PyFR: Heterogeneous Computing from a Homogeneous Codebase

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20th November 2014 (Antony's Birthday!)

Overview

- Motivation
- Flux Reconstruction
- Modern Hardware
- PyFR
- Results
- Summary

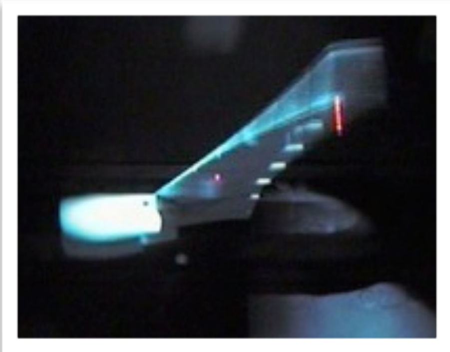
Motivation

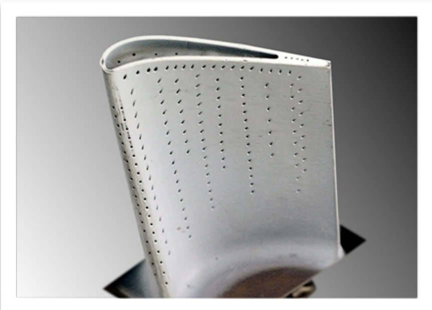
Current industry standard CFD tools have limited capabilities

Motivation

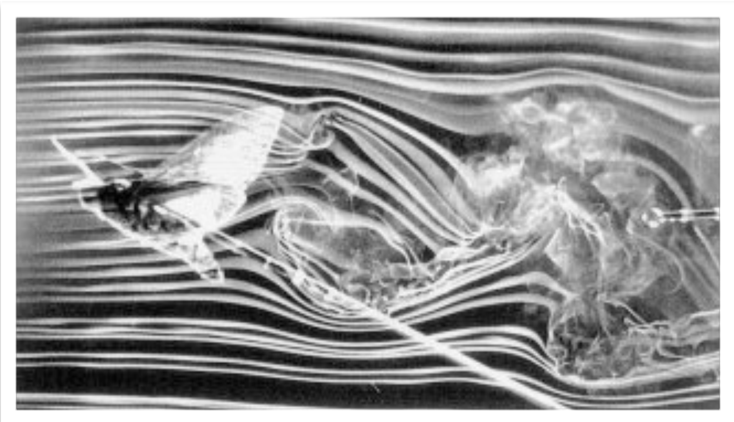
Technology is decades old and designed for solving steady flow problems (using RANS approach)

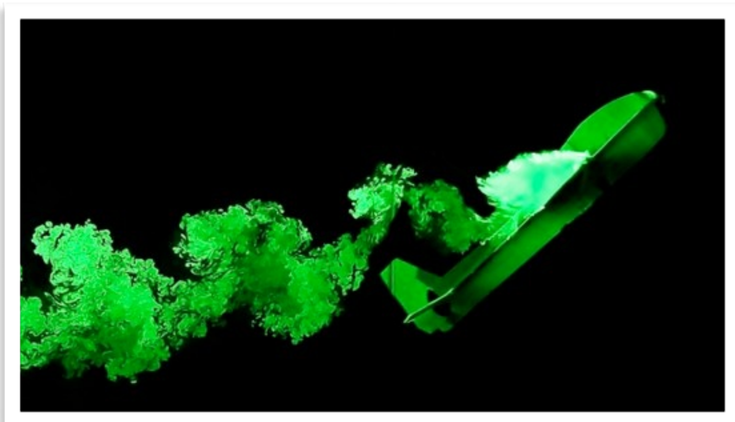
Motivation



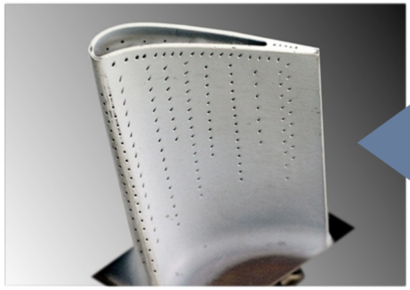


Technology is decades old and designed for solving steady flow problems (using RANS approach)

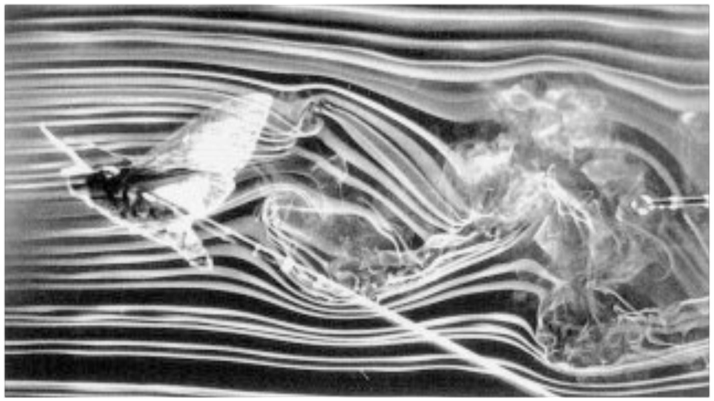


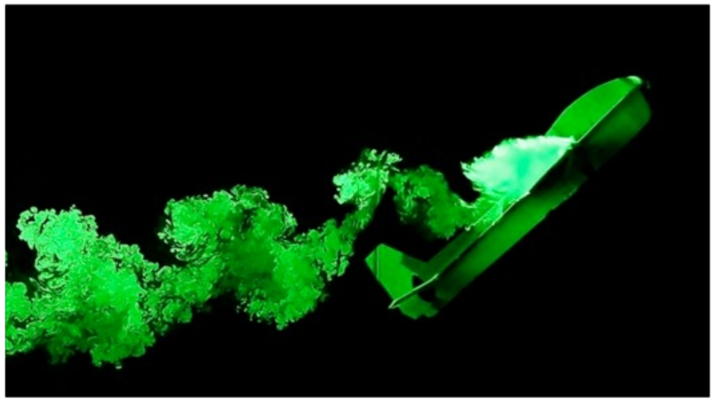


Motivation



Need to expand the ‘industrial CFD envelope’





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

Motivation

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

Motivation

- We aim to develop the *de facto* industry standard technology for affordable (and hence industrially relevant) high-fidelity scale-resolving simulations of unsteady flow phenomena within the vicinity of complex geometric configurations

Motivation

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

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 ...

$$\boxed{\text{High Accuracy + Complex Geometry}}$$

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 [4]
- A one-parameter family of provably stable FR schemes have been identified [5]

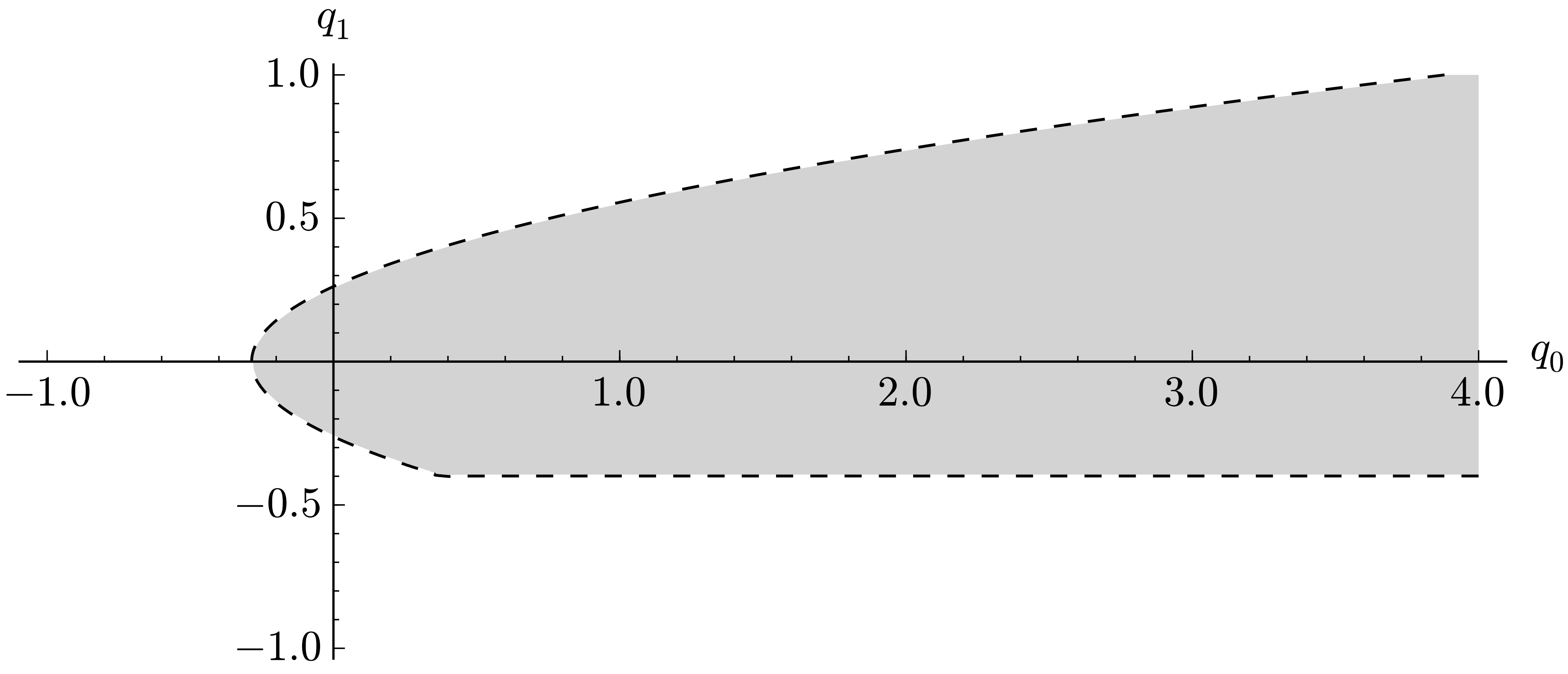
[4] H.T. Huynh. A flux Reconstruction Approach to High-Order Schemes Including Discontinuous Galerkin Methods. AIAA Paper 2007-4079. 2007
[5] P. E.Vincent, P. Castonguay, A. Jameson. A New Class of High-Order Energy Stable Flux Reconstruction Schemes. Journal of Scientific Computing. 2011

Flux Reconstruction

- We have recently identified a new multi-parameter family of stable FR schemes

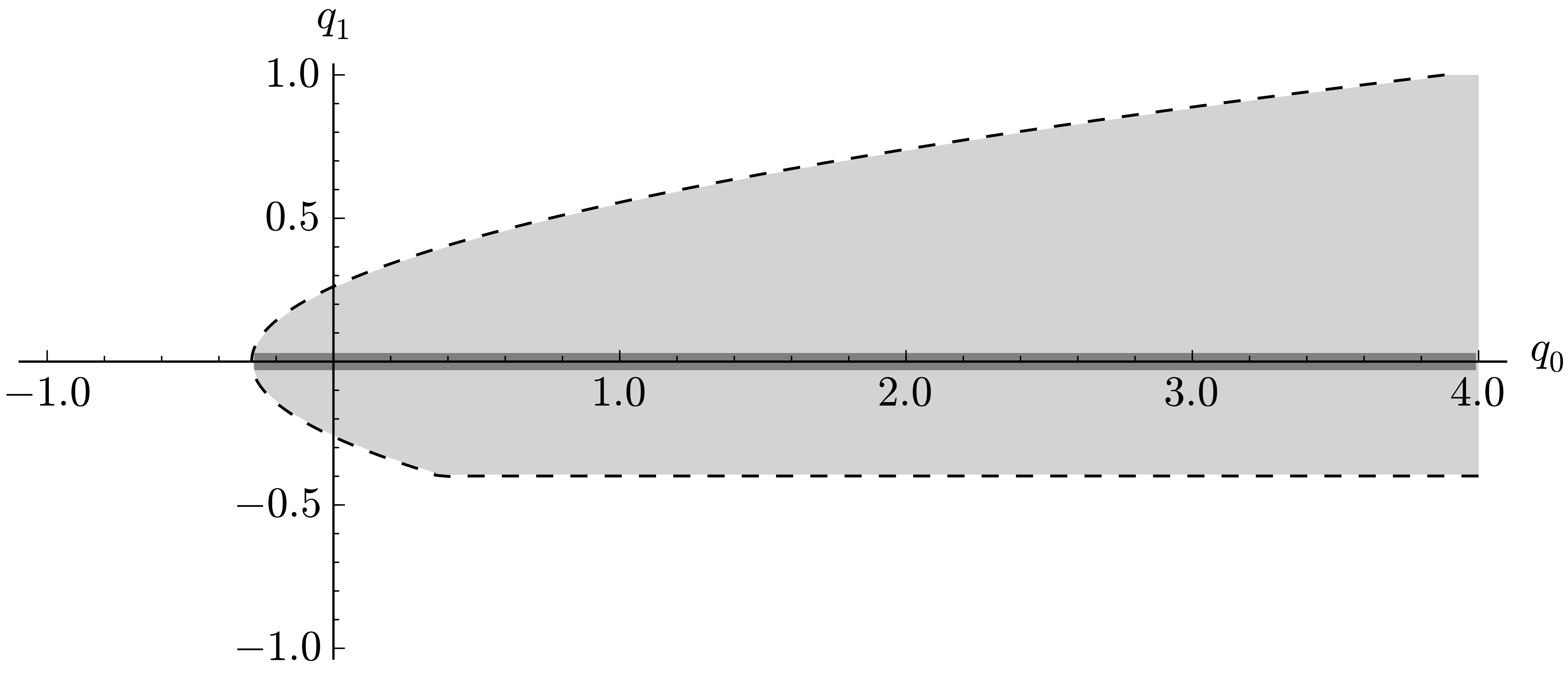
Flux Reconstruction

- Plot stable region of parameter space …



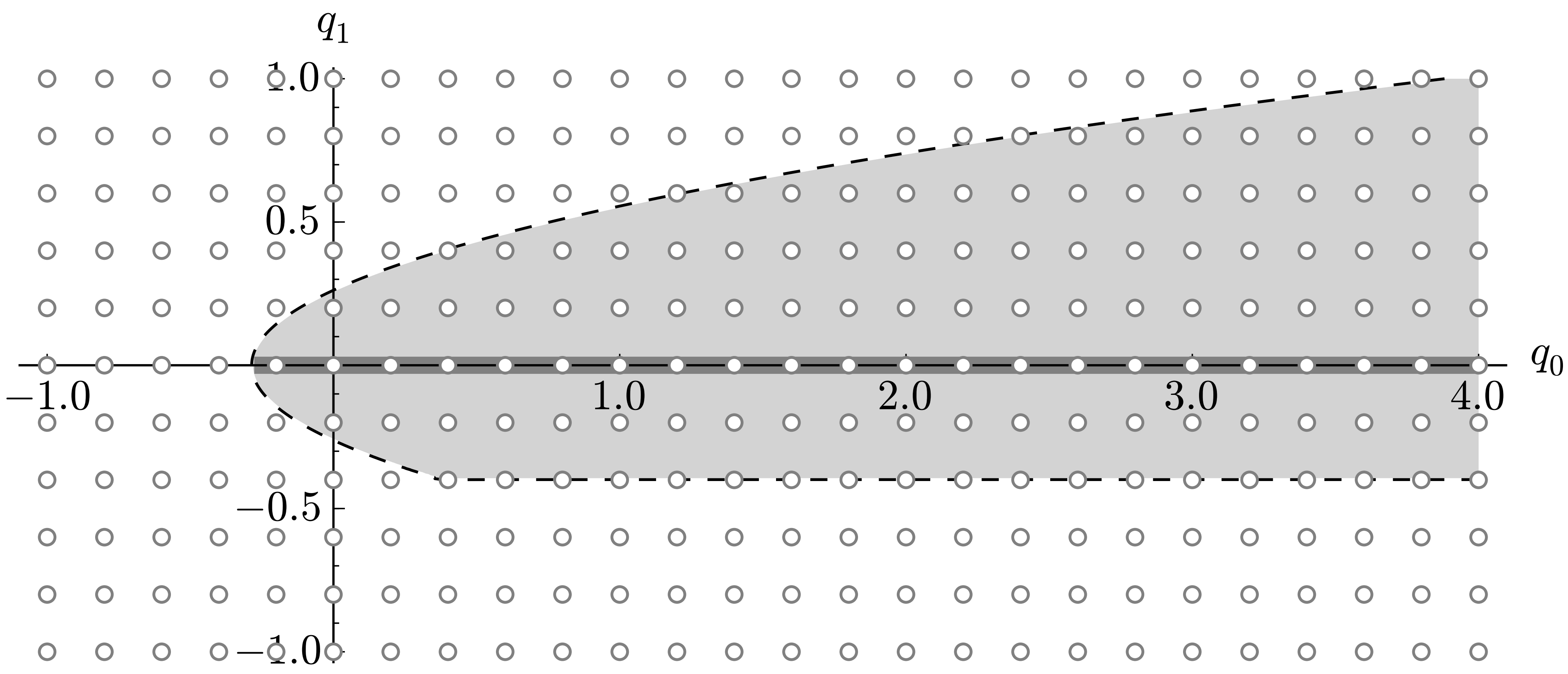
Flux Reconstruction

- Original one-parameter family …



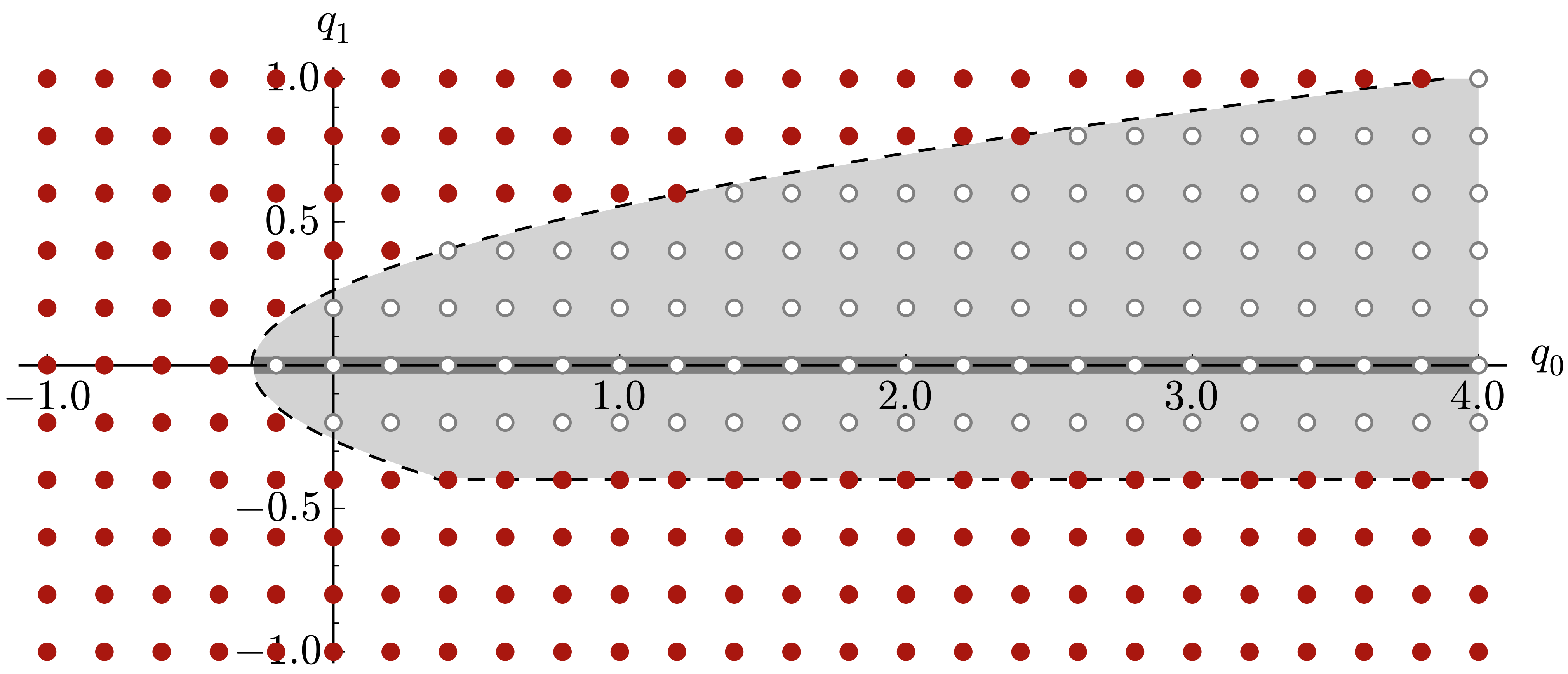
Flux Reconstruction

- Perform a whole bunch of numerical experiments …



Flux Reconstruction

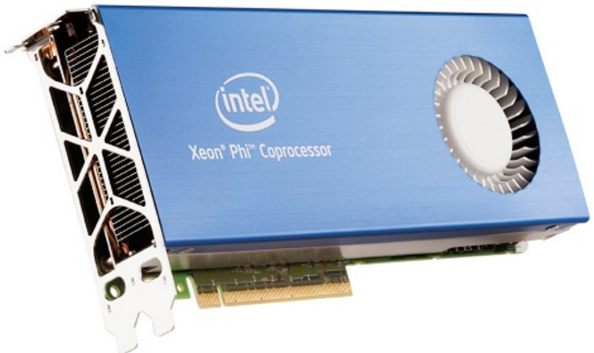
- And record which ones were stable/unstable …



