Direct numerical simulation of turbulent flows over acoustic liners

EUROHPC USER DAY 2023 Brussels 11.12.23

EuroHPC Joint Undertaking

Project: "ENTRAIN"

EuroHPC used: Meluxina

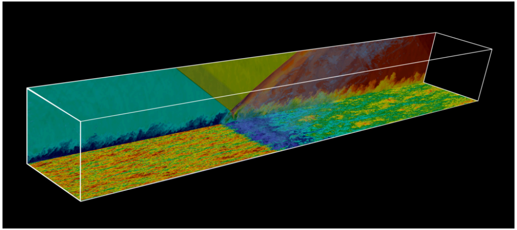
Speaker: *Davide Modesti (TU Delft)*

Introduction

Pre-exascale EU supercomputers

Rank	System	RPeak (ExaFlop/s)	Power (MW)
1.	Frontier (US)	1.6	23
2.	Aurora (US)	1.0	25
5.	LUMI (Finland)	0.4	7
6.	Leonardo (Italy)	0.3	7

The flow solver: STREAmS-2



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Documentation: `https://streams-cfd.github.io/STREAmS-2/`

Github: `https://github.com/STREAmS-CFD/STREAmS-2`

Main features:

- Open source GPL-3.0 license
- Direct numerical simulation of wall bounded fows
- Three different backends: CPU, NVIDIA GPU, AMD GPU
- Object oriented framework, modern Fortran

Developers team

Davide Modesti, TU Delft

Francesco Salvadore, Cineca

Matteo Bernardini, Sapienza

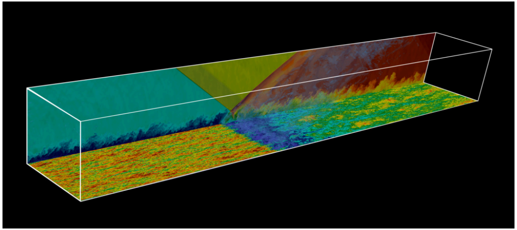
Srikanth Sathyanarayana, MPC

Sergio Pirozzoli, Sapienza

Research topics:

- Turbulent high-speed flows
- Wall turbulence
- Aeroacoustics
- Numerical methods
- High performance computing

STREAmS-2: numerics



Discretization:

- Hybrid energy conserving/shock capturing finite difference[1]
- High order WENO reconstruction close to discontinuities
- Arbitrary order of accuracy for spatial derivatives
- Explicit time step integration, 3rd order low storage R–K

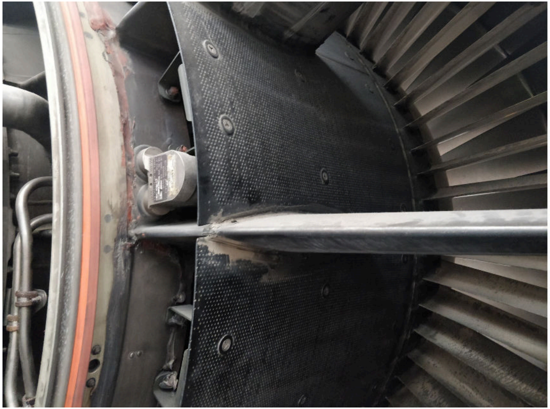
[1] S. Pirozzoli J. Comput. Phys. 229.19 (2010): 7180-7190.

Acoustic liners

Haris Shahzad Stefan Hickel
TU Delft

Acoustic liners

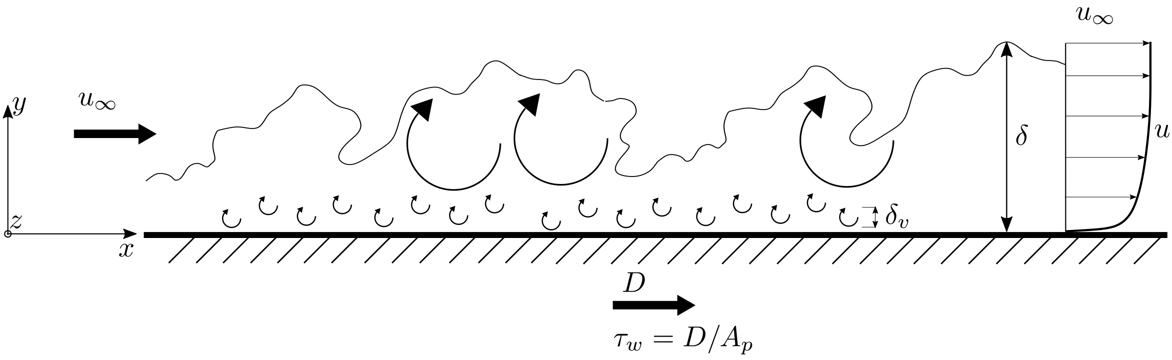
Acoustic liners



Acoustic liners

Acoustic liners

Effect of roughness: review



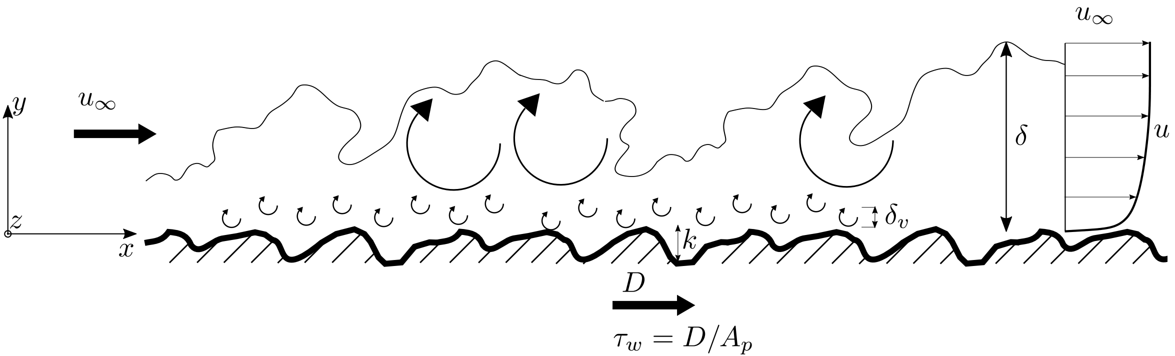
$u_\tau = \sqrt{\tau_w/\rho_w}$

$\delta_v = \nu_w/u_\tau$

$\boldsymbol{Re}_\tau = \delta/\delta_v$

$C_f = 2\tau_w/(\rho_\infty u_\infty^2)$

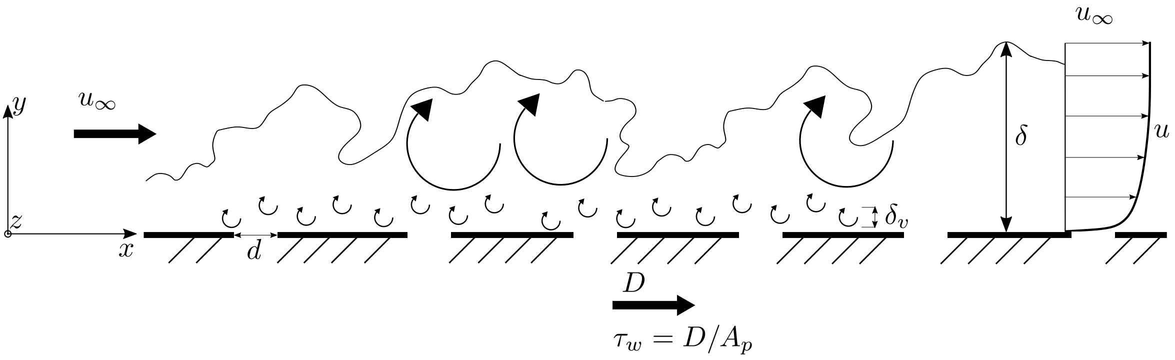
Effect of roughness: review



$u_\tau = \sqrt{\tau_w/\rho_w}$
$\delta_v = \nu_w/u_\tau$
$Re_\tau = \delta/\delta_v$

$k/\delta << 1$
$k^+ = k/\delta_v >> 1$
$k^+ > 5$ rough wall

Effect of roughness: review



$u_\tau = \sqrt{\tau_w/\rho_w}$
$\delta_v = \nu_w/u_\tau$
$\boldsymbol{Re}_\tau = \delta/\delta_v$

$k/\delta << 1$
$k^+ = k/\delta_v >> 1$
$k^+ > 5$ rough wall

$d/\delta = ?$
$d^+ = d/\delta_v = ?$

Effect of roughness: review

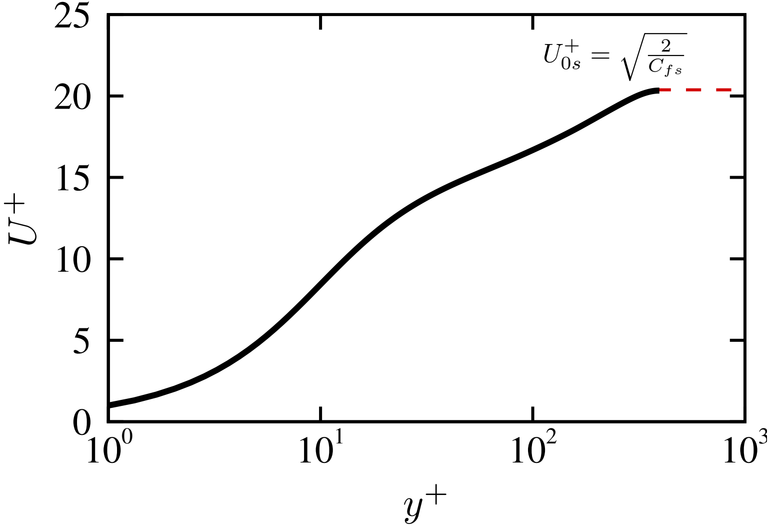
Noise reduction of about 8–10dB

$d/\delta \approx 0.1$

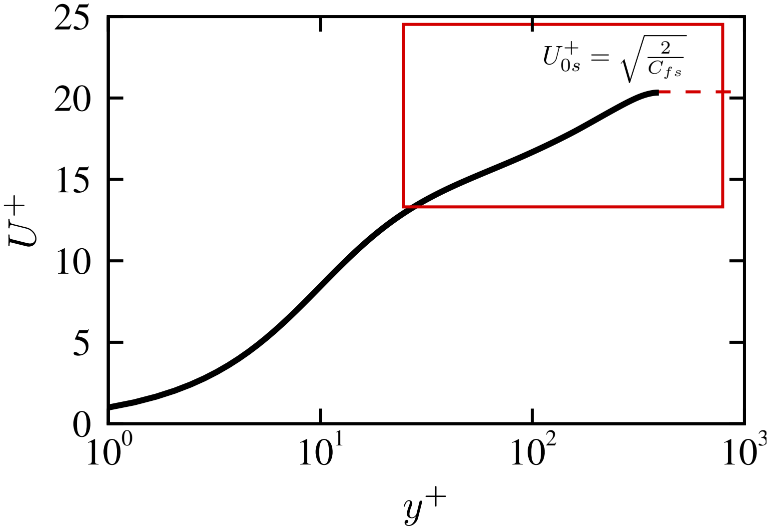
$d^{+} = d/\delta_v \approx 120$–$500$

$\sigma = 0.08$–0.3

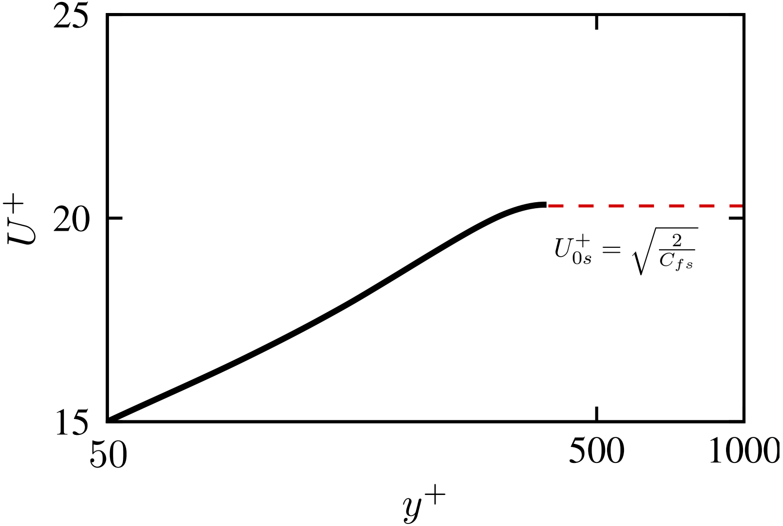
Effect of roughness: review



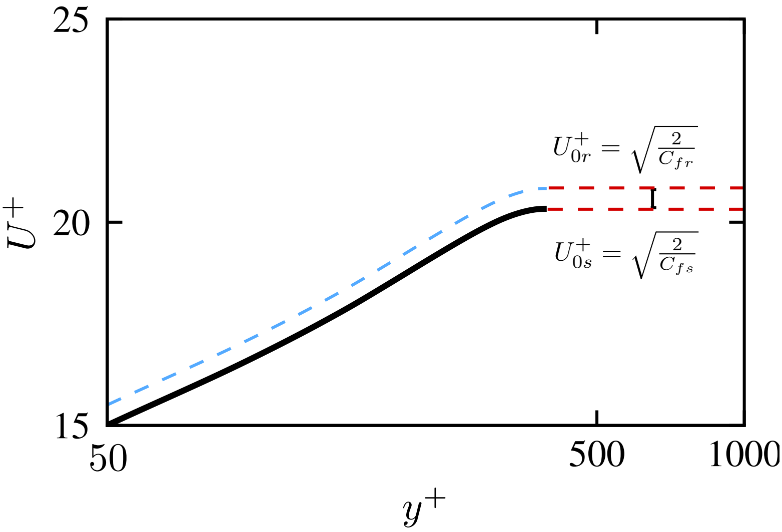
Effect of roughness: review



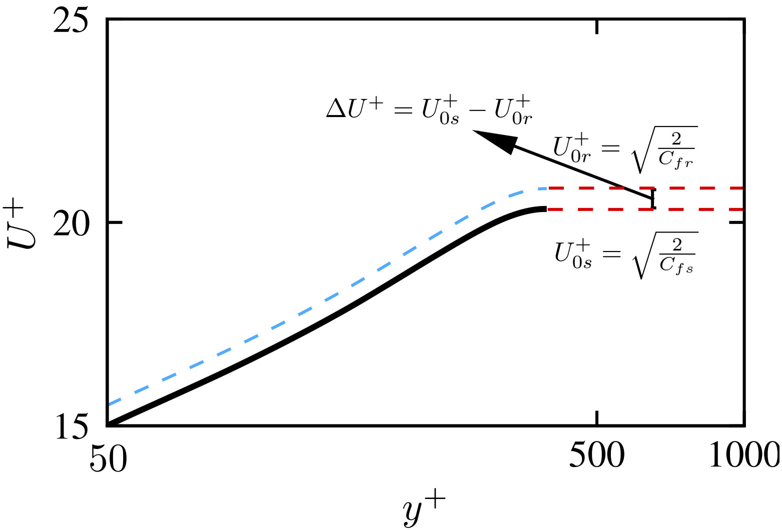
Effect of roughness: review



Effect of roughness: review

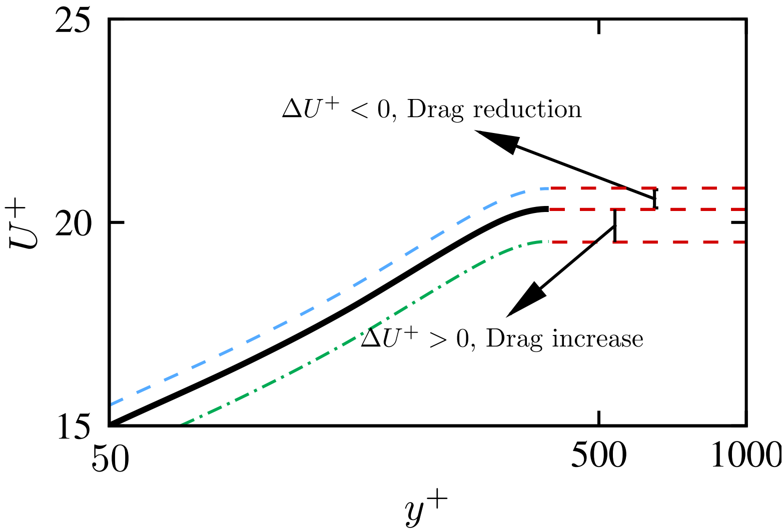


Effect of roughness: review

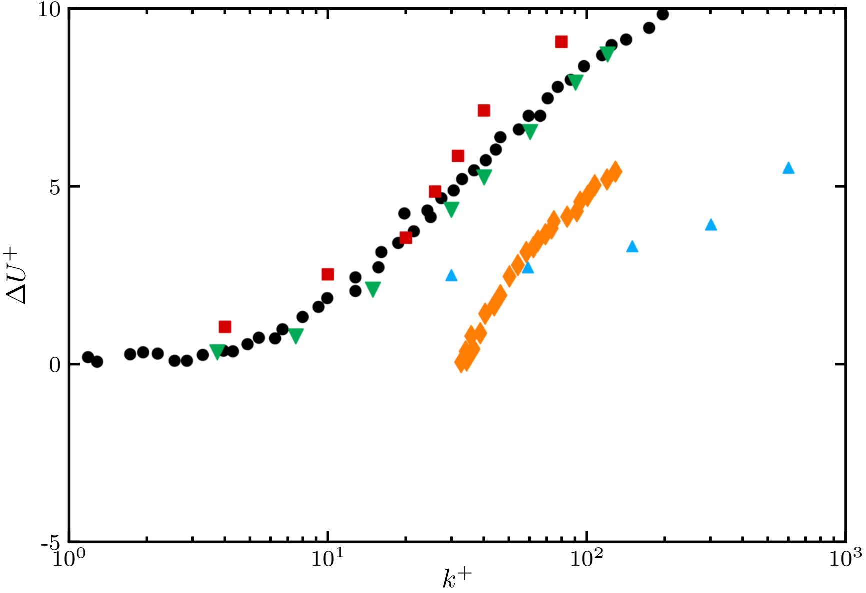


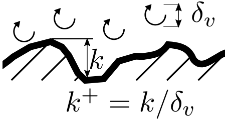
Effect of roughness: review

$$\mathcal{DV} = 1 - C_{fr}/C_{fs} \sim \sqrt{2C_{fs}}\Delta U^+$$

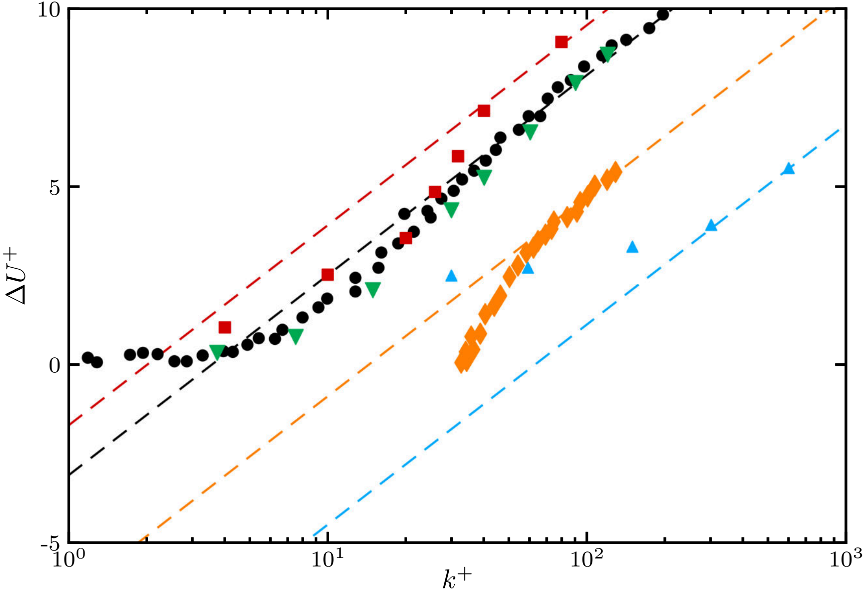


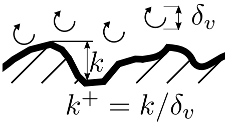
Effect of roughness: review



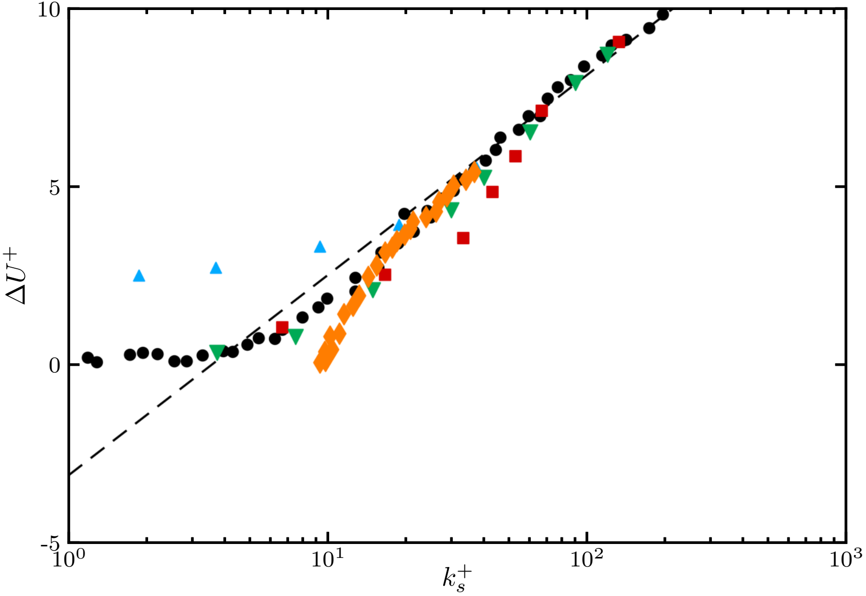


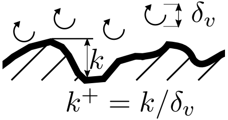
Effect of roughness: review



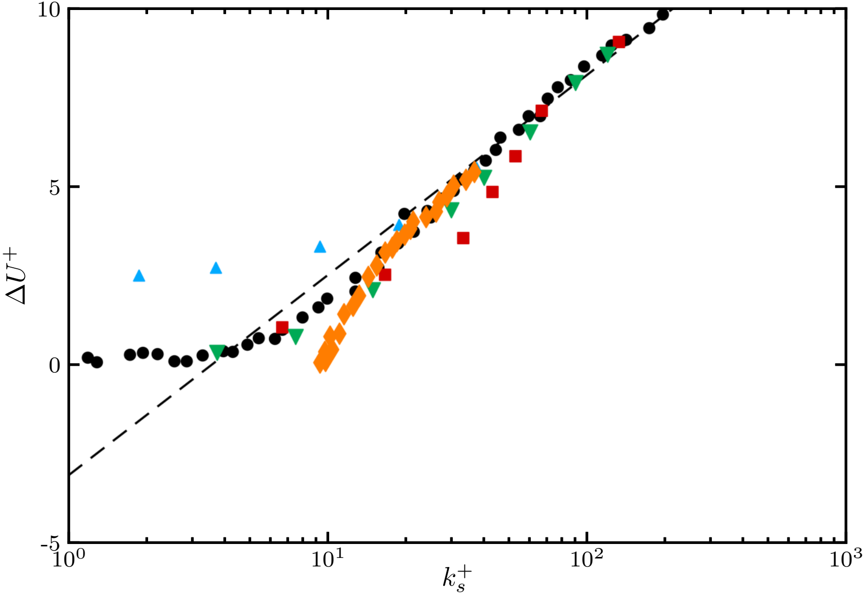


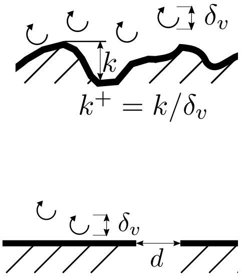
Effect of roughness: review





Effect of roughness: review





Effect of roughness: review

	d^+	σ	ΔD
GFIT[2,3,4]	$180 - 660$	$0.08 - 0.3$	$10 - 350\%$
Wilkinson (1983)[5]	$9 - 150$	$0.047 - 0.14$	$2 - 60\%$
Gustavsson *et al.* (2019)[6]	$350 - 550$	0.0853	$30 - 50\%$
Zhang and Bodony (2016)[7]	114	0.0099	$4 - 100\%$
Scalo *et al.* (2015)[8]	Impedance B.C		$\leq 325\%$
Sebastian *et al.* (2019)[9]	Impedance B.C		$\leq 575\%$

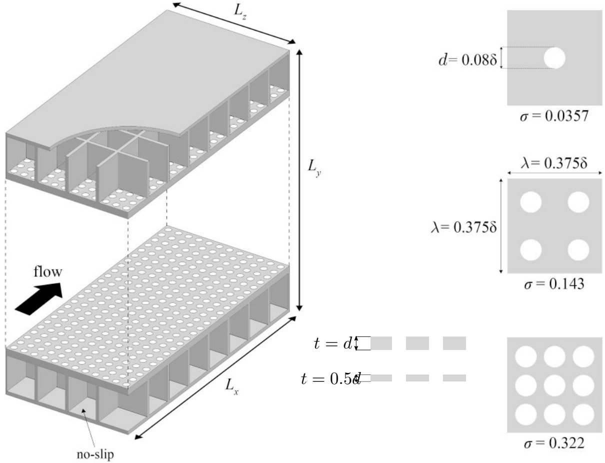
[2]B.M. Howerton and M.G. Jones (2015), AIAA Paper 2015-2230
[3]B.M. Howerton and M.G. Jones (2016), AIAA Paper 2016-2979
[4]B.M. Howerton and M.G. Jones (2017), AIAA Paper 2017-4190
[5]Wilkinson (1983), AIAA Paper 1983-0294
[6]Gustavsson *et al.* (2019), AIAA Paper 2019-2683
[7]Q. Zhang and D.J. Bodony (2016), J. Fluid Mech. 792, pp 936–980
[8]C. Scalo, J. Bodart, S.K. Lele (2015). Phys. Fluids 27.3, p. 035107
[9]R. Sebastian, D. Marx, and V. Fortuné (2019), J. Sound Vib. 306–330

Methodology and dataset

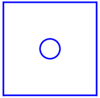
DNS of turbulent channel flow

Domain size $3\delta \times 2(\delta + h) \times 1.5\delta$

Bulk Mach number $M_b = 0.3$



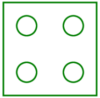
Methodology and dataset



$\sigma = 0.0357$

	Re_b	Re_τ	d^+	σ	t/d	$1/\alpha^+$	Δx^+	Δy^+_{min}	Δz^+
L_1	9139	503.5	40.3	0.0357	1	0.0528	1.1	0.80	1.1

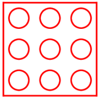
Methodology and dataset



$\sigma = 0.142$

	Re_b	Re_τ	d^+	σ	t/d	$1/\alpha^+$	Δx^+	Δy^+_{min}	Δz^+
L_1	9139	503.5	40.3	0.0357	1	0.0528	1.1	0.80	1.1
L_2	8794	496.4	39.7	0.142	1	0.859	1.0	0.80	1.0
L_4	19505	1038	83.0	0.142	1	1.80	2.1	0.81	2.1

Methodology and dataset



$\sigma = 0.322$

	Re_b	Re_τ	d^+	σ	t/d	$1/\alpha^+$	Δx^+	Δy^+_{min}	Δz^+
L_1	9139	503.5	40.3	0.0357	1	0.0528	1.1	0.80	1.1
L_2	8794	496.4	39.7	0.142	1	0.859	1.0	0.80	1.0
L_3	8264	505.3	40.4	0.322	1	5.14	1.0	0.81	1.0
L_4	19505	1038	83.0	0.142	1	1.80	2.1	0.81	2.1
L_5	17810	1026	82.1	0.322	1	10.4	2.1	0.82	2.1
L_6	35470	2044	164.0	0.322	1	20.8	4.1	0.82	4.1

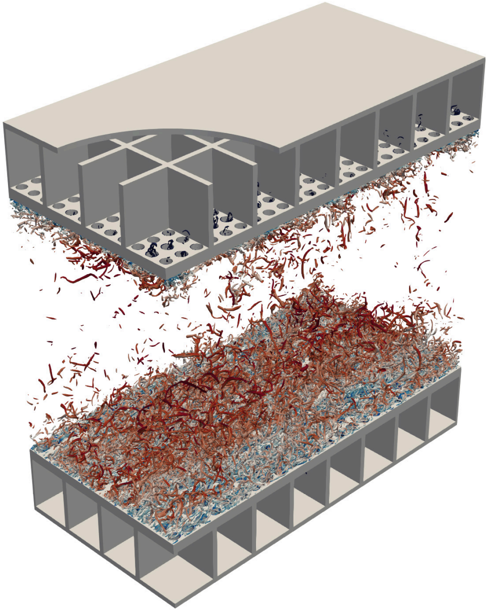
Methodology and dataset

	Re_b	Re_τ	d^+	σ	t/d	$1/\alpha^+$	Δx^+	$\Delta y^+_{\min}$	Δz^+
L_1	9139	503.5	40.3	0.0357	1	0.0528	1.1	0.80	1.1
L_{t1}	9139	508.8	40.7	0.0357	0.5	0.0533	1.5	0.81	1.1
L_2	8794	496.4	39.7	0.142	1	0.859	1.0	0.80	1.0
L_{t2}	8794	520.8	41.6	0.142	0.5	0.901	1.6	0.83	1.1
L_3	8264	505.3	40.4	0.322	1	5.14	1.0	0.81	1.0
L_4	19505	1038	83.0	0.142	1	1.80	2.1	0.81	2.1
L_{t4}	19505	1031	82.5	0.142	0.5	1.78	3.1	0.82	1.1
L_5	17810	1026	82.1	0.322	1	10.4	2.1	0.82	2.1
L_{t5}	17810	1057	84.6	0.322	0.5	10.7	3.2	0.85	1.1
L_6	35470	2044	164.0	0.322	1	20.8	4.1	0.82	4.1

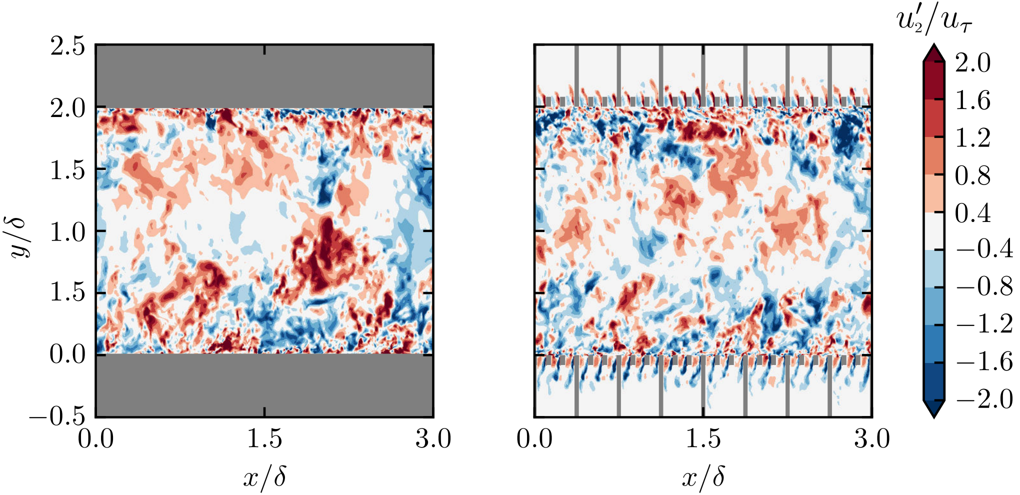
Methodology and dataset

	Re_b	Re_τ	d^+	σ	t/d	$1/\alpha^+$	Δx^+	Δy^+_{min}	Δz^+
S_1	9268	506.1	0	0	0	0	5.1	0.80	5.1
S_2	21180	1048	0	0	0	0	5.2	0.80	5.2
S_3	45240	2060	0	0	0	0	5.2	0.80	5.2
L_1	9139	503.5	40.3	0.0357	1	0.0528	1.1	0.80	1.1
L_{t1}	9139	508.8	40.7	0.0357	0.5	0.0533	1.5	0.81	1.1
L_2	8794	496.4	39.7	0.142	1	0.859	1.0	0.80	1.0
L_{t2}	8794	520.8	41.6	0.142	0.5	0.901	1.6	0.83	1.1
L_3	8264	505.3	40.4	0.322	1	5.14	1.0	0.81	1.0
L_4	19505	1038	83.0	0.142	1	1.80	2.1	0.81	2.1
L_{t4}	19505	1031	82.5	0.142	0.5	1.78	3.1	0.82	1.1
L_5	17810	1026	82.1	0.322	1	10.4	2.1	0.82	2.1
L_{t5}	17810	1057	84.6	0.322	0.5	10.7	3.2	0.85	1.1
L_6	35470	2044	164.0	0.322	1	20.8	4.1	0.82	4.1

