

New avenues in computational fluid dynamics

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@FerrerCfd



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UPM Collaborators:

E Valero, G Rubio, S Le Clainche, L Gonzalez, J Garicano...

Ext. Collaborators:

DA Kopriva (San Diego), C Hirsch (Numeca), Paniagua (Purdue), P. García (Zaragoza)  
R Vinuesa (KTH), S Sherwin (IC), R Willden (Oxford), H Blackburn (Monash)

Industrial collaborators:

Numeca-Cadence, Airbus, McLaren F1, Dassault Syst., Siemens-Gamesa...

## Students / Postdocs



L Botaro



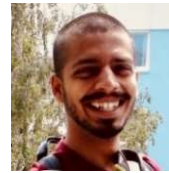
E Jané



G Ntoukas



O Marino



S Joshi,



J Kou



A Hurtado-Mendoza



W Laskowski



K Otmani



F Manrique de Lara



A Ballout



M de Frutos



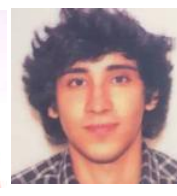
S Colombo



D Huergo



A Portillo



J Manzanero



A Rueda



M Chavez



Y Wang



M Kompenhan



O Browne

## Funding



Financiado por la Unión Europea  
NextGenerationEU



We acknowledge the funding received by the Grant DeepCFD (Project No. PID2022-137899OB-I00) funded by MICIU/AEI/10.13039/501100011033 and by ERDF, EU.

We thank the support of Agencia Estatal de Investigación for the grant "Europa Excelencia" for the project EUR2022-134041 funded by MCIN/AEI/10.13039/501100011033) y the European Union NextGenerationEU/PRTR

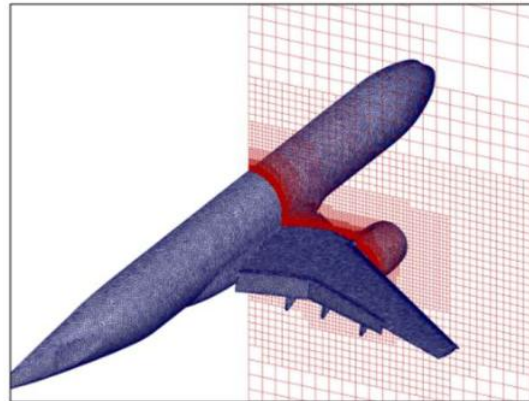


This research has been cofunded by the European Union (ERC, Off-coustics, project number 101086075). Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them

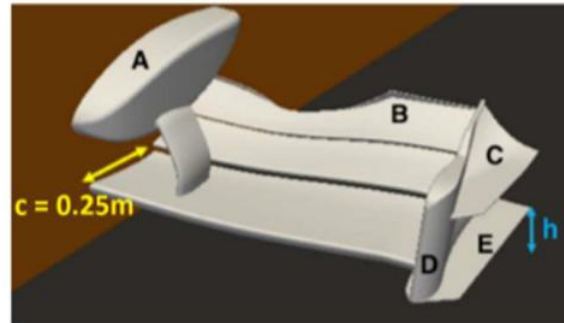
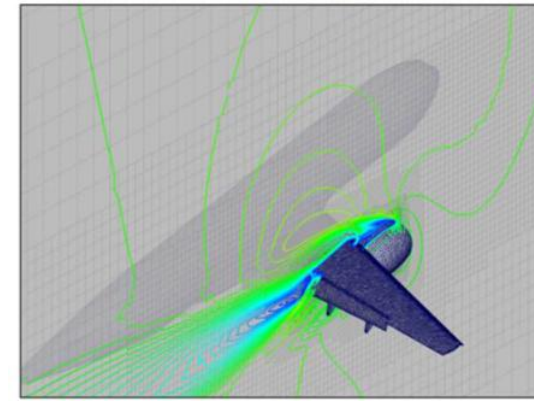
# Collaborations with Industry



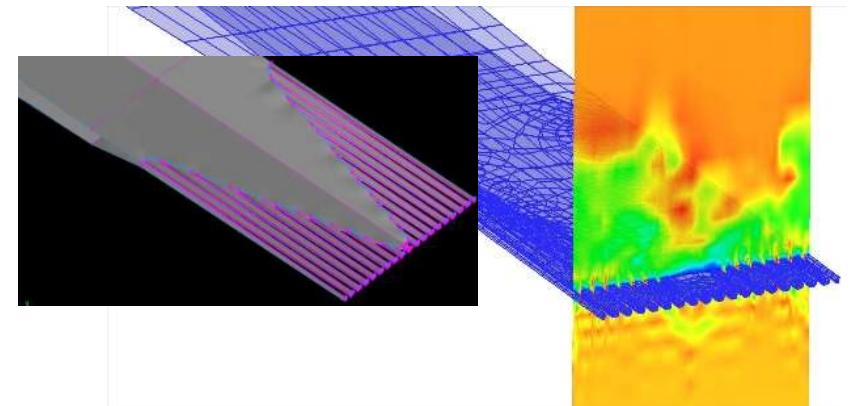
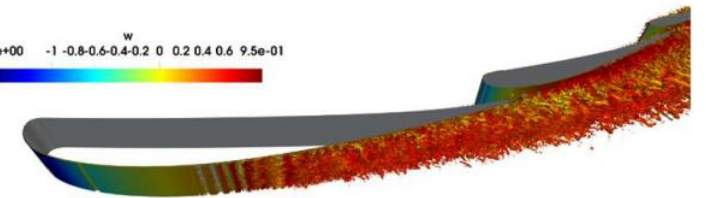
CRM Aircraft Mesh



CRM,  $\alpha = 8^\circ$ , VelocityMagnitude, Wall Model Deactivated



w  
-1.5e+00 -1 -0.8-0.6-0.4-0.2 0 0.2 0.4 0.6 9.5e-01



# Summary

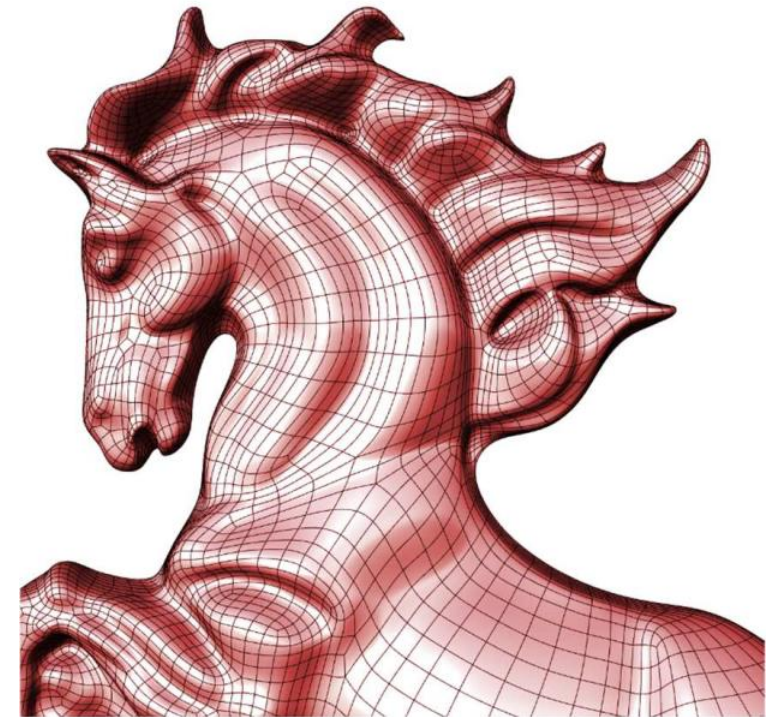
## 1- Introduction to DG & Horses3d

## 2- Multiphysics

- Wind turbines
- Turbulence

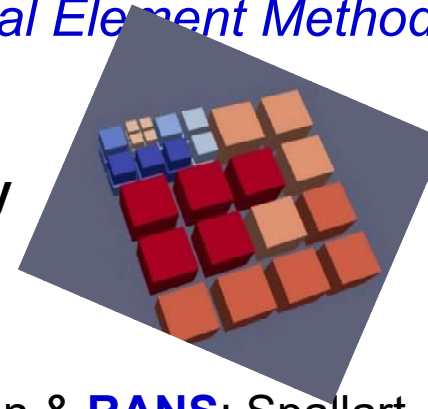
## 3. Machine Learning + CFD

- Mesh adaption
- NN acceleration
- RL for automation



## *DGSEM: nodal Discontinuous Galerkin Spectral Element Methods*

- **Compressible & Incompressible**
- **Entropy / Energy conserving schemes for stability**
- **Local p-adaption / h-adaption (hanging nodes)**
- **Explicit / implicit time stepping**
- **Turbulence models: LES:** SVV-Smag., Wale, Vreman & **RANS:** Spallart-Almaras
- **Multi-physics:** Multiphase, Immersed Boundaries, Shock etc..



**HORSES3D** <https://github.com/loganoz/horses3d>

Computer Physics Communications 287 (2023) 108700



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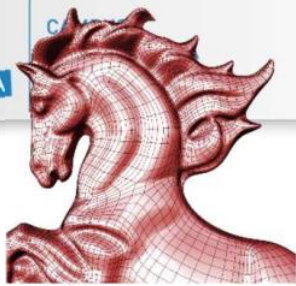
journal homepage: [www.elsevier.com/locate/cpc](http://www.elsevier.com/locate/cpc)



HORSES3D: A high-order discontinuous Galerkin solver for flow simulations and multi-physics applications ☆☆☆

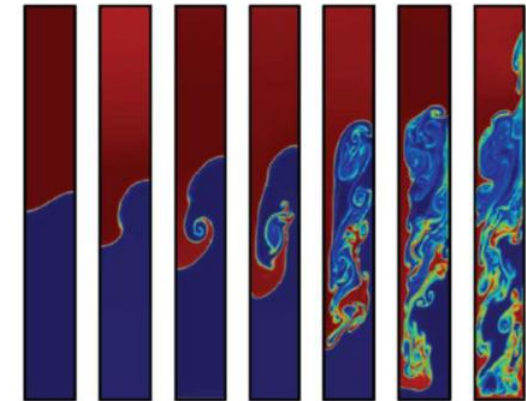
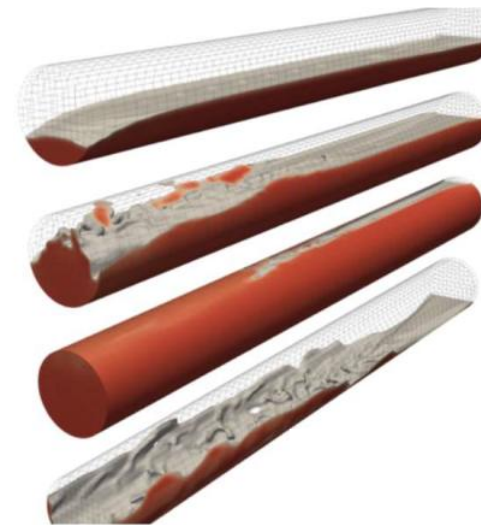
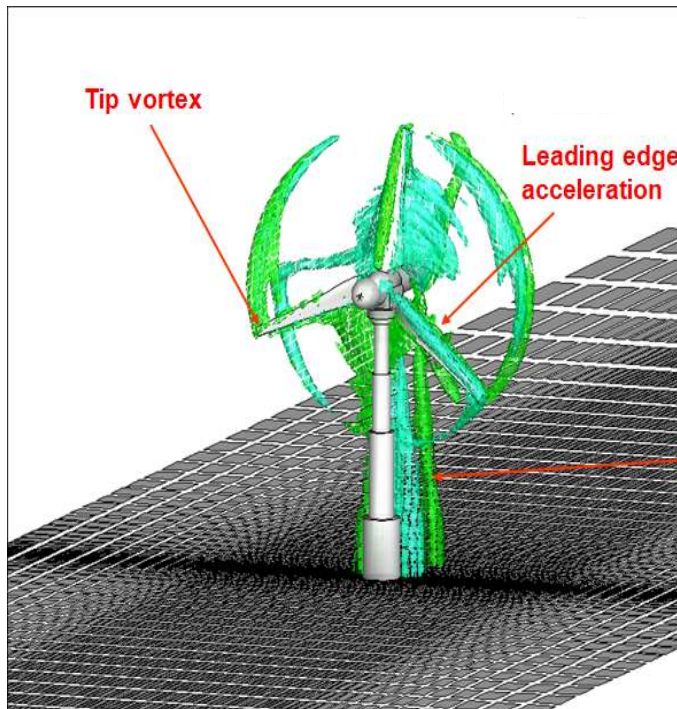


E. Ferrer<sup>a,b</sup>, G. Rubio<sup>a,b,\*</sup>, G. Ntoukas<sup>a</sup>, W. Laskowski<sup>a</sup>, O.A. Mariño<sup>a</sup>, S. Colombo<sup>a</sup>,  
A. Mateo-Gabín<sup>a</sup>, H. Marbona<sup>a</sup>, F. Manrique de Lara<sup>a</sup>, D. Huergo<sup>a</sup>, J. Manzanero<sup>e</sup>,  
A.M. Rueda-Ramírez<sup>c</sup>, D.A. Kopriva<sup>d</sup>, E. Valero<sup>a,b</sup>

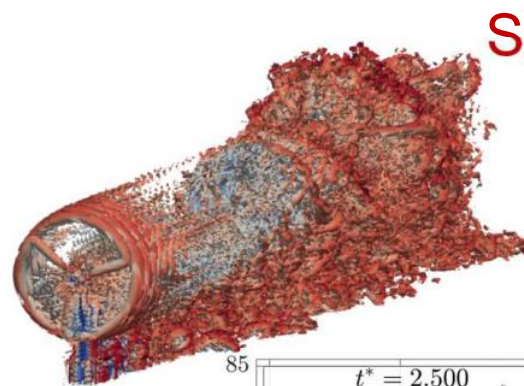


# HORSES3D

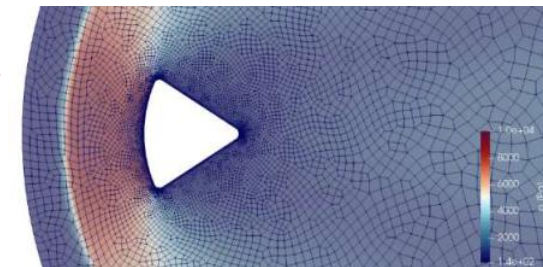
<http://github.com/loganoz/horses3d>



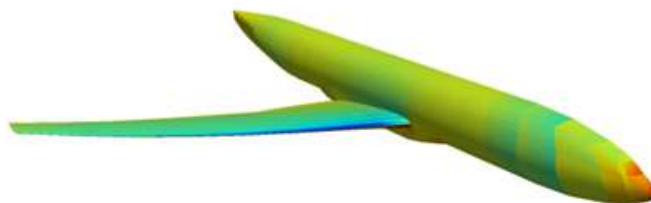
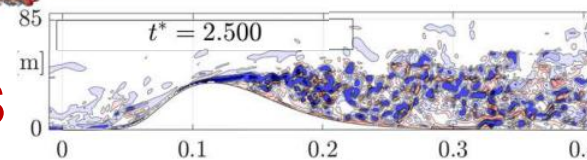
Multiphase



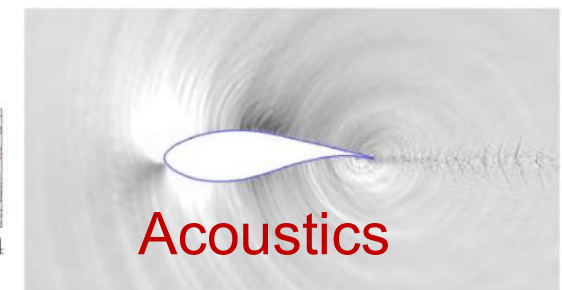
Shocks



LES



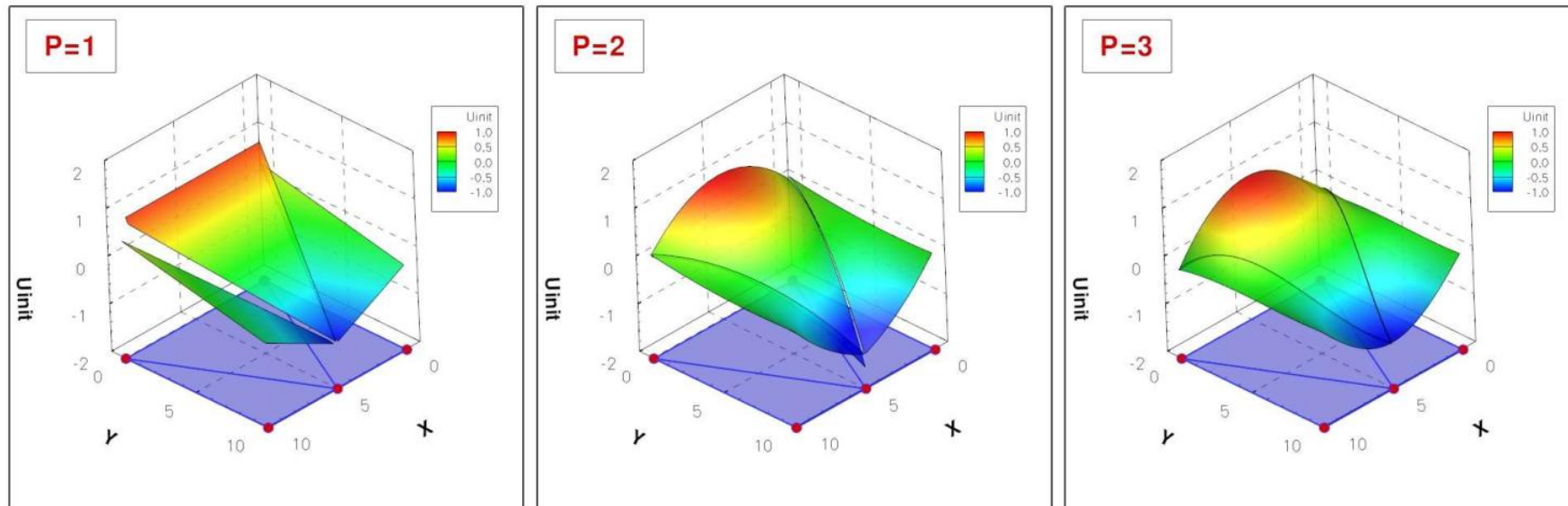
RANS



Acoustics

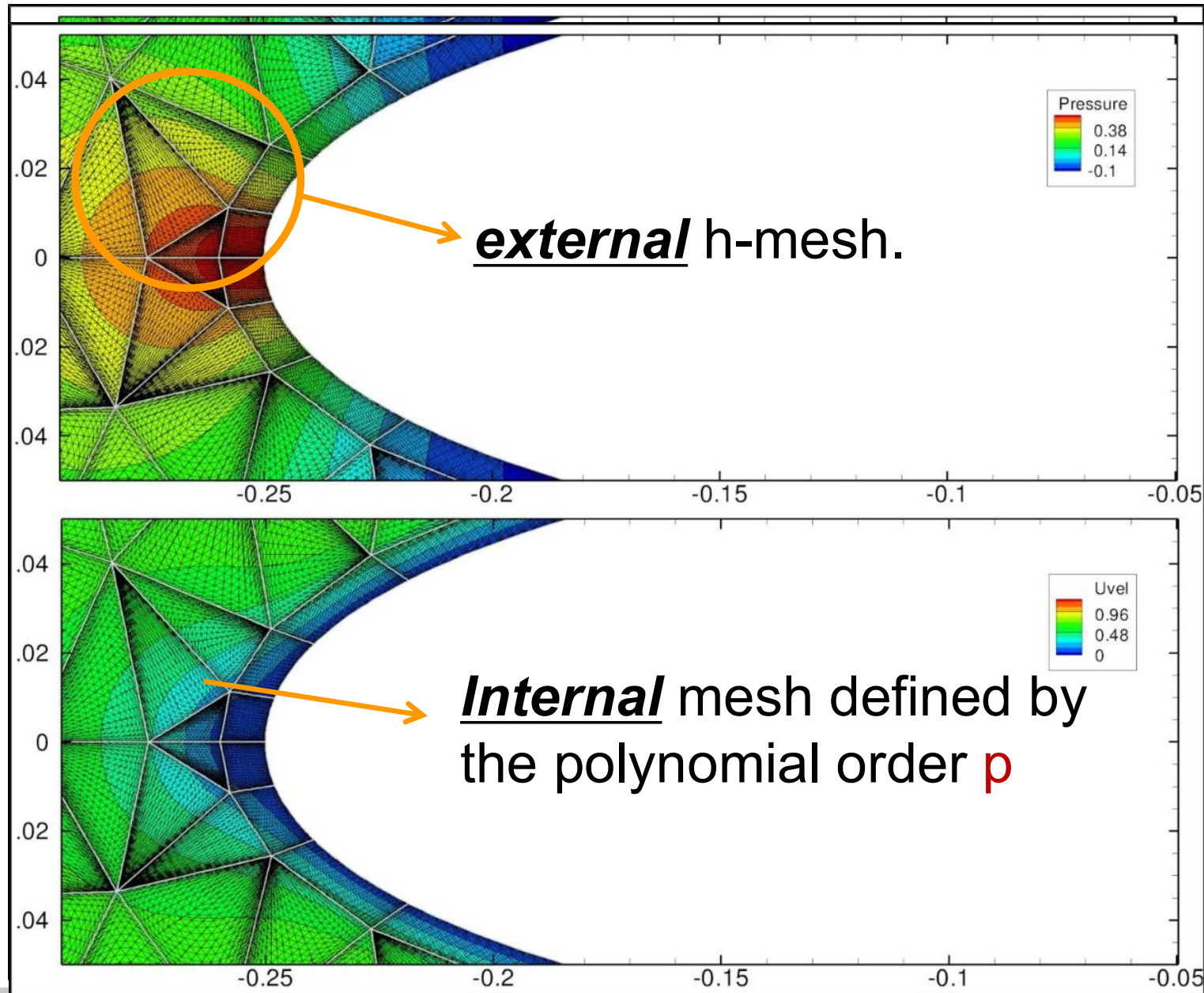
# High order methods

2D Discontinuous Galerkin Projection on triangular elements for various polynomial order



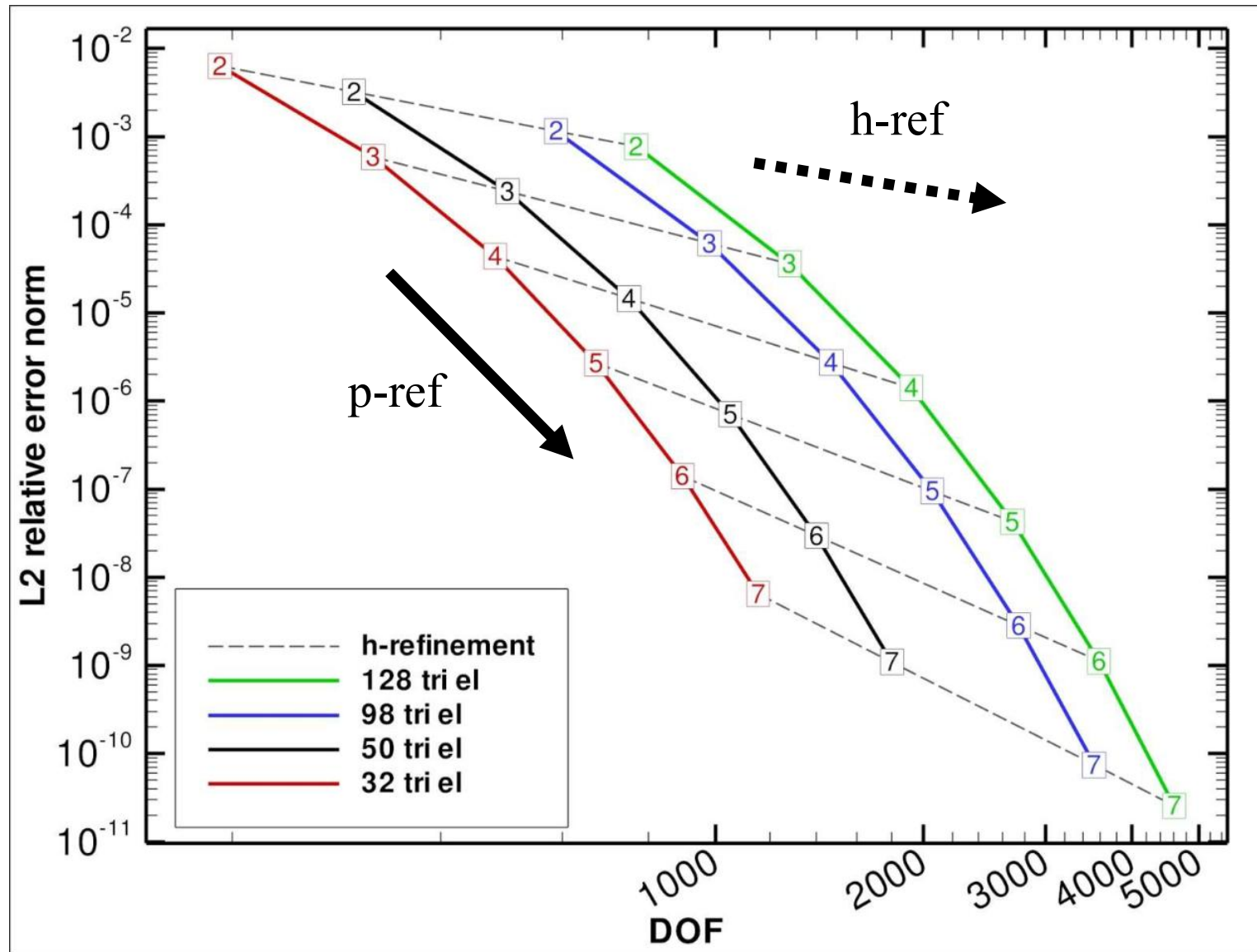
- **High order is generally defined for  $P \geq 2$**
- **High order allows  $h/p$  refinement**
  - $h$ -refinement offers constant decay of the error
  - $p$ -refinement offers exponential decay of the error

# High order methods

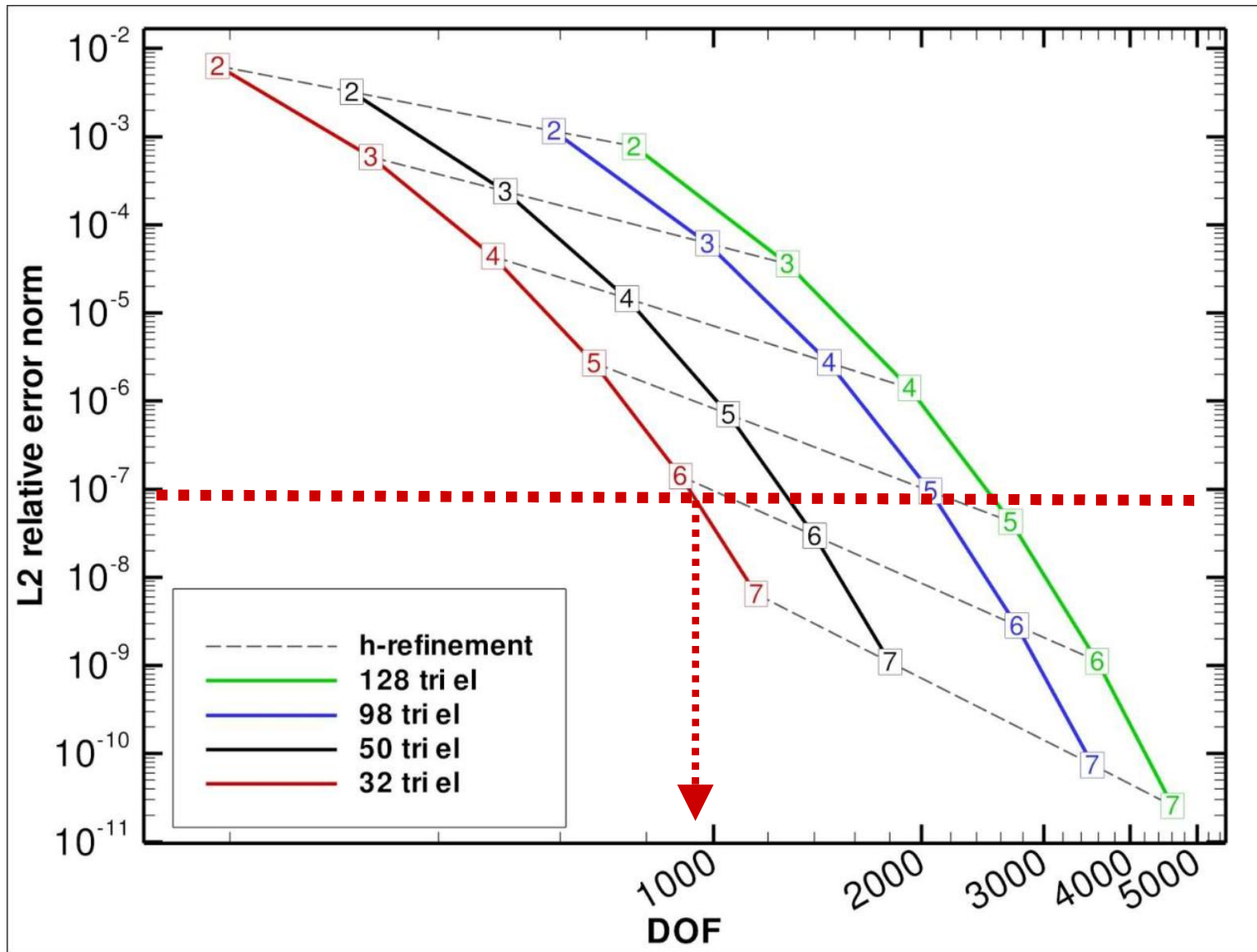




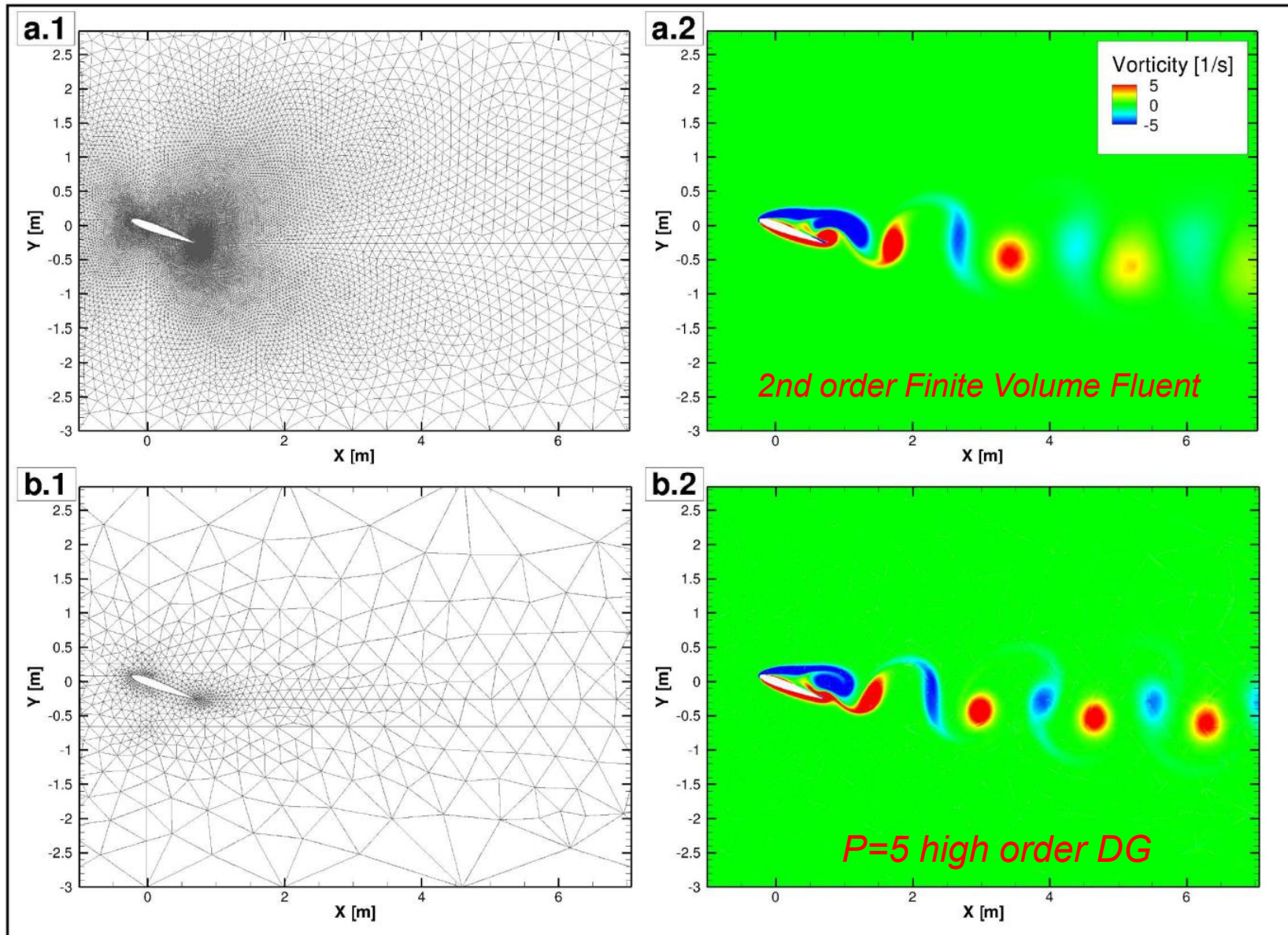
# High order methods (Poisson eq.)



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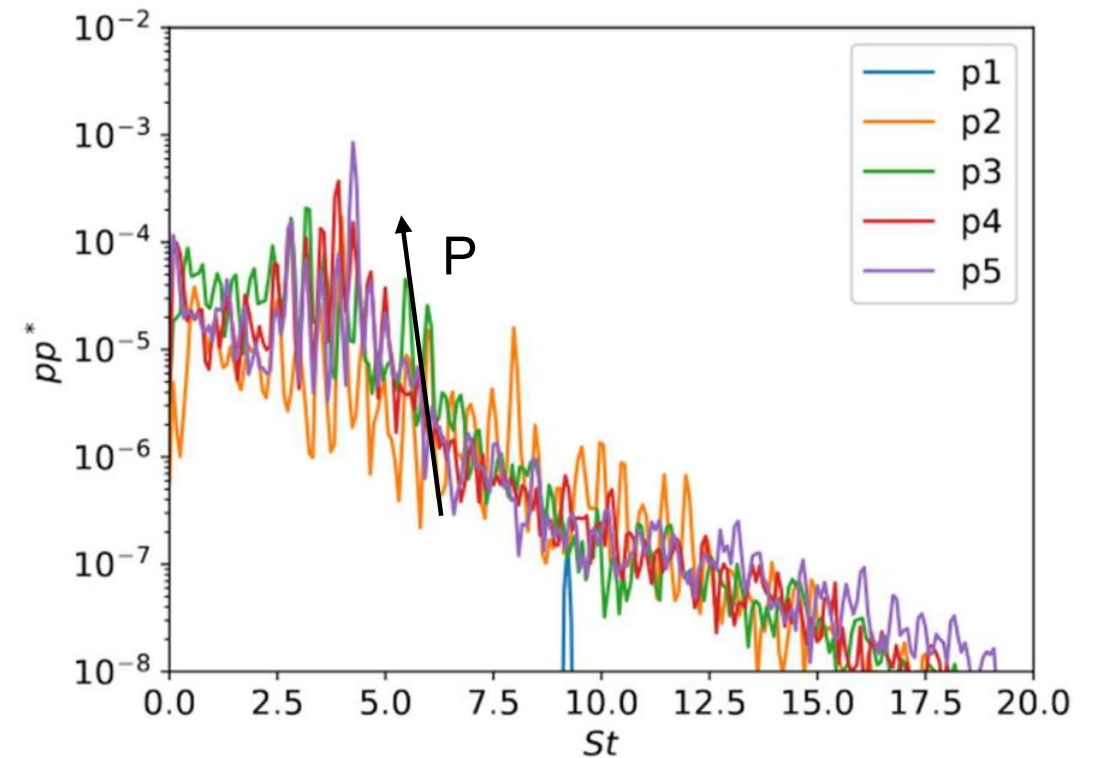
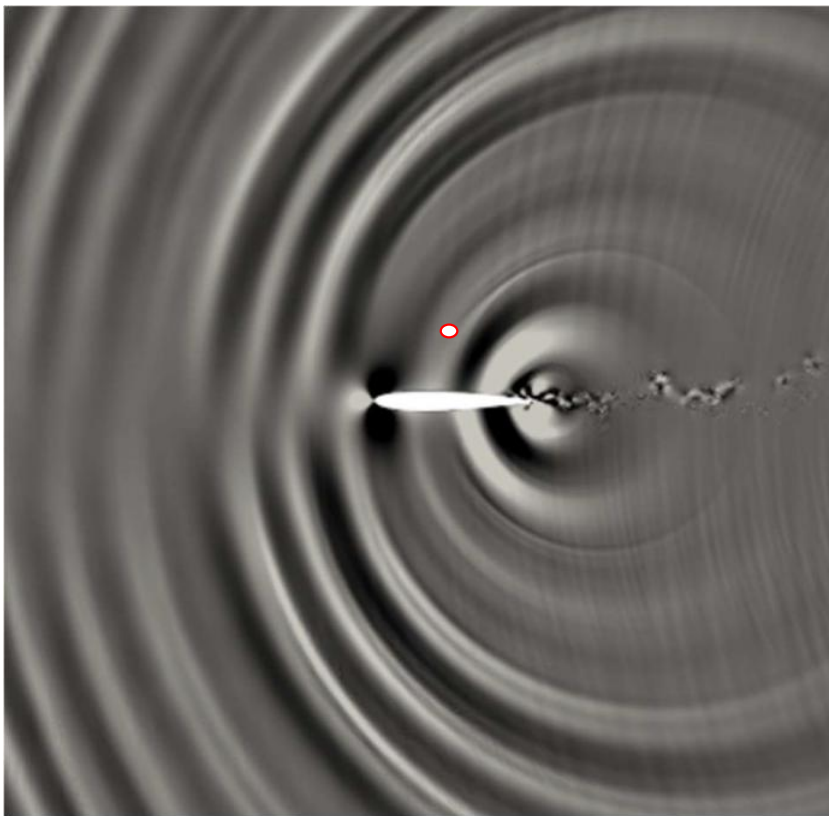
# NACA0012 - $Re=800$ - Laminar flow



# Horses: accuracy

NACA0012 airfoil at  $Re = 105$ ,  $M_0 = 0.4$  and  $AoA = 0^\circ$

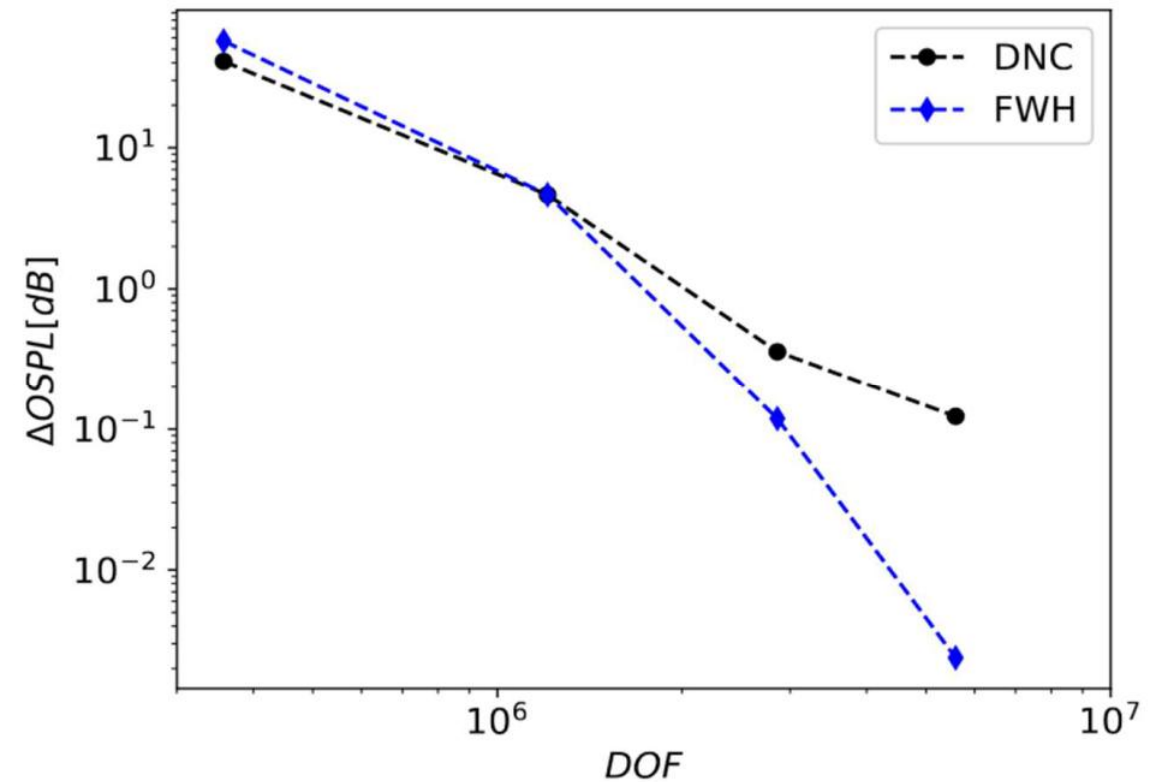
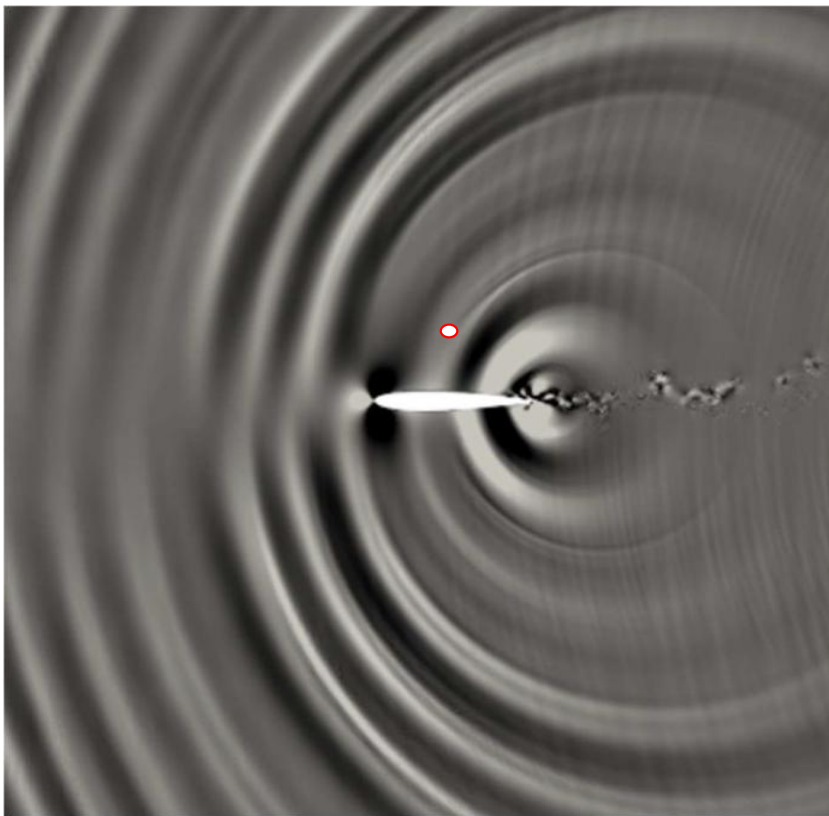
$P \uparrow$  : Error decreases **exponentially**



# Horses: accuracy

NACA0012 airfoil at  $Re = 10^5$ ,  $M_0 = 0.4$  and  $AoA = 0^\circ$

$P \uparrow$  : Error decreases **exponentially**

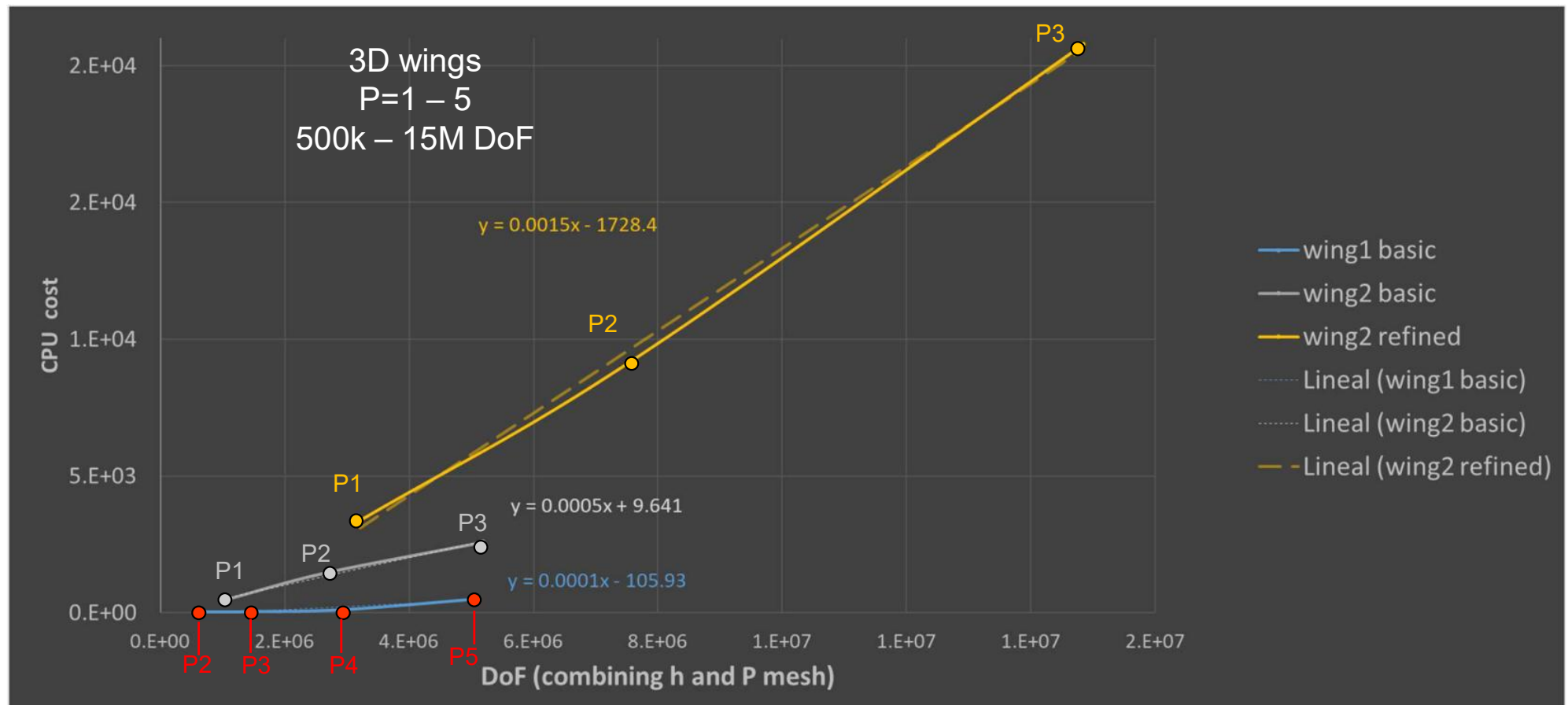


# Horses: cost



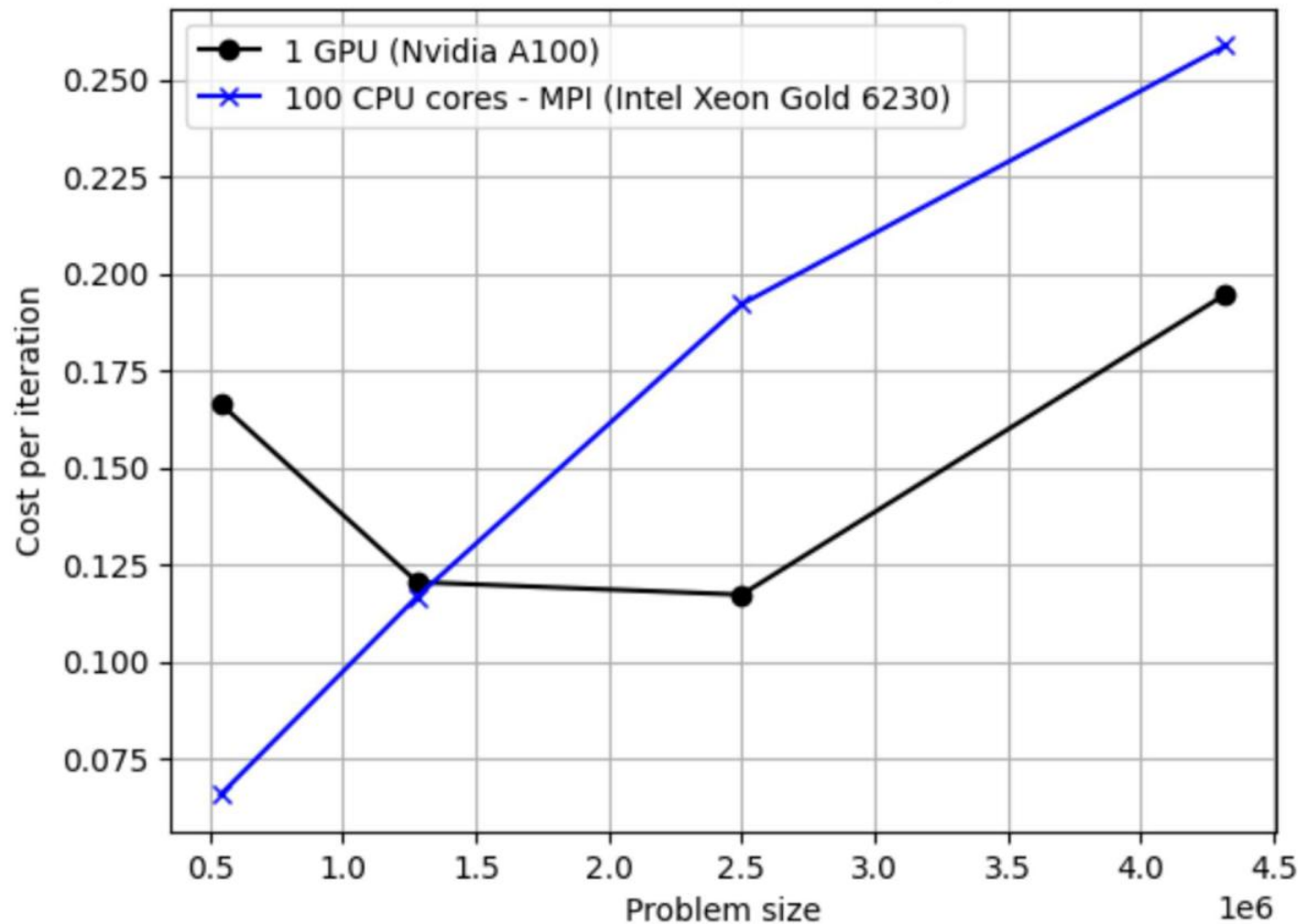
$P \uparrow$  : Error decreases **exponentially**

$P \uparrow$  : Cost increases **linearly**



Horses: cost → porting to GPUs (openACC on NVIDIA A100)  
..underway..