Modern Hardware

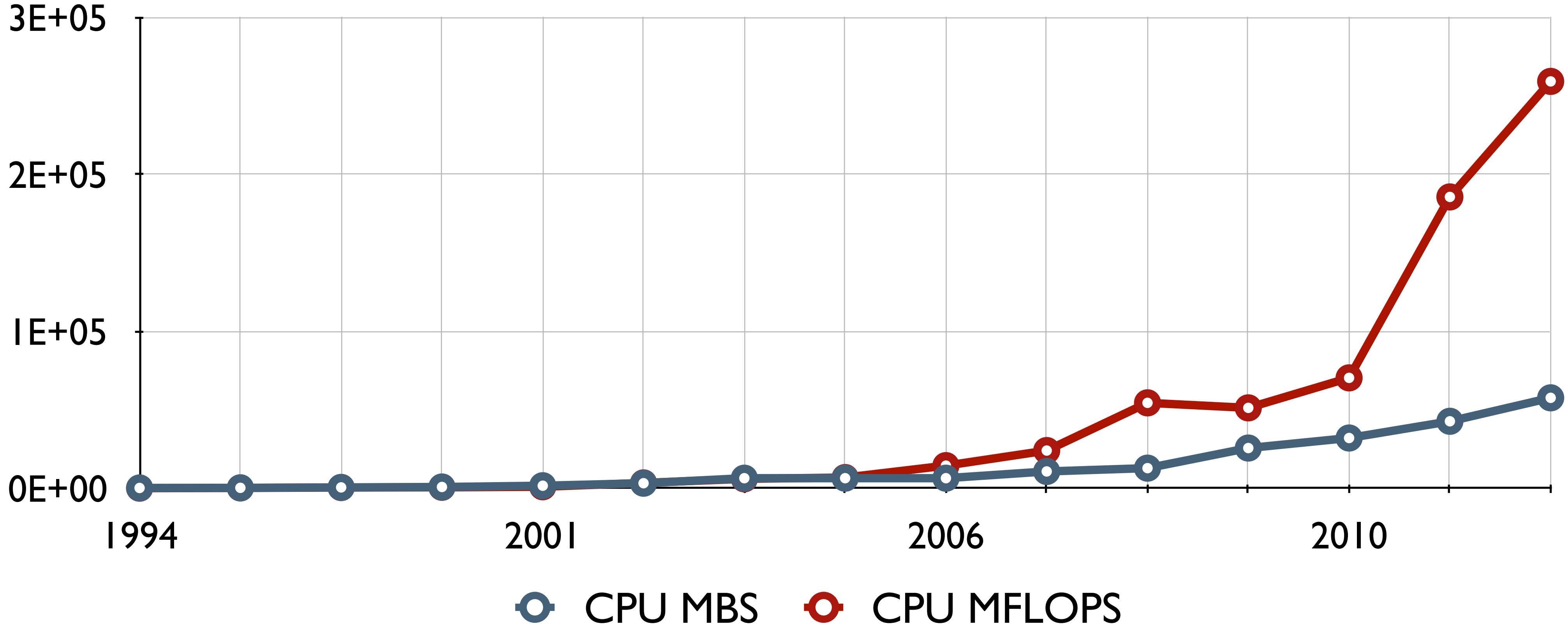
Modern Hardware

Modern Hardware



Modern Hardware

- FLOPS increasing faster than memory bandwidth



[2] 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

- Multiple Cores each with Vector Unit
- Parallelism exposed via MIMD (Multiple Instruction Multiple Data) + SMT (Simultaneous Multi Threading) + SIMD (Single Instruction Multiple Data) + ILP (Instruction Level Parallelism)

Modern Hardware

- Nvidia GPUs - multiple Streaming Multi-Processors each with CUDA Cores
- Parallelism exposed via SIMT (Single Instruction Multiple Thread)

Modern Hardware

- AMD GPUs - multiple Compute Units each with Stream Processors
- Parallelism exposed via SIMT (Single Instruction Multiple Thread)

Modern Hardware

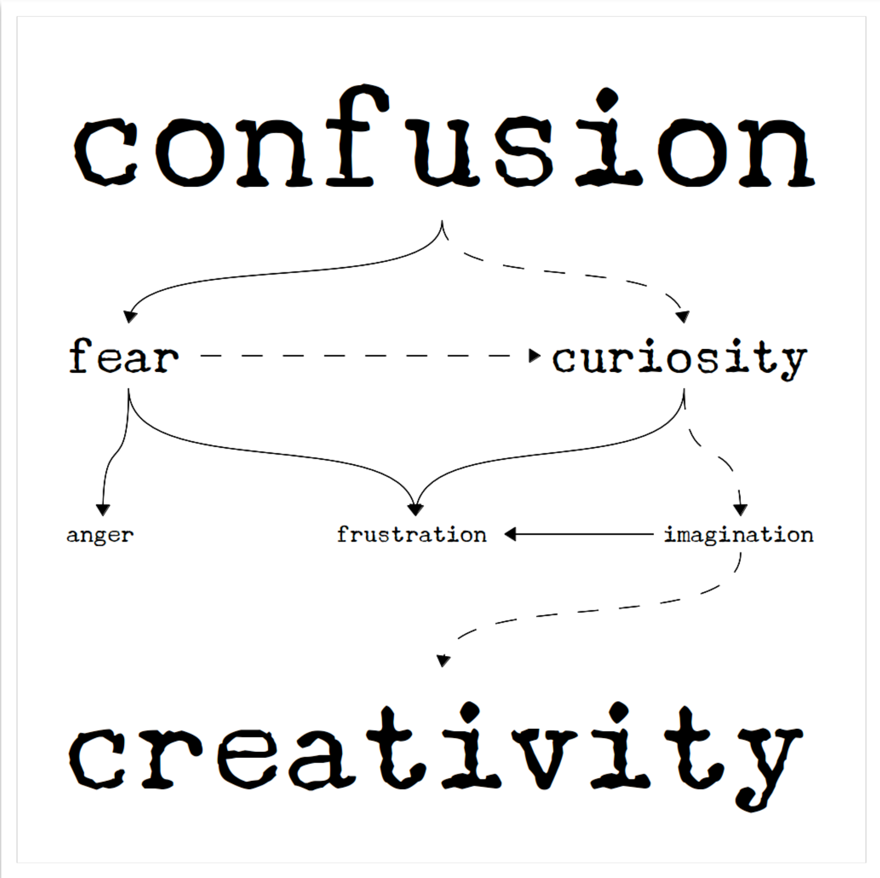
- Also, different programming languages for different devices

Modern Hardware

- So a challenging environment ...

Modern Hardware

- So a challenging environment ...



Modern Hardware

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

2.6TFLOPS
(Double Precision)

PyFR

Flux Reconstruction
+
Modern Hardware

PyFR

PyFR

PyFR

- Features (v0.2.3 - current release)

Governing Equations	Compressible Euler Compressible Navier Stokes
Spatial Discretisation	Arbitrary order FR on mixed unstructured grids (tris, quads, hexes, tets, prisms)
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.

Point-Wise Nonlinear Kernels

- Flux functions, Riemann solvers etc.

Use DGEMM from vendor supplied BLAS

PyFR

- Harder for point-wise nonlinear kernels …

Python Outer Layer (Hardware Independent)

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Matrix Multiply Kernels

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Point-Wise Nonlinear Kernels

- Flux functions, Riemann solvers etc.

Pass Mako derived kernel templates through Mako derived templating engine

PyFR

- These can now be called

Python Outer Layer
(Hardware Independent)

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Matrix Multiply Kernels

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C/OpenMP Hardware Specific Kernels

CUDA Hardware Specific Kernels

OpenCL Hardware Specific Kernels

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Hardware Specific Kernels

CUDA
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OpenCL
Hardware Specific Kernels

Use DGEMM from vendor supplied BLAS

Pass Mako derived kernel templates through Mako derived templating engine

PyFR

- ~5.5k lines of Python

PyFR

- Open source '3 Clause New Style BSD License'

PyFR

- Website: www.pyfr.org
- Twitter: @PyFR_Solver
- Paper: Computer Physics Communications [3]

[3] 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. Accepted for publication in Computer Physics Communications. 2014

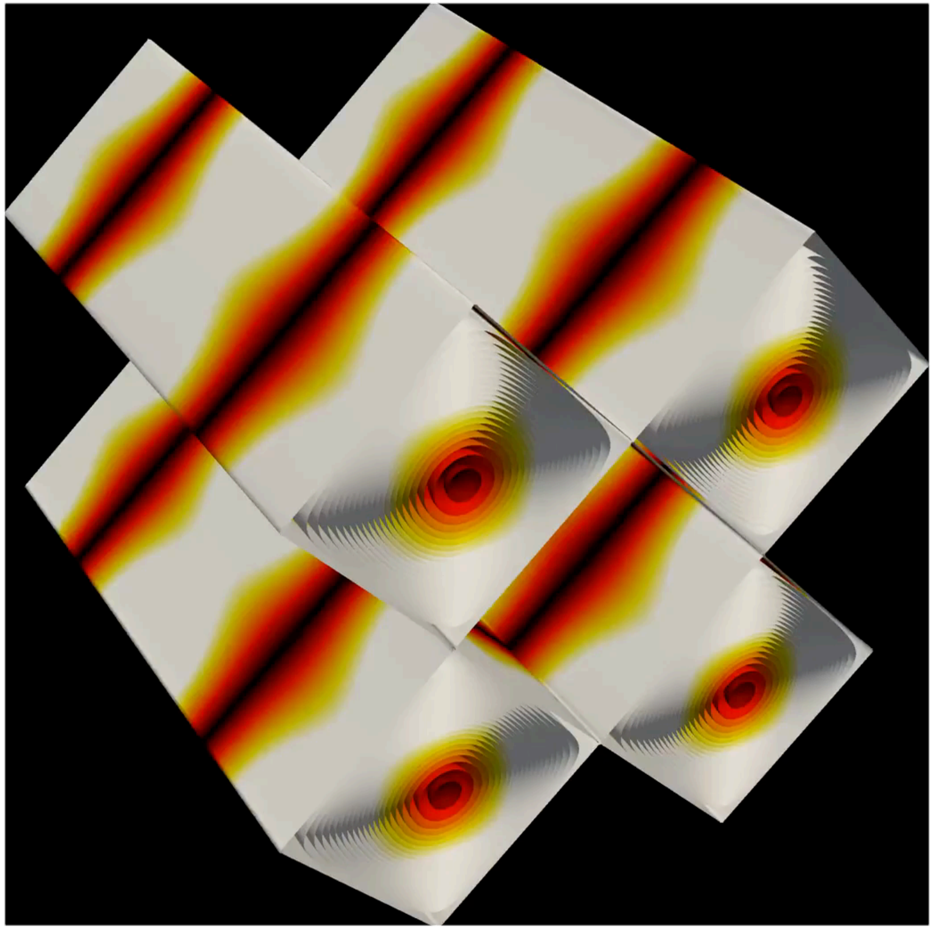
Results

- Taylor-Green vortex breakdown
- Re = 1600
- Ma = 0.1
- Compare with van Rees et al. [7]

[7] 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

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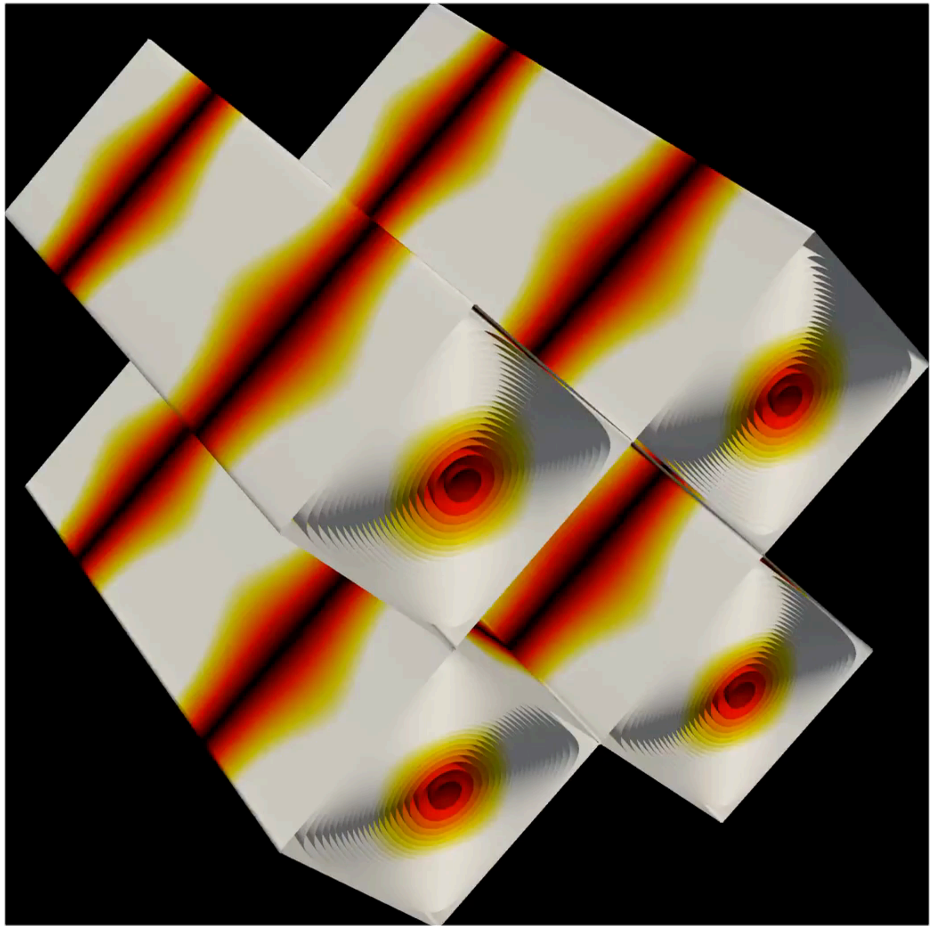
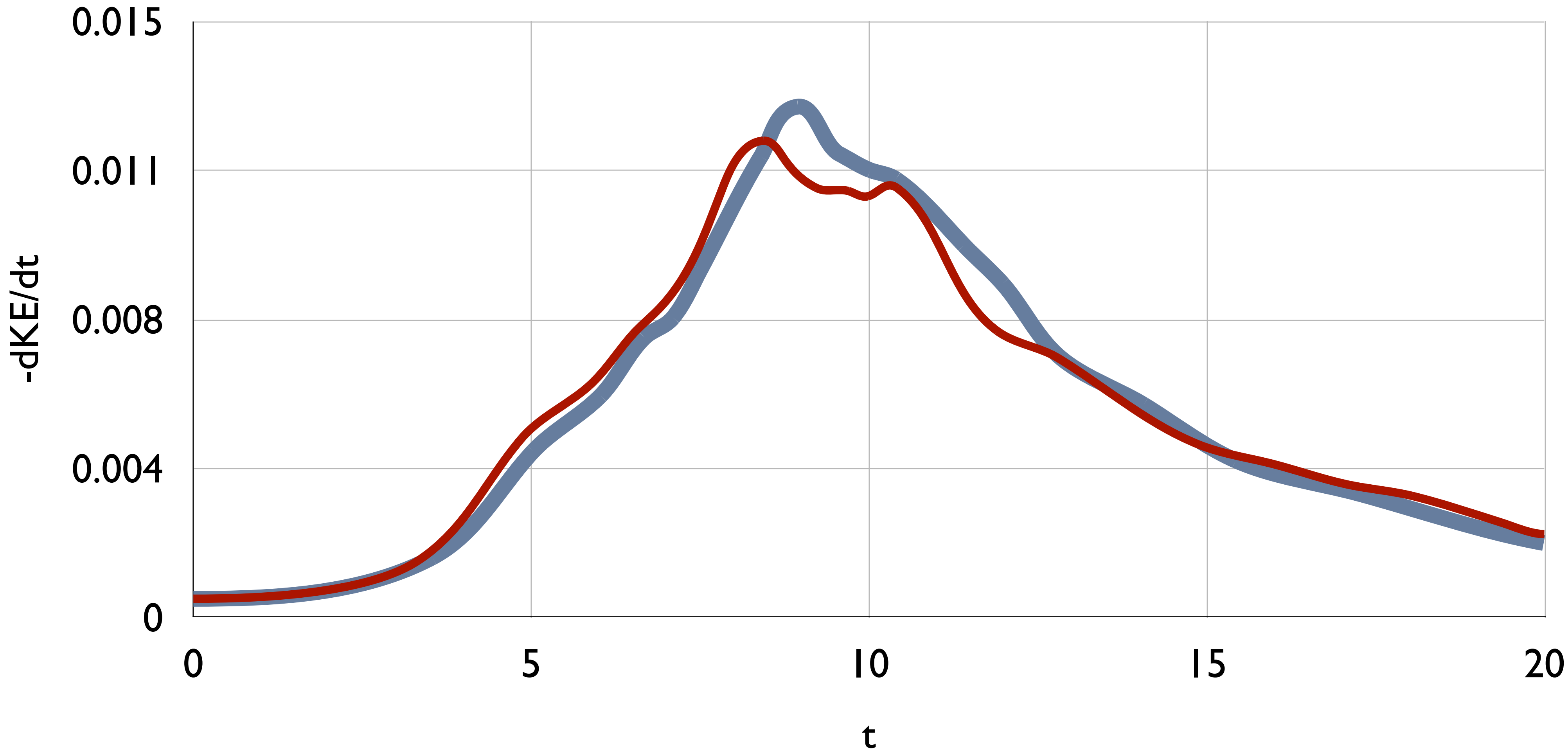


