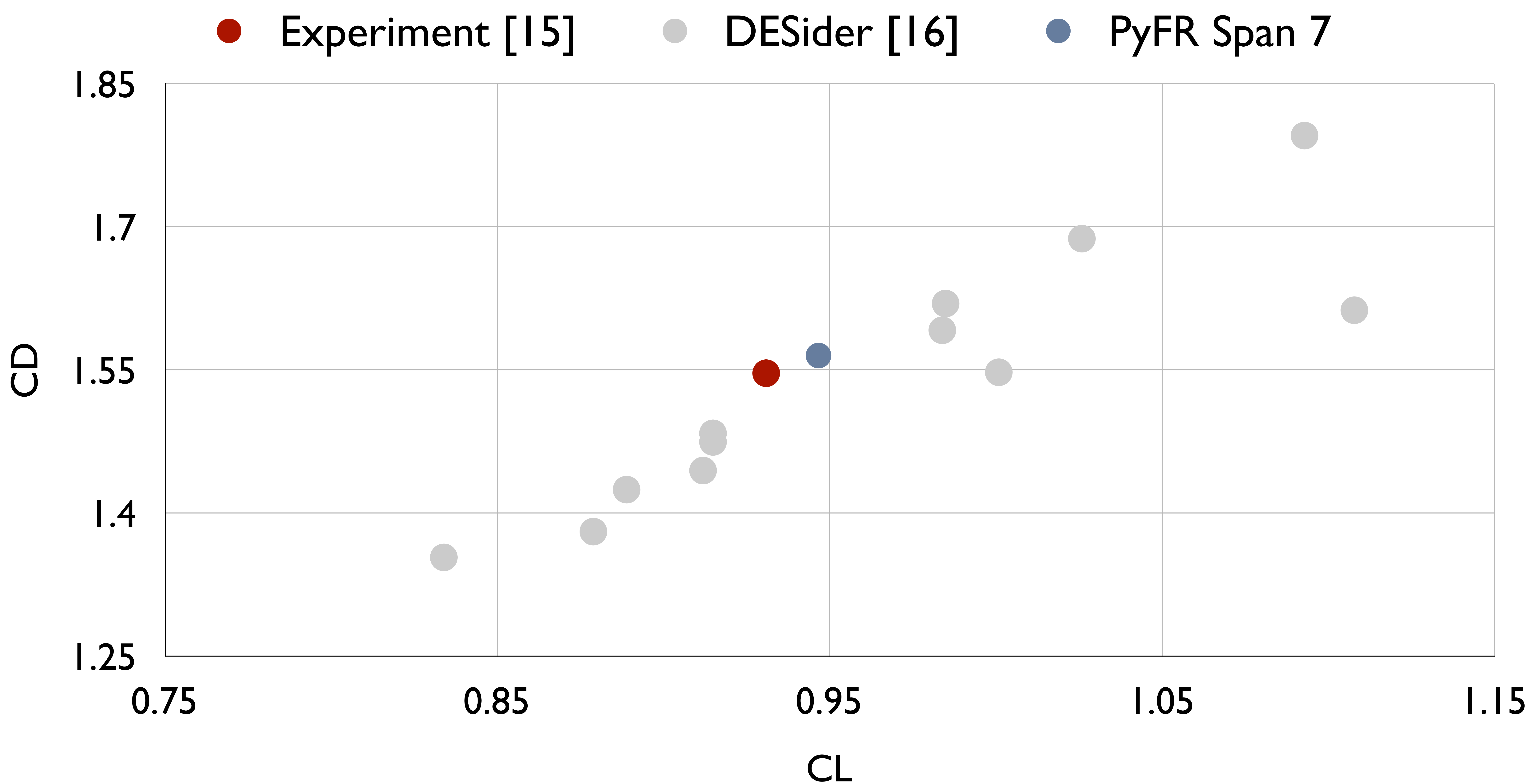

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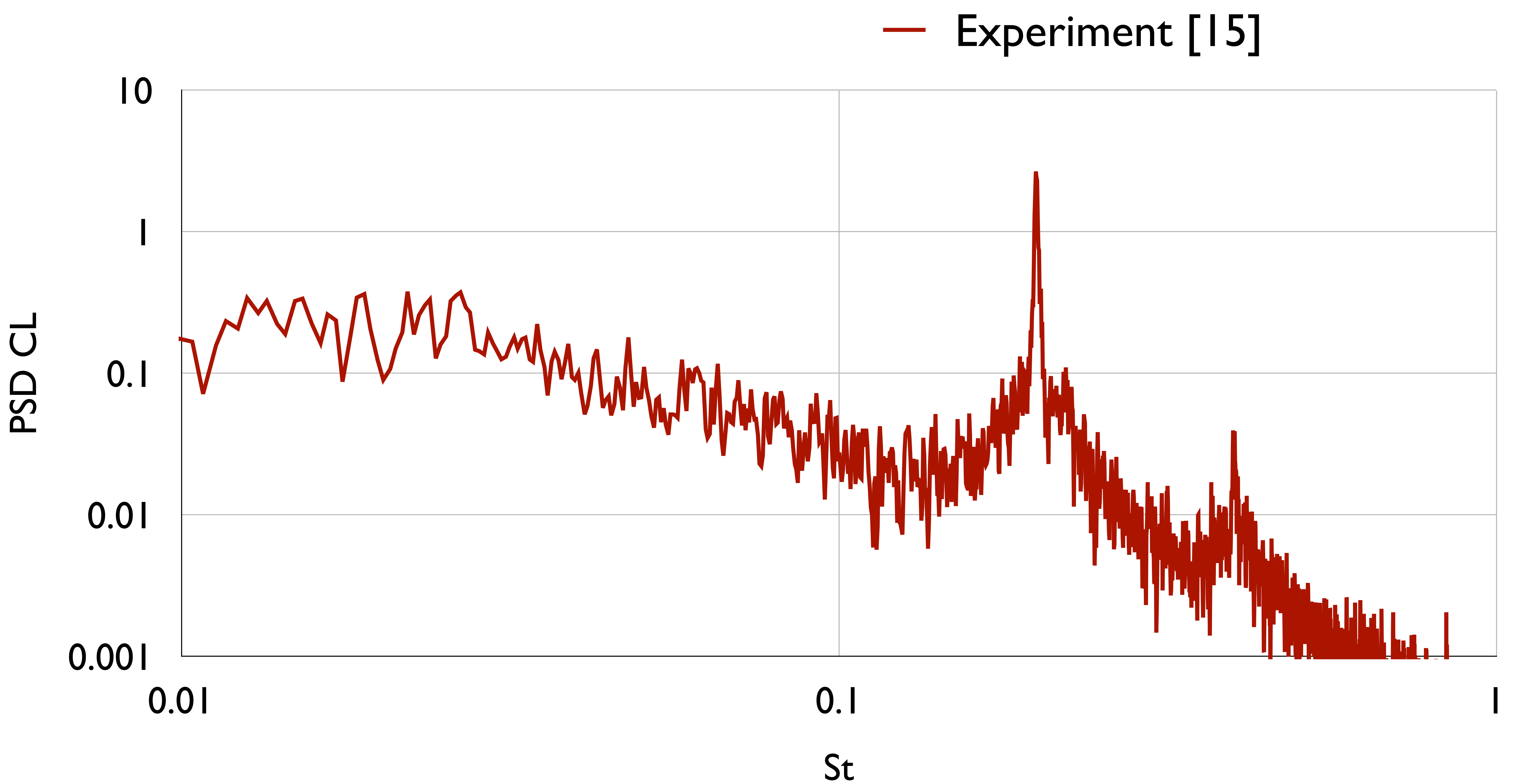