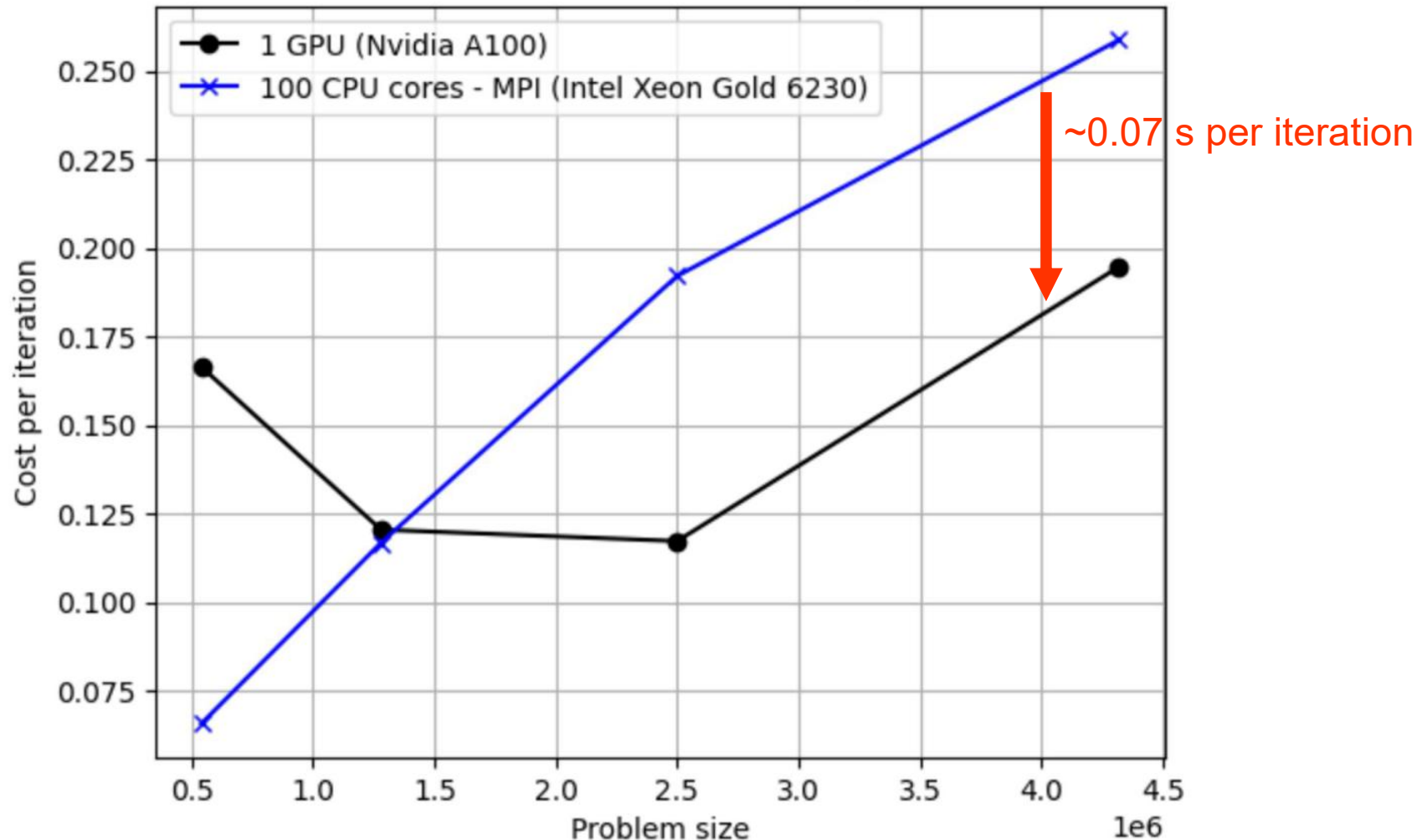
HORSES3D hardware cost comparison



*Better performance  
than 100 CPU cores*

# Horses: cost → porting to GPUs (openACC on NVIDIA A100) ..underway..

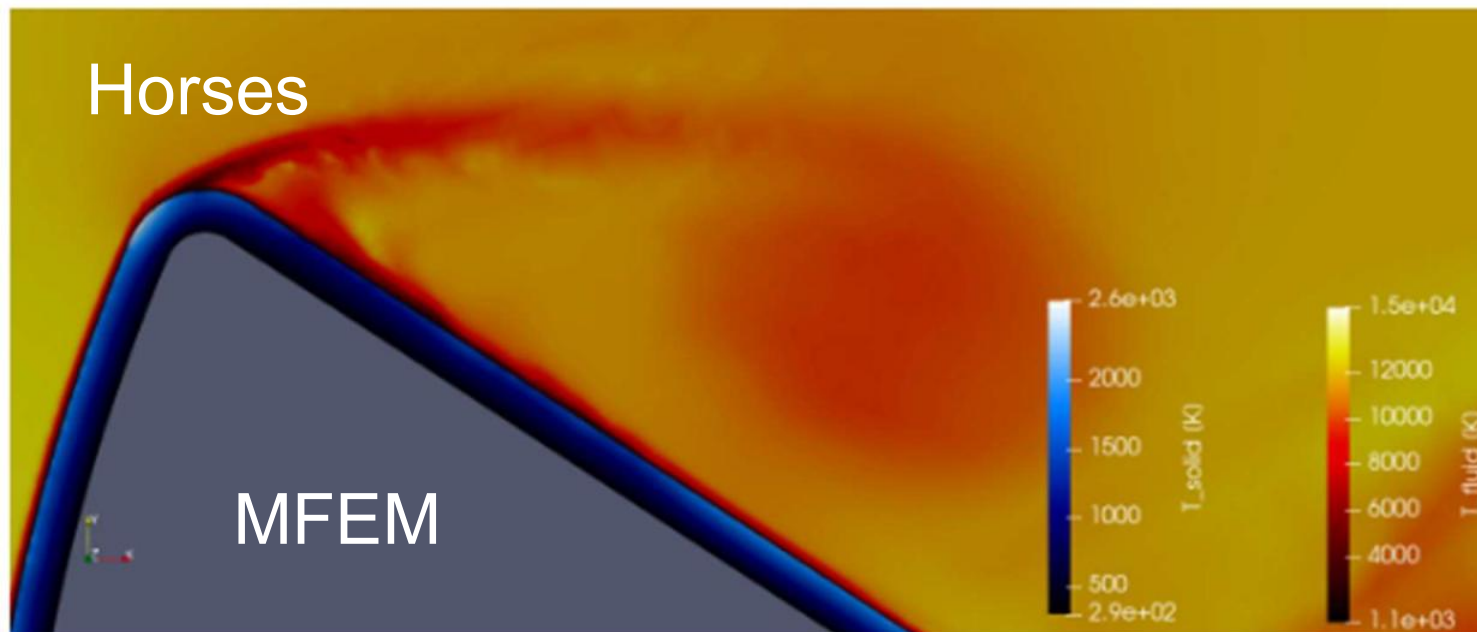
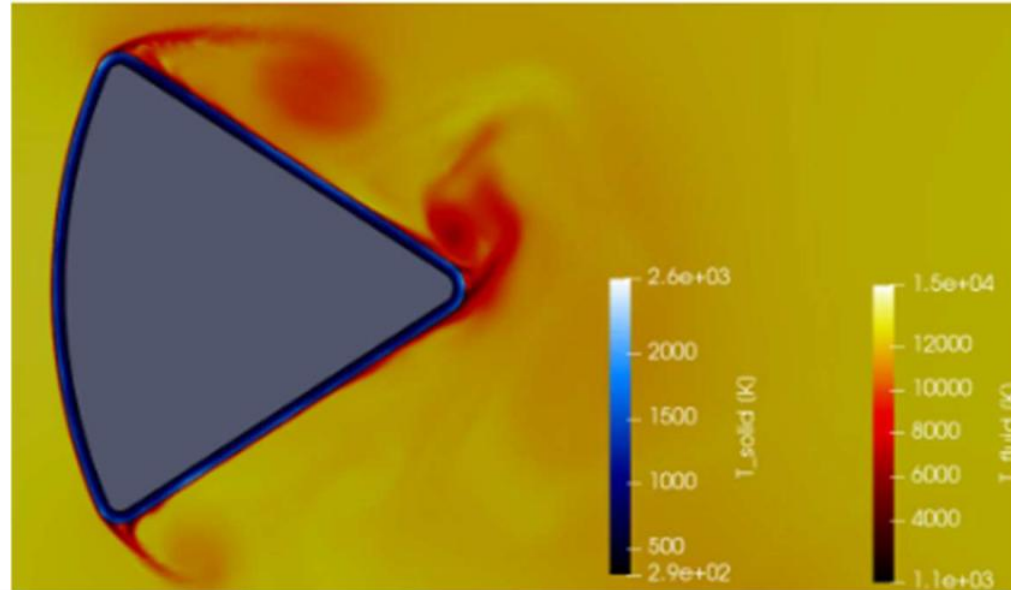
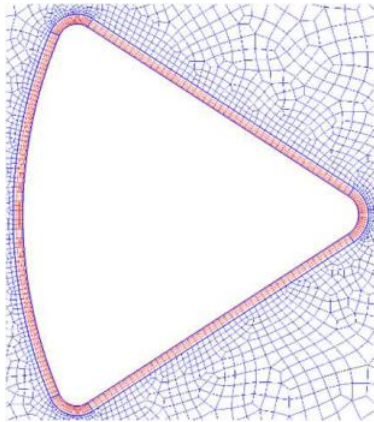
HORSES3D hardware cost comparison



*LES simulation → 1e8 time steps → 81 days faster than 100 CPUs*



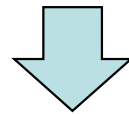
# Horses & MFEM (Python interface): example 1 - thermal coupling



## Horses & MFEM (*Python interface*): example 2 – incompressible solve

$$\frac{\partial \mathbf{u}}{\partial t} = -\nabla \cdot (\mathbf{u}\mathbf{u}) - \frac{1}{\rho_0} \nabla p - \nabla \cdot (\nu \nabla \mathbf{u}) + \frac{\mathbf{f}_{\text{ext}}}{\rho_0}$$

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



*Step 1*

$$\frac{\gamma_0 \mathbf{u}^* - \alpha_0 \mathbf{u}^n - \alpha_1 \mathbf{u}^{n-1}}{\Delta t} = -\beta_0 \mathbf{N}(\mathbf{u}^n) - \beta_1 \mathbf{N}(\mathbf{u}^{n-1}),$$

*DG/FR-horses*

*Step 2*

$$\nabla \cdot \left( \frac{1}{\rho_0} \nabla p^{n+1} \right) = -\frac{\gamma_0}{\Delta t} \nabla \cdot \mathbf{u}^*$$

*DG/CG-MFEM*

*Step 3*

$$-\nabla \cdot (\nu \nabla \mathbf{u}^{n+1}) + \frac{\gamma_0}{\Delta t} \mathbf{u}^{n+1} = \frac{\gamma_0}{\Delta t} \mathbf{u}^* - \frac{\nabla p^{n+1} + \mathbf{f}_{\text{ext}}^n}{\rho_0}$$

*DG/CG-MFEM*

# Summary

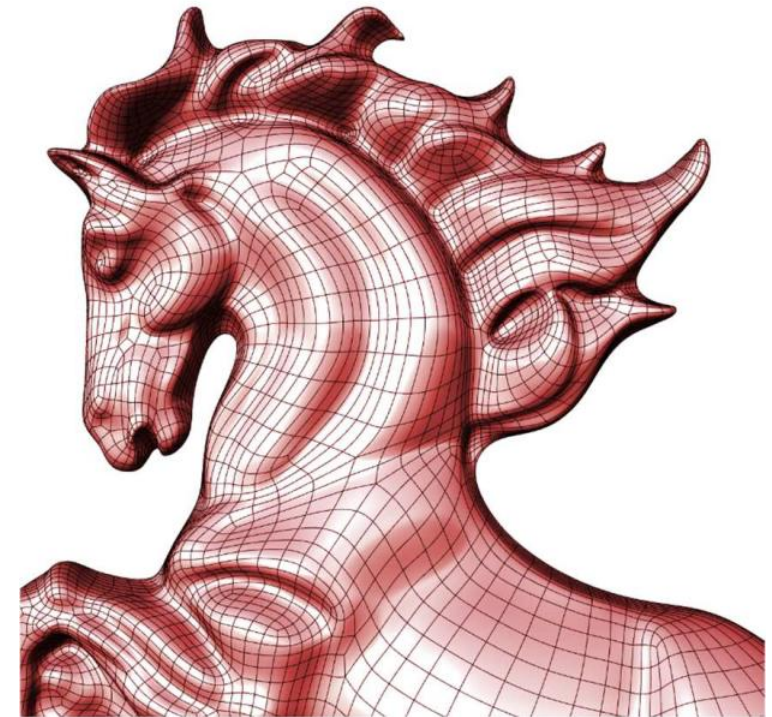
## 1- Introduction to DG & Horses3d

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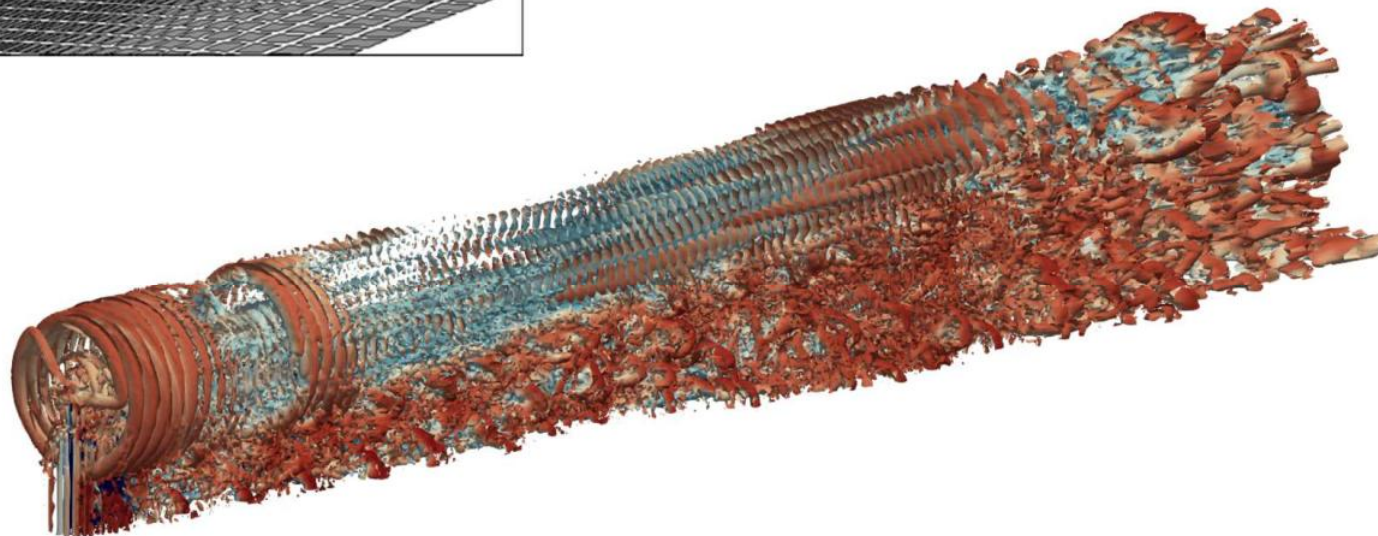
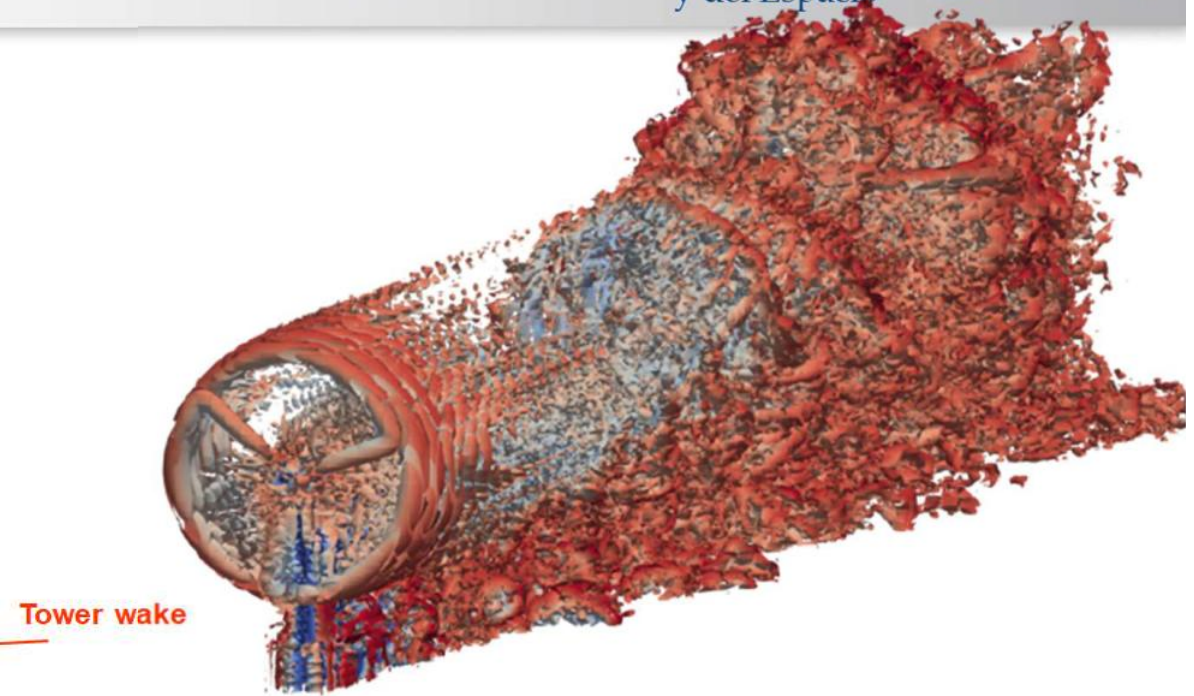
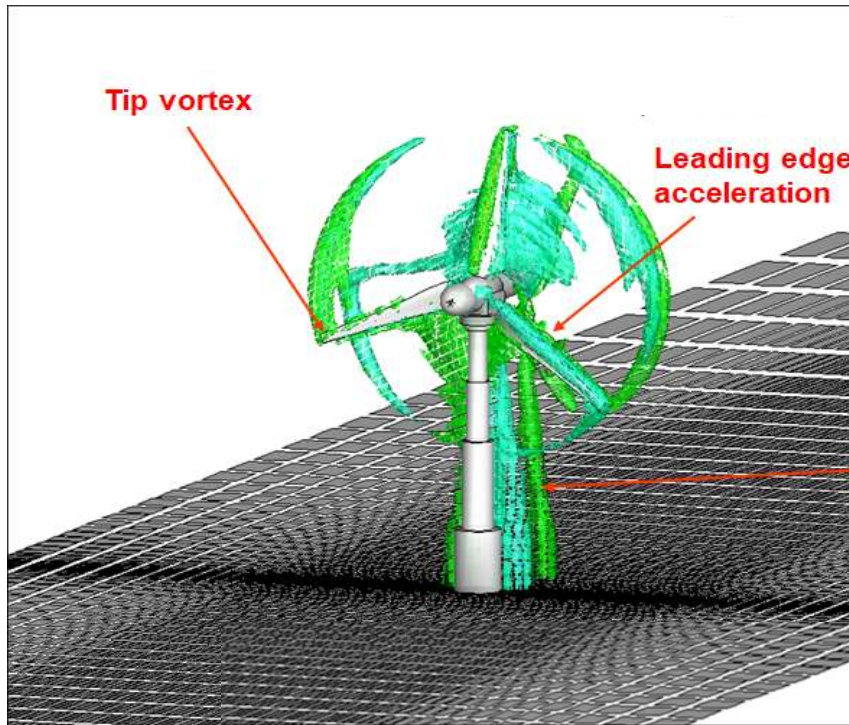
- Wind turbines
- Turbulence

## 3. Machine Learning + CFD

- Mesh adaption
- NN acceleration
- RL for automation

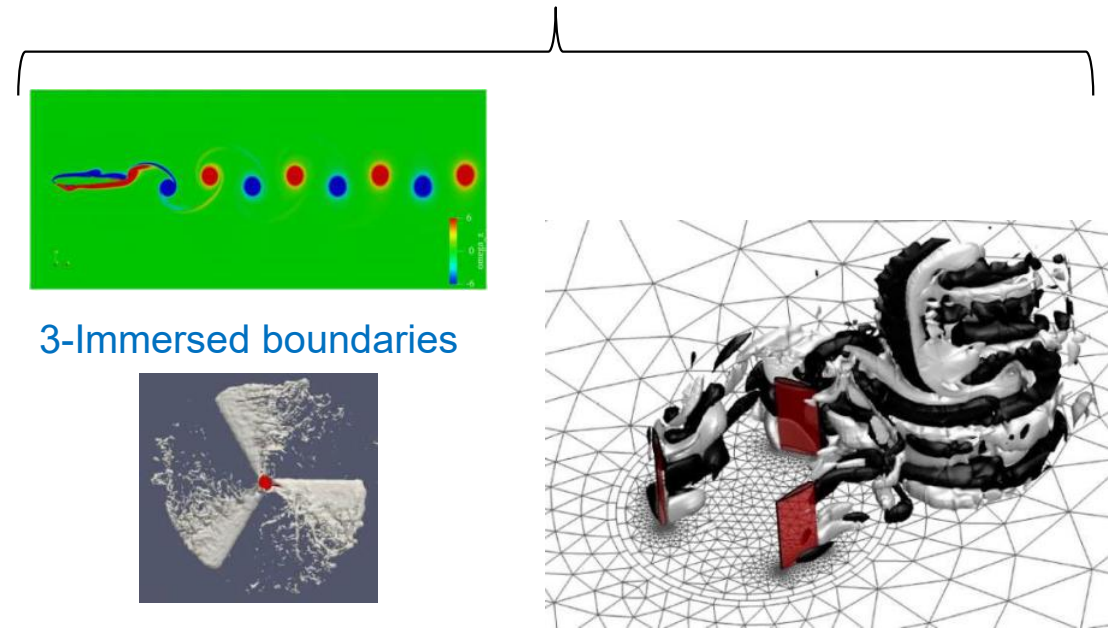
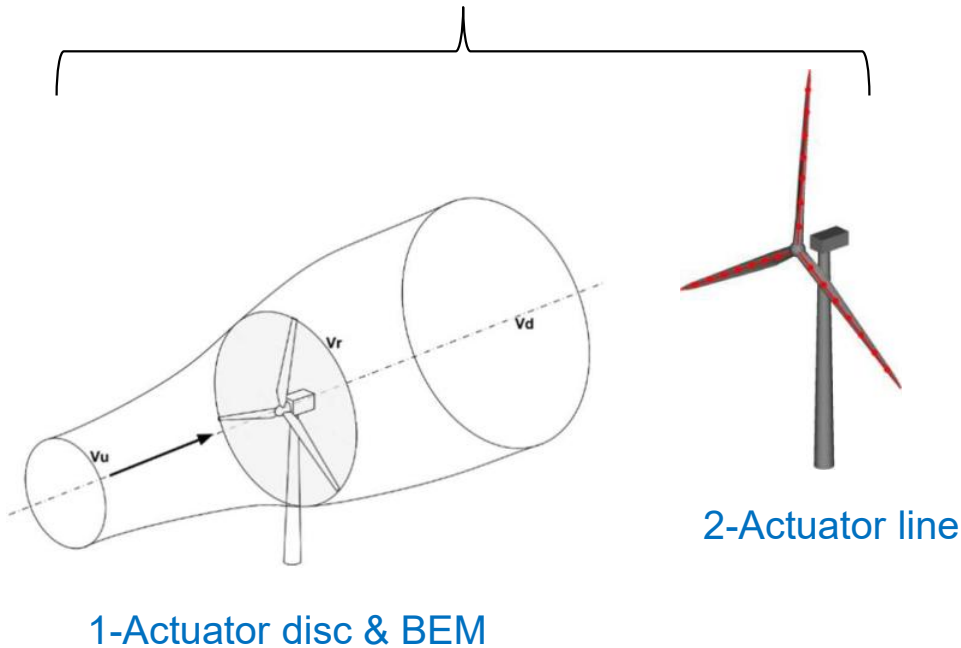


# High order wind turbines



Require 2D aerodynamic data

Explicit 3D geometry



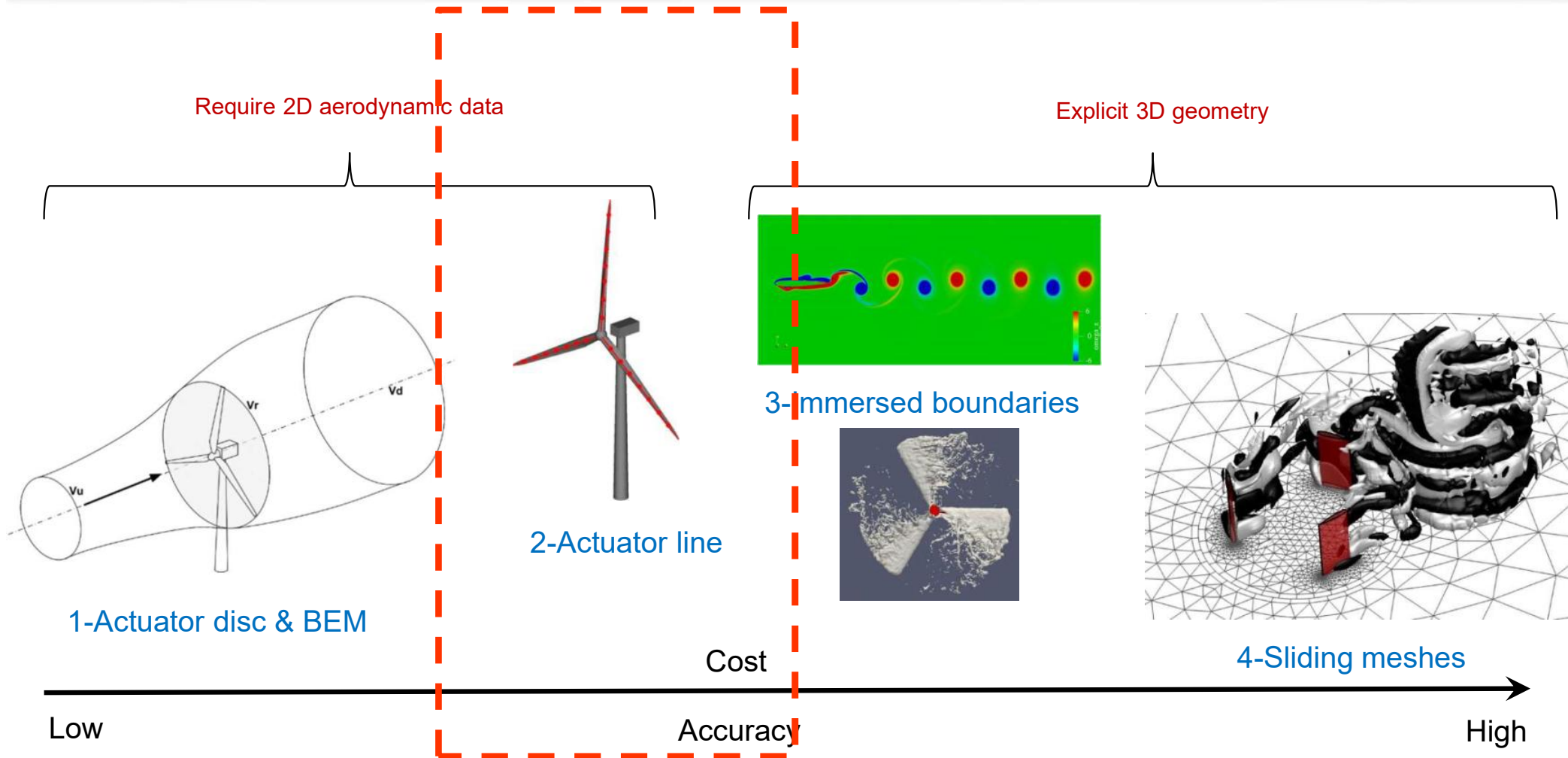
Cost

Accuracy

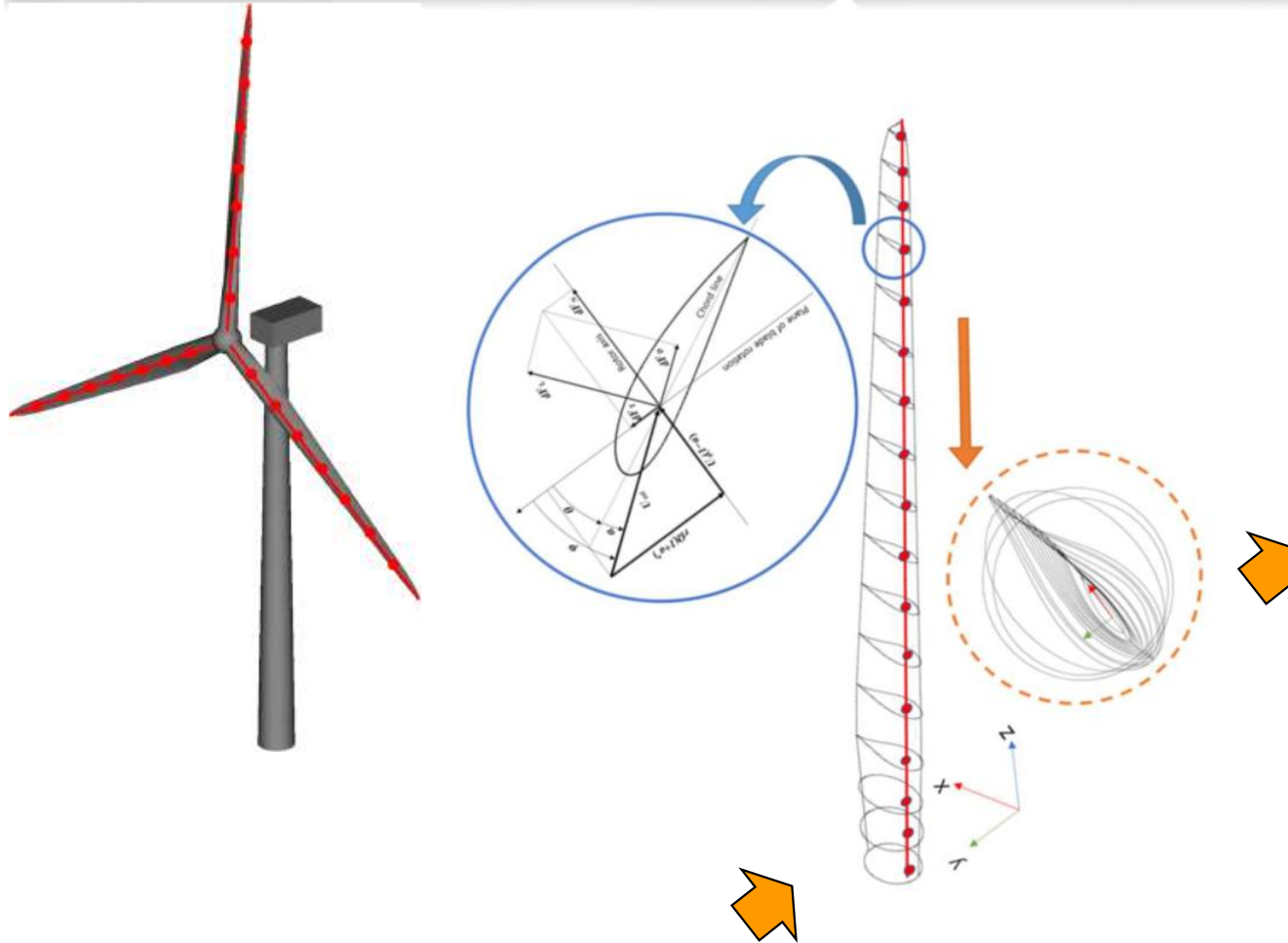
Low

High

- 4- E Ferrer and RHJ Willden, A high order Discontinuous Galerkin - Fourier incompressible 3D Navier–Stokes solver with **rotating sliding meshes**, *Journal of Computational Physics*, 2012
- 4- E Ferrer, RHJ Willden, Blade–wake interactions in **cross-flow turbines**, *International Journal of Marine Energy*, 2015
- 3- J Kou, A Hurtado-de-Mendoza, S Joshi, S Le Clainche, E Ferrer, Eigensolution analysis of **immersed boundaries** for high-order schemes, *Journal of Computational Physics*, 2022
- 3- J Kou, S Joshi, A Hurtado-de-Mendoza, K Puri, C Hirsch, E Ferrer, An **Immersed boundary** method for high–order flux reconstruction, *Journal of Computational Physics*, 2022
- 2 & 3- E Ferrer, S Colombo, O Marino, “Aeroacoustic predictions of wind turbines based on **actuator lines and immersed boundaries**”, *Under review at Wind Energy*
- 1- E Ferrer, S Le Clainche, **Simple models for cross flow turbines**, in *Recent advances in CFD for Wind and Tidal Offshore Turbines*, 2019
- 1- E Ferrer, OMF Browne, E Valero, Sensitivity analysis to control the far–wake unsteadiness behind **turbines**, *Energies*, 2017



- 4- E Ferrer and RHJ Willden, A high order Discontinuous Galerkin - Fourier incompressible 3D Navier–Stokes solver with **rotating sliding meshes**, *Journal of Computational Physics*, 2012
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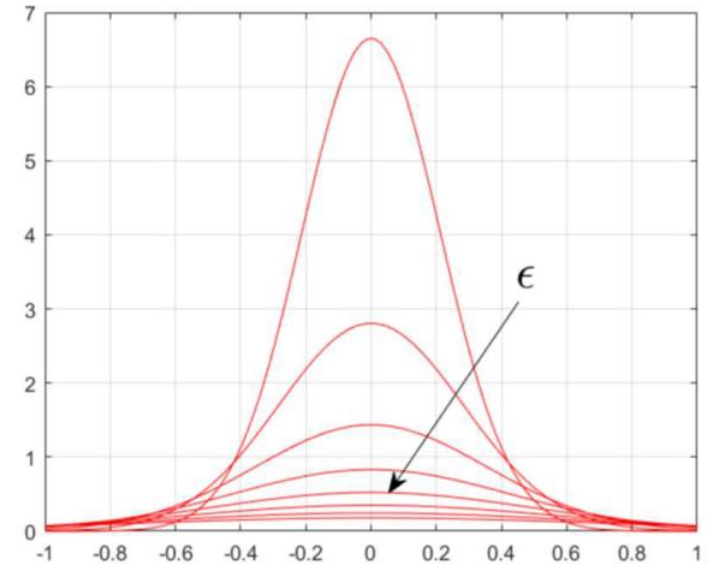


*Tabulated data*

$$f_L = \frac{1}{2} \rho U_{rel}^2 S C_l, \quad f_D = \frac{1}{2} \rho U_{rel}^2 S C_d,$$

$$\frac{d\mathbf{Q}}{dt} = \mathcal{R}(\mathbf{Q}, \nabla \mathbf{Q}) + \mathcal{S}(\mathbf{Q})$$

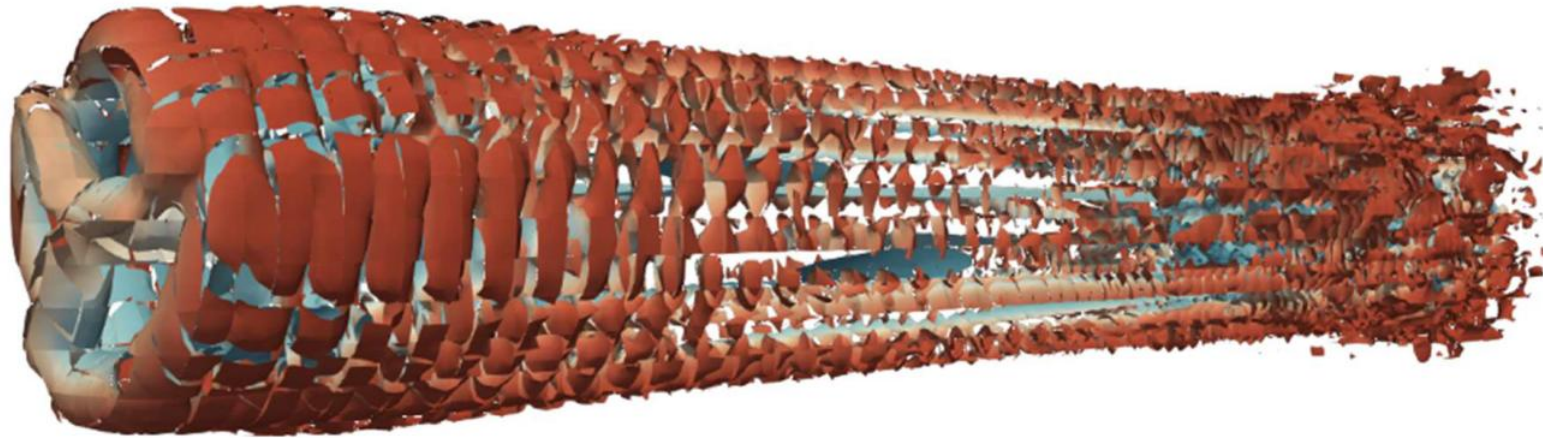
$$\mathcal{S}(\mathbf{Q}) = \eta_\epsilon \mathbf{F}$$



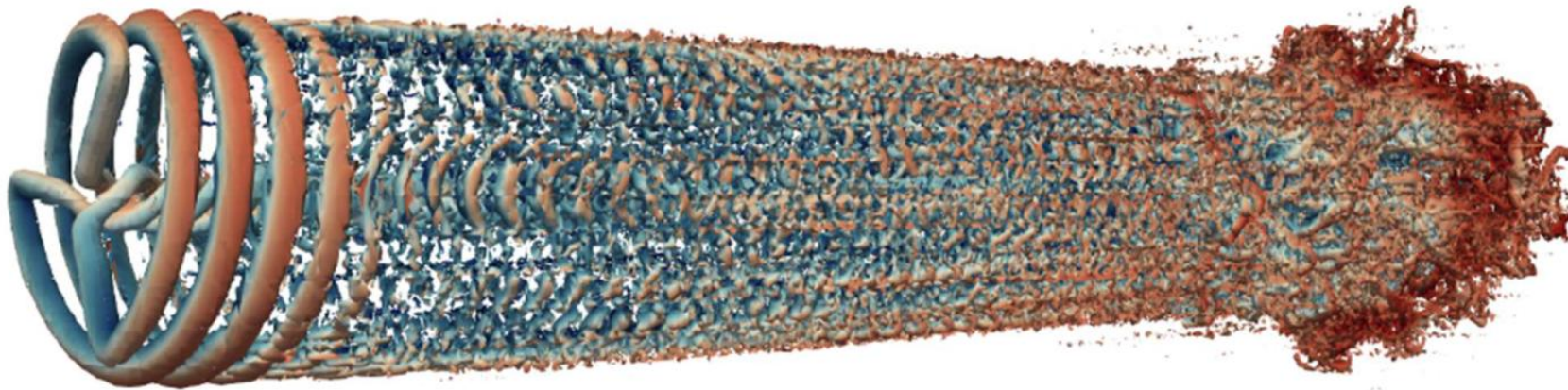
$$\eta_\epsilon = \frac{1}{\epsilon^3 \pi^{\frac{3}{2}}} e^{-\left(\frac{d}{\epsilon}\right)^2}$$

$$\epsilon_k = k \times \Delta_{grid} = k \times \frac{(\Delta_x \Delta_y \Delta_z)^{\frac{1}{3}}}{p+1}$$

## Improved solution using the same h-mesh



$P = 2$

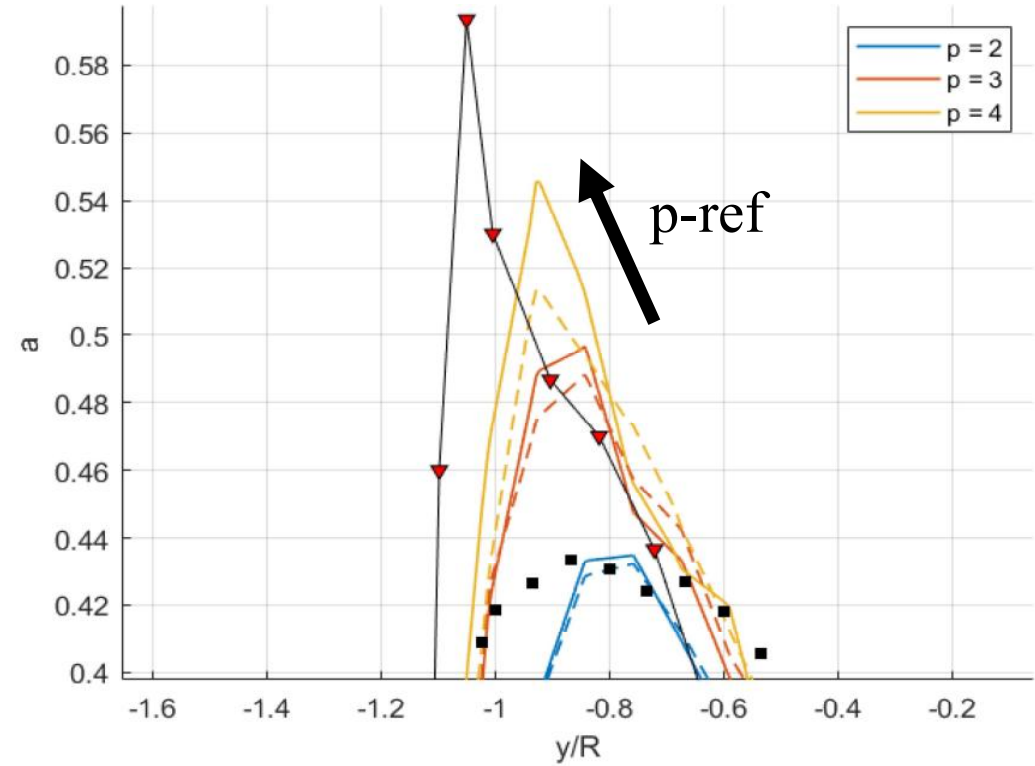
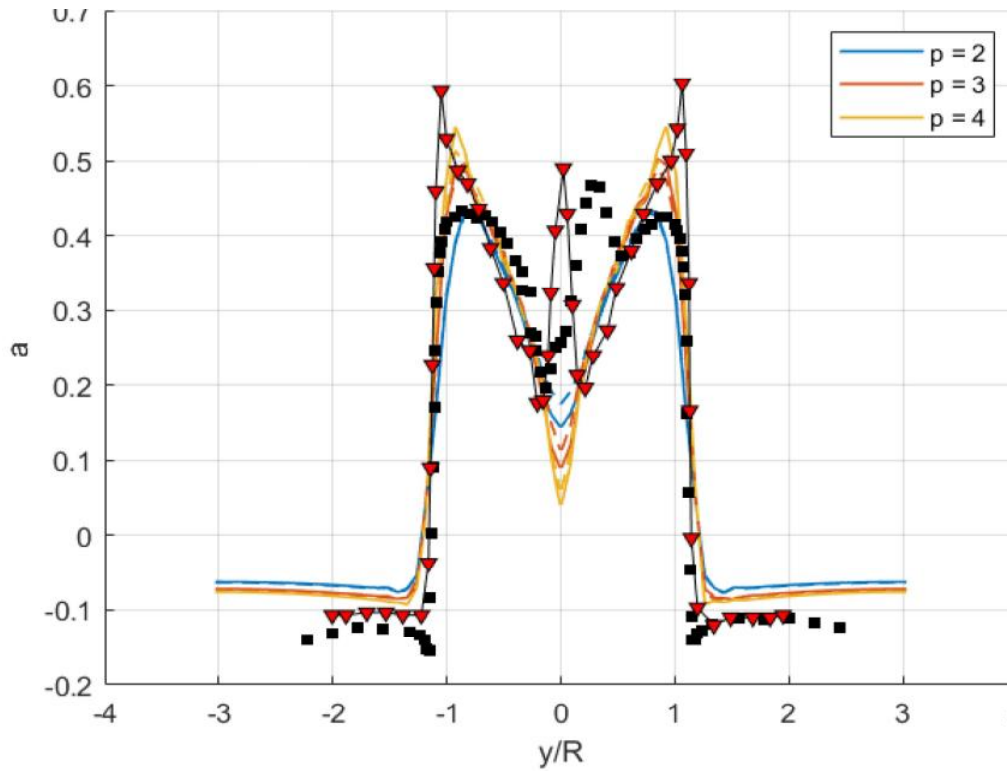
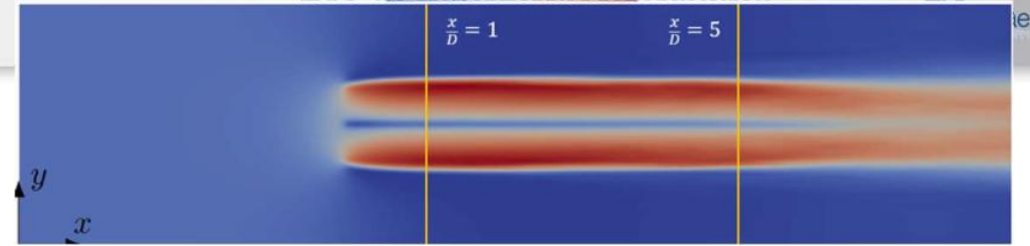