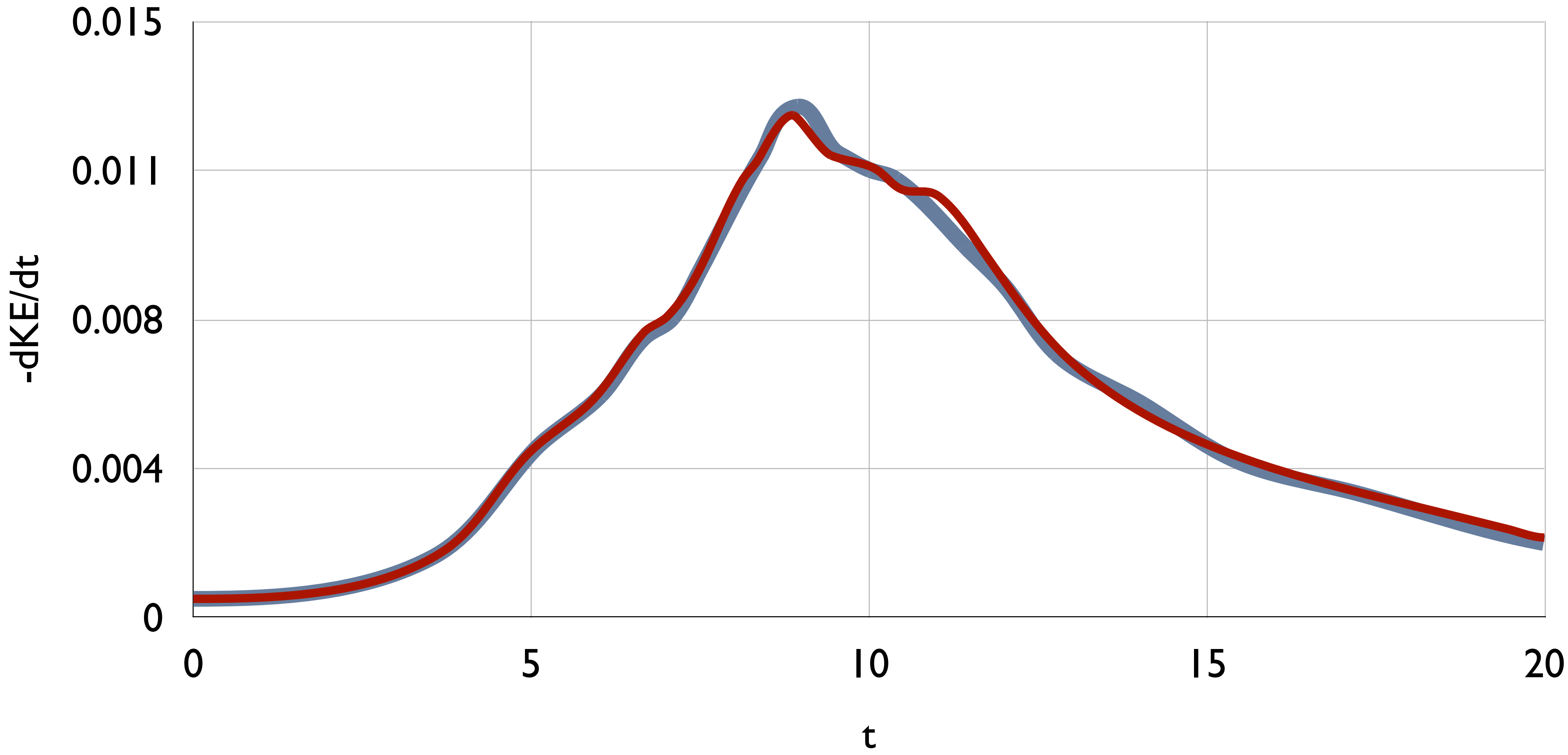
Results

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



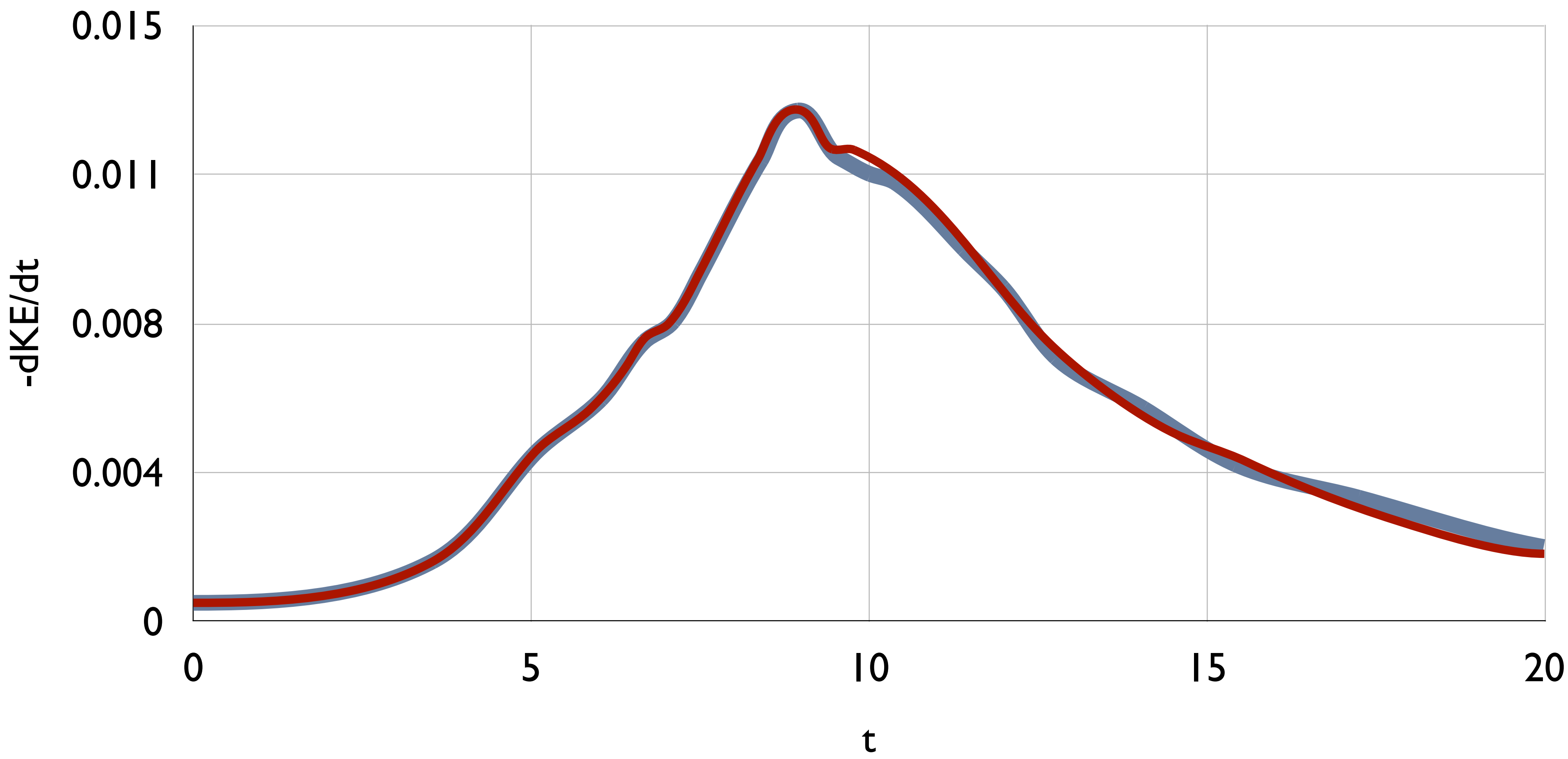
Results

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



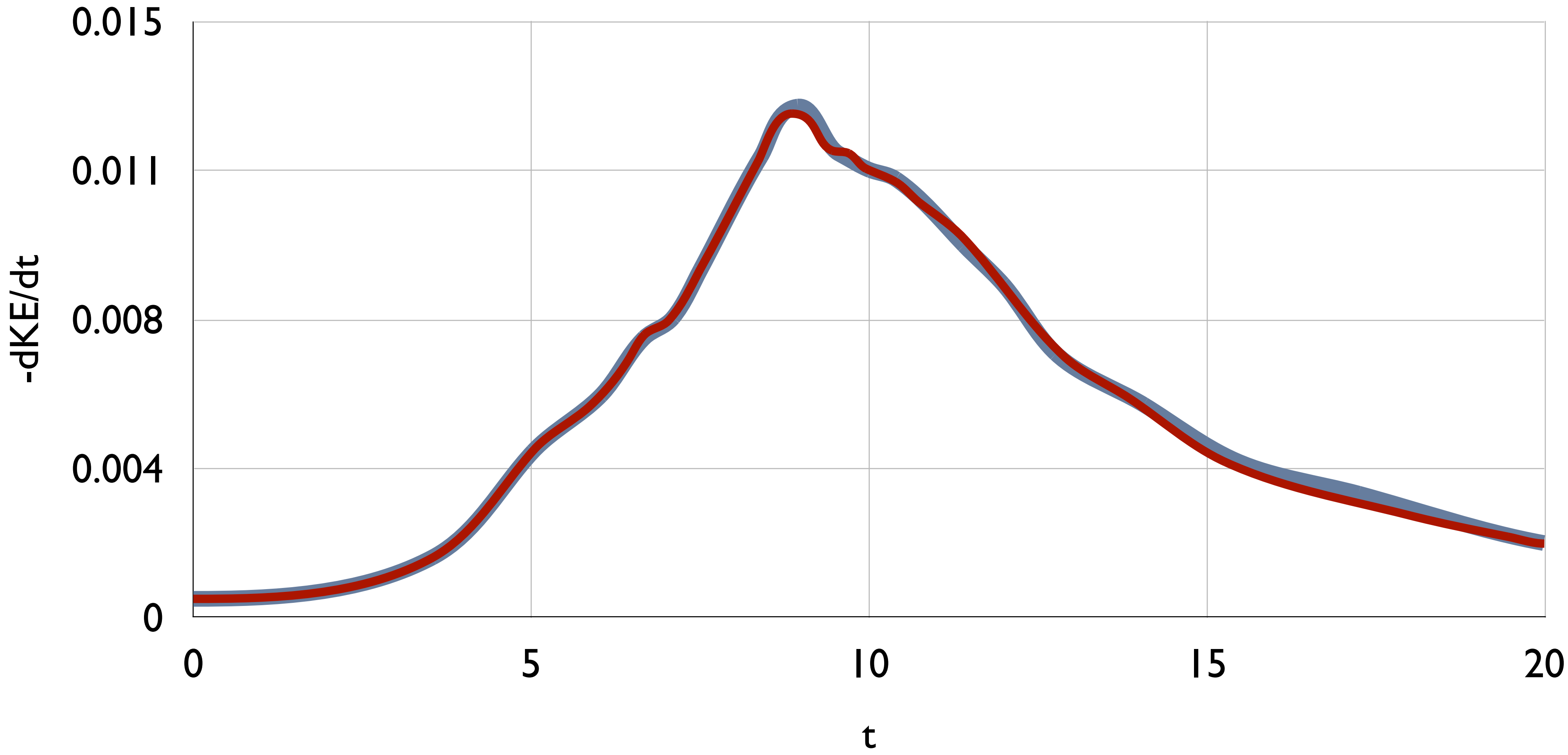
Results

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



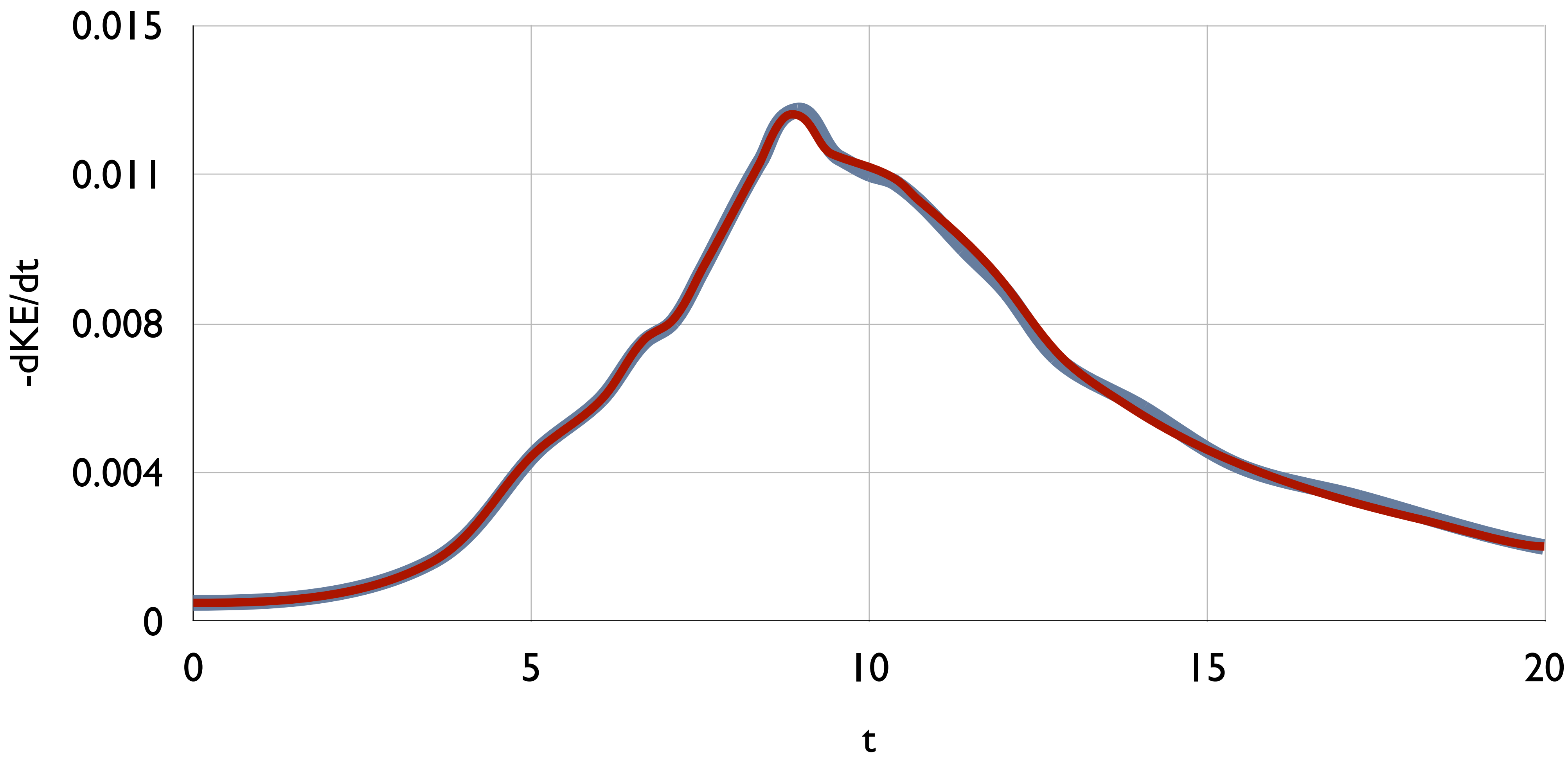
Results

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



Results

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



Results

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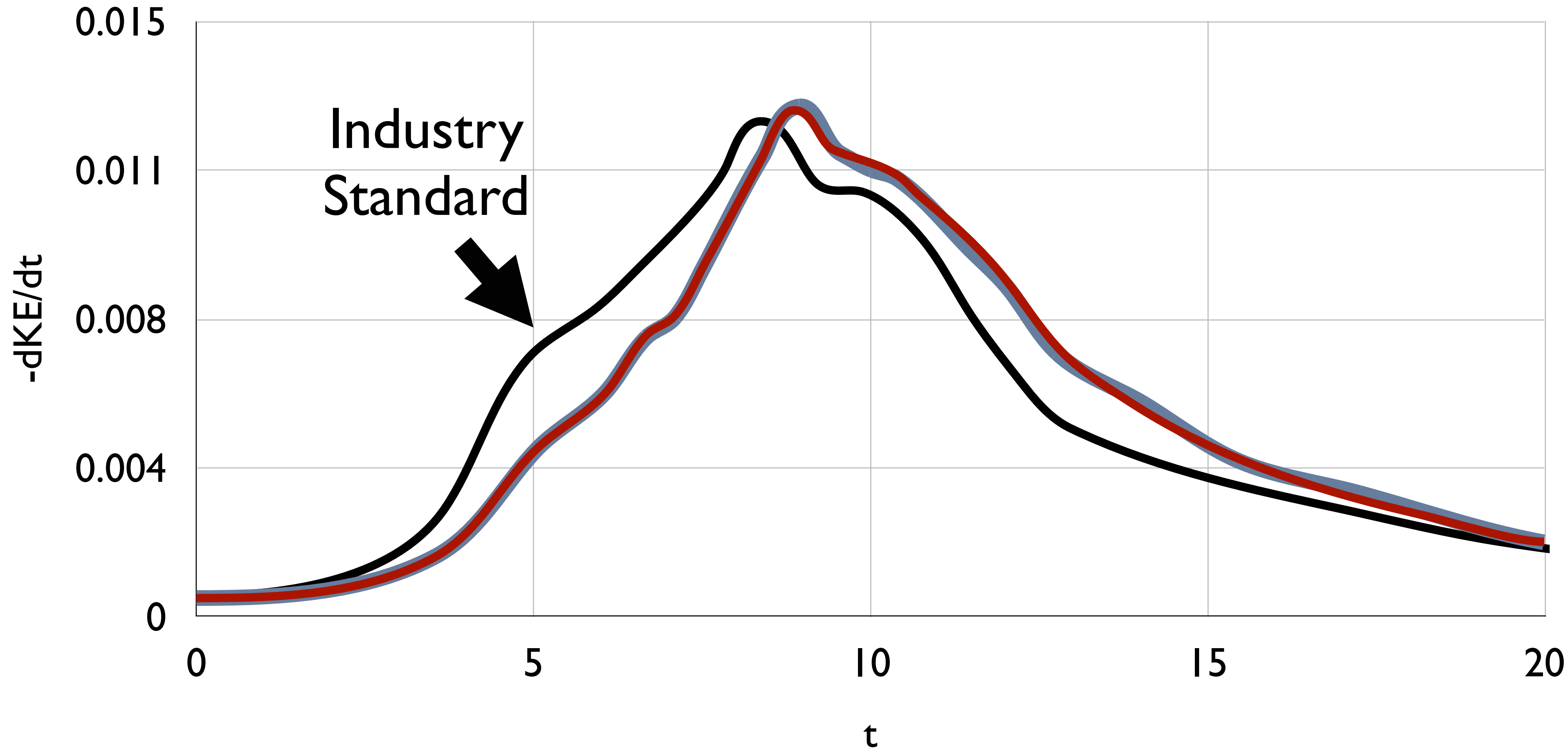
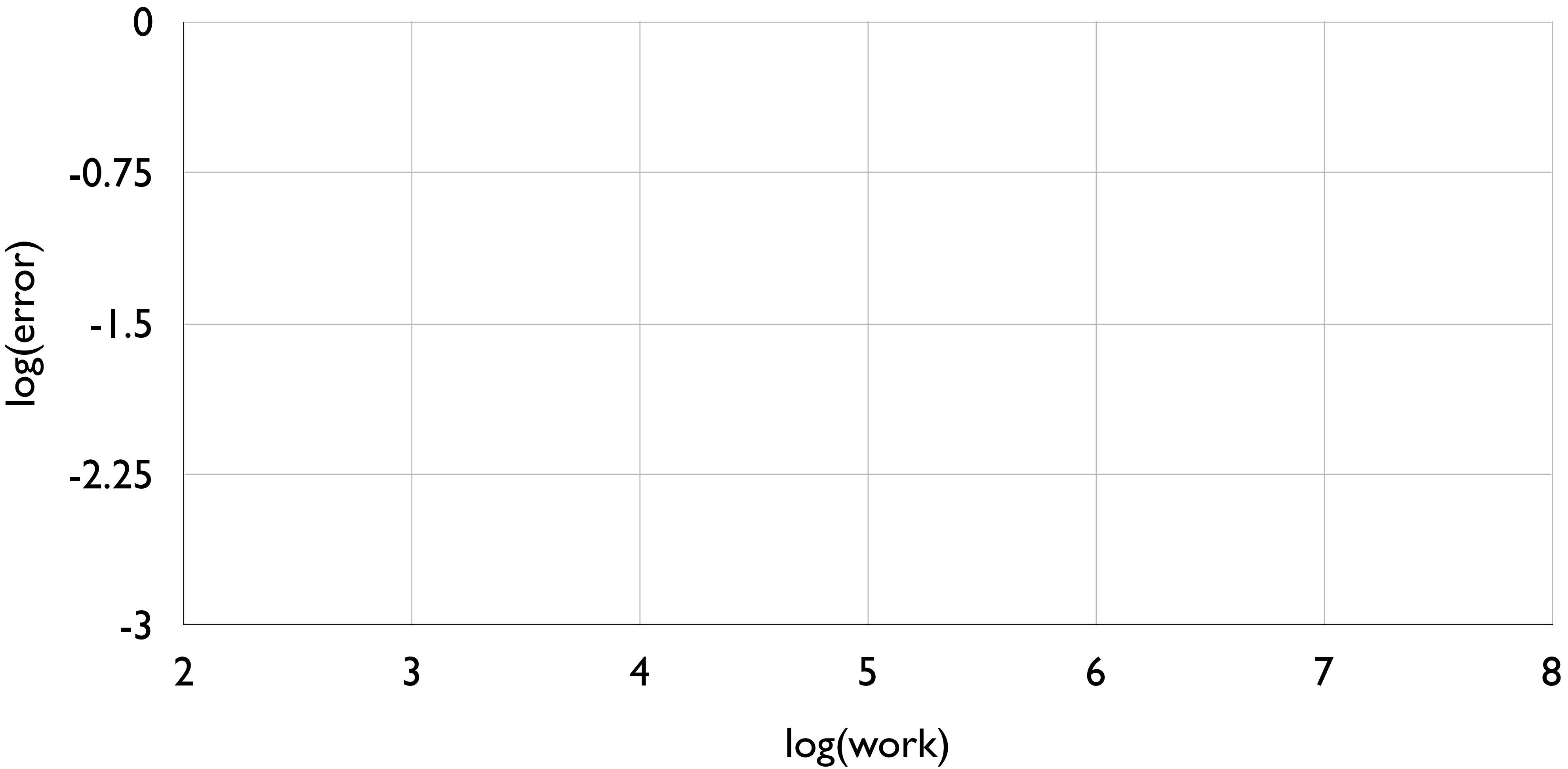


Results

- L_∞ error in decay rate



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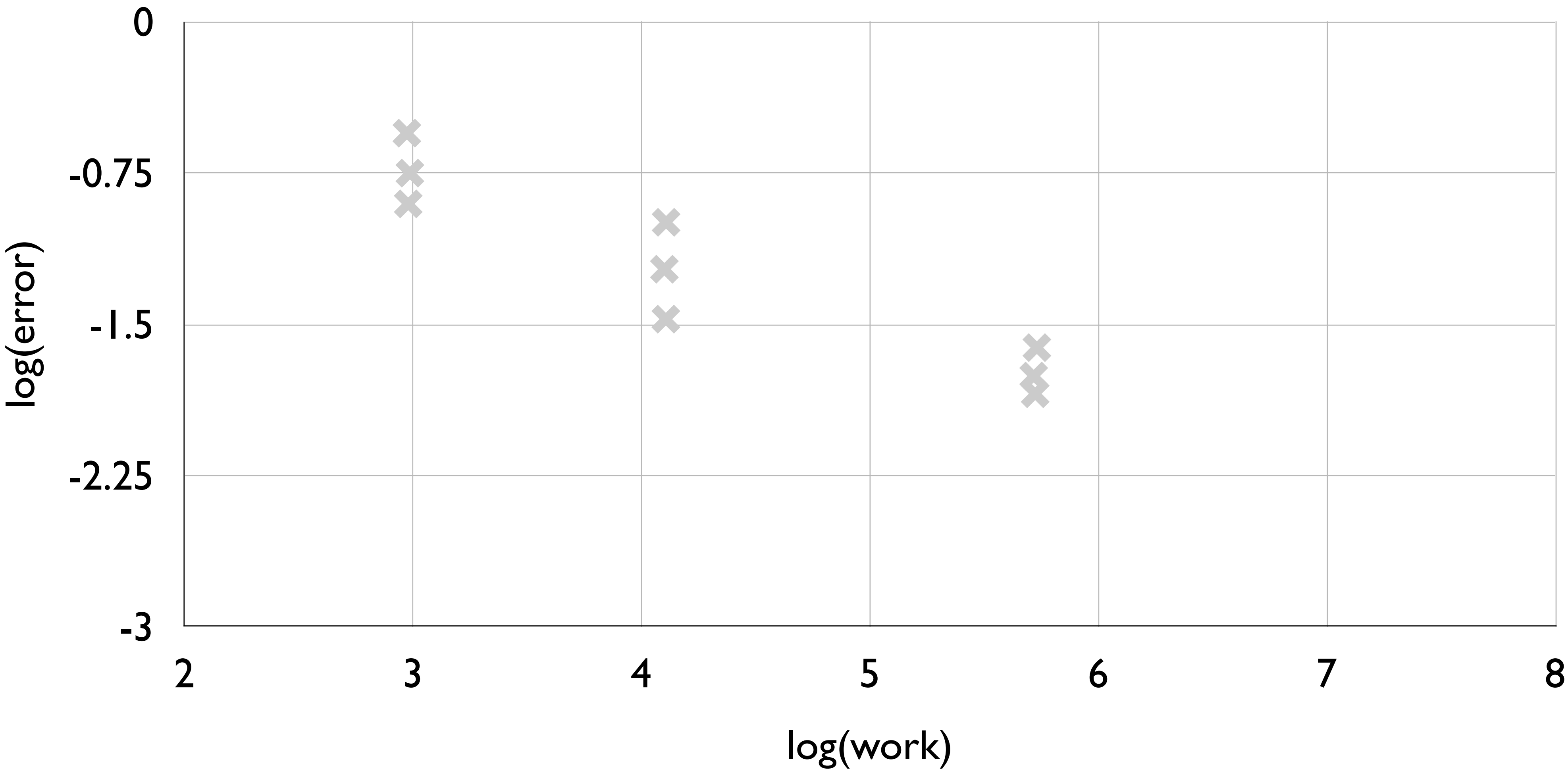