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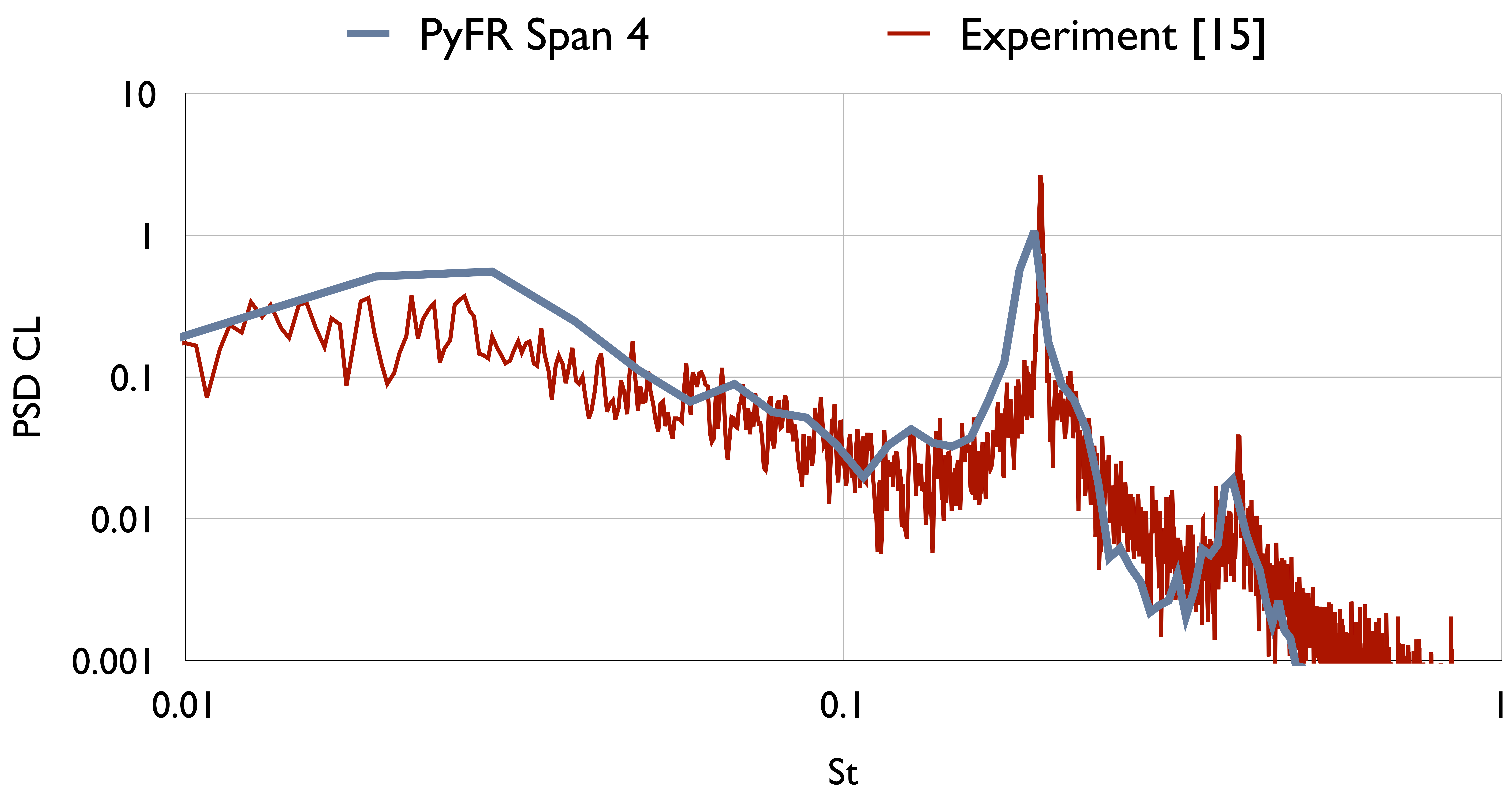
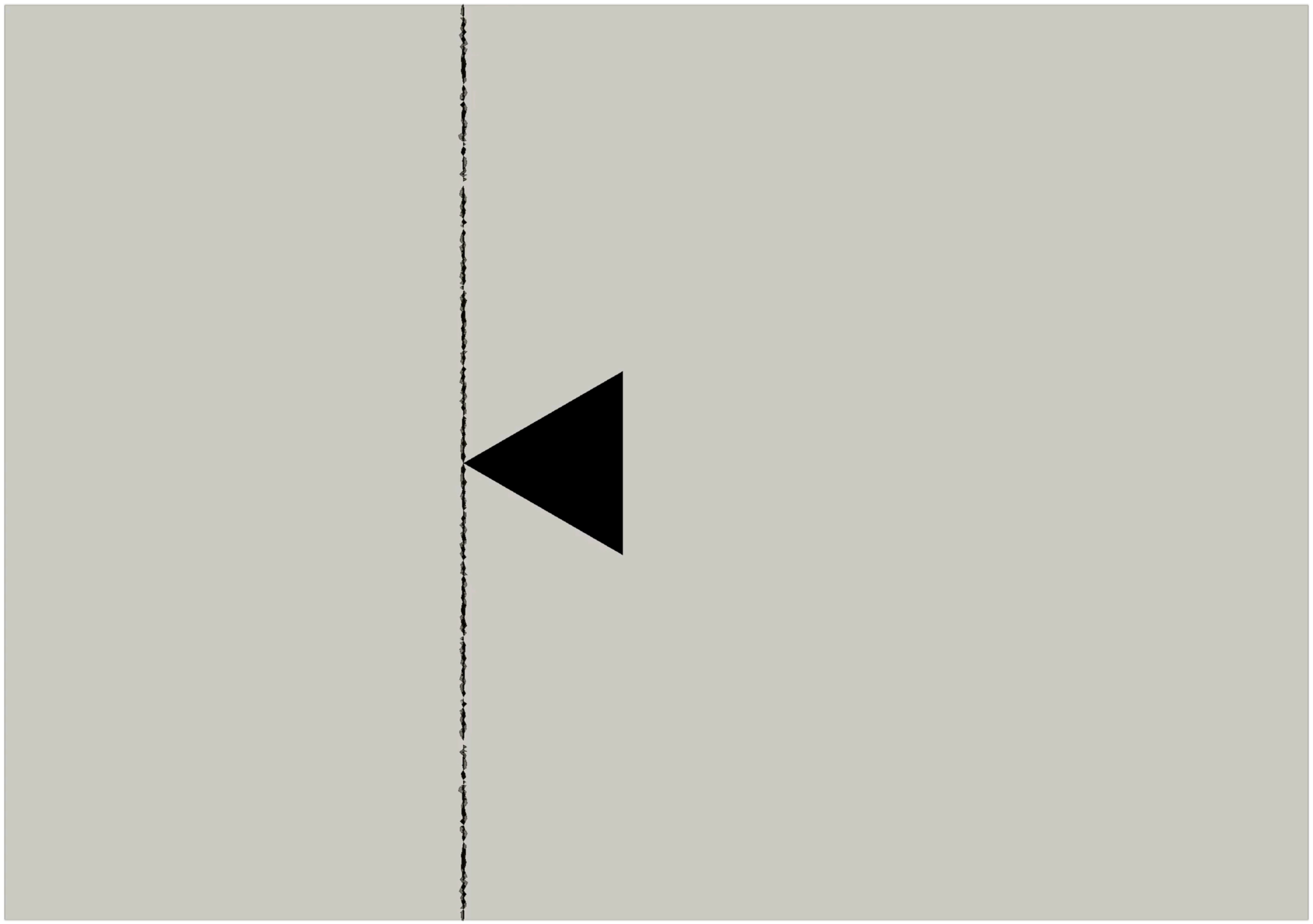