$P = 5$





# Averaged velocity deficit



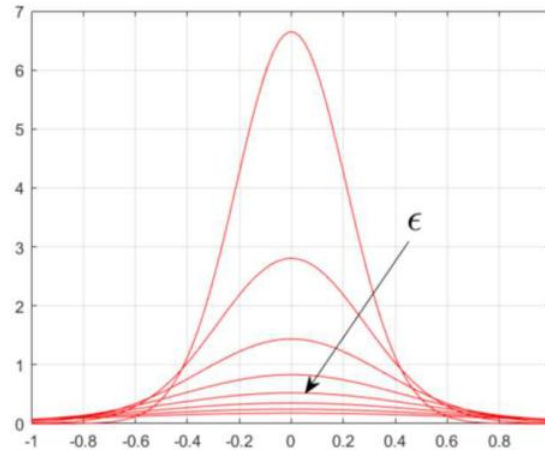
■ Experimental

▽ OpenFoam-Oxford Fine mesh → 190M elements

$$f_L = \frac{1}{2} \rho U_{rel}^2 S C_l, \quad f_D = \frac{1}{2} \rho U_{rel}^2 S C_d,$$

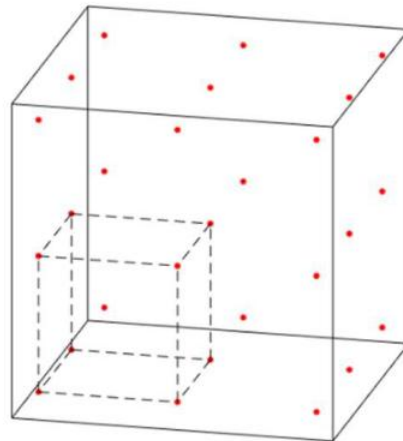
cell averaged velocity

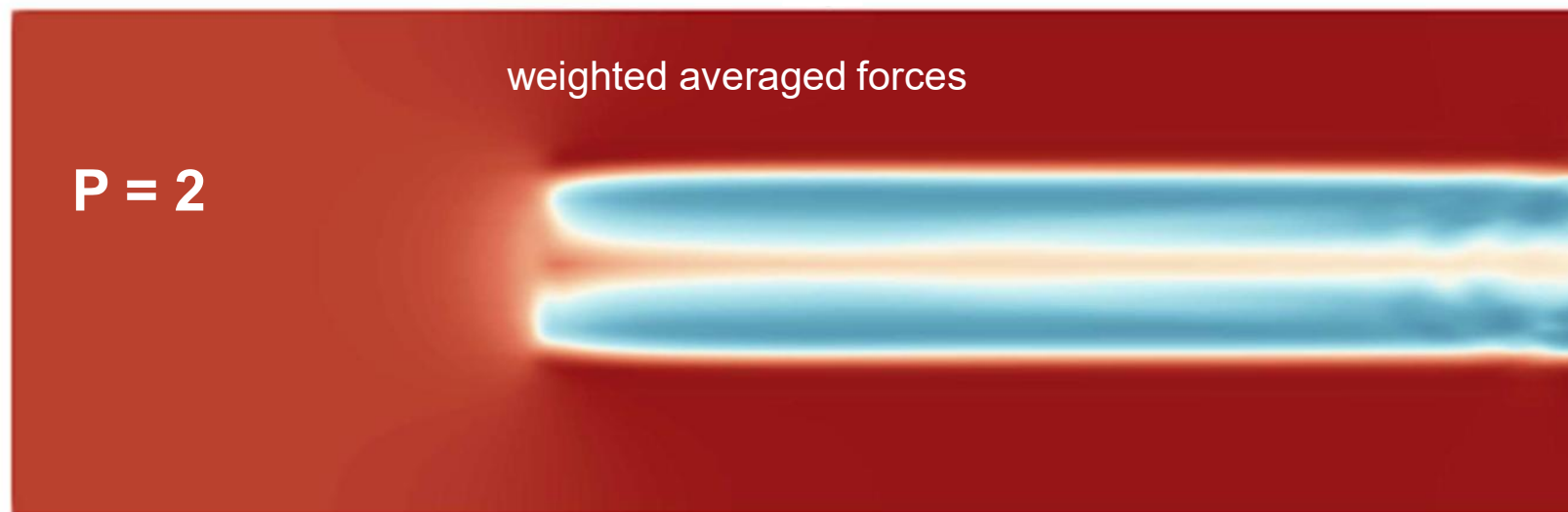
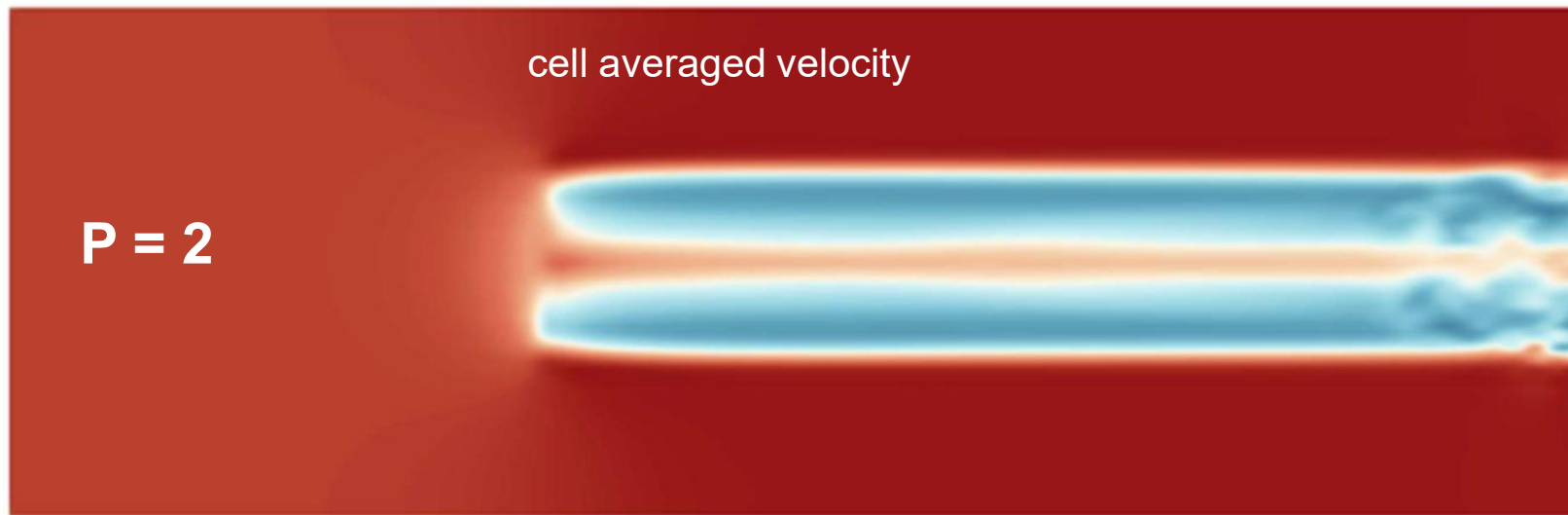
$$\bar{\mathbf{q}}_t = \frac{1}{N} \sum_{i=1}^N \mathbf{q}_{t_i}$$

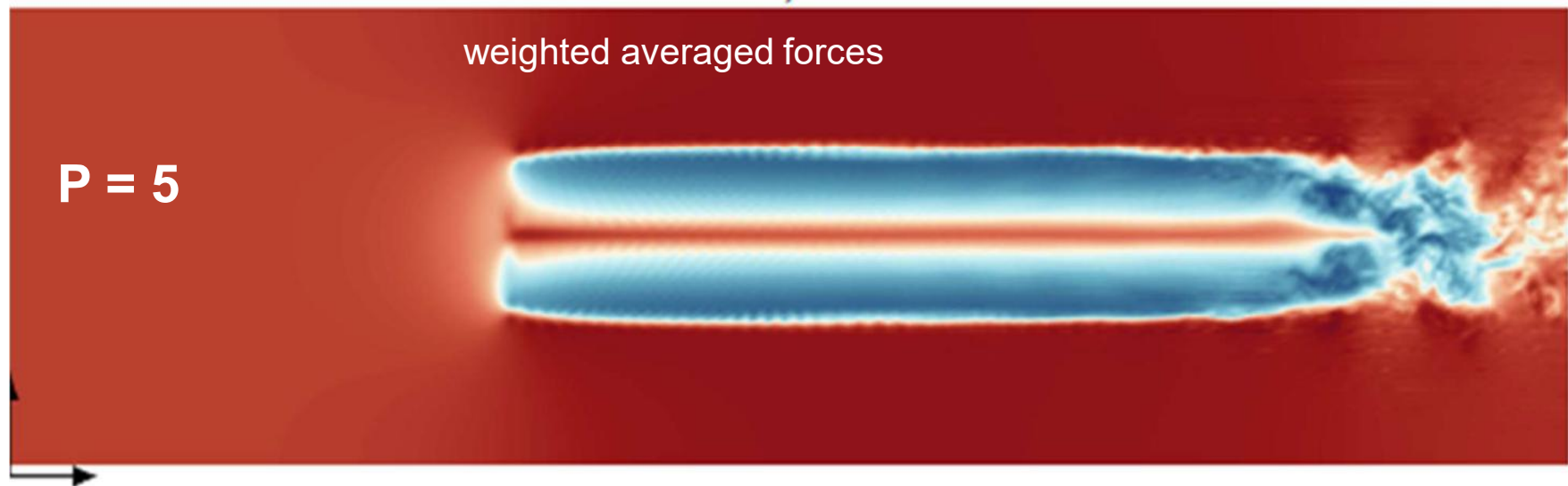
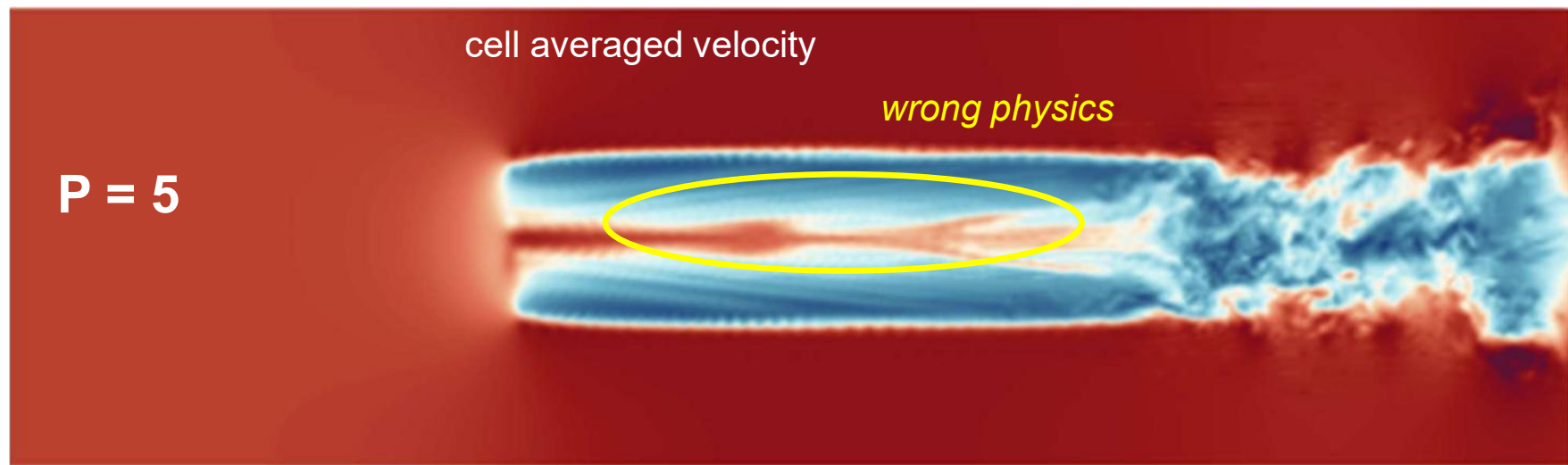


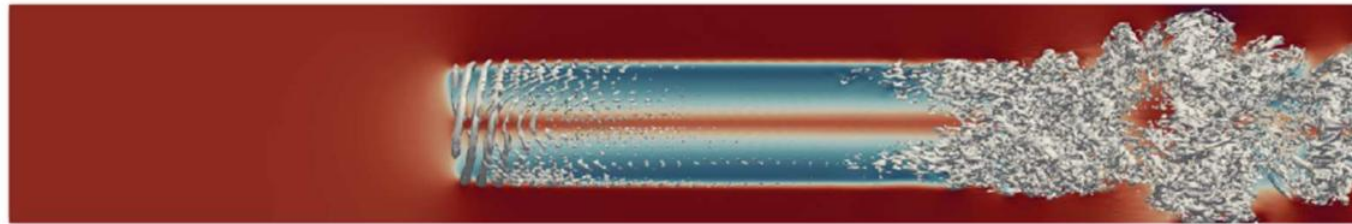
weighted averaged forces

$$\bar{\mathbf{f}}_j = \frac{\sum_{i=1}^N \eta_{ji}(d) \cdot \mathbf{f}_i}{\sum_{j=1}^{N_a} \sum_{i=1}^N \eta_{ji}(d)}$$

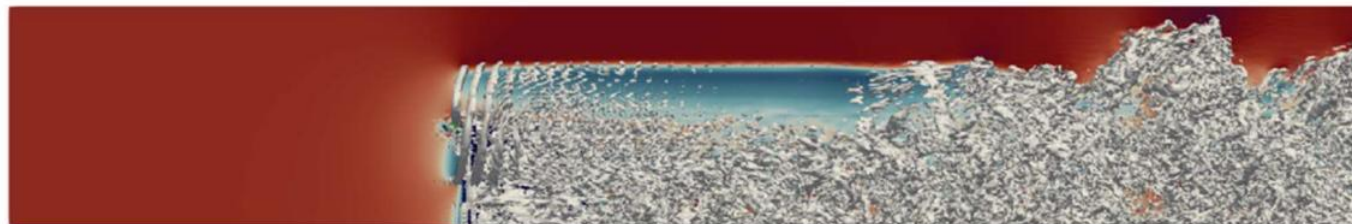




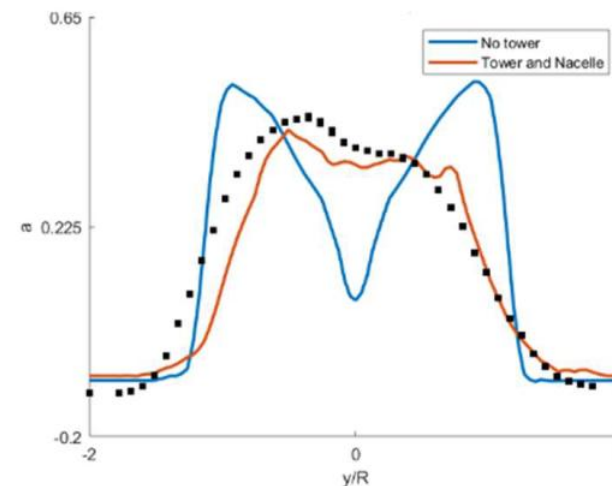
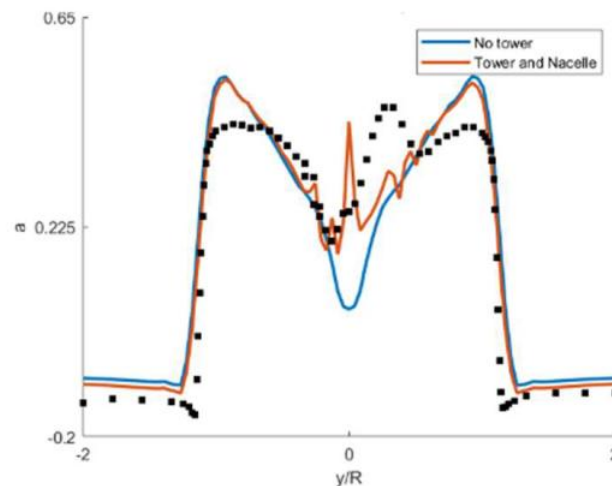


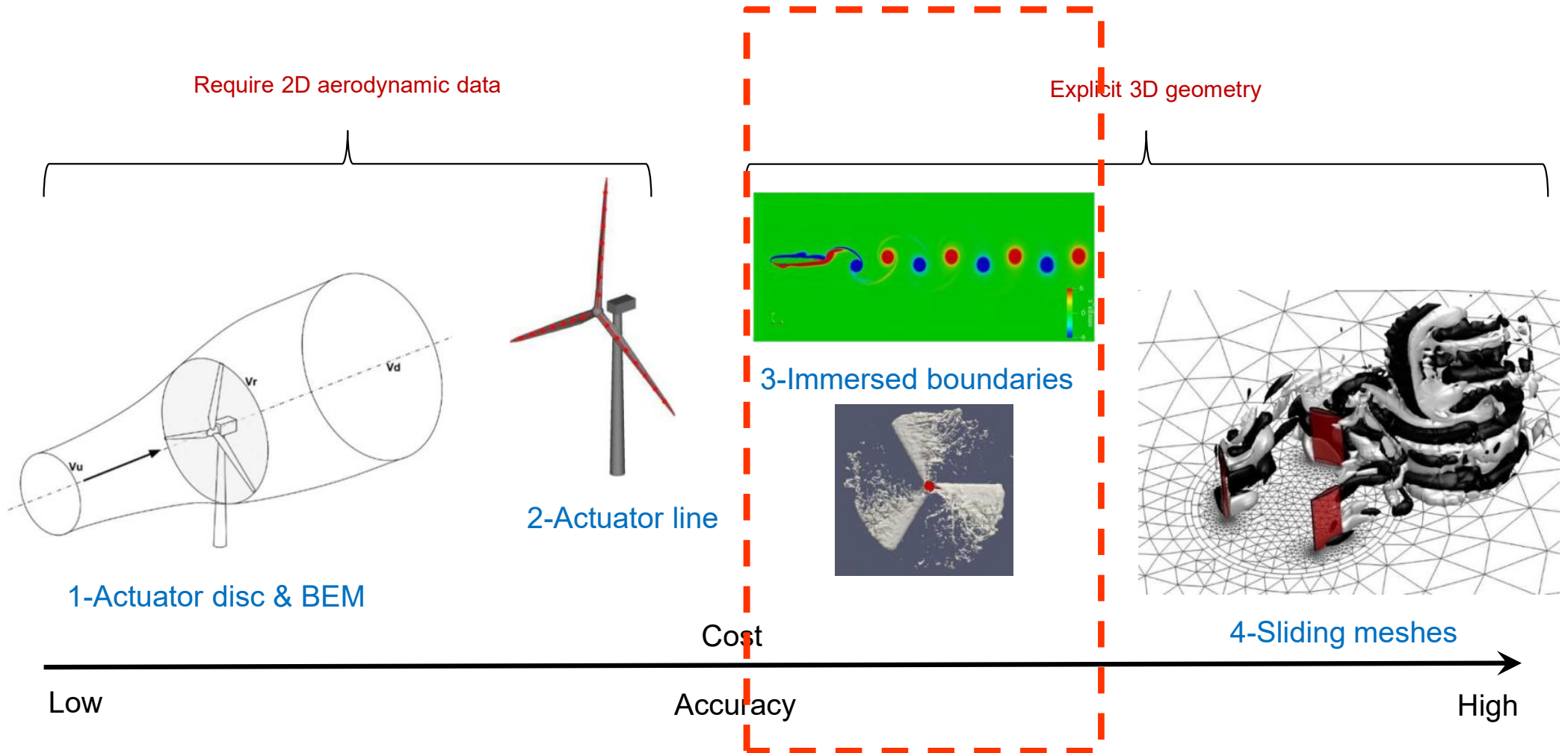


a) Actuator line without tower and nacelle.



b) Actuator line with tower and nacelle, which are modeled using immersed boundaries.

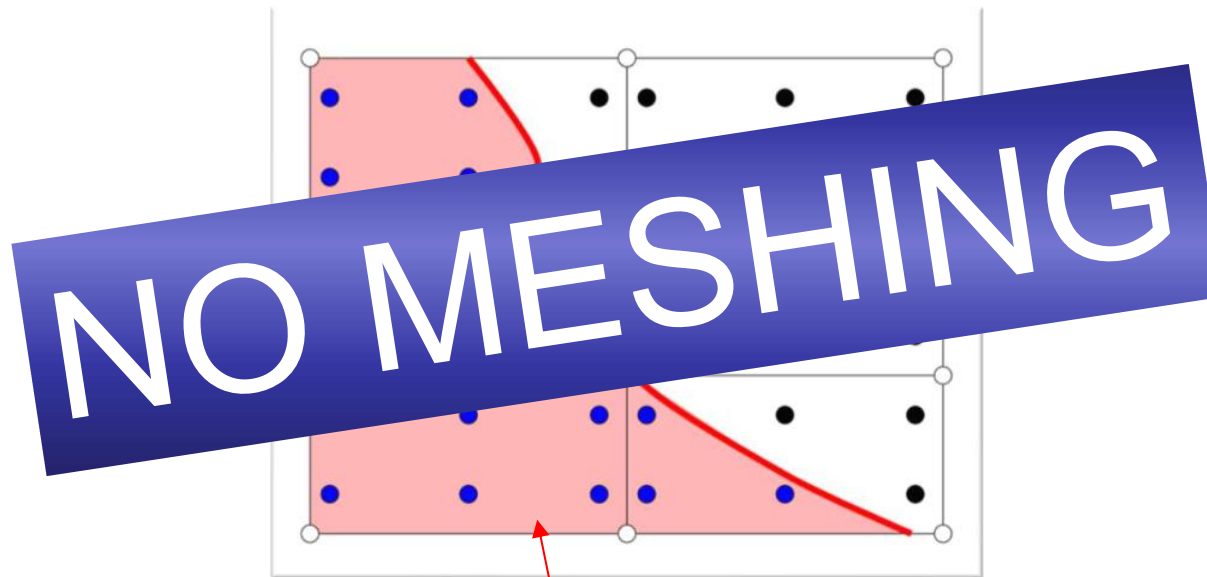




- 4- E Ferrer and RHJ Willden, A high order Discontinuous Galerkin - Fourier incompressible 3D Navier–Stokes solver with **rotating sliding meshes**, *Journal of Computational Physics*, 2012
- 4- E Ferrer, RHJ Willden, Blade–wake interactions in **cross-flow turbines**, *International Journal of Marine Energy*, 2015
- 3- J Kou, A Hurtado-de-Mendoza, S Joshi, S Le Clainche, E Ferrer, Eigensolution analysis of **immersed boundaries** for high-order schemes, *Journal of Computational Physics*, 2022
- 3- J Kou, S Joshi, A Hurtado-de-Mendoza, K Puri, C Hirsch, E Ferrer, An **Immersed boundary** method for high–order flux reconstruction, *Journal of Computational Physics*, 2022
- 2 & 3- E Ferrer, S Colombo, O Marino, “Aeroacoustic predictions of wind turbines based on **actuator lines and immersed boundaries**”, *Under review at Wind Energy*
- 1- E Ferrer, S Le Clainche, **Simple models for cross flow turbines**, in *Recent advances in CFD for Wind and Tidal Offshore Turbines*, 2019
- 1- E Ferrer, OMF Browne, E Valero, Sensitivity analysis to control the far–wake unsteadiness behind **turbines**, *Energies*, 2017

## Immersed boundary method (penalty) → Mesh Free method

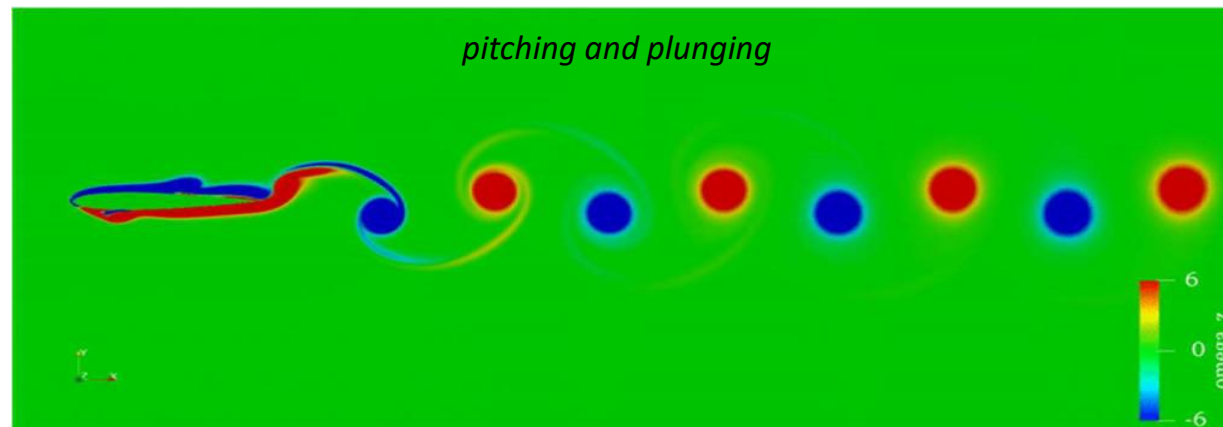
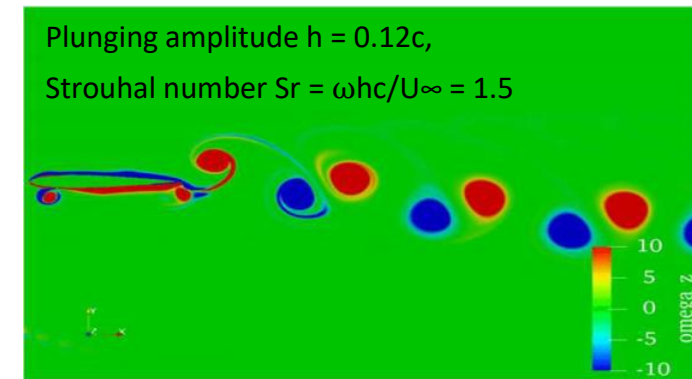
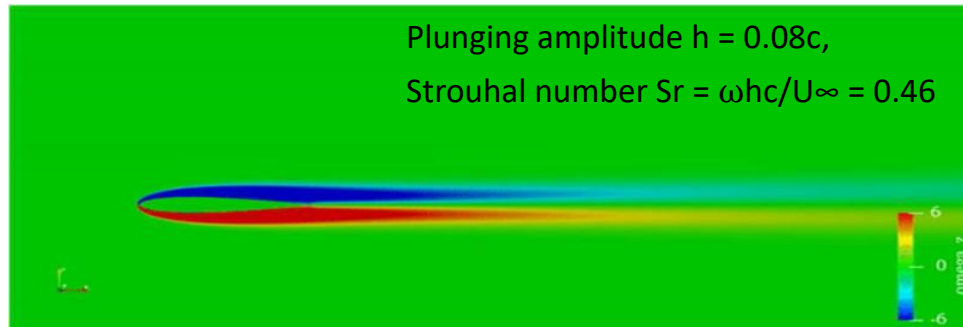
- Simple 'Cartesian' grids (with local P refinement)
- Complex geometries
- Moving geometries



$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \vec{\mathbf{F}}(\mathbf{U}) = \nabla \cdot \vec{\mathbf{G}}(\mathbf{U}, \nabla \mathbf{U}) + \mathbf{S}(\mathbf{U}).$$

$$\mathbf{S}(\mathbf{U}) = a \times \begin{pmatrix} 0 \\ \rho u_0 - \rho u \\ \rho v_0 - \rho v \\ \rho w_0 - \rho w \\ \frac{\rho}{2}(u_0^2 + v_0^2 + w_0^2) - \frac{\rho}{2}(u^2 + v^2 + w^2) \end{pmatrix}$$

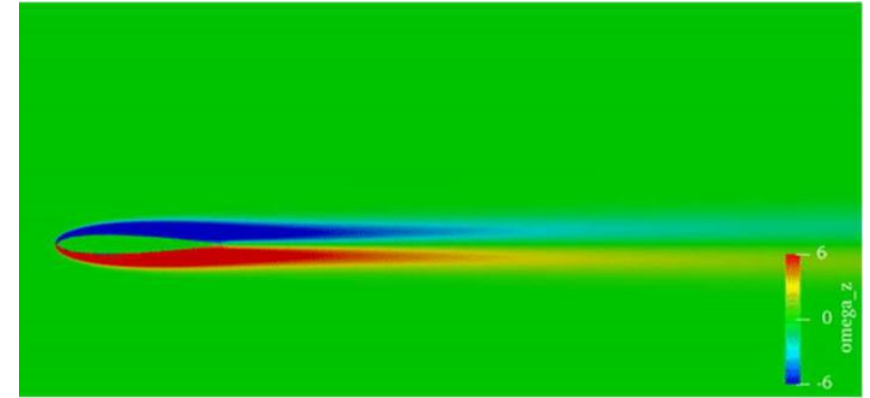
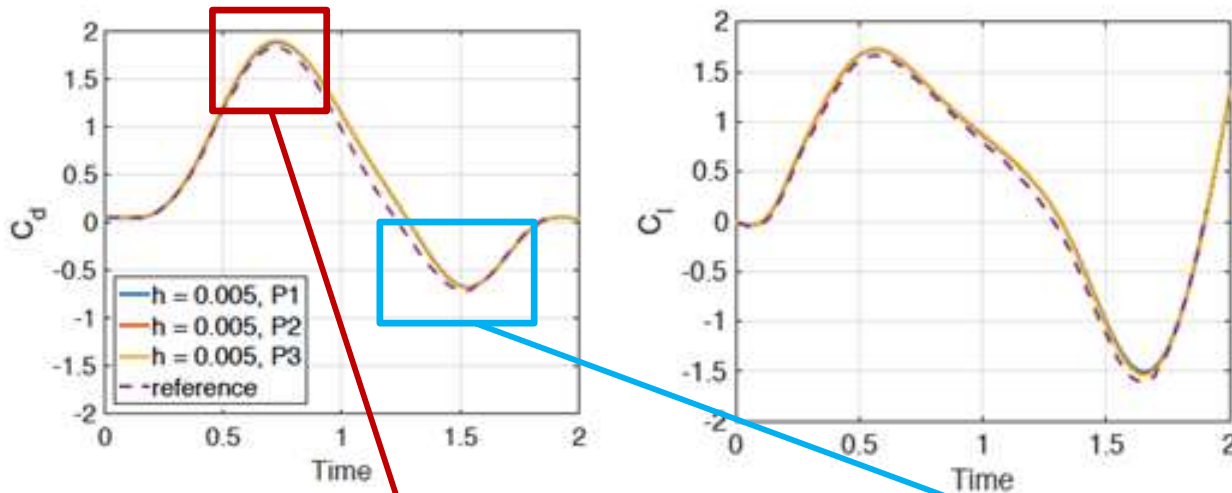
## Moving NACA0012 at Reynolds number 1000, *pitching and plunging*:



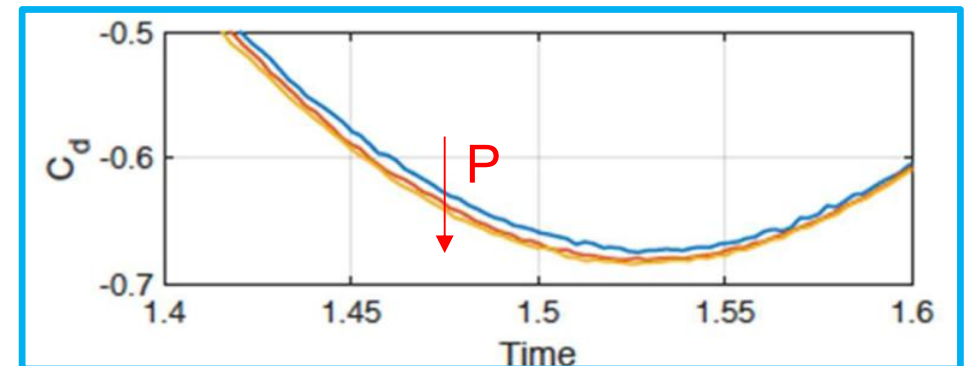
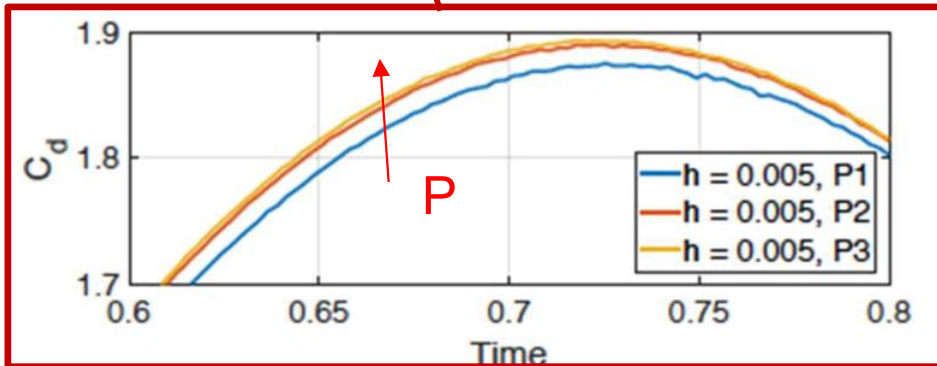
- J Kou, A Hurtado-de-Mendoza, S Joshi, S Le Clainche, **E Ferrer**, "Eigensolution analysis of immersed boundary method based on volume penalization: applications to high-order schemes", *Journal of Computational Physics*, Vol 449, 110817, 2022
- J Kou, S Joshi, A Hurtado-de-Mendoza, K Puri, C Hirsch, **E Ferrer**, "An Immersed boundary method for high-order flux reconstruction based on volume penalization", *Journal of Computational Physics*, Vol 448, 110721, 2022
- J Kou, VJ Llorente, E Valero, **E Ferrer**, "A Modified Equation Analysis for Immersed Boundary Methods based on Volume Penalization: Applications to Linear Advection-Diffusion and High-Order Discontinuous Galerkin Schemes" *Computers & Fluids*, Vol 257, 105869, 2023
- J Kou, **E Ferrer**, "A combined volume penalization / selective frequency damping for immersed boundary methods applied to high-order schemes" *Journal of Computational Physics*, Vol 472, 111678, 2023



## Moving NACA0012 at Reynolds number 1000, *pitching and plunging*:



P-adaption increases accuracy



- J Kou, A Hurtado-de-Mendoza, S Joshi, S Le Clainche, **E Ferrer**, "Eigensolution analysis of immersed boundary method based on volume penalization: applications to high-order schemes", *Journal of Computational Physics*, Vol 449, 110817, 2022
- J Kou, S Joshi, A Hurtado-de-Mendoza, K Puri, C Hirsch, **E Ferrer**, "An Immersed boundary method for high-order flux reconstruction based on volume penalization", *Journal of Computational Physics*, Vol 448, 110721, 2022
- J Kou, VJ Llorente, E Valero, **E Ferrer**, "A Modified Equation Analysis for Immersed Boundary Methods based on Volume Penalization: Applications to Linear Advection-Diffusion and High-Order Discontinuous Galerkin Schemes" *Computers & Fluids*, Vol 257, 105869, 2023
- J Kou, **E Ferrer**, "A combined volume penalization / selective frequency damping for immersed boundary methods applied to high-order schemes" *Journal of Computational Physics*, Vol 472, 111678, 2023

## Immersed boundary method (penalty)

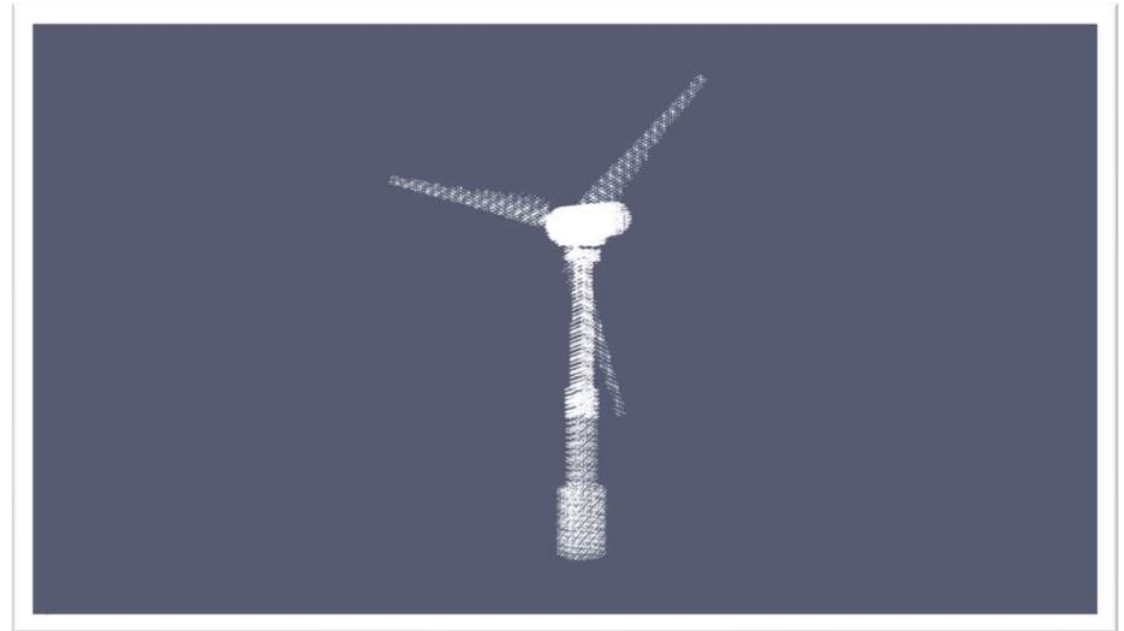
IB for rotating Wind turbine



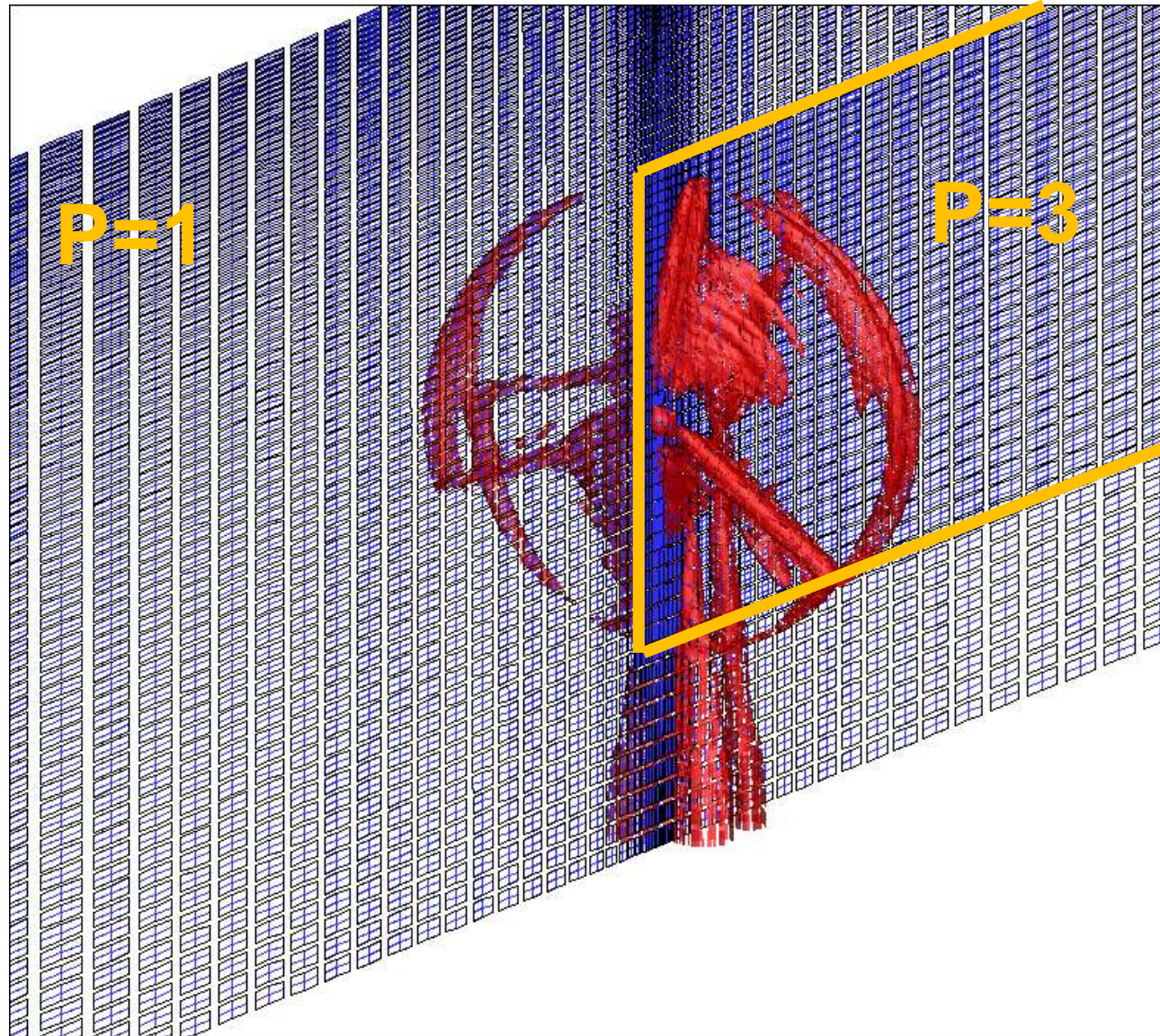
**Only CAD '.stl' file**  
for the wind turbine