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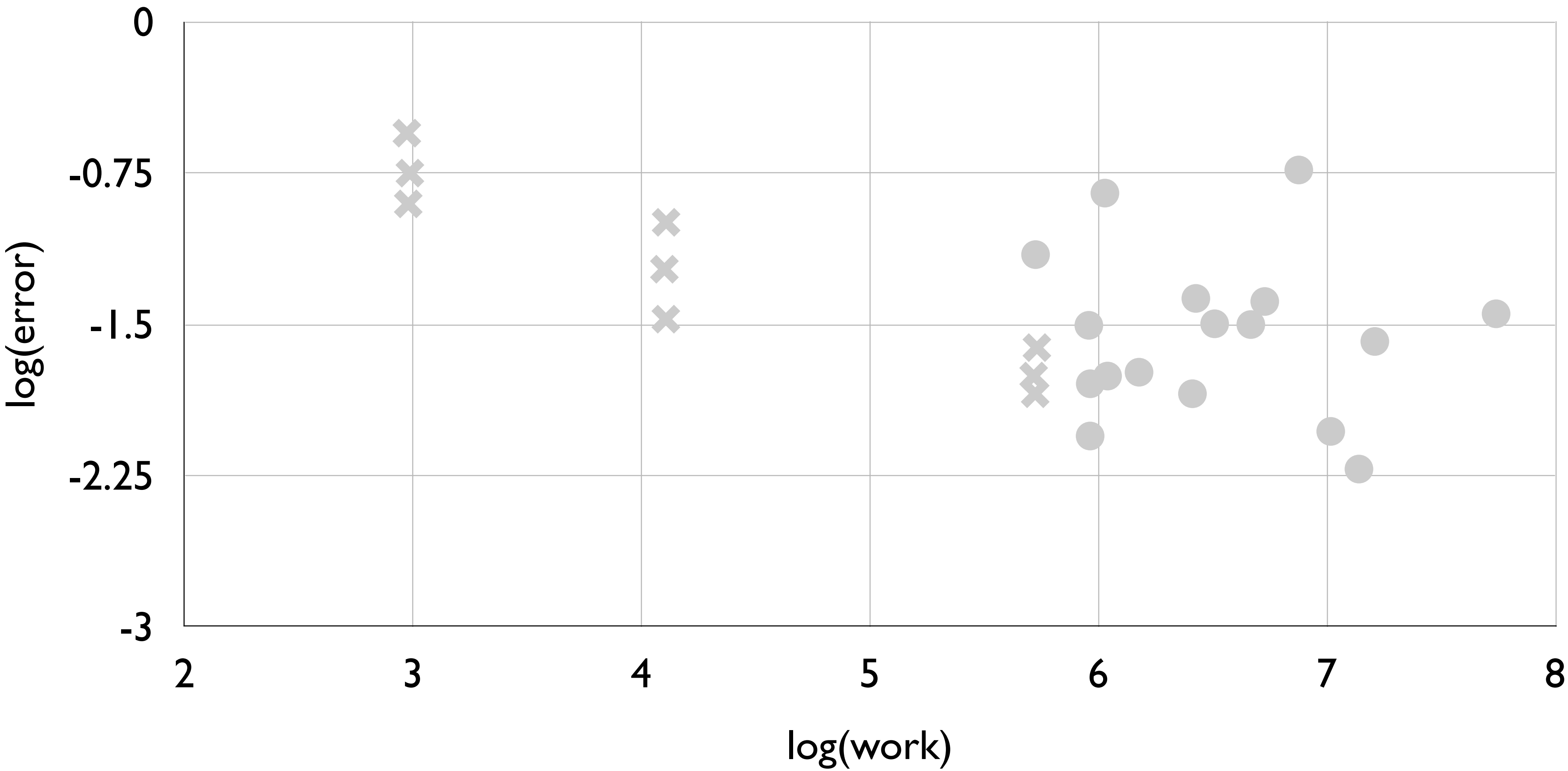

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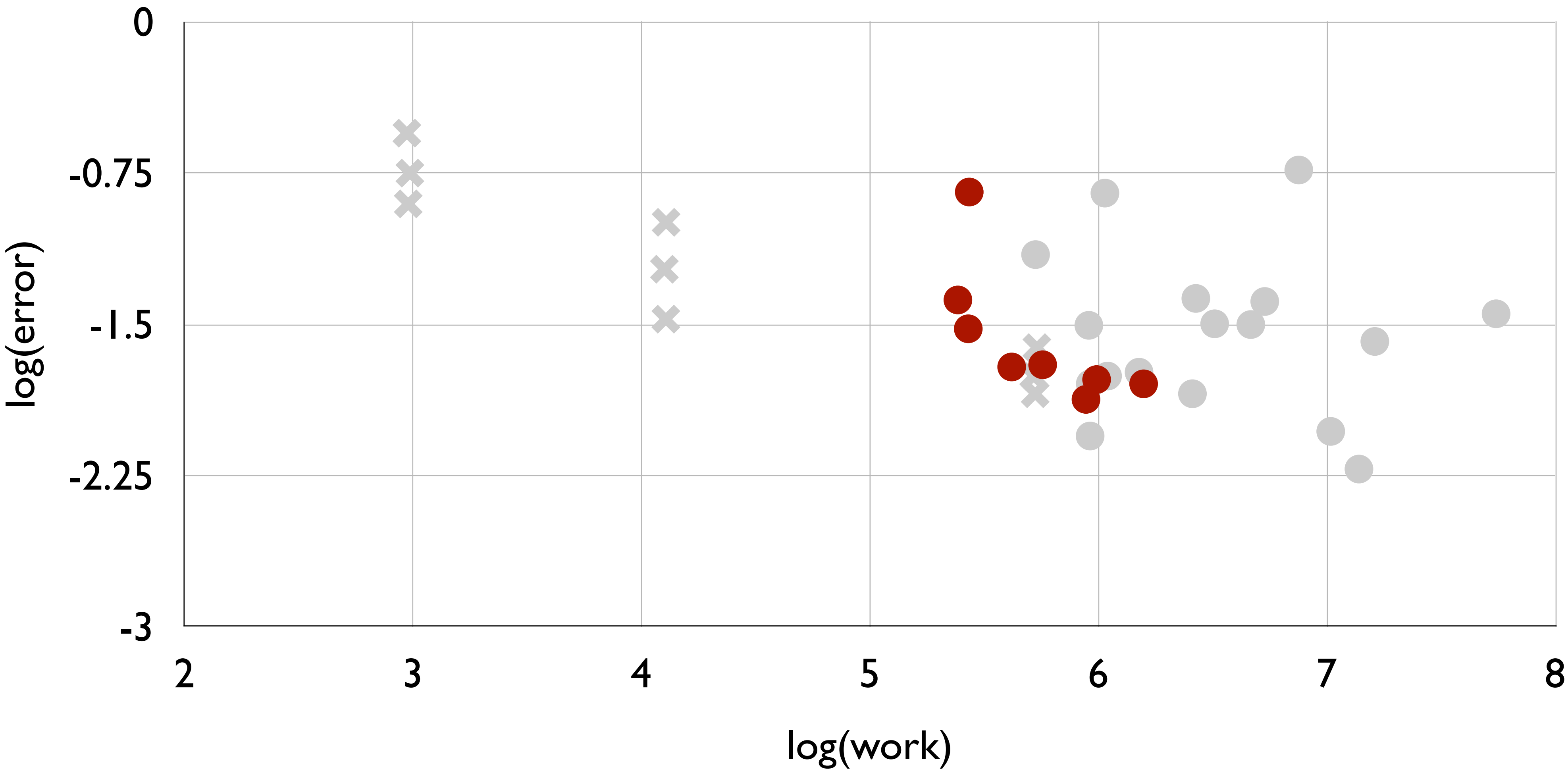

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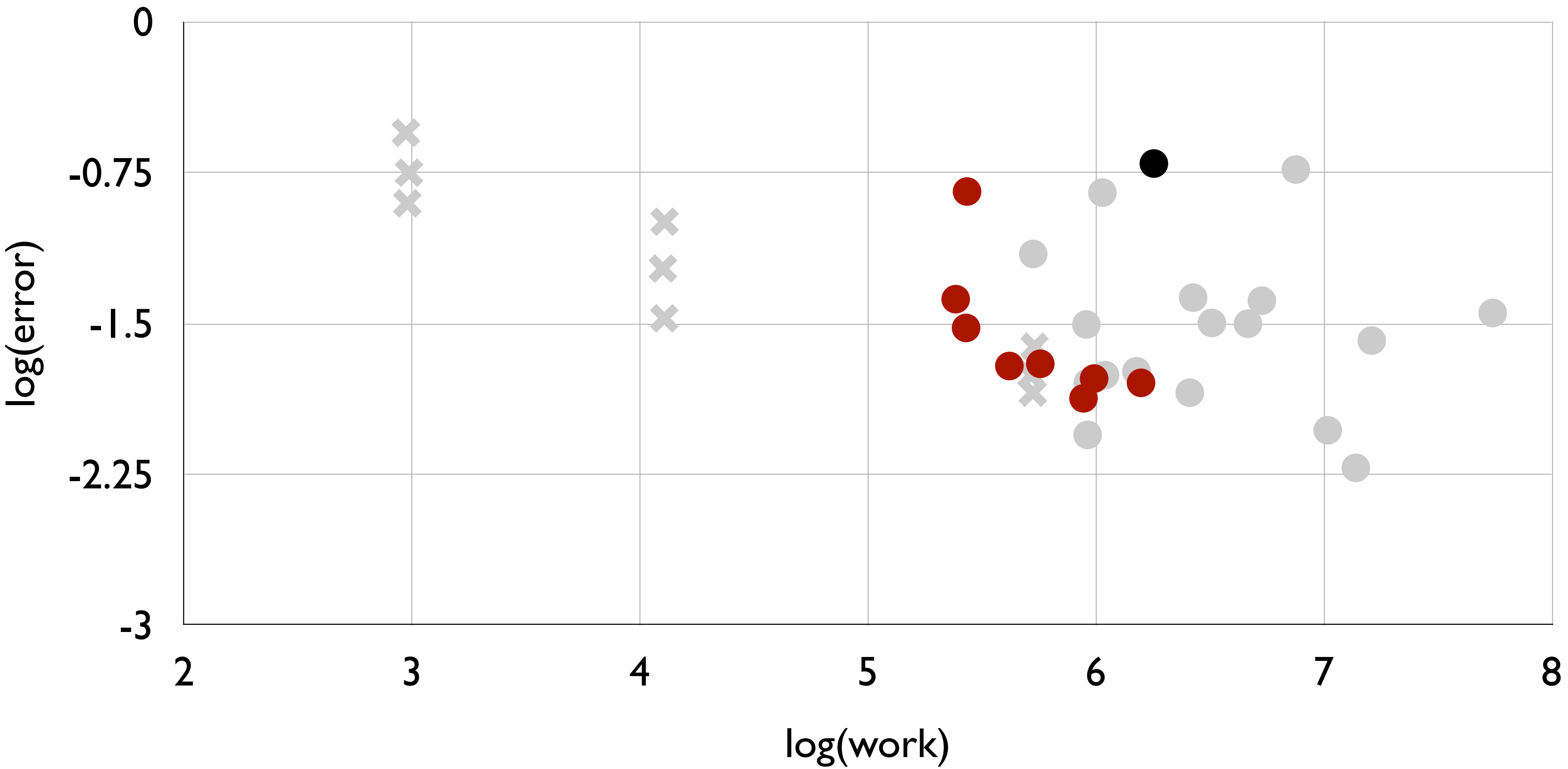

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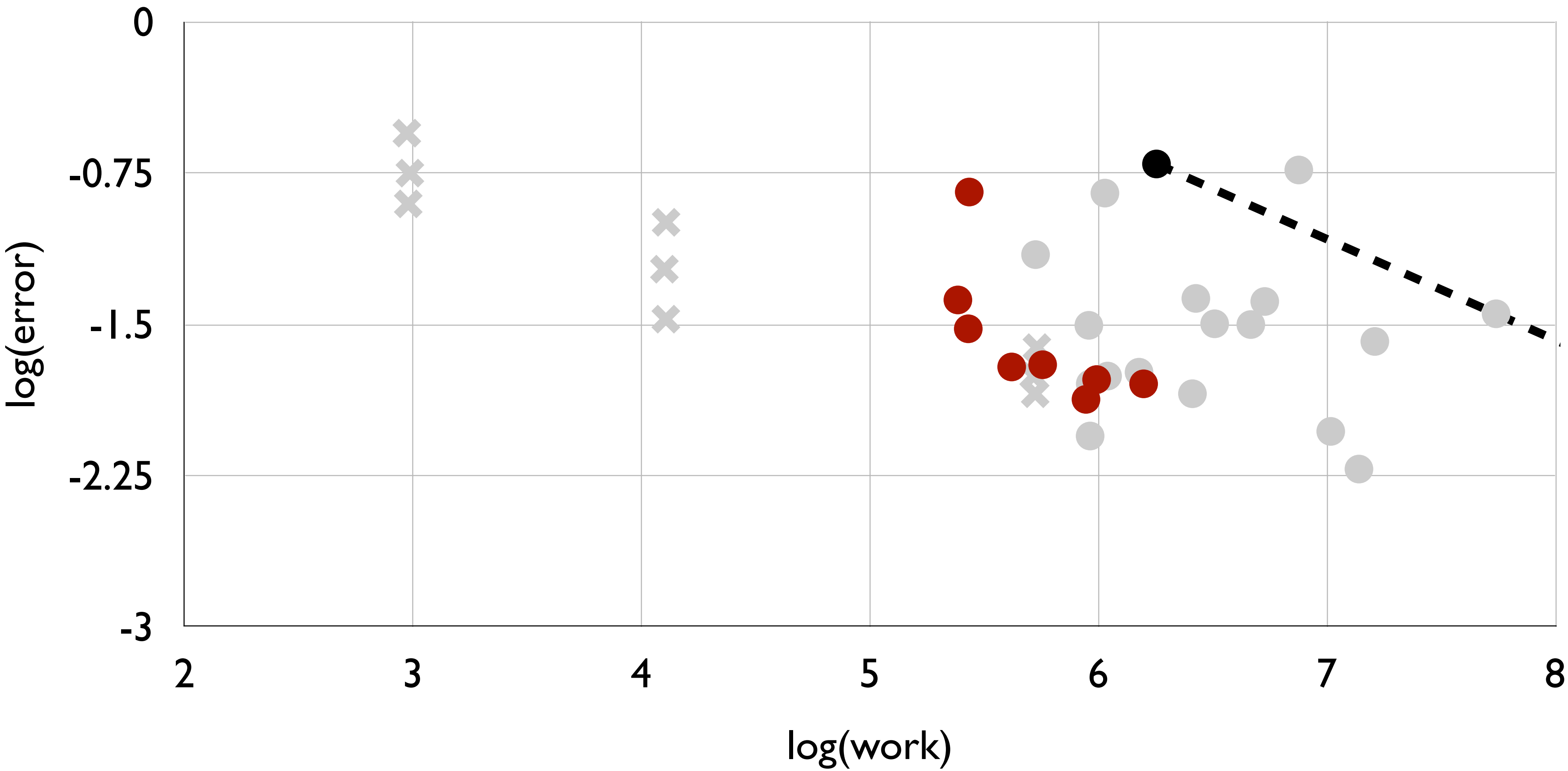
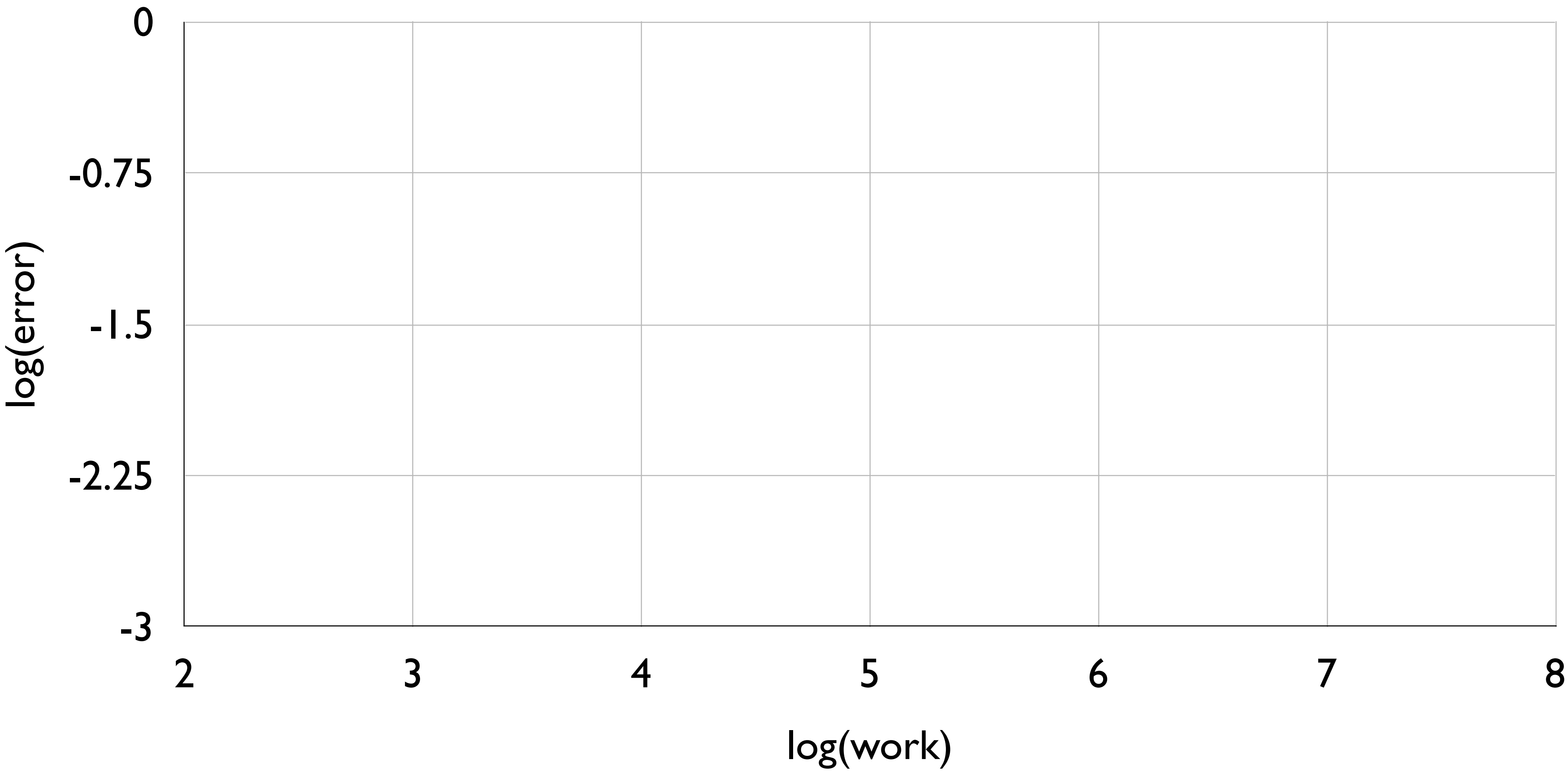