[15] K. Swalwell. The Effect of Turbulence on Stall of Horizontal Axis Wind Turbines. PhD Thesis. 2005.

Results

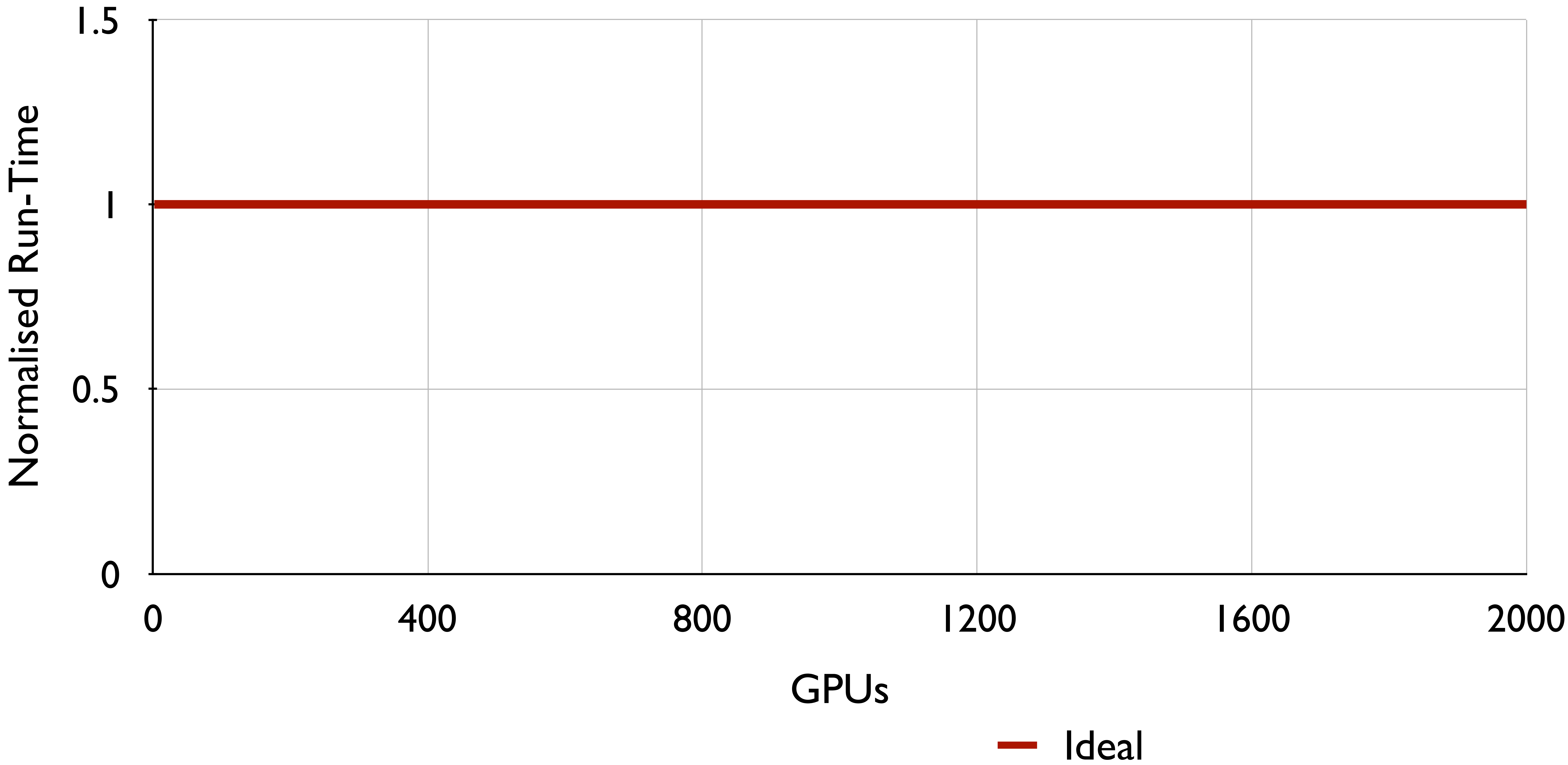
- Flow over a wedge
- Ma = 1.34

Results



Results