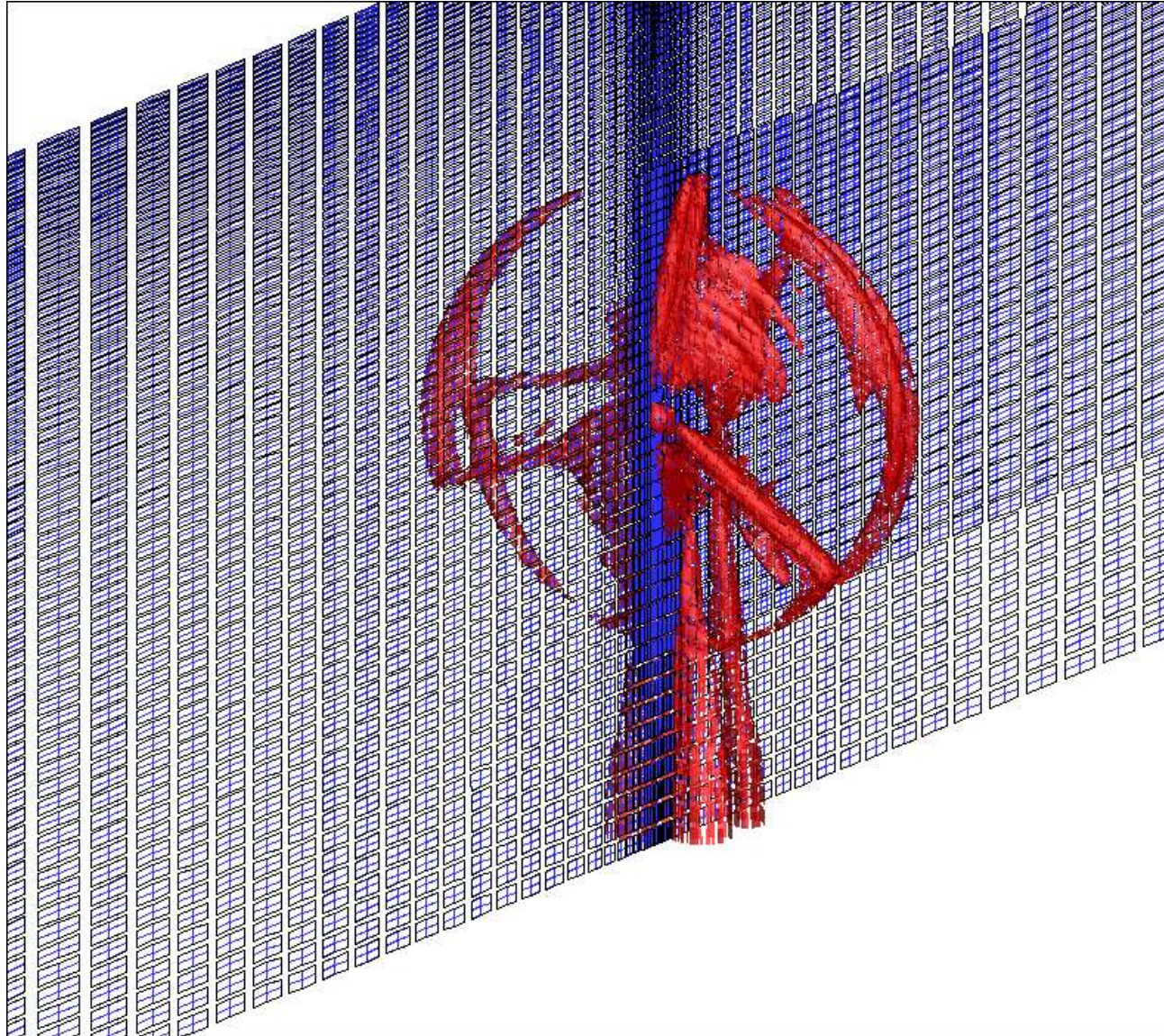
&

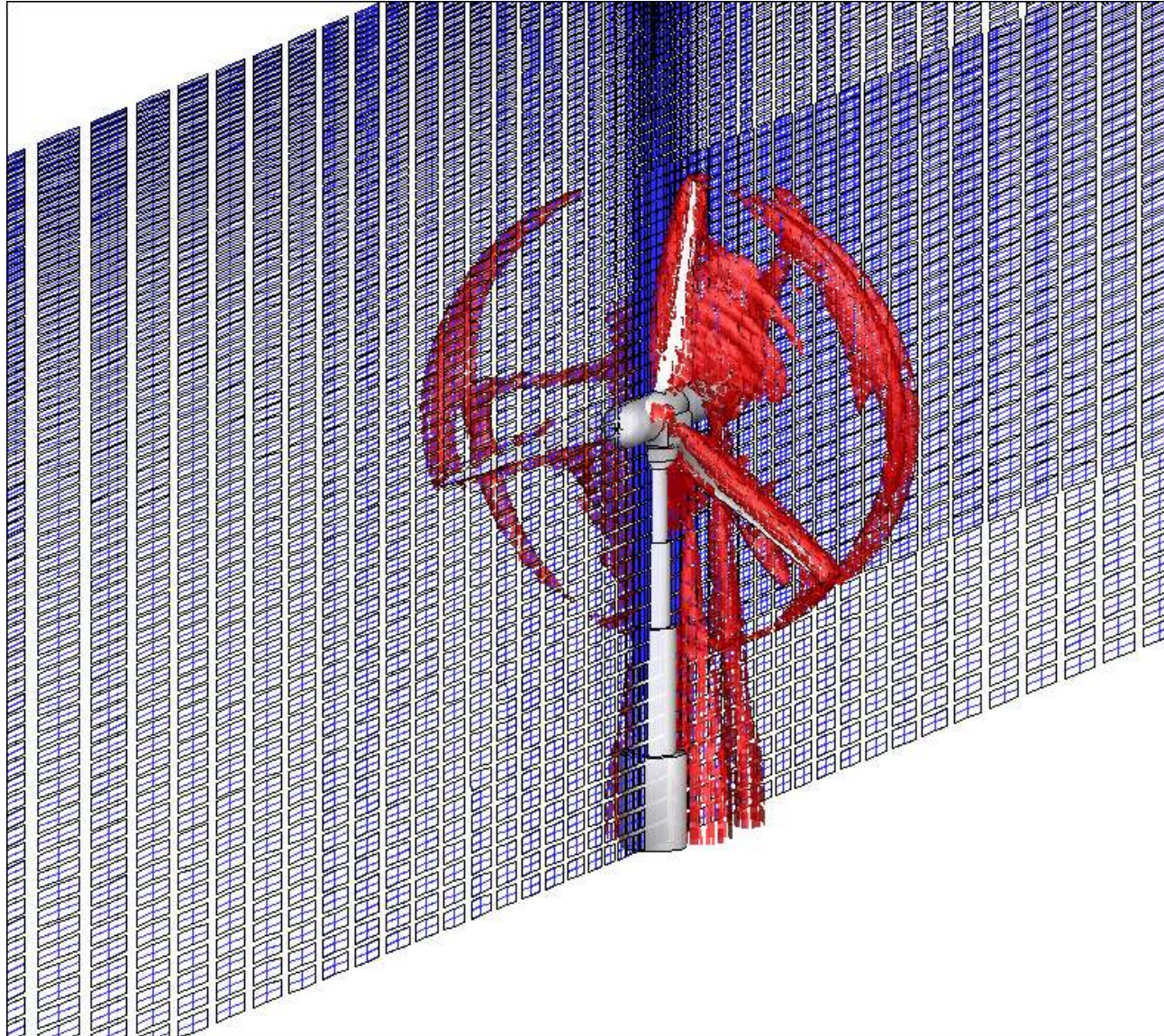
**Simple Cartesian mesh**

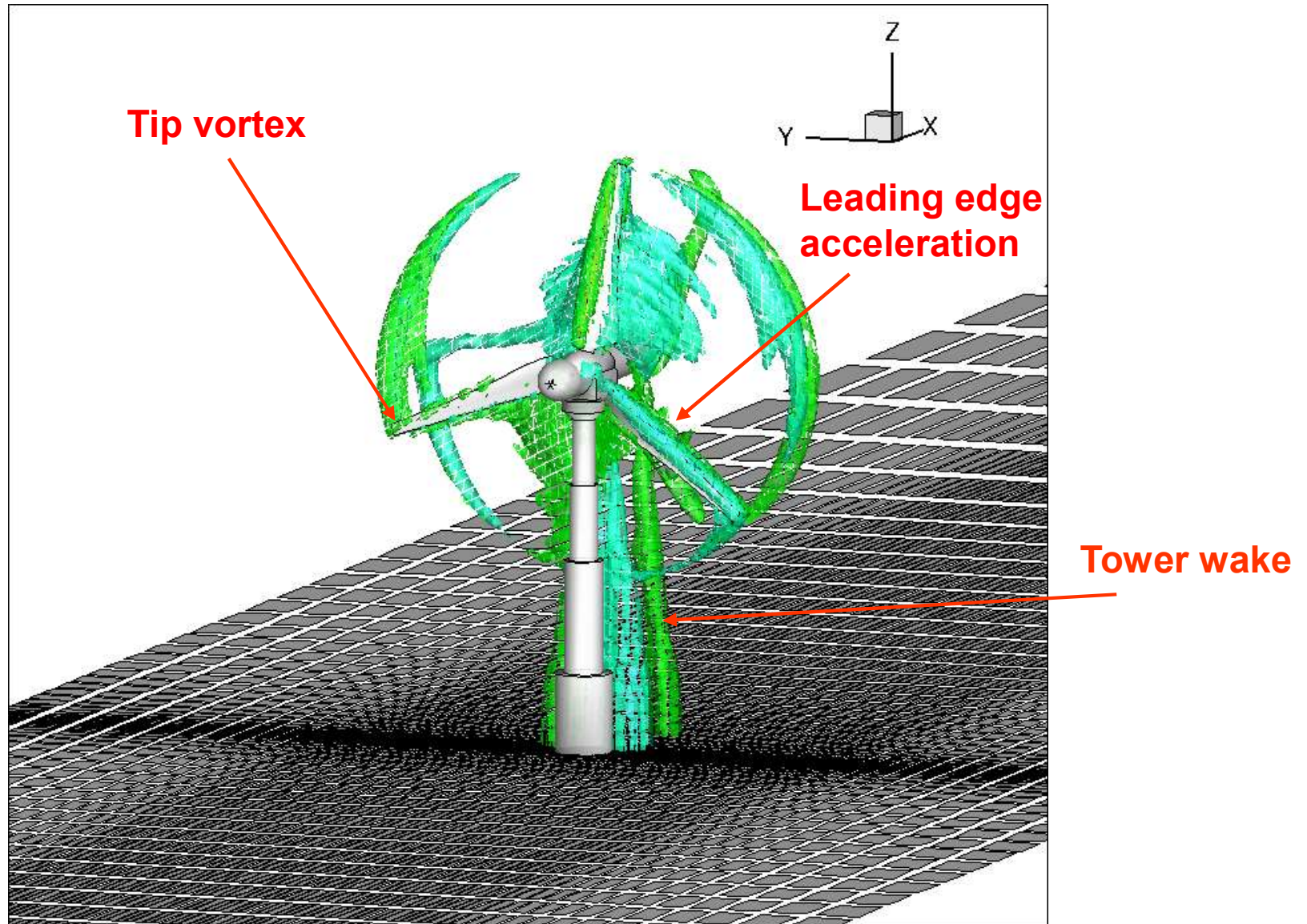


Penalty points for the wind turbine



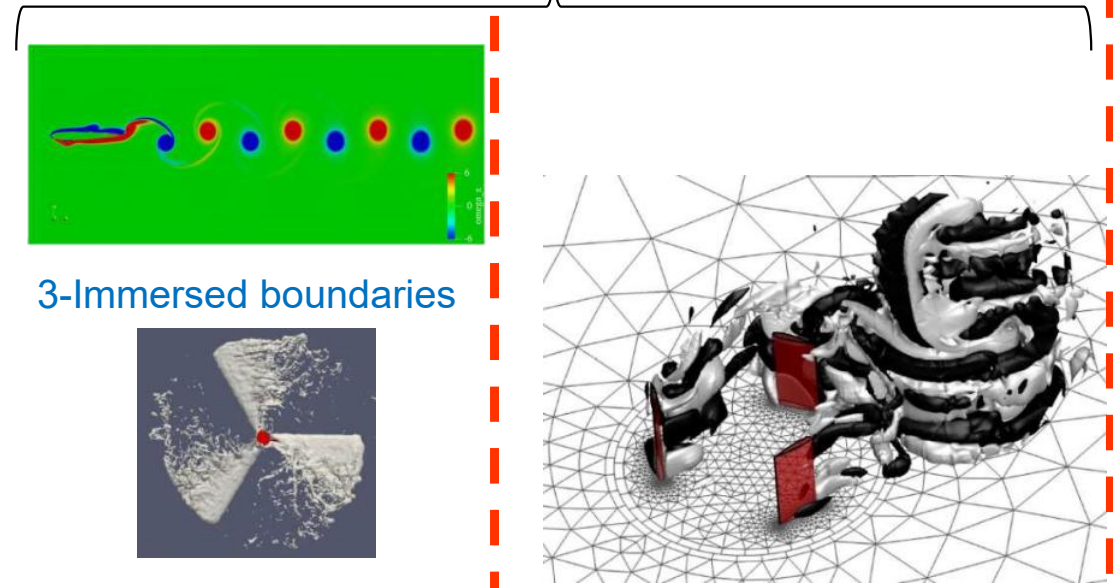
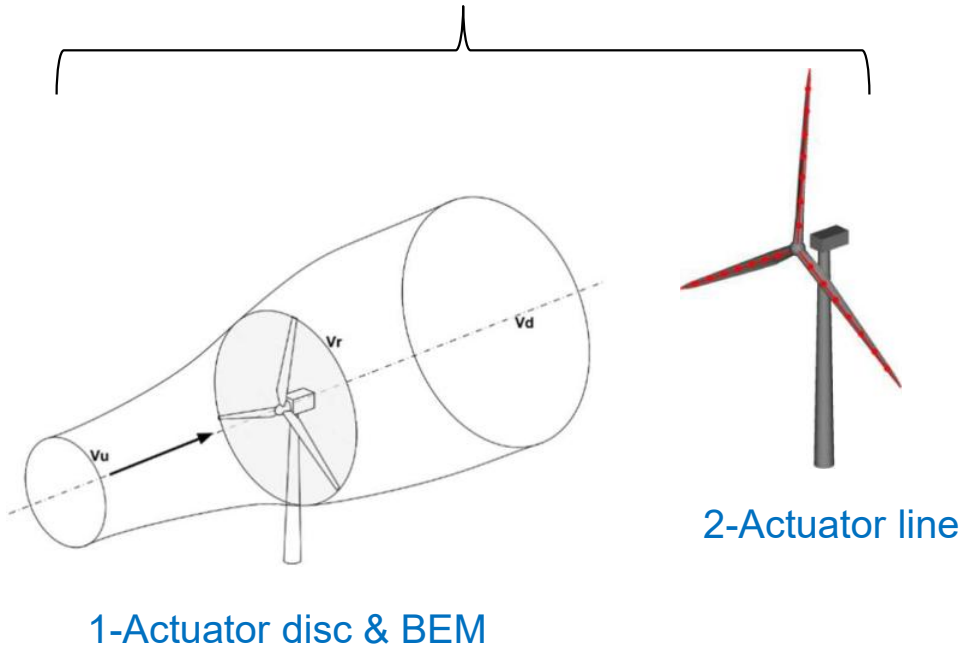






Require 2D aerodynamic data

Explicit 3D geometry



Cost

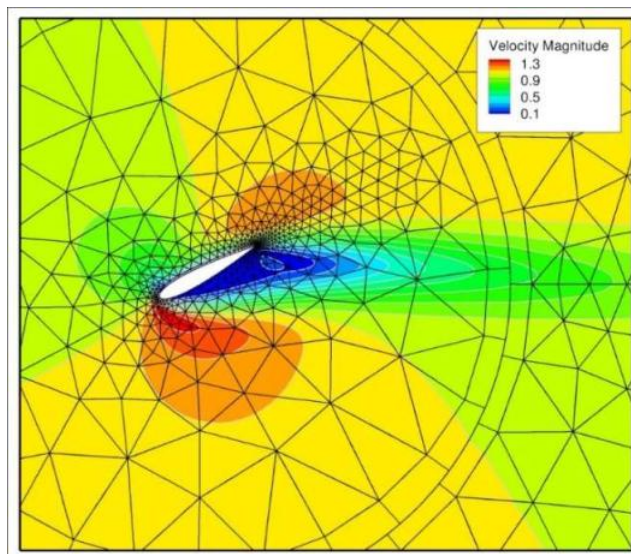
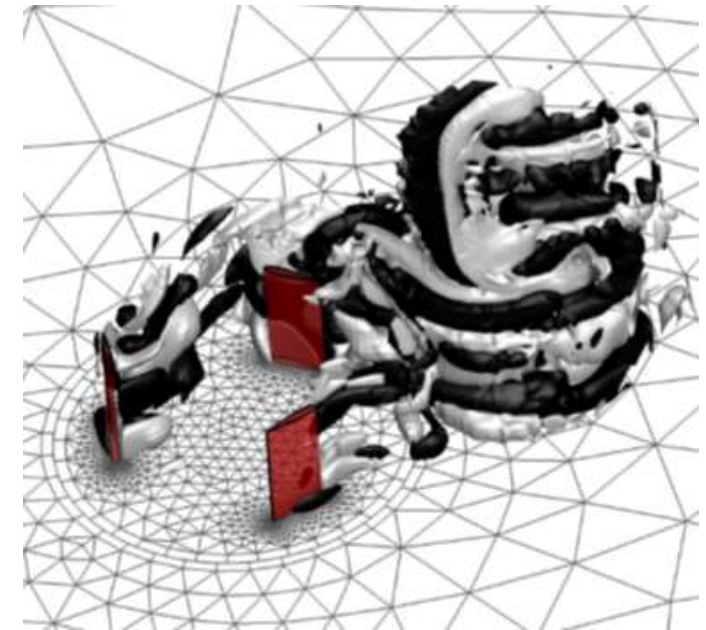
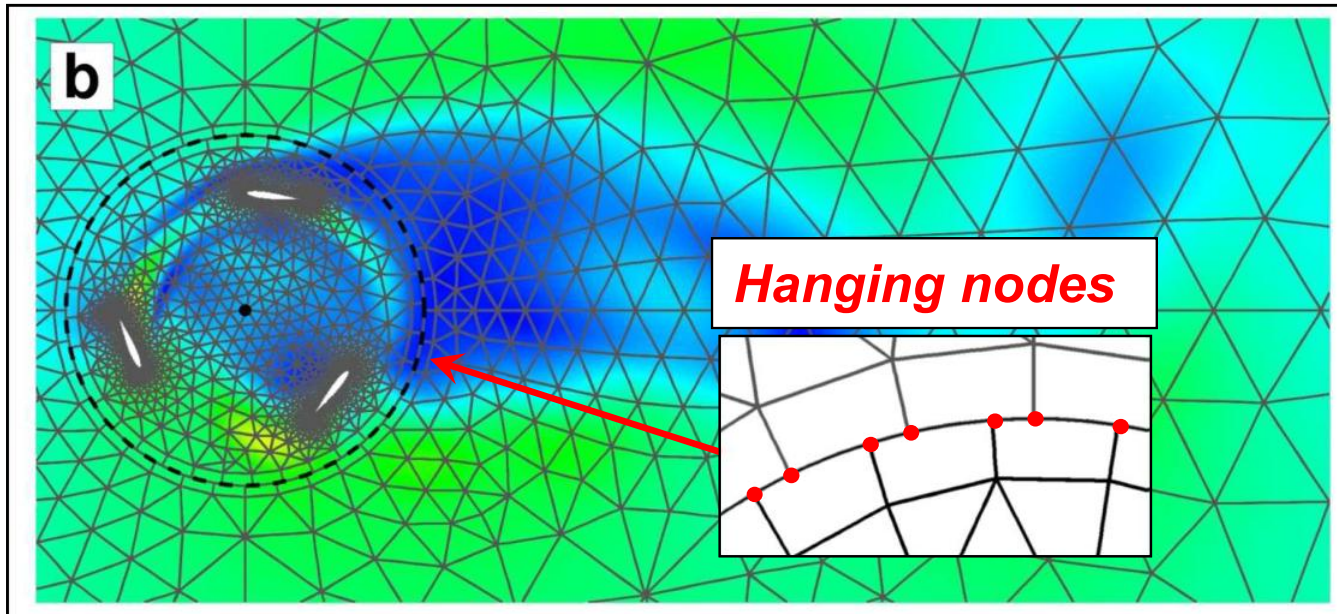
Accuracy

Low

High

- 4- E Ferrer and RHJ Willden, A high order Discontinuous Galerkin - Fourier incompressible 3D Navier–Stokes solver with **rotating sliding meshes**, *Journal of Computational Physics*, 2012
- 4- E Ferrer, RHJ Willden, Blade–wake interactions in **cross-flow turbines**, *International Journal of Marine Energy*, 2015
- 3- J Kou, A Hurtado-de-Mendoza, S Joshi, S Le Clainche, E Ferrer, Eigensolution analysis of **immersed boundaries** for high-order schemes, *Journal of Computational Physics*, 2022
- 3- J Kou, S Joshi, A Hurtado-de-Mendoza, K Puri, C Hirsch, E Ferrer, An **Immersed boundary** method for high–order flux reconstruction, *Journal of Computational Physics*, 2022
- 2 & 3- E Ferrer, S Colombo, O Marino, “Aeroacoustic predictions of wind turbines based on **actuator lines and immersed boundaries**”, *Under review at Wind Energy*
- 1- E Ferrer, S Le Clainche, **Simple models for cross flow turbines**, in *Recent advances in CFD for Wind and Tidal Offshore Turbines*, 2019
- 1- E Ferrer, OMF Browne, E Valero, Sensitivity analysis to control the far–wake unsteadiness behind **turbines**, *Energies*, 2017

## High order sliding meshes



DG solution  
Rotating NACA0015  
Re=100  
Rot speed=0.3  
polynomial order  
k=5



# Summary

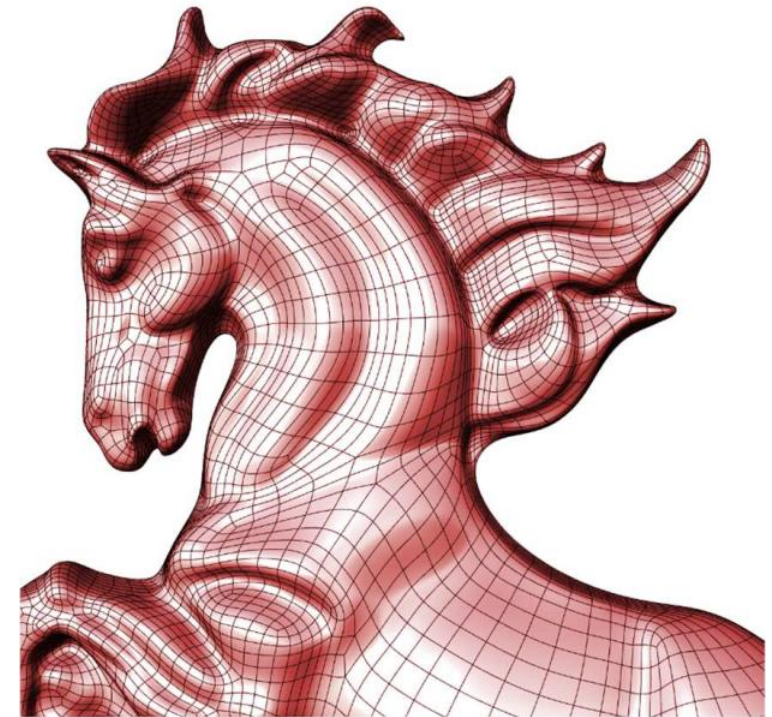
## 1- Introduction to DG & Horses3d

## 2- Multiphysics

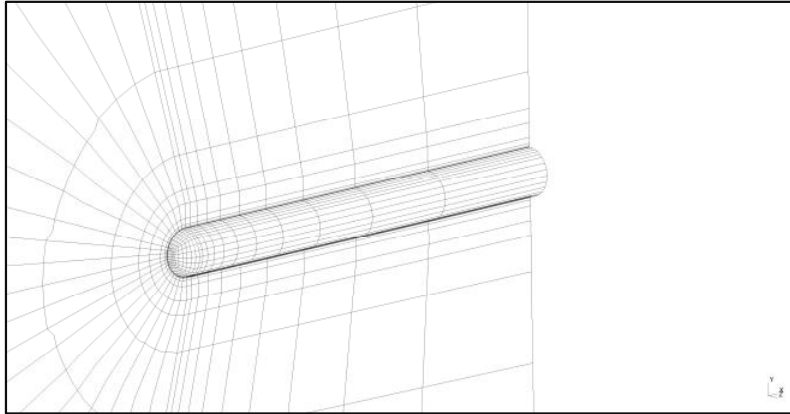
- Wind turbines
- Turbulence

## 3. Machine Learning + CFD

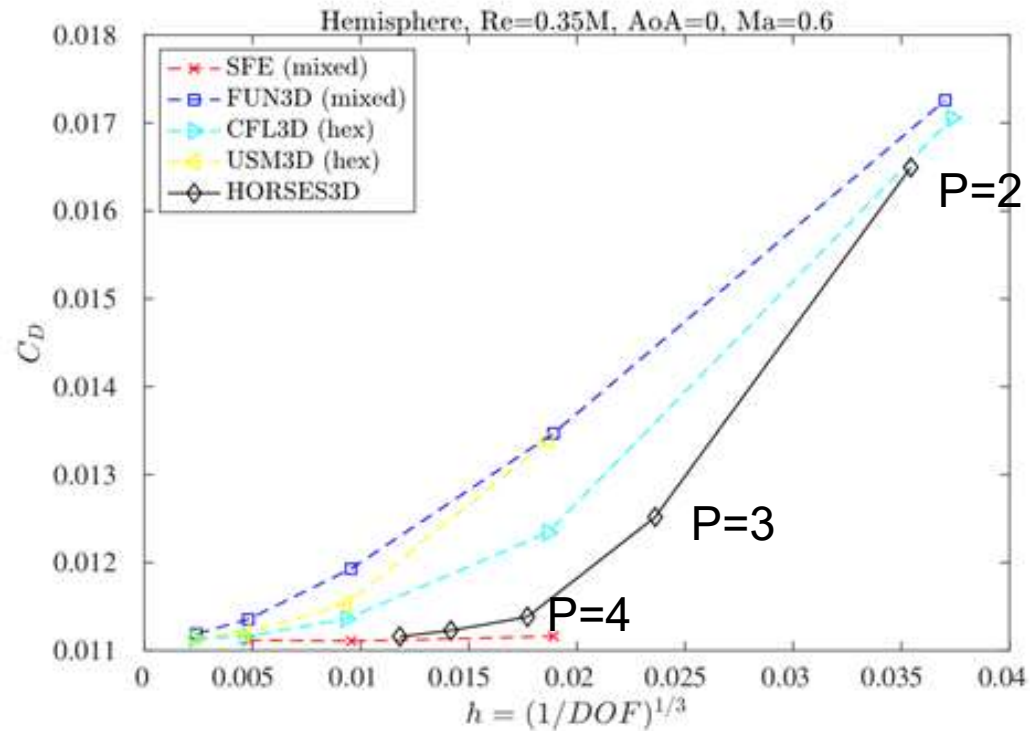
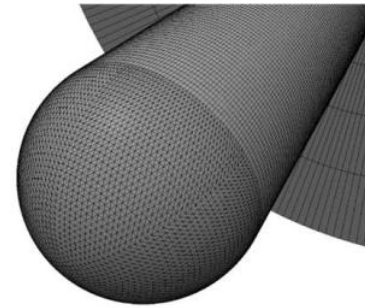
- Mesh adaption
- NN acceleration
- RL for automation



# High order RANS (SAneg)

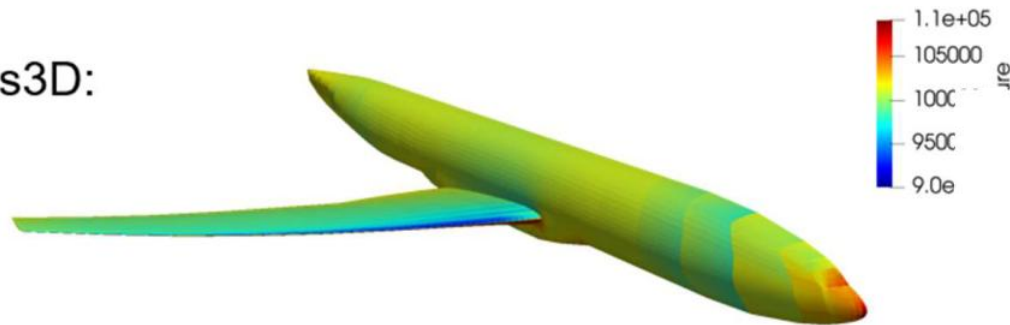


NASA workshop  
[https://turbmodels.larc.nasa.gov/hc3dnumerics\\_val.html](https://turbmodels.larc.nasa.gov/hc3dnumerics_val.html)

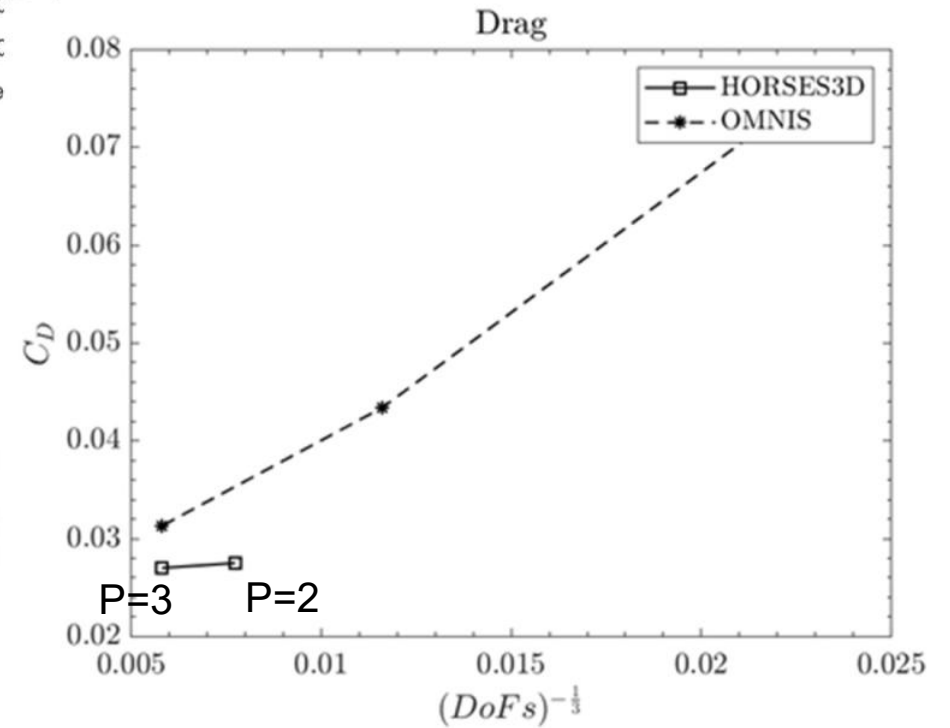
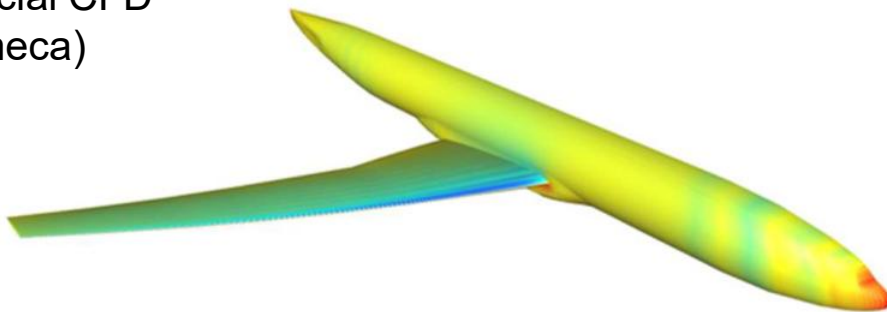


# High order RANS (SAneg)

Horses3D:



Commercial CFD (Numeca)



CRM Family Of Models

From Left to Right: High-Speed CRM, High-Lift CRM, CRM with NLF wing and Icing Research Tunnel CRM.

Re=1.000.000  
AoA = 0 deg



Re=1.000.000  
AoA = 5 deg

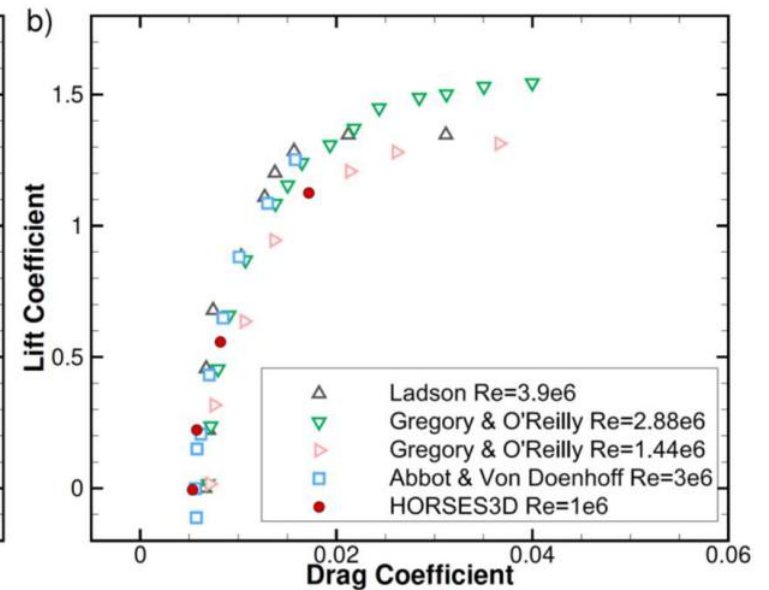
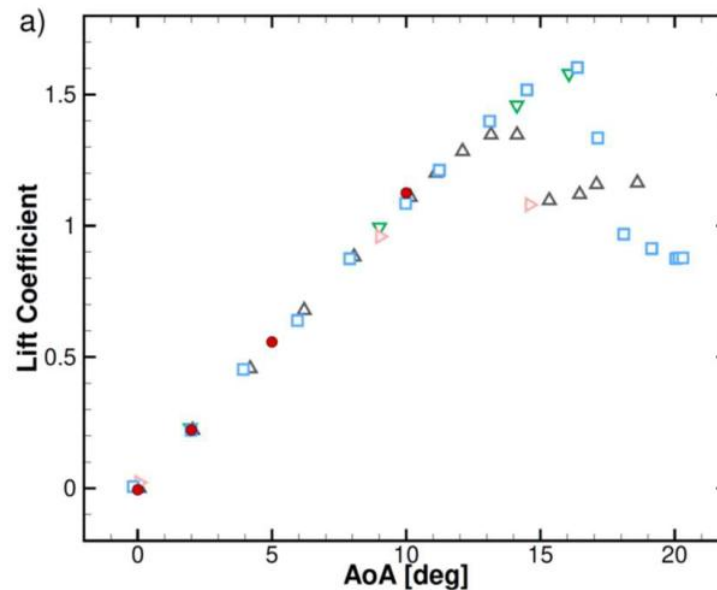


contours of velocity: [0.85; 1.2]

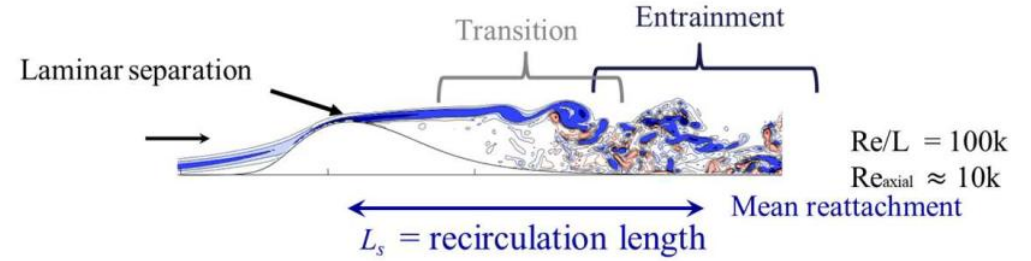
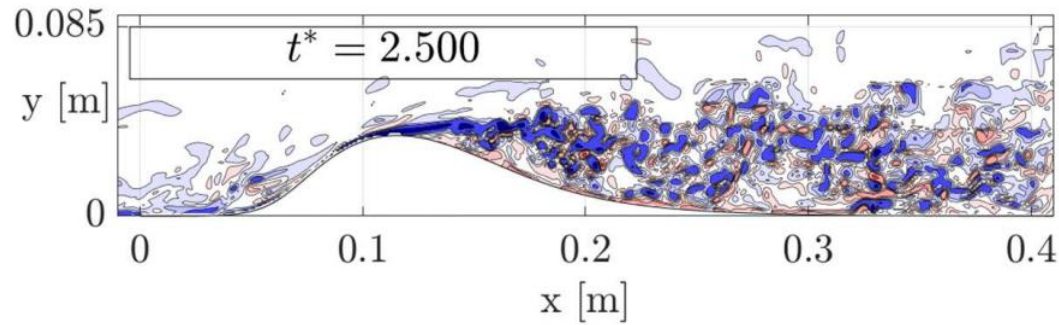
## Implicit LES

### NACA0012 at various AoAs

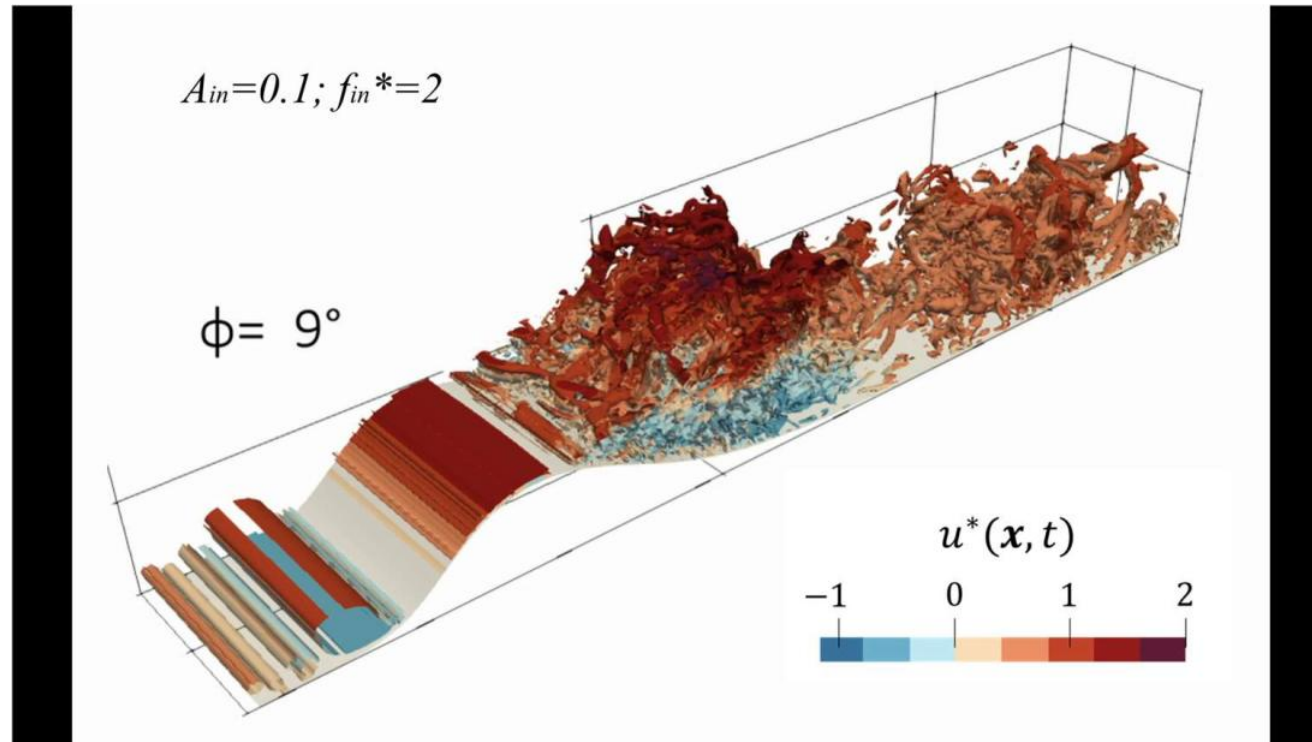
Re=1.000.000  
AoA = 10 deg



HORSES3D: Compressible DGSEM – energy-stable - SBP-SAT & Roe fluxes & BR1

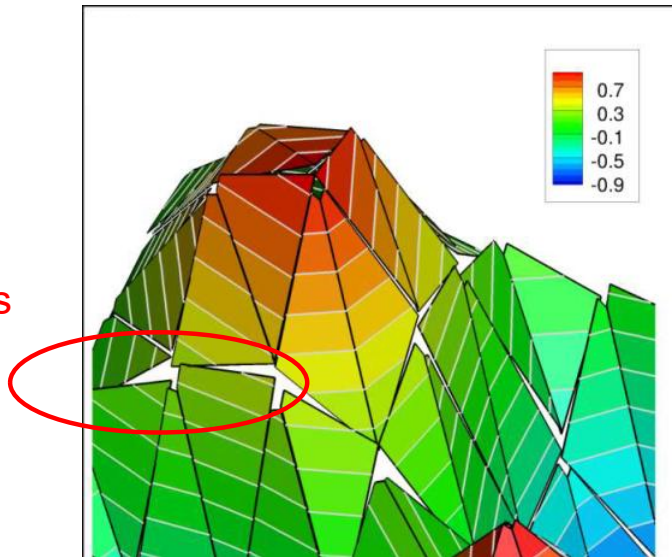


## Implicit LES

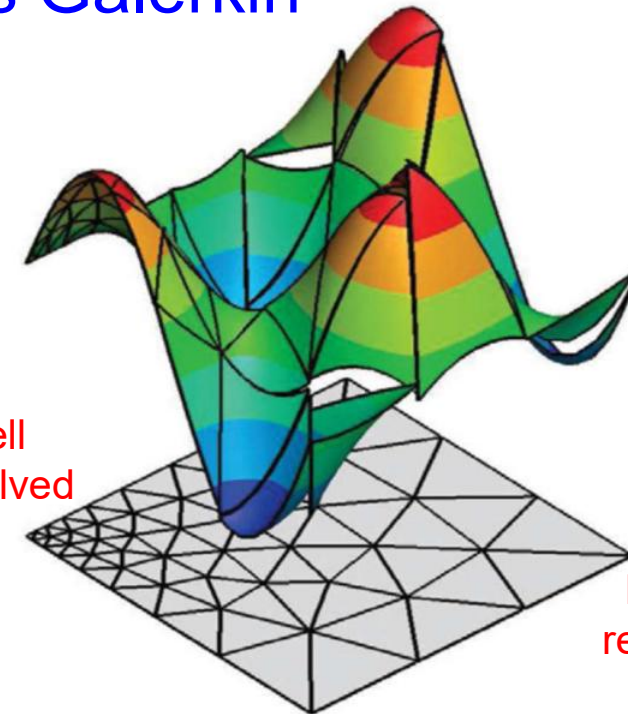


# New turbulent models for discontinuous Galerkin

Discontinuous  
solutions



well  
resolved

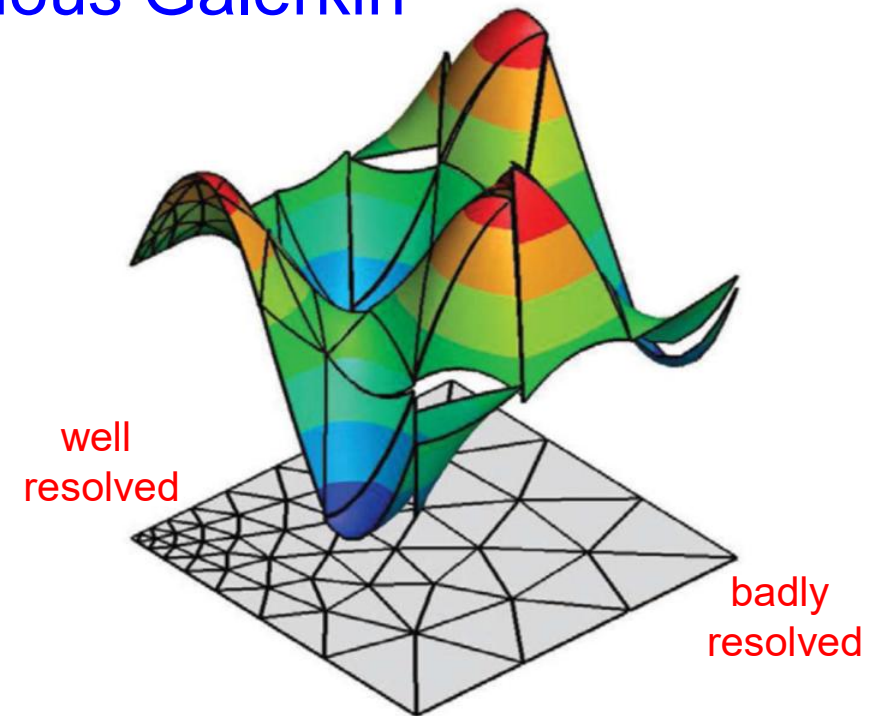
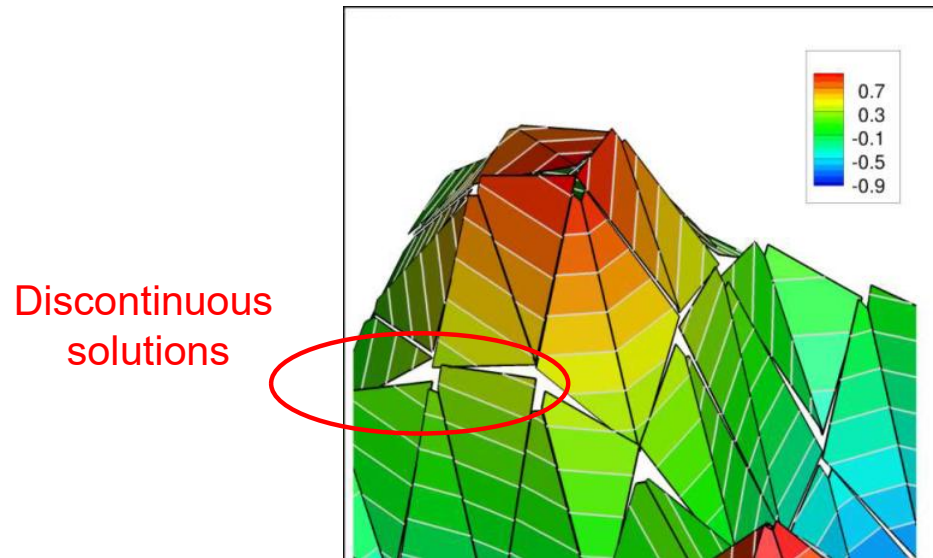


badly  
resolved

J Kou, OA Marino, **E Ferrer**, "Jump penalty stabilisation techniques for under-resolved turbulence in DG schemes" *Journal of Computational Physics*, Vol 491, 112399, 2023

**E Ferrer**, "An interior penalty stabilised incompressible DG–Fourier solver for implicit Large Eddy Simulations", *Journal of Computational Physics*, Vol 348, 2017

# New turbulent models for discontinuous Galerkin



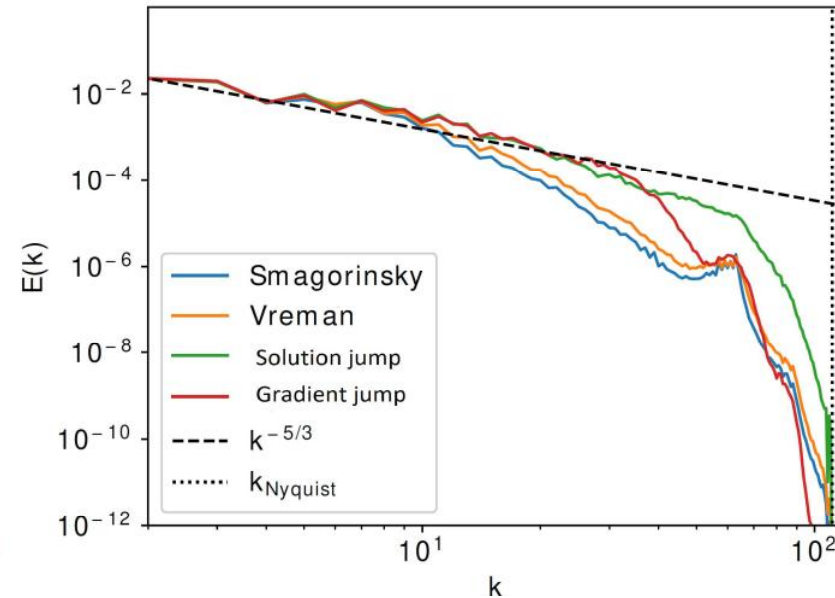
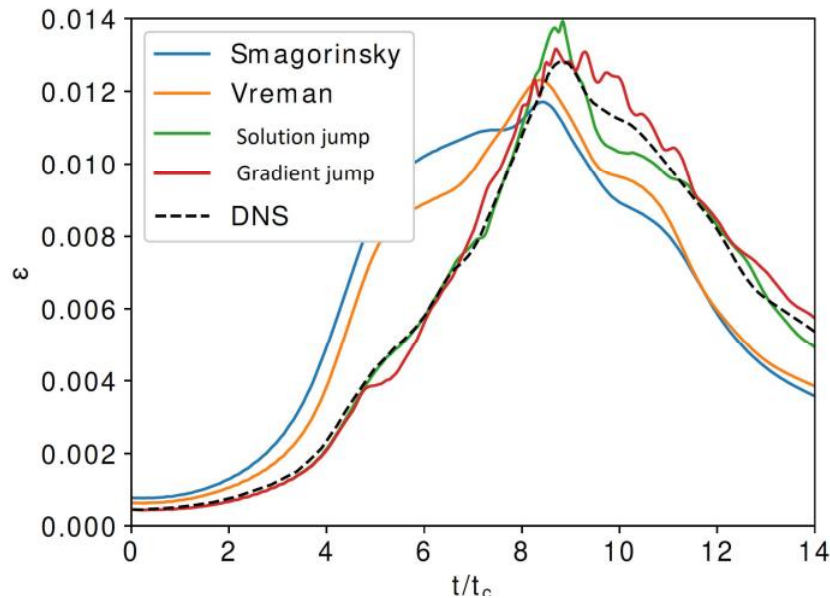
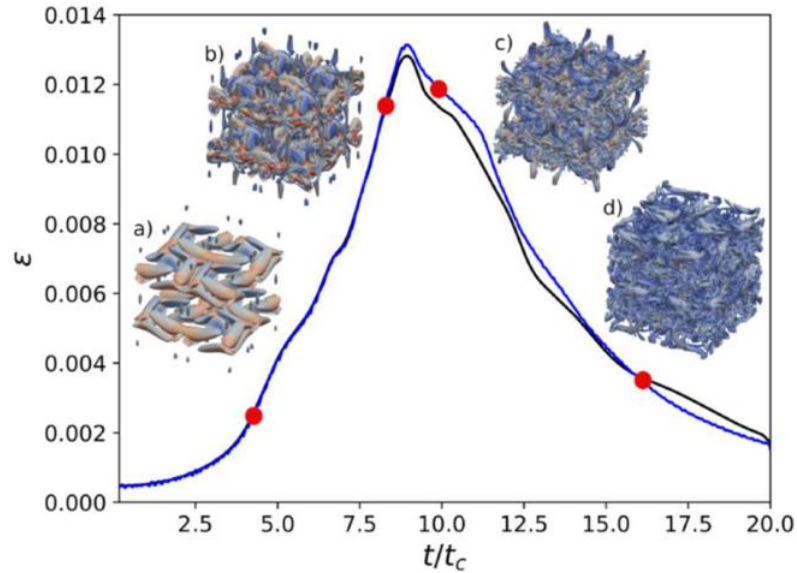
Viscosity proportional to jumps (associated to under-resolution)

Solution:  $\frac{\tau_s}{Re} \int_{\partial\Omega_n} [\tilde{\mathbf{q}}] \phi_i$  Ferrer 2017

Gradients:  $-\frac{\tau_g h^2}{Re} \int_{\partial\Omega_n} [\nabla \tilde{\mathbf{q}}] \nabla \phi_i \cdot \mathbf{n}$  Burman et al 2010  
Moura et al 2022