Results

- L_∞ difference between decay rate and enstrophy



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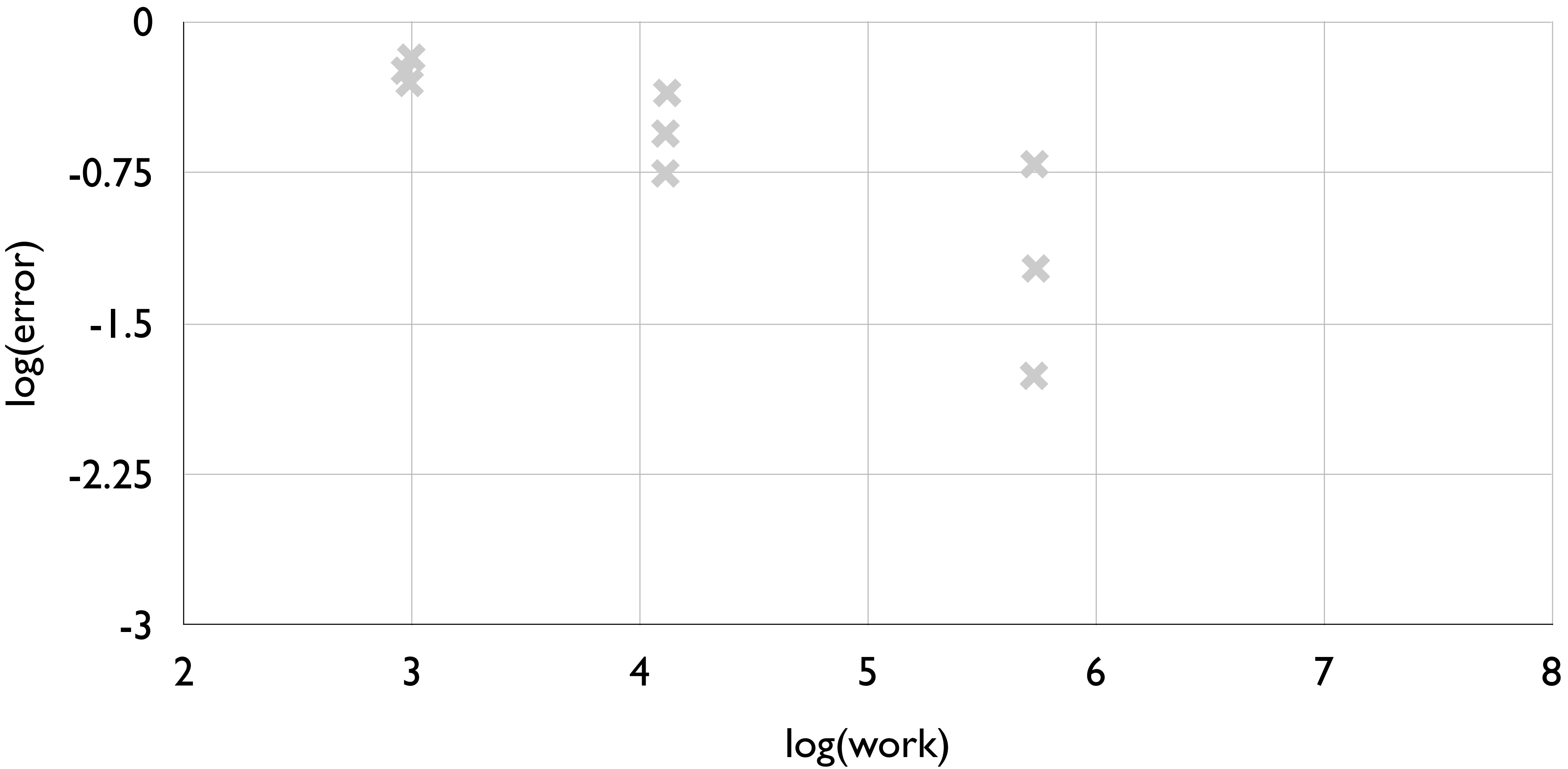

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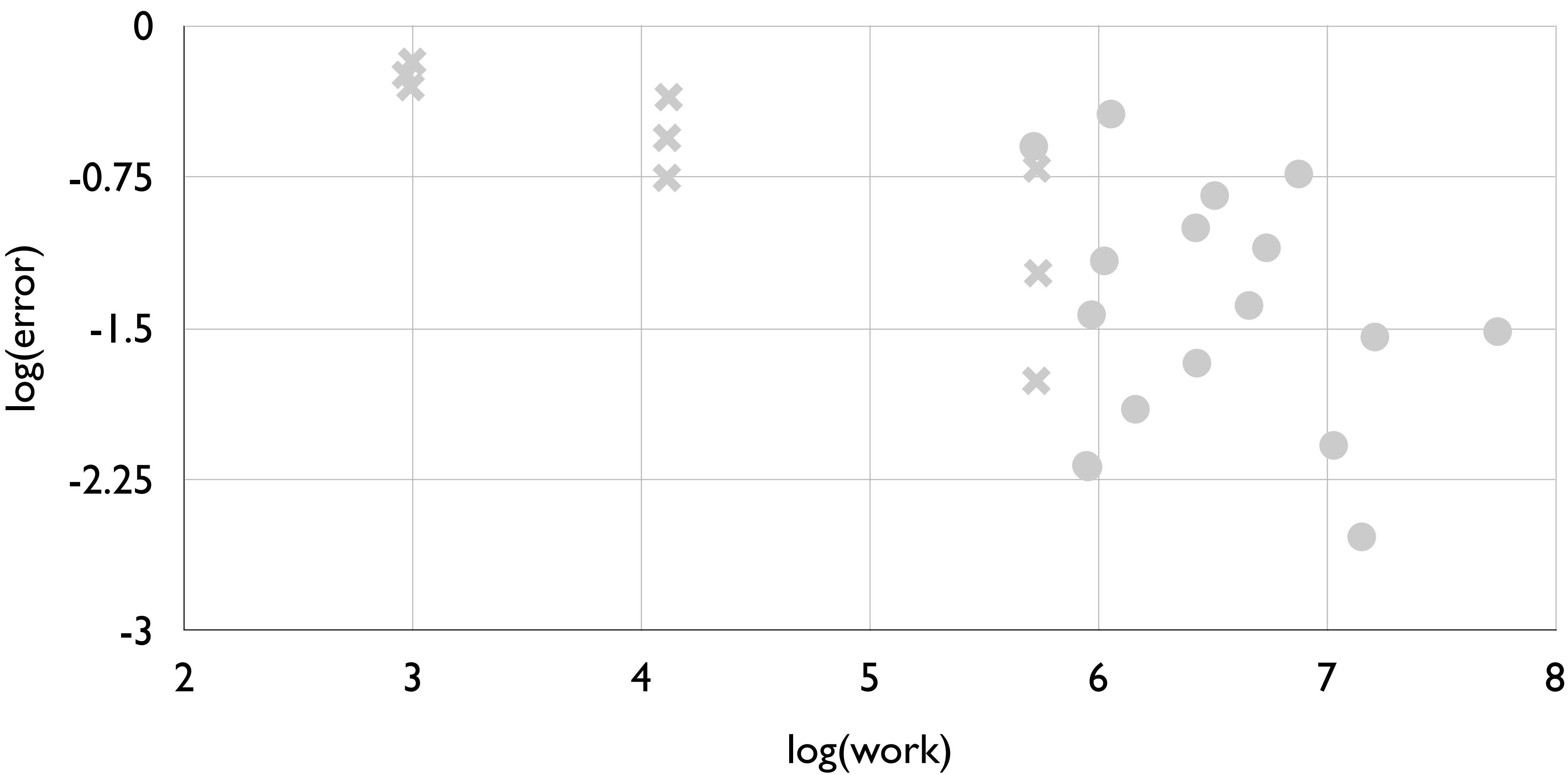

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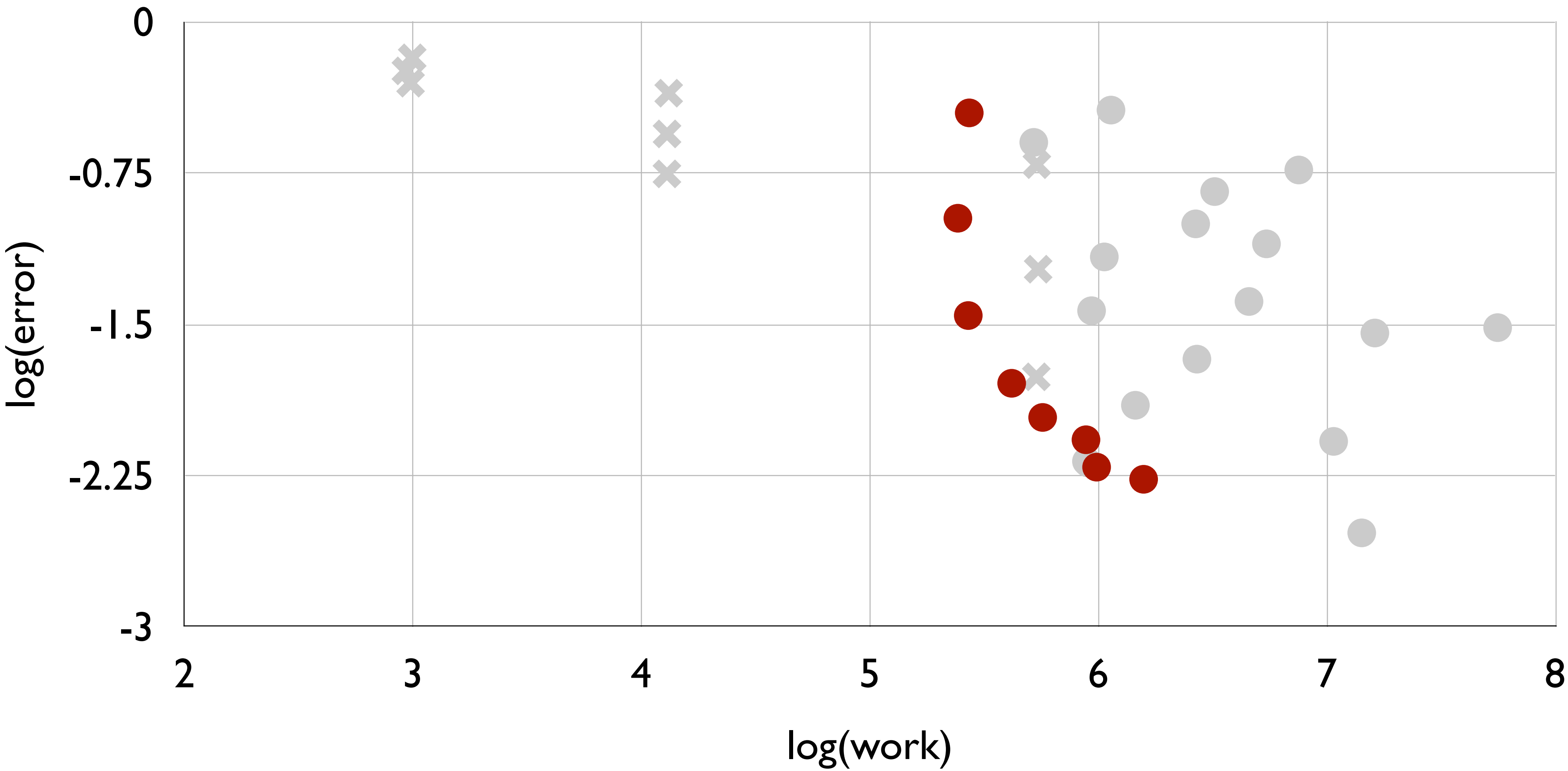

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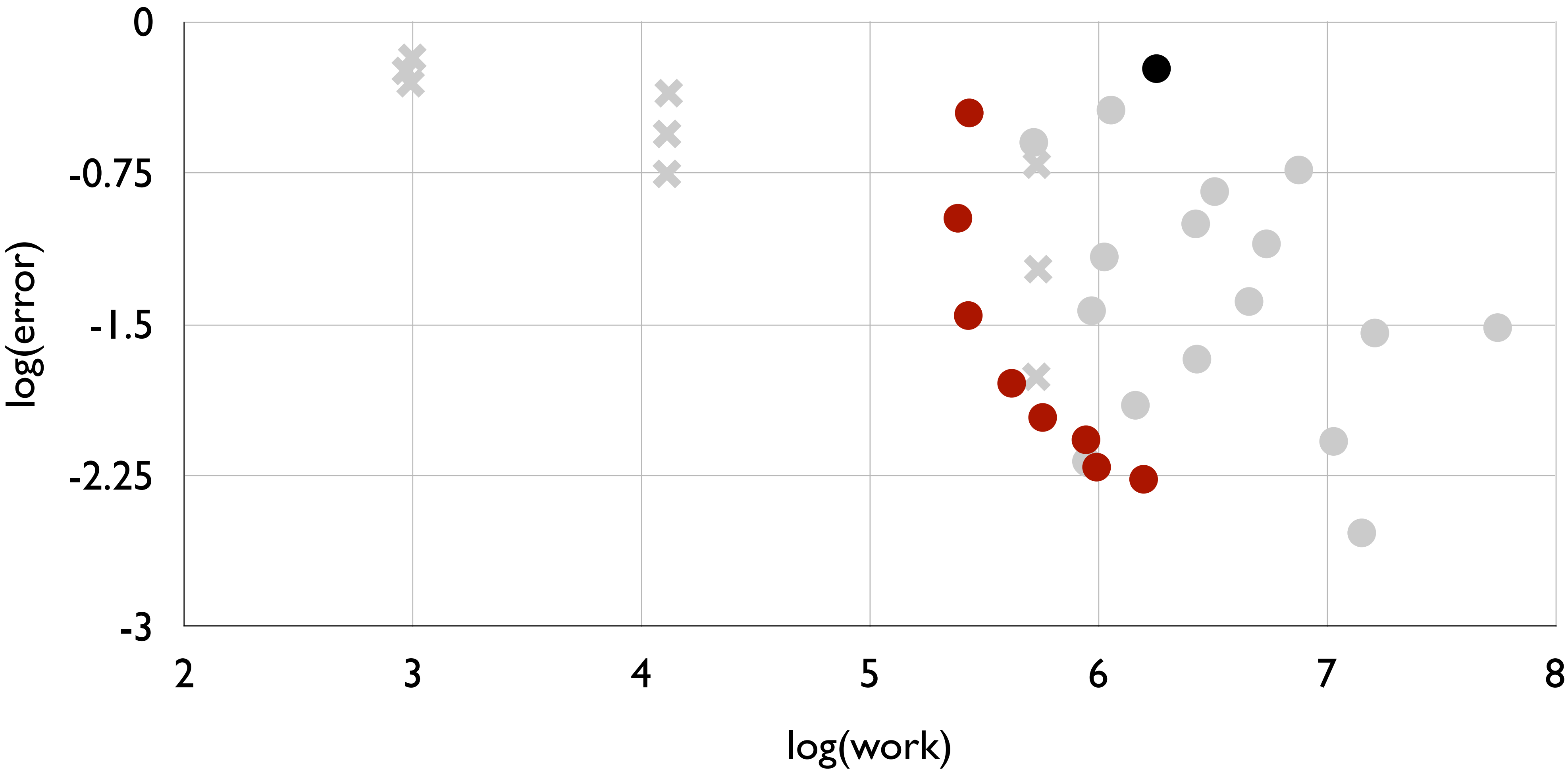

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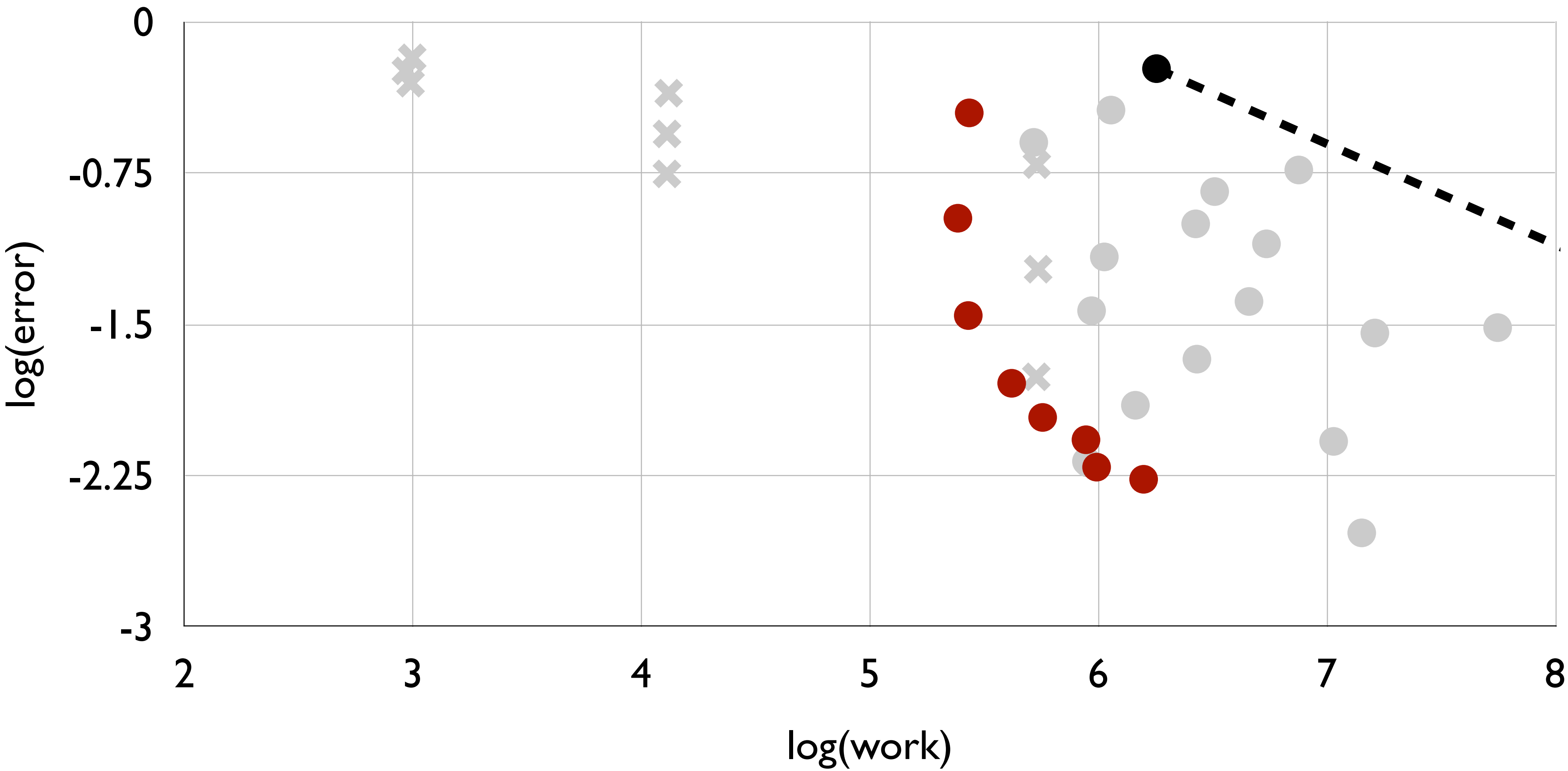


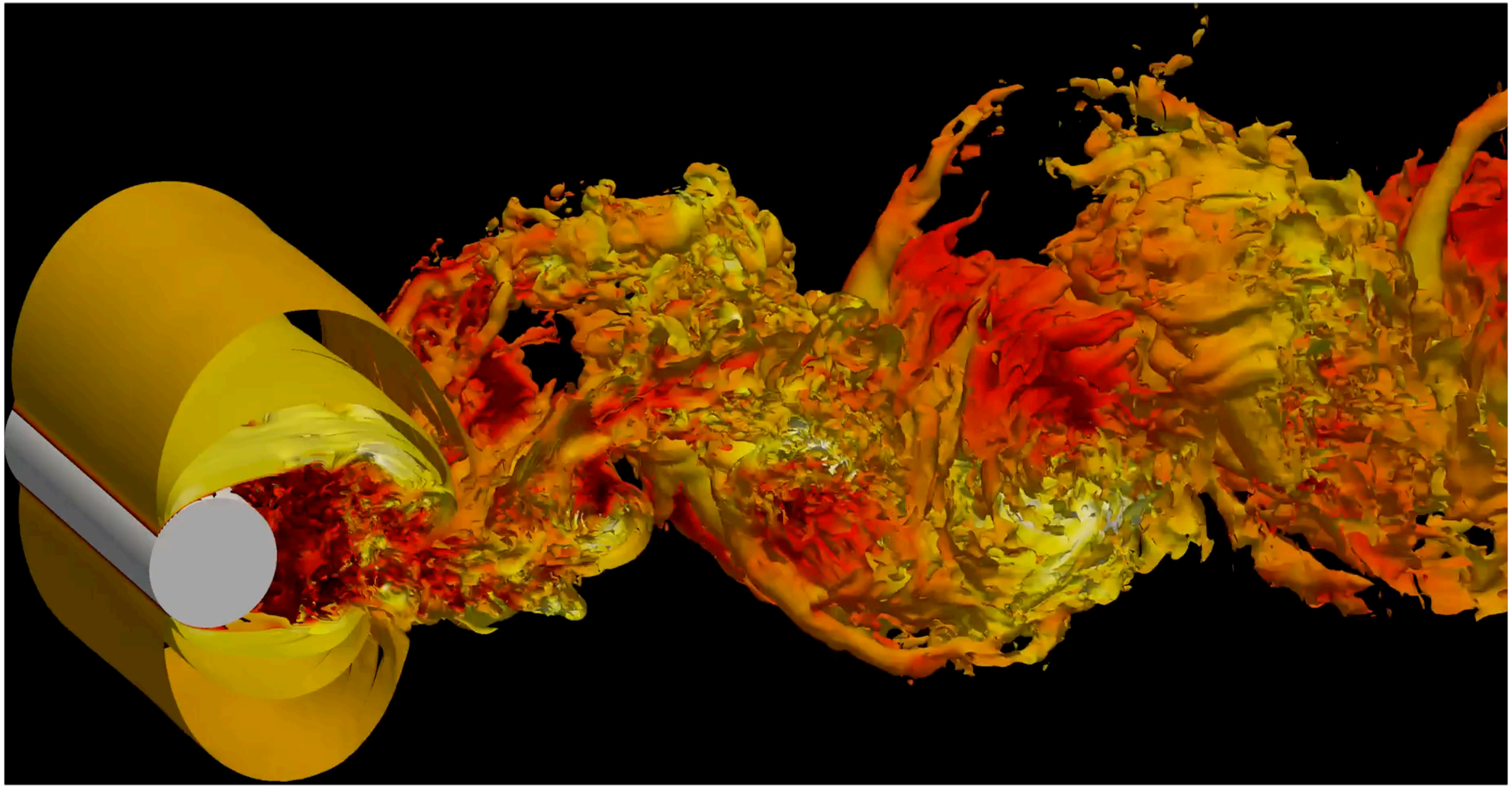
Results

- Flow over a circular cylinder
- Re = 3900
- Ma = 0.2
- Compare with Parnaudeau et al. [6]