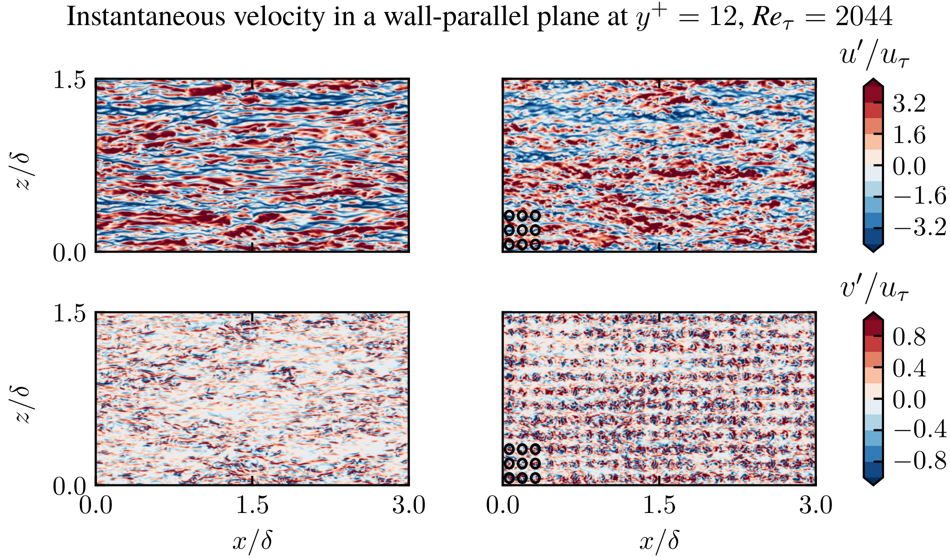
Instantaneous flow field channel flow



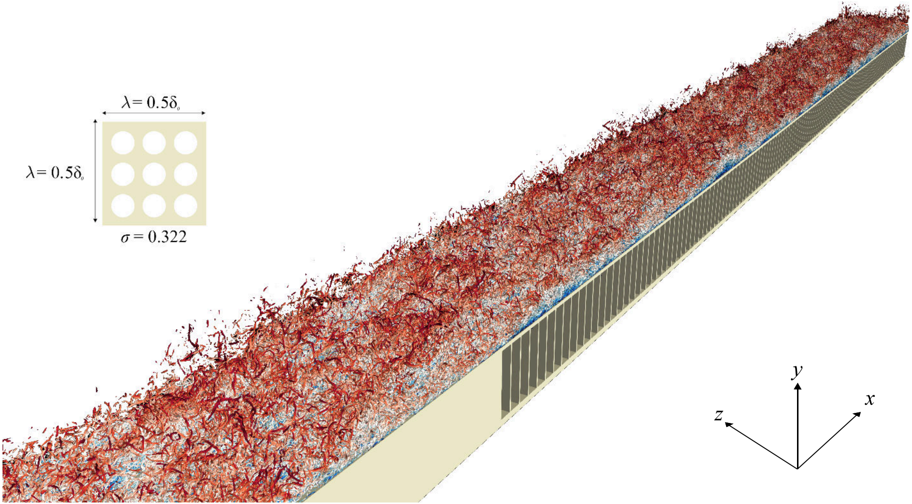
Instantaneous flow field channel flow



Instantaneous flow field channel flow

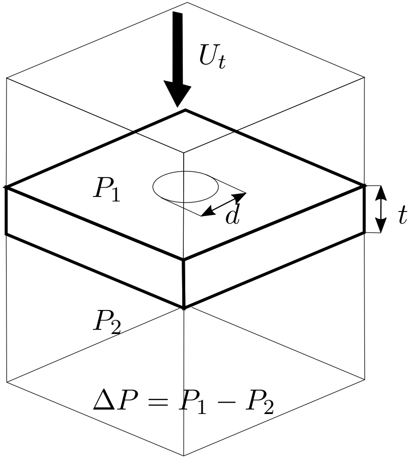


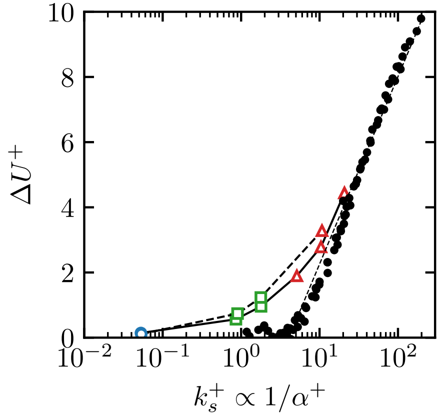
Turbulent boundary layer over acoustic liners[10]



Added drag

ΔU^+ depends on wall-normal permeability of the plate[11] [12].

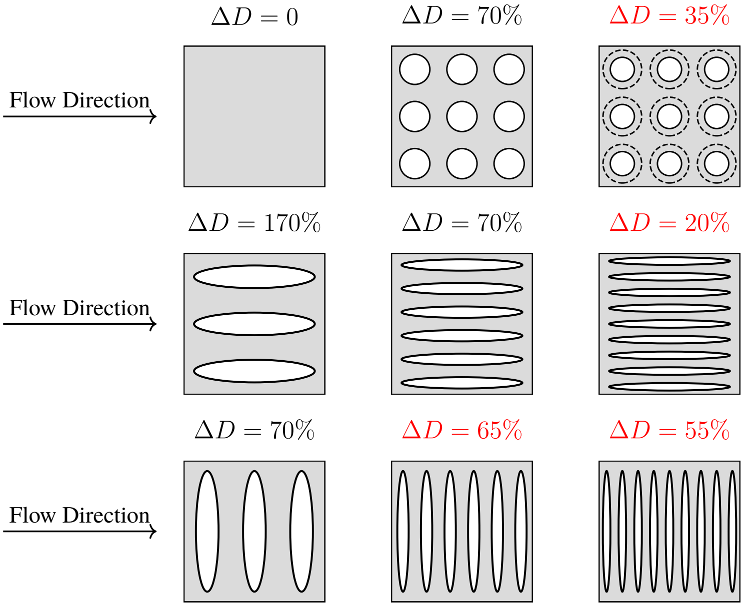




[11] H. Shahzad, S. Hickel, D. Modesti Flow Turbul. Combust. 109.4 (2022): 1241-1254.

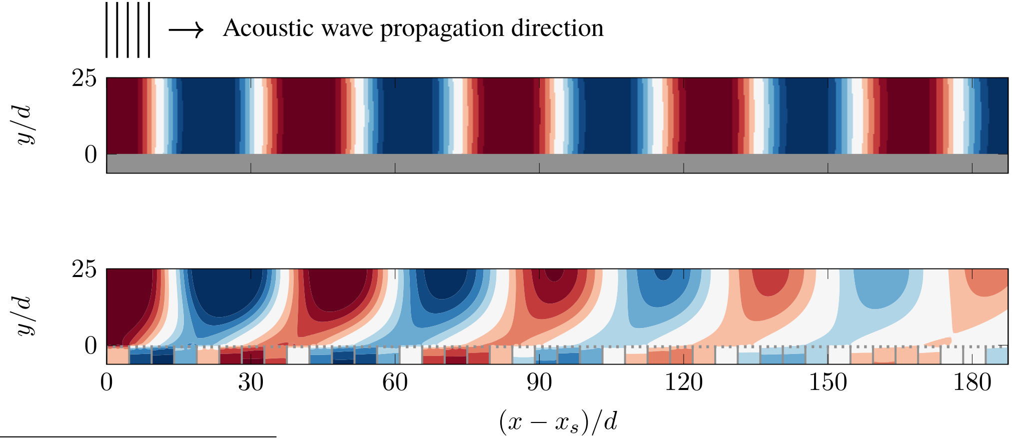
[12] H. Shahzad S. Hickel D. Modesti J. Fluid Mech. 965 (2023): A10.

Acoustic liners: optimized geometries



Acoustic Performance

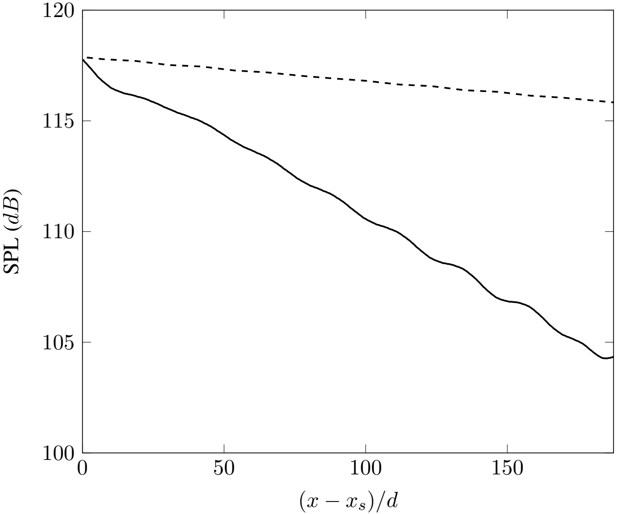
No grazing flow, array of 40 cavities[13]

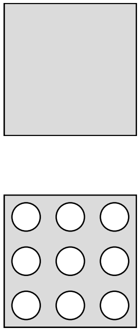


[13]H. Shahzad, S. Hickel, D. Modesti AIAA J. (Under review)

Acoustic liners: optimized geometries

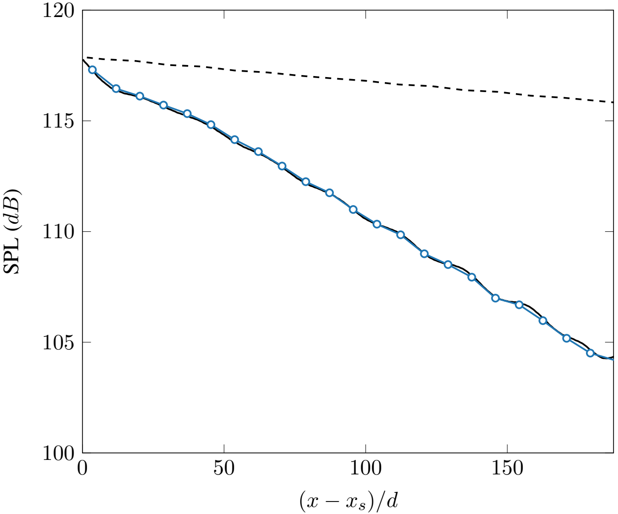
SPL Loss

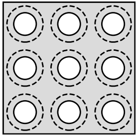




Acoustic liners: optimized geometries

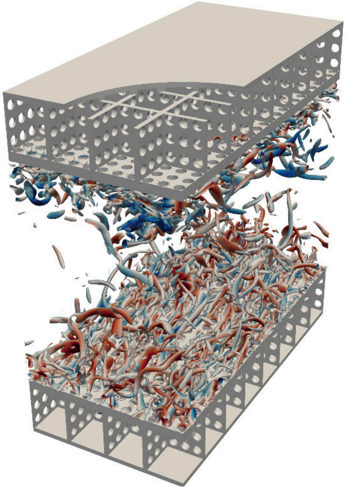
SPL Loss





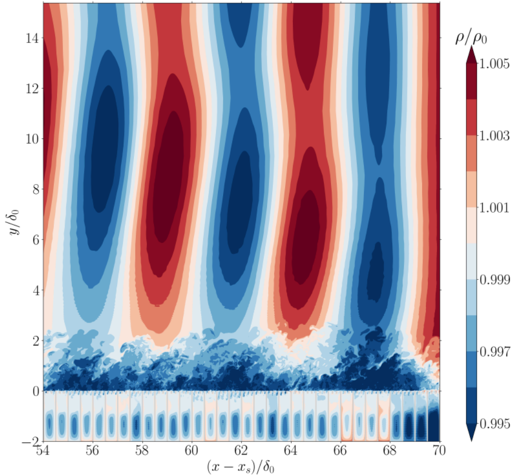
Ongoing work

Broadband acoustic liners



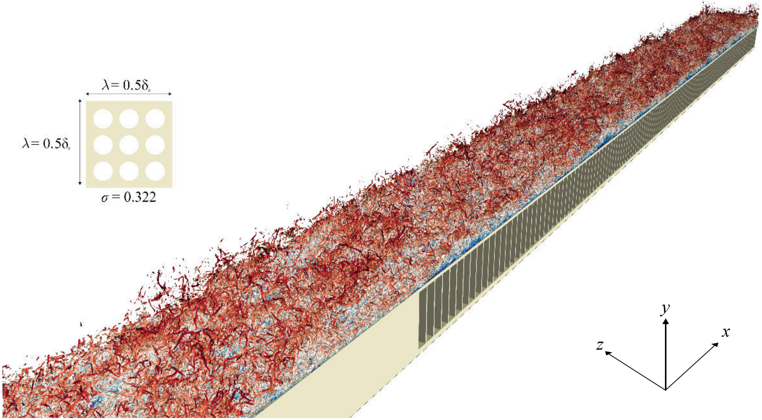
Ongoing work

Turbulent boundary layer with incoming sound wave, currently running on Meluxina



Final Remarks

- STREAmS-2 targets CPU and multiple GPU backends
- DNS at engineering Reynolds numbers are becoming accessible
- EuroHPC facilities are key



Final Remarks

Interview for the general public

Science | Mechanics +… | 2022

Quiet Query: Scientists model how noise-reducing aircraft liners are a drag on efficiency

Aircraft noise is reduced by acoustic liners covering the inner surfaces of its engines. However, these components also add to aerodynamic drag — but by how much, and how this can be mitigated, was unclear. Thanks to simulations performed on the CSCS supercomputer “Piz Daint”, scientists have now deciphered the acoustic liners’ impact and how to improve them.

November 21, 2022 - by Santina Russo

QR code

Scale-resolving flow simulations for gaining physical insight in the flow and improving turbulence models for turbomachinery applications

EUROHPC USER DAY 2023 Brussels 11.12.23

EuroHPC Joint Undertaking

Projects: *RoundedStepData4ML* + BE share on LUMI + Early access on LUMI + *TurbData4ML* (PRACE)

EuroHPC used: VEGA@IZUM, LUMI@CSC

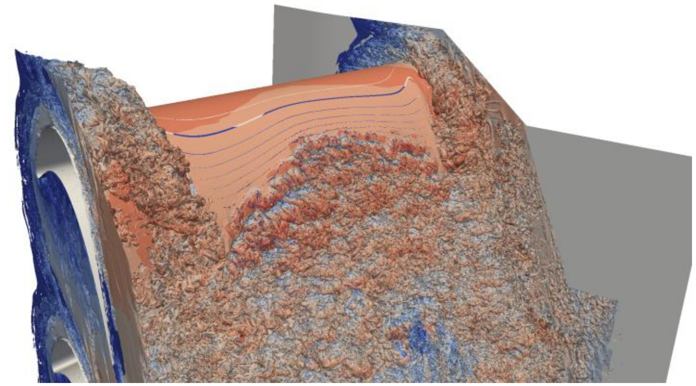
Speaker: *Michel RASQUIN (Cenaero)*

High-fidelity CFD @ Cenaero

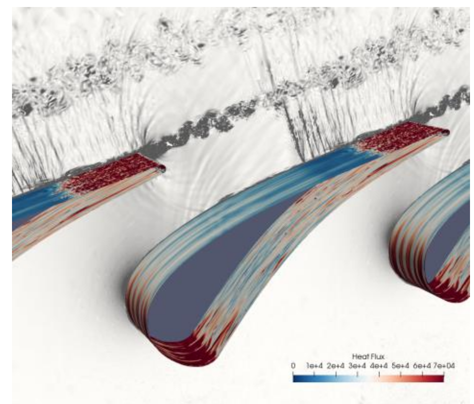
- **Author list: M. Rasquin, T. S. Cação Ferreira, T. Toulorge, K. Hillewaert**

Cenaero · VON KARMAN INSTITUTE · UCLouvain · LIÈGE université

- **High-resolution DNS and wall-resolved LES on realistic geometries**
  - **Accurate representation of flow phenomena in boundary layers near solid surfaces**
    - Separation
    - Shocks
    - Transition and turbulence
  - **Main enablers**
    - Superior accuracy of high-order methods like DGM
    - Access to and efficient exploitation of supercomputers



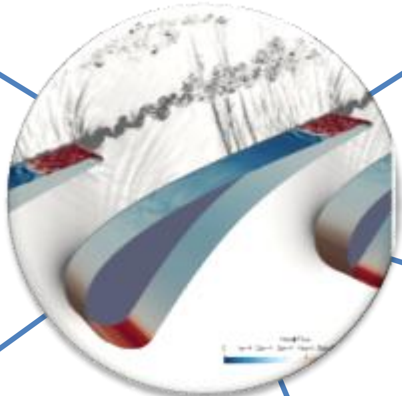
- **Research themes for the application of DNS and LES**
  - **Development of high-resolution numerical methods & tools**
  - **Applications: high fidelity CFD of complex flows**
    - High-pressure turbine vane LS89
  - **Data-driven turbulence modeling**
    - HiFi-Turb-DLR rounded step



PROD-F-015-02

Development of high-resolution numerical tools

Highly accurate numerical wind tunnel for turbulence in turbomachinery



Turbo-machinery

- Generic frame of reference
- Parallel periodicity
- Dedicated BC (moving wall, total conditions, radial equilibrium, …)
- High order accurate non-matching connections

HPC capabilities

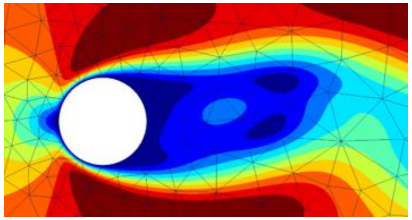
- Algorithmic efficiency
- Extreme scalability, including NMC
- Optimised IO
- *GPU implementation (ongoing)*

Lumi@CSC

Vega@IZUM

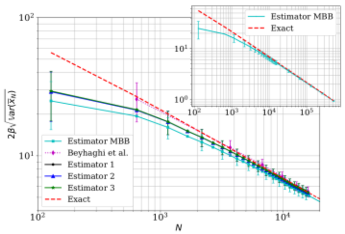
Advanced numerics

- DGM: high-accuracy on unstructured meshes
- High order time integrators
- *Dissipation-free shock capturing (ongoing)*
- *Mesh and order adaptivity (ongoing)*



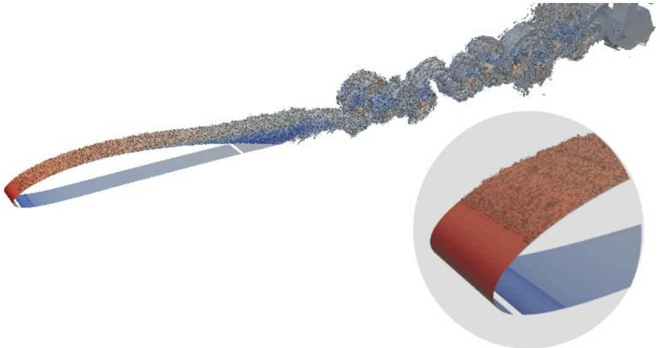
Co-processed analysis

- In-situ visualisation Catalyst
- Spatio-temporal statistics
- *Confidence intervals on statistics (ongoing)*



Resolved turbulence

- DNS, LES and wmLES
- Turbulence injection
- RANS turbulence budgets
- *Adaptation on TKE budget (ongoing)*
- *ML-based wall modeling (ongoing)*
- *Quality criteria for statistics (ongoing)*



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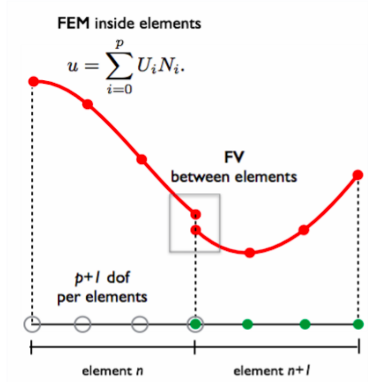
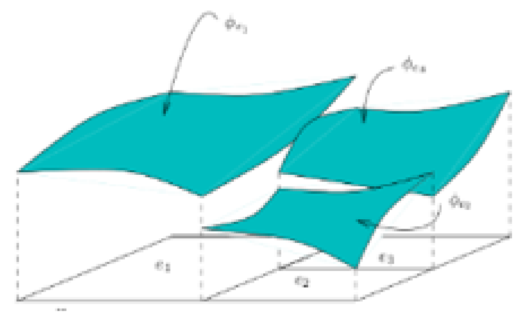
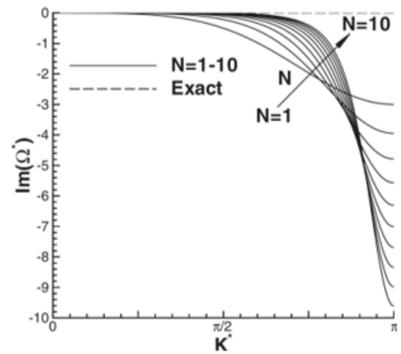
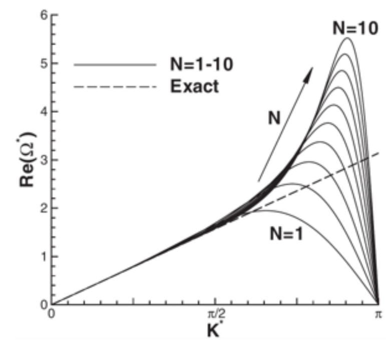
High-order Discontinuous Galerkin Method
Why DG?

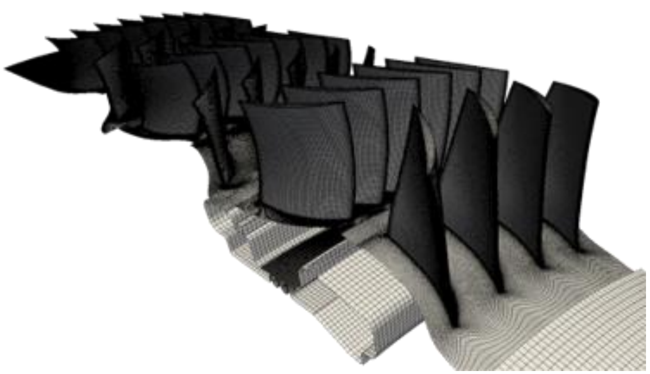
- **Unstructured meshes and complex geometries**
- **High accuracy**
  - **Guaranteed order of convergence p+1**
  - **No degradation near size jumps/walls**
  - **Low dissipation/dispersion error**
- **High efficiency**
  - **Data locality**
  - **Compact matrix-matrix operations**
  - **High scalability (MPI/OpenMP/GPU)**

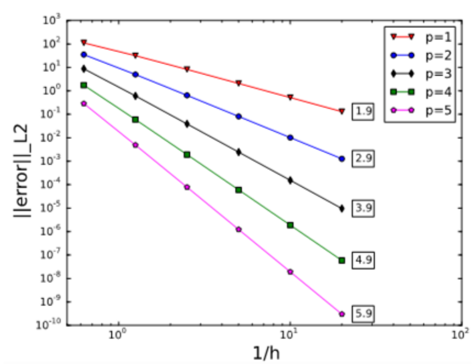


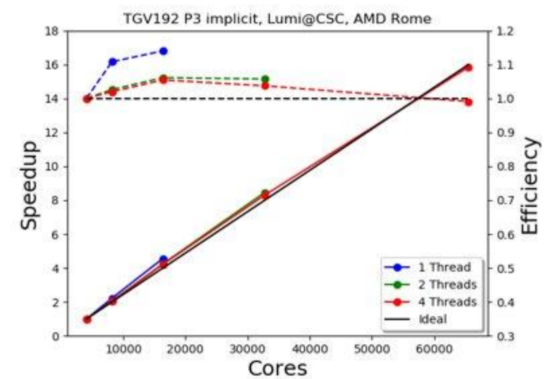








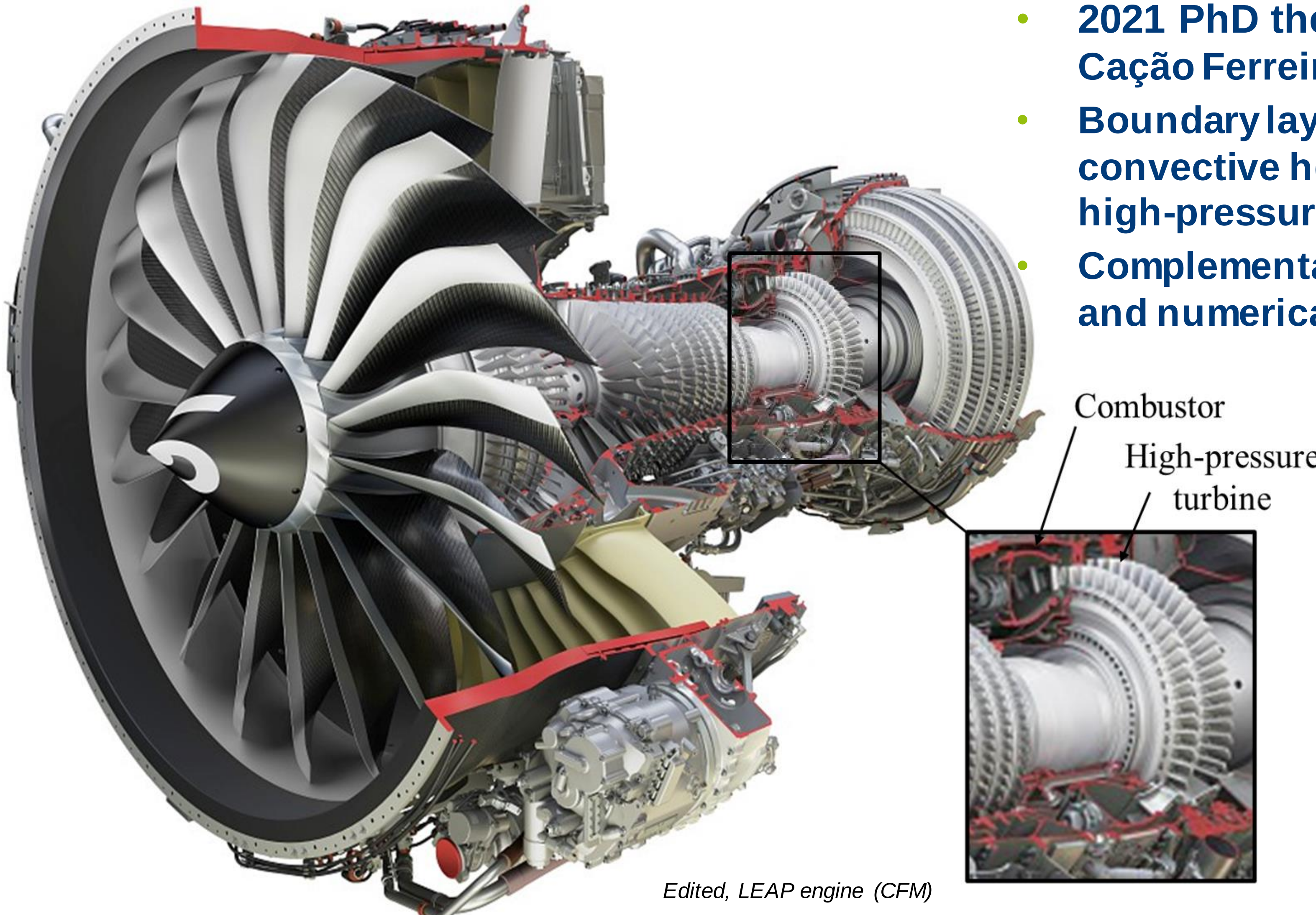




Cenaero

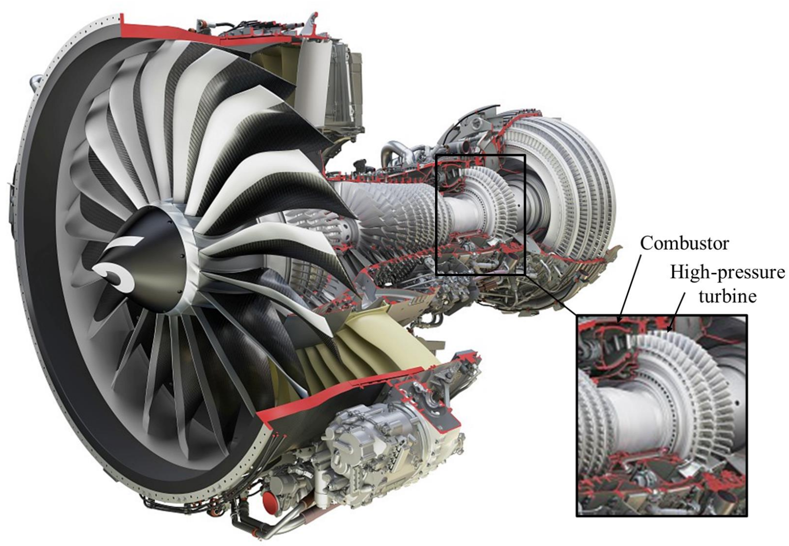
Aircraft gas turbine engine
High pressure turbine vane LS89

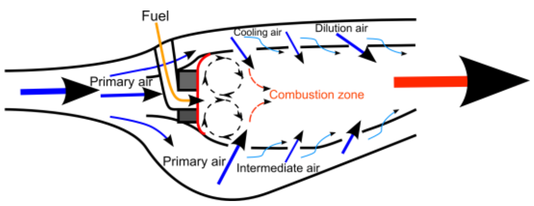
- **2021 PhD thesis Tânia Sofia Cação Ferreira + follow up**
- **Boundary layer transition and convective heat transfer of the high-pressure turbine vane LS89**
- **Complementary experimental and numerical work**

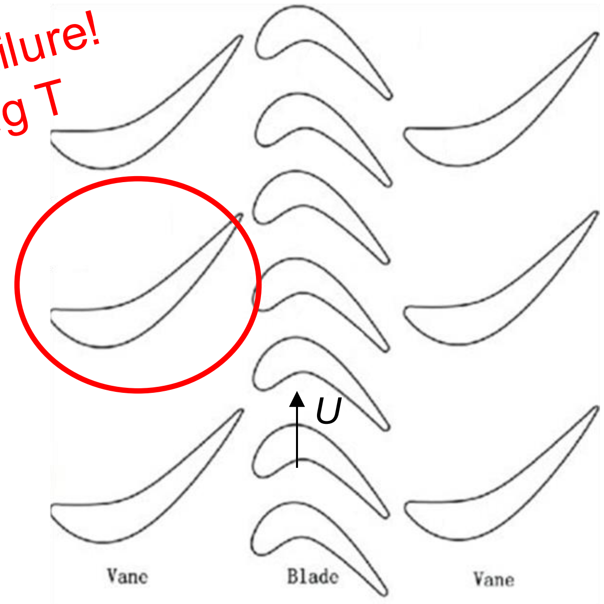


Edited, LEAP engine (CFM)

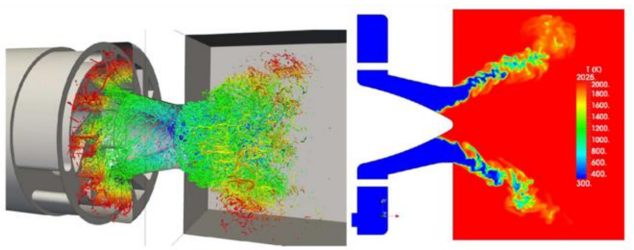
High-pressure aircraft gas turbine
Highest temperature during engine cycle







DNS of an isothermal and reacting combustion swirler (Moureau et al. 2010)



Combustor exit/HPT inlet flow:

- **Temperature = 500-2000K**
- **Turbulence intensity = 10-30%**

1st turbine stator

faces the **hot turbulent combustion flow**

- **Accurate heat transfer predictions are crucial for efficiency and safety!**
- **Requires accurate prediction of the boundary layer**