# New turbulent models for discontinuous Galerkin

## Taylor Green Vortex Re=1600





# Summary

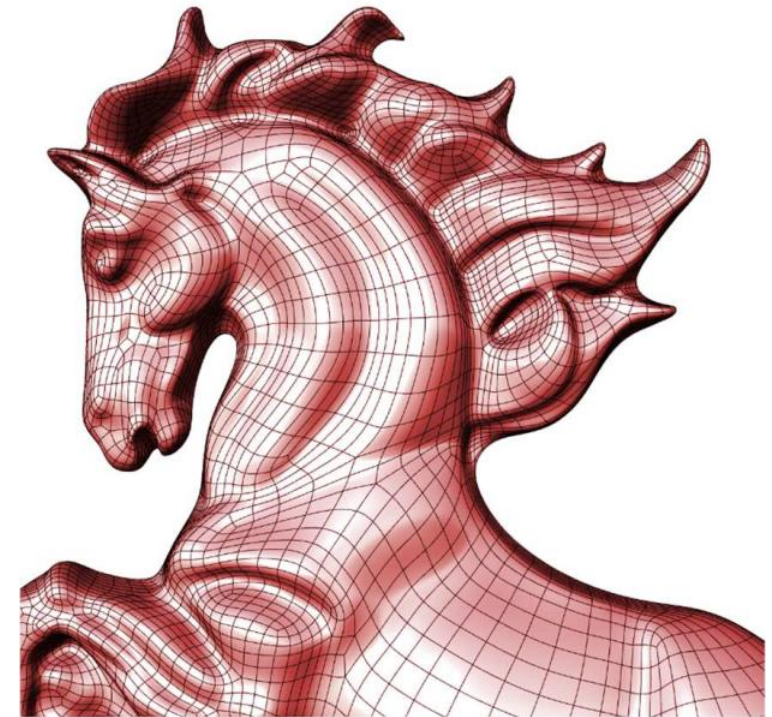
## 1- Introduction to DG & Horses3d

## 2- Multiphysics

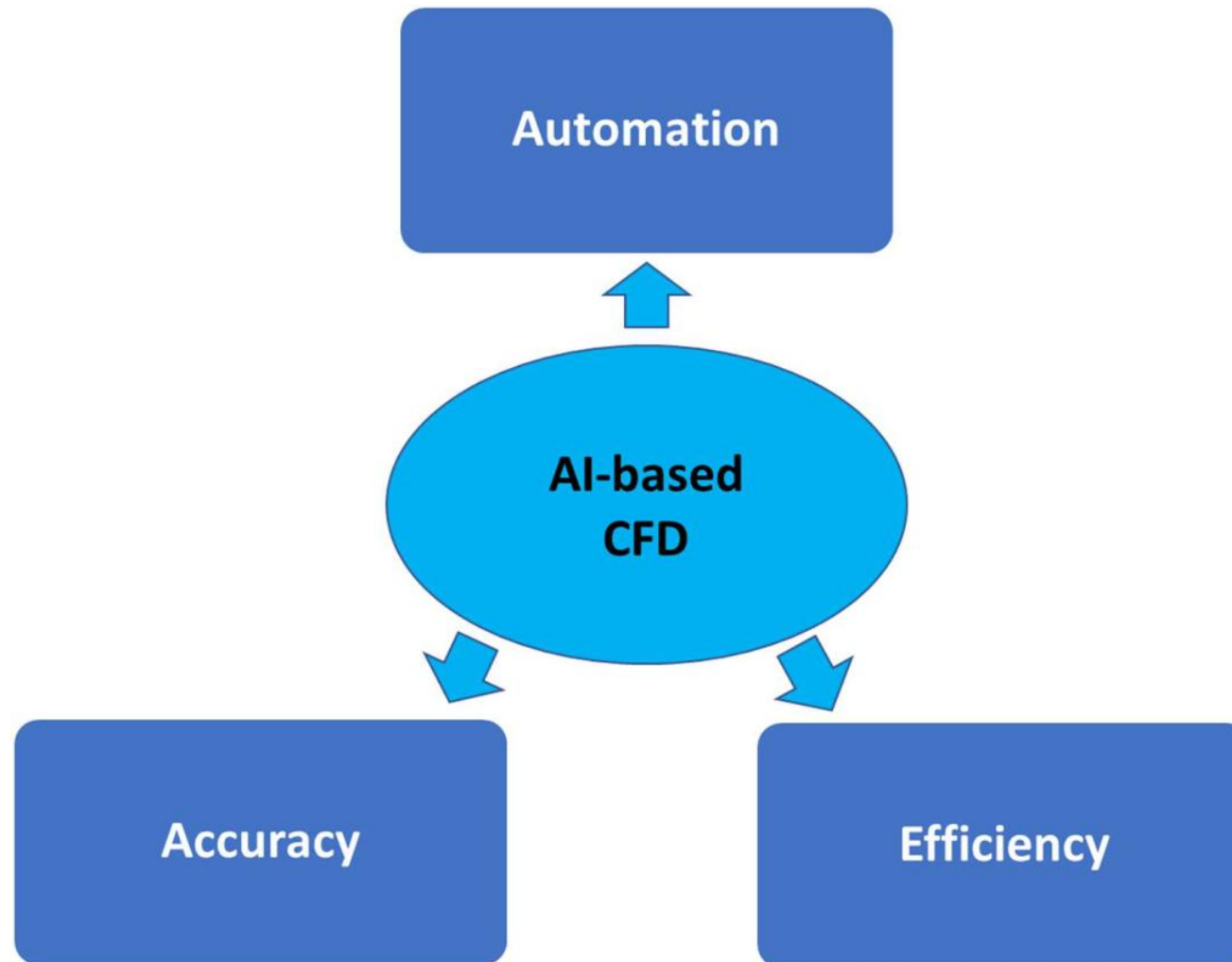
- Wind turbines
- Turbulence

## 3. Machine Learning + CFD

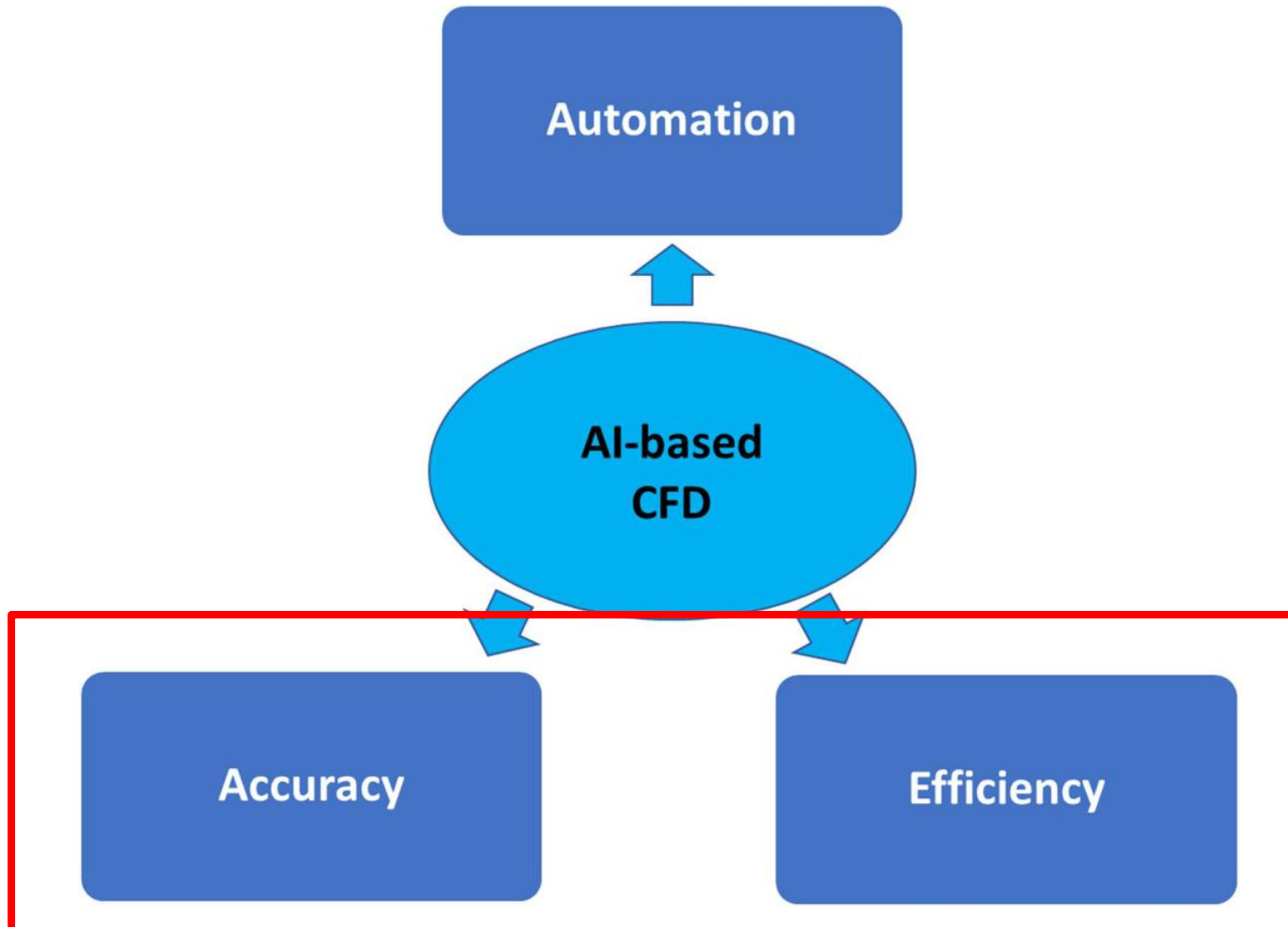
- Mesh adaption
- NN acceleration
- RL for automation



# Towards AI-based Computational Fluid Dynamics

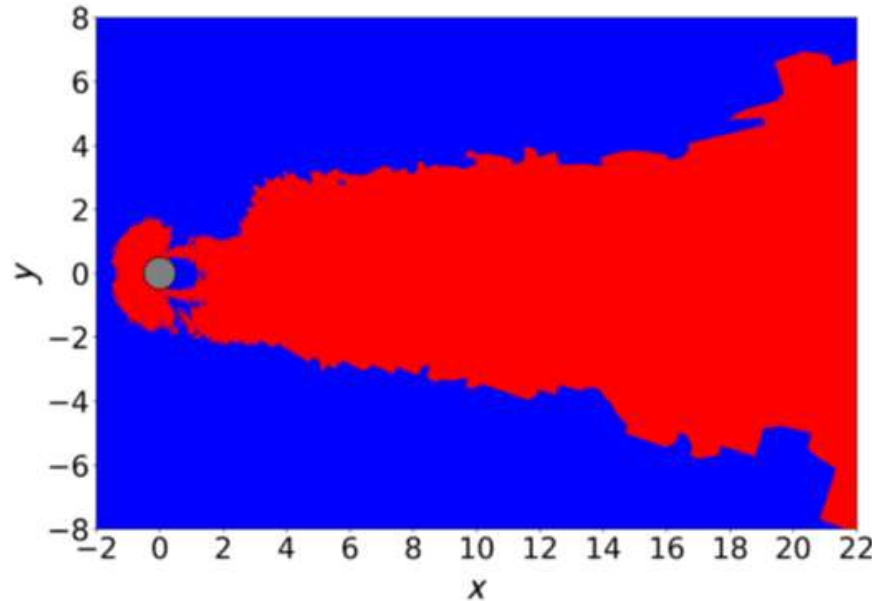


# Towards AI-based Computational Fluid Dynamics

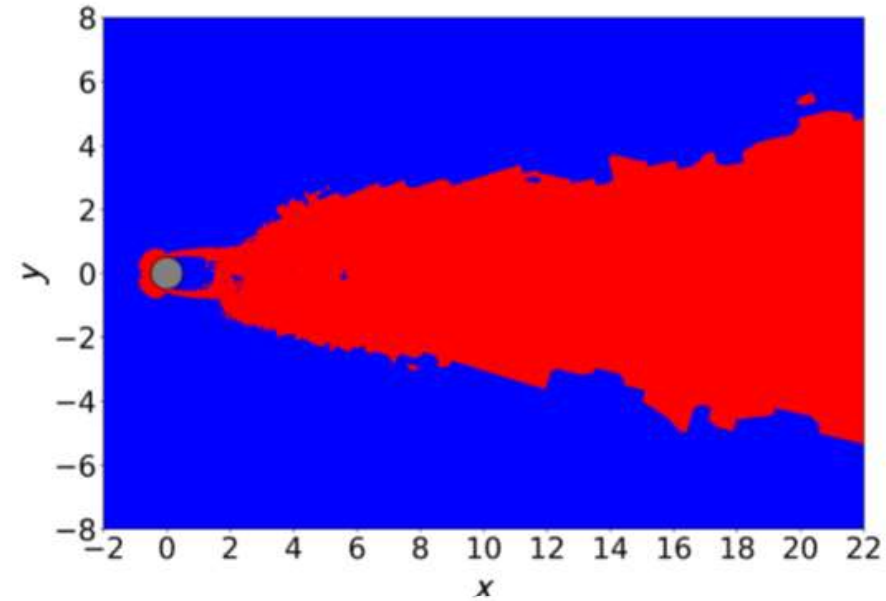


# Machine Learning to detect flow regions

$F=1.25$

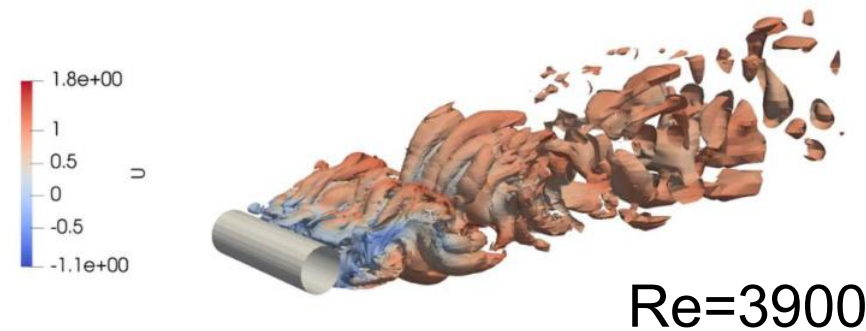


$F=1.5$



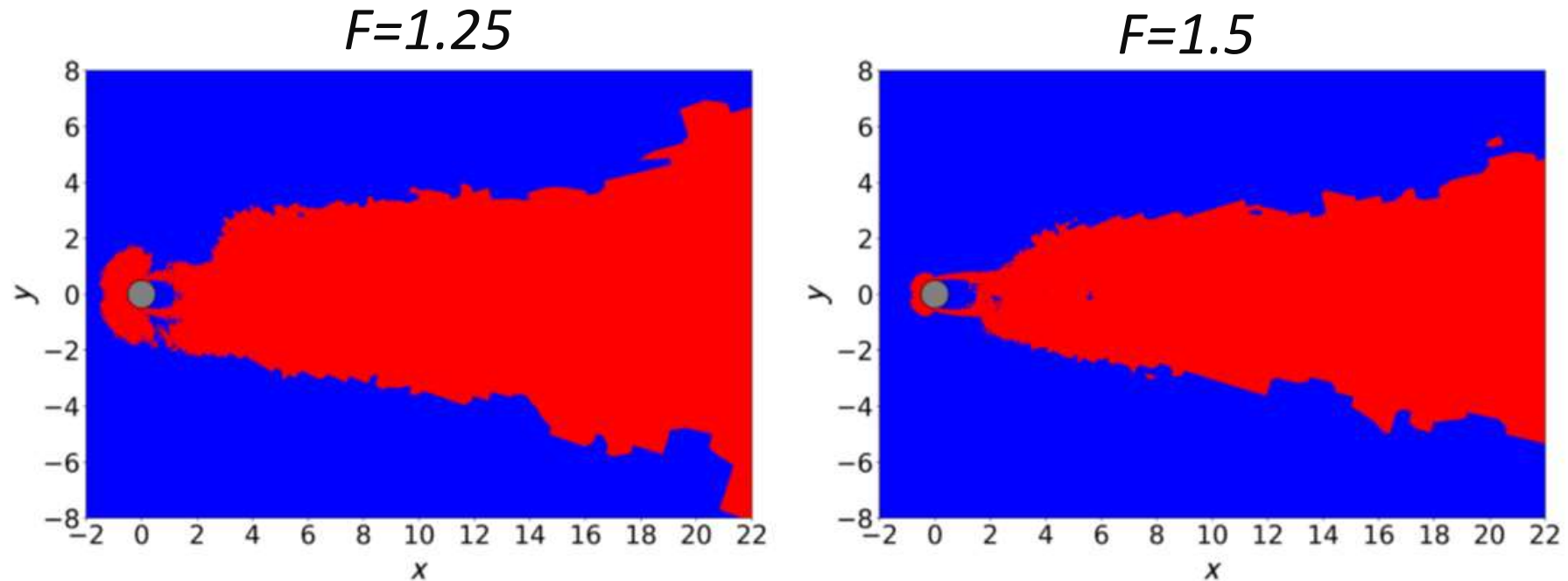
Feature based sensors  
Eddy viscosity sensor

$$F_{\mu_t} = \frac{\mu + \mu_t}{\mu}$$



$Re=3900$

## Machine Learning to detect flow regions



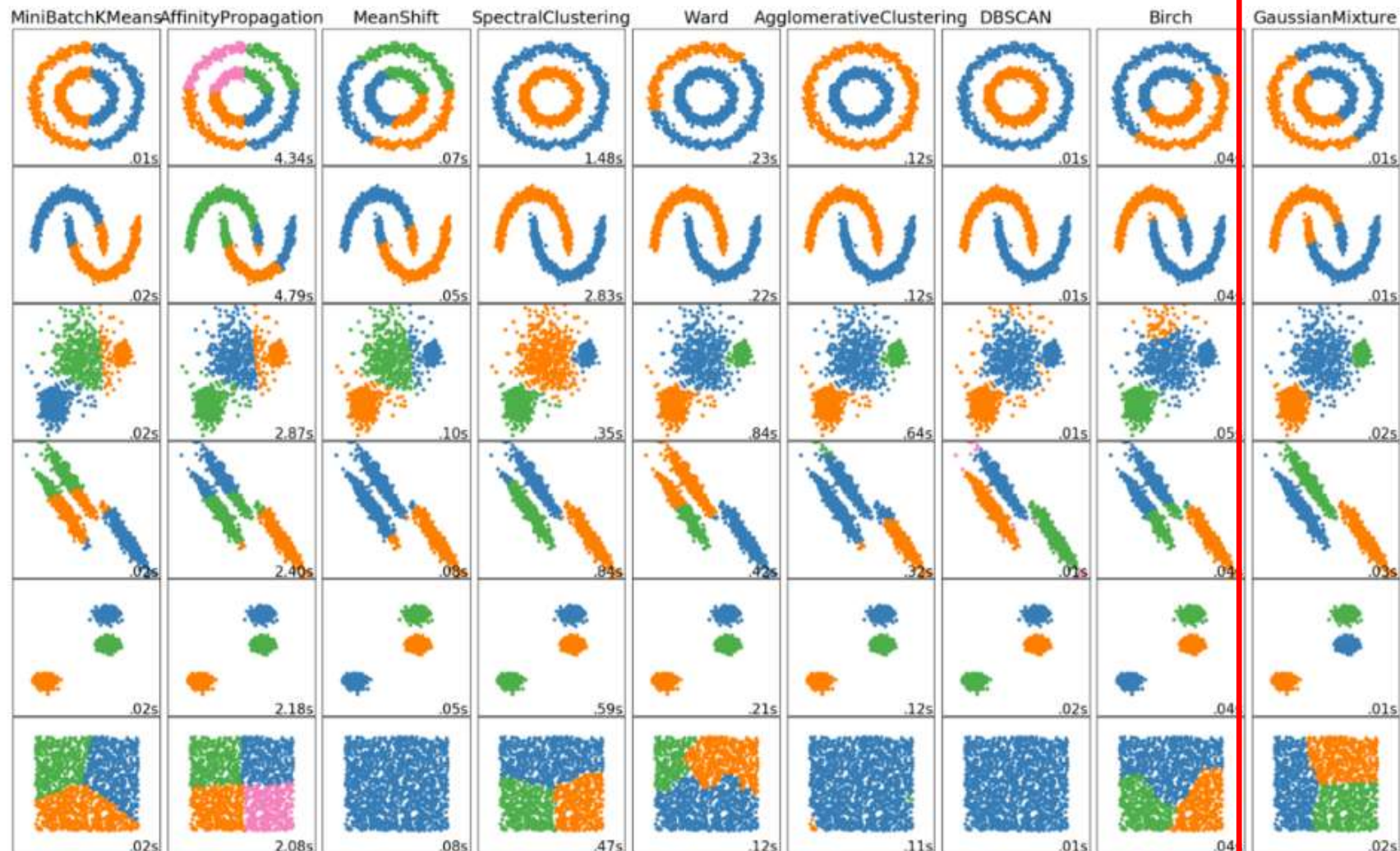
**Feature based sensors**  
**Eddy viscosity sensor**

$$F_{\mu_t} = \frac{\mu + \mu_t}{\mu}$$

- Very sensitive to **threshold**
- Cannot detect **mixed regions**  
**(e.g. laminar-turbulent)**

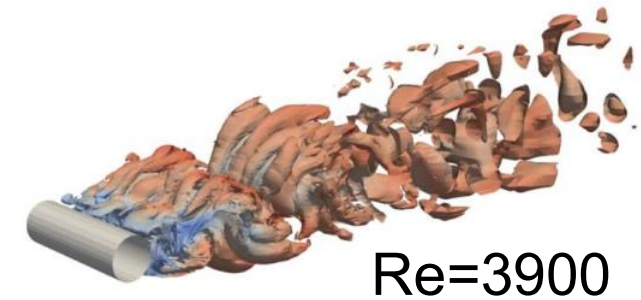
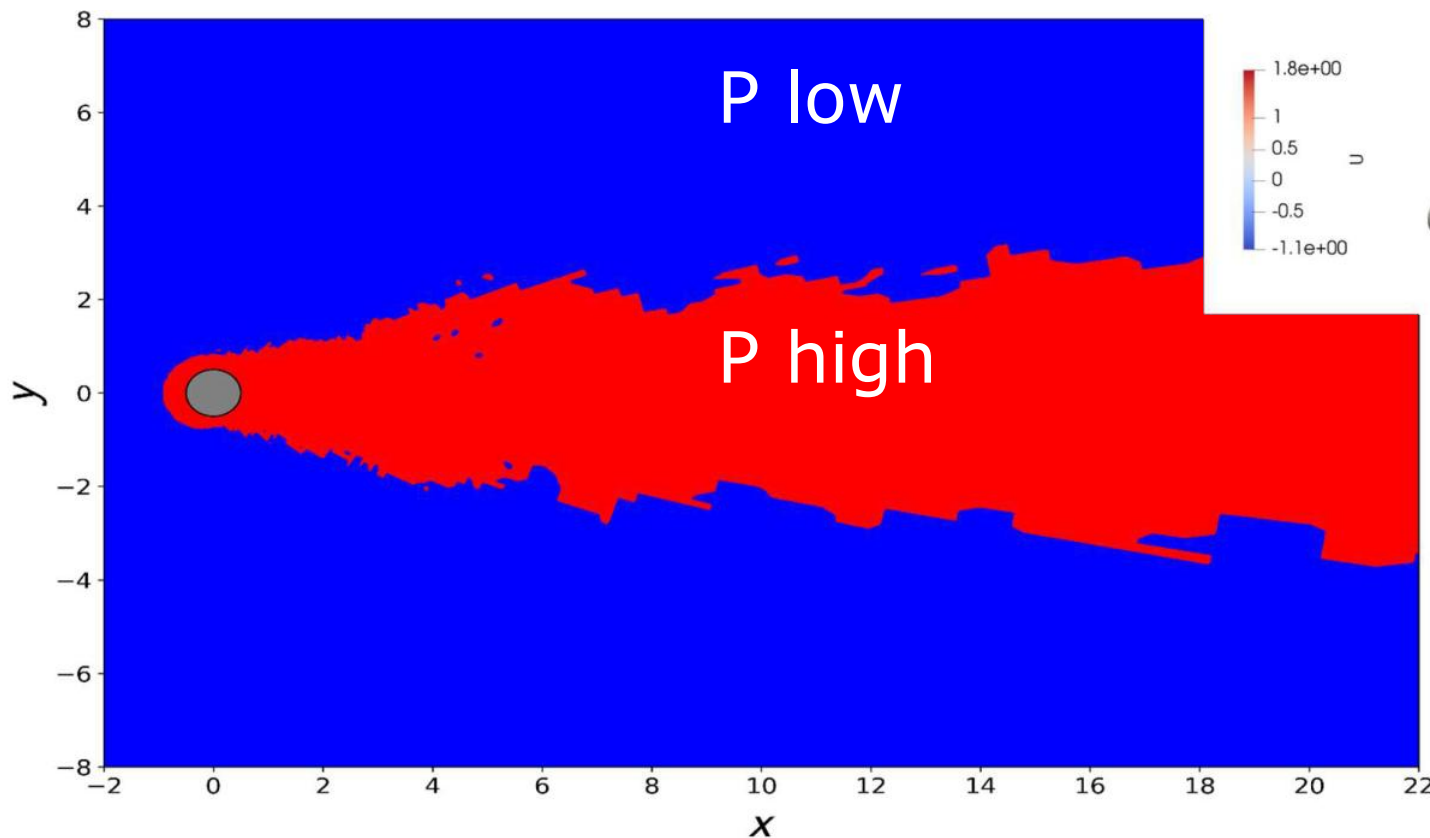
# Machine Learning to detect flow regions

## Clustering (classify data): Gaussian mixture model



# Machine Learning to detect flow regions

## Clustering (classify data): Gaussian mixture model



Automate the detection  
(no thresholds)

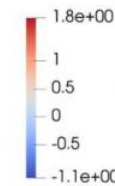
**Use a robust feature space  
for a variety of Re**

Invariants of strain and rotational  
rate tensors

# Machine Learning to detect flow regions

## Clustering: Gaussian mixture model

	St	$C_d$	$L_r$	$L_z \setminus D$
Uniform P3	0.202	0.7844	1.36	$\pi$
Uniform P4	0.203	0.9513	1.64	$\pi$
Cluster-Adapt P4-P2	0.204	0.9506	1.63	$\pi$
Parnadeau et al. [40]	0.208	-	1.56	$\pi$
Snyder and Degrez [45]	0.207	1.09	1.30	$\pi$
Kravchenko and Moin [46]	0.210	1.04	1.35	$\pi$
Breuer [47]	-	1.07	1.20	$\pi$
Franke and Frank [48]	0.209	0.98	1.64	$\pi$
(DNS) Ma et al. [41]	0.219	1.59	-	$\pi$
Ouvrard et al. [49]	0.223	0.94	1.56	$\pi$

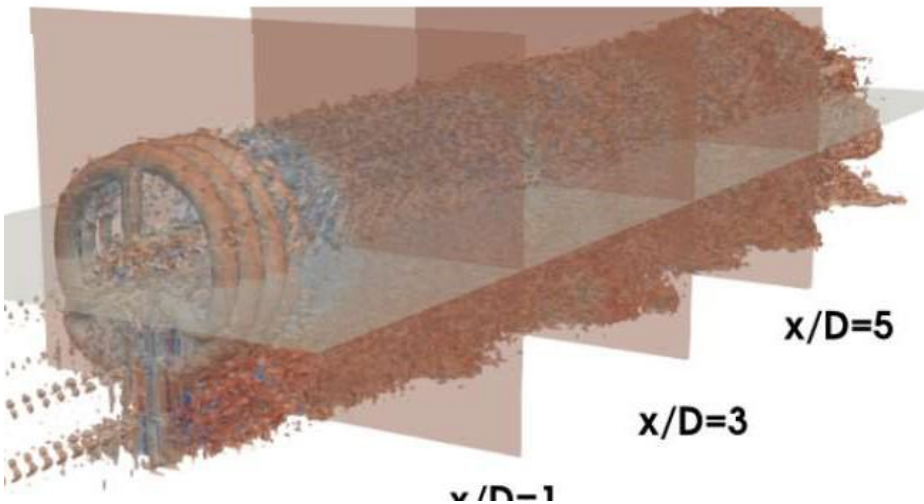
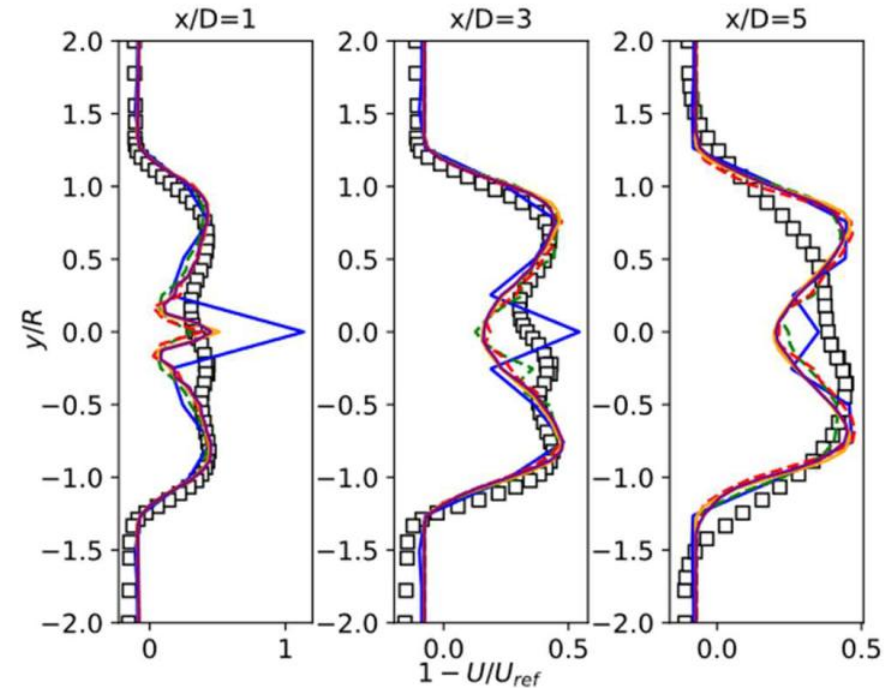
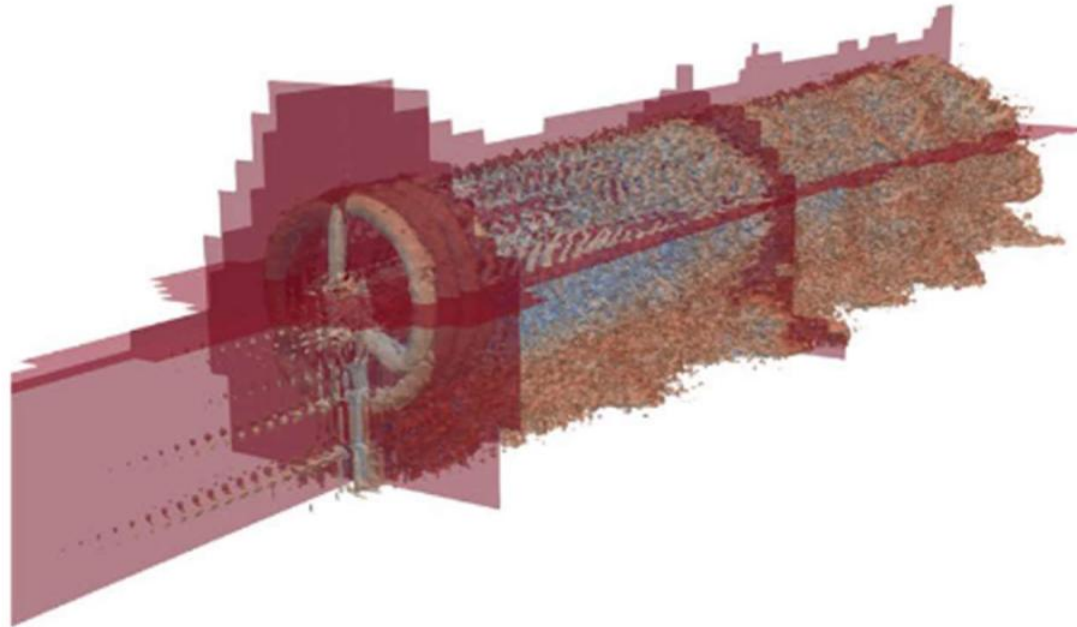


Re=3900

	DoFs	reduction of DoFs	reduction of comp. time
Cluster-Adapt P4-P2	1.55M	41%	33%

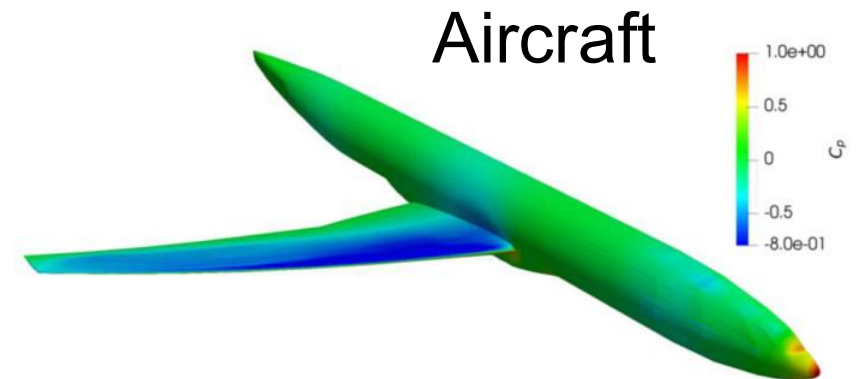
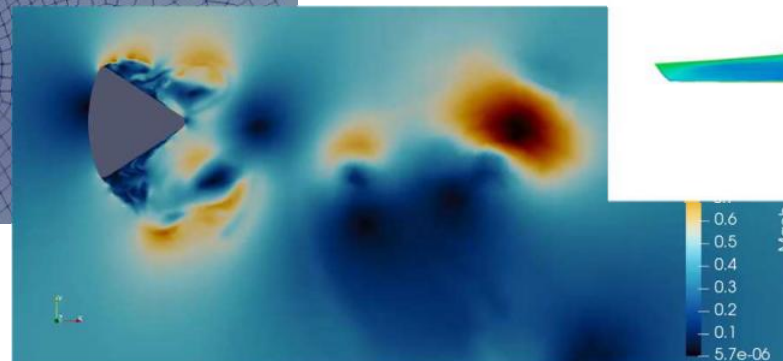
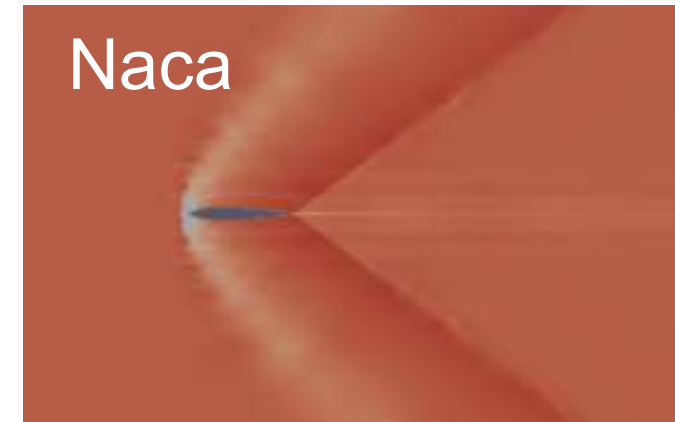
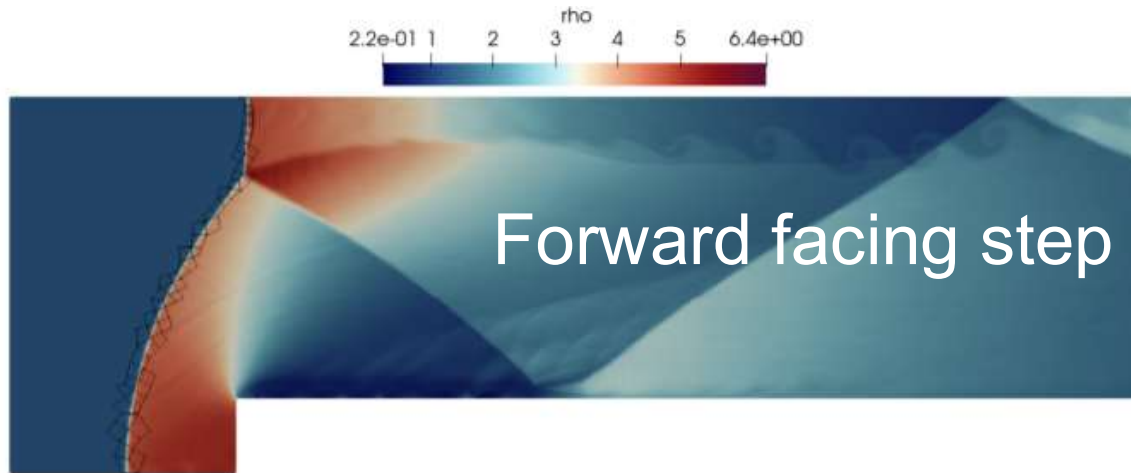


# Machine Learning to detect flow regions



	DoFs	reduction of DoFs	reduction of comp. time
Uniform P1	0.59M	93.6%	92.7%
Uniform P2	1.99M	78.2%	86.5%
Uniform P3	4.72M	48.7%	54.1%
Uniform P4	9.22M	-	-
Cluster-Adapt P4-P1	3.58M	61%	43%

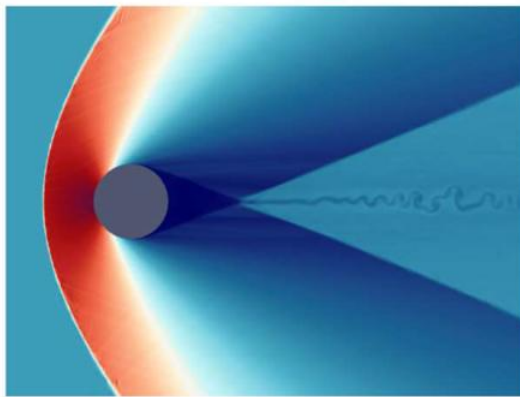
# Supersonic & Shock capturing



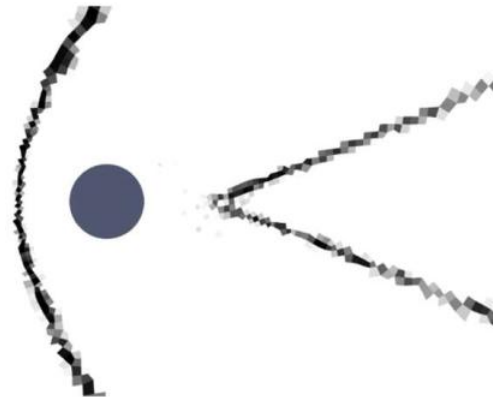
## What about shocks?

Classic feature based sensors (fine tuned)

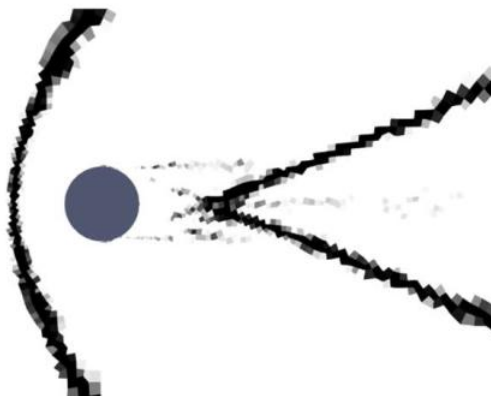
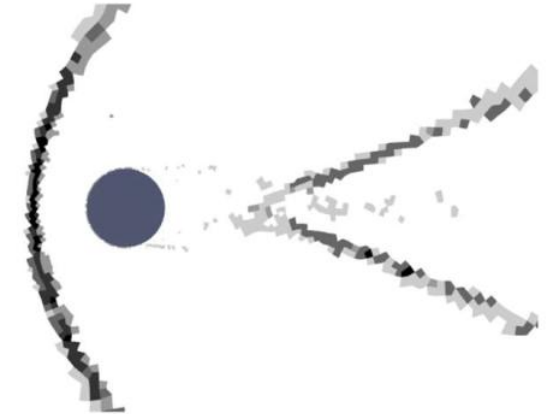
GMM  
(no tuning)



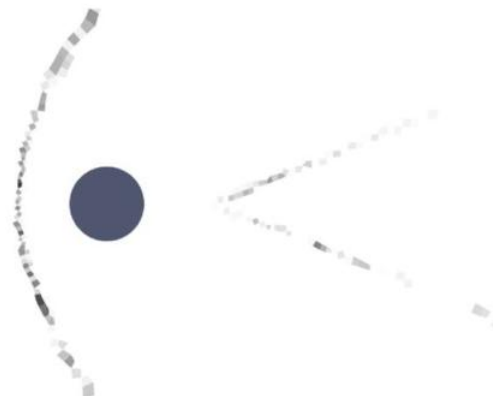
(a)



(b)



(c)

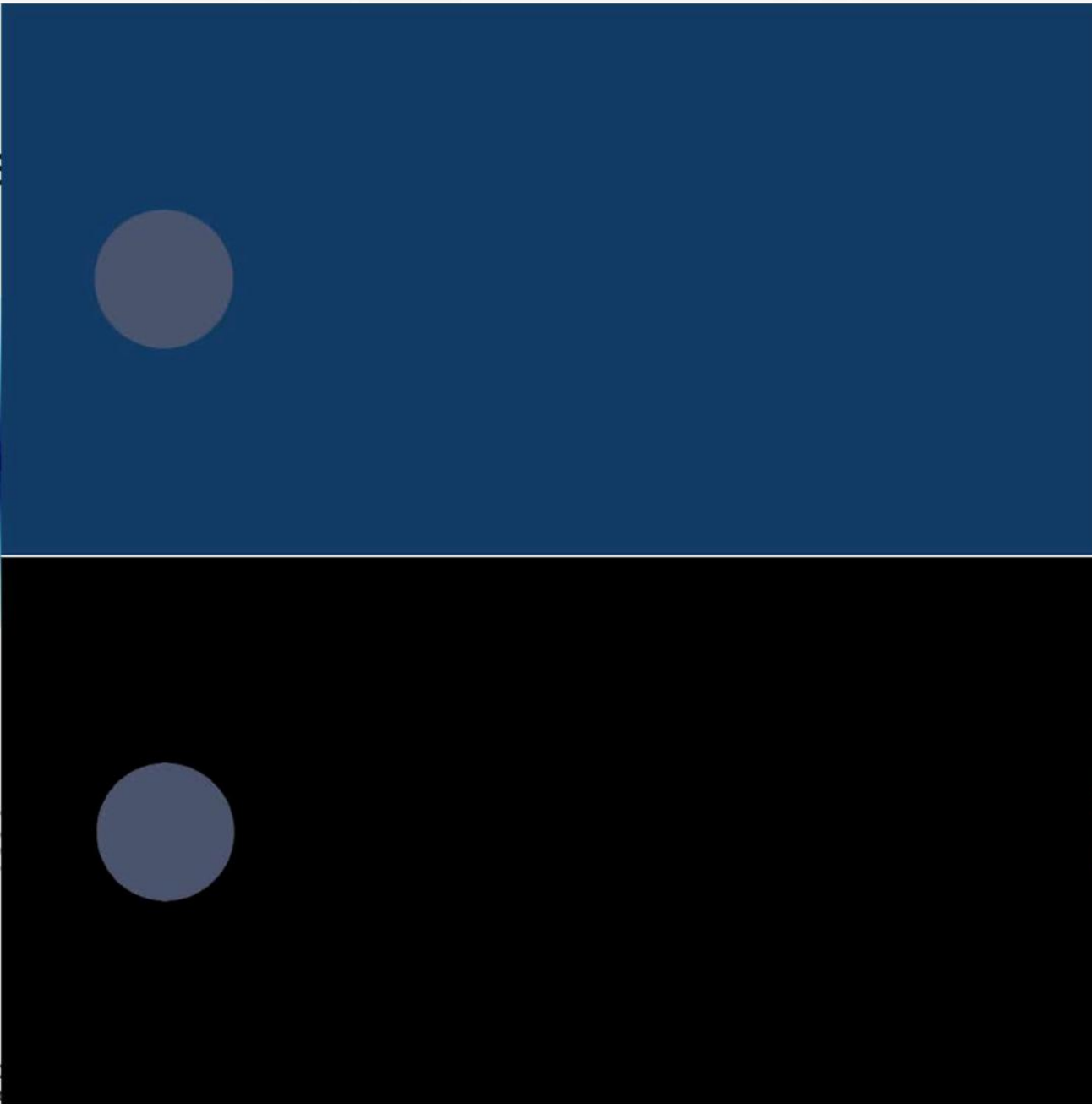
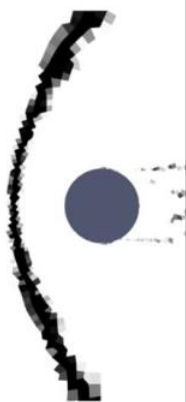
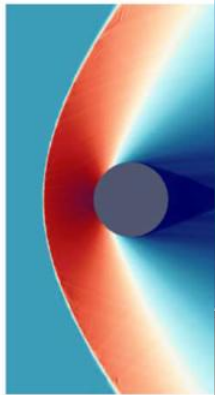


(d)

Similar result to  
state of the art  
without tuning!

FIG. 10. Viscous case after 300,000 iterations with the modal sensor of section IV A, using  $pp$ . a) density field, b) sensor with  $s_0 = -2.5$  and  $\Delta s = 1$ . Sensor applied to the last iteration with  $s_0 = -3.5$ ,  $\Delta s = 1$  (c), and with  $s_0 = -1.5$ ,  $\Delta s = 1$  (d).

Classic fe



MM  
(no tuning)

Similar result to  
state of the art  
without tuning!