[6] 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

- A movie …



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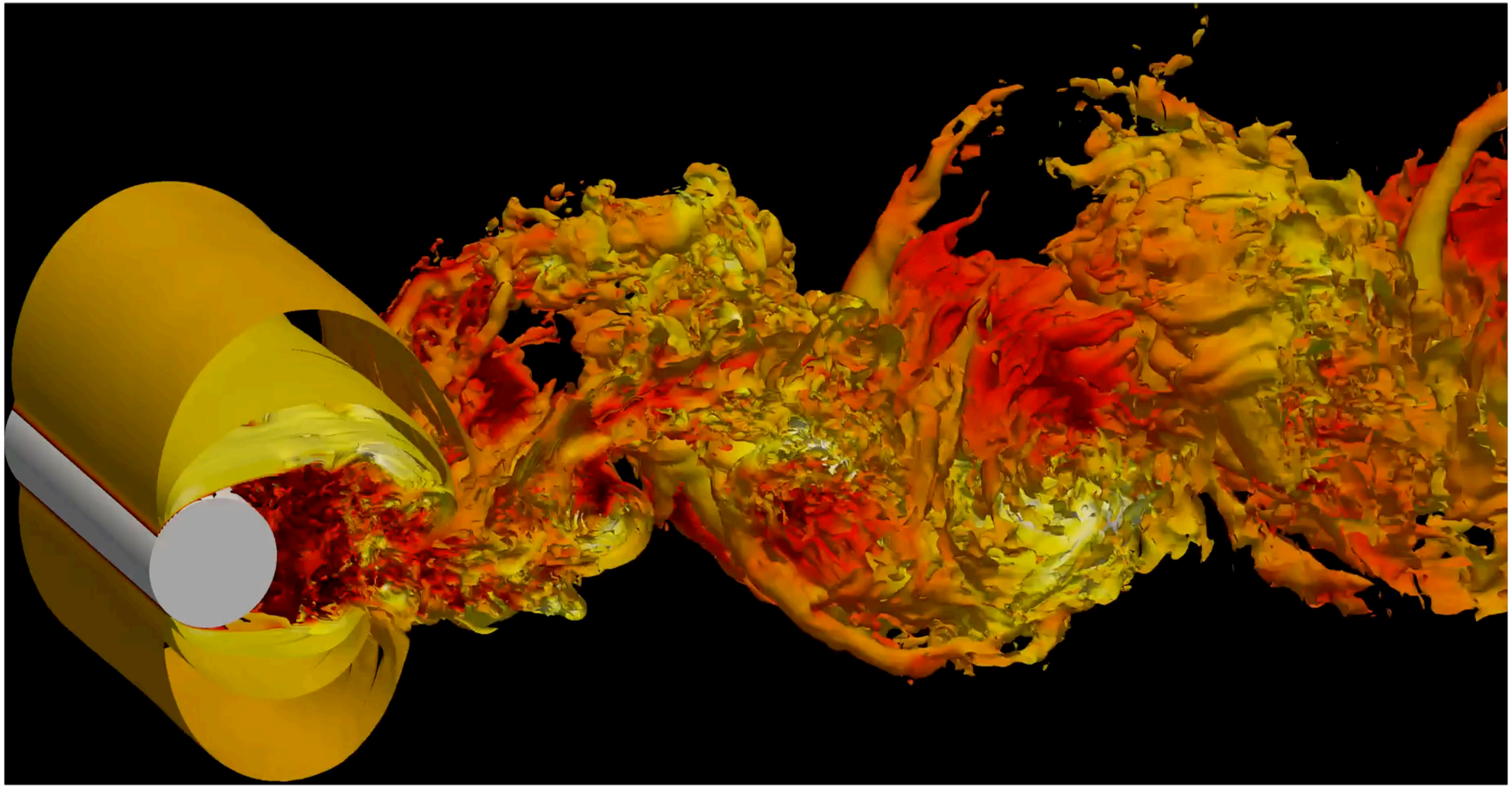
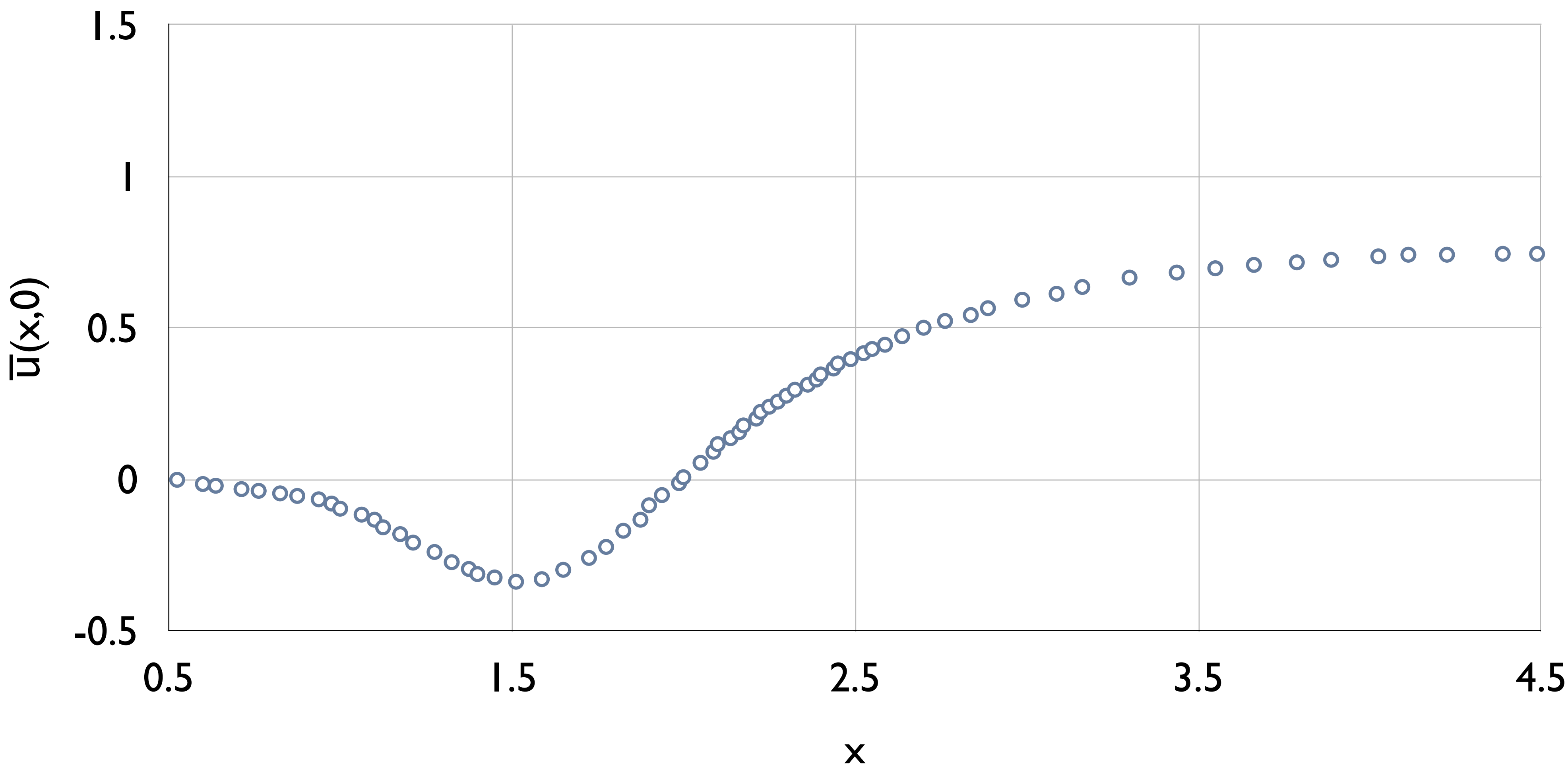


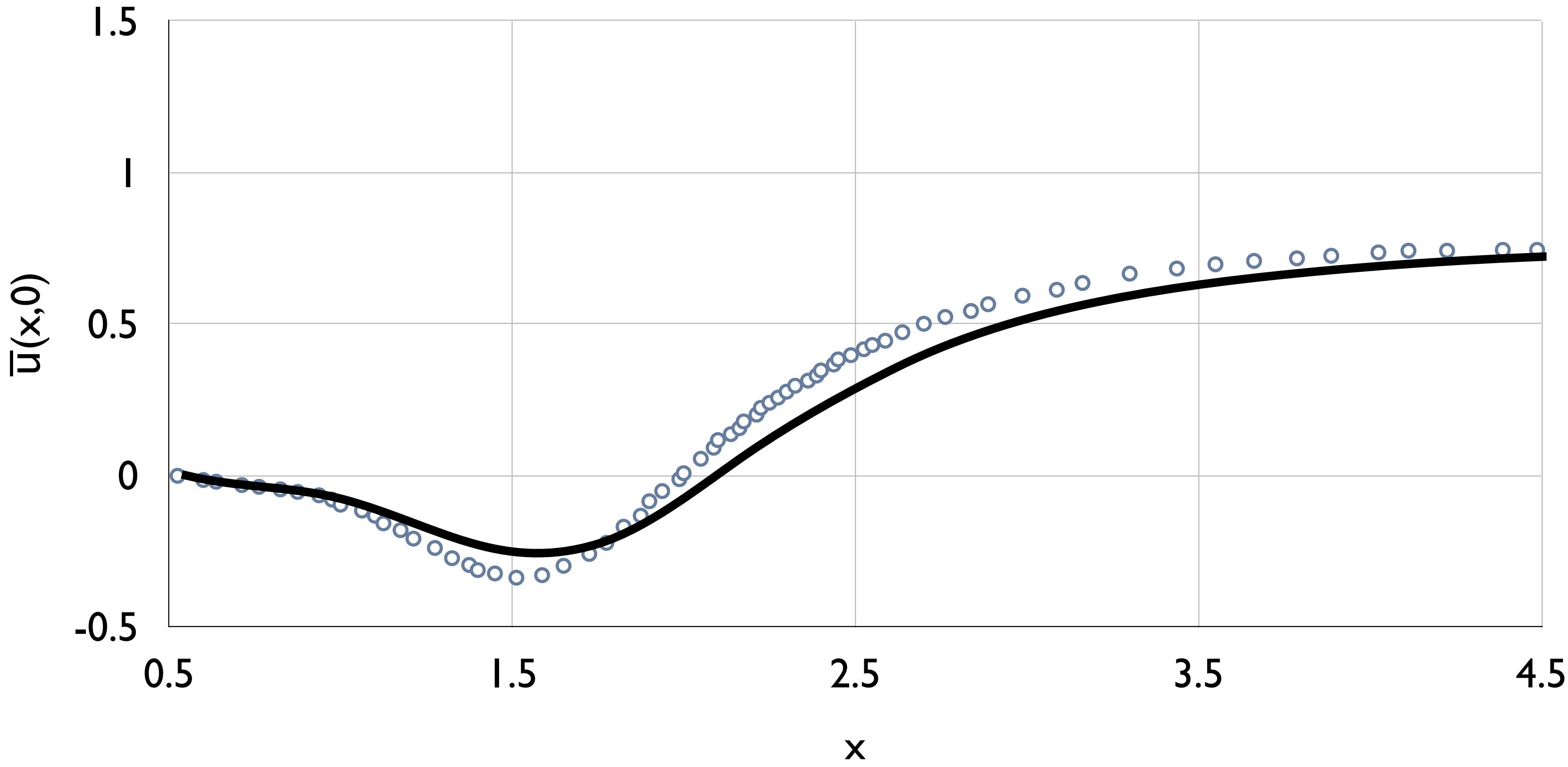
Results

- Parnaudeau et al. experiment



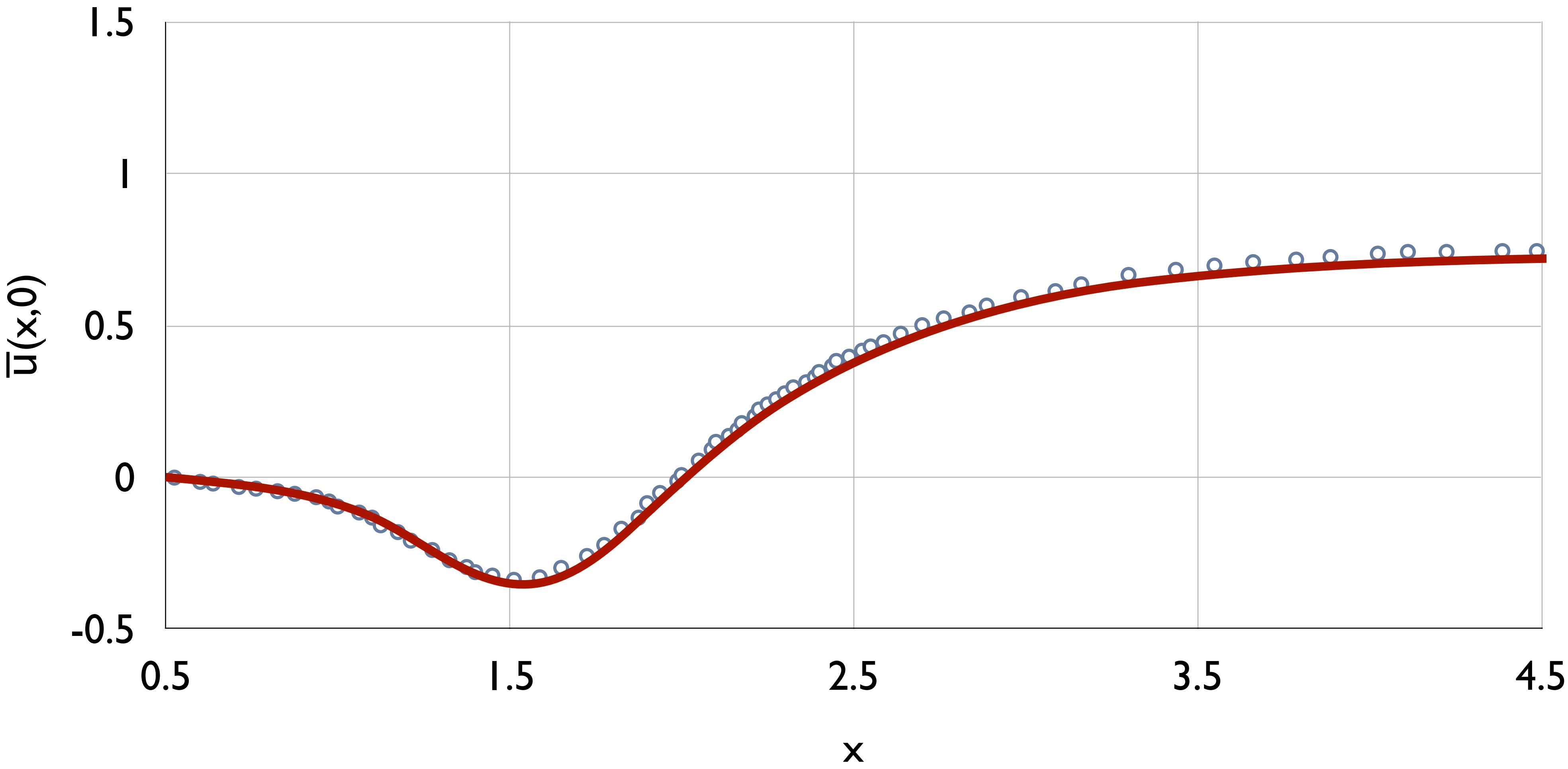
Results

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



Results

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



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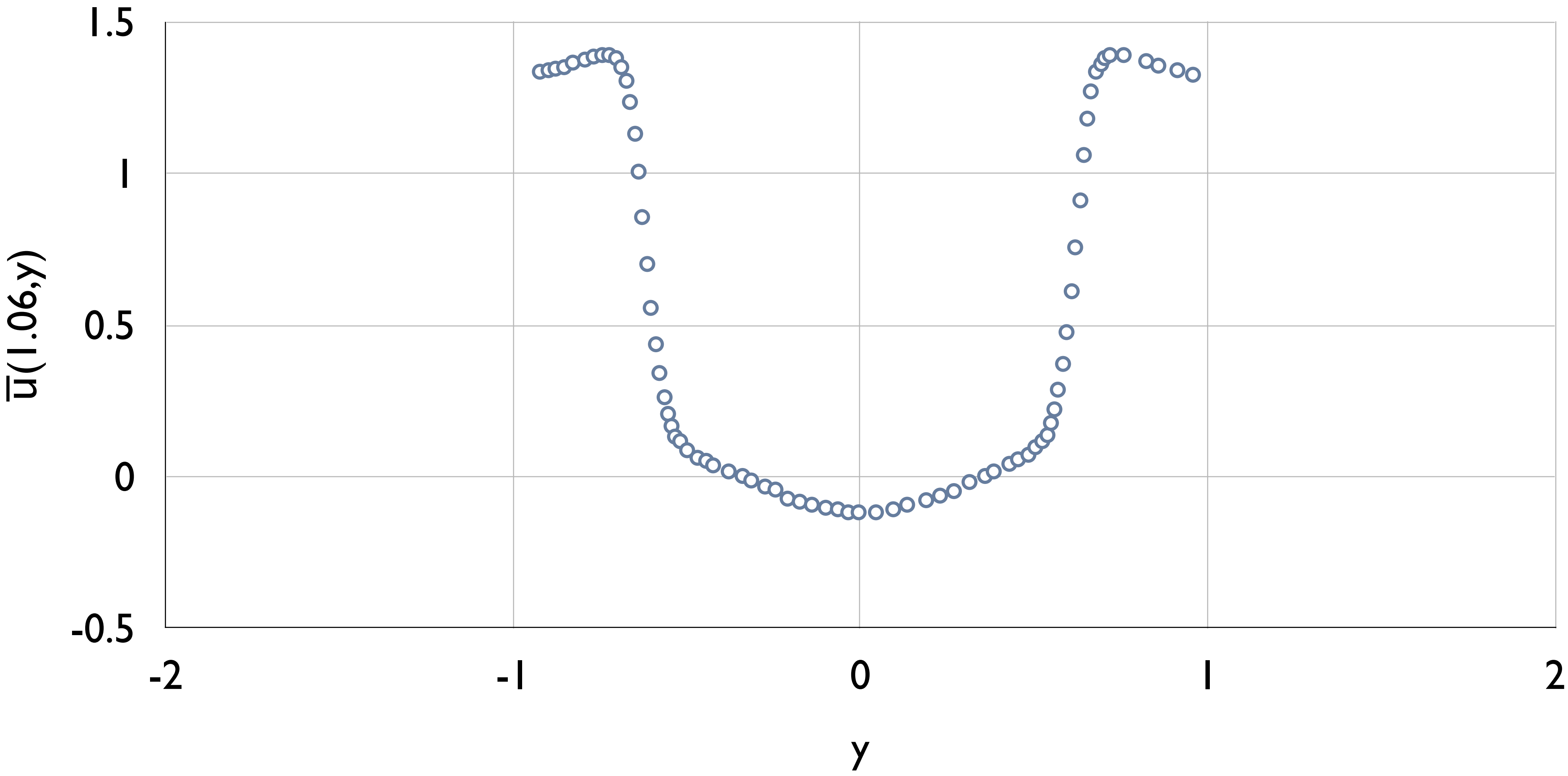