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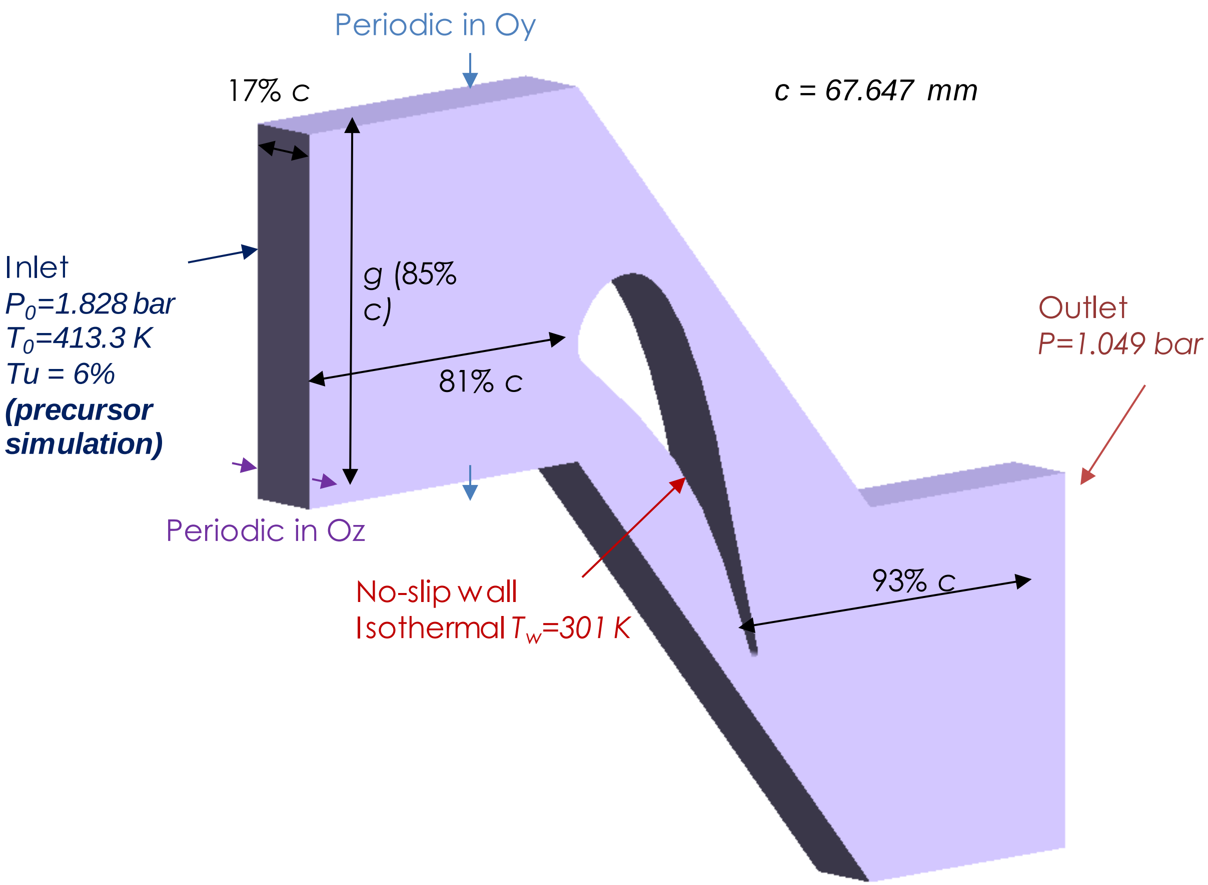
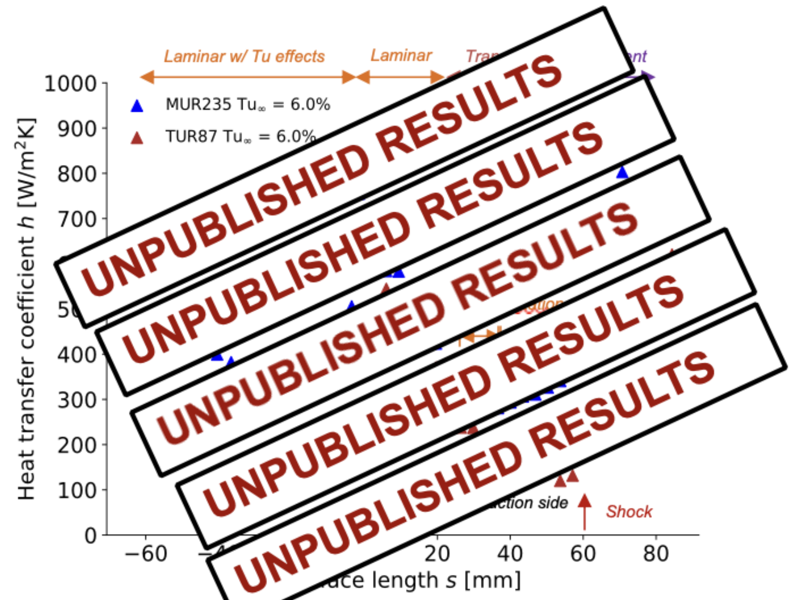
Cenaero

Domain and boundary conditions
MUR235/TUR87 configuration



Experiments	MUR235	TUR87
$M_{is,out}$	0.93	0.92
$Re_{is,out}$	$1.15\text{x}10^6$	$1.15\text{x}10^6$
$T_{0,in}/T_{s,wall}$	1.37	1.37
Tu_∞	6%	6%
	Arts et al. 1990	*Ferreira & Arts 2021*

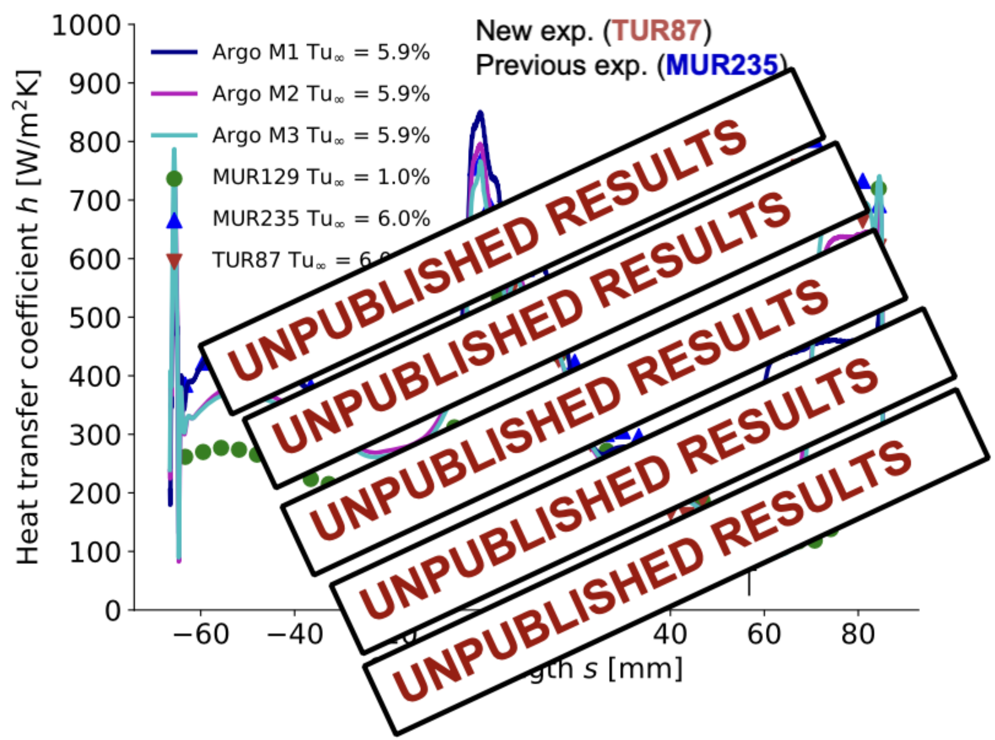


(*edited*, *Arts et al., 1990*)

EuroHPC Joint Undertaking · PRACE · Wallonie

Parameters				*New mesh!*
Mesh	M1	M2	M3	M4
Oz layers	40	74	85	153
Prism elements	80	148	510	918
Hexahedron elements	2M	3.7M	3.3M	10.9M
Degrees of freedom	127M	236M	212M	700M
x^+	83	83	50	25
y^+ (max)	~1	~1	~1	~1
z^+	~100	~50	~45	25
Partitions	2160	3960	3456	9984
CPU hours/flow over inlet + chord**	1M Zenobe	0.95M Galileo	0.8M Zenobe + Lumi	Lumi

Heat transfer for **meshes M1, M2, M3**



- **Observations:**
  - **Experiments: highly sensitive boundary layer to the facility environment**
  - **Simulations: strong dependence on the mesh resolution (and on the artificial viscosity)**
  - **2nd experimental campaign with updated facility (TUR87) and refined numerical simulations tend to converge towards the same heat flux prediction**

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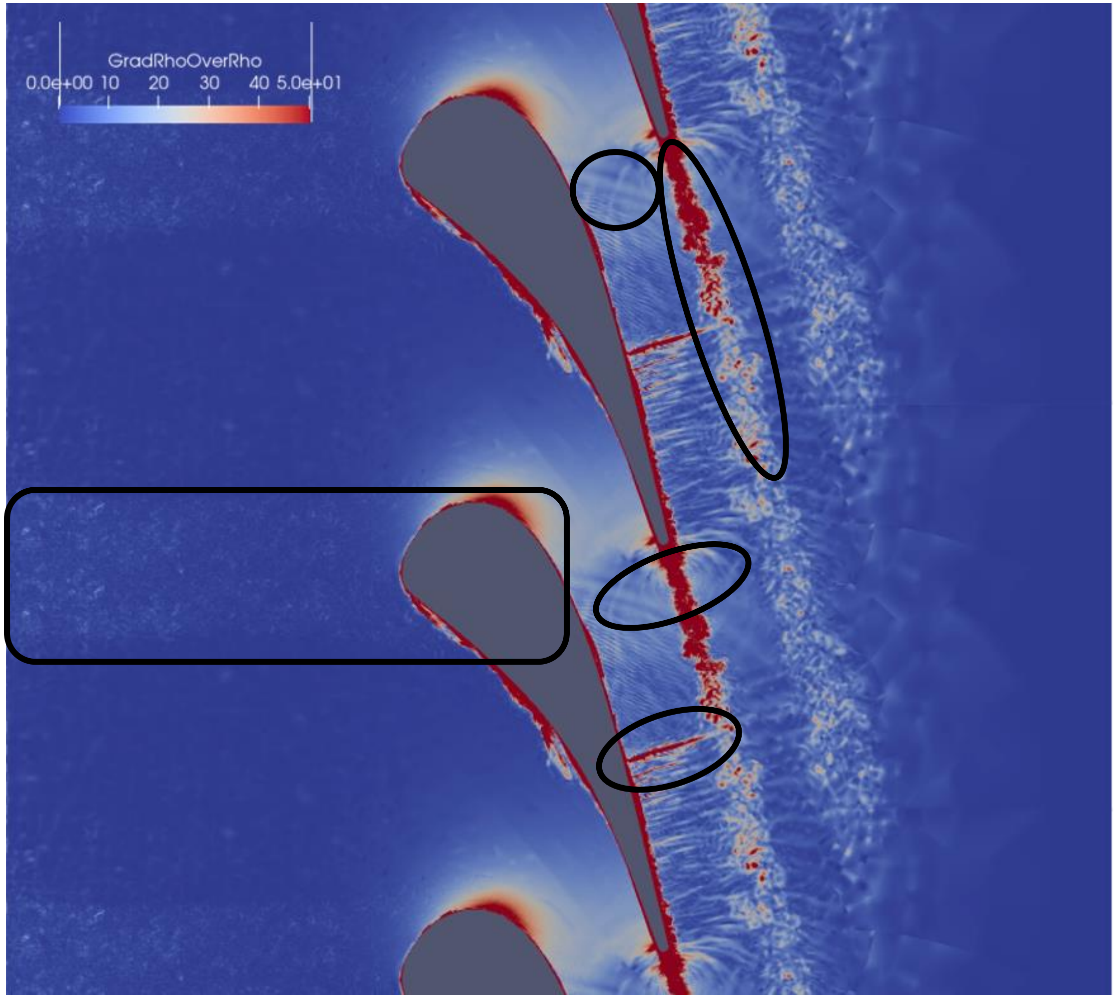
Flow visualisation
Density gradient

Refined inlet turbulent structures



Acoustic waves reflection on the suction side

Wake vortex shedding

Acoustic waves formation at the trailing edge

Normal shock

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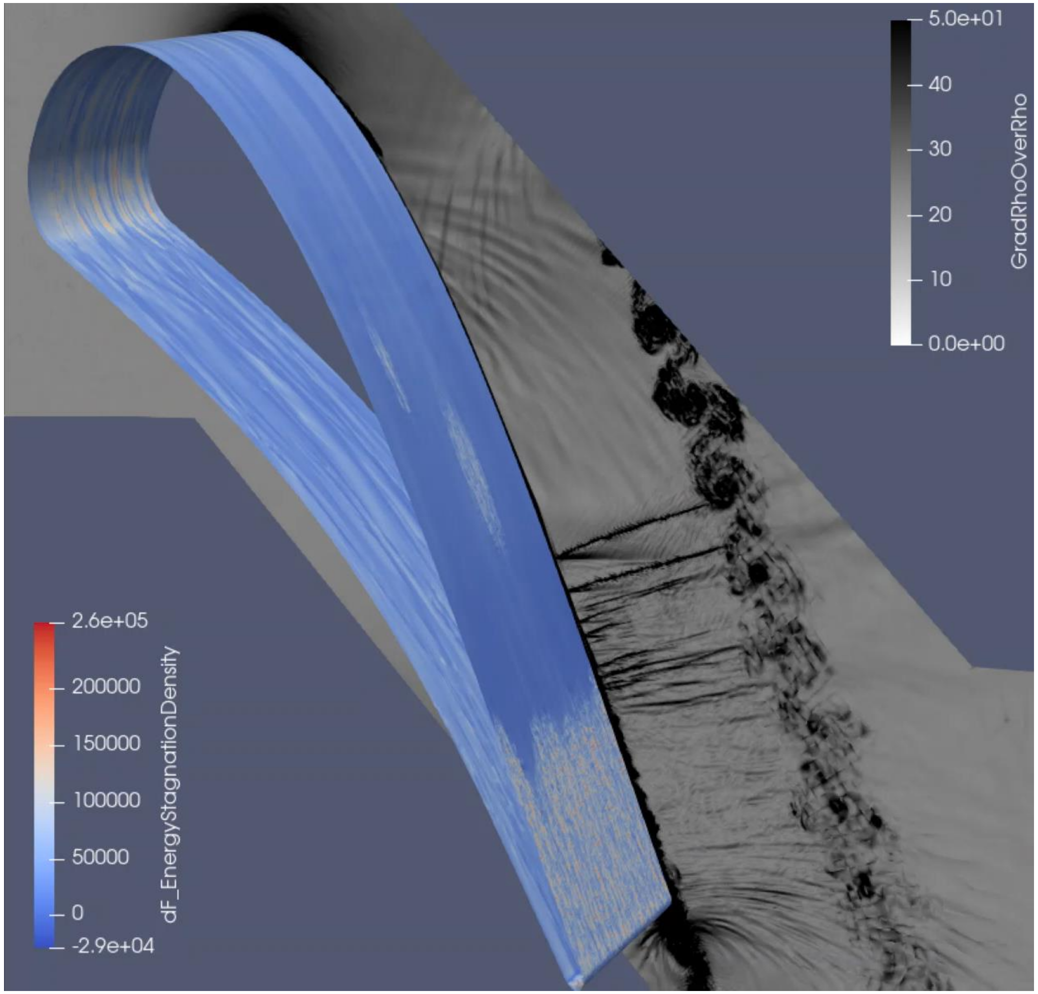
Heat transfer
Mesh M2



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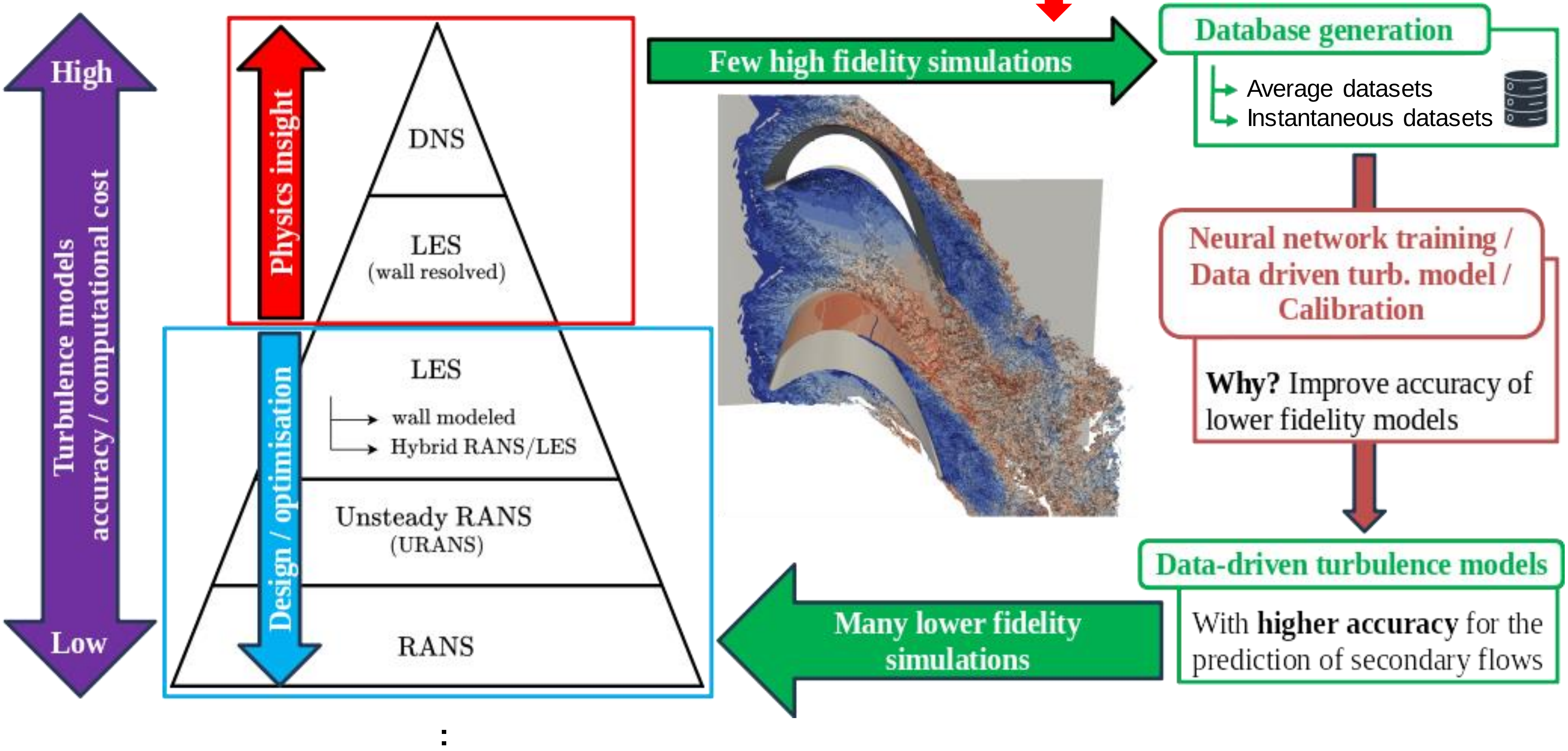
Cenaero

Data-driven turbulence modeling
Generic methodology

Access to EuroHPC systems is essential



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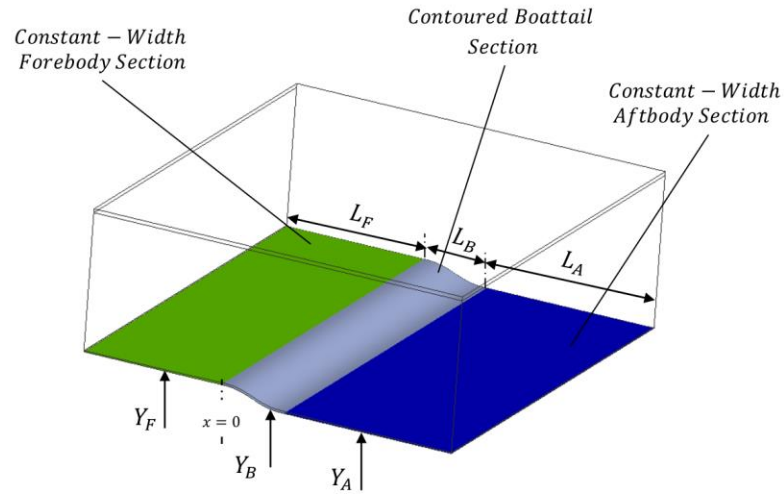
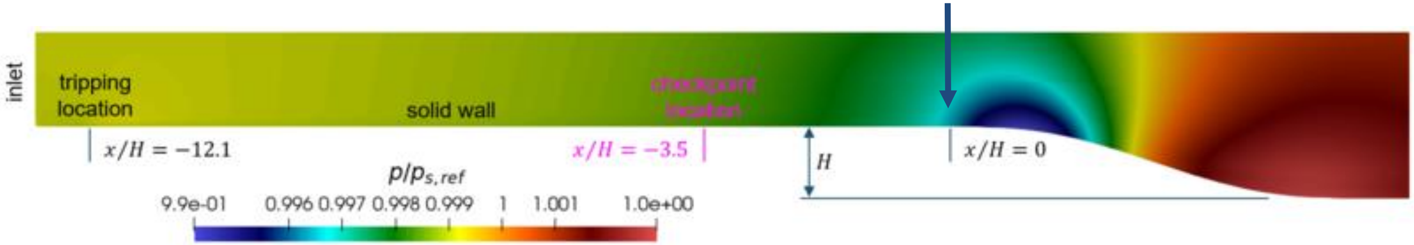
Cenaero

HiFi-Turb-DLR rounded step

Test case definition

- **Test case proposed within H2020 HiFi-Turb project**
  - **Documented in the ERCOFTAC Knowledge Base wiki**
  - https://www.kbwiki.ercoftac.org/w/index.php/DNS_1-5
- **Features an adverse pressure gradient on a turbulent boundary layer**
  - **3 step heights**
  - **Incipient, moderate (Re_h=98113) and full separation**





Courtesy of UniBG and ERCOFTAC

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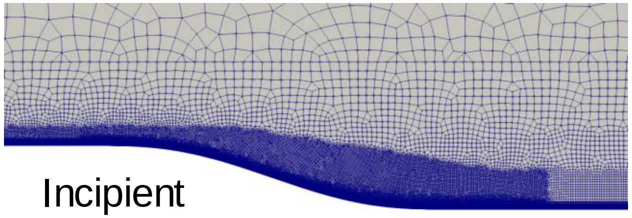
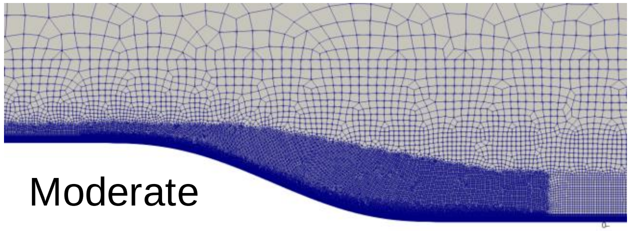
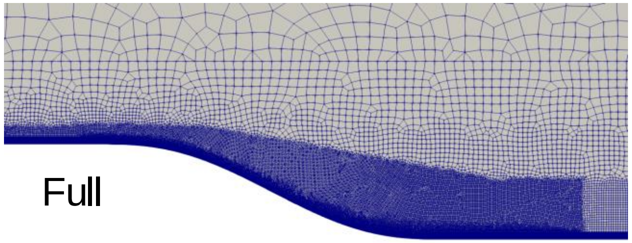
Cenaero

HiFi-Turb-DLR rounded step
Mesh characteristics

	Incipient	Moderate	Full
Hexes	10.3 M	10.8 M	11.6 M
Dof	1.30 B	1.35 B	1.45 B
Height (m)	2.90e-2	3.62e-2	4.38e-2
Span (m)	8.69e-2		
Span/height	3	2.4	2
Nz	188		
Δz	4.10e-4 m		
Upstream bump			
Δx^+	<20		
Δy_1+	<1		
$\Delta z+$	<14.8		
Bump			
Δx	*0.5 w.r.t. upstream bump		







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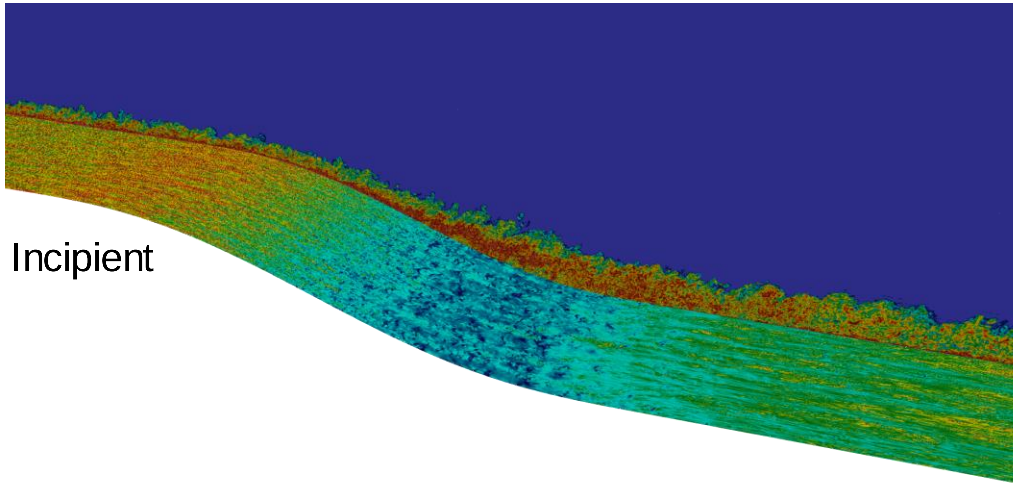
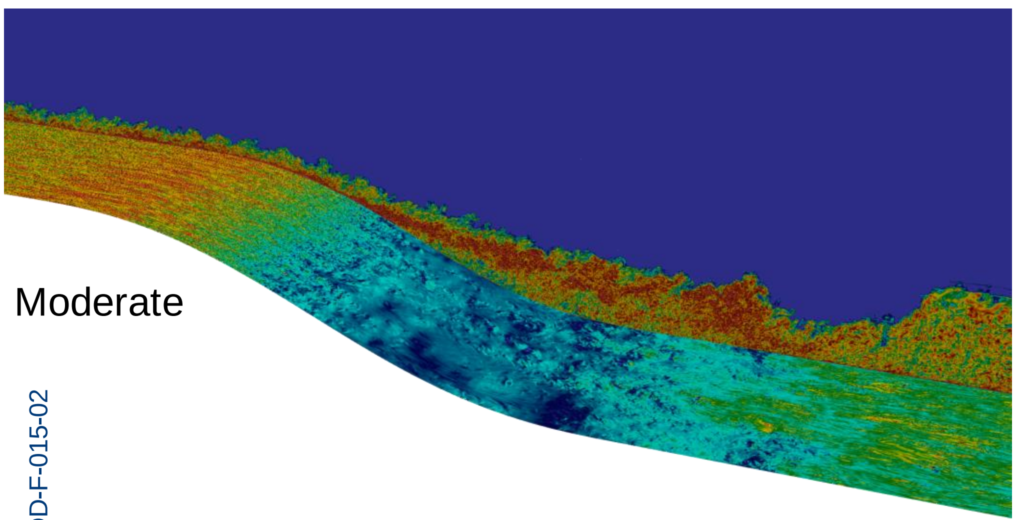
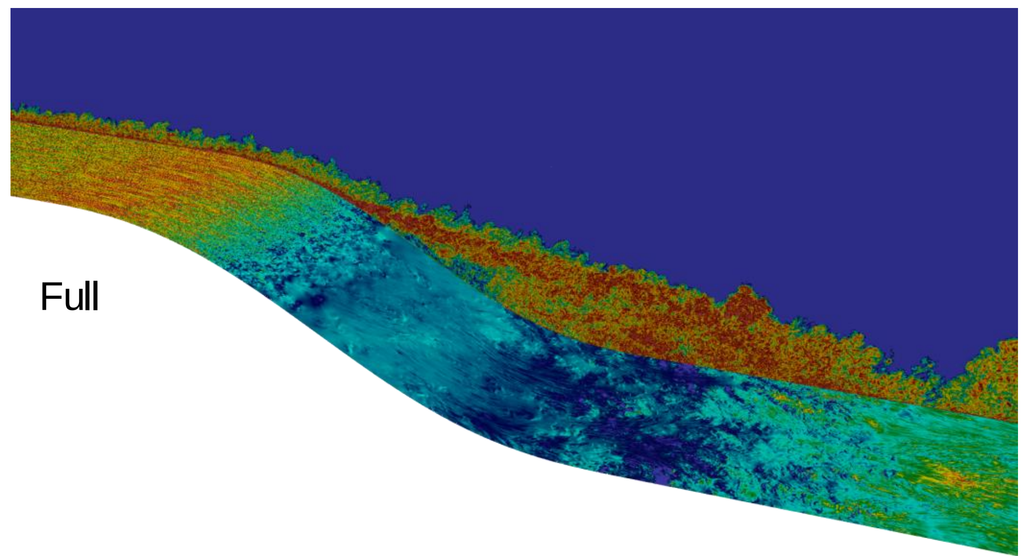
Flow visualisation
Wall shear stress + Vorticity







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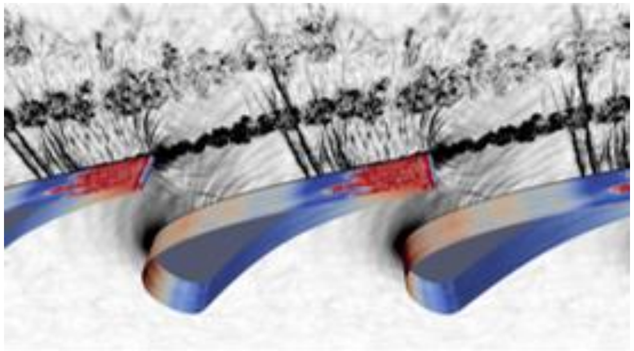
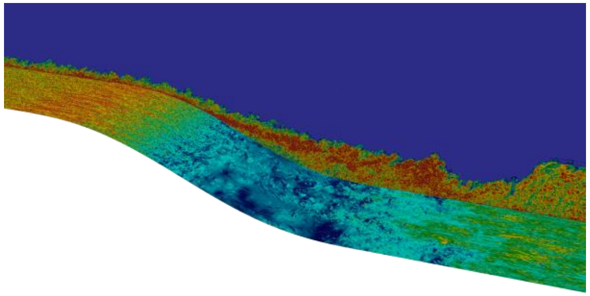
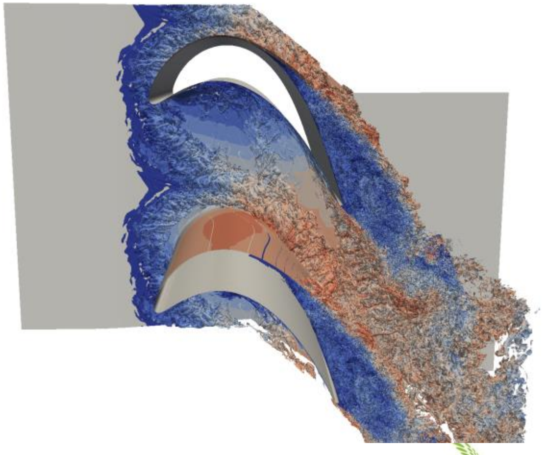
Summary

- **High-resolution simulations as part of a "multi-fidelity" paradigm**
  - Physical understanding to support and complement experimental testing
  - Performance prediction in off-design conditions
  - Data generation for lower-fidelity model calibration (RANS, wall models)
- **Advanced numerical framework**
  - High-order numerical scheme
  - Scalable
  - Post-processing and statistical analysis
- **Applications**
  - Academic aerodynamic flows
  - Turbomachinery flows







→ Access to large computational resources is essential

PROD-F-015-02

Acknowledgments

- We acknowledge **EuroHPC JU** for awarding us access to
  - LUMI hosted by CSC in Kajaani, Finland
  - VEGA hosted by IZUM in Maribo, Slovenia

- We acknowledge **PRACE** for awarding us access to
  - Galileo hosted by CINECA in Bologna, Italy
  - Hawk hosted by HLRS in Stuttgart, Germany

- The present research benefited from computational resources made available on the Tier-1 supercomputer of the Fédération Wallonie-Bruxelles, infrastructure funded by the **Walloon Region** under grant agreement numbers 1117545 and 1910247