- 3D Navier-Stokes weak scaling on Piz Daint



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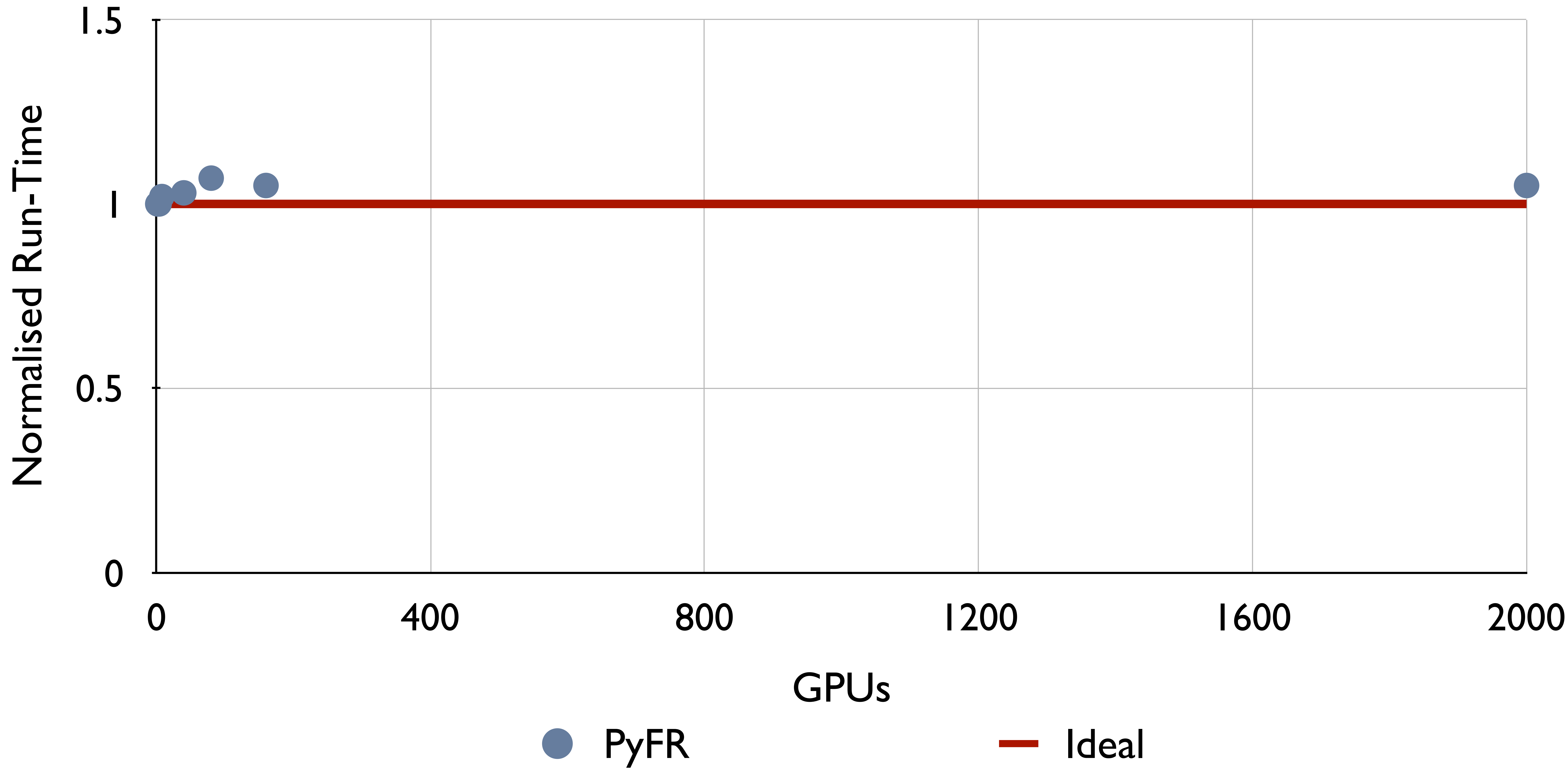

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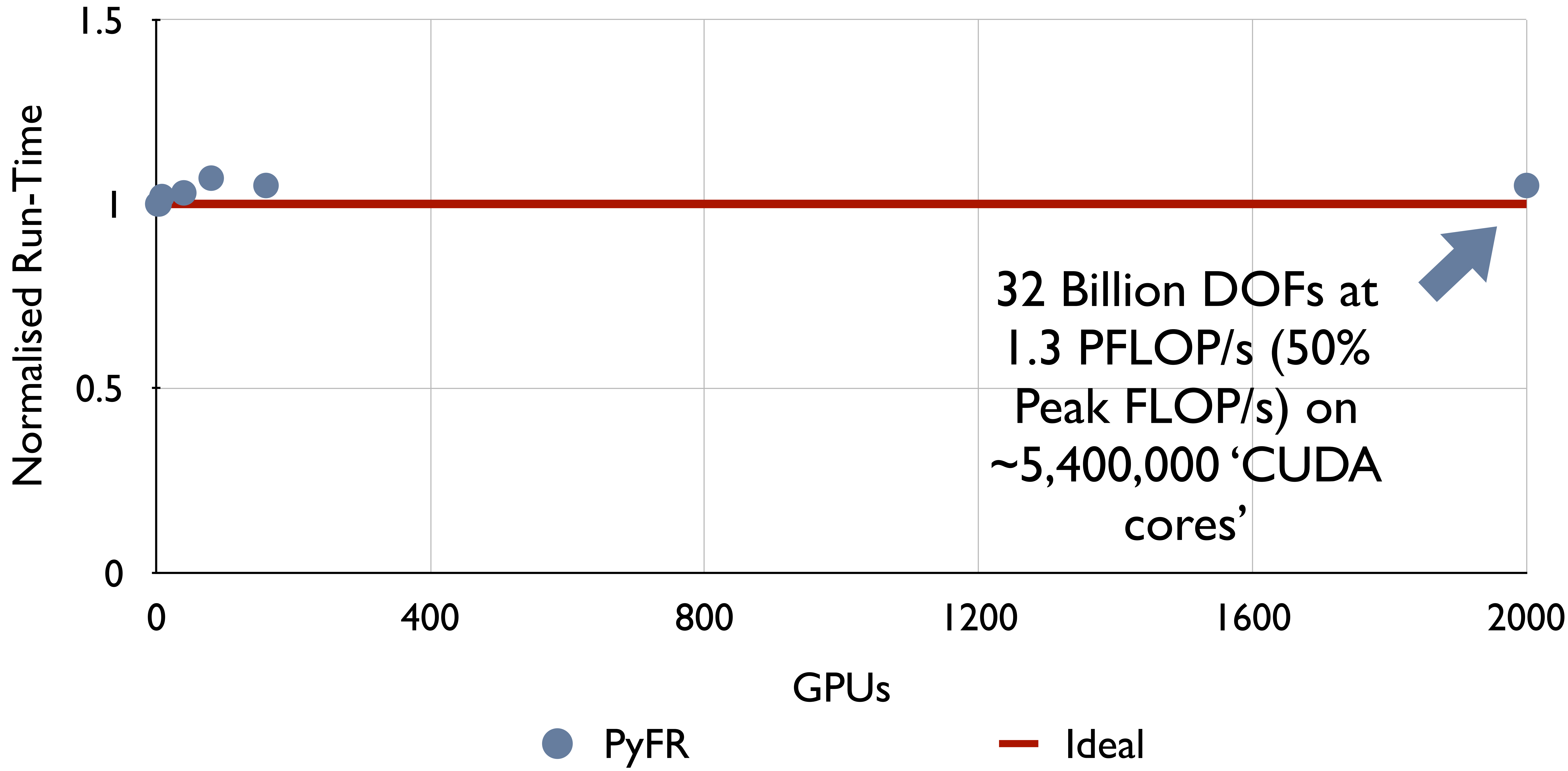