FIG. 10. Viscous case after 30  
 $s_0 = -2.5$  and  $\Delta s = 1$ . Sensor

RESEARCH ARTICLE | FEBRUARY 08 2023

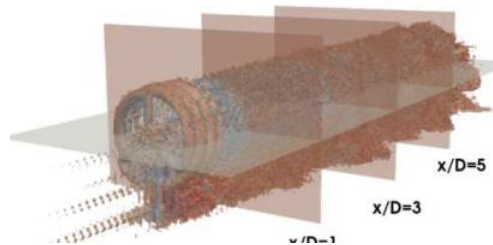
## Toward a robust detection of viscous and turbulent flow regions using unsupervised machine learning

Kheir-Eddine Otmani  ; Gerasimos Ntoukas ; Oscar A. Mariño ; Esteban Ferrer 



*Physics of Fluids* 35, 027112 (2023)

<https://doi.org/10.1063/5.0138626>



Engineering with Computers  
<https://doi.org/10.1007/s00366-024-01950-y>

ORIGINAL ARTICLE



## Machine learning mesh-adaptation for laminar and turbulent flows: applications to high-order discontinuous Galerkin solvers

Kenza Tlales<sup>1</sup> · Kheir-Eddine Otmani<sup>1</sup> · Gerasimos Ntoukas<sup>1</sup> · Gonzalo Rubio<sup>1,2</sup> · Esteban Ferrer<sup>1,2</sup>

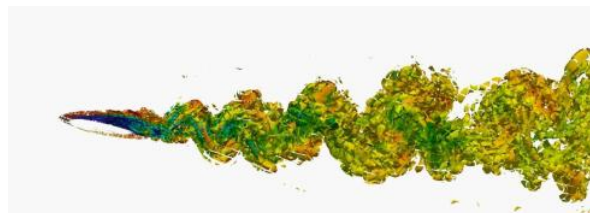
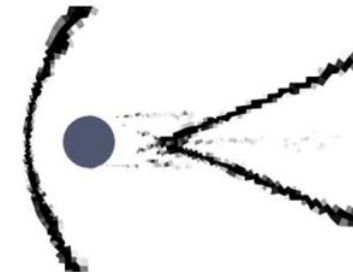
## An unsupervised machine-learning-based shock sensor for high-order supersonic flow solvers

Andrés Mateo-Gabín,<sup>1</sup>  Kenza Tlales,<sup>1</sup> Eusebio Valero,<sup>1,2</sup> Esteban Ferrer,<sup>1,2</sup> and Gonzalo Rubio<sup>1,2</sup>

<sup>1</sup>*ETSIAE-UPM-School of Aeronautics, Universidad Politécnica de Madrid, Madrid-Spain*

<sup>2</sup>*Center for Computational Simulation, Universidad Politécnica de Madrid, Madrid-Spain*

(Dated: 10 October 2023)



Accelerating high order discontinuous Galerkin solvers through a clustering-based viscous/turbulent-inviscid domain decomposition

Kheir-Eddine Otmani\*<sup>1</sup>, Andrés Mateo-Gabín<sup>1</sup>, Gonzalo Rubio<sup>1,2</sup>, and Esteban Ferrer<sup>1,2</sup>

<sup>1</sup>*ETSIAE-UPM-School of Aeronautics, Universidad Politécnica de Madrid, Plaza Cardenal Cisneros 3, E-28040 Madrid, Spain*

<sup>2</sup>*Center for Computational Simulation, Universidad Politécnica de Madrid, Campus de Montegancedo, Boadilla del Monte, 28660 Madrid, Spain*

# Summary

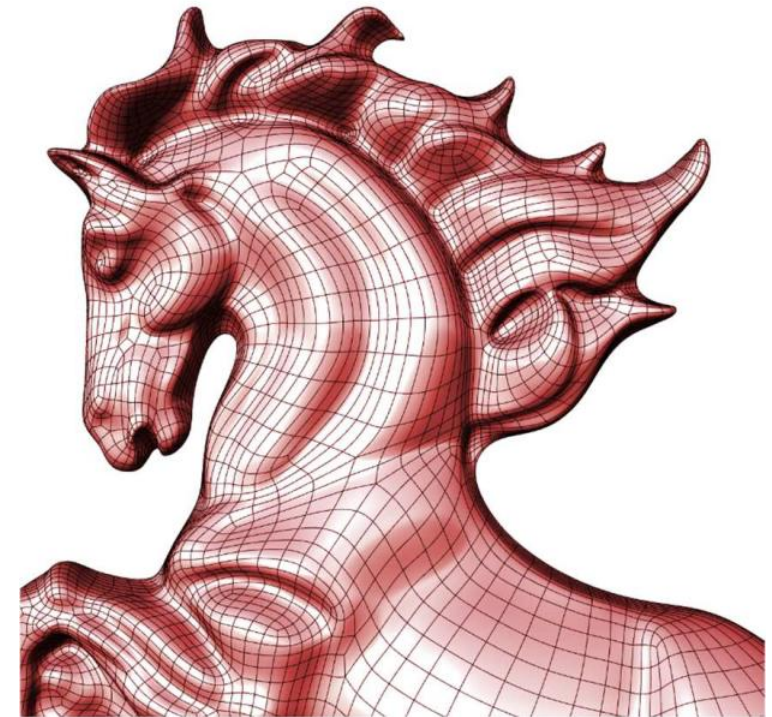
## 1- Introduction to DG & Horses3d

## 2- Multiphysics

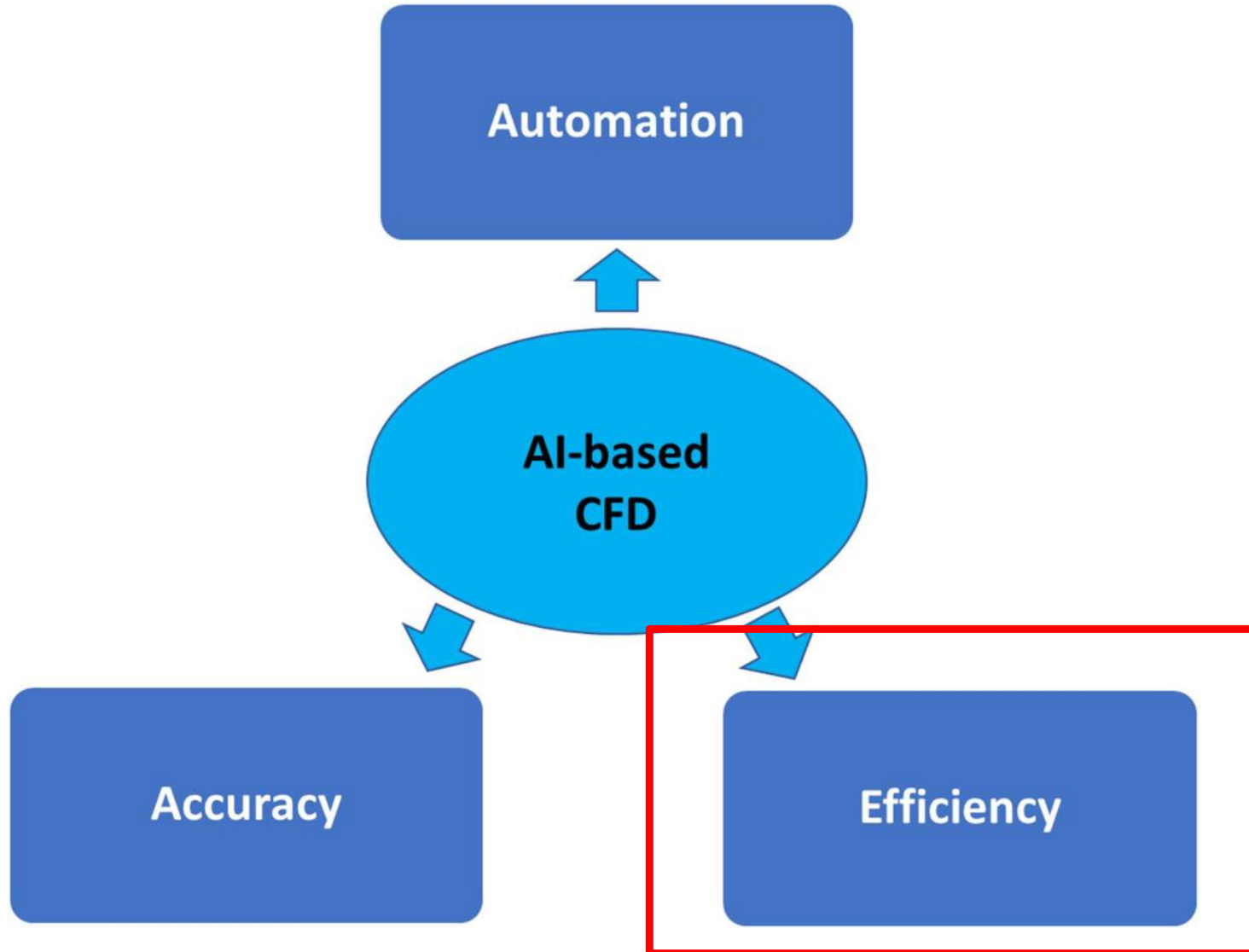
- Wind turbines
- Turbulence

## 3. Machine Learning + CFD

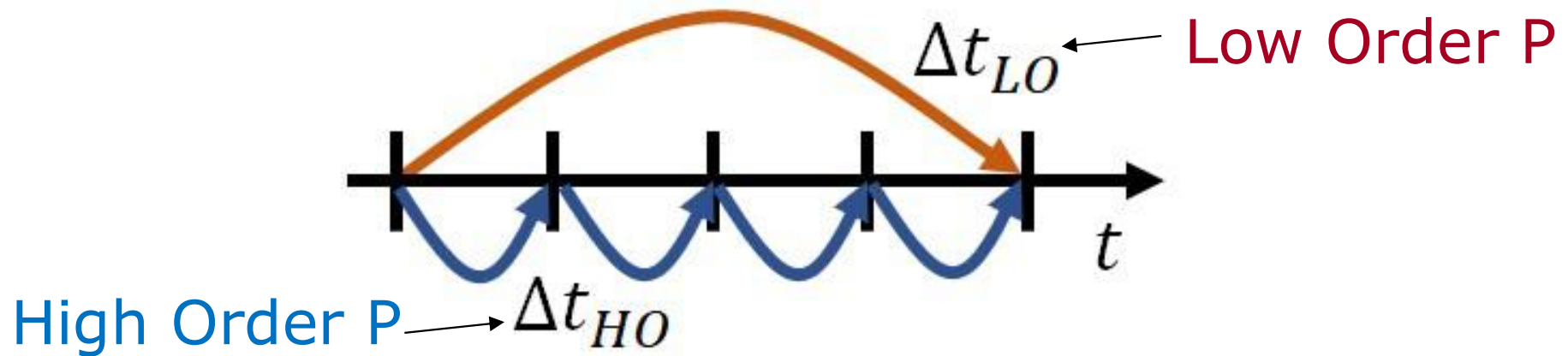
- Mesh adaption
- NN acceleration
- RL for automation



# Towards AI-based Computational Fluid Dynamics

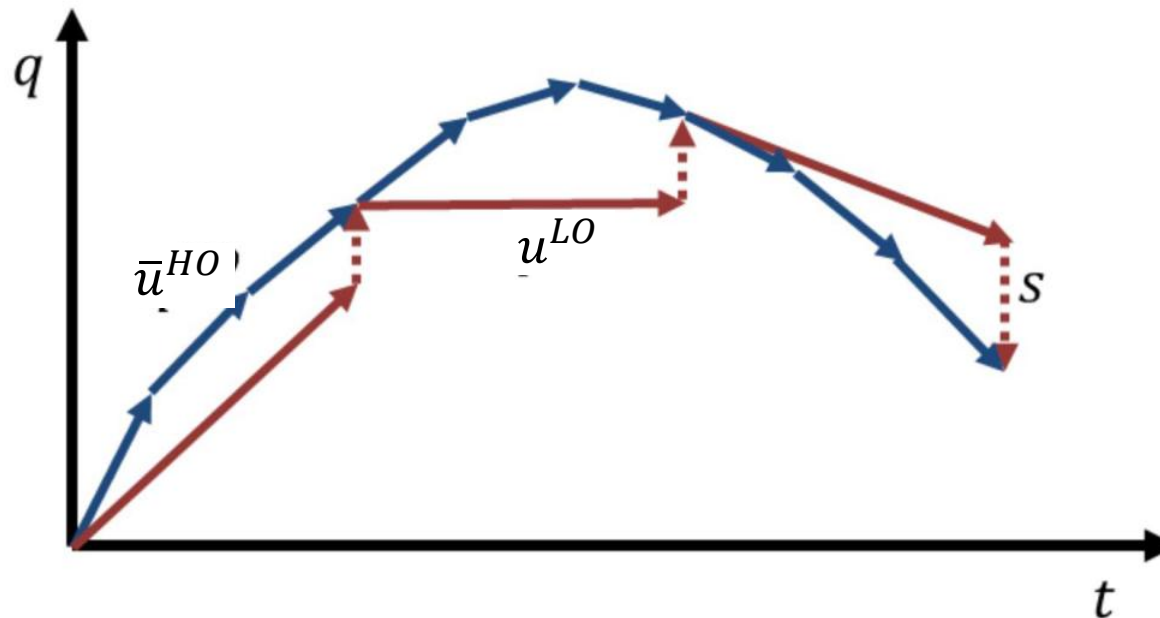
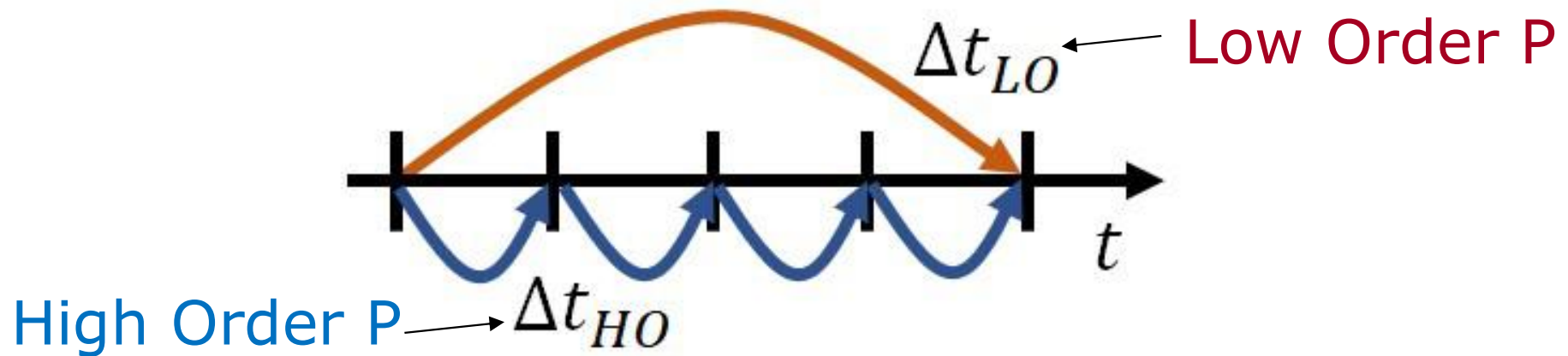


## Machine Learning to accelerate CFD





# Machine Learning to accelerate CFD



# Machine Learning to accelerate CFD

LO evolution:

$$u_{n+1}^{LO} = u_n^{LO} + \Delta t_n q^{LO}(u_n^{LO}; t_n)$$

Filtered HO:

$$\bar{u}_{n+1}^{HO} = \bar{u}_n^{HO} + \Delta t_n \bar{q}^{HO}(u_n^{HO}; t_n)$$

# Machine Learning to accelerate CFD

LO evolution:

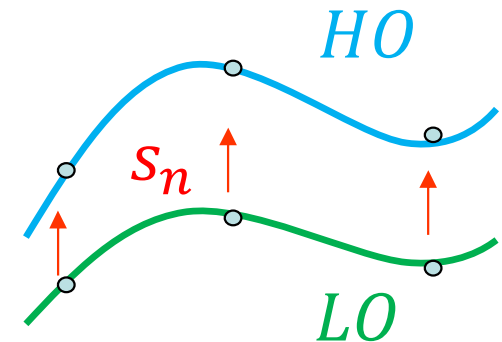
$$u_{n+1}^{LO} = u_n^{LO} + \Delta t_n q^{LO}(u_n^{LO}; t_n)$$

Filtered HO:

$$\bar{u}_{n+1}^{HO} = \bar{u}_n^{HO} + \Delta t_n \bar{q}^{HO}(u_n^{HO}; t_n)$$

LO-NN corrected:

$$u_{n+1}^{NN} = u_n^{NN} + \Delta t_n [q^{LO}(u_n^{NN}; t_n) + s_n]$$



# Machine Learning to accelerate CFD

LO evolution:

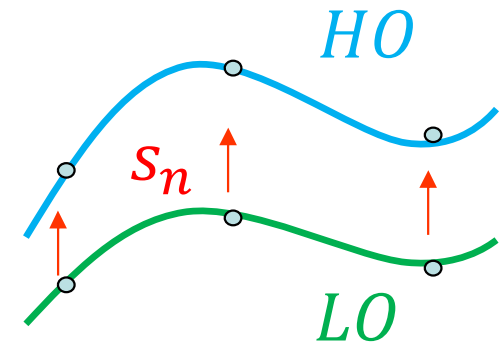
$$u_{n+1}^{LO} = u_n^{LO} + \Delta t_n q^{LO}(u_n^{LO}; t_n)$$

Filtered HO:

$$\bar{u}_{n+1}^{HO} = \bar{u}_n^{HO} + \Delta t_n \bar{q}^{HO}(u_n^{HO}; t_n)$$

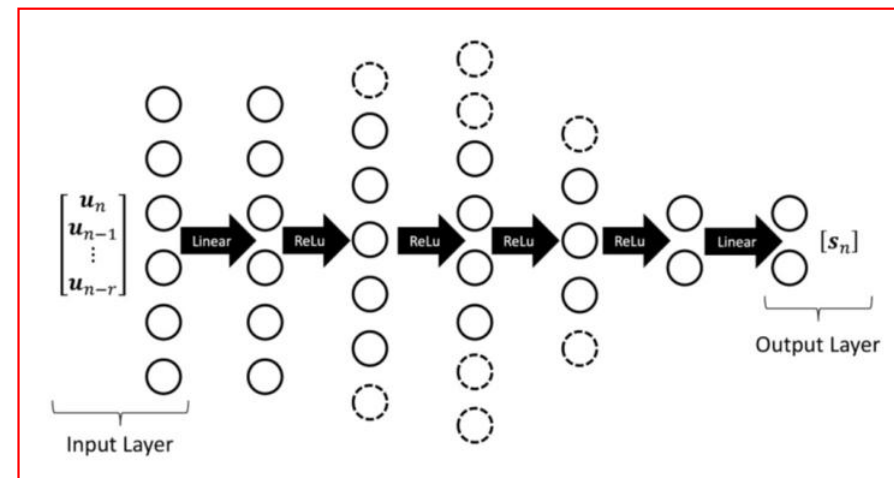
LO-NN corrected:

$$u_{n+1}^{NN} = u_n^{NN} + \Delta t_n [q^{LO}(u_n^{NN}; t_n) + s_n]$$



$$s_n = f(u_n^{NN}, u_{n-1}^{NN}, u_{n-r}^{NN}, \bar{u}^{HO})$$

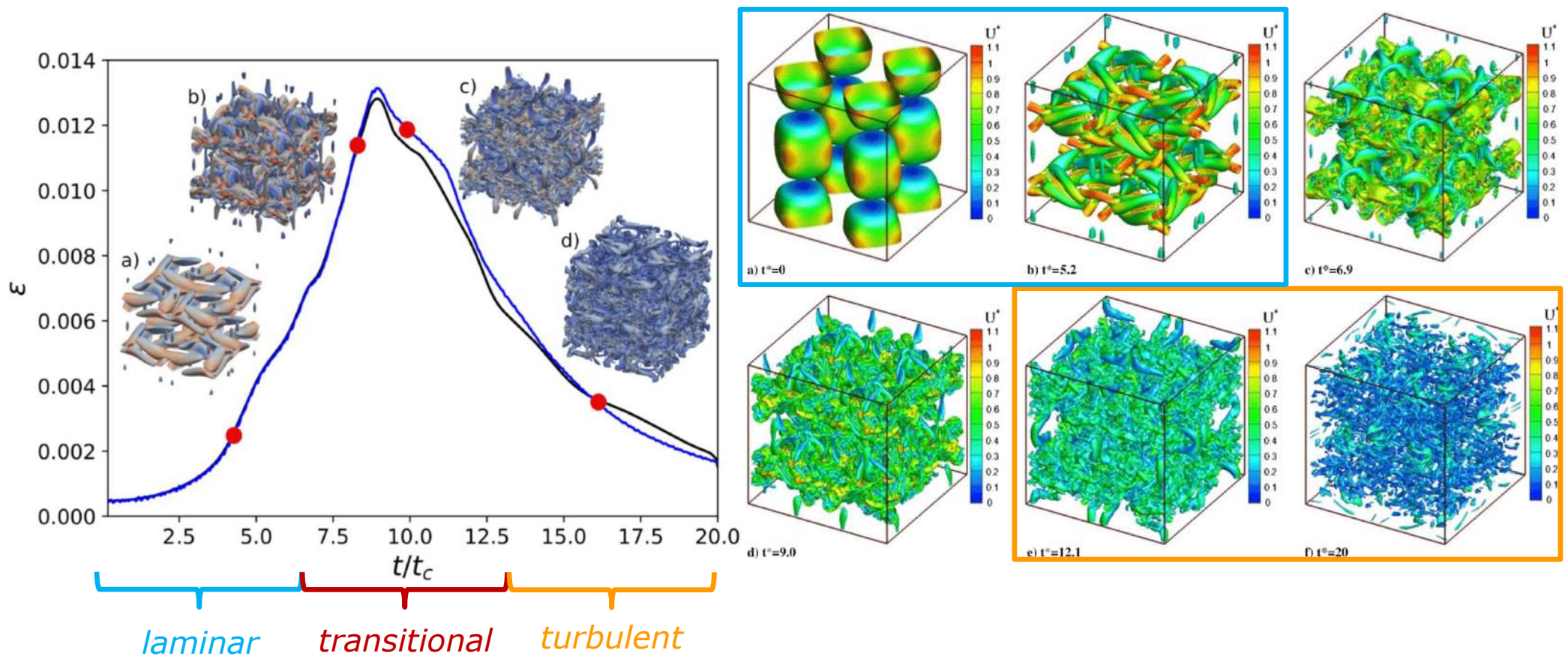
Trained to give HO solution



# Machine Learning to accelerate CFD

## 3D Navier-Stokes - LES

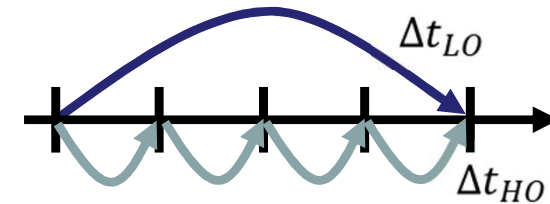
### Taylor-Green – Reynolds 1600



# Machine Learning to accelerate CFD

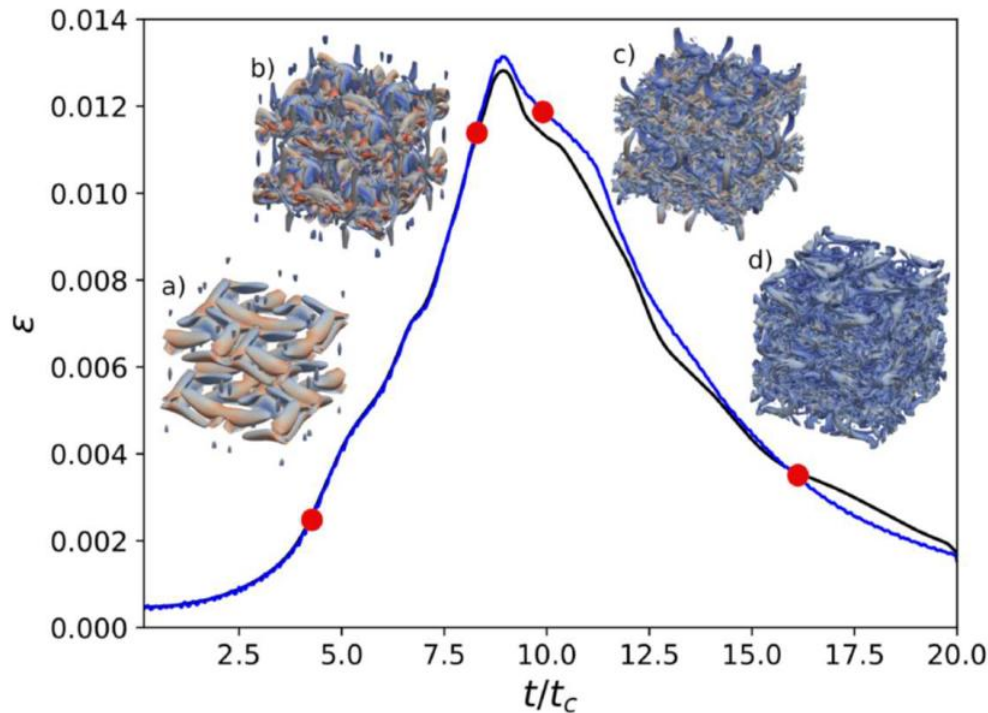
## 3D Navier-Stokes - LES

Taylor-Green – Reynolds 1600



$$P8 \rightarrow P3$$

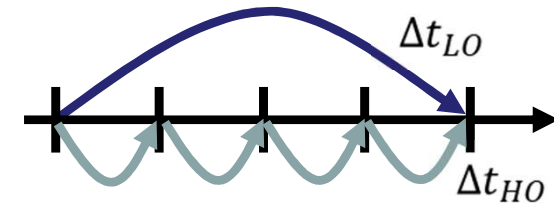
$$\Delta t_{LO} / \Delta t_{HO} = 3$$



# Machine Learning to accelerate CFD

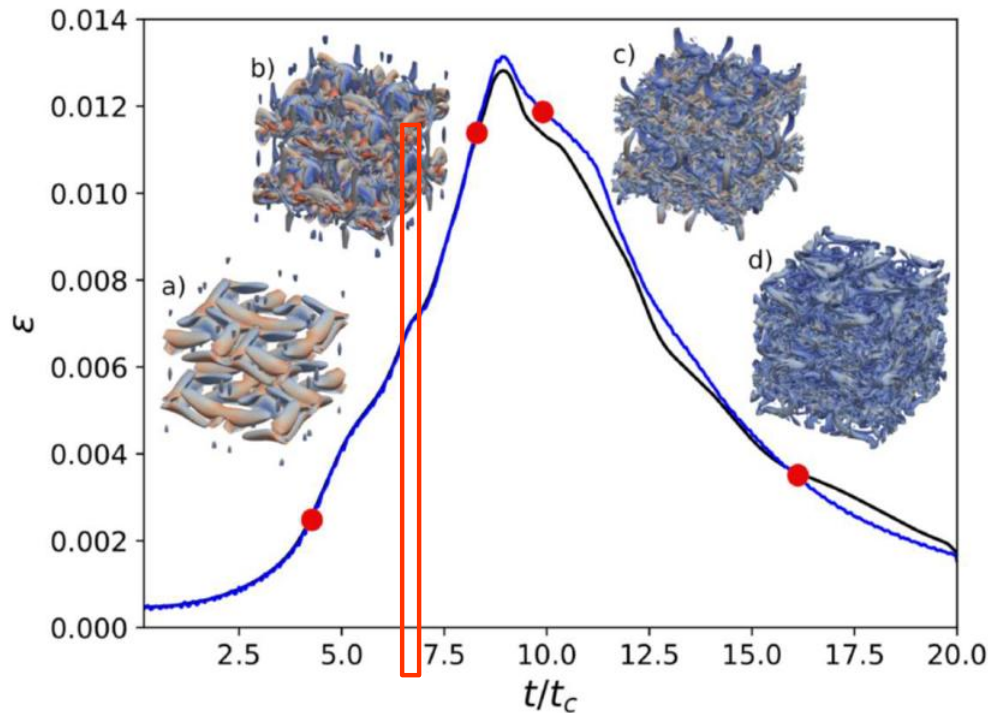
## 3D Navier-Stokes - LES

### Taylor-Green – Reynolds 1600



$$P8 \rightarrow P3$$

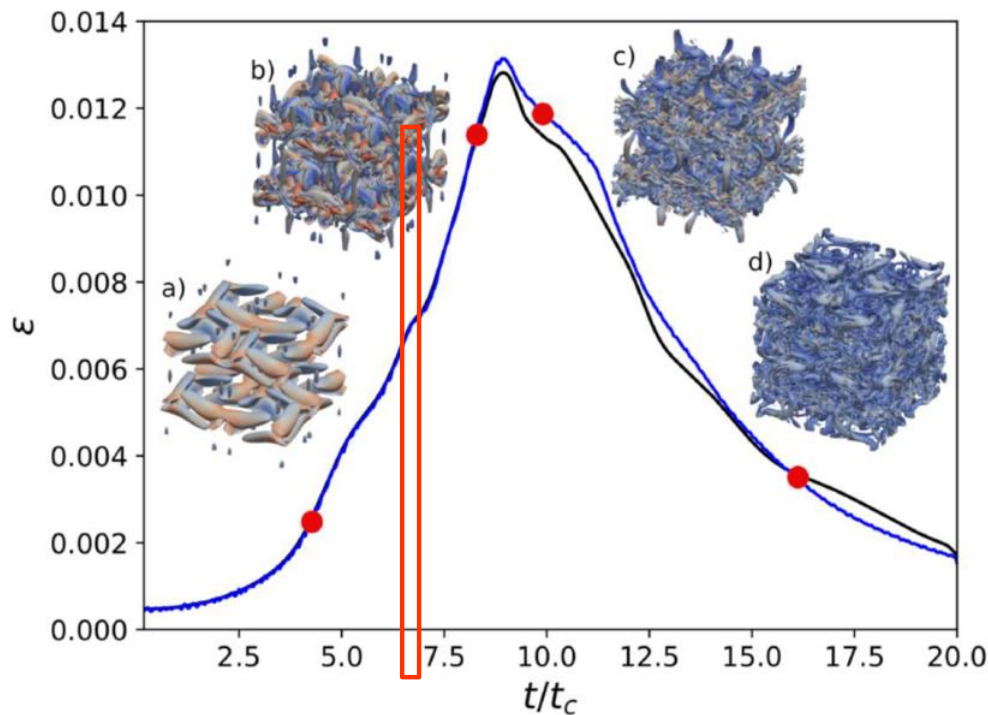
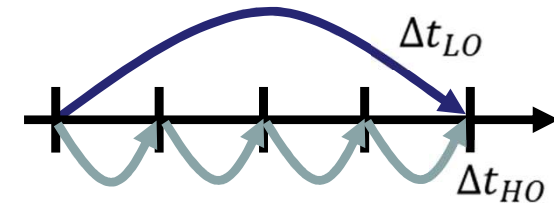
$$\Delta t_{LO} / \Delta t_{HO} = 3$$



*training*

# Machine Learning to accelerate CFD

## 3D Navier-Stokes - LES Taylor-Green – Reynolds 1600

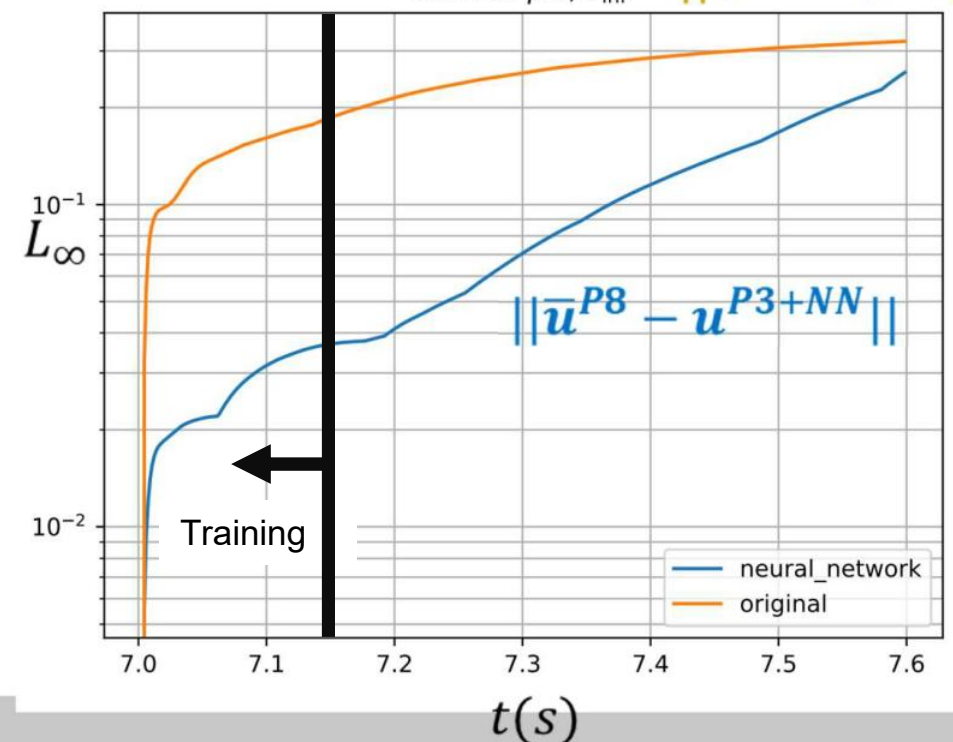


12 times faster

$$P8 \rightarrow P3$$

$$\Delta t_{LO} / \Delta t_{HO} = 3$$

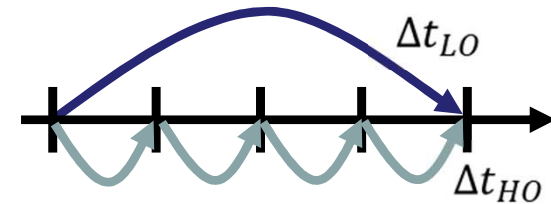
error in  $\rho w$ ,  $L_{inf}$   $\|\bar{u}^{P8} - u^{P3}\|$





# Machine Learning to accelerate CFD

3D Navier-Stokes - LES  
Taylor-Green – Reynolds 1600



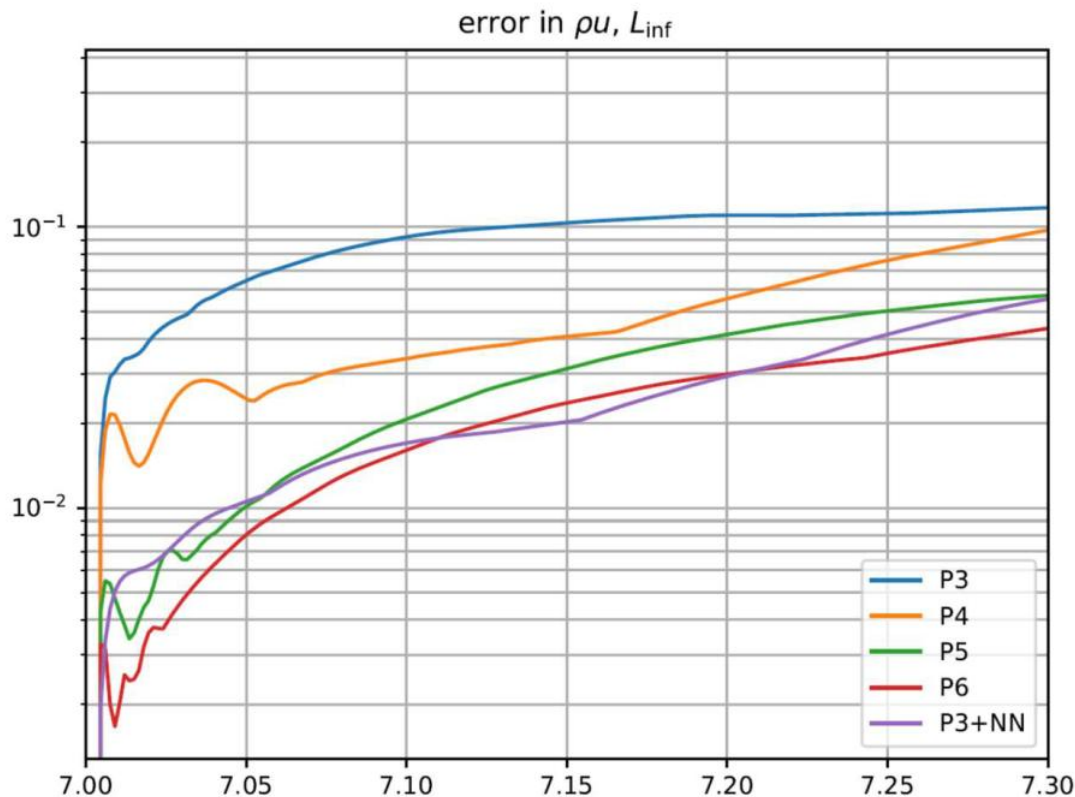
$$P8 \rightarrow P3$$

$$\Delta t_{LO} / \Delta t_{HO} = 3$$

What is the real accuracy?

**Probably P=6**

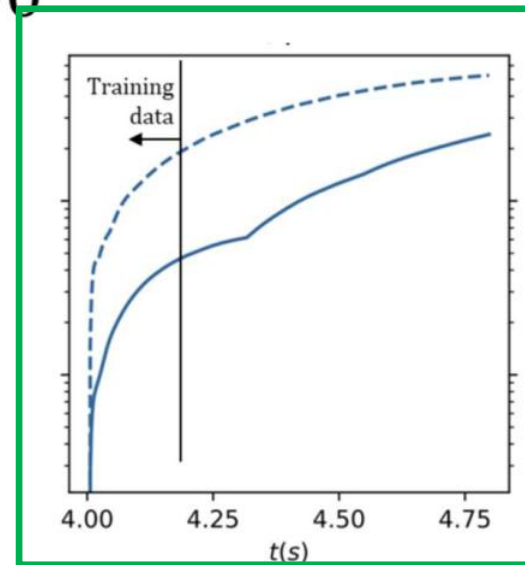
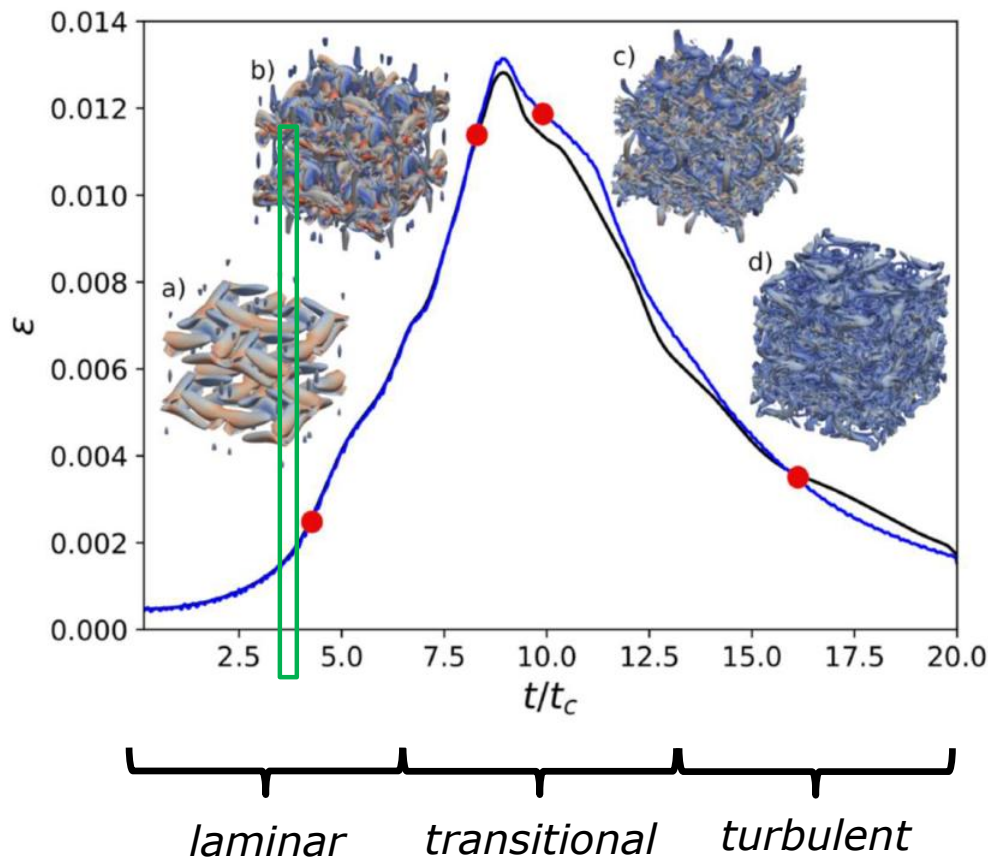
**P3+NN is 4-5 times faster**  
(compared to P6)



# Machine Learning to accelerate CFD

## 3D Navier-Stokes - LES

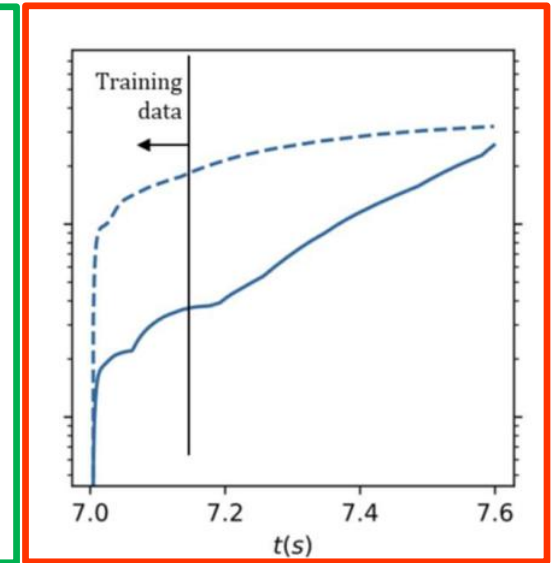
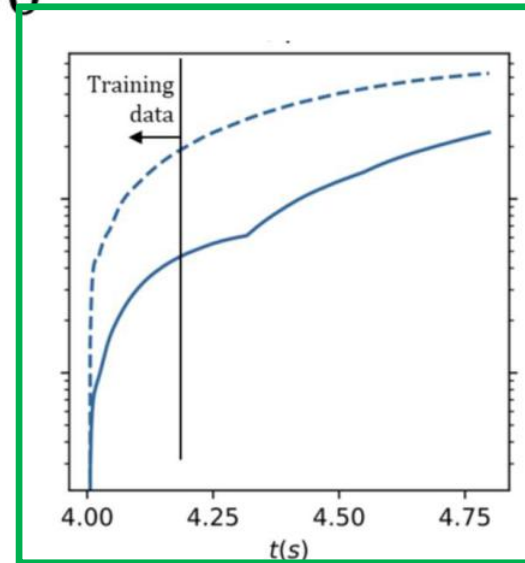
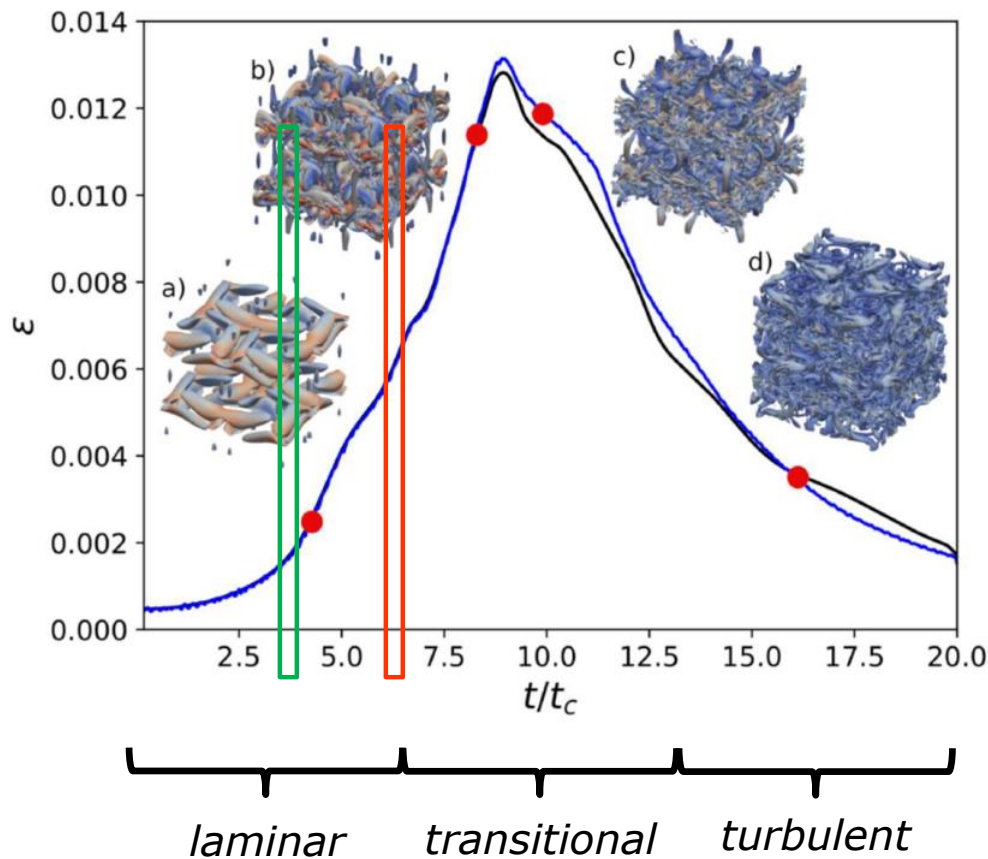
### Taylor-Green – Reynolds 1600



# Machine Learning to accelerate CFD

## 3D Navier-Stokes - LES

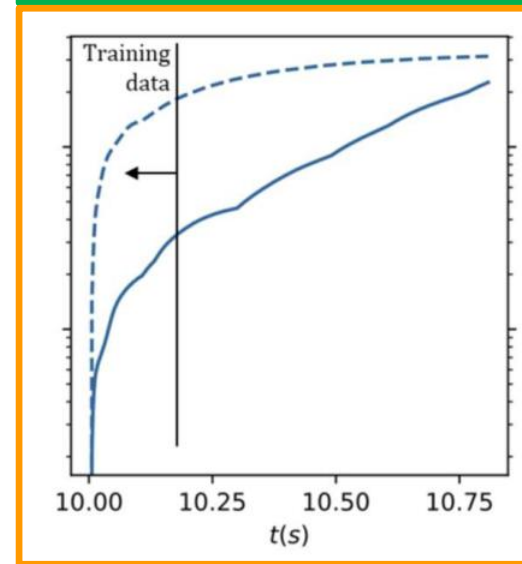
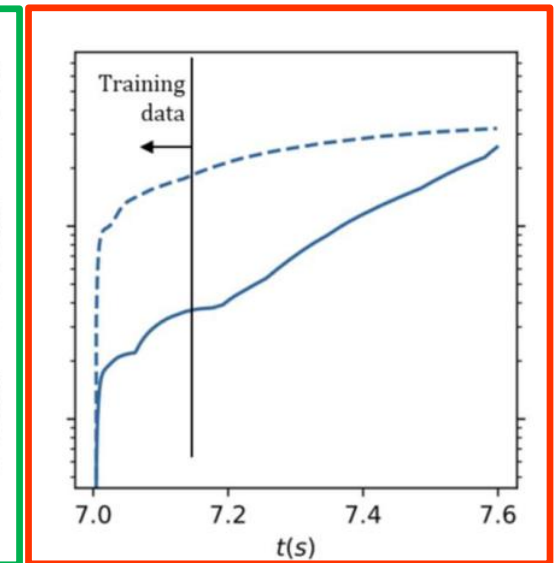
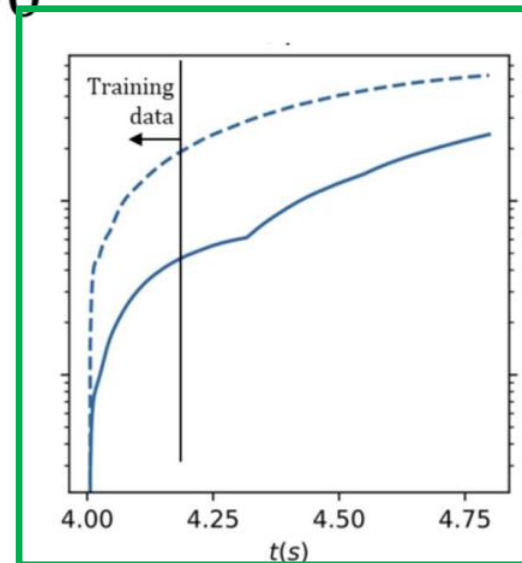
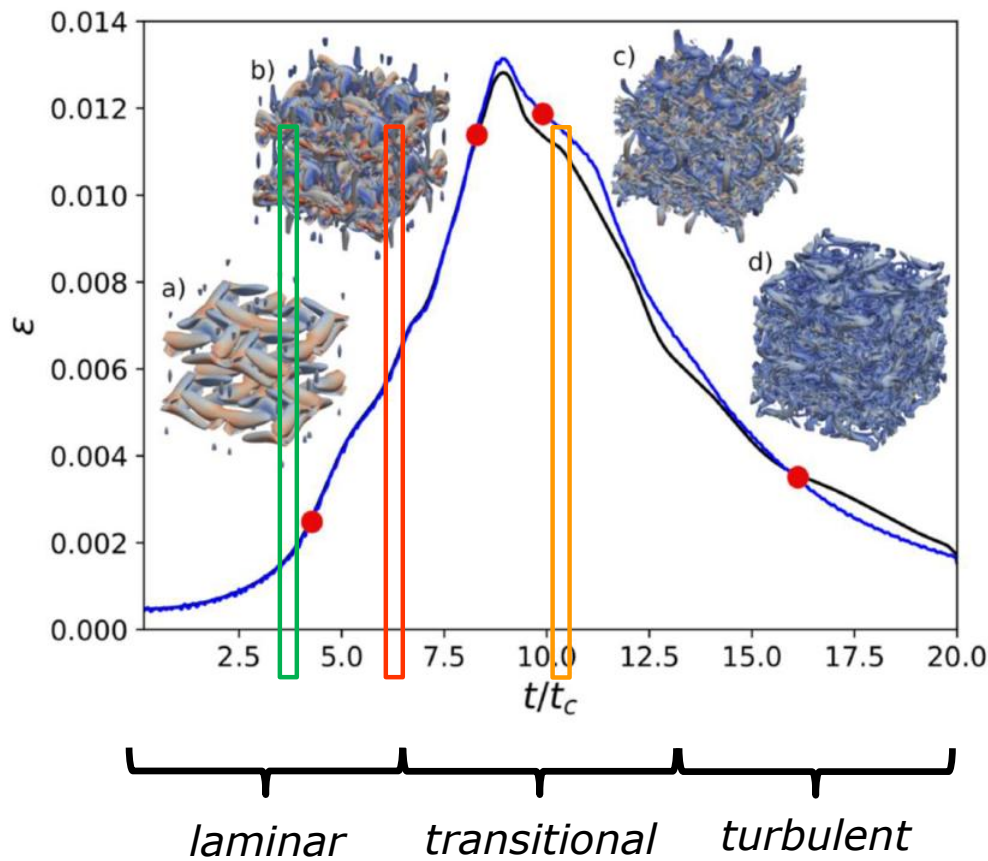
### Taylor-Green – Reynolds 1600