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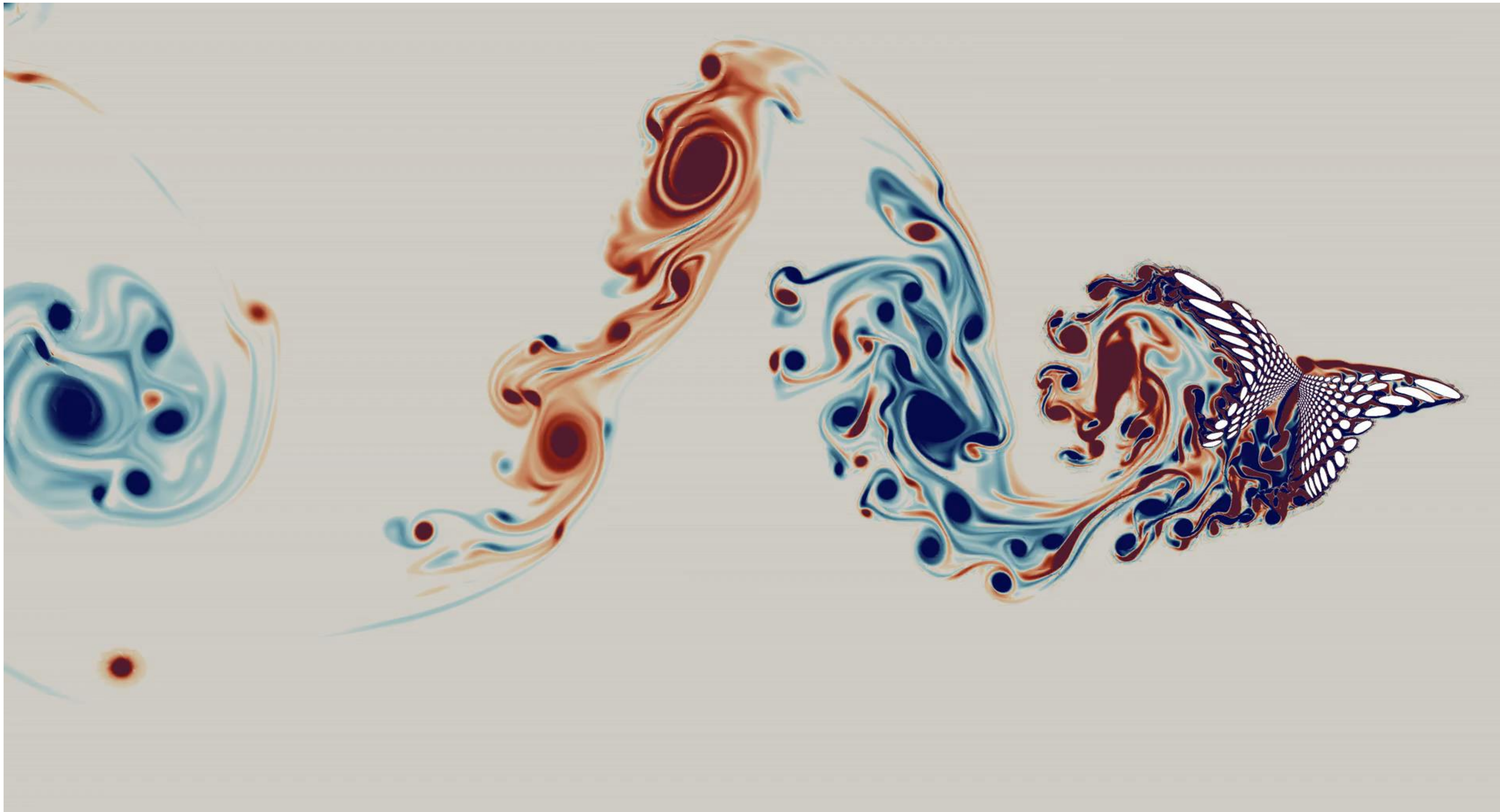
Thank you for your attention



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Cenaero

A Portable Drug Discovery Platform for Urgent Computing

EUROHPC USER DAY 2023 Brussels 11.12.23

EuroHPC Joint Undertaking

Project: *EHPC-BEN-2022B12-001*

EuroHPC used: LUMI-G

Speaker: *Davide GADIOLI (Politecnico di Milano)*

Drug discovery

- Target at least one protein that represents the disease
- The goal is to find a small molecule that has a strong interaction
  - Expected to yield a therapeutic effect in clinical trials

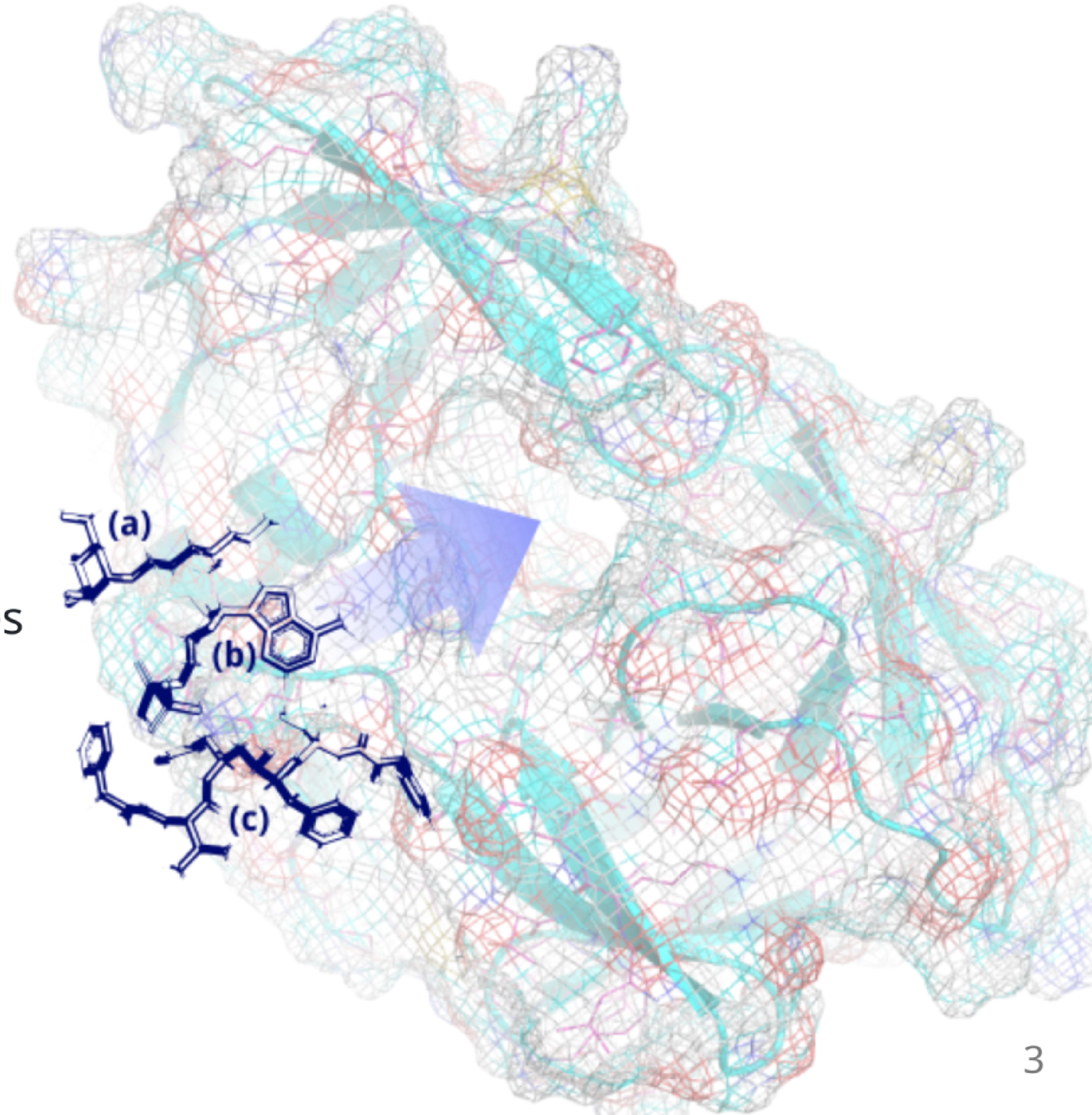
Virtual screening

Problem input

- Target protein
- Huge databse of virtual molecules

Expected output

- Molecules to test *in-vitro*



Why High Performance Computing?

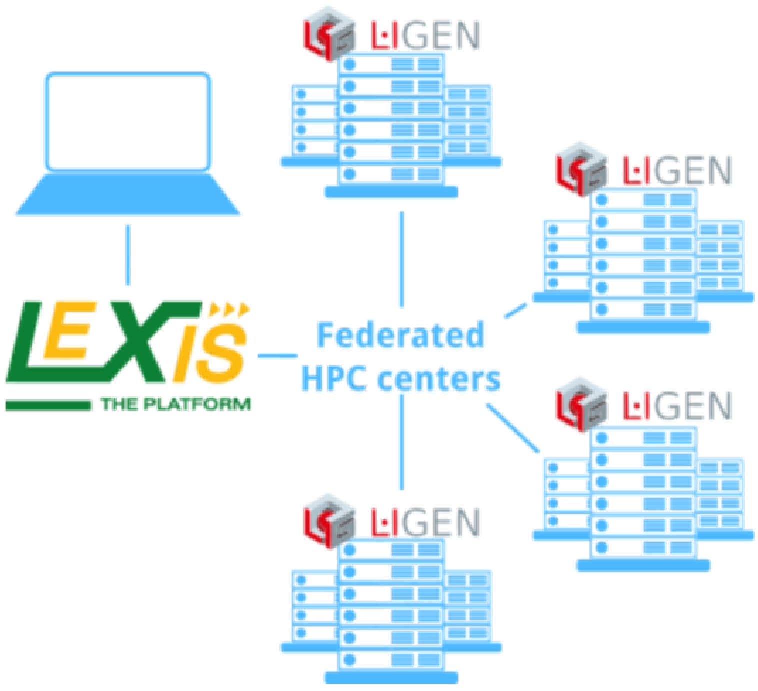
- The interaction strength estimation is complex
- The evaluation of each molecule-protein pair is independent
  - Embarrassing parallel problem
- Simulation of known chemical reactions grants access to huge chemical space
  - increasing the probability of finding good candidates

LiGen Virtual Screening Application

- Component of the EXSCALATE drug discovery platform
- Designed from scratch to hinge on modern supercomputer nodes
- Used to perform extreme-scale virtual screening campaign

HPCaaS: The Urgent Computing Scenario

- LiGen deployed on multiple EU HPC centers
- Integration in the LEXIS platform
- Virtual screening on multiple locations

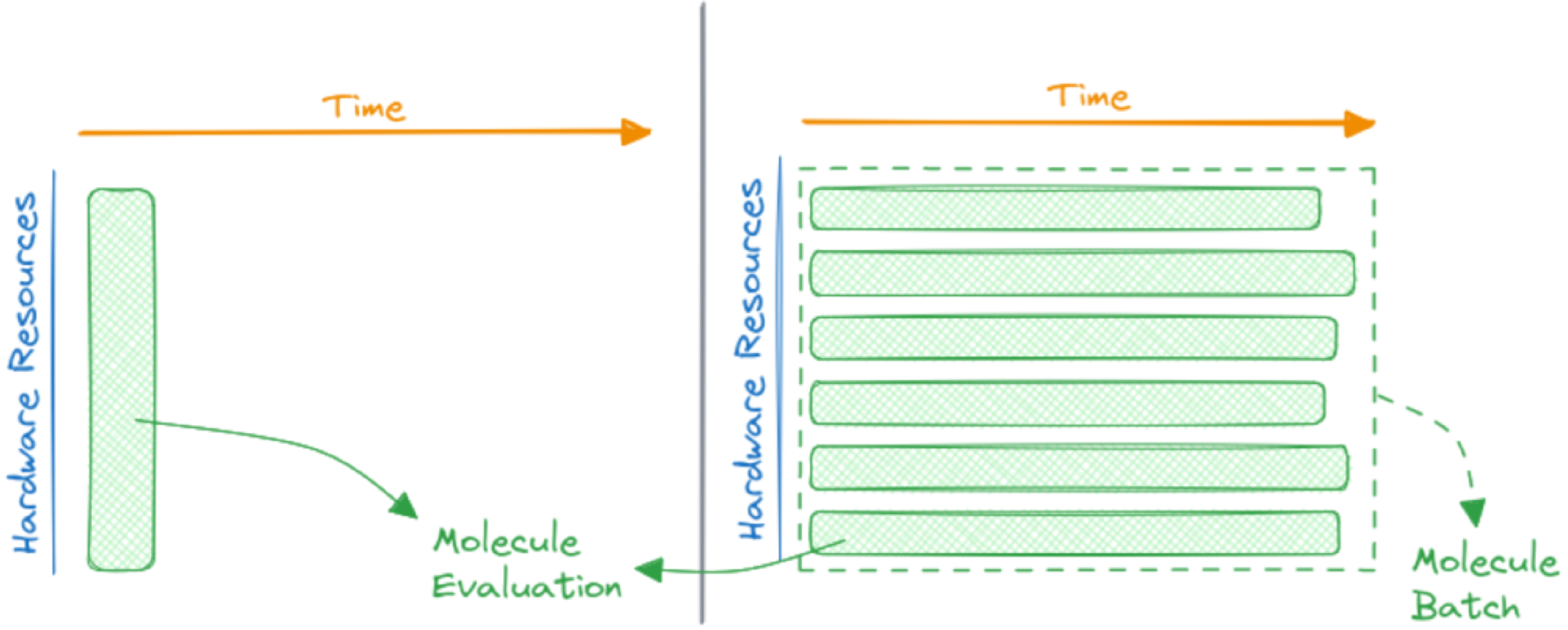


Manage Hardware Heterogeneity

- Efficient CUDA implementation
  - Support from NVIDIA engineers
- We introduced a SYCL porting
  - Computation kernels
  - Out-of-order input computation

LIGATE

LiGen Computation parallelism



POLITECNICO MILANO 1863

LiGen Batched Approach

1. Write kernels with non-type template parameters for atom number
    - Different hardware requirements

```
template<size_t num_atoms>
__global__ void kernel( ... ) {
  ...
}
```

LiGen Batched Approach

1. Write kernels with non-type template parameters for input features
2. Define input features clusters that impact the kernel's complexity
    - The ligands computation should last for a similar period

LiGen Batched Approach

1. Write kernels with non-type template parameters for input features
2. Define input features clusters that impact the kernel's complexity
3. Use Hardware characteristics to size each ligand batch at runtime
    - Automatic tuning using CUDA or SYCL query API

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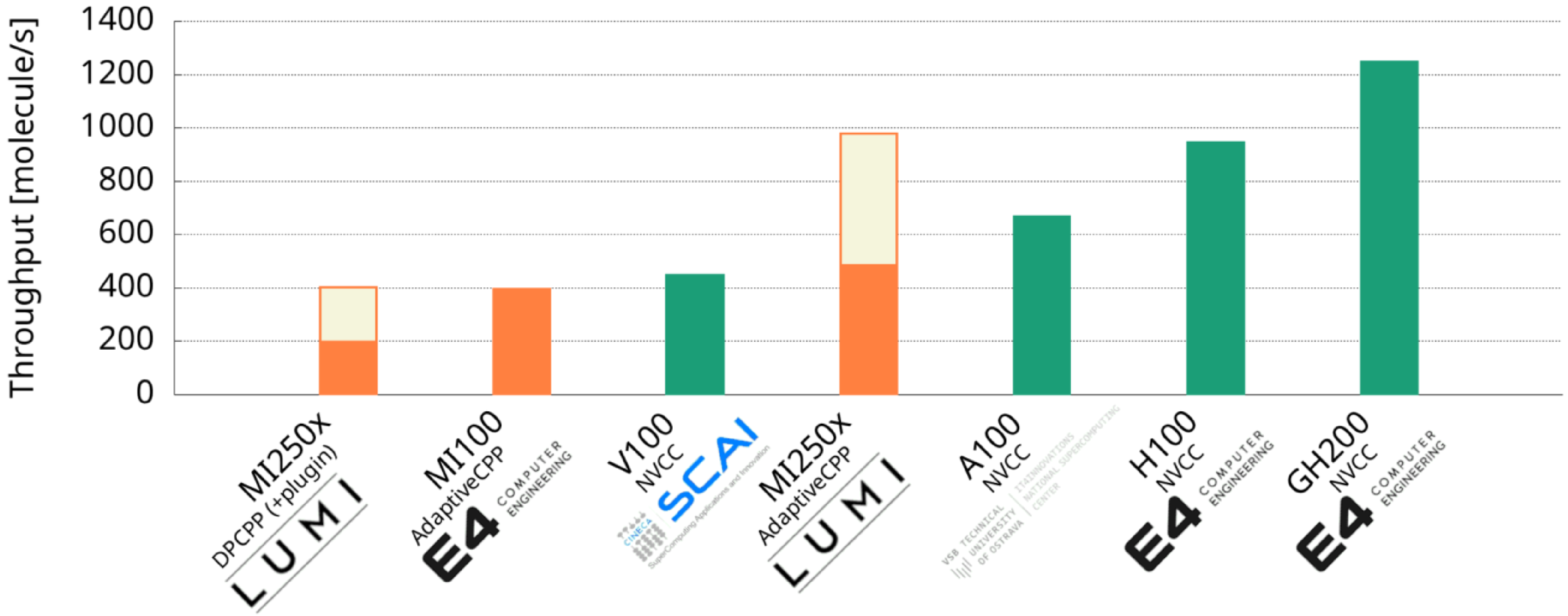
Performance on the single logical GPU card

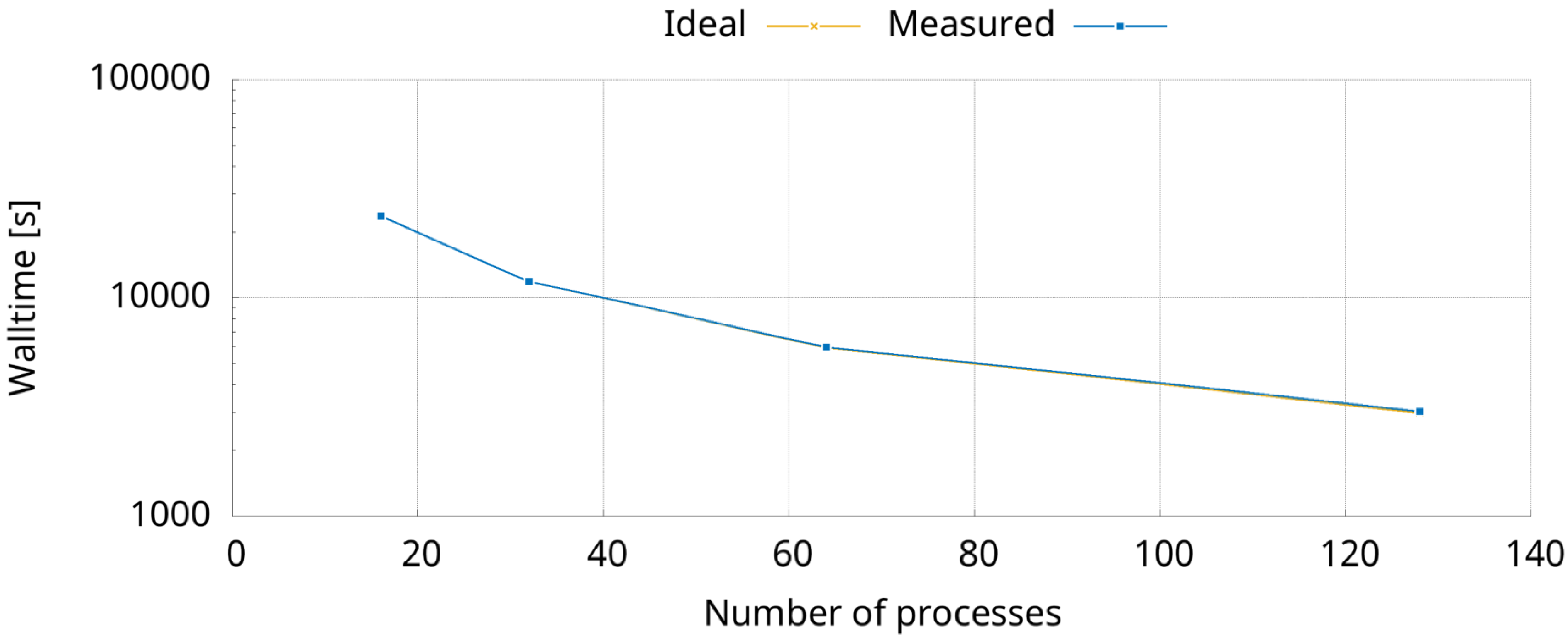


POLITECNICO
MILANO 1863

Scaling on the number of GPUs (LUMI-G)

Num nodes	Num GPUs/node	Throguhput [molecule/s]	Speed-up
16	1	7'808.96	1
16	8	60'566.672	7.756

Strong Scaling on the number of nodes (LUMI-G)



> **NOTE**: due to a technical problem with the FS, we used only 1 GPU per node

POLITECNICO MILANO 1863

Acknowledgement

EuroHPC JU for awarding this project access to LUMI and Karolina

- We could optimize LiGen software-knobs
- We benchmarked on the LUMI machine
  - Ready to run a virtual screening campaign
- In the LIGATE context, we can provide access to LiGen through the LEXIS platform

References

- "EXSCALATE: an extreme-scale virtual screening platform for drug discovery targeting polypharmacology to fight SARS-CoV-2." IEEE Transactions on Emerging Topics in Computing
- "Understanding the I/O impact on the performance of high-throughput molecular docking." 2021 IEEE/ACM Sixth International Parallel Data Systems Workshop (PDSW).
- "Exploiting OpenMP and OpenACC to accelerate a geometric approach to molecular docking in heterogeneous HPC nodes." The Journal of Supercomputing
- "Improving computation efficiency using input and architecture features for a virtual screening application", arxiv, minor revision
- "GPU-optimized Approaches to Molecular Docking-based Virtual Screening in Drug Discovery: A Comparative Analysis", arxiv, minor revision

Large Eddy Simulations (LES) of a Three-Element High-Lift Wing: Exploring the Active Flow Control (AFC) Capabilities.

EUROHPC USER DAY 2023 Brussels 11.12.23

EuroHPC Joint Undertaking

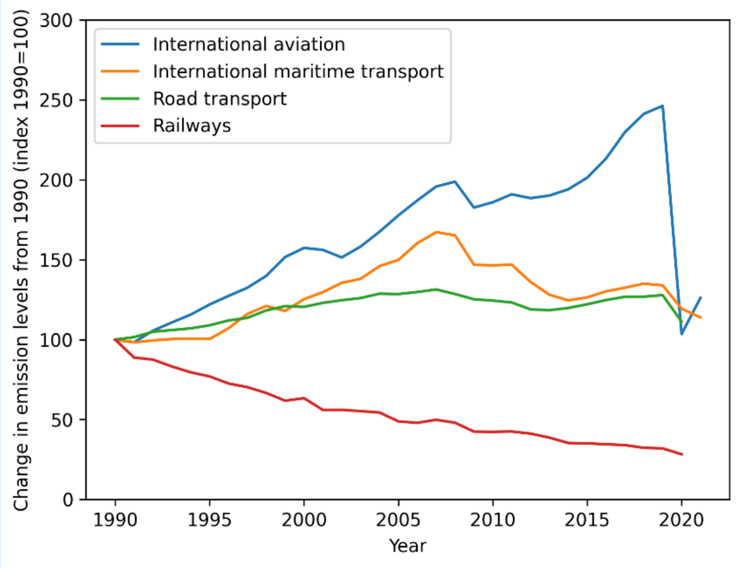
Project: "*Active Flow Control of a 3-Element High-Lift Wing: The Role of Coherent Structures*"

EuroHPC used: Vega CPU (IZUM)

Motivation

GOAL

Reduce drag in wings

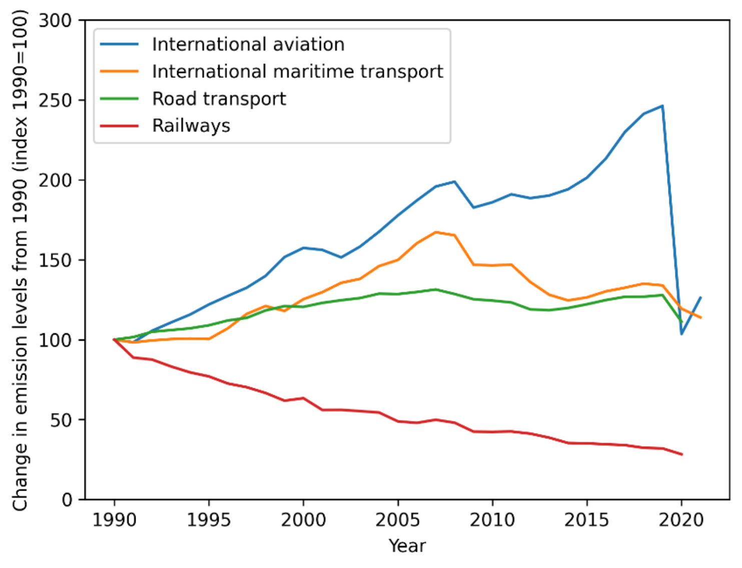


[1] European Environment Agency, Greenhouse gas emissions from transport in Europe, accessed 6 June 2023, https://www.eea.europa.eu/ims/greenhouse-gas-emissions-from-transport
[2] B. Eiximeno, A. Miró, J.C. Cajas, O. Lehmkuhl, I. Rodriguez (2022). DOI: https://doi.org/10.3390/fluids7090292
[3] O. Lehmkuhl, A. Lozano-Durán, I. Rodriguez (2020). DOI: 10.1088/1742-6596/1522/1/012017

Motivation

GOAL

Reduce drag in wings



[1] European Environment Agency, Greenhouse gas emissions from transport in Europe, accessed 6 June 2023, https://www.eea.europa.eu/ims/greenhouse-gas-emissions-from-transport

[2] B. Eiximeno, A. Miró, J.C. Cajas, O. Lehmkuhl, I. Rodriguez (2022). DOI: https://doi.org/10.3390/fluids7090292

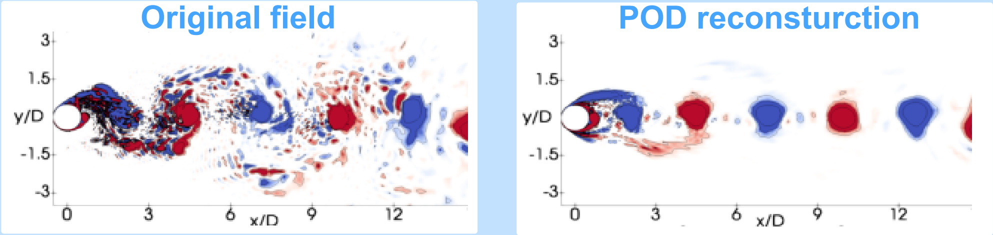
[3] O. Lehmkuhl, A. Lozano-Durán, I. Rodriguez (2020). DOI: 10.1088/1742-6596/1522/1/012017

METHODOLOGY

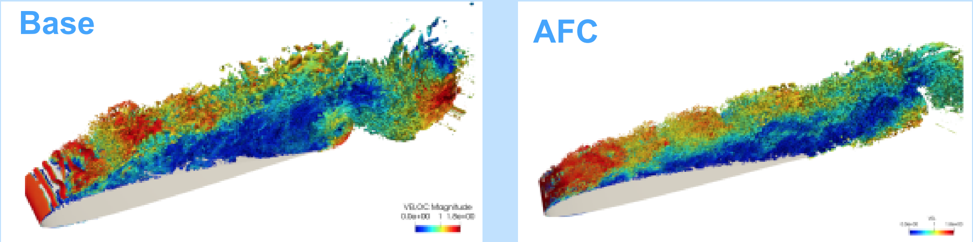
LES simulations of the baseline configuration

Understand the underlying physics of the problem

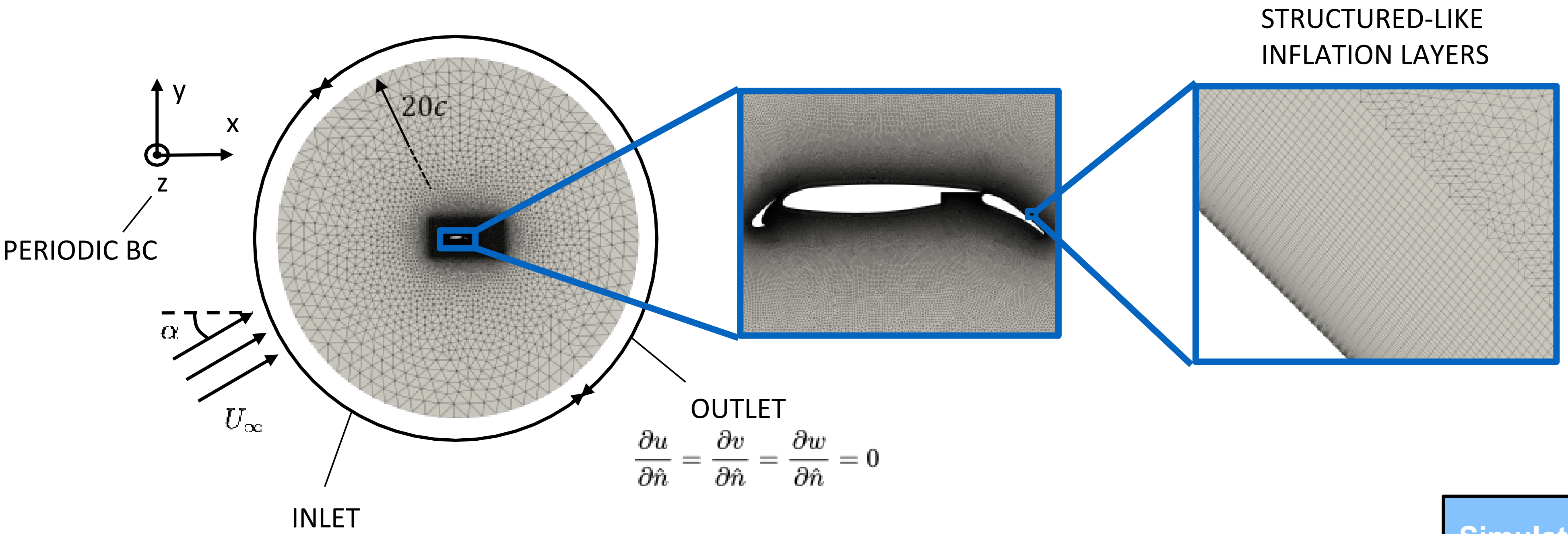
Apply reduce order models (ROMs): POD, DMD, Autoencoders…



Propose Active Flow Control (AFC) actuations



Baseline LES – Case Configuration



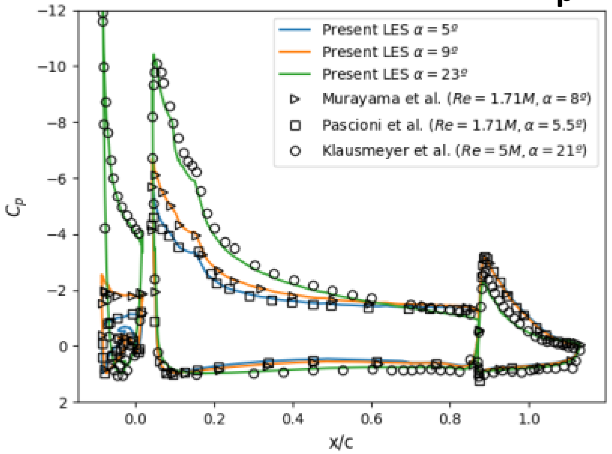
Simulation Code:

ALYA (FEM)

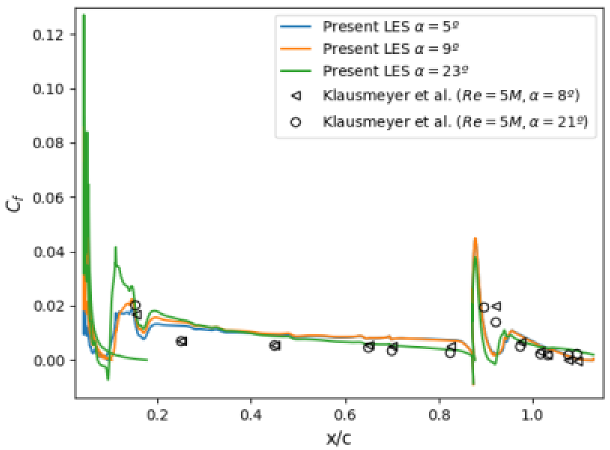
Flow Conditions		Domain			Mesh				
Re_c	α	Airfoil	$L_x = L_y$	L_z	N_{points}	N_{planes}	Δx^+_{max}	Δy^+_{max}	Δz^+_{max}
750,000	5, 9 and 23º	30P30N	20c	0.1c	58M	128	80	1	50