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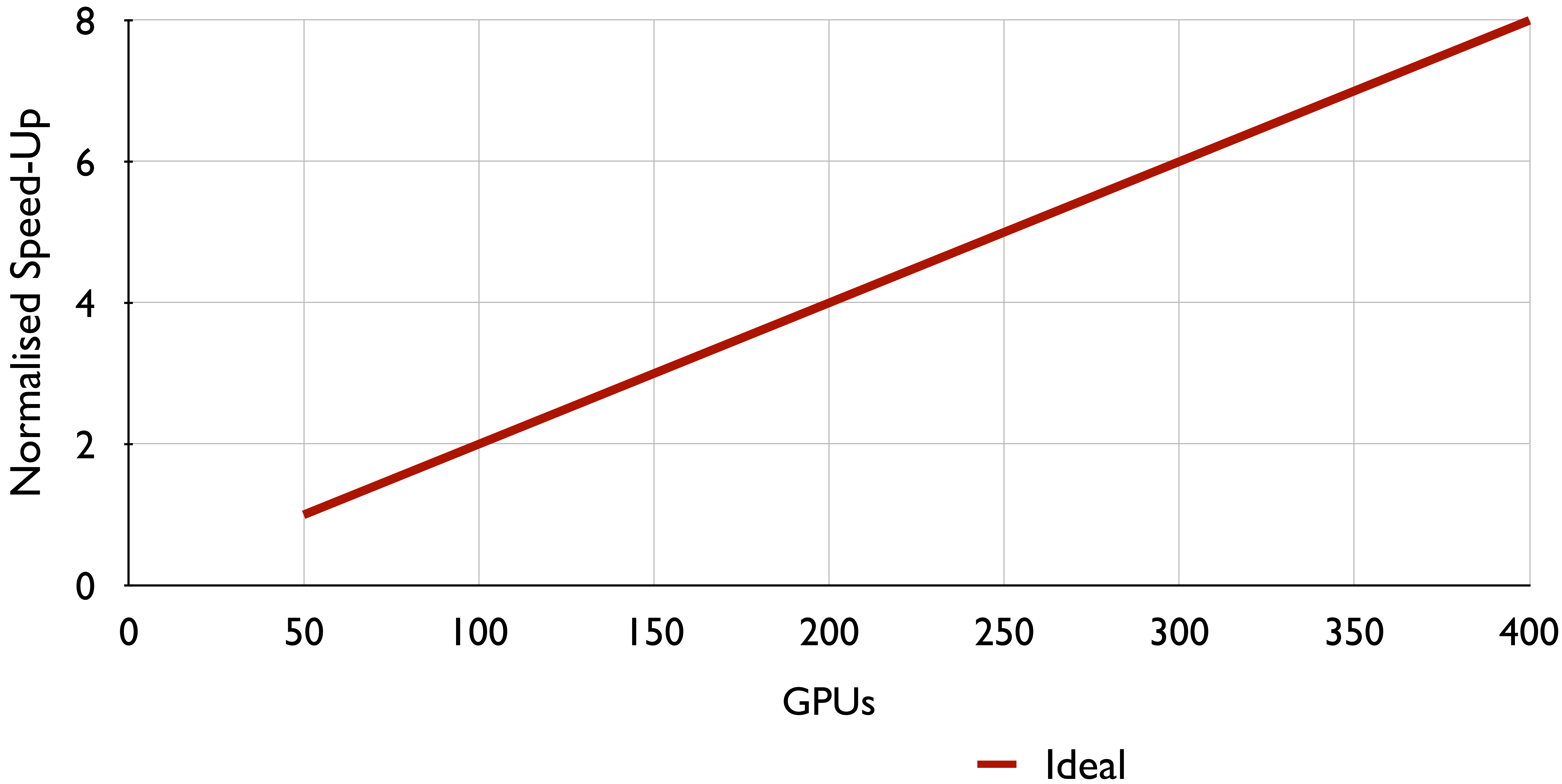