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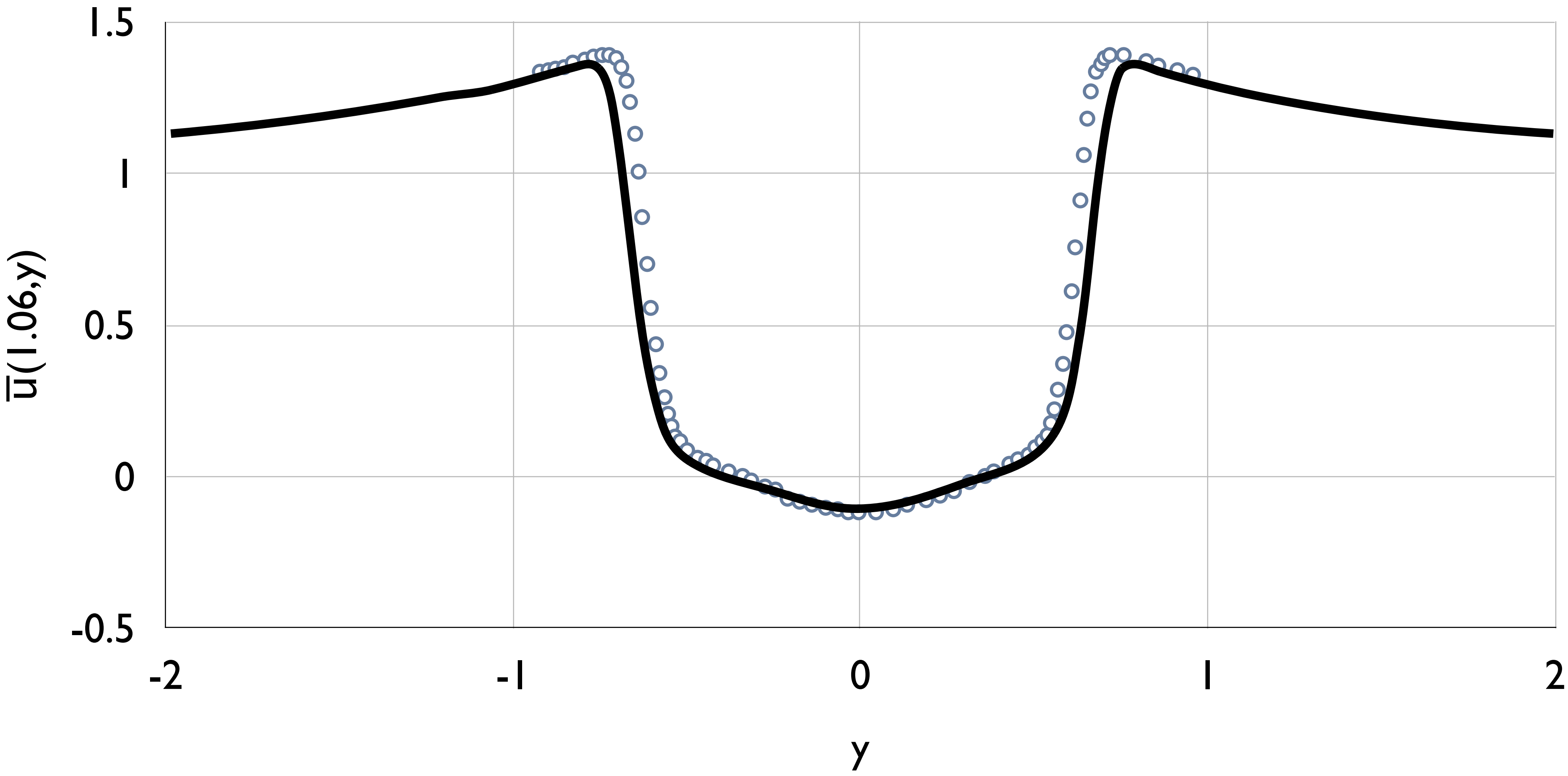

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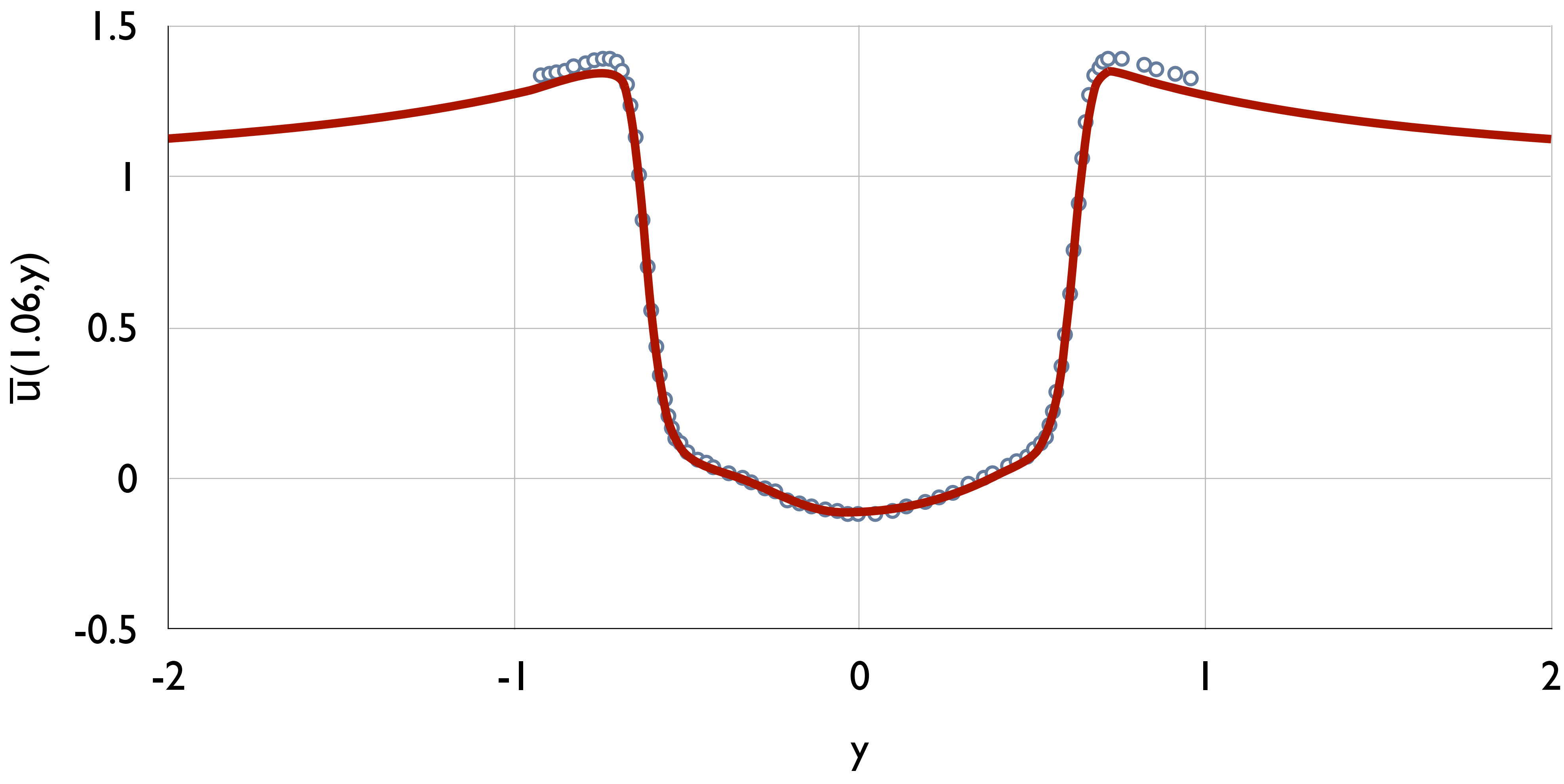

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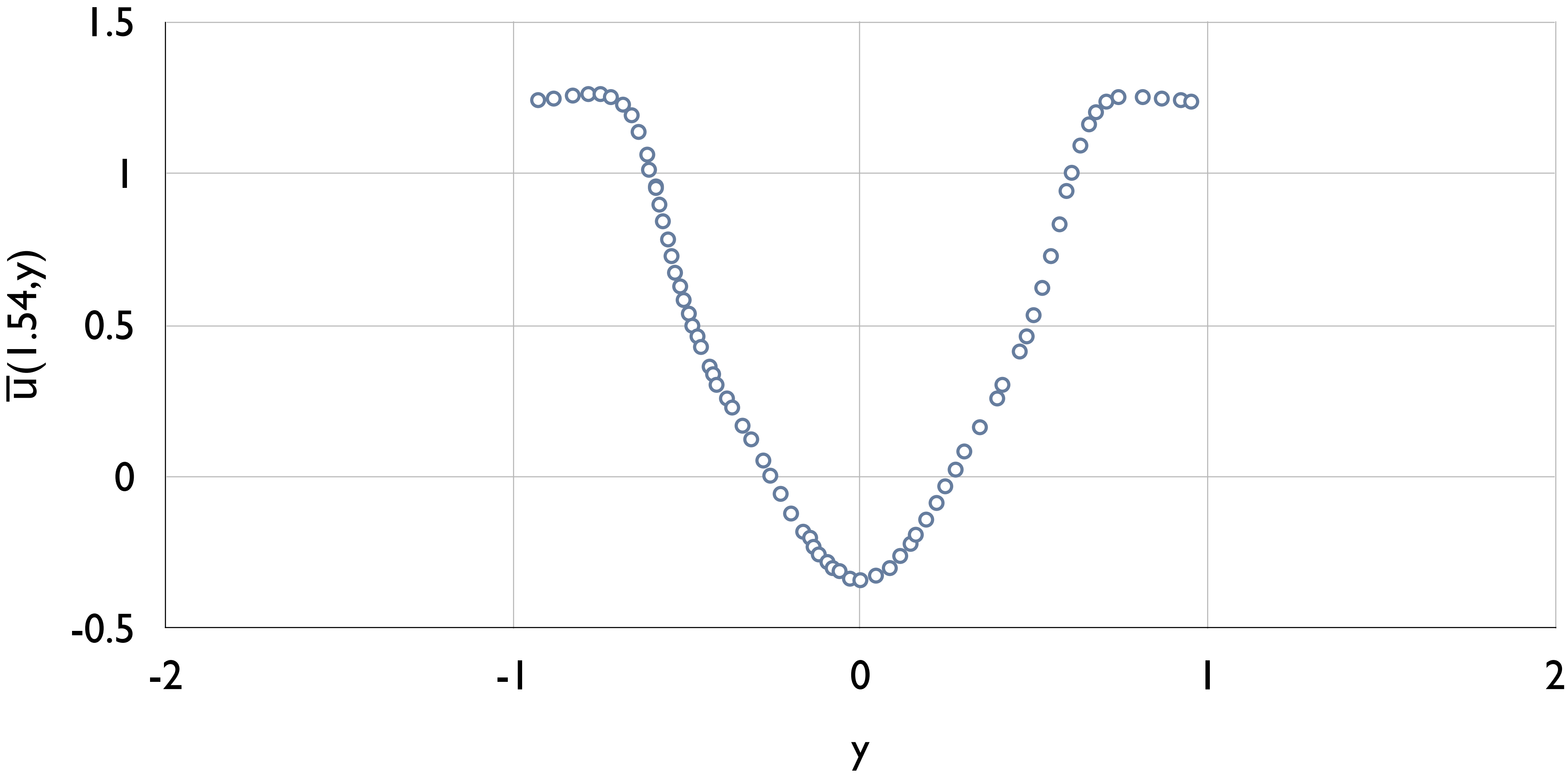

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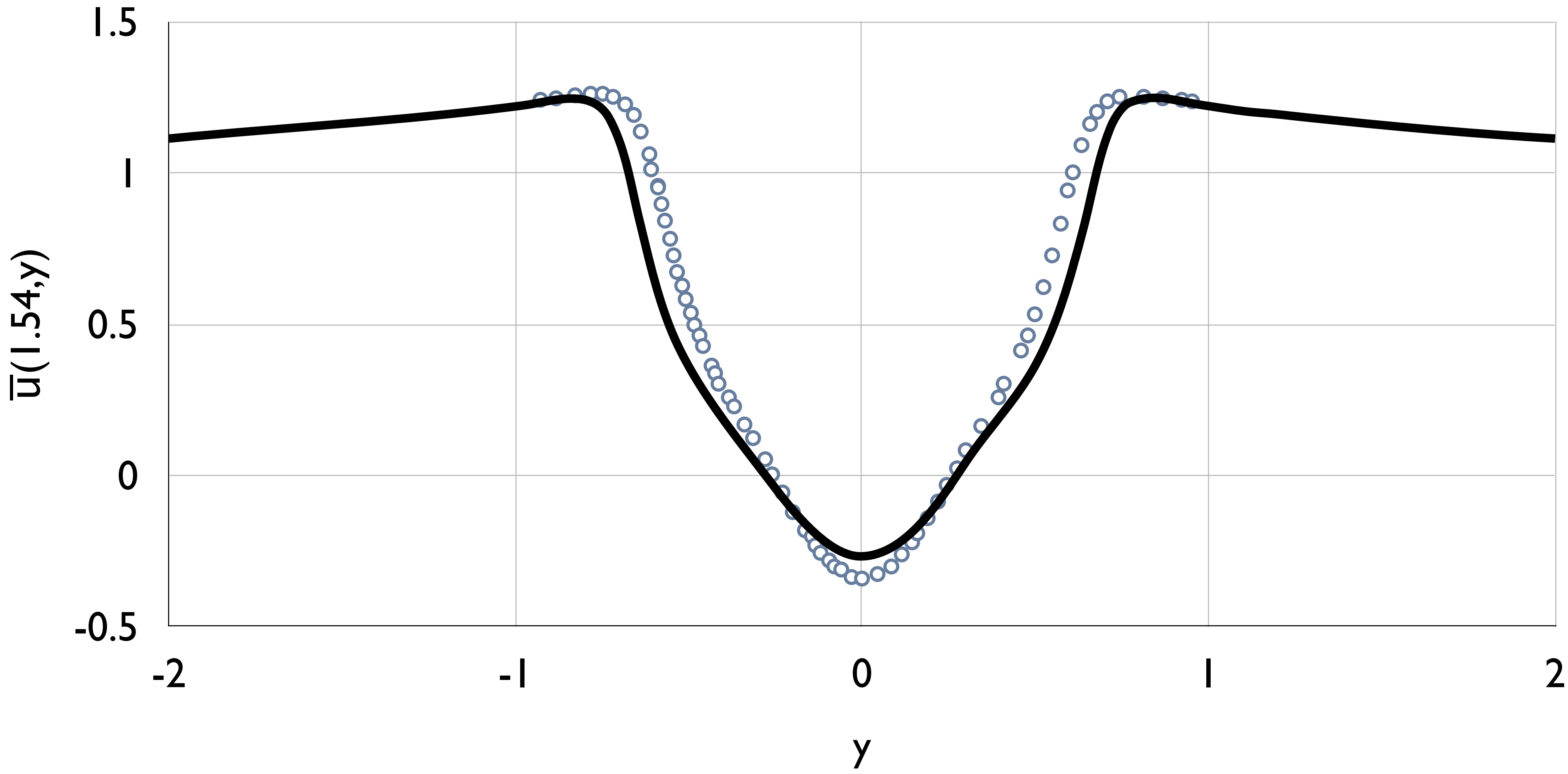

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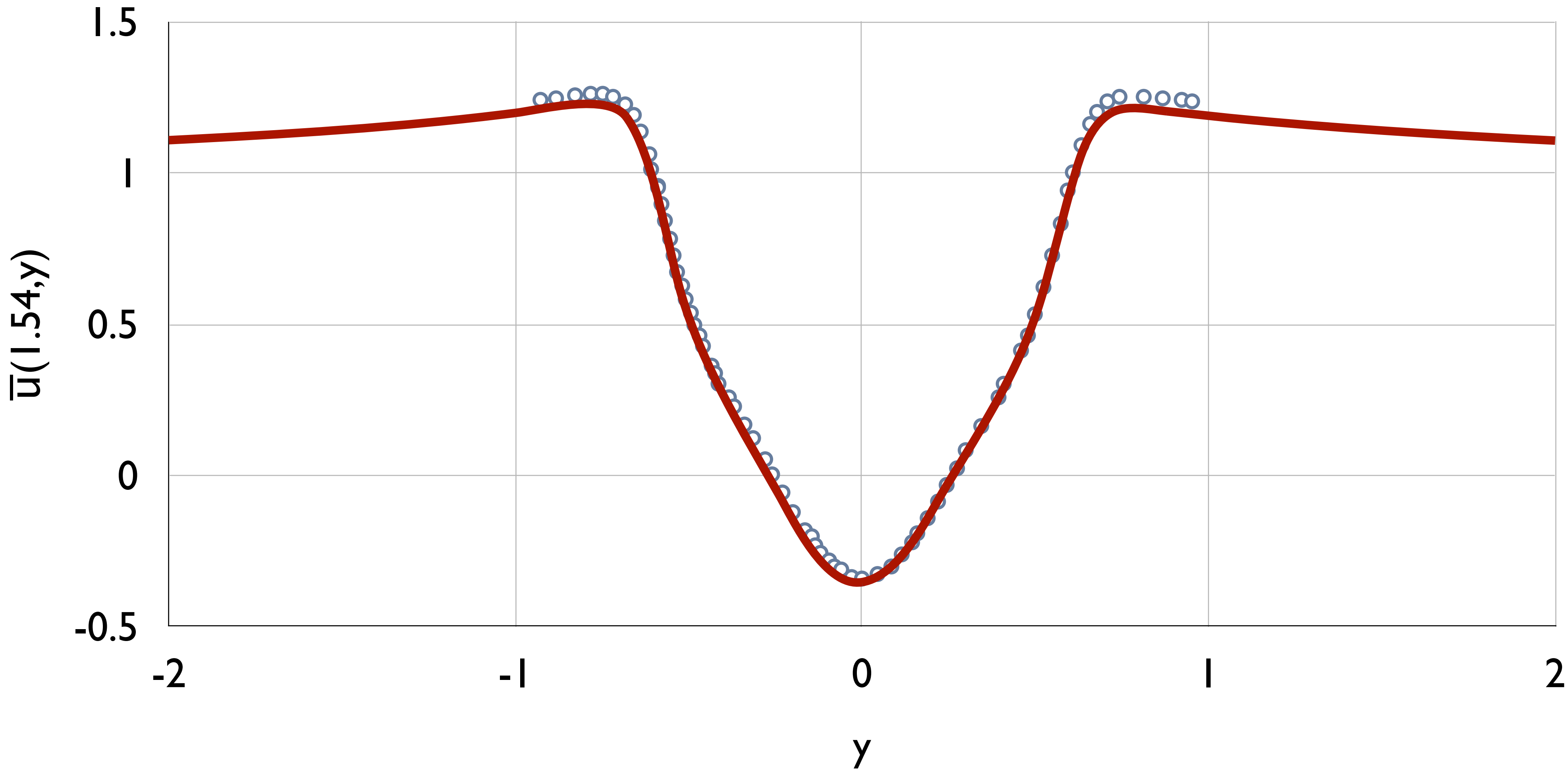
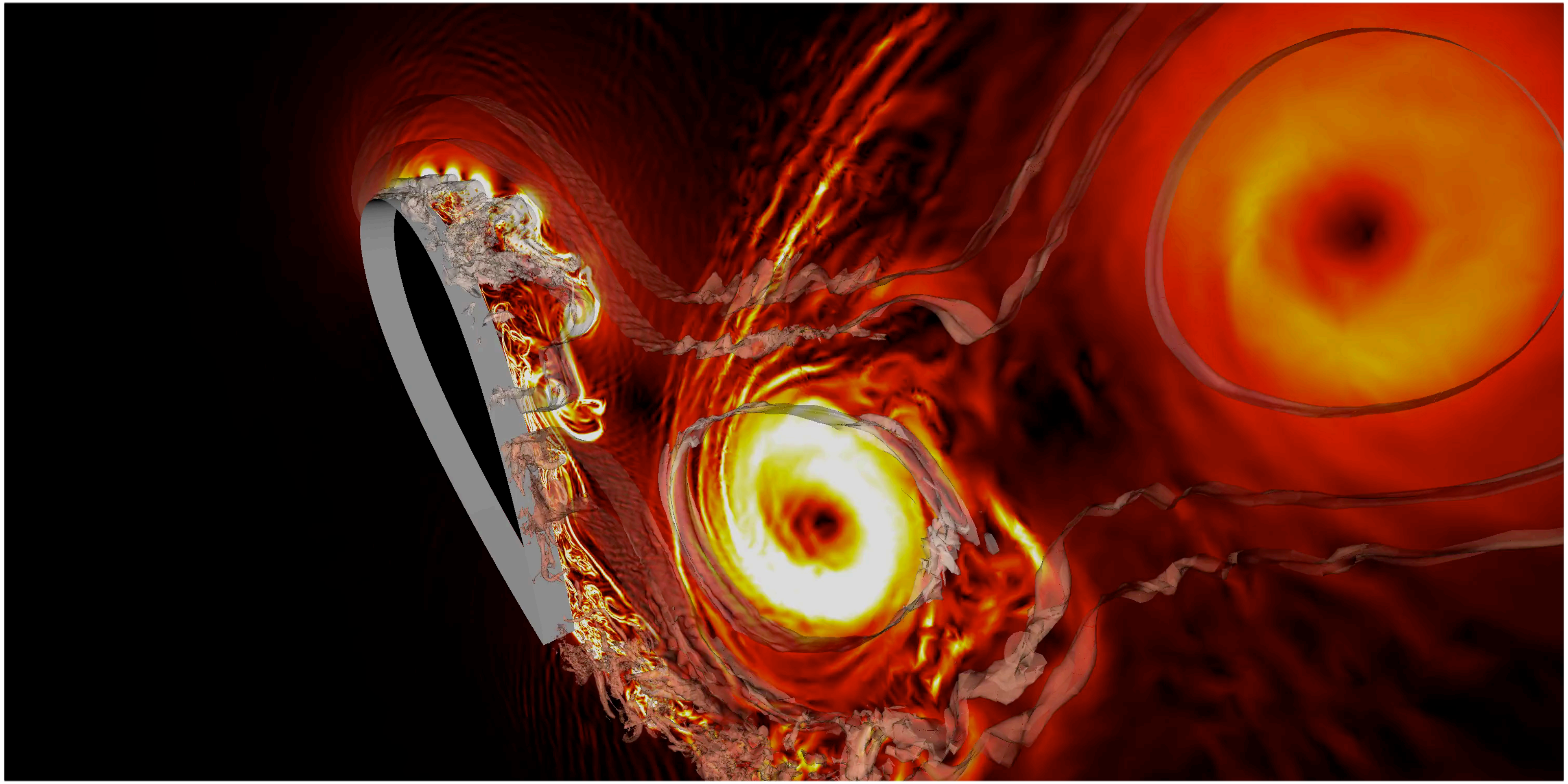


Results

- Flow over a NACA 0021 at 60 degree AoA
- Re = 270,000
- Ma = 0.2

Results

- A movie ...