Baseline LES – Validation

Pressure Coefficient (C_p)



Skin Friction Coefficient(C_f)



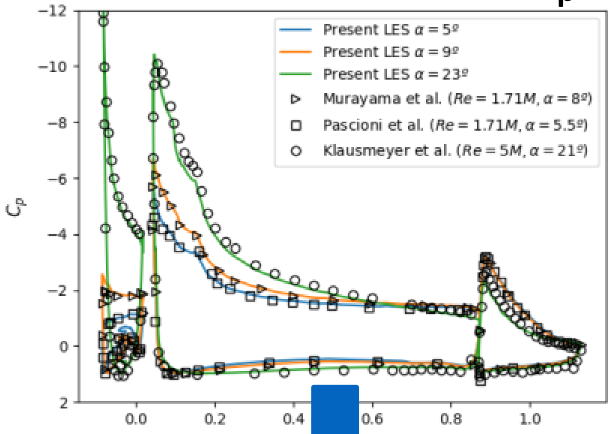
[6] M. Murayama, K. Nakakita, K. Yamamoto, H. Ura, Y. Ito, M. Choudhari (2014). DOI: https://doi.org/10.2514/6.2018-3460

[7] K. Pascioni, L.N. Cattafesta, M. Choudhari (2014). DOI: https://doi.org/10.2514/6.2014-3062

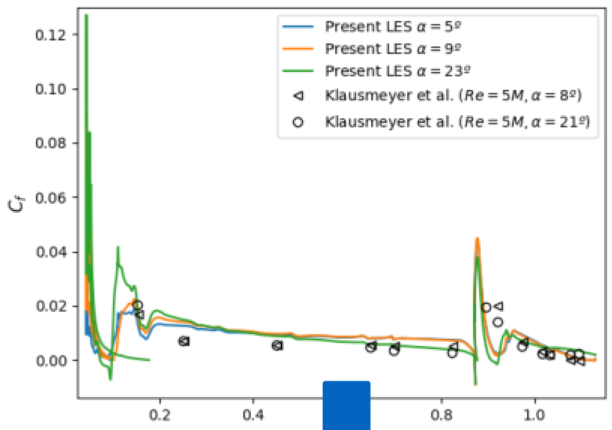
[8] S. Klausmeyer, J. Lin (1994). DOI: https://doi.org/10.2514/6.1994-1870

Baseline LES – Validation

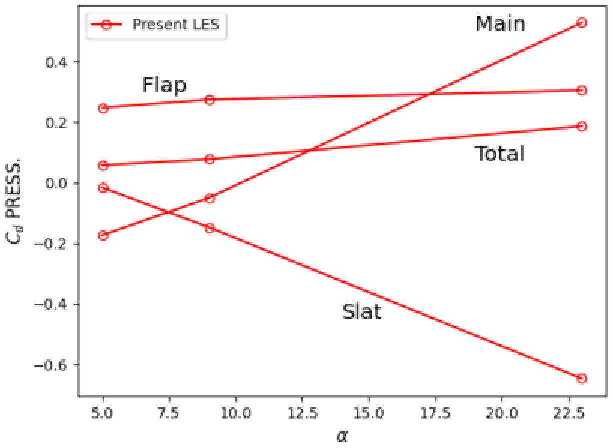
Pressure Coefficient (C_p)



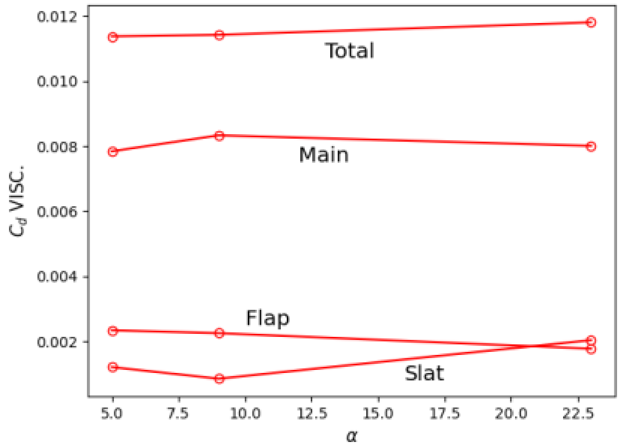
Skin Friction Coefficient(C_f)



Pressure Drag Coefficient ($C_{d,\ pres.}$)



Viscous Drag Coefficient ($C_{d,\ visc.}$)



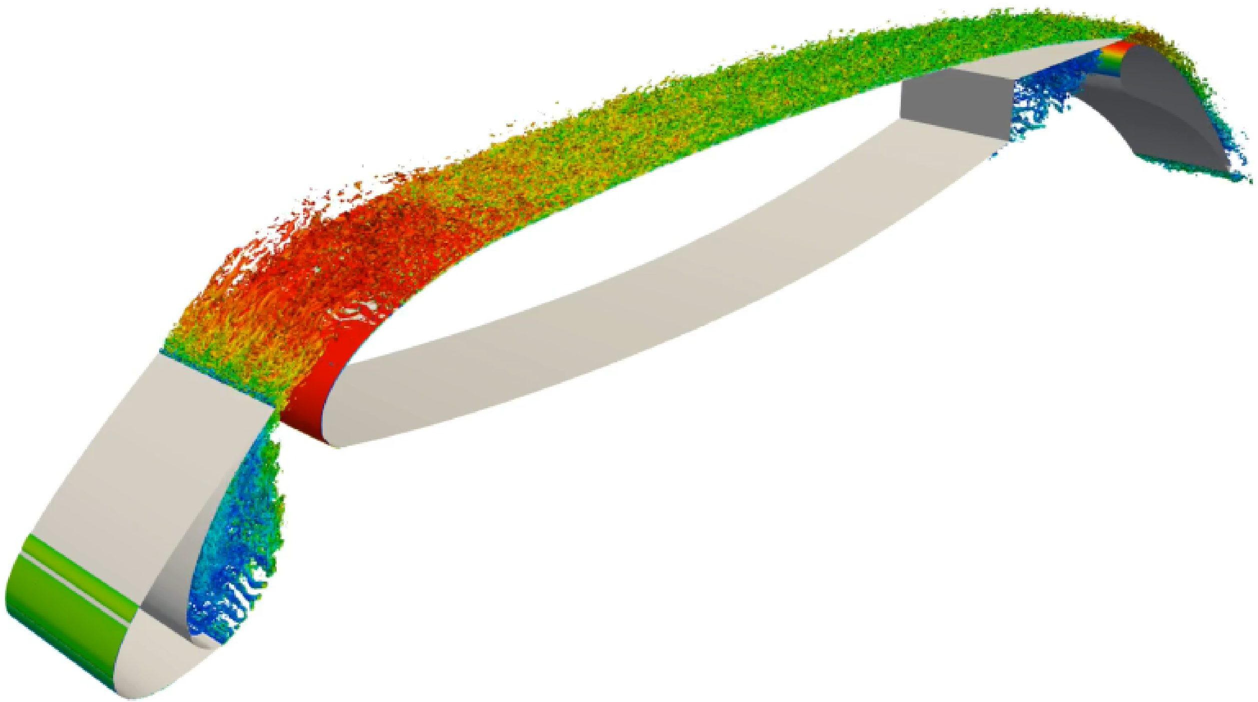
[6] M. Murayama, K. Nakakita, K. Yamamoto, H. Ura, Y. Ito, M. Choudhari (2014). DOI: https://doi.org/10.2514/6.2018-3460

[7] K. Pascioni, L.N. Cattafesta, M. Choudhari (2014). DOI: https://doi.org/10.2514/6.2014-3062

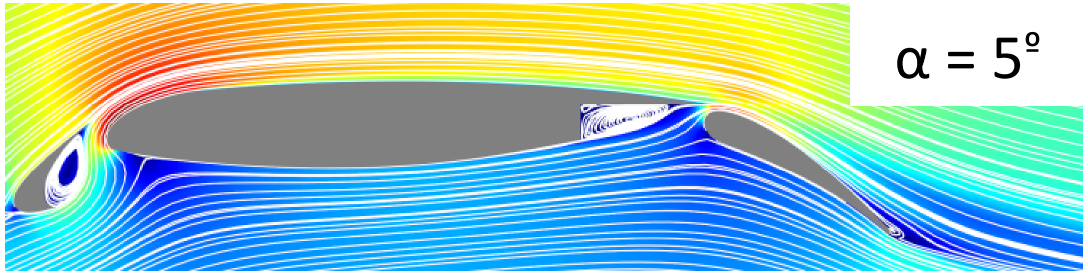
[8] S. Klausmeyer, J. Lin (1994). DOI: https://doi.org/10.2514/6.1994-1870

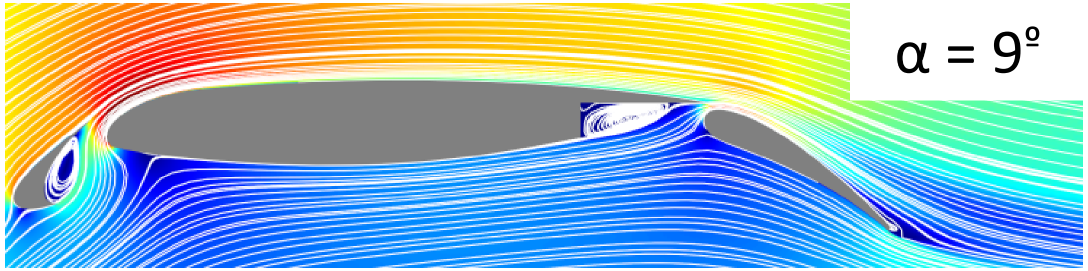
Baseline LES – Flow Overview

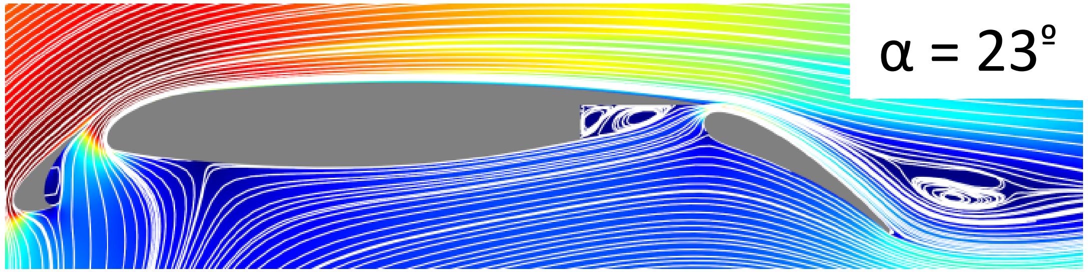
Q-criterion isocontours at $\alpha = 5^{\circ}$



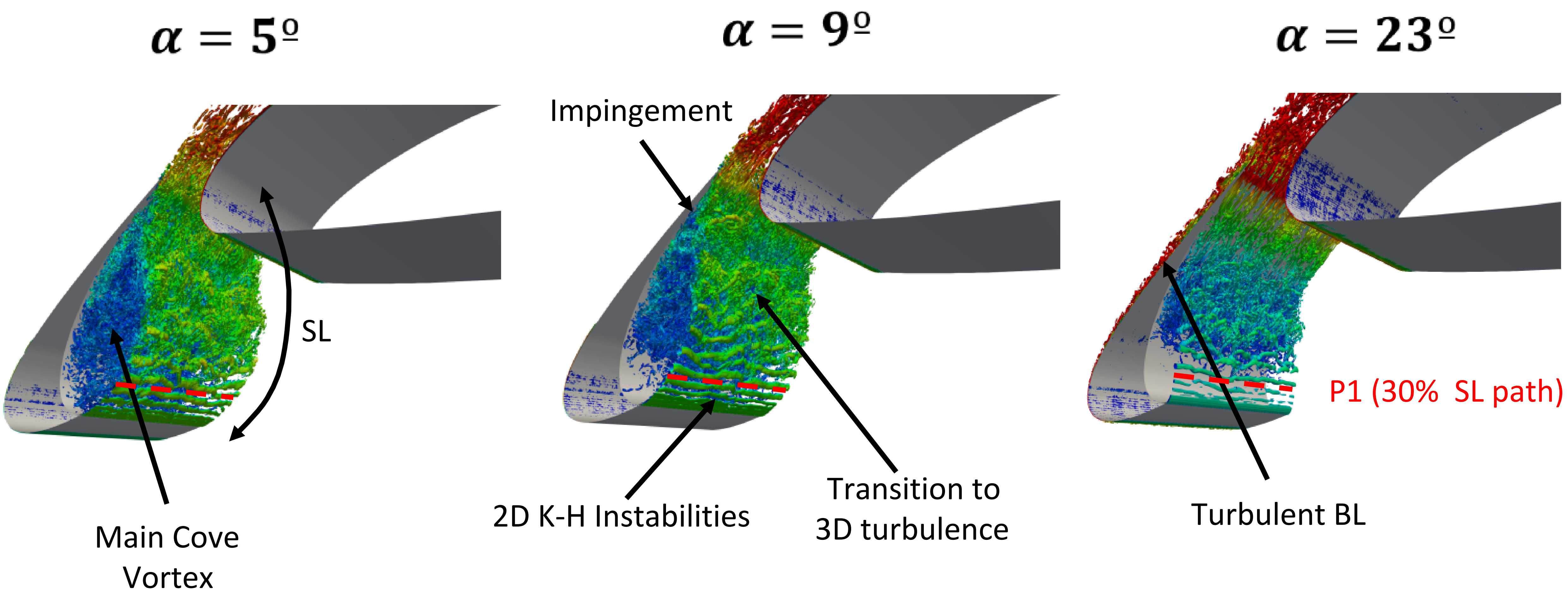
Streamlines Coloured by Velocity Magnitude





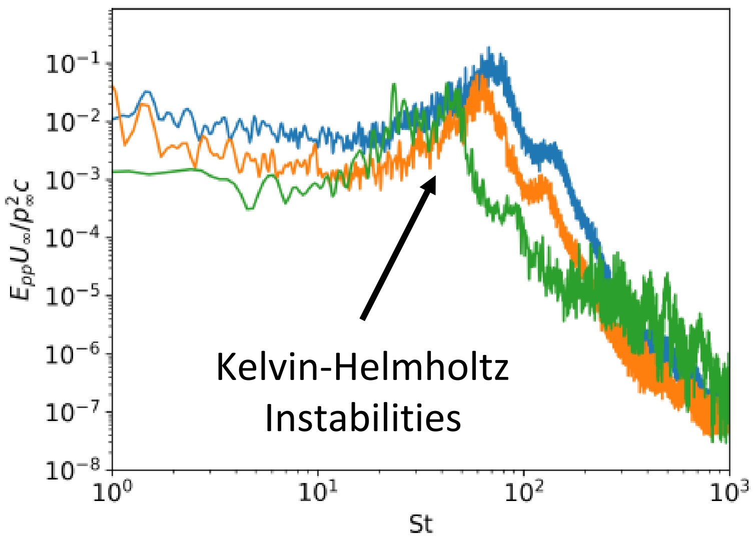


Baseline LES – Slat Cove Dynamics



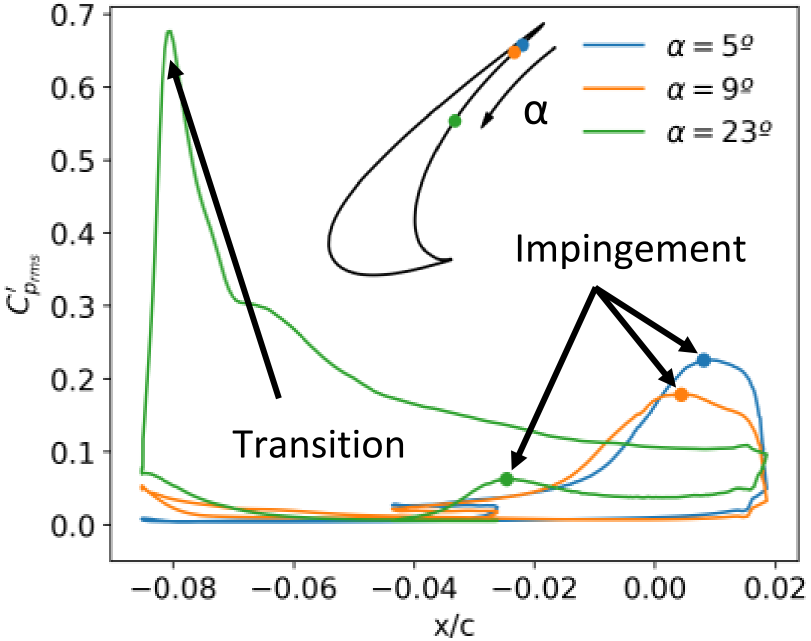
Baseline LES – Slat Cove Dynamics

Pressure Spectra at P1

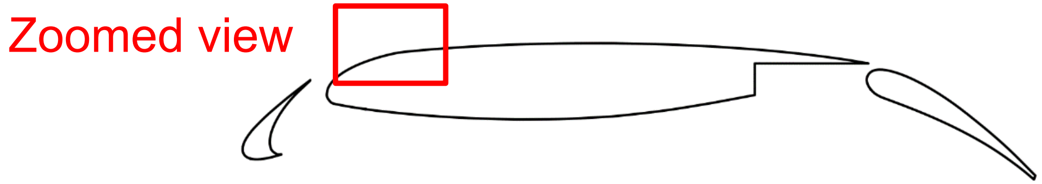


α [º]	St [-]
5	70
9	64
23	35

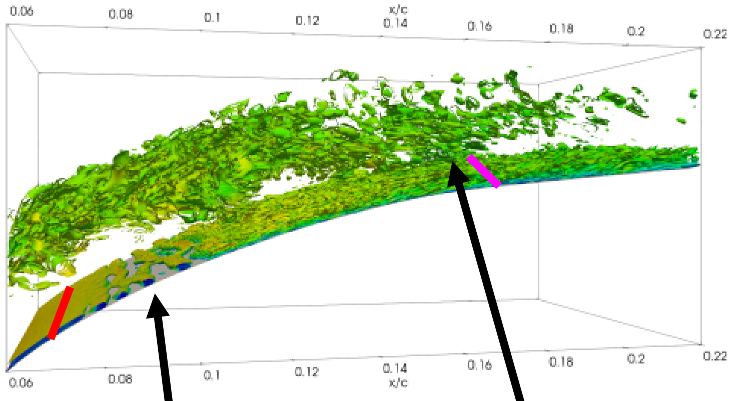
RMS of Cp’