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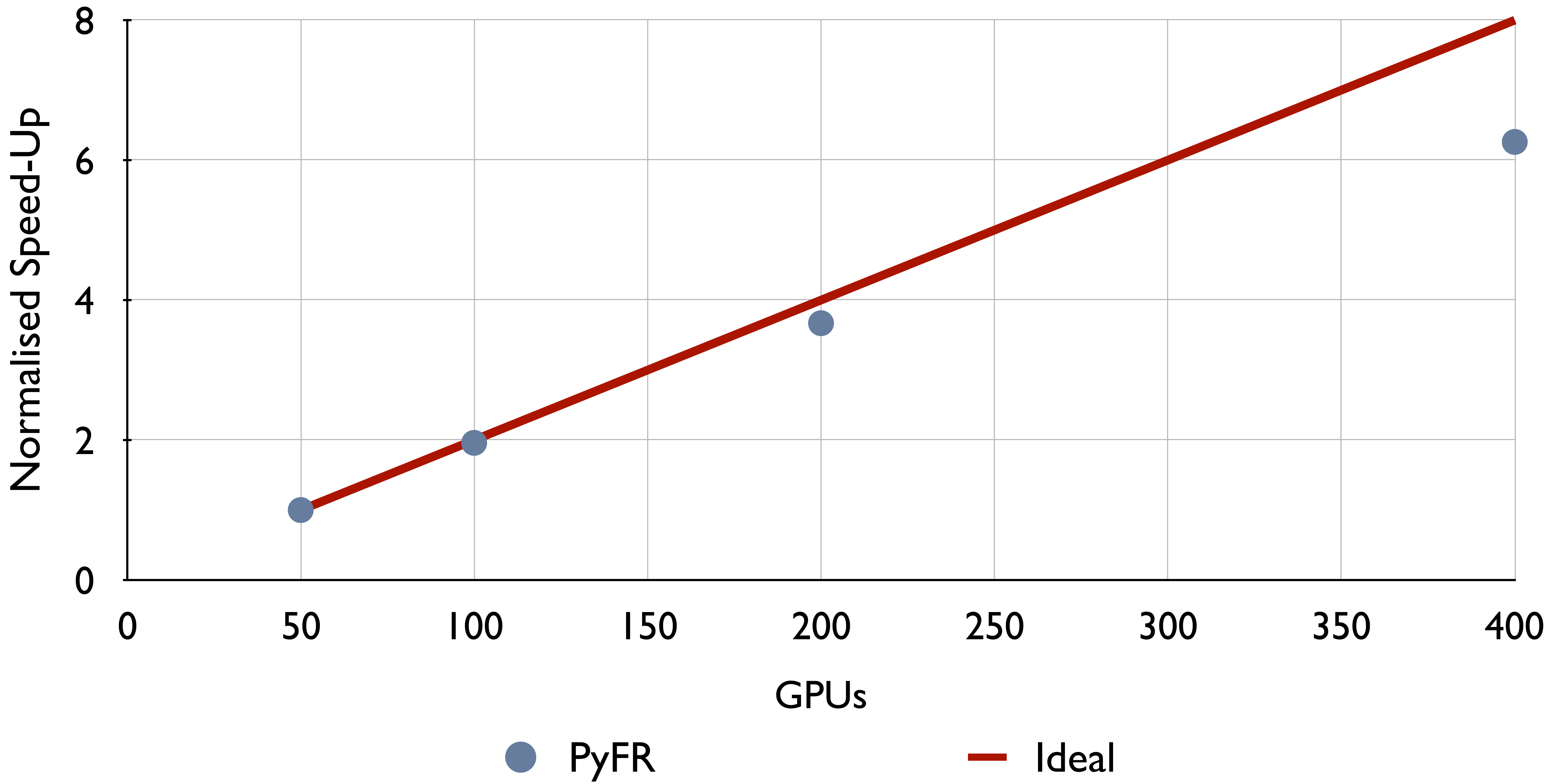

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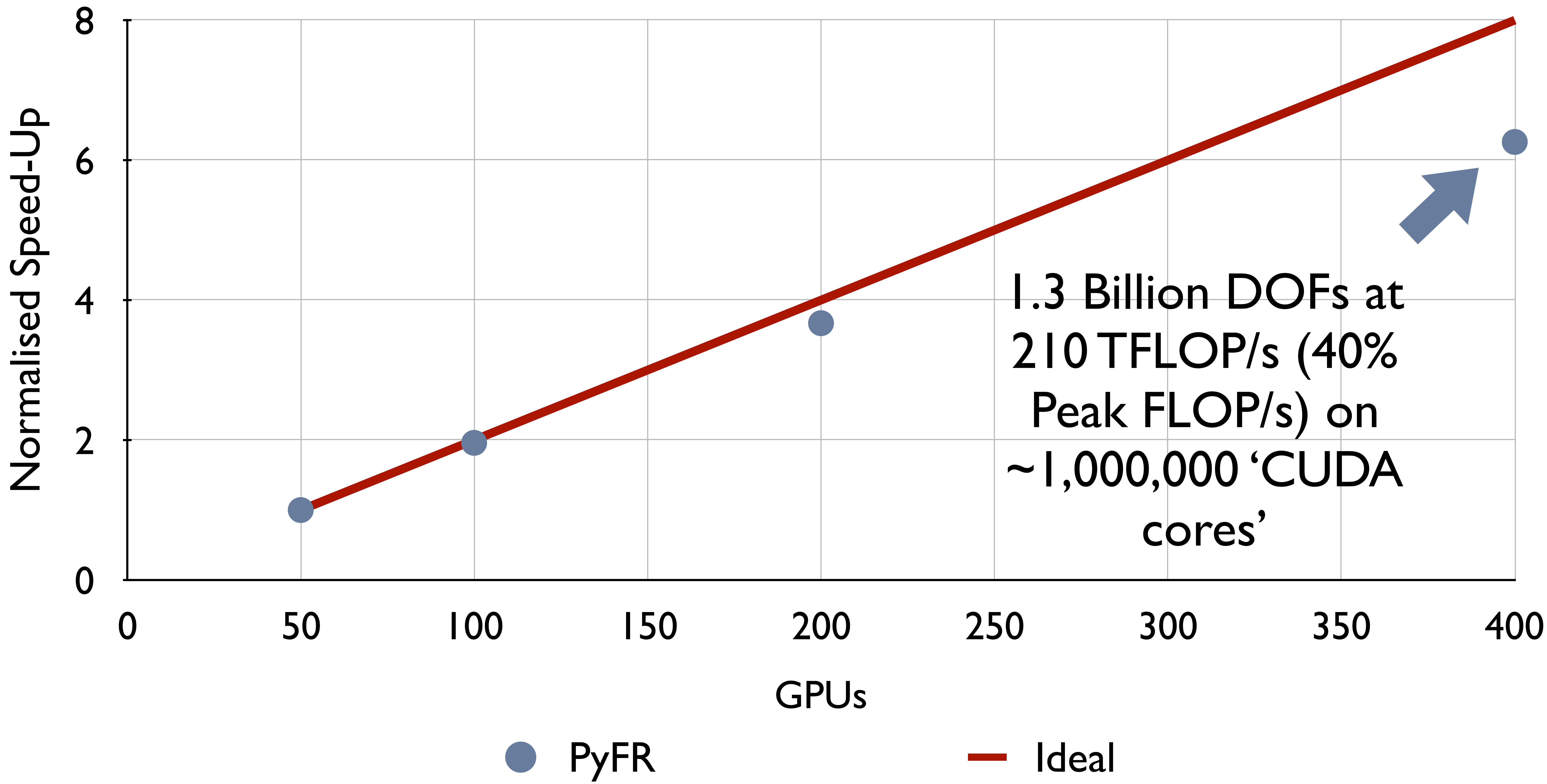