# Machine Learning to accelerate CFD

## 3D Navier-Stokes - LES

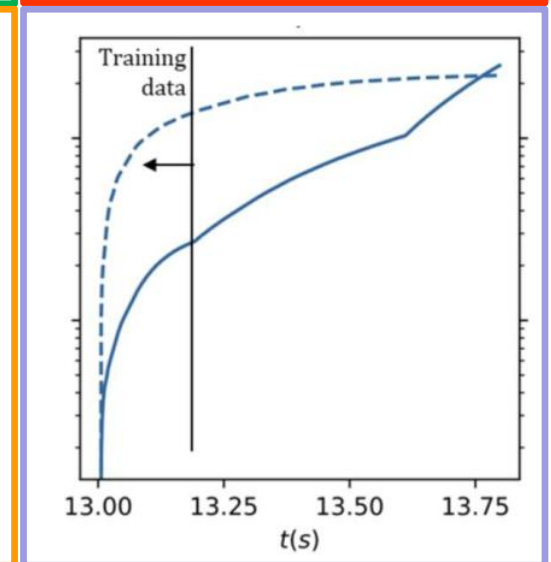
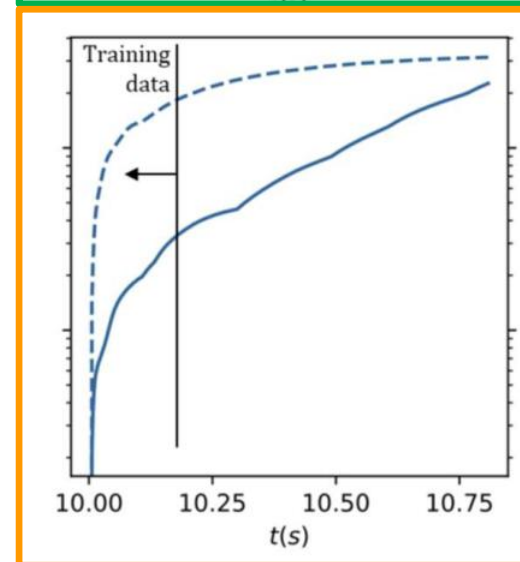
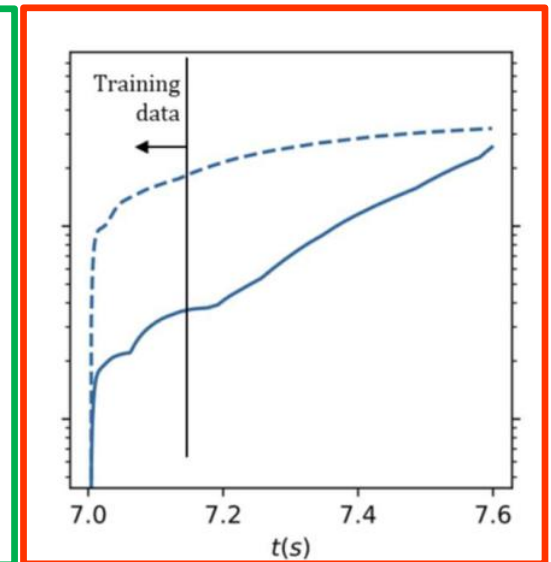
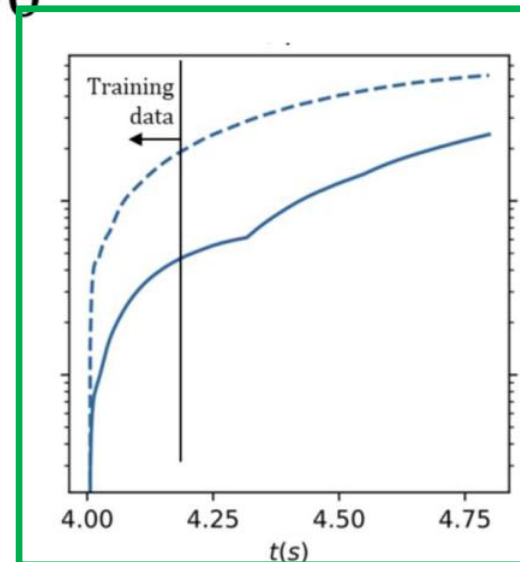
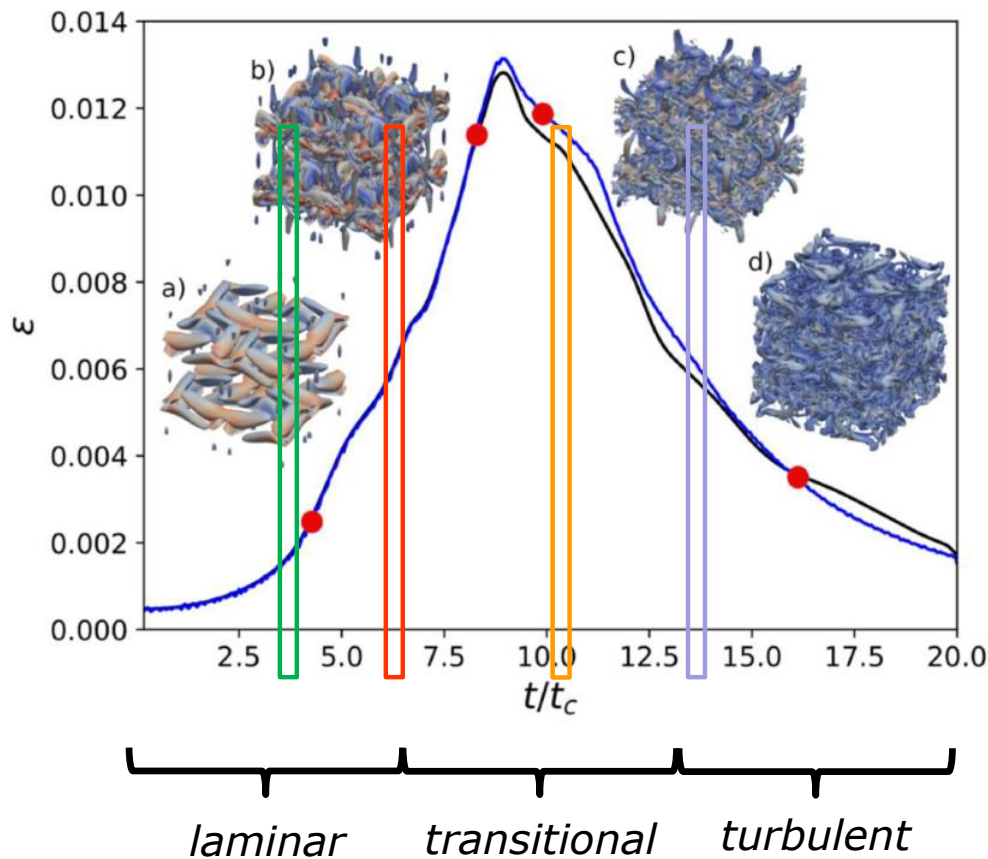
### Taylor-Green – Reynolds 1600



# Machine Learning to accelerate CFD

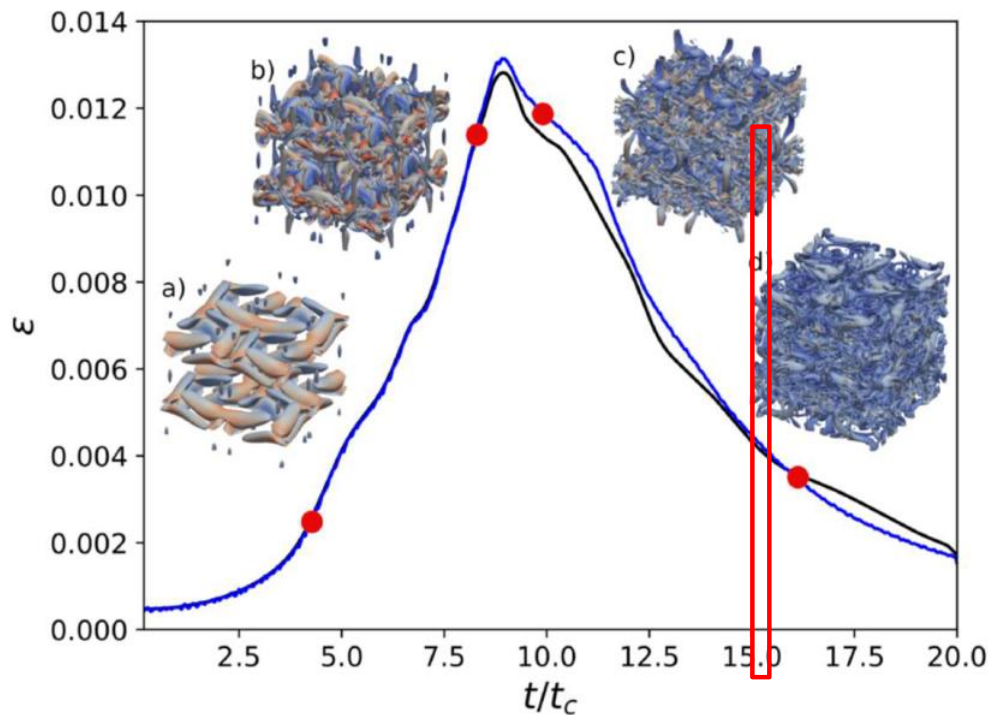
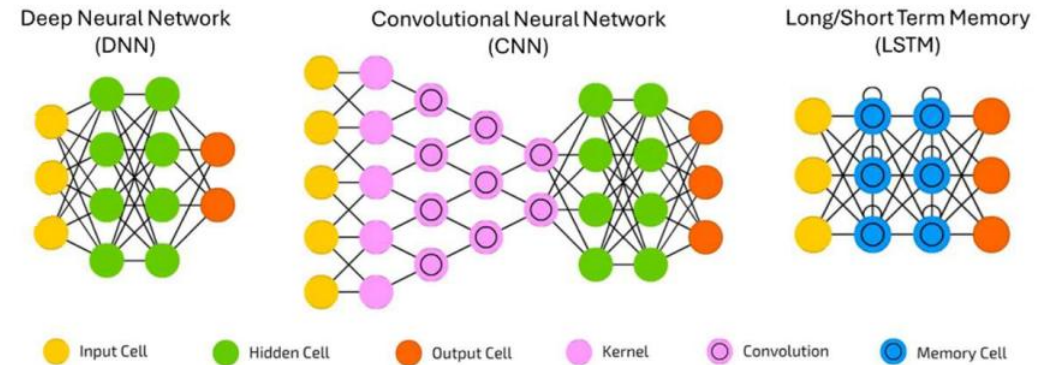
## 3D Navier-Stokes - LES

### Taylor-Green – Reynolds 1600

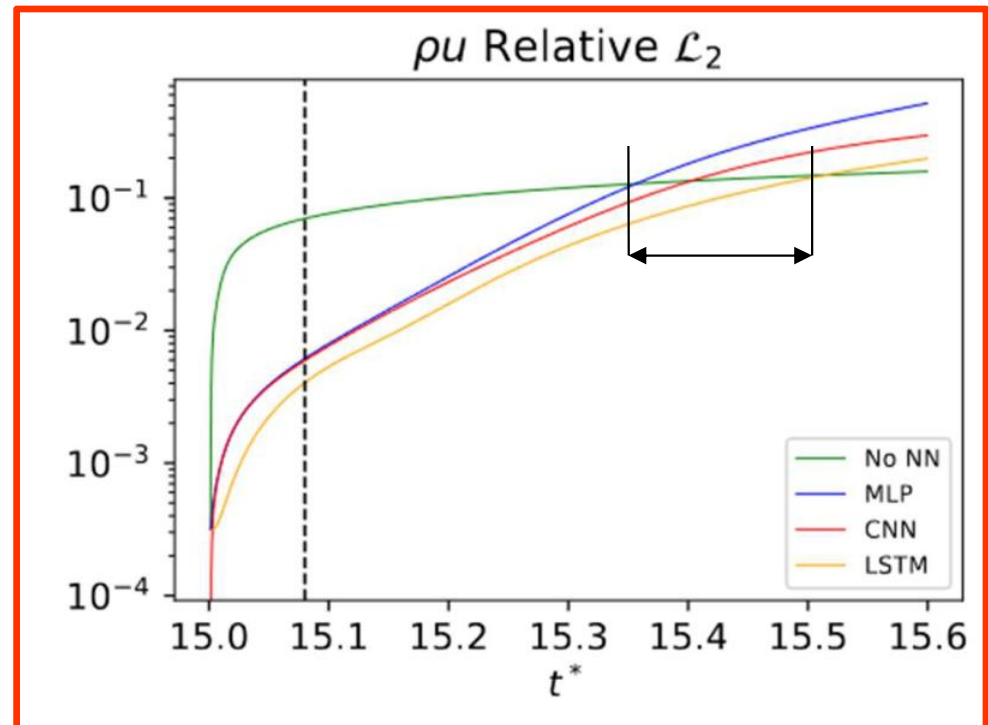


# Machine Learning to accelerate CFD

## 3D Navier-Stokes - LES Taylor-Green – Reynolds 1600



*training*



# Summary

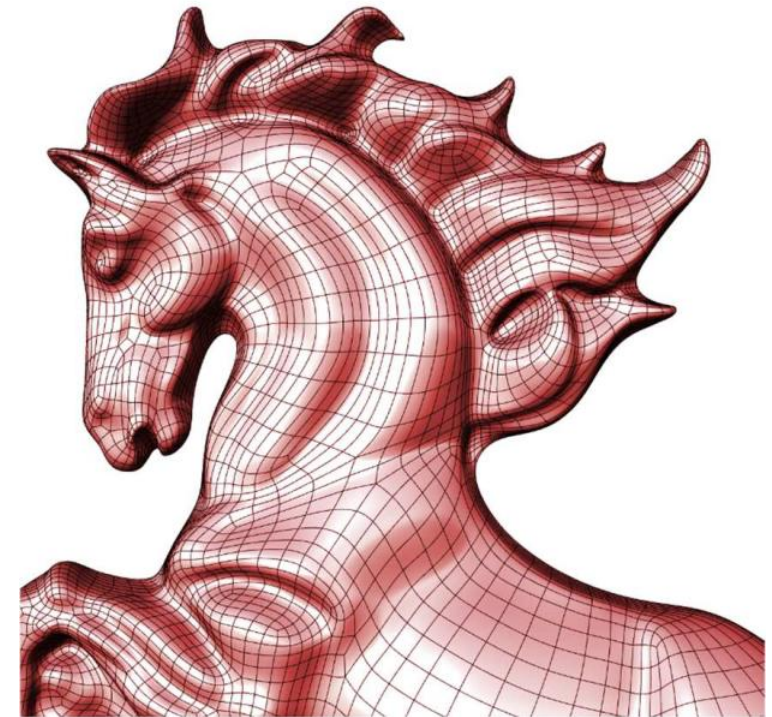
## 1- Introduction to DG & Horses3d

## 2- Multiphysics

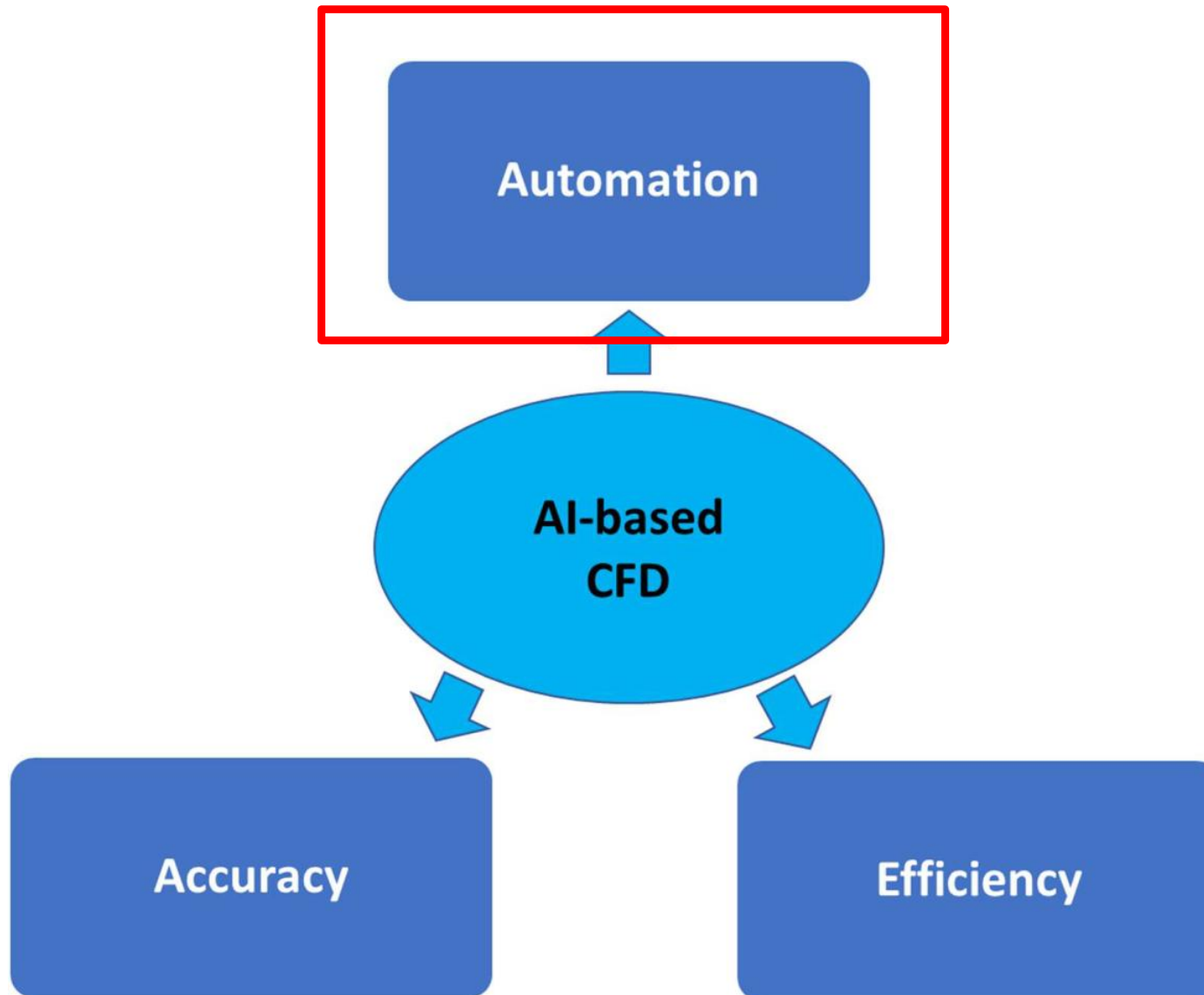
- Wind turbines
- Turbulence

## 3. Machine Learning + CFD

- Mesh adaption
- NN acceleration
- RL for automation

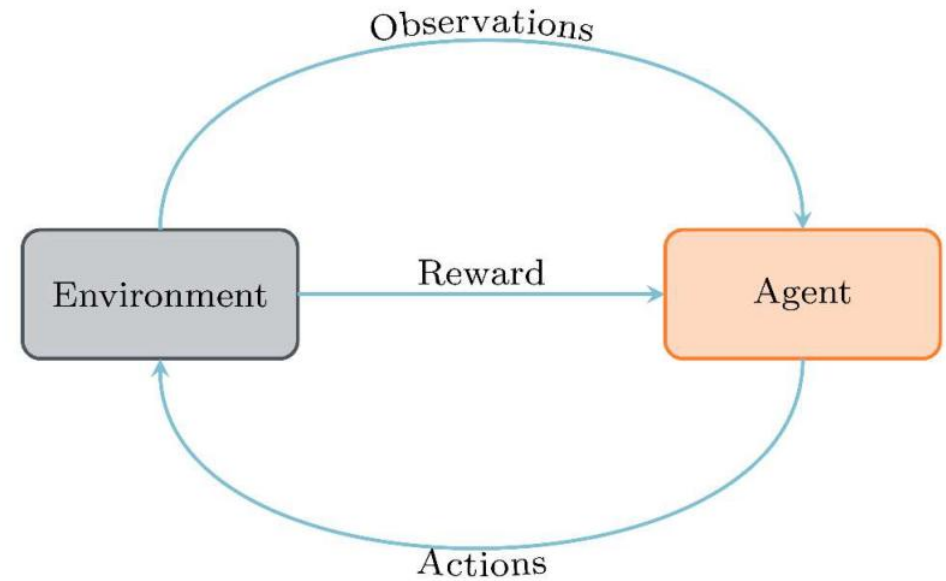


# Towards AI-based Computational Fluid Dynamics





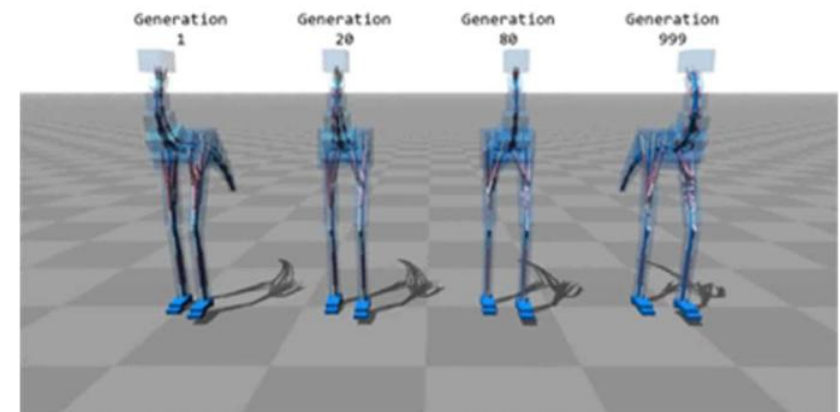
# Machine Learning and Reinforcement Learning



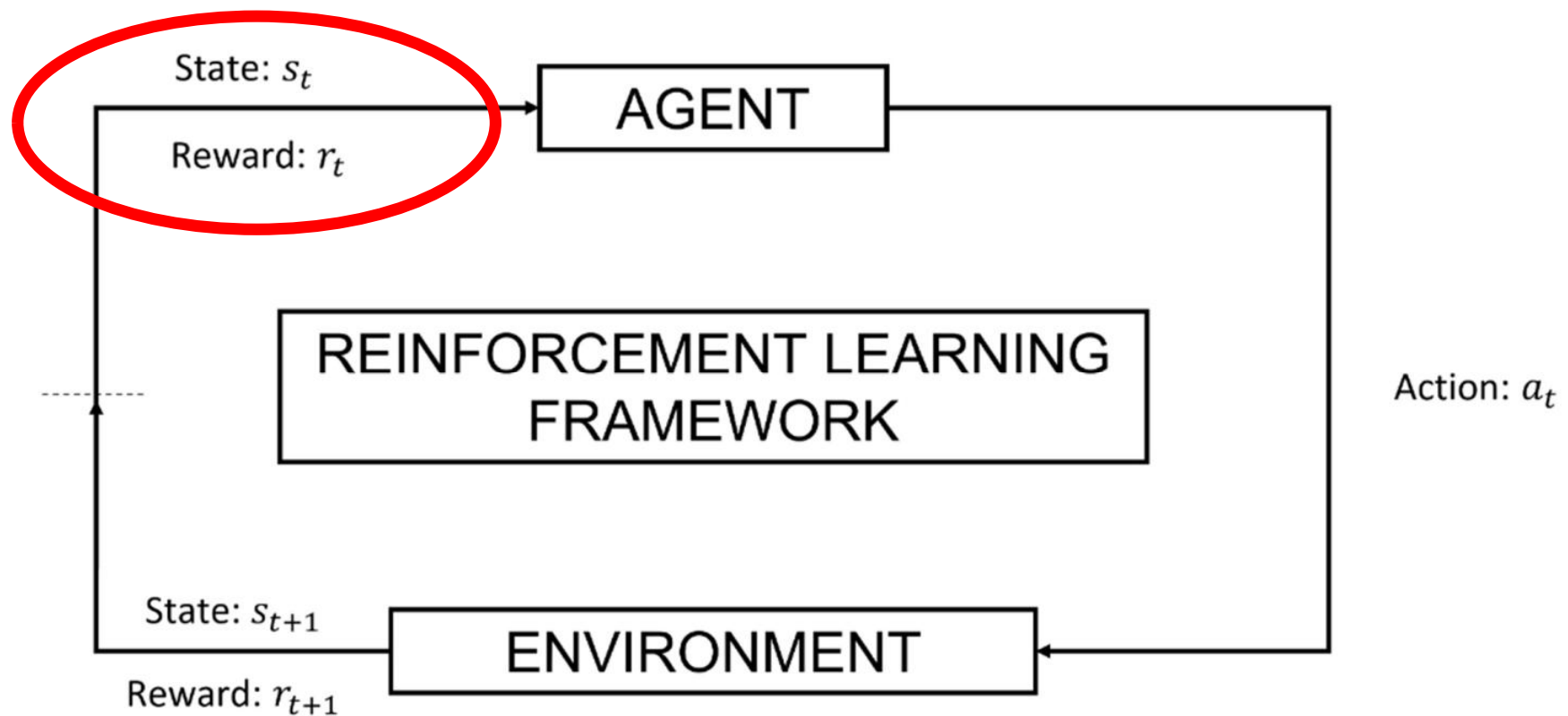
Go game



Chess game

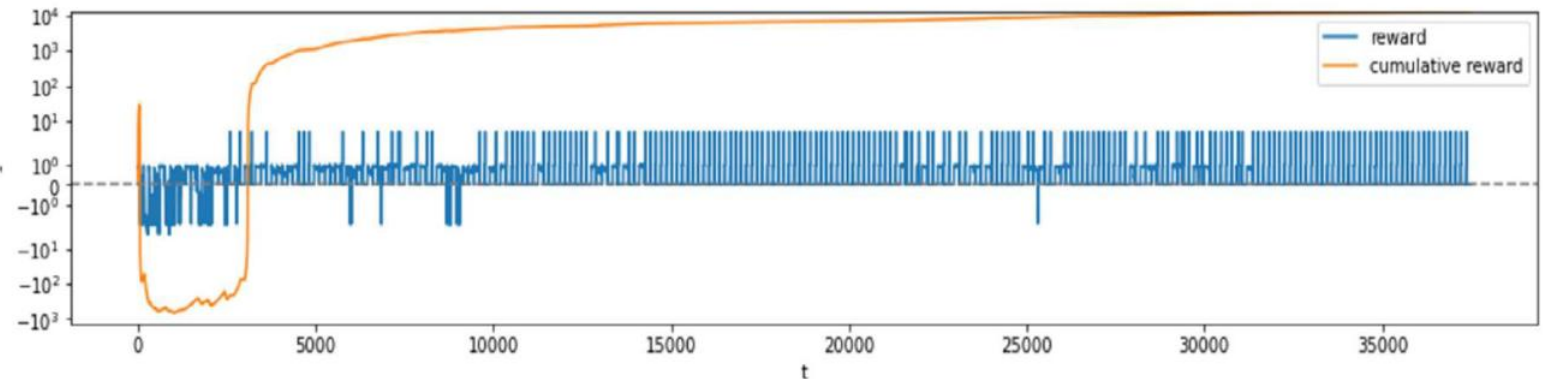
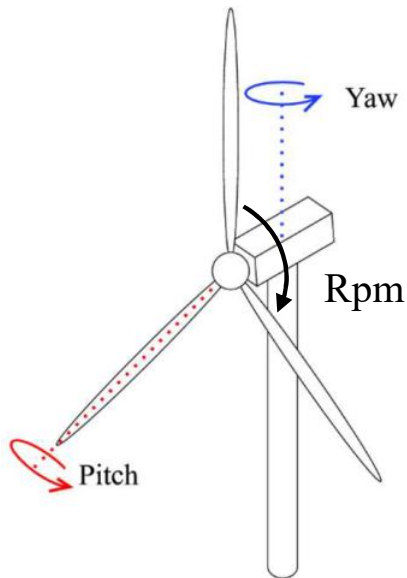


Defining the state, actions and rewards are the key aspects of RL

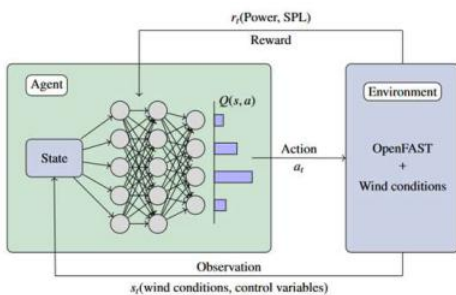


# Deep reinforcement learning for wind turbine control

## Training with simple winds



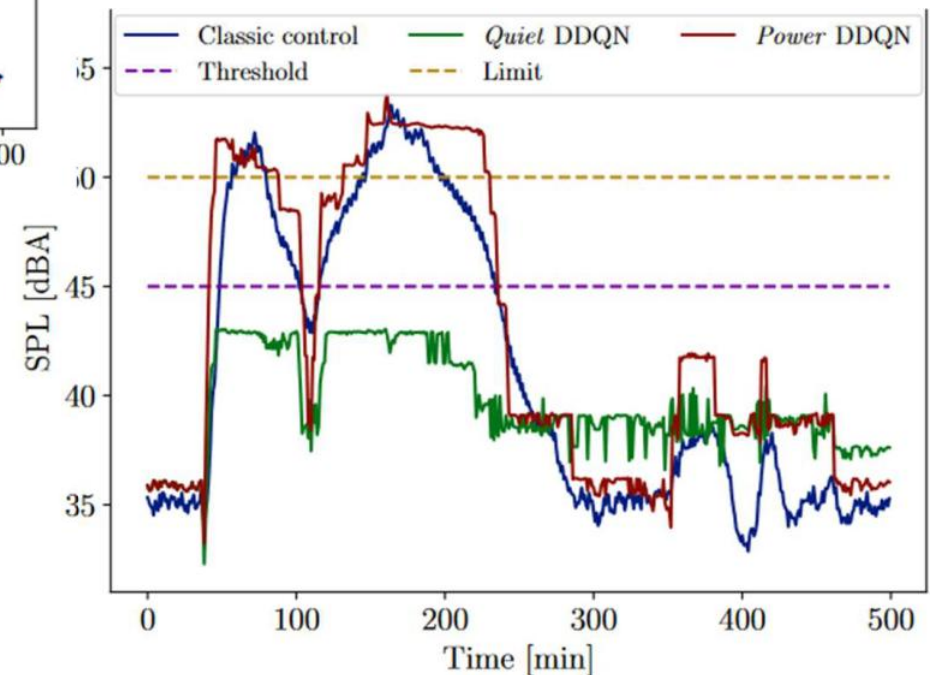
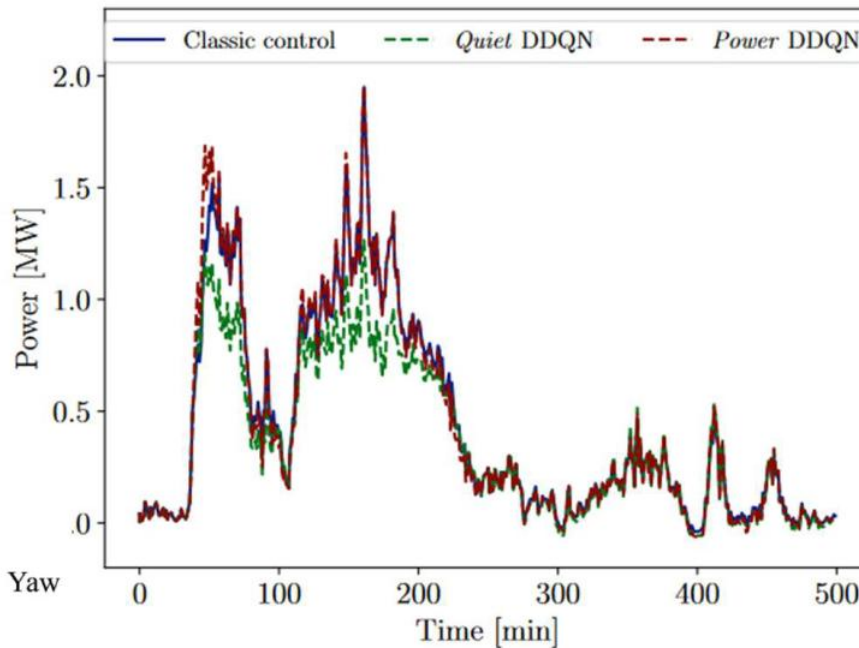
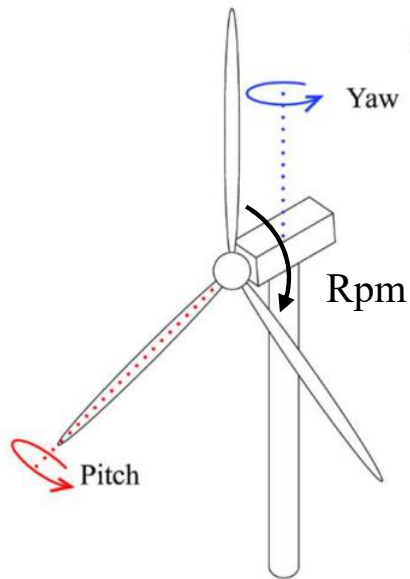
## Validation with turbulent real winds



Metric	DDQN1	VI	PID	Uncontrolled
Control Capacity Factor (%)	91.31	87.50	57.60	12.77
Capacity Factor (%)	20.95	20.50	12.49	1.59
Yearly Production (MWh)	4162.95	4073.45	2481.97	316.12

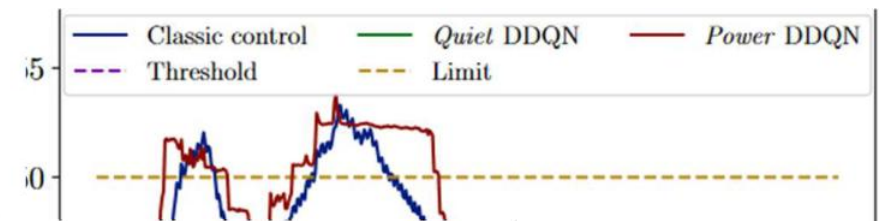
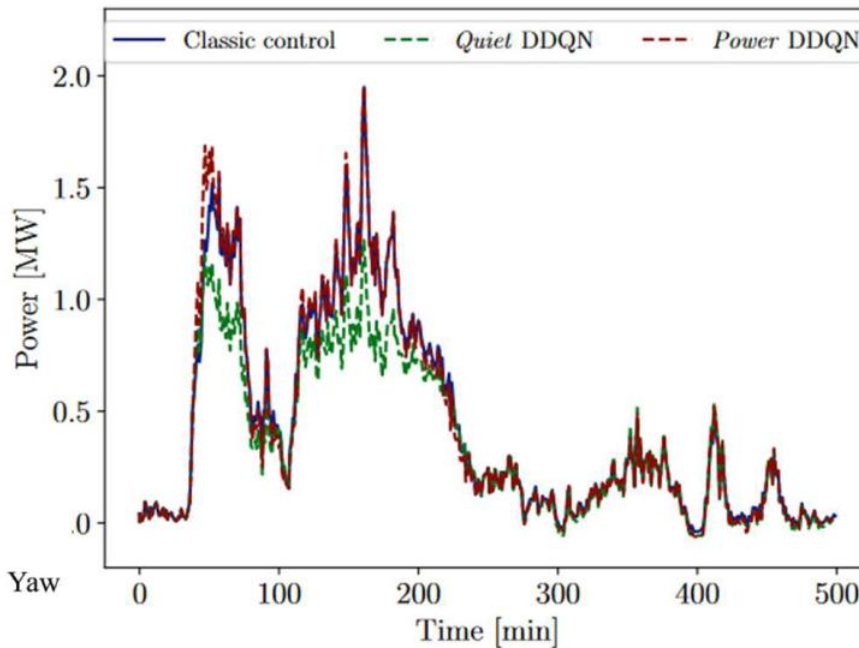
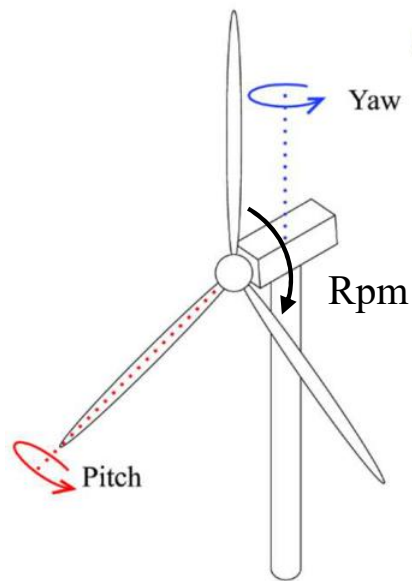
# Deep reinforcement learning for wind turbine control

## *Adding Noise Constraints*

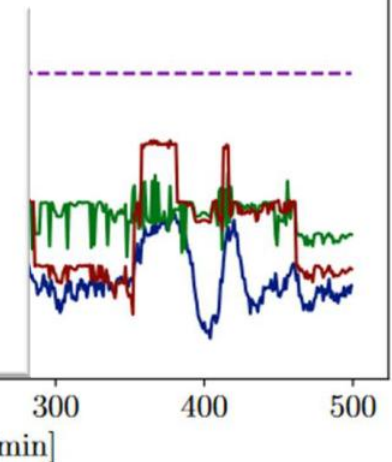


# Deep reinforcement learning for wind turbine control

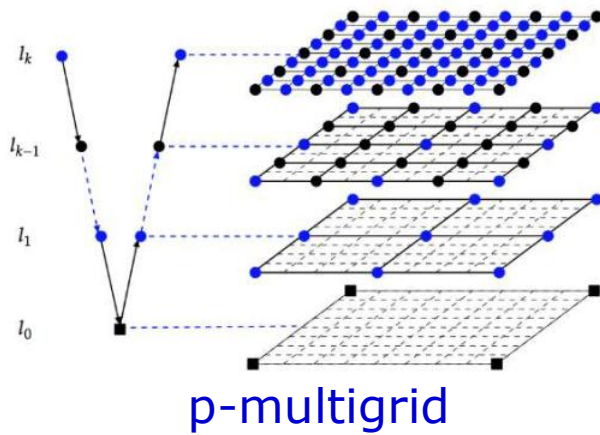
## *Adding Noise constraint*



Controller	$E_w$ [MWh]	$\hat{\sigma}_{C_p}$
<i>Quiet DDQN</i>	2722	0.024
<i>Power DDQN</i>	3541	0.042
Classic Controller	3458	0.057



# Reinforcement learning for p-multigrid



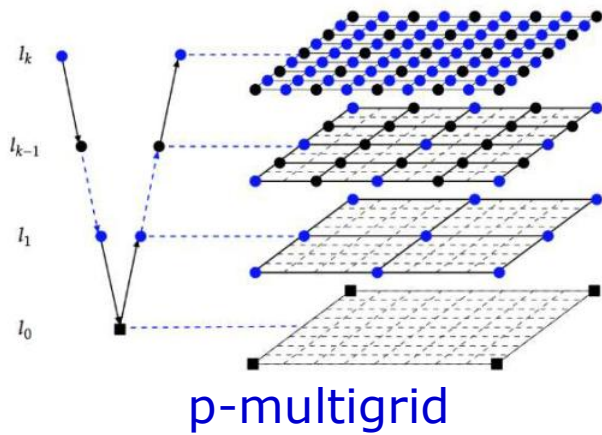
Cases			0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1	
Advection-diffusion	P3	IC: Sine7		135	126	121	121	123	124	1186	U	U	
		IC: sine				121				1186	U	U	
		IC: exp				121				1186	U	U	
	P5	IC: Sine7				471					U	U	U
		IC: sine				471					U	U	U
		IC: exp				471					U	U	U
	P7	IC: Sine7				1207					1205	U	U
		IC: sine				1207					1205	U	U
		IC: exp				1207					1205	U	U
	P9	IC: Sine7				2466					U	U	U
		IC: sine				2466					U	U	U
		IC: exp				2466					U	U	U
P3	R10	IC: Sine7	229	146	144	142	140	138	136	1188	U	U	

$$u_t + au_x - \nu u_{xx} = S$$

## Optimal parameters in p-multigrid multigrid?

- Sweeps
- Relaxation between levels

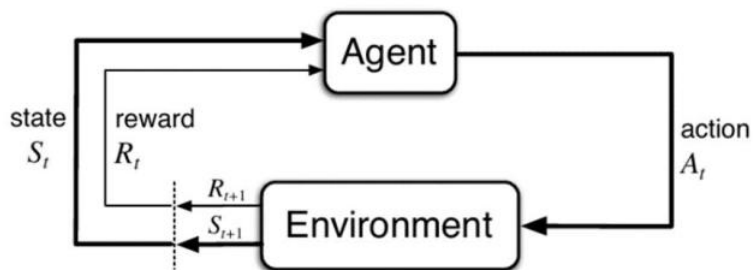
# Reinforcement learning for p-multigrid



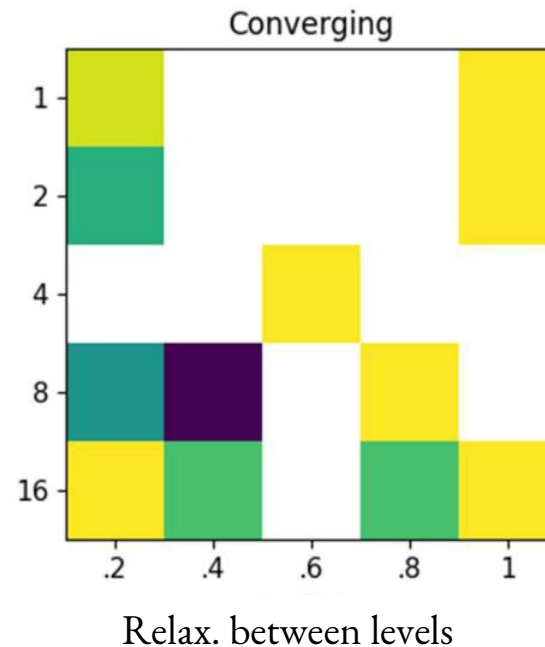
Cases		0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1	
Advection-diffusion	P3	IC: Sine7										
		IC: sine	135	126	121	121	123	124	1186	U	U	
		IC: exp								1186	U	U
	P5	IC: Sine7				471				U	U	U
		IC: sine				471				U	U	U
		IC: exp				471				U	U	U
	P7	IC: Sine7				1207				1205	U	U
		IC: sine				1207				1205	U	U
		IC: exp				1207				1205	U	U
	P9	IC: Sine7				2466				U	U	U
IC: sine					2466				U	U	U	
IC: exp					2466				U	U	U	
P3	R10	IC: Sine7	229	146	144	142	140	138	136	1188	U	U

$$u_t + au_x - \nu u_{xx} = S$$

Reward:  $f$  (Relative drop in residual, time taken)

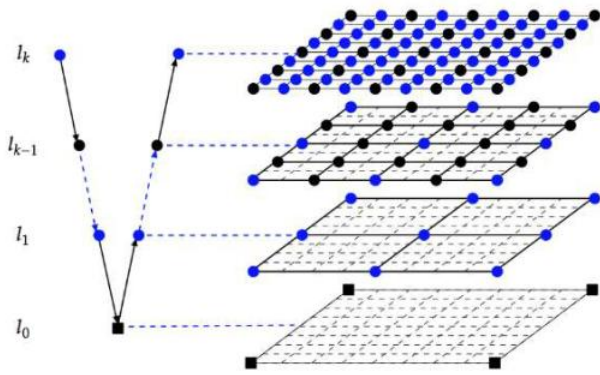


sweeps



Yellow → action taken  
Blue do not take it

# Reinforcement learning for p-multigrid



p-multigrid

Cases		0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1	
Advection-diffusion	P3	IC: Sine7										
		IC: sine	135	126	121	121	123	124	1186	U	U	
		IC: exp								1186	U	U
	P5	IC: Sine7				471				U	U	U
		IC: sine				471				U	U	U
		IC: exp				471				U	U	U
	P7	IC: Sine7				1207				1205	U	U
		IC: sine				1207				1205	U	U
		IC: exp				1207				1205	U	U
	P9	IC: Sine7				2466				U	U	U
IC: sine					2466				U	U	U	
IC: exp					2466				U	U	U	
P3	R10	IC: Sine7	229	146	144	142	140	138	136	1188	U	U

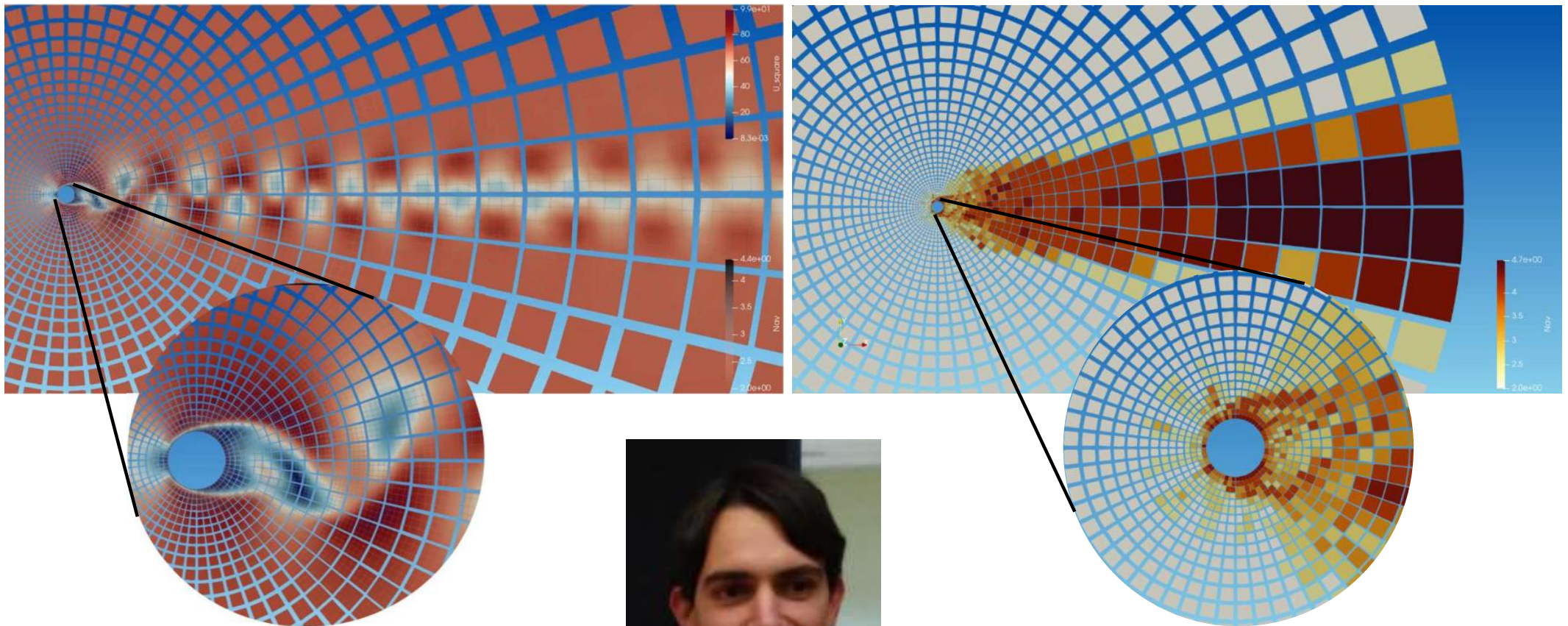
$$u_t + au_x - \nu u_{xx} = S$$

"Arbitrary"		MC		PPO		
runtime	iter	runtime	iter	runtime	iter	res
AD - Order 2						
a = 1., v = 0.01						
69.7168839	197	49.38292694	197	31.02763486	626	9.67E-09
a = 0.5., v = 0.01						
80.01094651	207	51.54315066	207	31.81400156	651	8.33E-09
a = 0.5., v = 0.5						
808.6031666	2178	480.8234568	2178	33.21327591	652	9.31E-09
a = 0.4, v = 0.6						
634.2691302	3166	582.4802358	3166	31.52360582	654	9.29E-09
a = 0.2, v = 0.8						
1476.47674	8063	1278.344407	7163	31.47797155	648	9.98E-09



# Reinforcement learning for p-adaptation

Cylinder  $Re = 200$

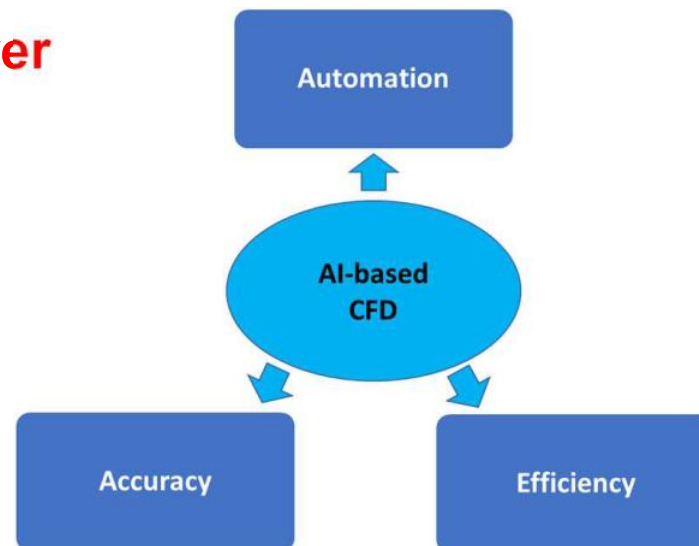


# Conclusions



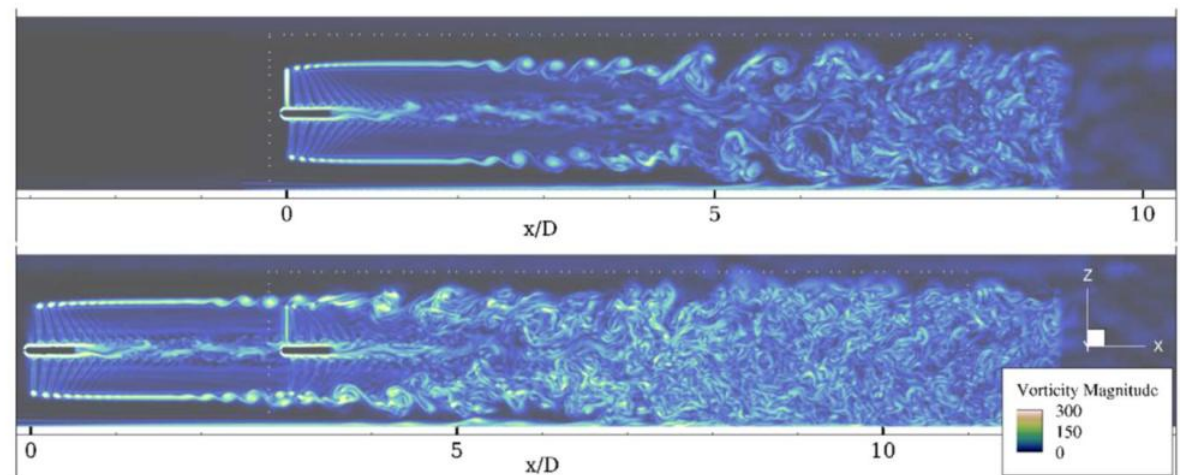
- **High order DG methods fairly well developed**
  - Incompressible flows & Compressible flows
- **Multiphysics:**
  - Wind turbines with various methods
  - Turbulence (iLES & explicit LES)
  - Aero-acoustics
  - Supersonic & Shocks