Baseline LES – Turbulent Transition



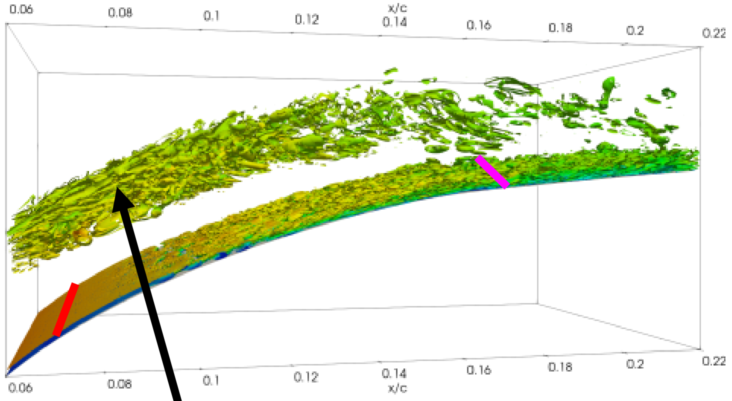
$\alpha = 5^{\text{o}}$



T-S Instabilities

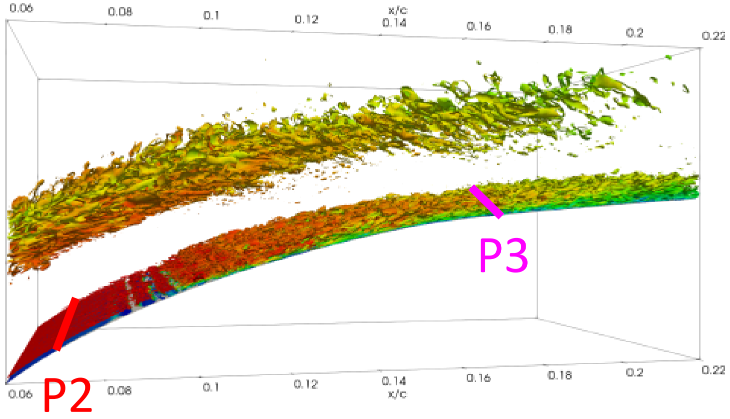
Slat Wake Interaction

$\alpha = 9^{\text{o}}$



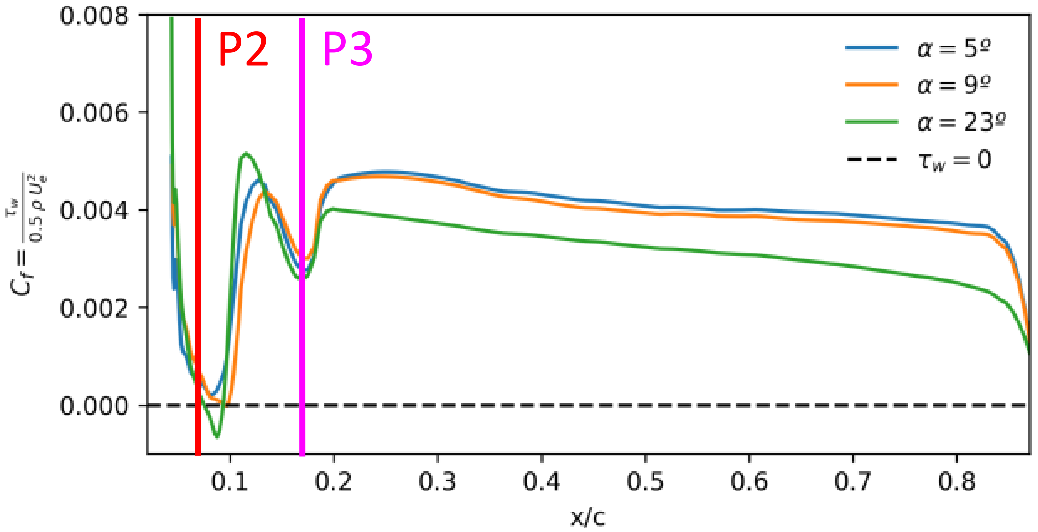
Slat Wake

$\alpha = 23^{\text{o}}$



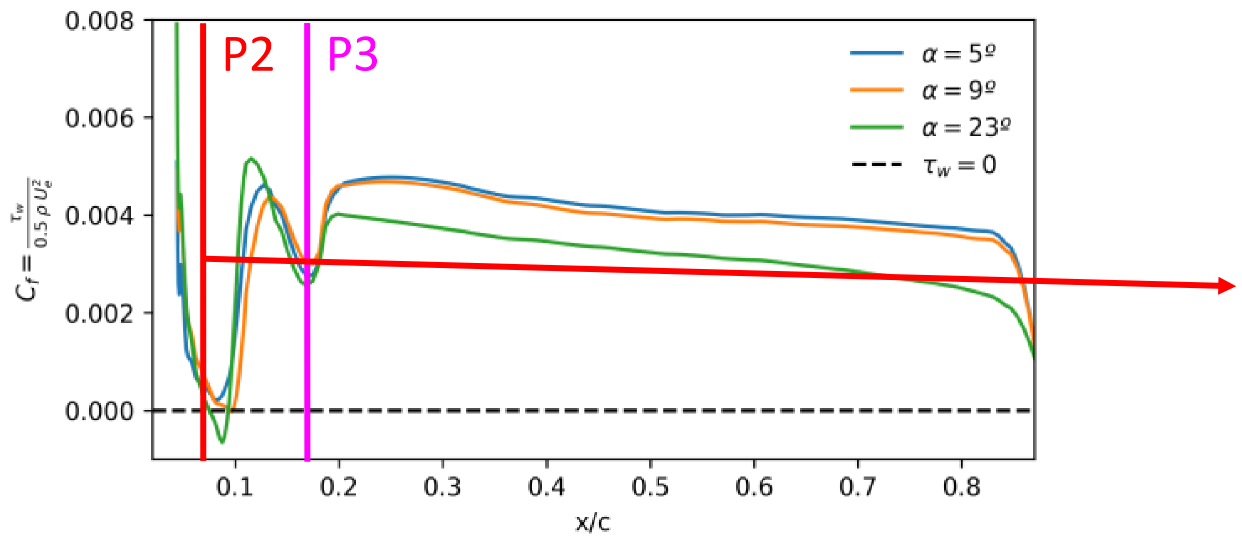
Baseline LES – Turbulent Transition

Skin Friction Coefficient

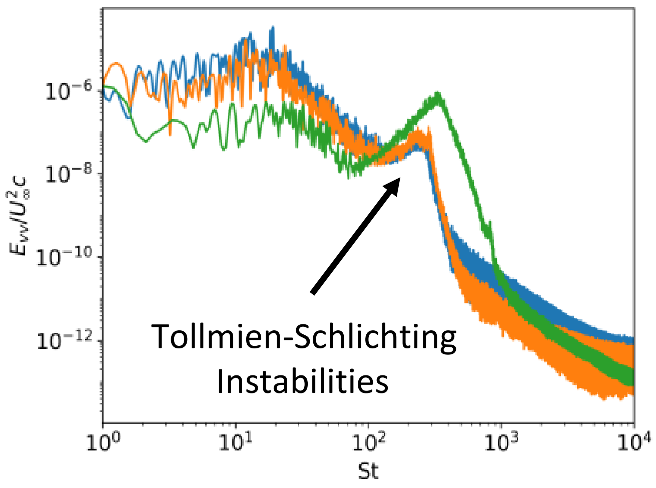


Baseline LES – Turbulent Transition

Skin Friction Coefficient



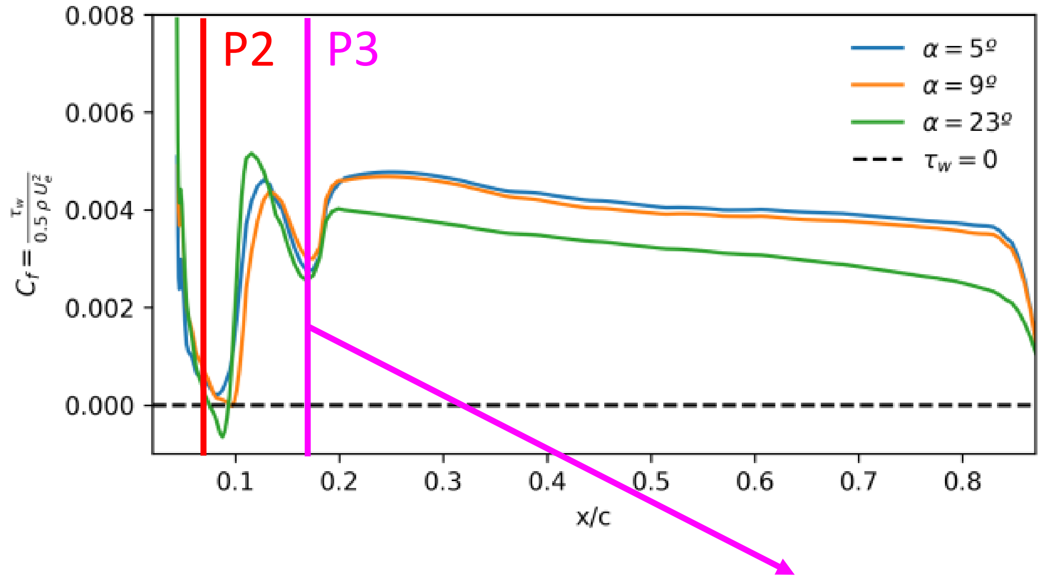
Velocity Magnitude Spectra at P2



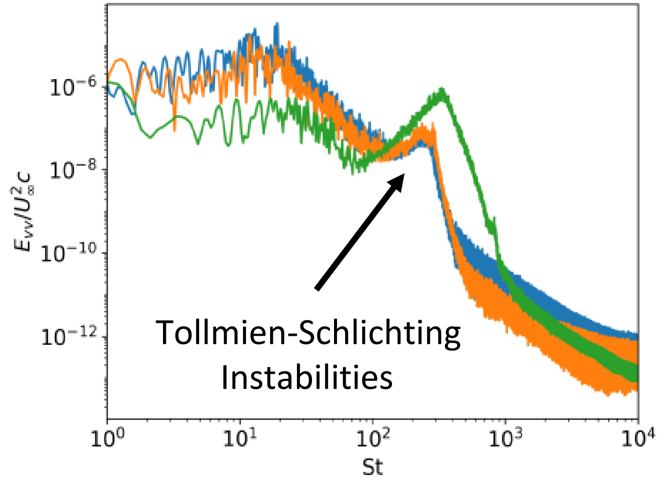
α [º]	St [-]
5	255
9	285
23	340

Baseline LES – Turbulent Transition

Skin Friction Coefficient

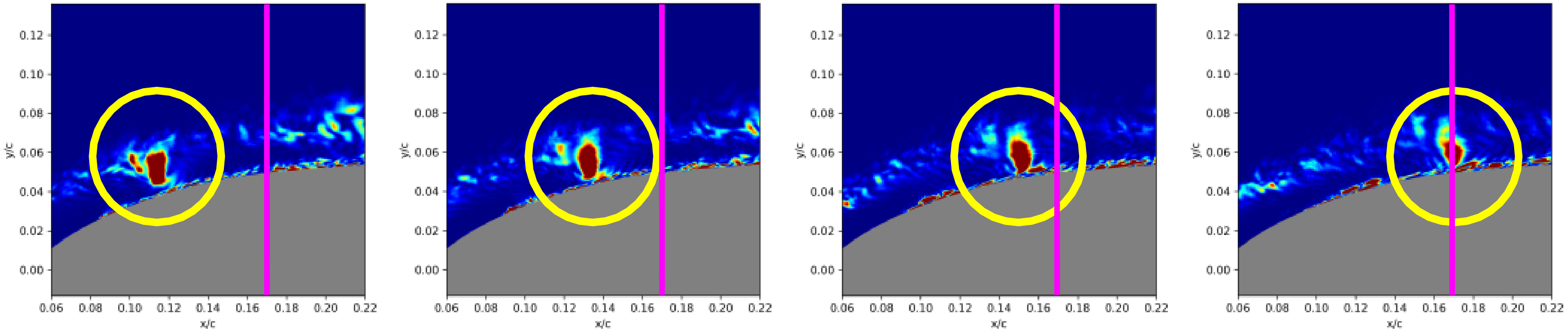


Velocity Magnitude Spectra at P2



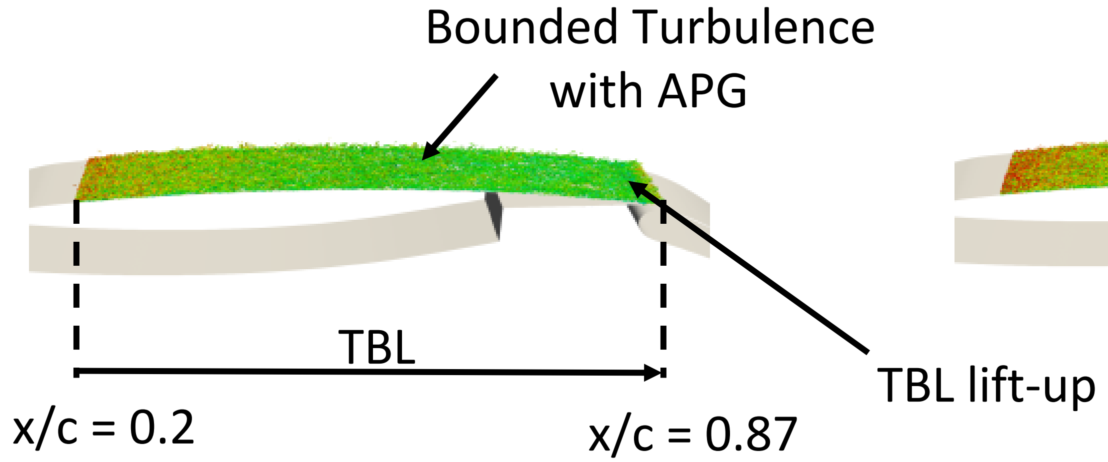
α [º]	St [-]
5	255
9	285
23	340

Instantaneous TKE

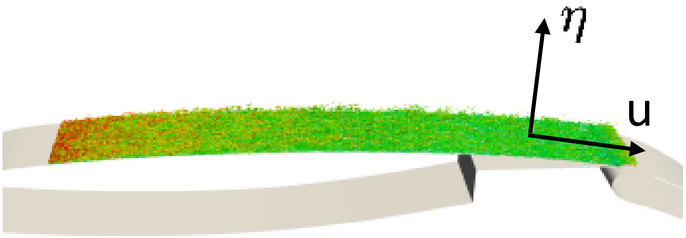


Baseline LES – Trubulent Boundary Layer

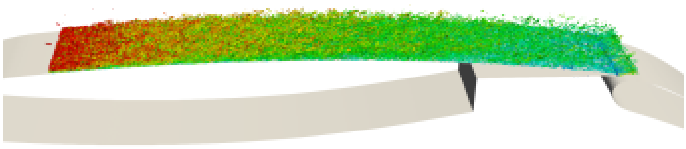
$\alpha = 5º$



$\alpha = 9º$

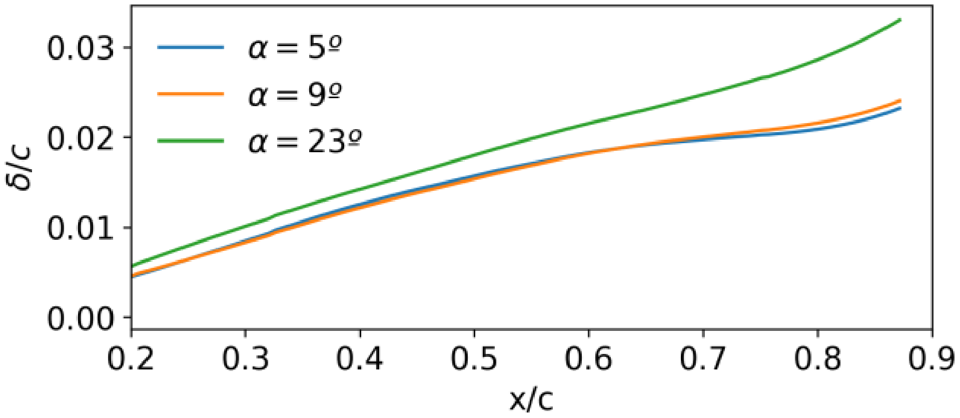


$\alpha = 23º$

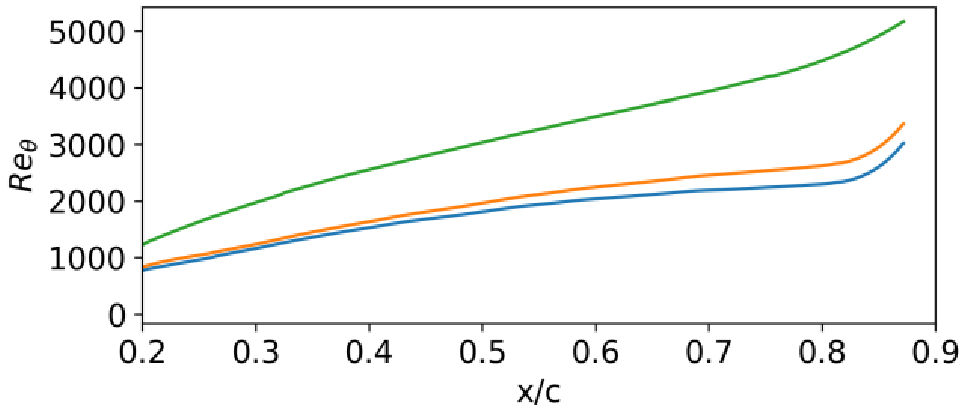


Baseline LES – Trubulent Boundary Layer

Boundary Layer Thickness

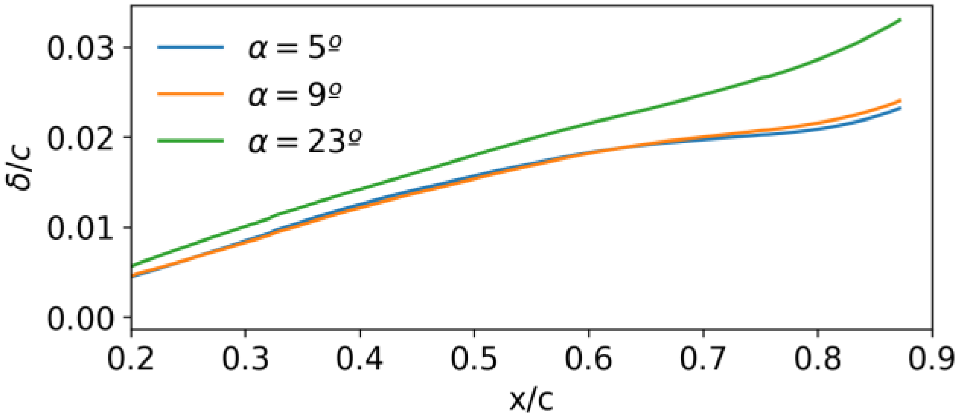


Momentum Thickness Reynolds

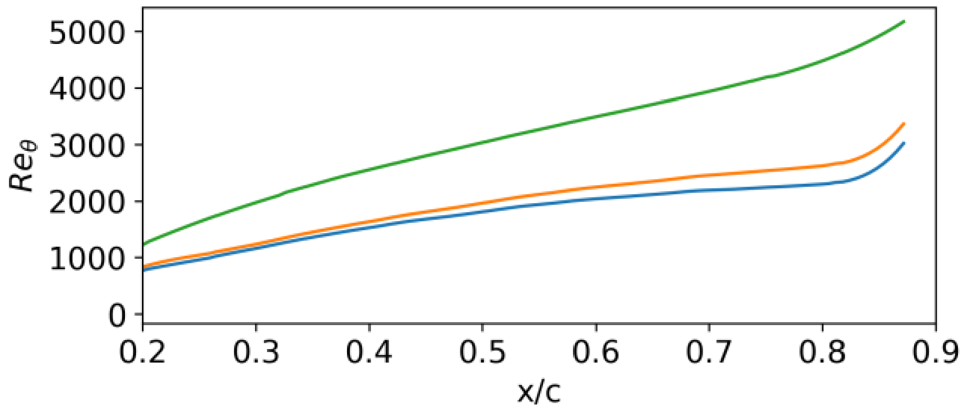


Baseline LES – Trubulent Boundary Layer

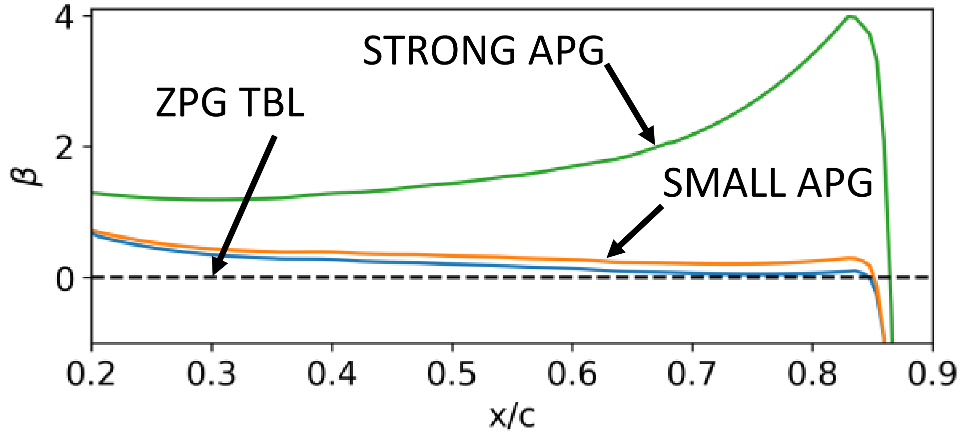
Boundary Layer Thickness



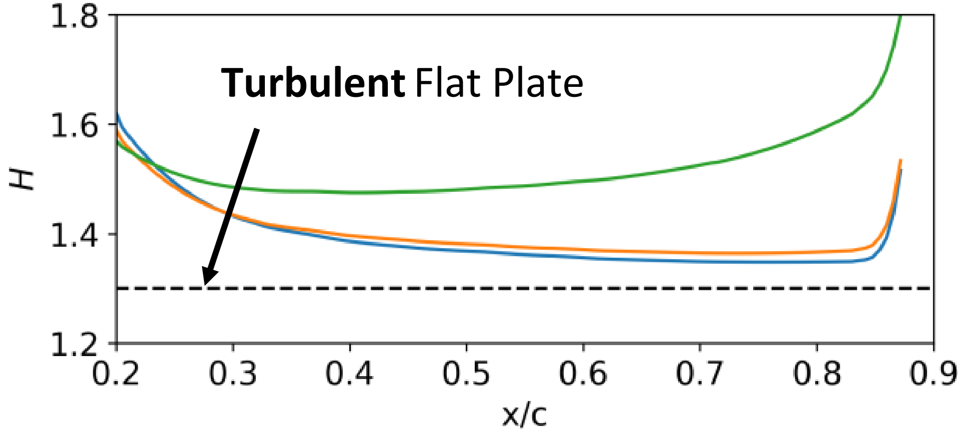
Momentum Thickness Reynolds



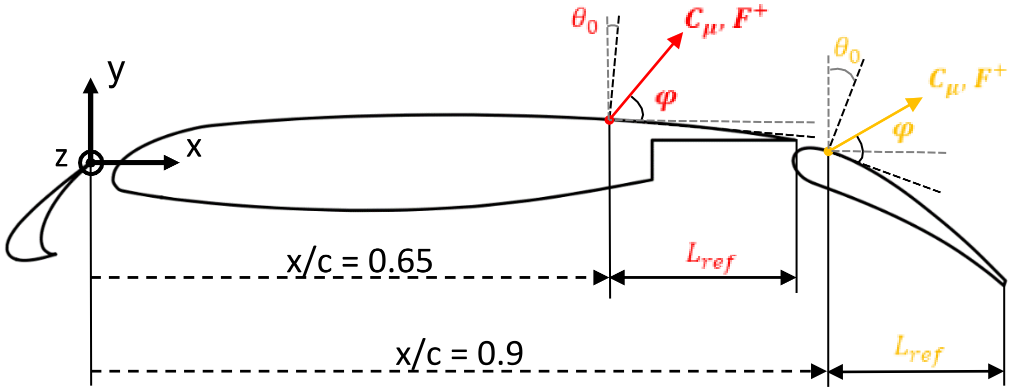
Clauser Pressure-Gradient Parameter



Shape Factor



AFC LES – Case Configuration

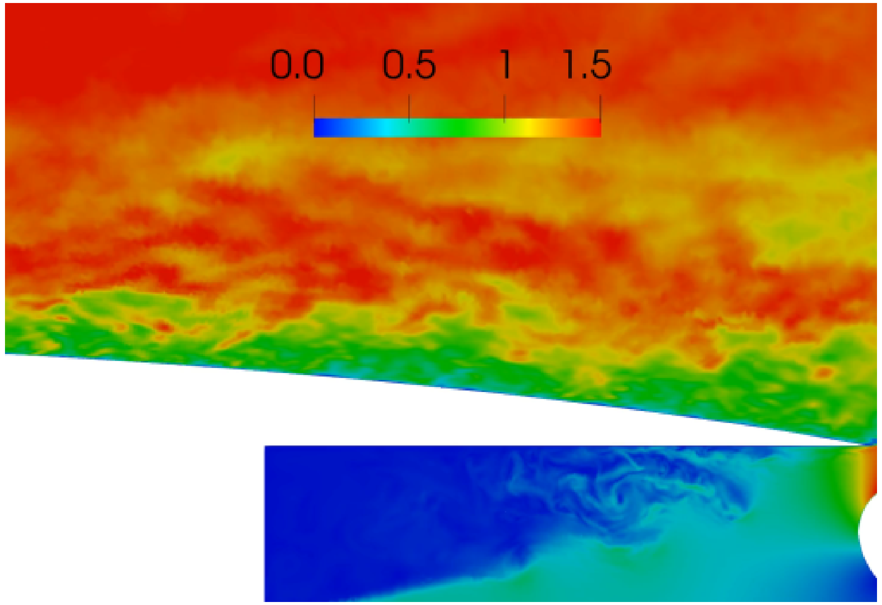


$$\begin{bmatrix} u \\ v \\ w \end{bmatrix}_{xyz,\,act} = U_\infty \sqrt{\frac{c}{h} C_\mu} \sin\left(2\pi \frac{F^+ U_\infty}{L_{ref}} t\right) \begin{bmatrix} \cos(\varphi - \theta_0) \\ \sin(\varphi - \theta_0) \\ 0 \end{bmatrix} = f(C_\mu, F^+, \varphi)$$

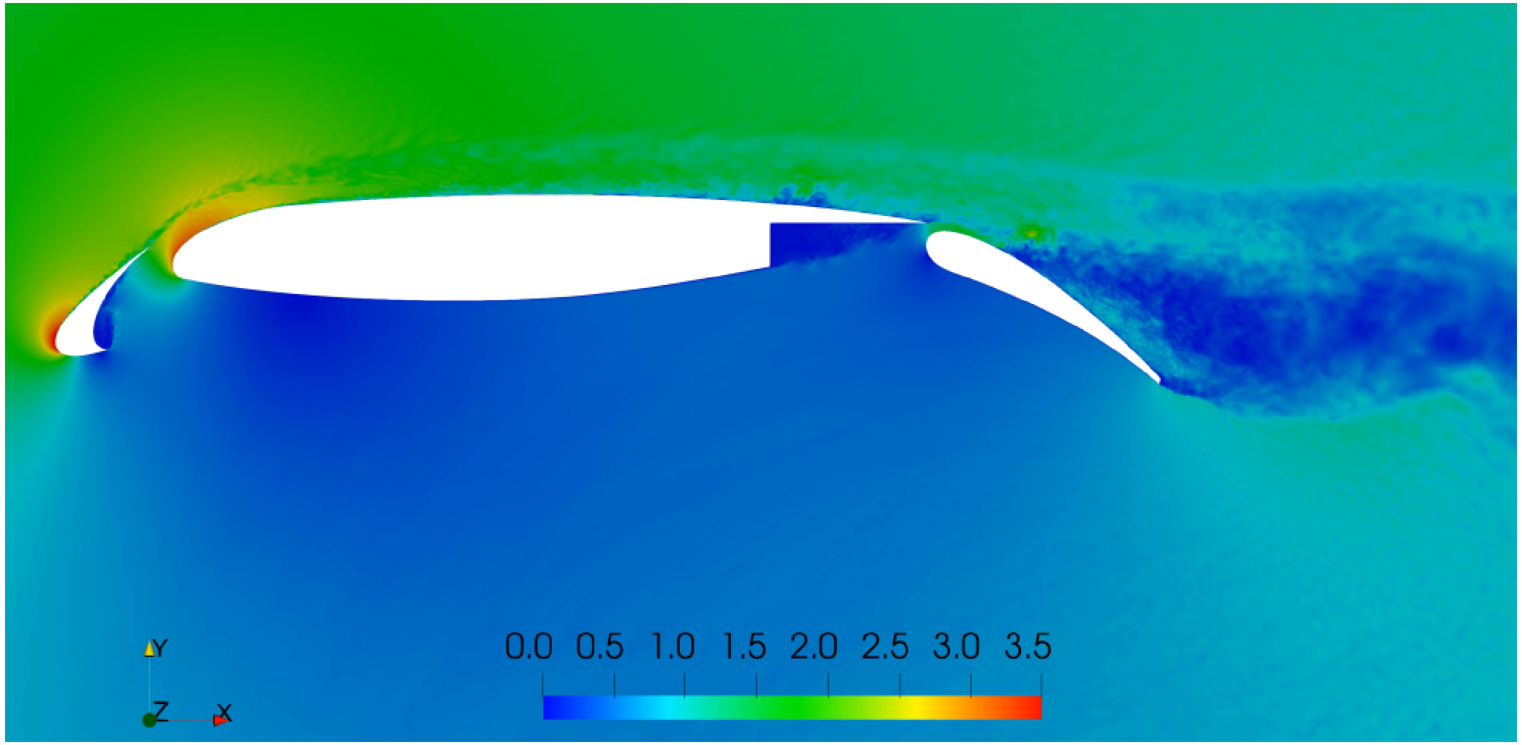
	CASE ID	Main Actuation			Flap Actuation		
		C_μ	F^+	φ	C_μ	F^+	φ
$Re_c =$ 750,000 $\alpha = 23^{\circ}$	1	0.015	0.34	20º	*- Not actuated -*		
	2	*- Not actuated -*			0.025	0.34	20º
	3	0.015	1.52	90º	*- Not actuated -*		
	4	*- Not actuated -*			0.025	1.52	90º
	5	0.015	1.52	45º	0.025	1.52	90º

AFC LES - Results

Case ID 1



Case ID 5



Work in Progress!

Conclusions

- Computational data shows **good agreement** with the experimental observations.
- Evolution of flow dynamics **at increasing α**:
  - **Slat SL:** (i) Smaller recirculation area. (ii) Lower K-H frequencies. (iii) Weaker impingement strength. (iv) More pronounced wake (TBL on suction side).
  - **Main turb. transition**: (i) Nearly at constant locations. (ii) Higher T-S frequencies.
  - **Main TBL:** (i) Stronger APG. (ii) More pronounced main wake. (iii) Recirculation region (Stall conditions).
- **Viscous drag** remains nearly **constant** with α (from $C_{d\ visc.}$= 0.0114 to 0.0118); while **pressure drag increases** noticeably (from $C_{d\ press.}$= 0.0580 to 0.1865).
- **Pressure is the main contributor** to drag (Half or even one order of magnitude higher):
  - **Flap** has the highest $C_{d\ press.}$ at lower α (curvature → APG), but it remains approximately constant with α (constrained flow → main-flap gap jet).
  - In the **slat**, $C_{d\ press}$ diminishes with α (Higher suction peak + element inclination → Positive force).
  - The $C_{d\ press.}$ in the **main** goes from the lowest value (behaves nearly as a flat plate) to the highest one (Strong APG along suction side).
- Two **actuations strategies** tested **with the idea of**:
  - **Main actuator:** Reduce the APG in the main TBL → reduce its wake.
  - **Flap actuator:** Increase the vertical mixing of the main-flap gap jet flow.

Future Work

- Analyse the **AFC results** and assess the differences with the baseline case: Why /Why not improved?
- Build **ROMs models** (POD, DMD, Autoencoders…): Fruther understand the Flow features contributed by the actuations.
- **Exploit** the capabilities of machine learning (**Deep Reinforcement Learning**) to optimize the actuation parameters.

Thank you for your attention

EuroHPC
Joint Undertaking

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Heat-transfer in drop-laden turbulence

EUROHPC USER DAY 2023 Brussels 11.12.23

EuroHPC Joint Undertaking

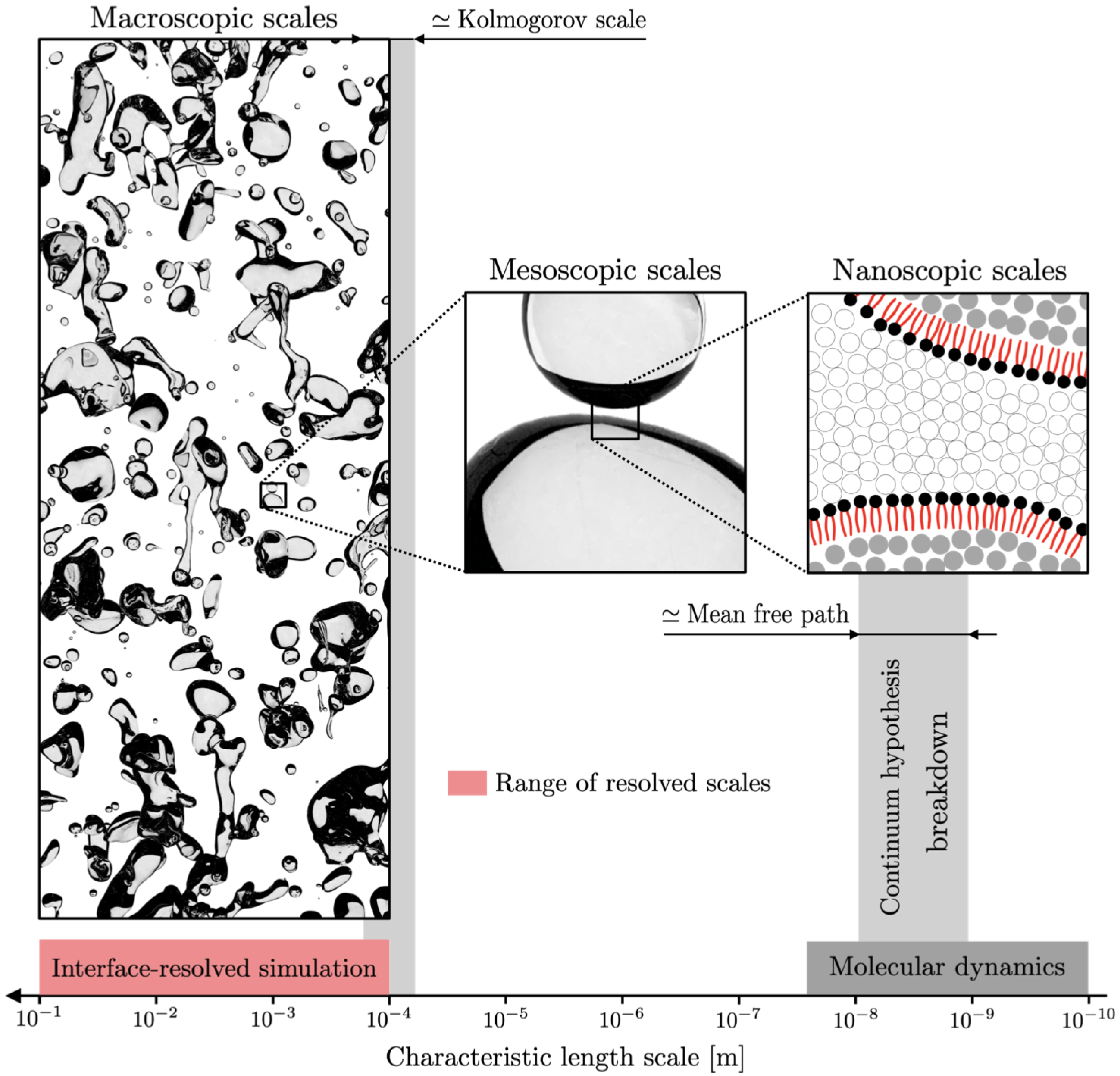
Project: “*BubbLe-modUlated Mixing in turbulENce (BLUMEN)*”

EuroHPC used: Discoverer

Speaker: *Alessio ROCCON (Univ. Udine)*

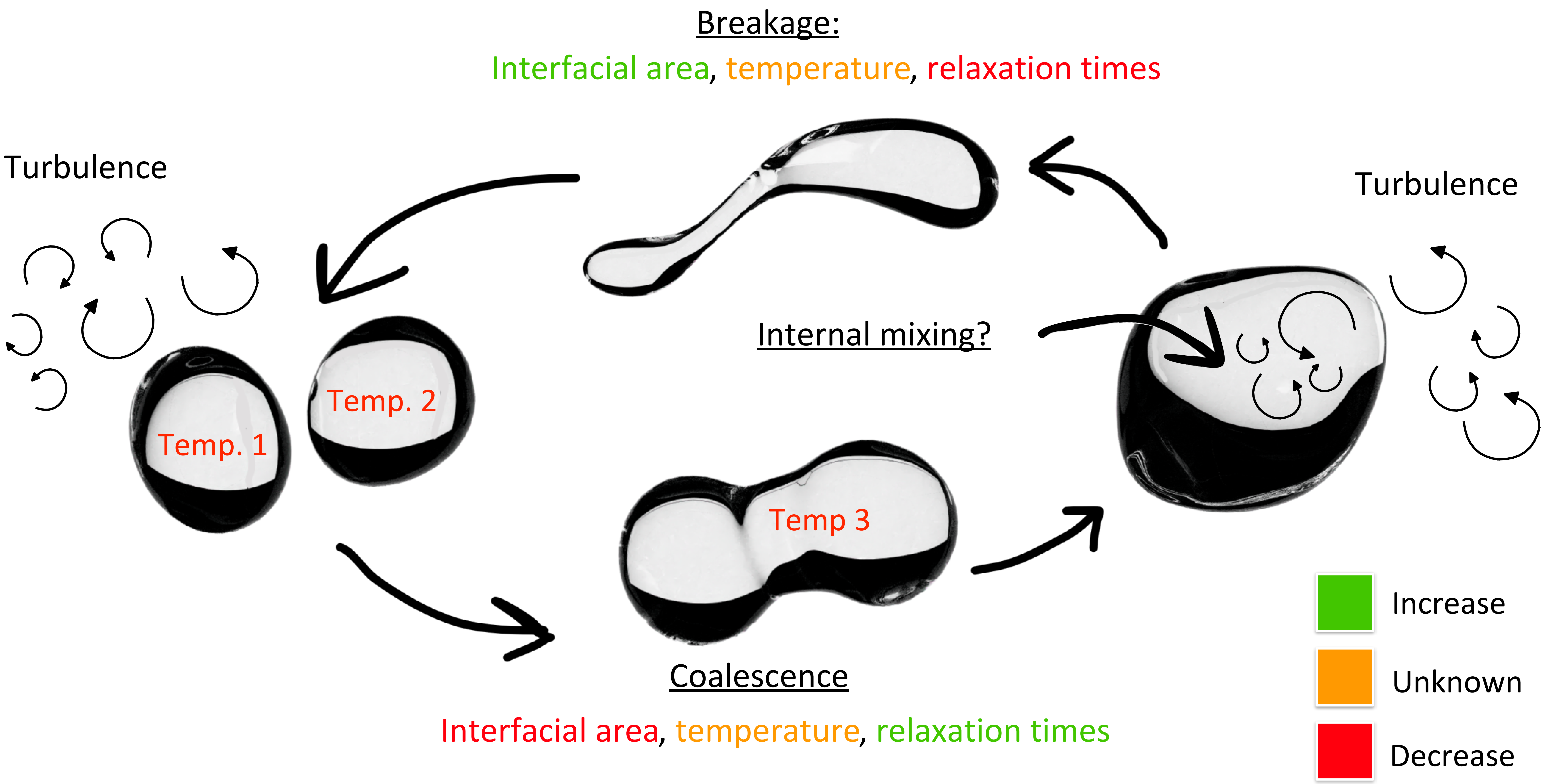
The problem involves a wide range of spatial and temporal scales:

- Largest scale of problem
- Kolmogorov scale
- Molecular scale of the interface



Roccon et al., "Phase-field modeling of complex interface dynamics in drop-laden turbulence, PRF (2023).

How does a passive scalar (e.g. temperature) behave in multiphase turbulence?
Internal/external turbulent transport and turbulence-interface interactions can modify the mixing:



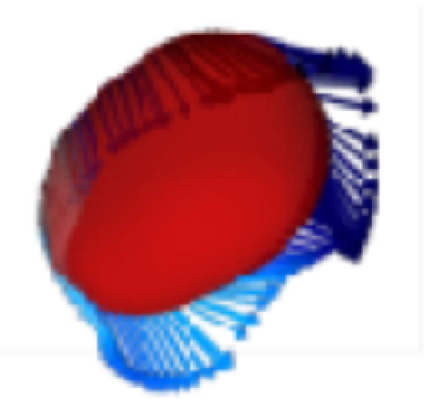
Heat transfer?

Assumptions:
- Same density/viscosity
- Small temperature difference
- Same thermal diffusivity

Prandtl number

$$Pr = \frac{\nu}{a} = \frac{\text{Momentum diffusivity}}{\text{Thermal diffusivity}}$$

Flow:

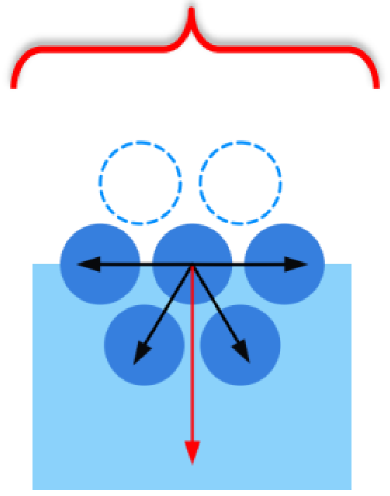


$$\nabla \cdot \mathbf{u} = 0$$

$$\rho(\phi)\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right] = -\nabla p + \frac{1}{Re_\tau}\nabla\cdot\left[\eta(\phi)(\nabla\mathbf{u}+\nabla\mathbf{u}^T)\right] + \frac{3}{\sqrt{8}}\frac{Ch}{We}\nabla\cdot\tau_c$$

Interface:

$$\frac{\partial \phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \frac{1}{Pe_\phi}\nabla^2\mu_\phi$$



Surface tension forces

Temperature:

$$\frac{\partial \theta}{\partial t} + \mathbf{u}\cdot\nabla\theta = \frac{1}{Re_\tau Pr}\nabla^2\theta$$

Transport equation for a passive scalar, no feedback on NS

Cahn and Hilliard ‚Free energy of a non-uniform system I, Interfacial free energy, JCP (1958) Roccon et al., "Phase-field modeling of complex interface dynamics in drop-laden turbulence, PRF (2023). Mangani et al., “Heat-transfer in drop-laden turbulence”, JFM (2023)

The **Cahn-Hilliard equation** is the principal governing equation in the phase-field method and includes all important physical phenomena: **phase-change and surface tension**.
CH equation is a fourth-order non linear partial differential equation.

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \frac{1}{Pe_\phi} \nabla^2 \mu_\phi$$

Chemical potential (Ginzburg-Landau theory)

$$\mu_\phi = \phi^3 - \phi - Ch^2 \nabla^2 \phi$$

Dimensionless parameters:

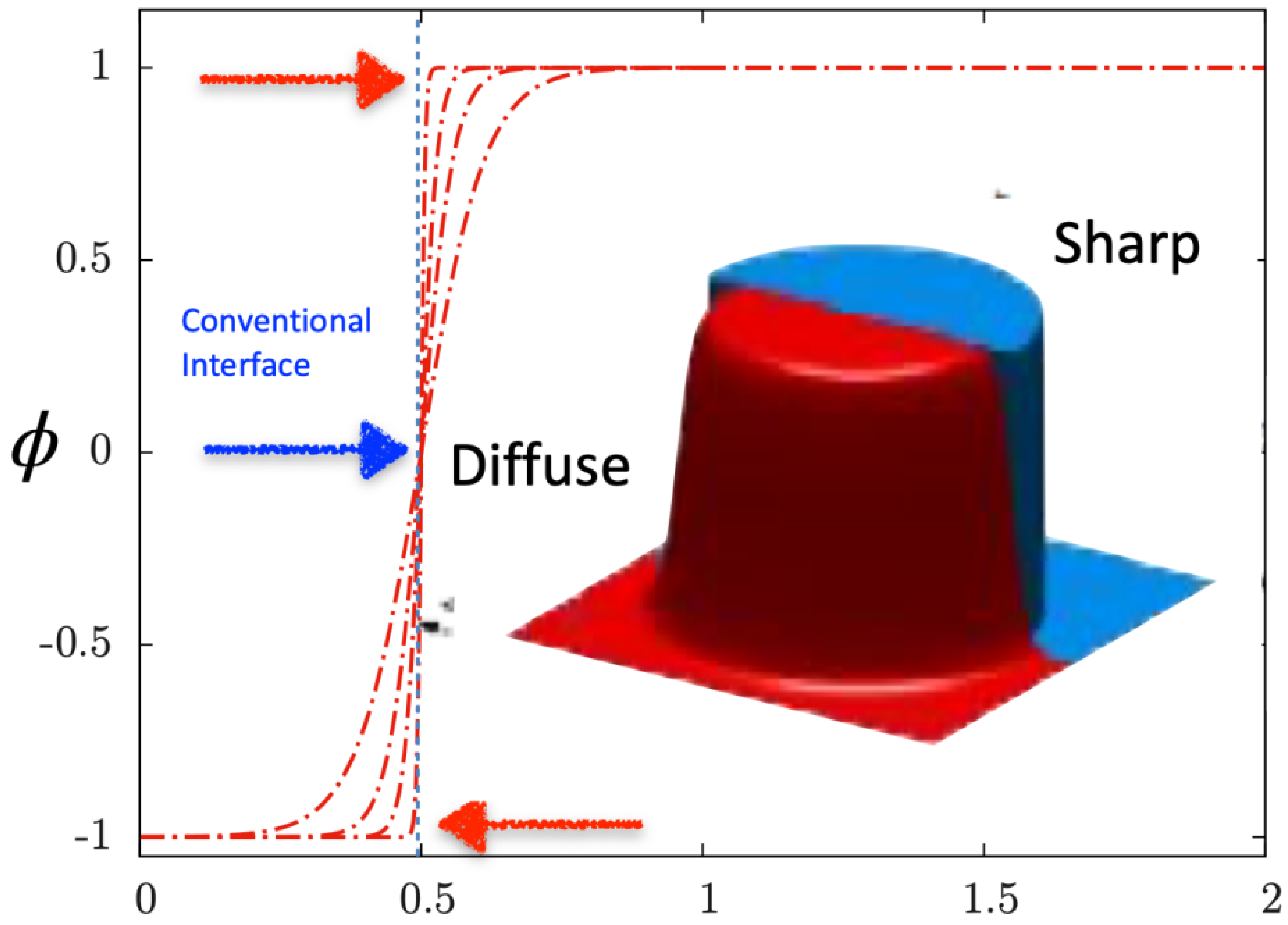
$$Ch = \frac{\epsilon}{h} \qquad Pe_\phi = \frac{u_\tau h}{\mathcal{M}\beta}$$

$Ch = \mathcal{O}(10^{-9})$ *Cahn number*

$Pe = \mathcal{O}(10^{9})$ *Peclet number*

To reduce the computational effort, the interface must be fictitiously enlarged to the point that it becomes computationally tractable (3-5 grid poir

Phase indicator ϕ



At equilibrium:

$$\phi = \tanh\left(\frac{x}{\sqrt{2}Ch}\right)$$

Jacqmin, Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modeling, JCP (1999)
Cahn and Hilliard ,Free energy of a non-uniform system I, Interfacial free energy, JCP (1958)
Roccon et al. "Phase-field modeling of complex interface dynamics in drop-laden turbulence, PRF (2023).