Pathways to Impact

Imperial College London

PyFR

Pathways to Impact

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Pathways to Impact

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PyFR

→ open source →

AIRBUS

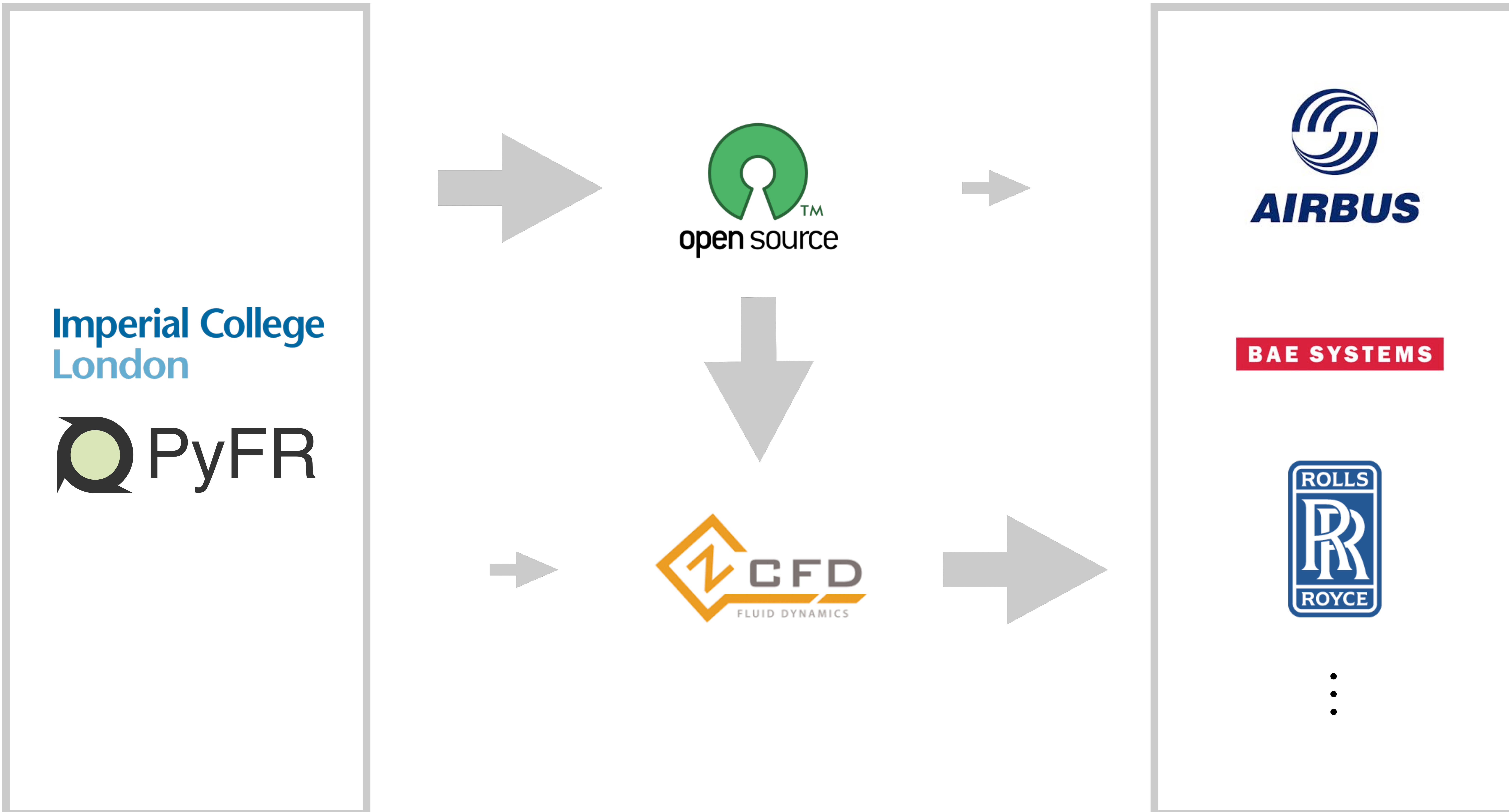
BAE SYSTEMS

ROLLS ROYCE

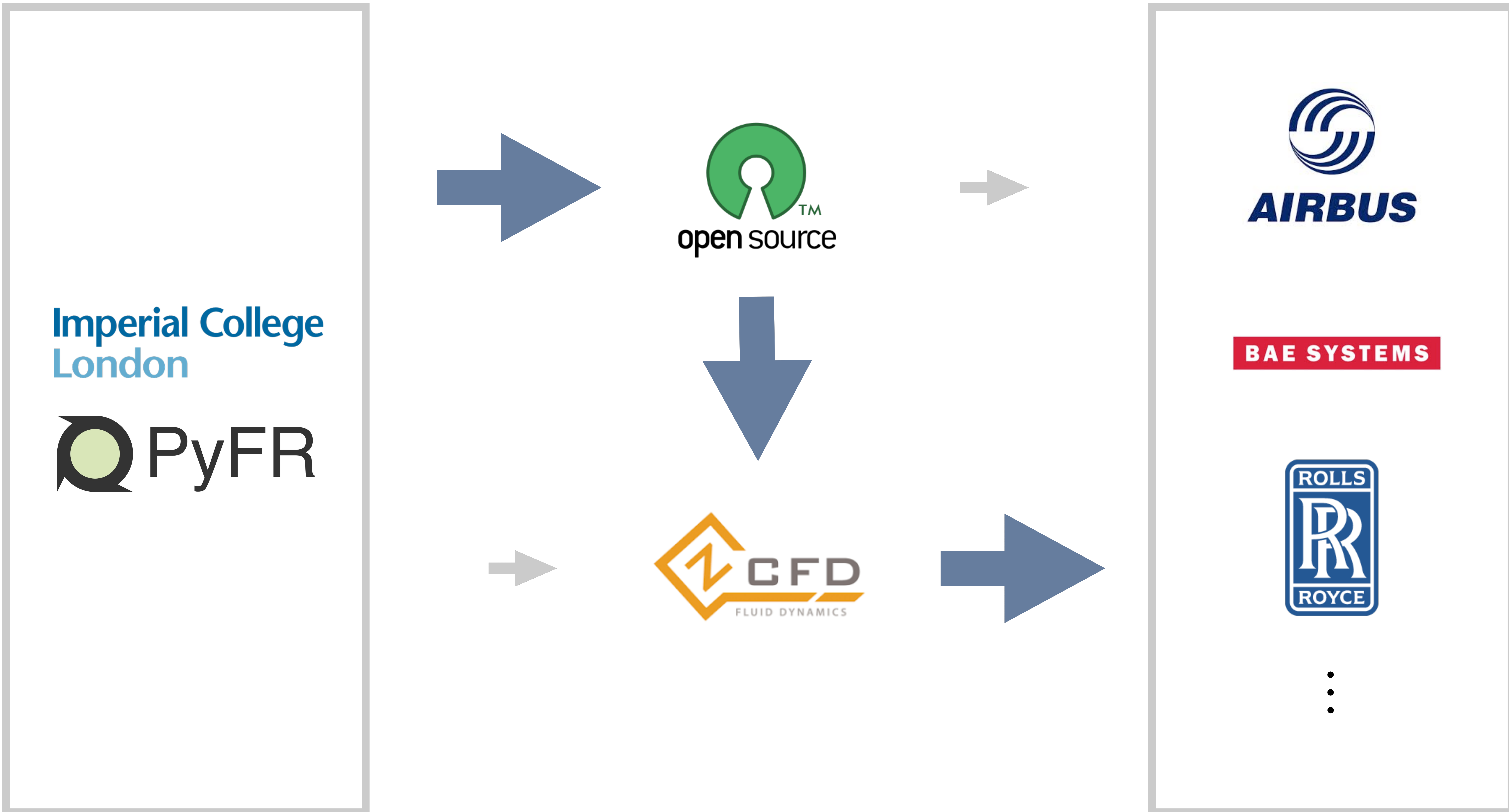
⋮

Pathways to Impact

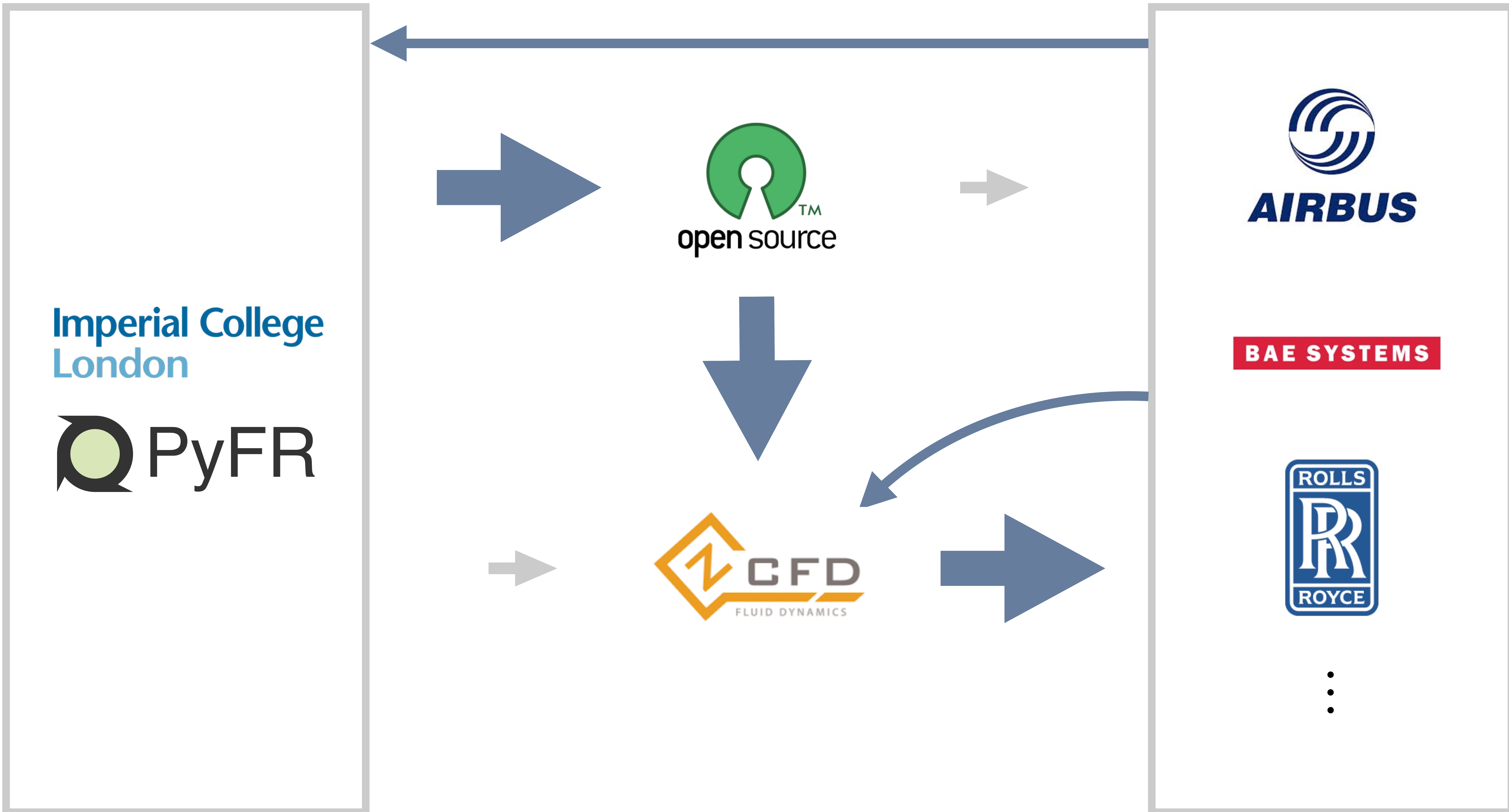
Pathways to Impact



Pathways to Impact



Pathways to Impact



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PRISM

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BAE SYSTEMS

NVIDIA

AMD
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- Emerald (CFI - UK)
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- Piz Daint (CSCS - Switzerland)
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