Results

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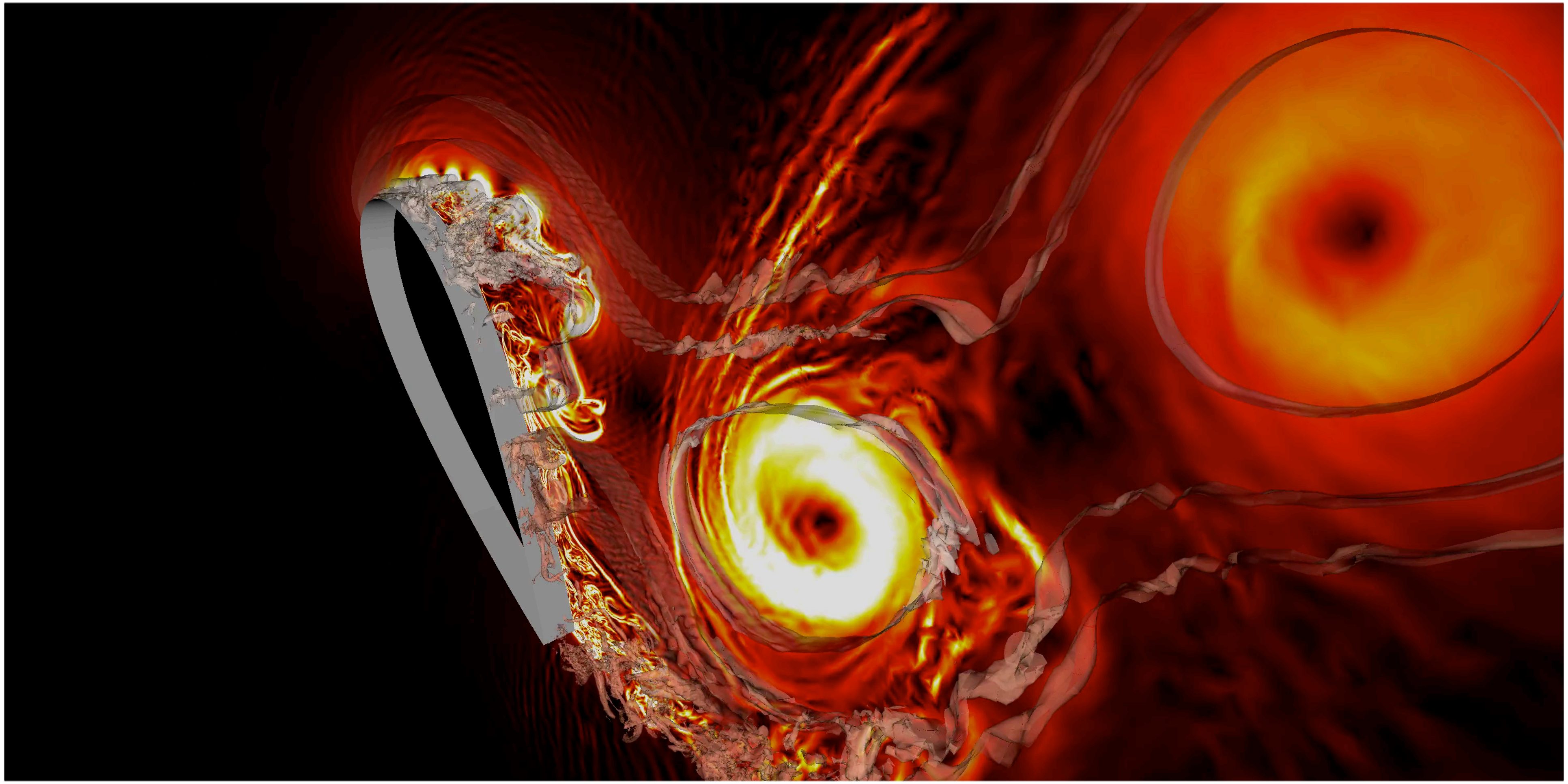
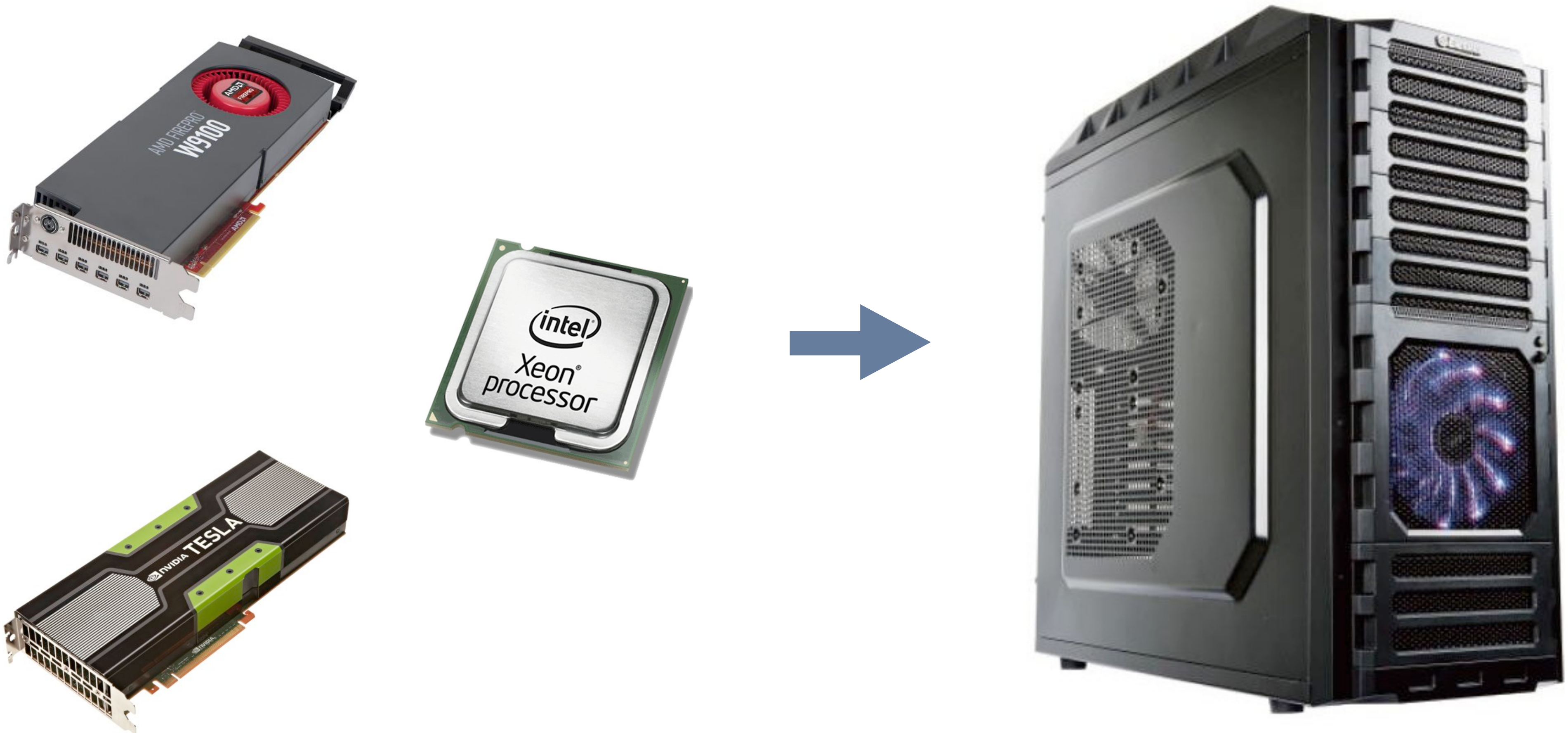


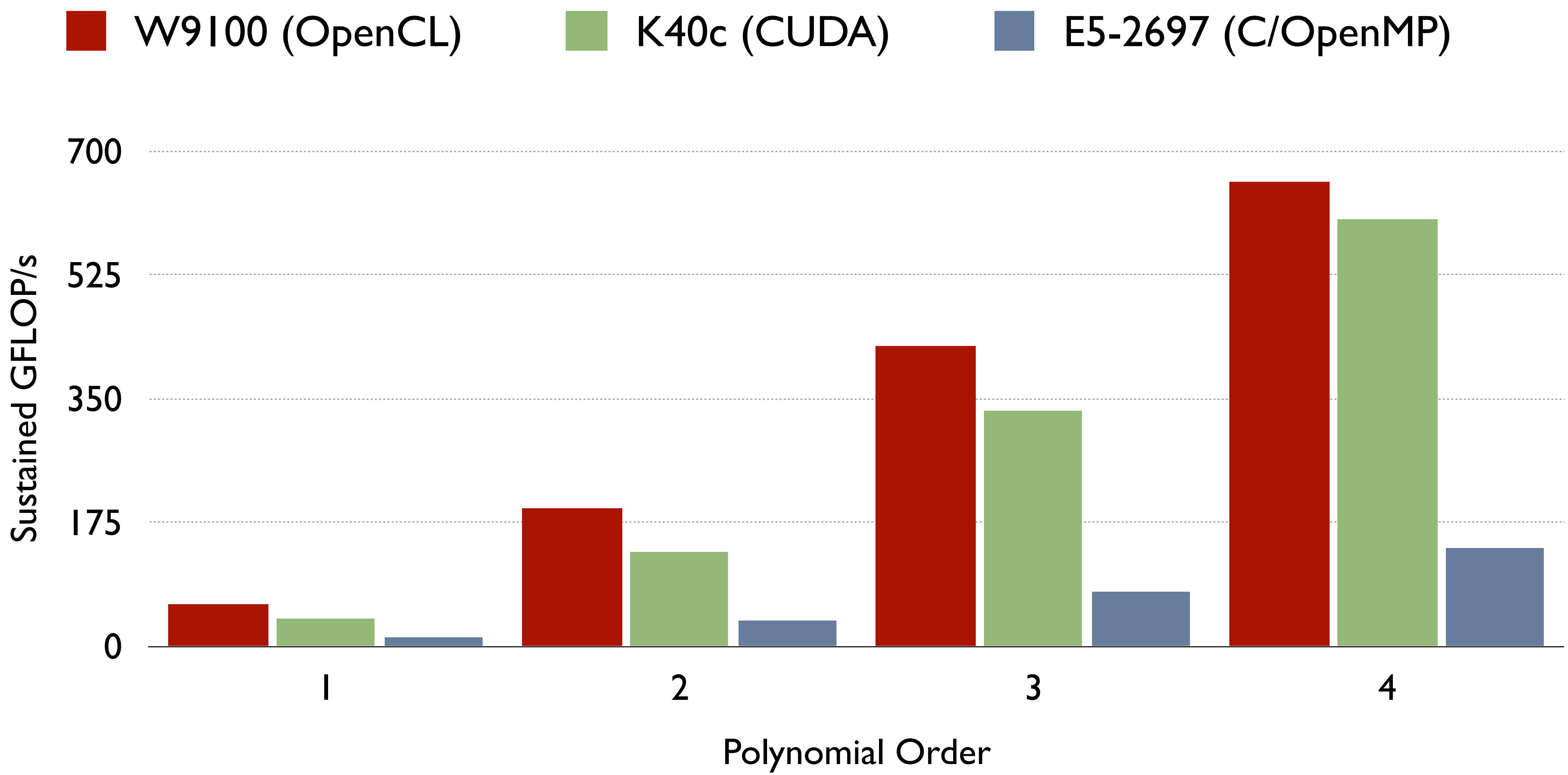
Results

- Performance on a heterogeneous workstation



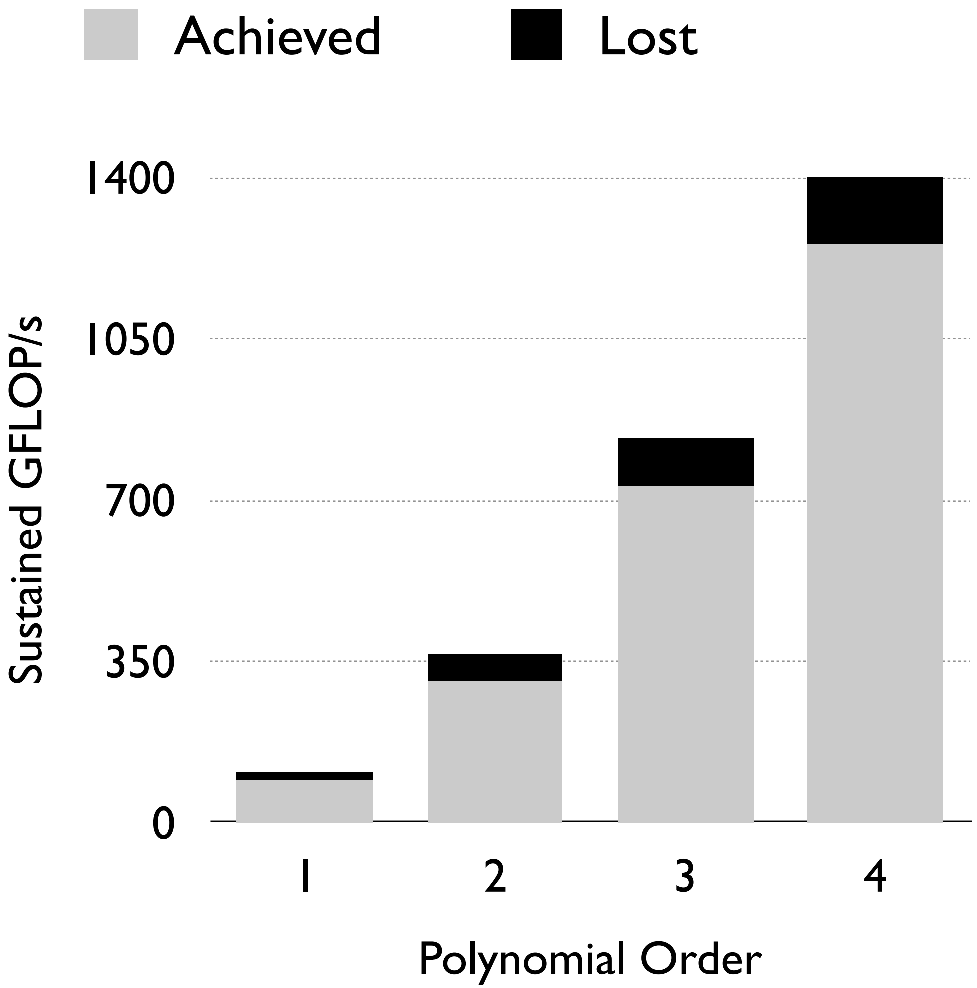
Results

- Single-node on prism/tetrahedral mesh



Results

- Multi-node heterogeneous on prism/tetrahedral mesh



Summary

Flux Reconstruction

+

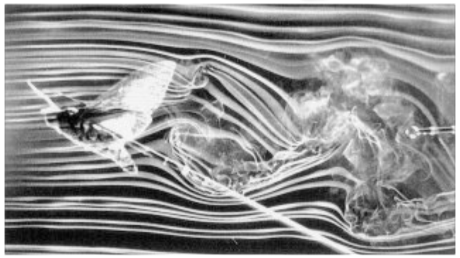
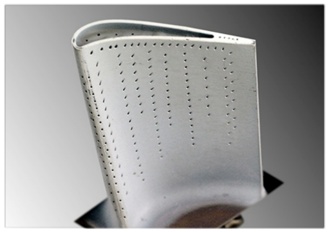
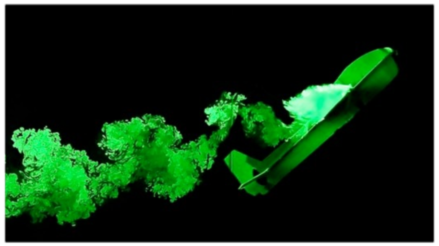
Modern Hardware

Summary

PyFR





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AIRBUS

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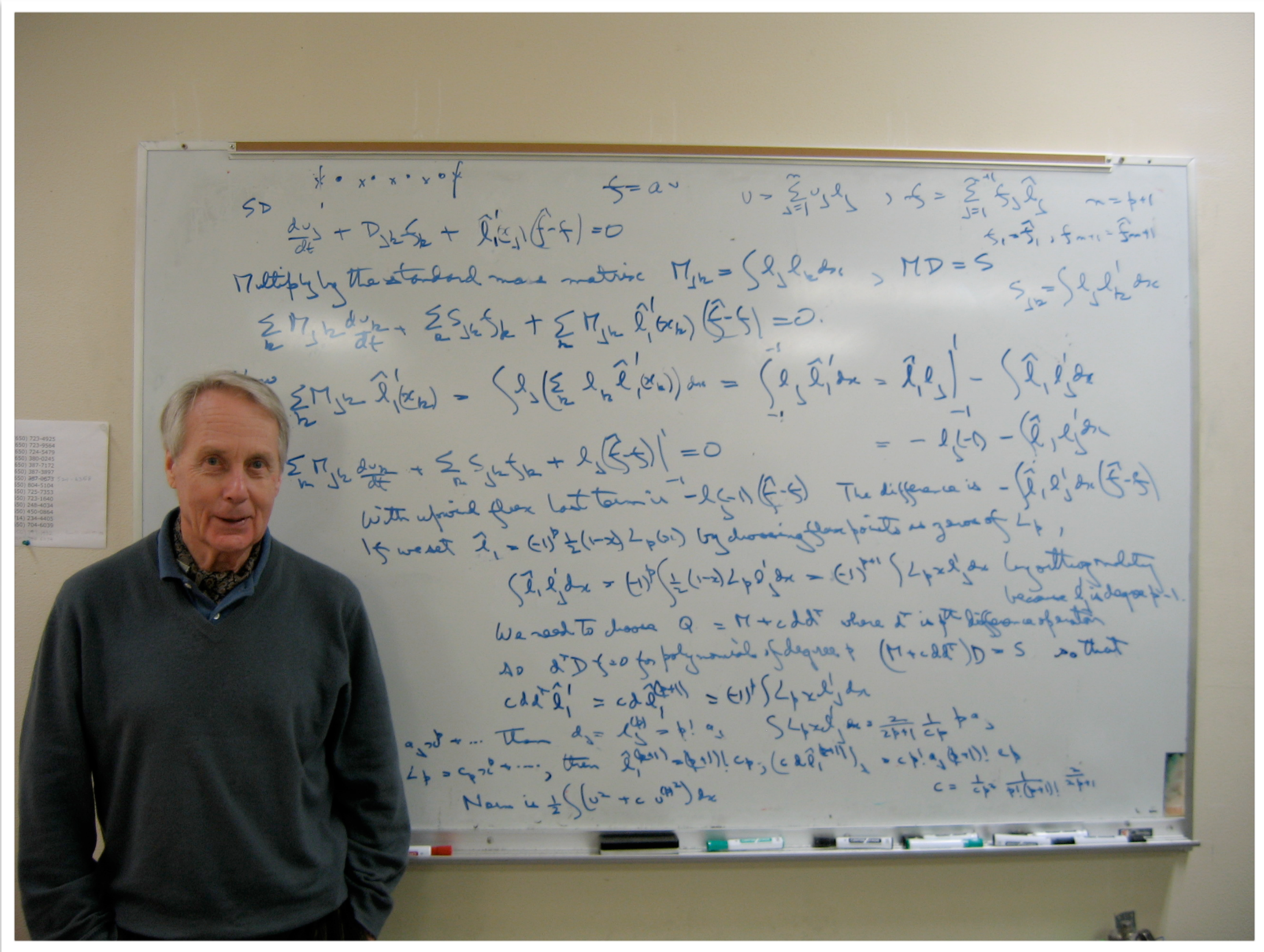
Antony

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