Numerical method, parallelisation + GPU-acceleration and initial conditions

Numerical method:

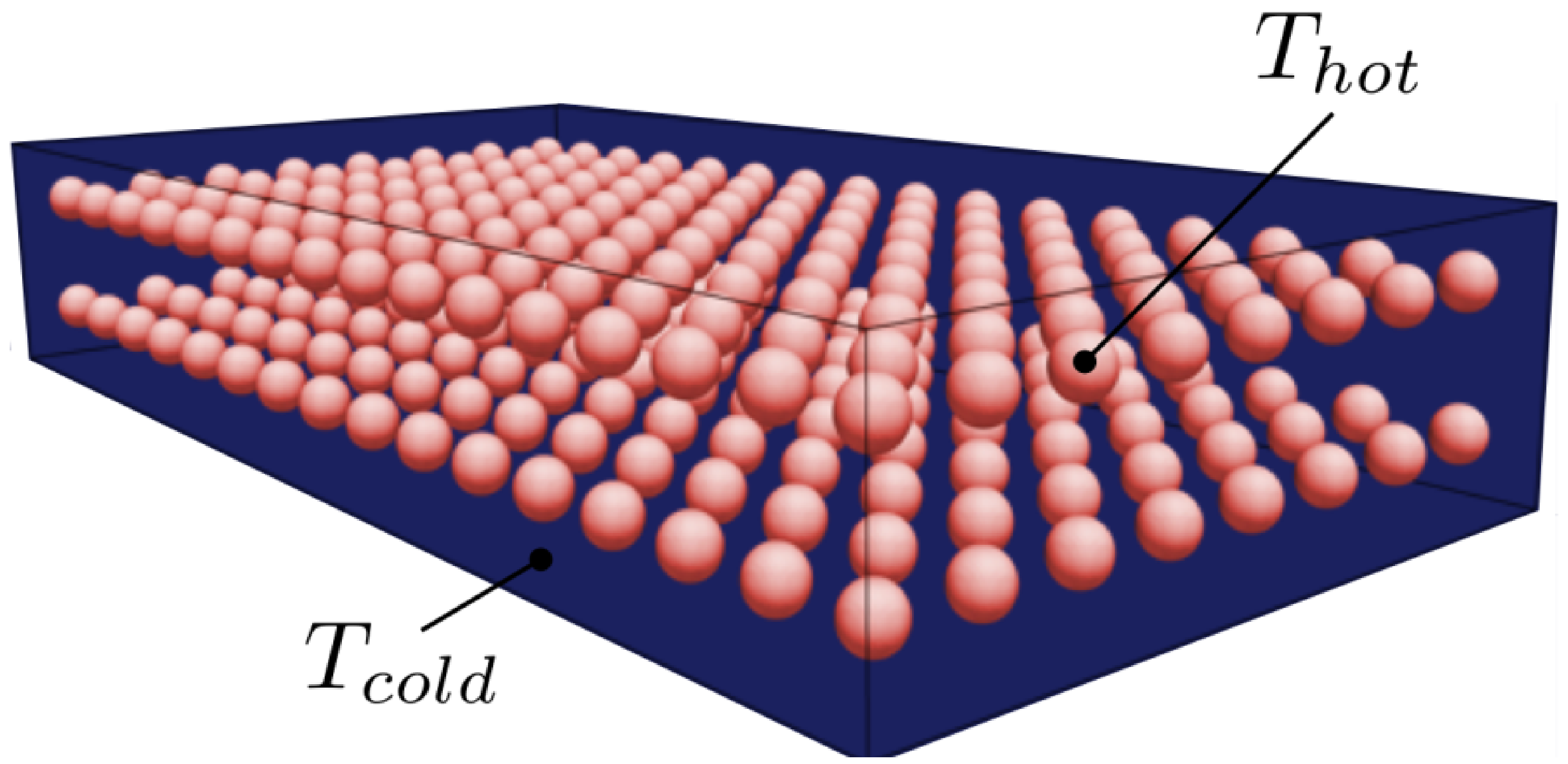
- Wall-normal velocity formulation for the Navier-Stokes equations.
- Pseudo-spectral method (Fourier for the homogenous directions and Chebychev for the wall-normal direction)
- For Cahn-Hilliard equation, splitting technique (recasted in two 2nd order equations)

Parallelization strategy:

- First layer of parallalization that relies on MPI (2D domain decomposition), in -house library for pencil rotations. Used for CPU-based machines (Discoverer, LUMI-C, etc.) + FFTW.
- Second layer of parallelisation that relies on openACC directives and CUDA Fortran instructions for GPU-based machines (Leonardo) + cuFFT.

Initial conditions:

- Flow Field:
  Fully developed turbulent channel flow (Shear Reynolds Re= 300)
- Phase Field and temperature:
  256 spherical hot drops in a cold channel (adiabatic)



Simulation parameters:

We=3.0

Four different Prandtl numbers:

- Pr=1, 2, 4, 8 (obtained reducing therm. diff.)

Multi resolution strategy to resolve the Batchelor scale.

$Pr \rightarrow$

$$\eta_B = \frac{\eta_k}{\sqrt{Pr}}$$

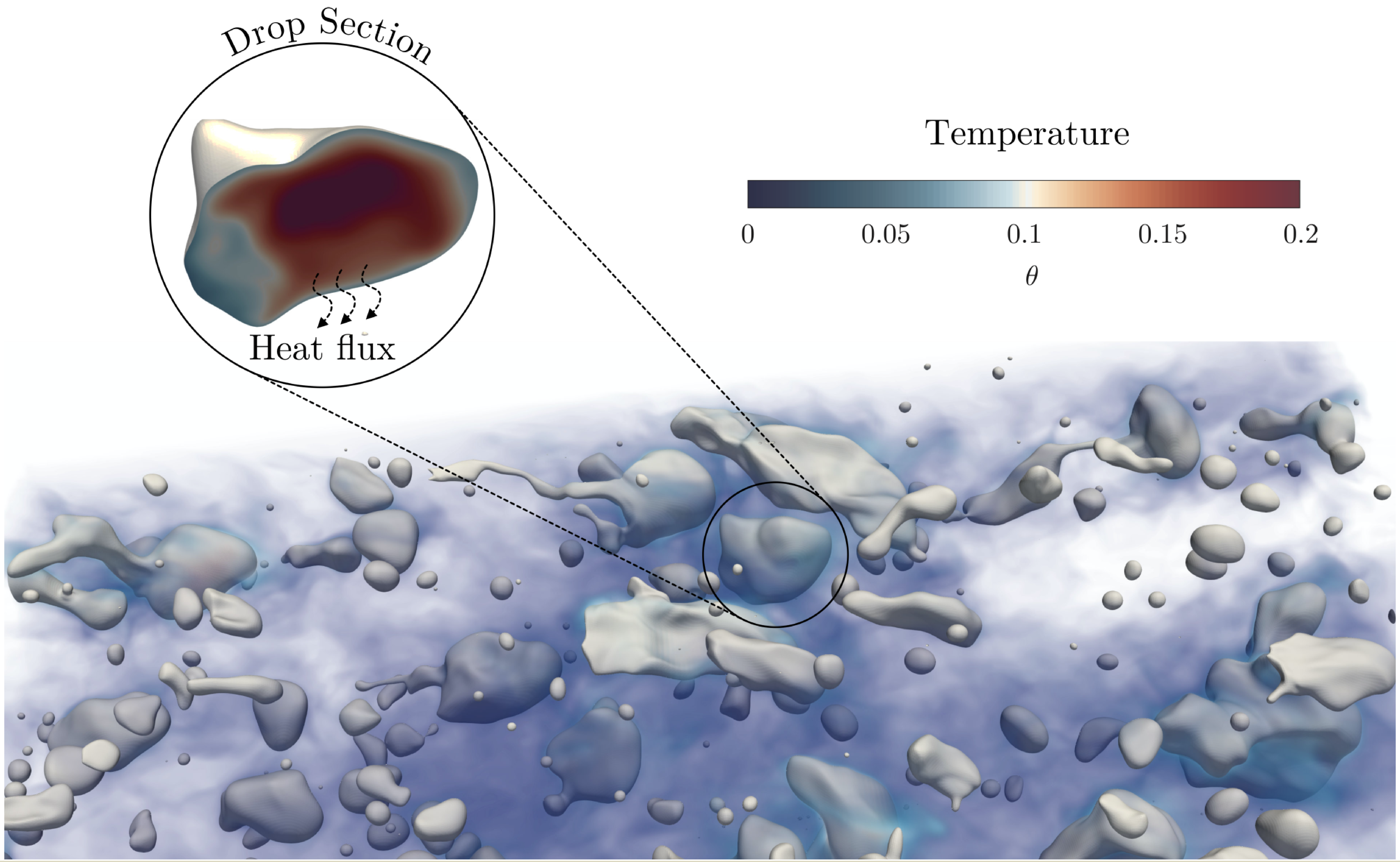
Batchelor scale

Pr	η_B	
1	η_k	grid 1
2	$0.71\eta_k$	grid 1
4	$0.50\eta_k$	grid 2
8	$0.35\eta_k$	grid 2

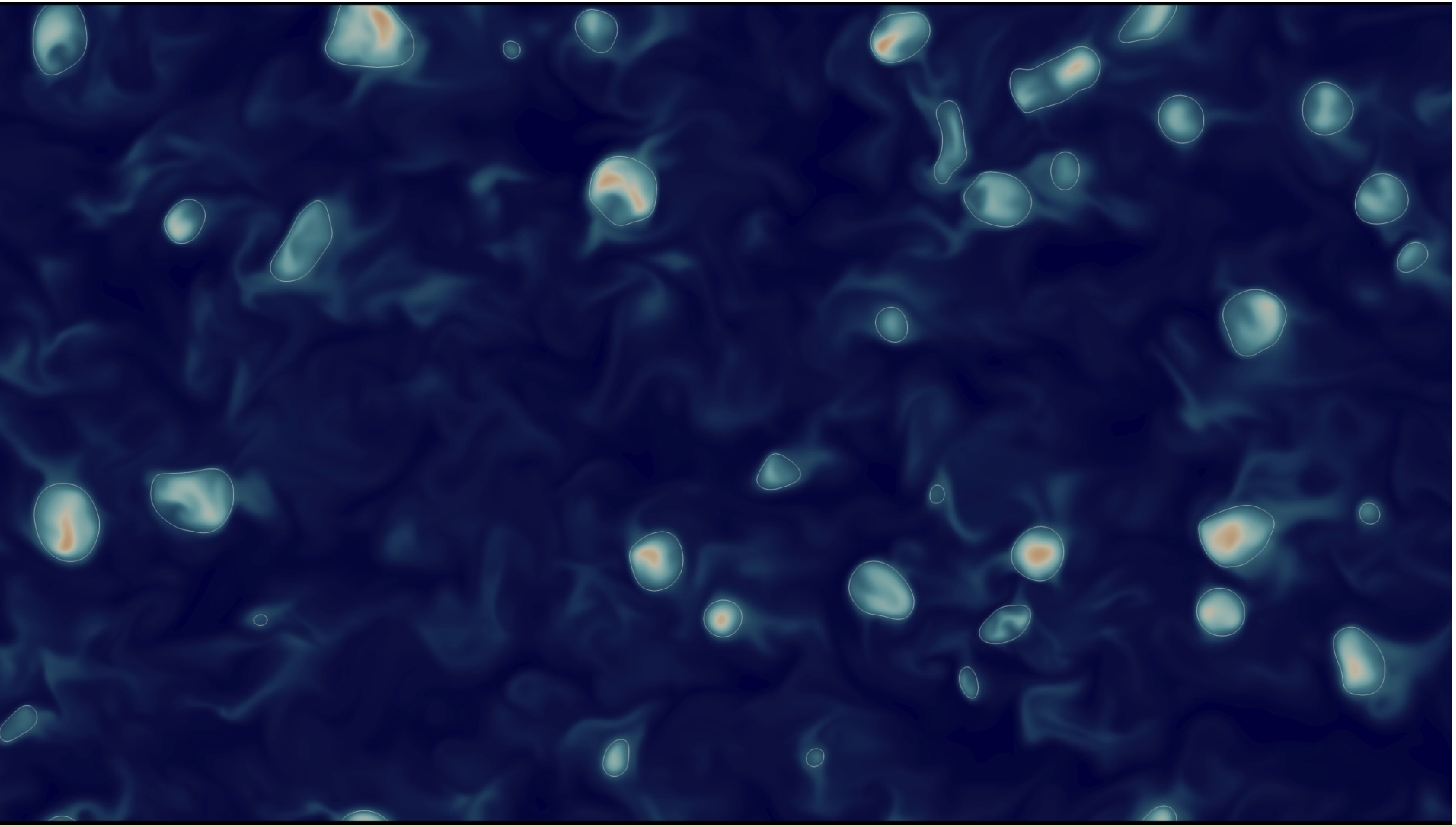
Grid 1: 1024 x 512 x 513
Grid 2: 2048 x 1204 x 513

Mangani et al., "Heat-transfer in drop-laden turbulence", JFM (2023)

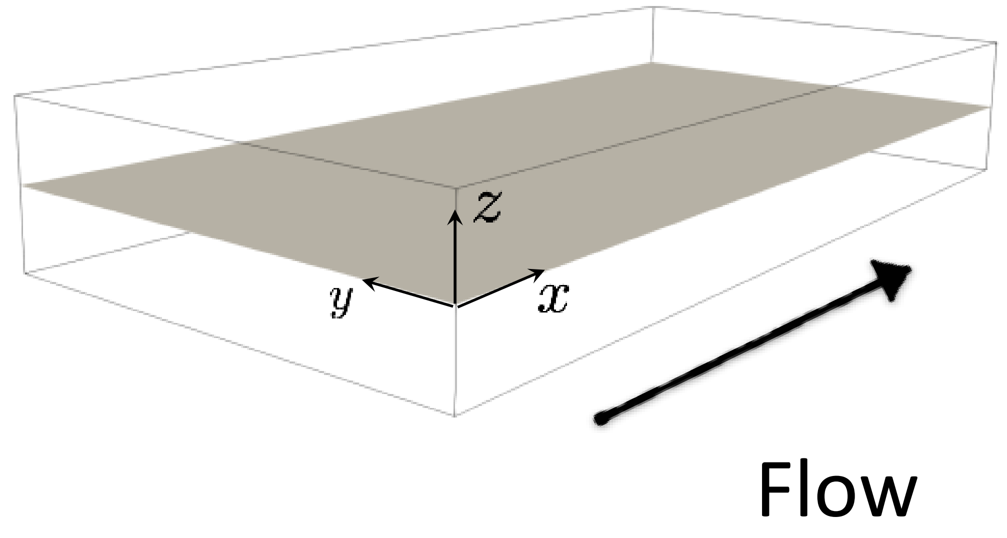
EUROHPC USER DAY 2023 Brussels 11.12.23



Roccon et al., "Phase-field modeling of complex interface dynamics in drop-laden turbulence, PRF (2023).
Mangani et al., "Heat-transfer in drop-laden turbulence", JFM (2023).



Channel mid plane

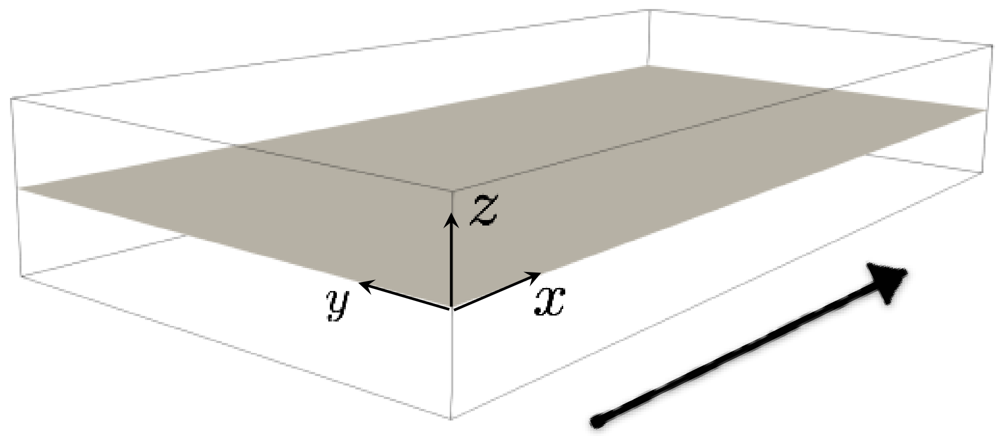


Roccon et al., "Phase-field modeling of complex interface dynamics in drop-laden turbulence, PRF (2023).
Mangani et al., "Heat-transfer in drop-laden turbulence", JFM (2023)

$$Pr = \frac{\nu}{a} = \frac{\text{Momentum diffusivity}}{\text{Thermal diffusivity}}$$

Qualitative view
Time evolution (Pr=8)

Channel mid plane



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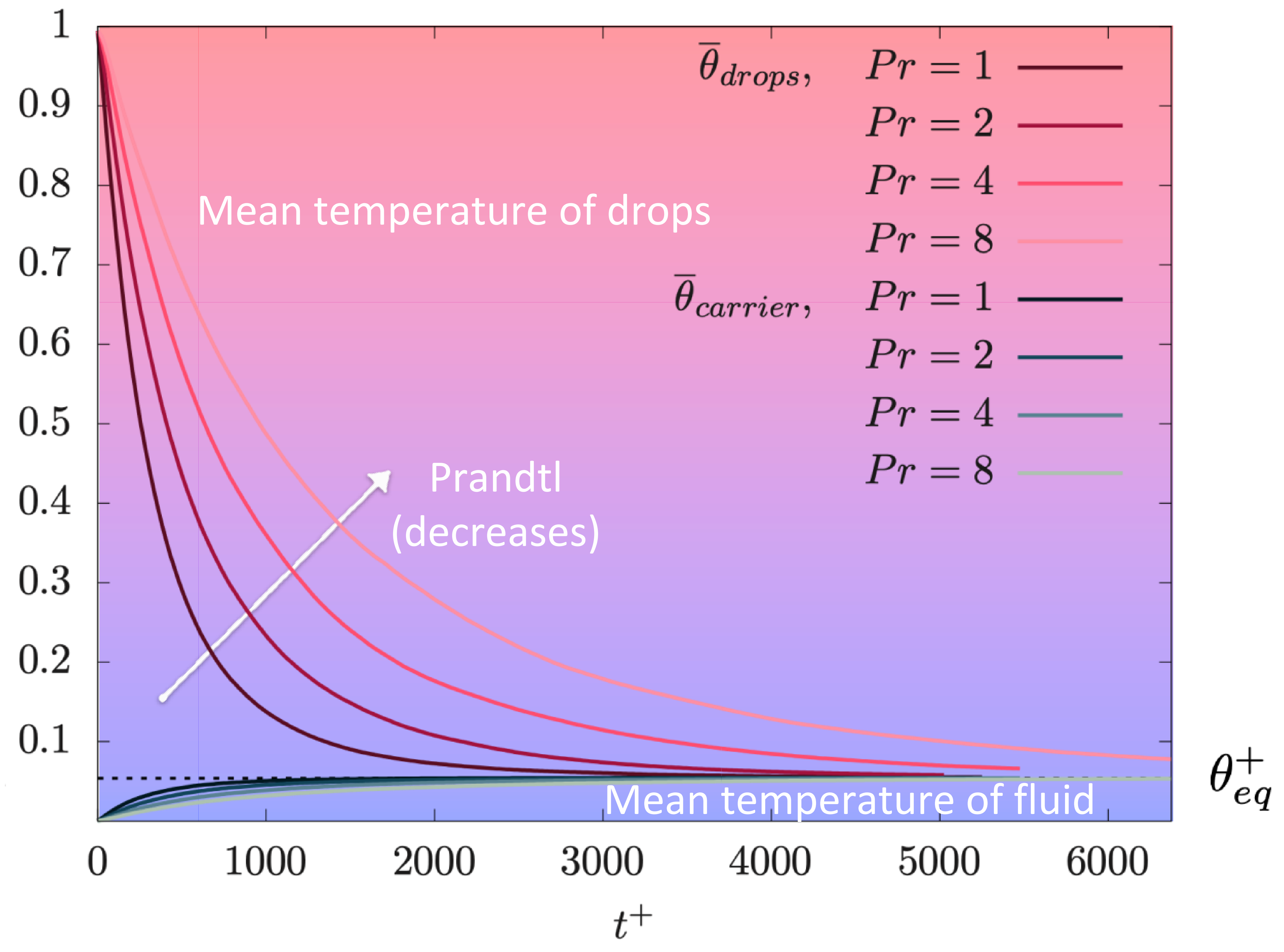
$$Pr = \frac{\nu}{a} = \frac{\text{Momentum diffusivity}}{\text{Thermal diffusivity}}$$

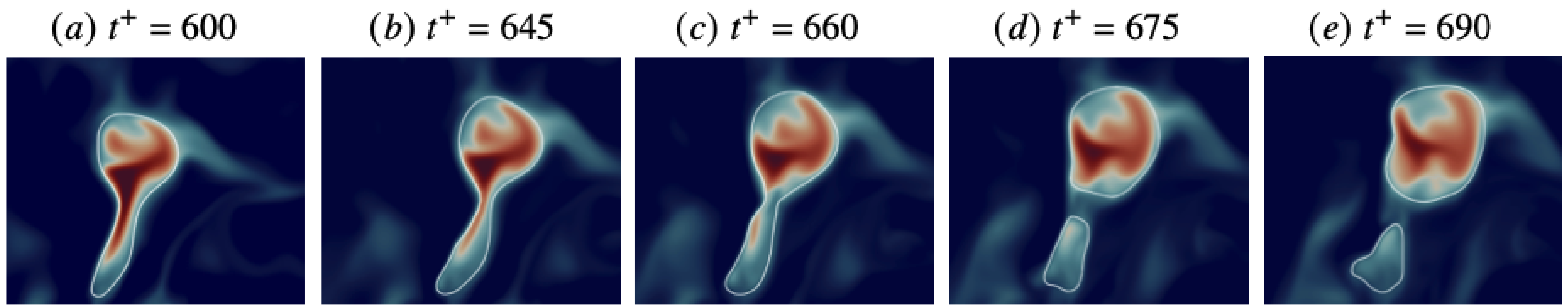


Steady average temperature of the mixture

$$\theta^+_{eq} = \theta^+_{c,0}(1 - \Phi) + \theta^+_{d,0}\Phi$$

Volume fraction: $\Phi = 5.4\%$

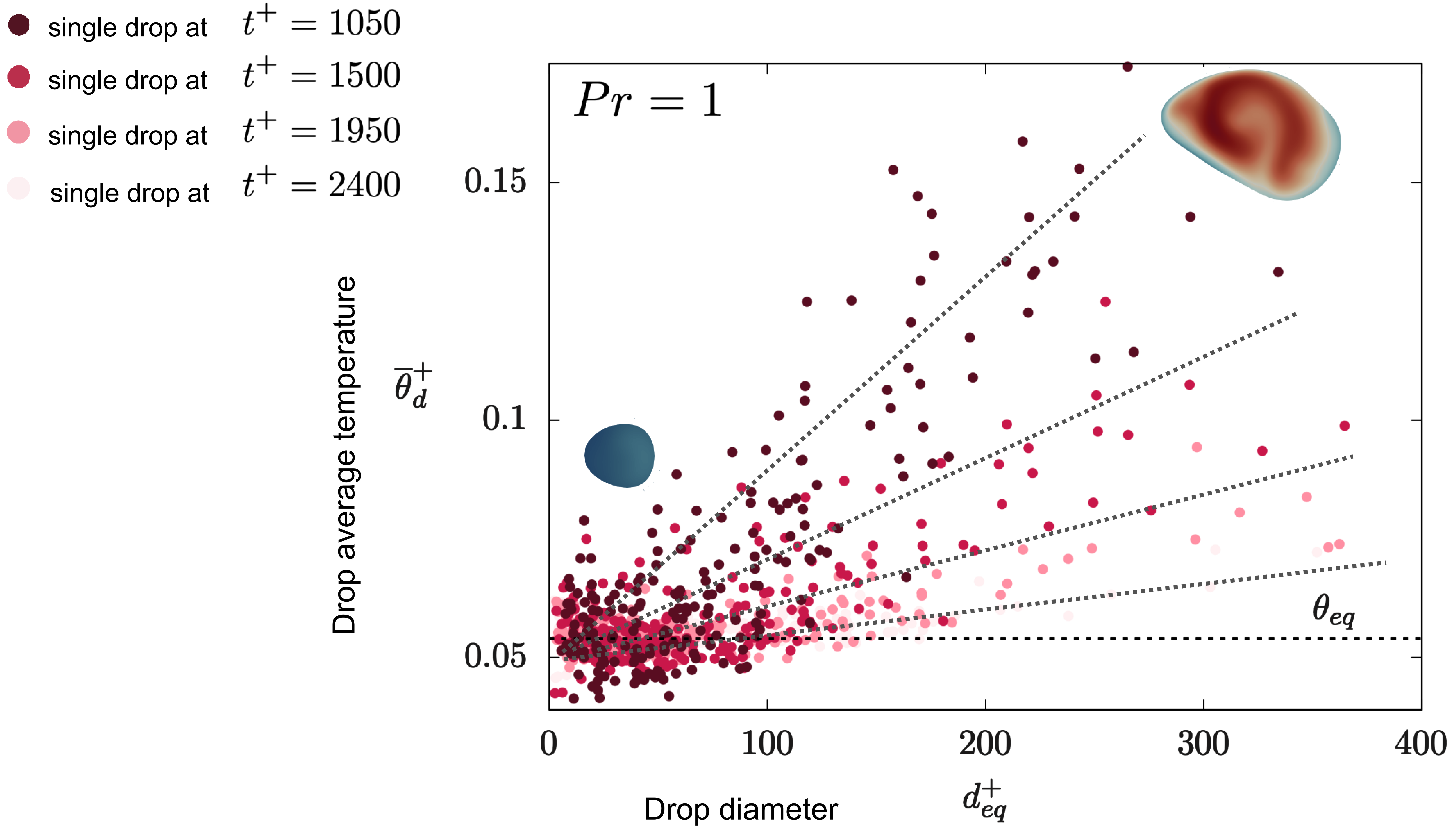
Drops can coalescence and break, and thus can have different sizes..
What is the effect of drop size on temperature evolution?



Small drops tend to cool down faster (small heat capacity).

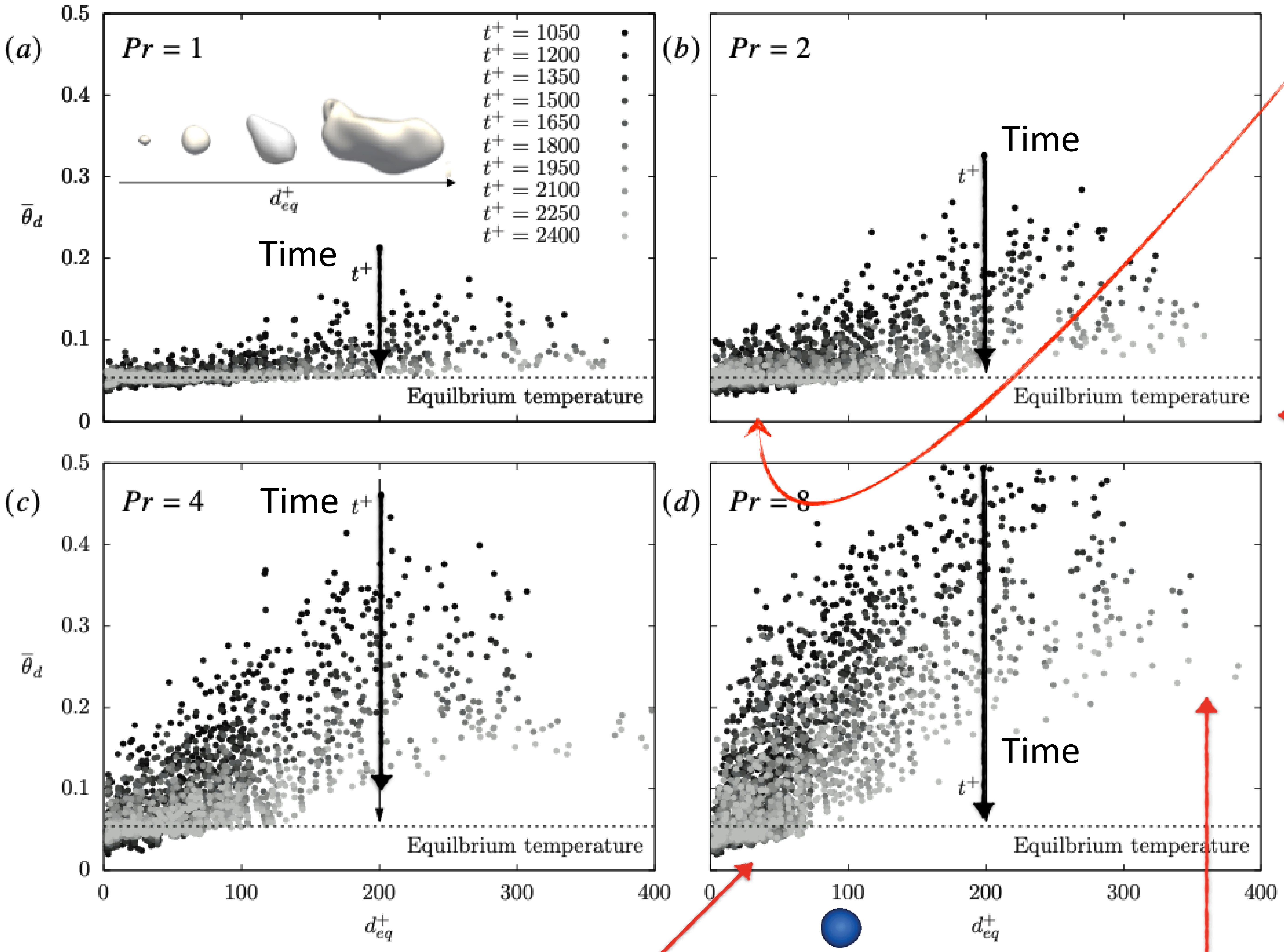
$$Pr = \frac{\nu}{a} = \frac{\text{Momentum diffusivity}}{\text{Thermal diffusivity}}$$

Mean temperature and drop size (I)



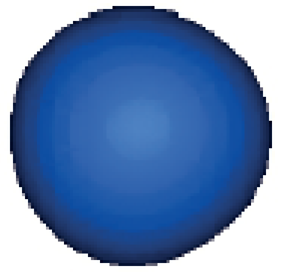
Mangani et al., “Heat-transfer in drop-laden turbulence”, JFM (2023)

Time evolution of average drop temperature for different drop sizes.



Small drops temperature?

Initial temperature of the carrier flow

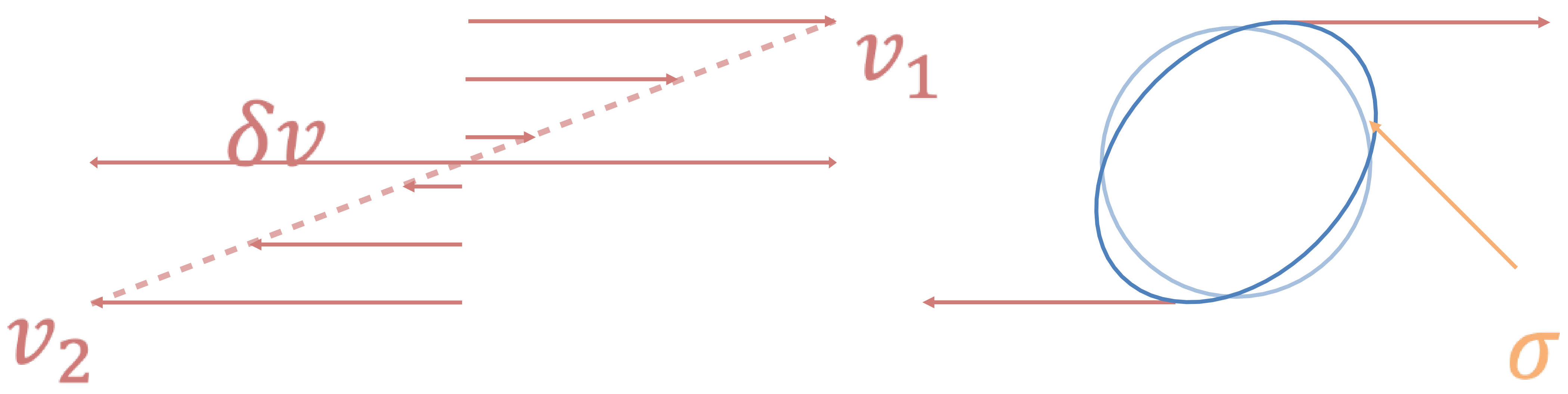


$$Pr = \frac{\nu}{a} = \frac{\text{Momentum diffusivity}}{\text{Thermal diffusivity}}$$

Small drops: low heat capacity; cool down is faster

Large drops: large heat capacity cool down is slower.

Bubbles/Drops break if stresses win over restoring surface tension



Kolmogorov-Hinze Critical radius

$$r_H \propto \left(\frac{\rho}{\sigma}\right) \varepsilon^{-2/5} \propto We^{-3/5} \varepsilon^{-2/5}$$

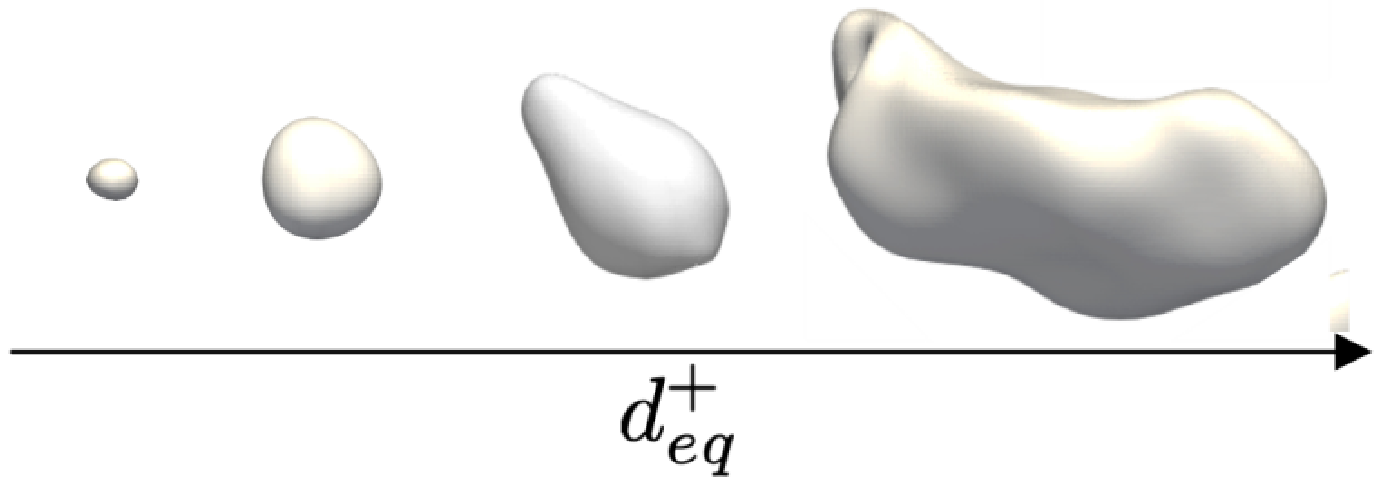
$$We = \rho u_\tau^2 h/\sigma_0$$

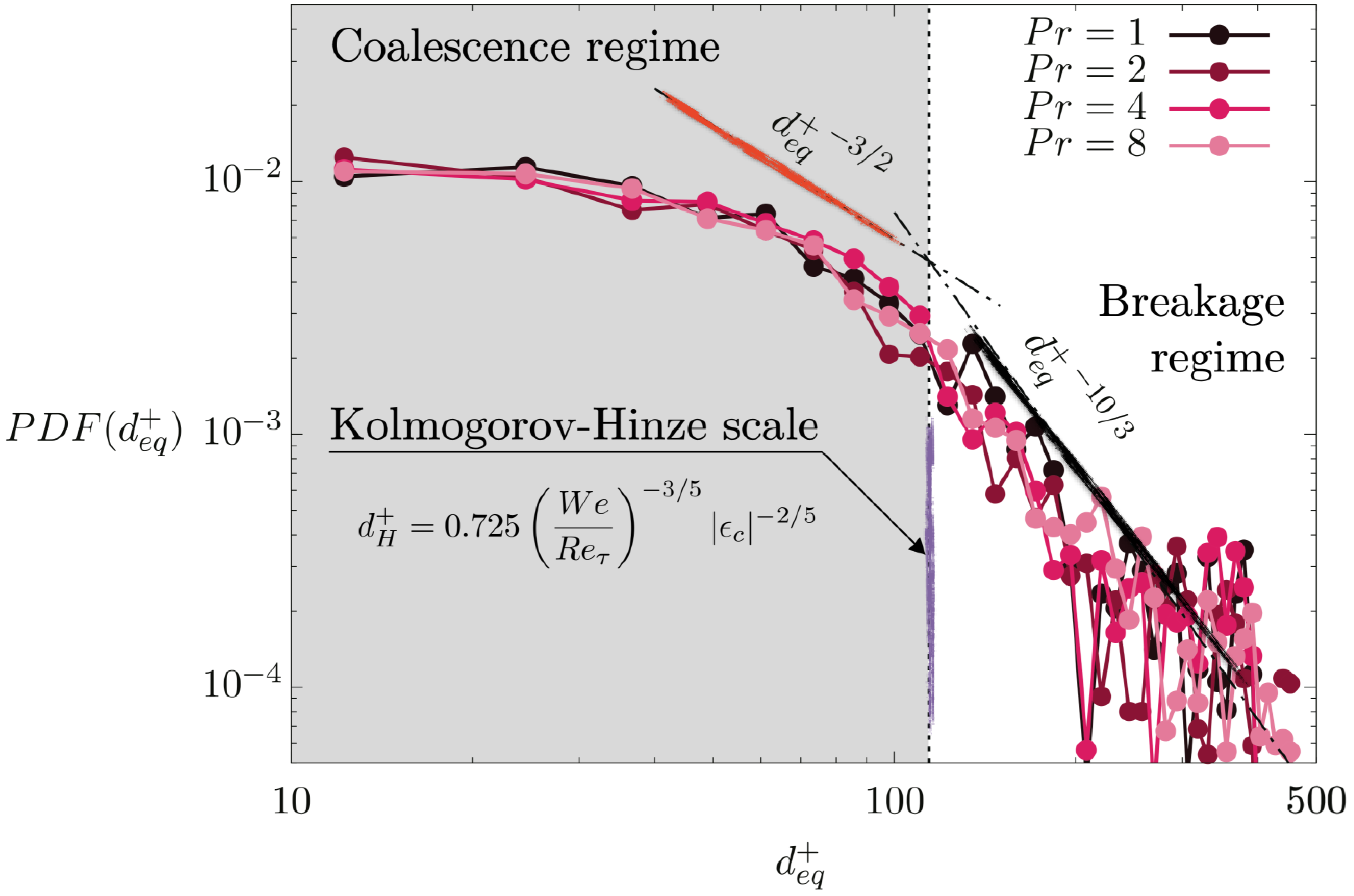
Small drops/bubbles

$$N(r) \propto Q \left(\frac{\sigma}{\rho}\right)^{-3/2} u^2 r^{-3/2}$$

Large drops/bubbles

$$N(r) \propto Q \varepsilon^{-1/3} r^{-10/3}$$





Roccon et al., "Phase-field modeling of complex interface dynamics in drop-laden turbulence, PRF (2023).
Mangani et al., "Heat-transfer in drop-laden turbulence", JFM (2023)

The steady-state size distribution well matches with the analytical scaling laws proposed in literature.

Results
Simple model for mean temperature evolution (I)

Thermal balance for an isolated drop:

$$m_d^* c_p^* \frac{\partial \theta_d^*}{\partial t^*} = \mathcal{H}^* A_d^* \left(\theta_c^* - \theta_d^*\right)$$

$$\frac{\partial \theta_d^*}{\partial t^*} = \frac{6\nu^* \rho_c^*}{\rho_d^* d^* \delta_t^* Pr} \left(\theta_c^* - \theta_d^*\right)$$

Temperature evolution for a single droplet:

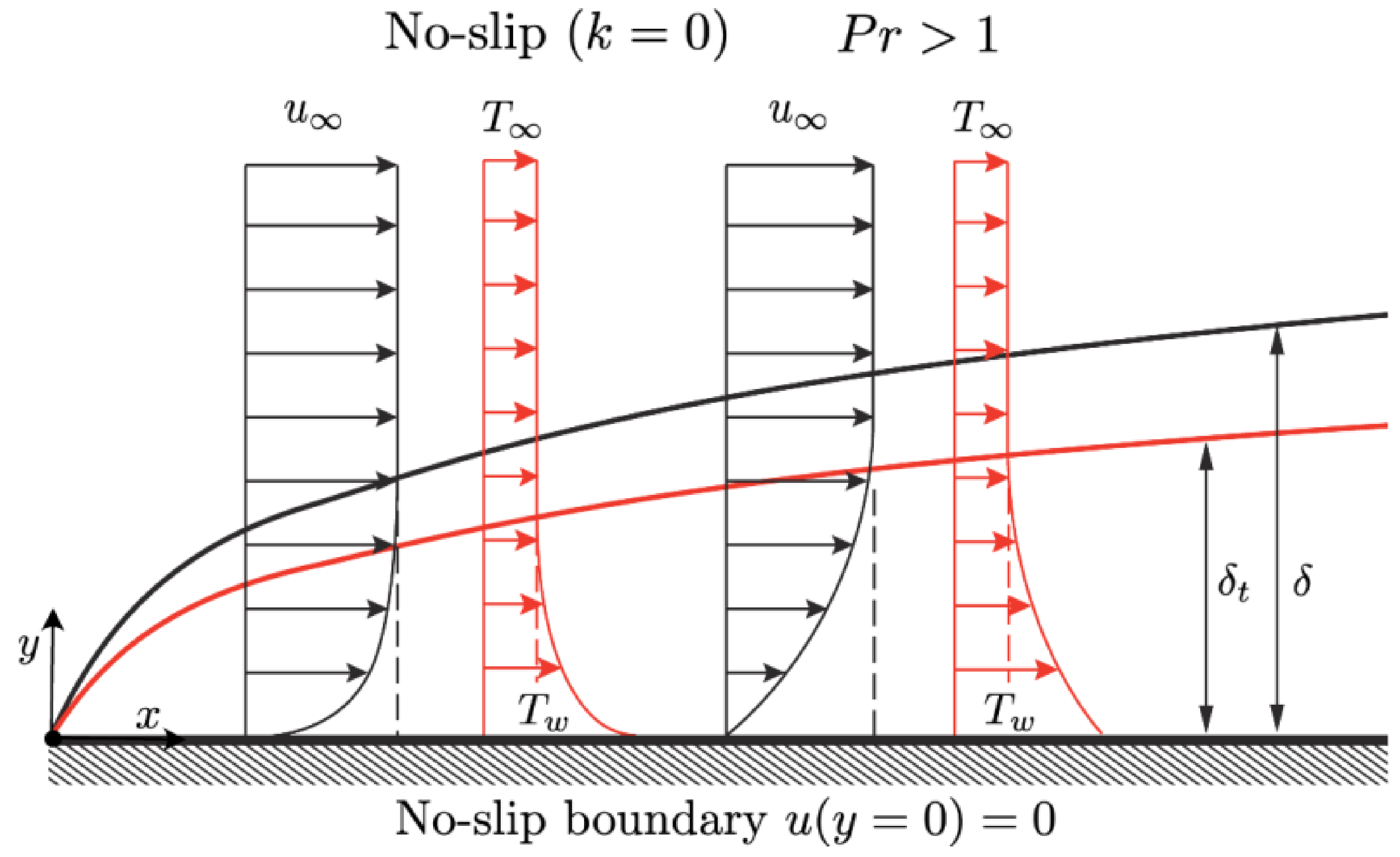
$$\frac{\partial \theta_d^+}{\partial t^+} = \mathcal{C} Pr^{-2/3} \left(D_d^+\right)^{-1} \left(\theta_f^+ - \theta_d^+\right)$$

We can now integrate this temperature evolution equation over different class of diameters (DSD) so as to obtain the evolution of the mean temperature of the drops and of the carrier flow.

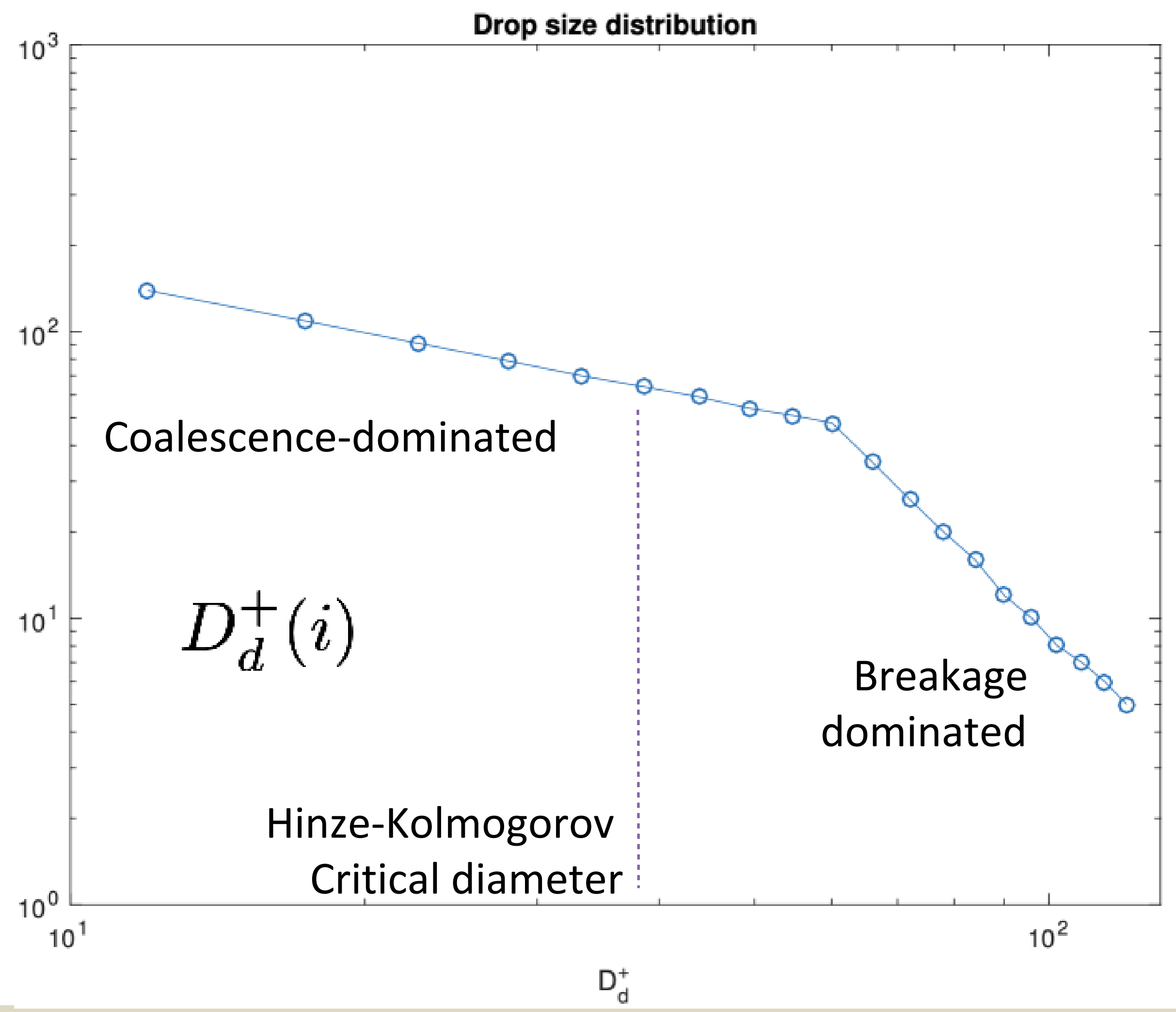
Boundary layer theory (heat transfer coefficient):

$$\mathcal{H}^* \sim \lambda^* / \delta_t^*$$

$$\delta_t = \delta Pr^{-1/3}$$



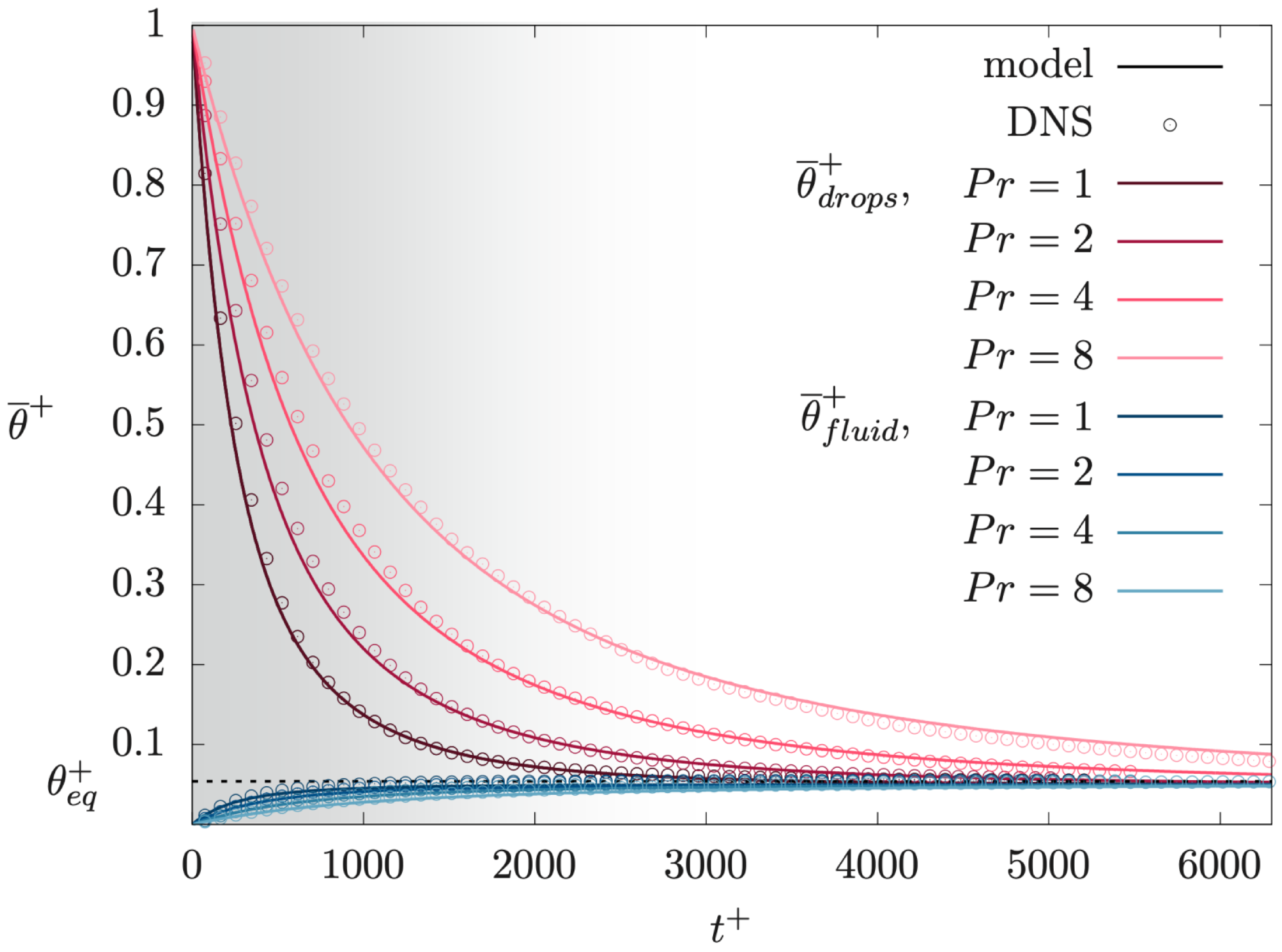
Drop size distribution:



$$Pr = \frac{\nu}{a} = \frac{\text{Momentum diffusivity}}{\text{Thermal diffusivity}}$$

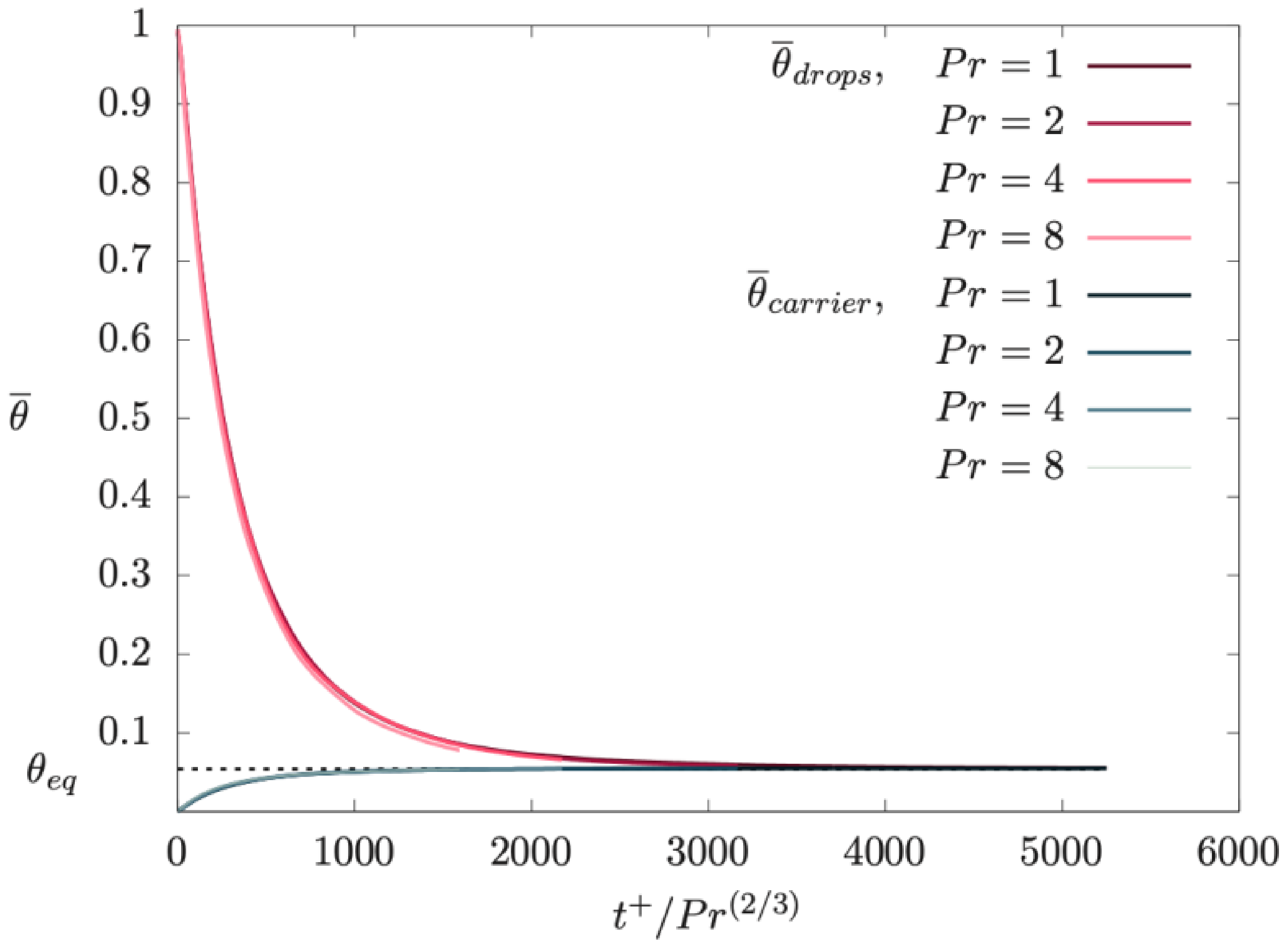
Schlichting, Boundary Layer Theory, 7th ed., McGraw Hill (1979).

Simple model for mean temperature evolution (II)



Excellent agreement between the numerical results and the phenomenological model…!!

We can also rescale everything using the Pr^2/3 exponent and collapse all the curves:



Roccon et al., "Phase-field modeling of complex interface dynamics in drop-laden turbulence, PRF (2023).
Mangani et al., "Heat-transfer in drop-laden turbulence", JFM (2023)

Conclusions & Future developments

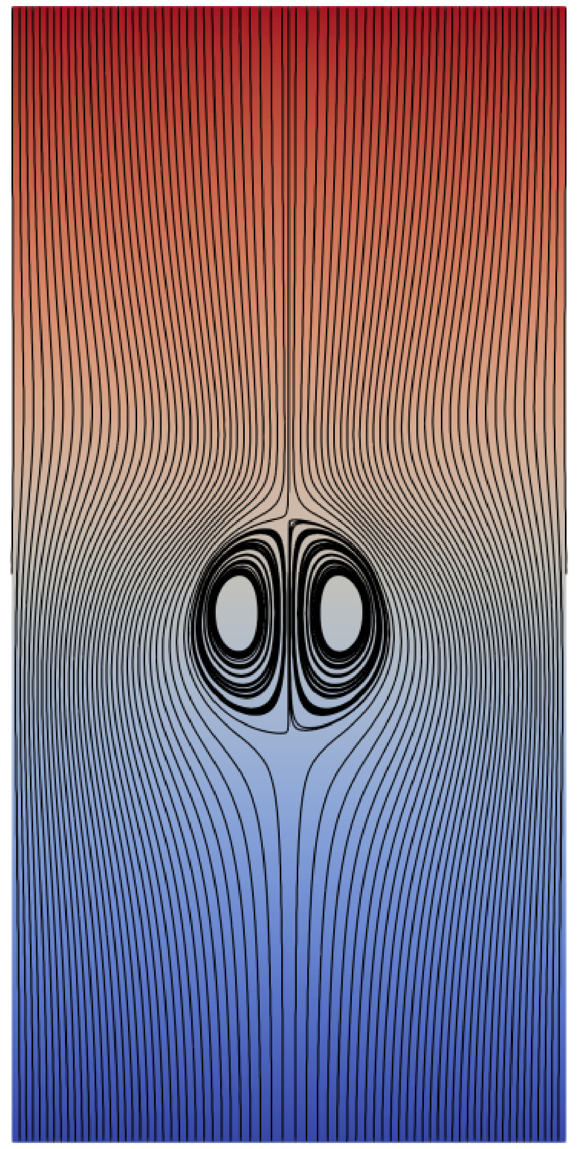
Conclusions:

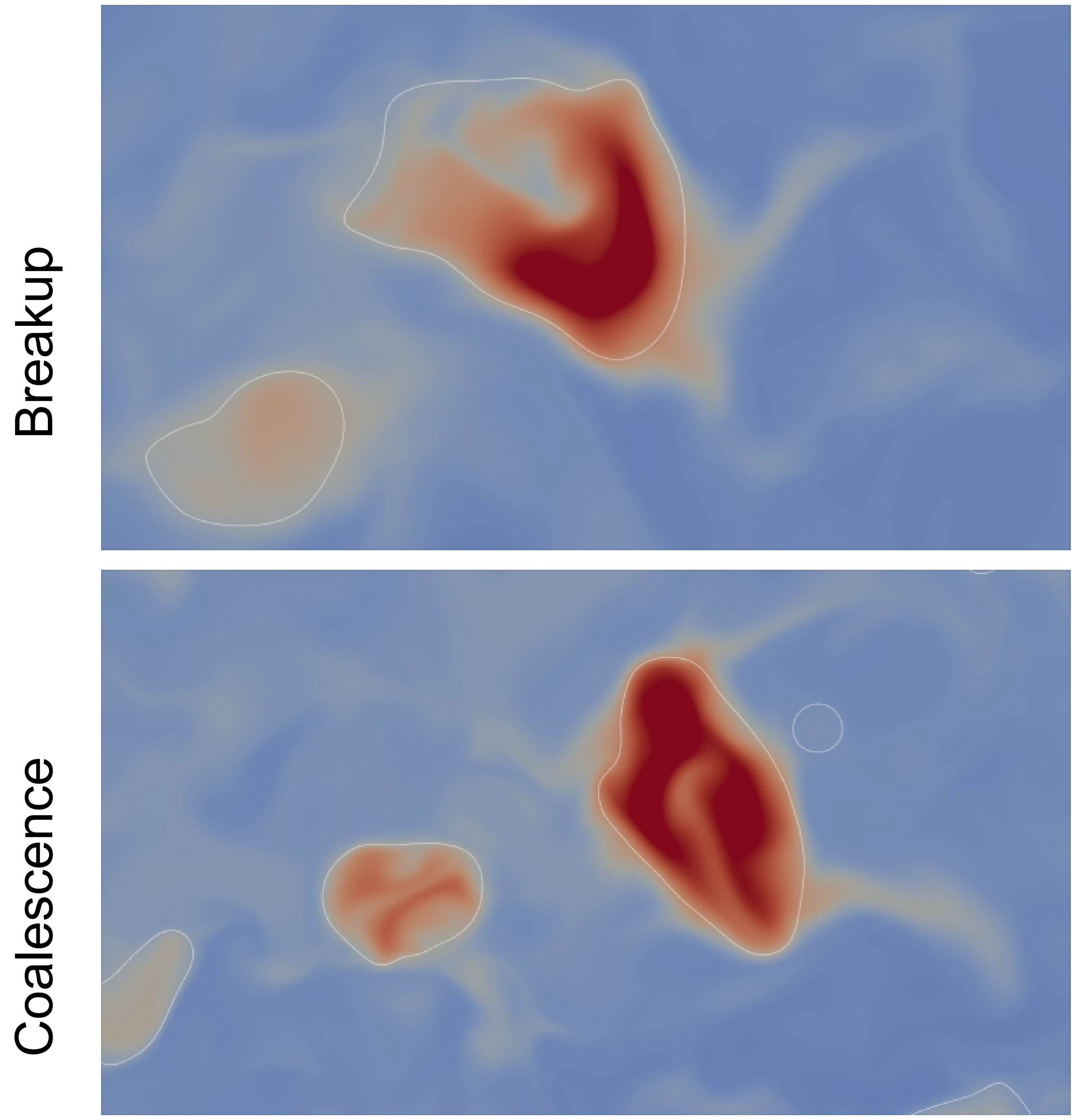
- The heat transfer from the drops to the carrier fluid shows an expected dependency on ***Prandtl:*** the higher is the Pr, the slower is the diffusion and thus the heat transfer between the phases
- We developed an analytical model which can well predict the average temperature of the two phases
- We found a scaling for the time (diffusive time)
- We found a correlation between the diameter and the average temperature

Future developments:

- Extend the simulations to mass/species transfer.
- Thermocapillary Marangoni effects
- Phase Change/Boiling (MIT Collaboration)

Thermocapillarity





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