- **AI-based Solver**



# Doc & PostDoc disponibles in the group

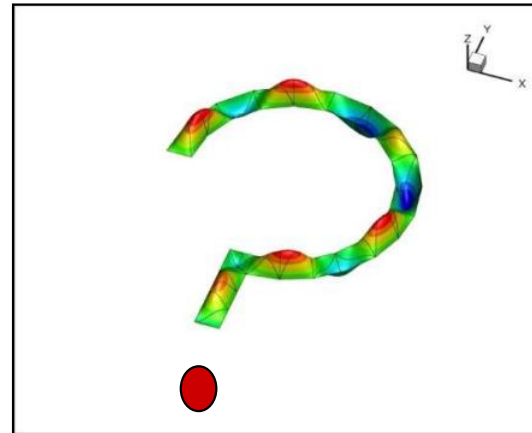
[esteban.ferrer@upm.es](mailto:esteban.ferrer@upm.es)



*If you like computers (like B. Gates), fluids, wind turbines, etc.*

# Thank you very much

esteban.ferrer@upm.es



@FerrerCfd



Esteban Ferrer

<http://sites.google.com/site/eferrerdg/publications>



Financiado por la Unión Europea  
NextGenerationEU



*We acknowledge the funding received by the Grant DeepCFD (Project No. PID2022-137899OB-I00) funded by MICIU/AEI/10.13039/501100011033 and by ERDF, EU.*

*We thank the support of Agencia Estatal de Investigación for the grant "Europa Excelencia" for the project EUR2022-134041 funded by MCIN/AEI/10.13039/501100011033) y the European Union NextGenerationEU/PRTR*



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*This research has been cofunded by the European Union (ERC, Off-coustics, project number 101086075). Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them*



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# Reinforcement Learning for Anisotropic p-Adaptation and Error Estimation in High-order Solvers

David Huergo Perea

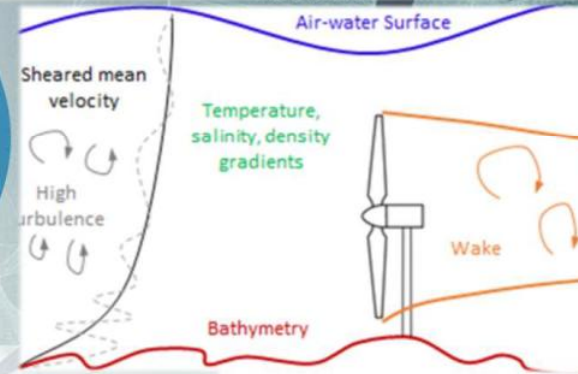
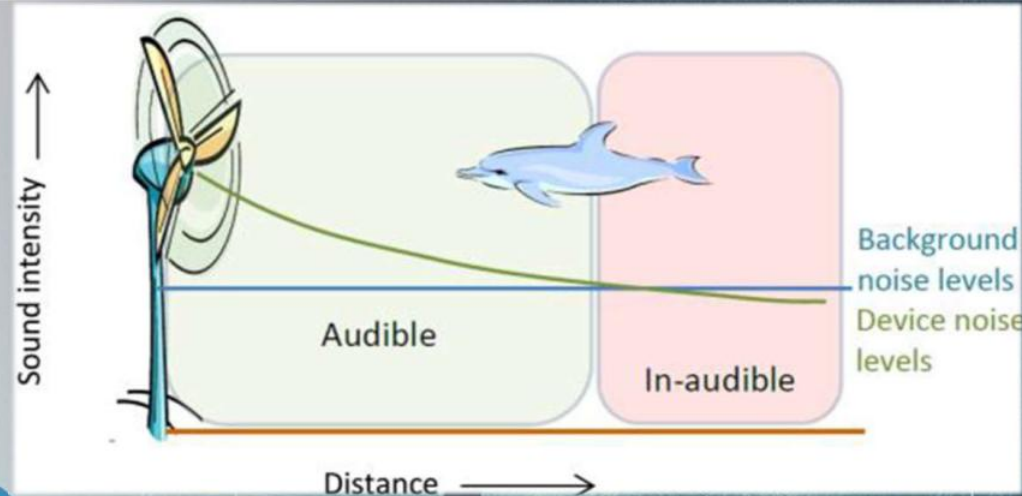
**UPM Collaborators:**

M. de Frutos, E. Jané, O. Mariño, G. Rubio, E. Ferrer





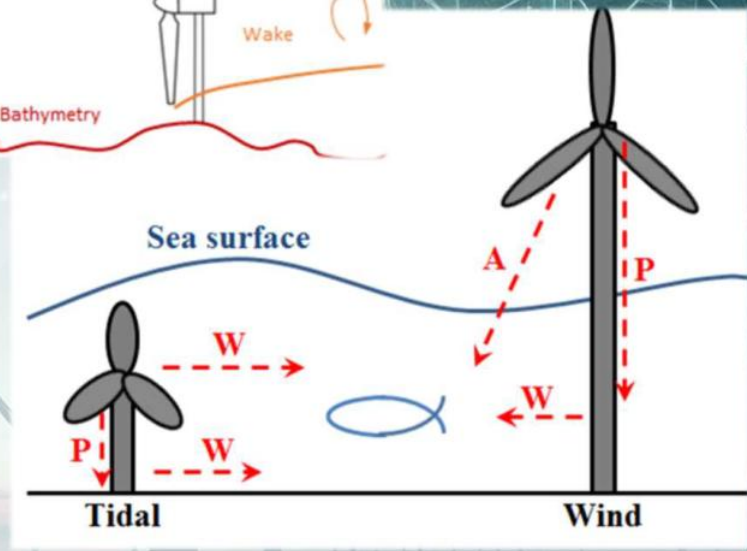
POLITÉCNICA



# Funding



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# Contents



- p-Adaptation in DGSEM solvers
- Reinforcement Learning for p-adaptation
- Results
- Ongoing Work
- Conclusions

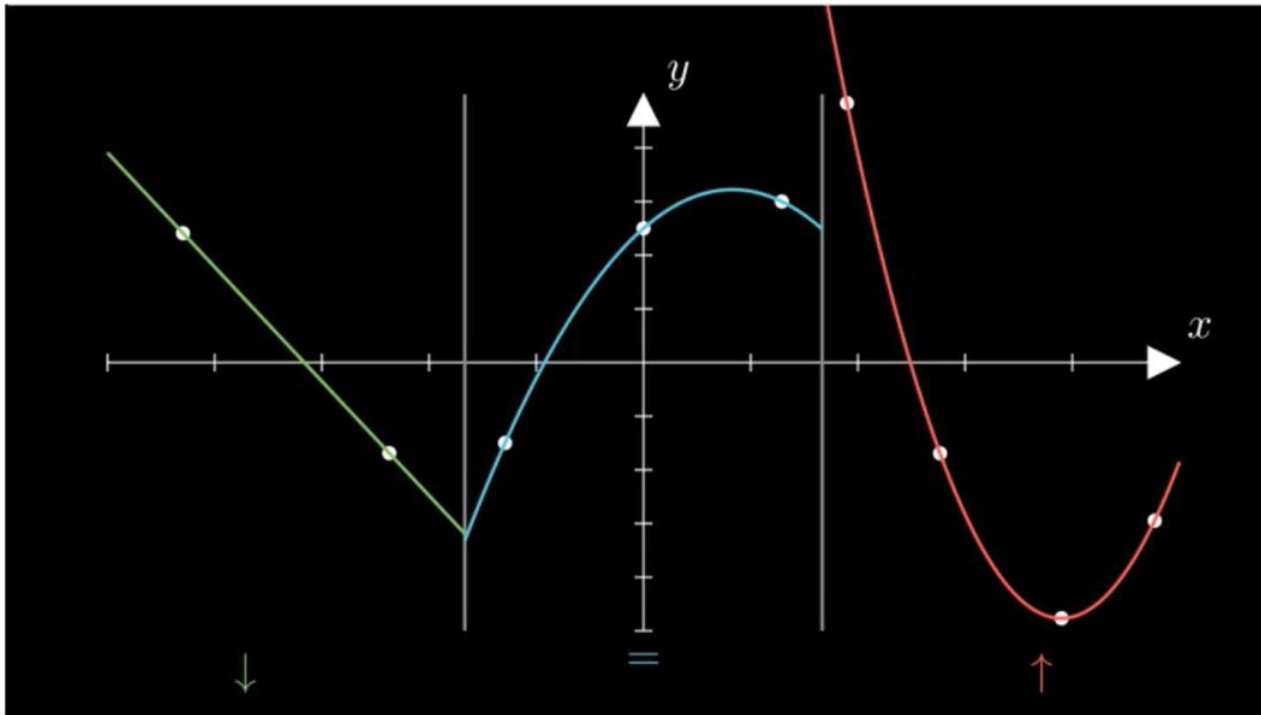
# **p-Adaptation in DGSEM solvers**

---



# 1.1. p-Adaptation for DGSEM

## Discontinuous Galerkin Spectral Element Method



- The solution is approximated in each element using **Lagrange polynomials** based on **Legendre-Gauss nodes**.
- p-Adaptation allows to select the **optimal polynomial in each element** of the mesh to obtain **accurate solutions** with a **reduced computational cost**.
- Manual p-adaptation requires to know beforehand the behaviour of the solution.

# 1.2. p-Adaptation with Truncation Error

## DGSEM simulation

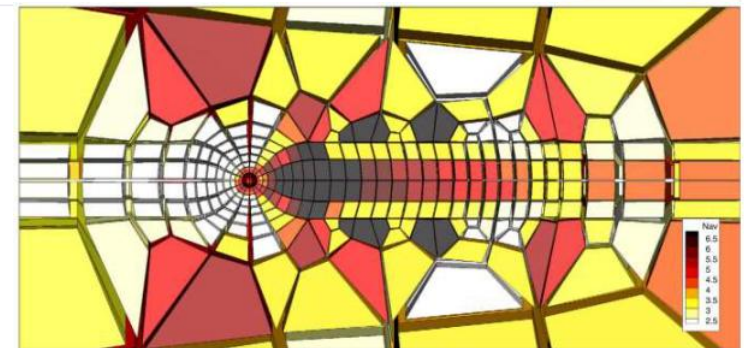
Example of a p-adapted mesh, based on the **Truncation Error**, for the flow around a sphere at Reynolds 200.

The contours indicate the average polynomial order ( $N_{av}=(N1 +N2 +N3)/3$ ). [1, 2]

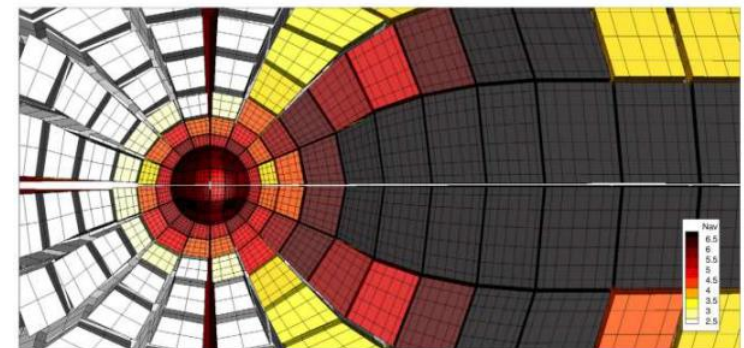
Simulated using HORSES3D

<https://github.com/loganoz/horses3d>

[3] E. Ferrer, G. Rubio, W. Laskowski, O.A. Mariño, S. Colombo, A. Mateo-Gabín, H. Marbona, F. Manrique de Lara, D. Huergo, J. Manzanero, A.M. Rueda-Ramírez, D.A. Kopriva and E. Valero, HORSES3D: A high-order discontinuous Galerkin solver for flow simulations and multi-physics applications, Computer Physics Communications 287 (2023): 108700.



(a) Average polynomial order ( $N_{av}$ ).



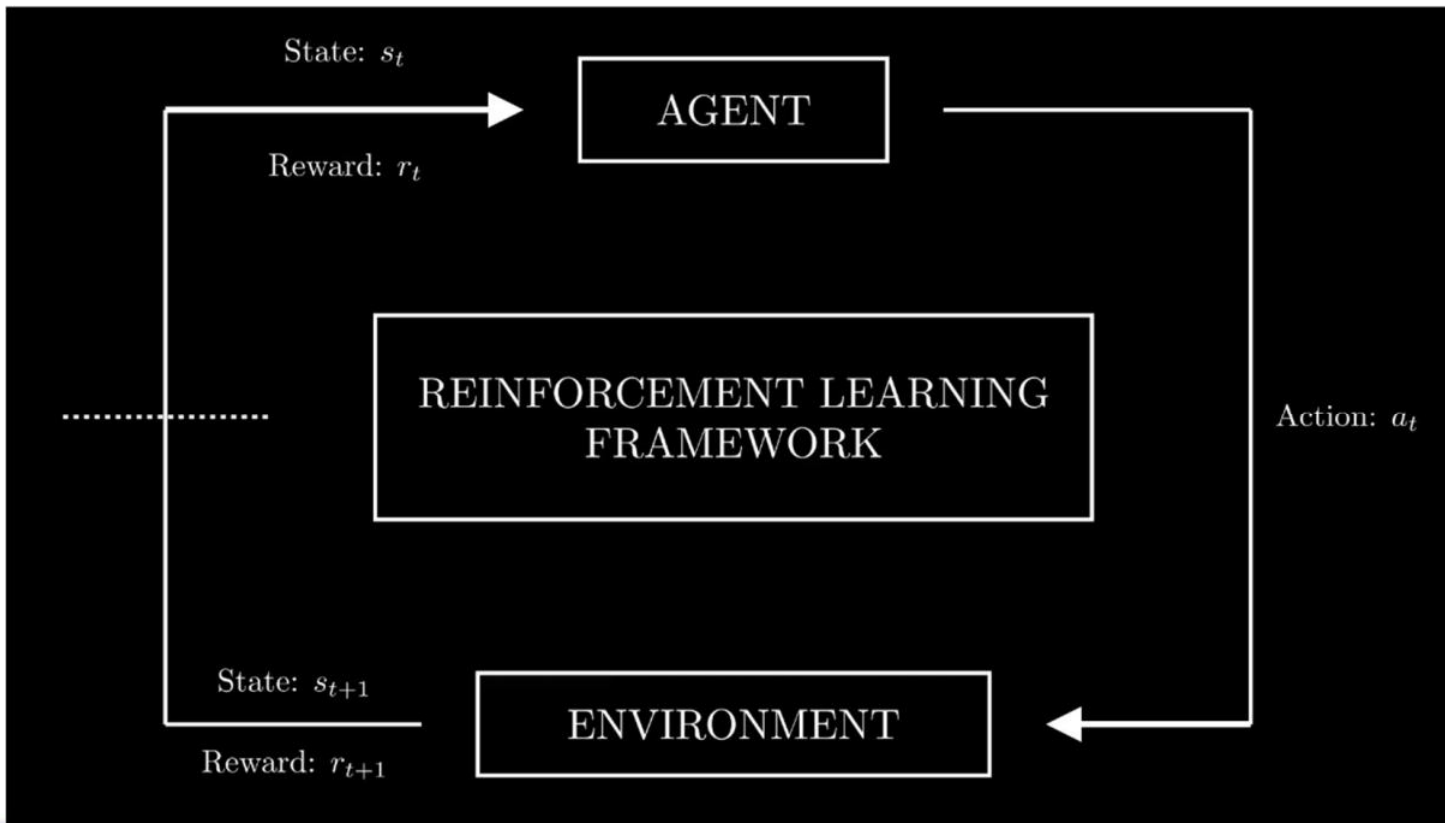
[1] A. M. Rueda-Ramírez, J. Manzanero, E. Ferrer, G. Rubio, E. Valero, A p-multigrid strategy with anisotropic p-adaptation based on truncation errors for high-order discontinuous Galerkin methods, Journal of Computational Physics 378 (2019).

[2] A. M. Rueda-Ramírez, G. Ntoukas, G. Rubio, E. Valero, E. Ferrer, Truncation Error-Based Anisotropic p-Adaptation for Unsteady Flows for High-Order Discontinuous Galerkin Methods, International Journal of Computational Fluid Dynamics, 37(6), 430–450 (2024).

# **Reinforcement Learning for p-adaptation**



# 2.1. The RL framework

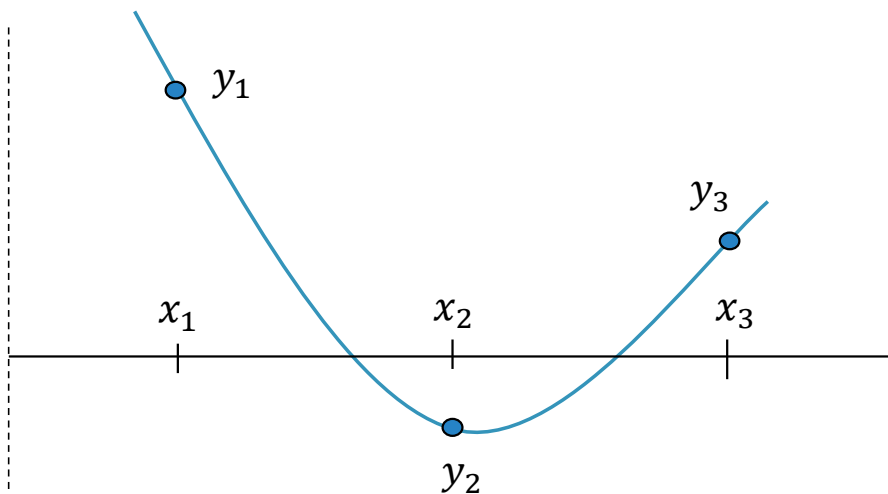


- **Agent:** Decides the action.
- **Environment:** Current problem (our DGSEM solver).
- **Action:** Increment or decrement the polynomial order  $p$ .
- **State:** To be defined.
- **Reward:** To be defined.

## 2.2. State and Reward

### State

$$s = [y_1, y_2, \dots, y_n]$$



The size of the state depends on the polynomial order.

### Reward

Two main objectives:

- **Minimum polynomial order:** Computational cost is reduced.
- **High accuracy:** High order required if strong gradients are present.

$$reward = \left( \frac{p_{max}}{p} \right)^\alpha e^{-\frac{rmse^2}{2\sigma^2}}$$

- $rmse$  : Between the solution and the analytical function in 14 points.
- $\sigma = 0.05$ : Standard deviation.
- $p_{max} = 6$ : Maximum order allowed.
- $\alpha = 0.9$ : Control parameter.

## 2.3. Training

### Drawbacks

**Expensive** training when coupled with a CFD solver

Reward function based on **analytical solution**



### Solution

Training based on **polynomial functions** in a single element



### Advantages

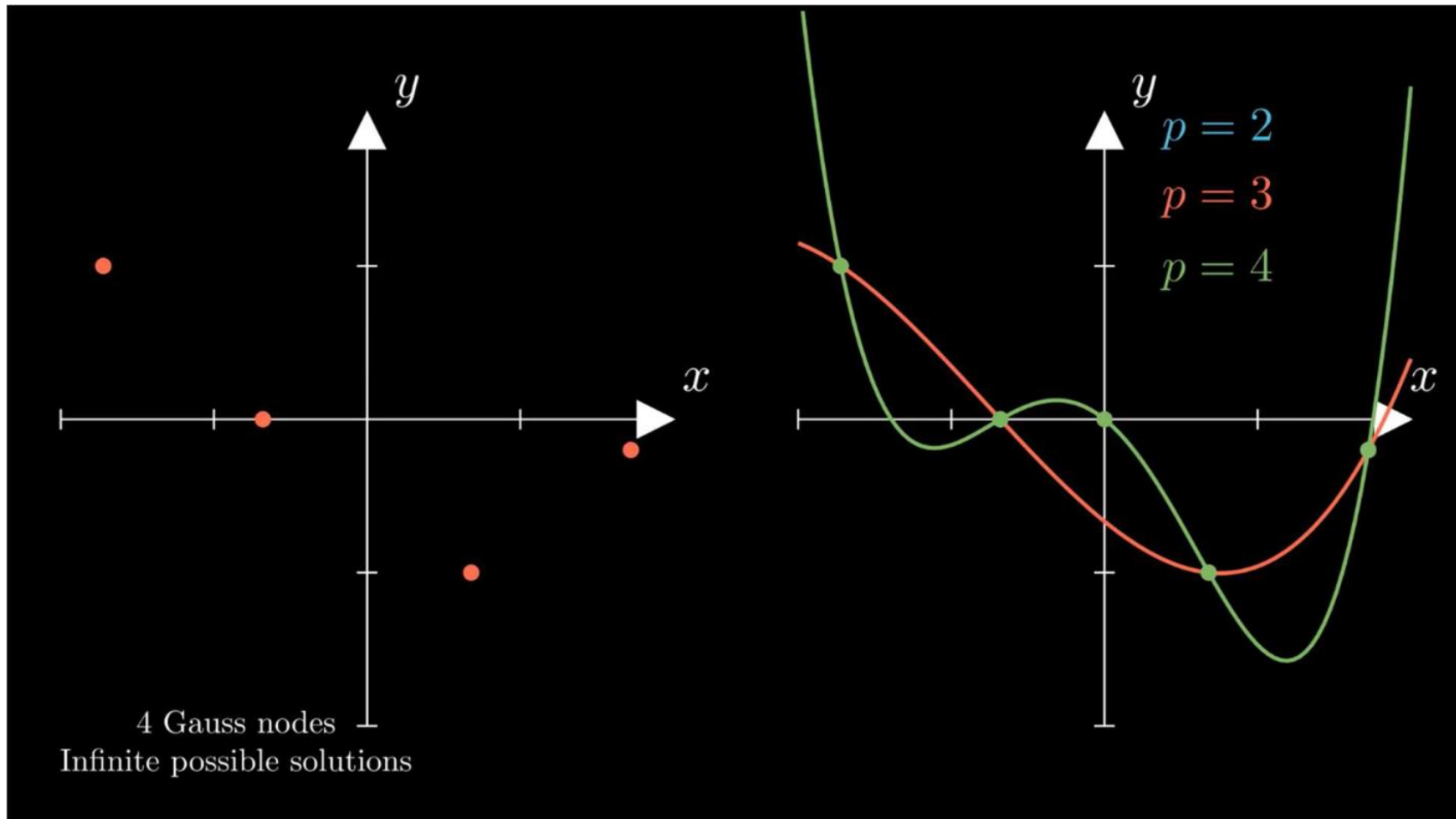
**CFD not required** during the training

**Analytical solution known** during the training

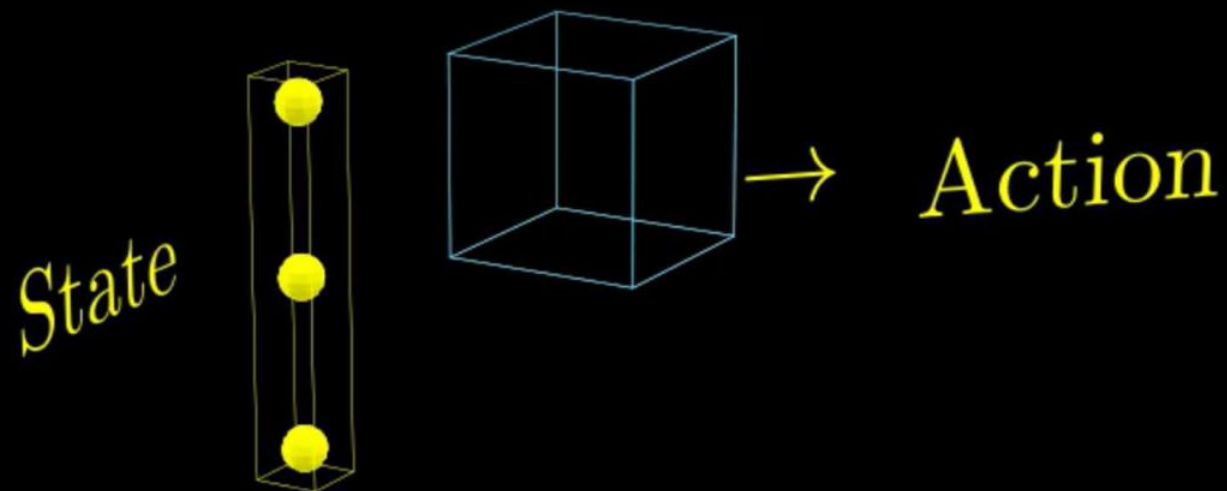
The resulting agent:

- Has to be **trained only once**.
- **Can be potentially applied to any PDE** solved with a DGSEM solver.
- **Can be used in an arbitrary mesh**: the agent chooses the optimum polynomial order individually for each element.

## 2.3. Training



## 2.4. Extrapolation for 3D cases





## 2.5. Error Estimation

### Bellman Optimality Equation

$$V^*(s) = \max_a \sum_{s', r} p(s', r | s, a) [r + \gamma V^*(s')]$$



$$\widehat{rmse} = \sqrt{-2\sigma^2 \log \left( \frac{V^*(s) - \bar{r} - \gamma \bar{r}'}{\gamma^2 V_{\max, p}} \right)}$$

- **V-values**
- **Reward**
- **Discount factor**
- **Probability transition function**

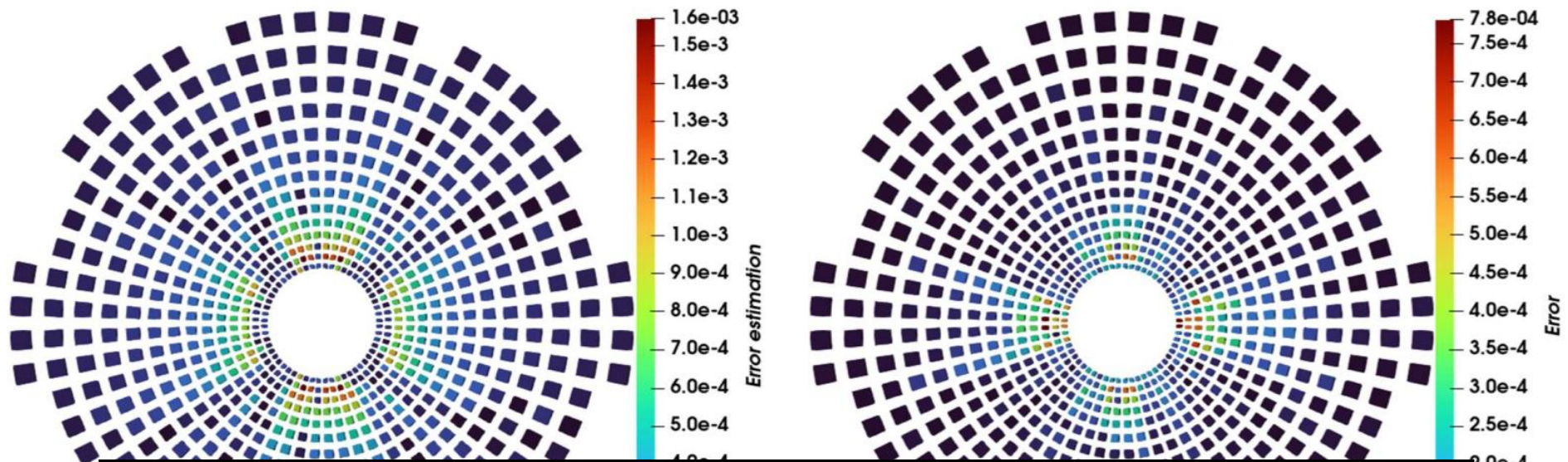
The error estimation:

- Provides the **spatial error that the RL agent believes to be real** inside each element.
- **Is learned during the training** and can be applied without additional knowledge of the problem to be solved.
- **Is more accurate if coupled with p-adaptation.**

# Results

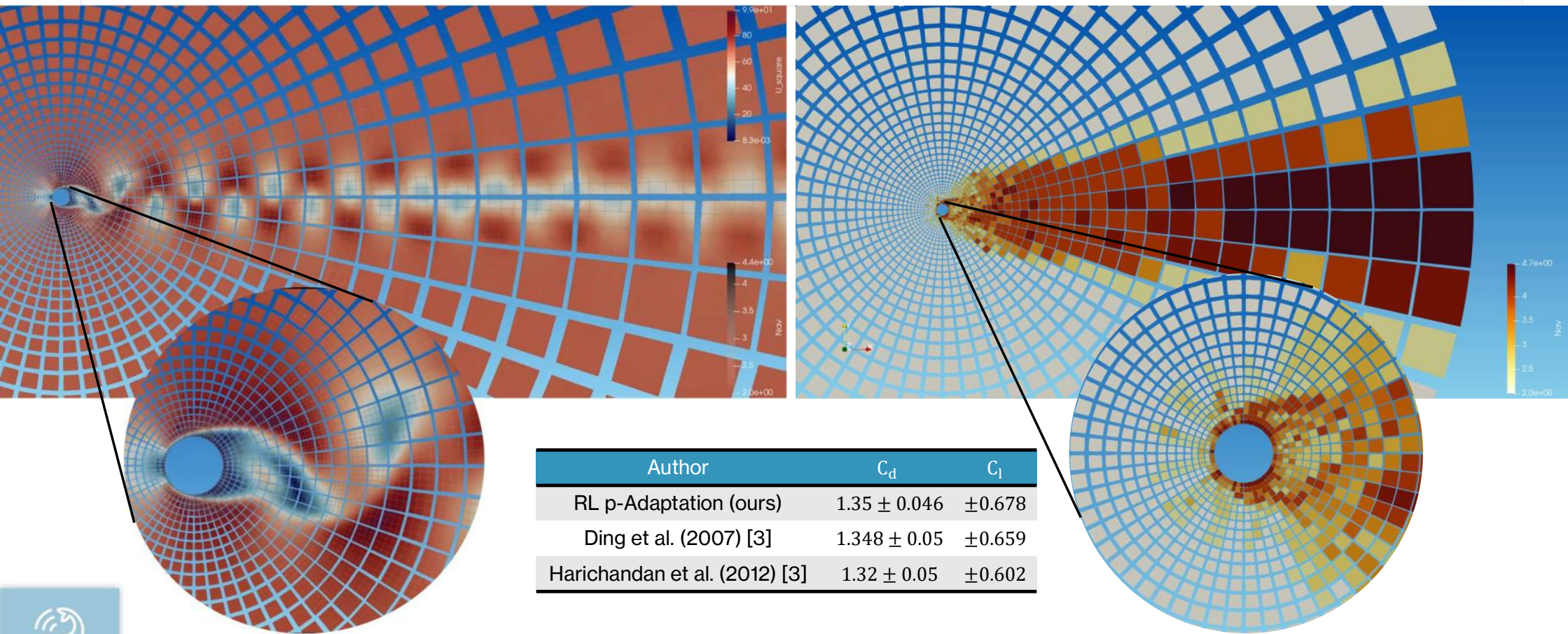
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# 3.1. Euler Flow around a cylinder



Polynomial order	DOFs	Computational cost (s)	Real Error	Error Estimation
$p = 2$	58968	252	$8.1 \cdot 10^{-3}$	$2.1 \cdot 10^{-3}$
$p = 3$	139776	431	$6.7 \cdot 10^{-4}$	$2.8 \cdot 10^{-4}$
$p = 4$	273000	737	$6.5 \cdot 10^{-5}$	$3.0 \cdot 10^{-5}$
$p = 5$	471744	1181	0.0 (reference)	0.0 (reference)
<b>p – adapted</b>	<b>27708</b>	<b>197</b>	<b><math>7.8 \cdot 10^{-4}</math></b>	<b><math>1.6 \cdot 10^{-3}</math></b>

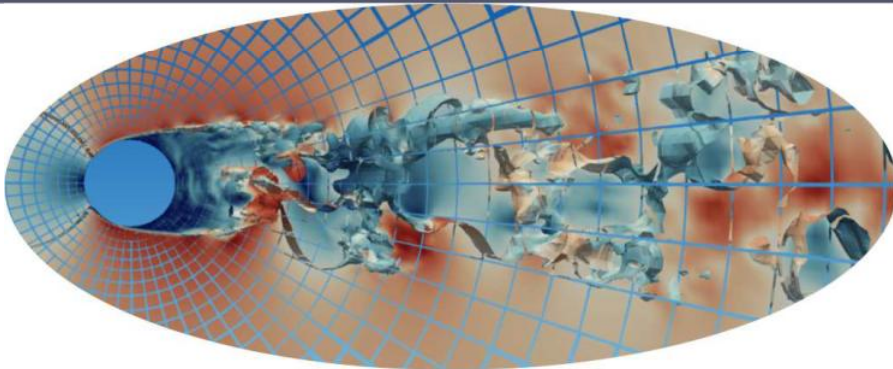
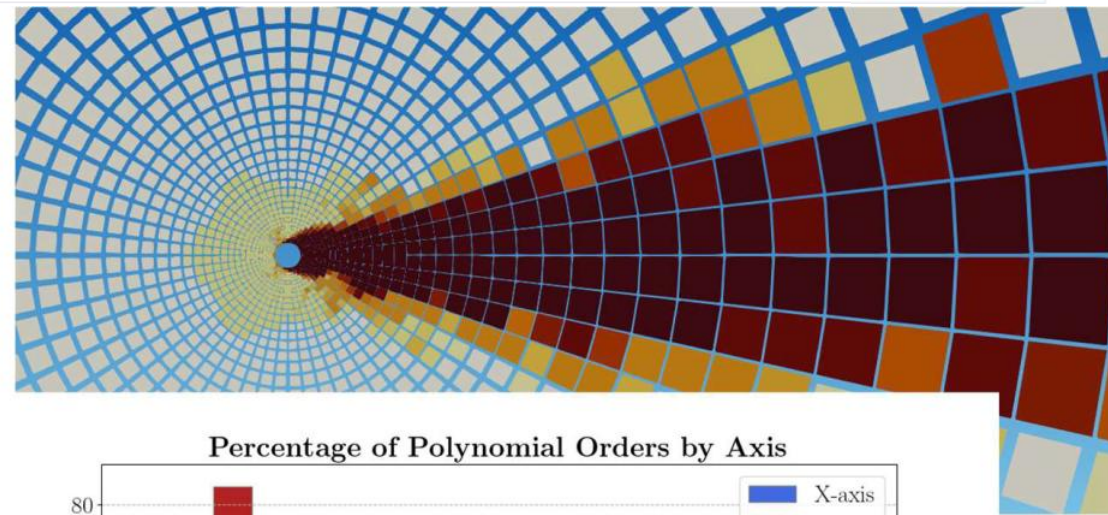
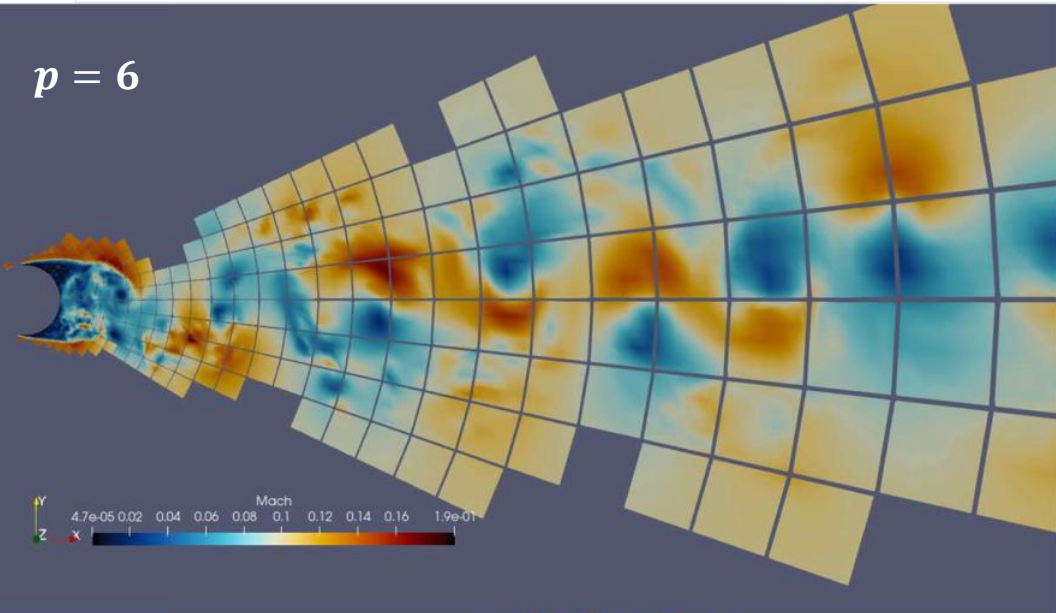
## 3.2. Cylinder $Re = 200$



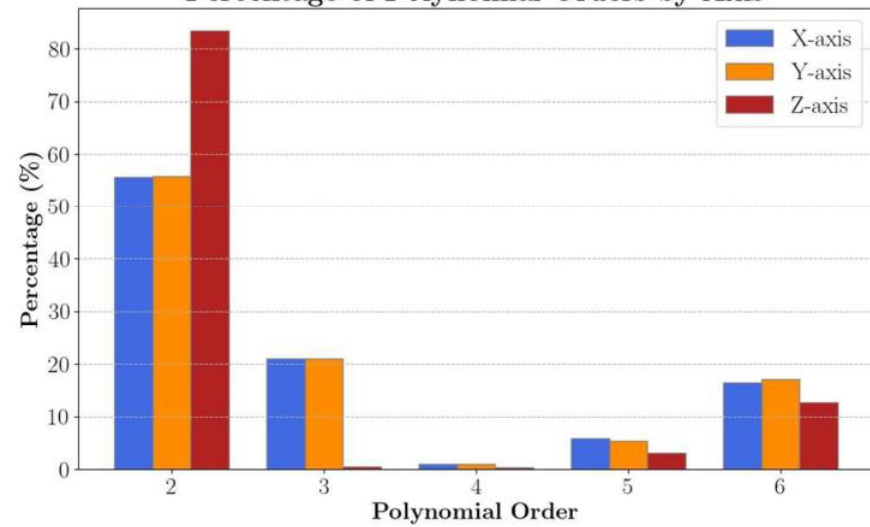
[3] AB Harichandan and A Roy. Numerical investigation of flow past single and tandem cylindrical bodies in the vicinity of a plane wall. Journal of Fluids and Structures, 33:19–43, 2012.

# 3.3. Cylinder $Re = 3900$

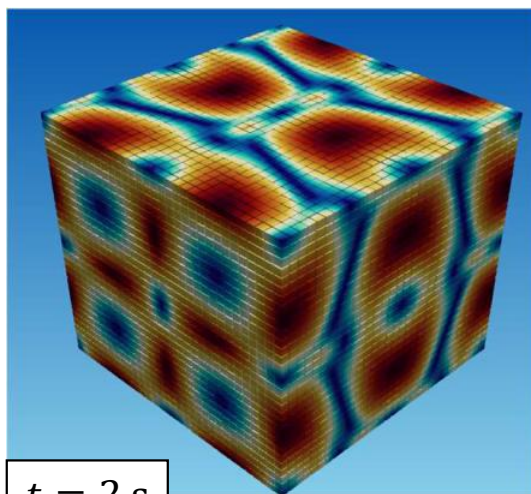
$p = 6$



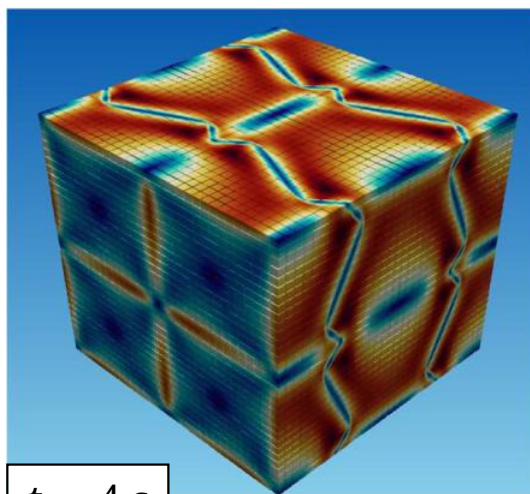
Percentage of Polynomial Orders by Axis



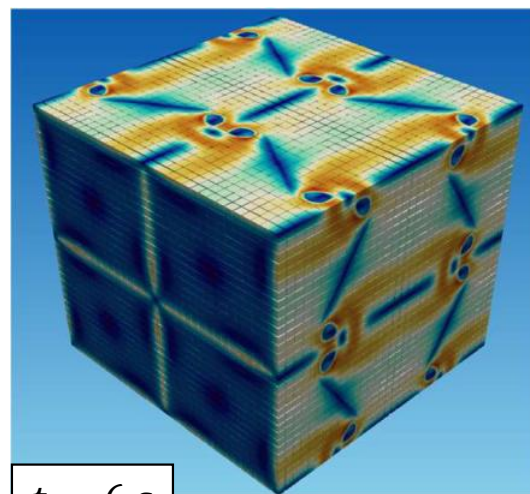
# 3.4. Taylor Green Vortex



$t = 2 \text{ s}$

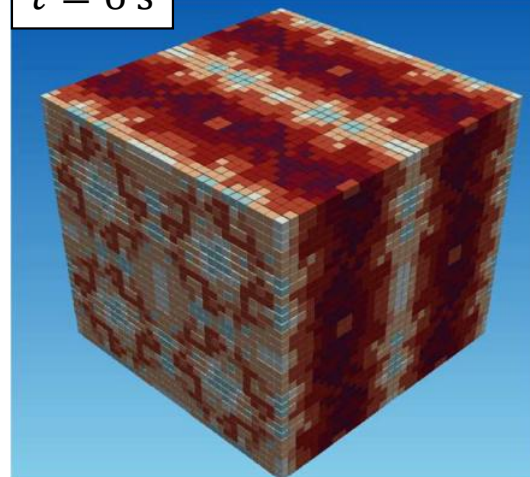
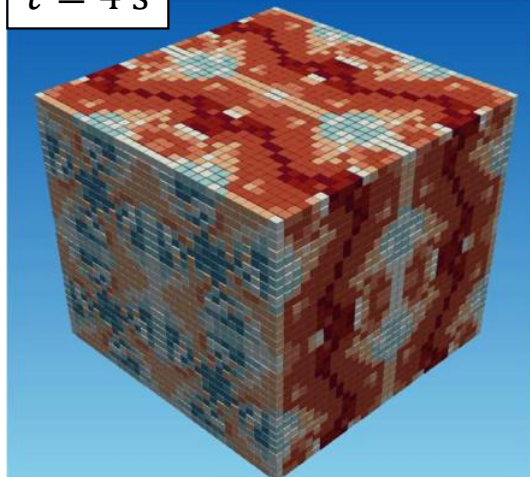
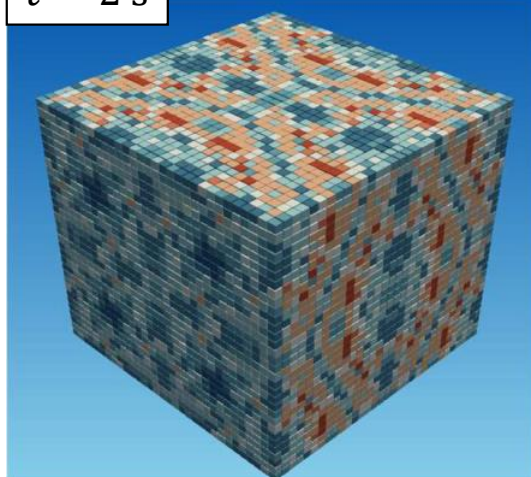


$t = 4 \text{ s}$



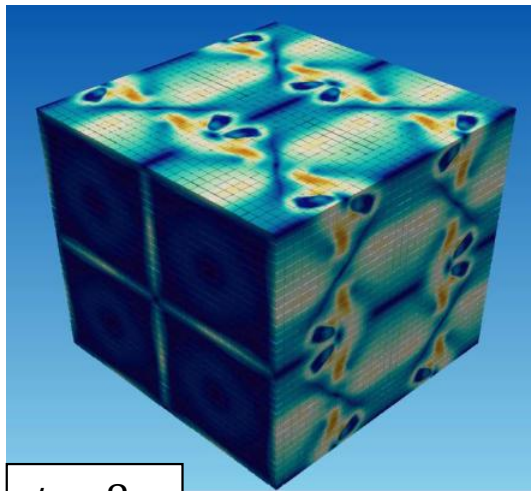
$t = 6 \text{ s}$

Velocity magnitude

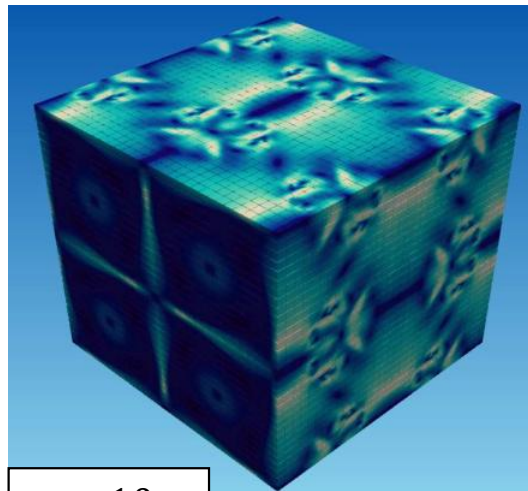


$p_{av}$

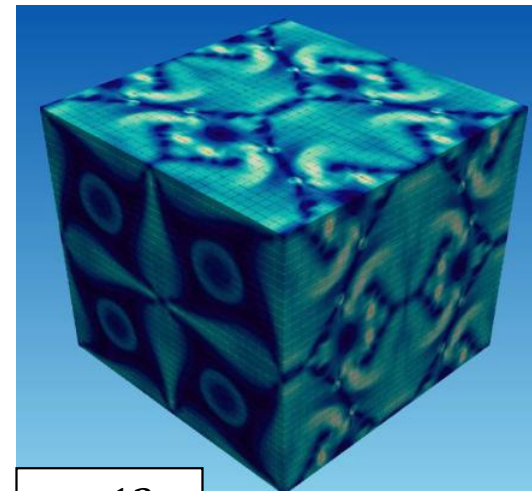
# 3.4. Taylor Green Vortex



$t = 8 \text{ s}$

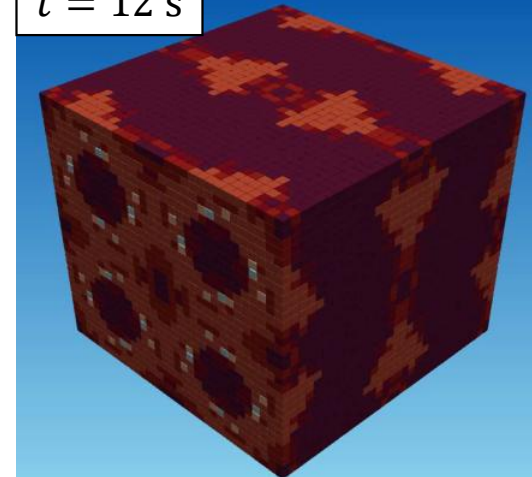
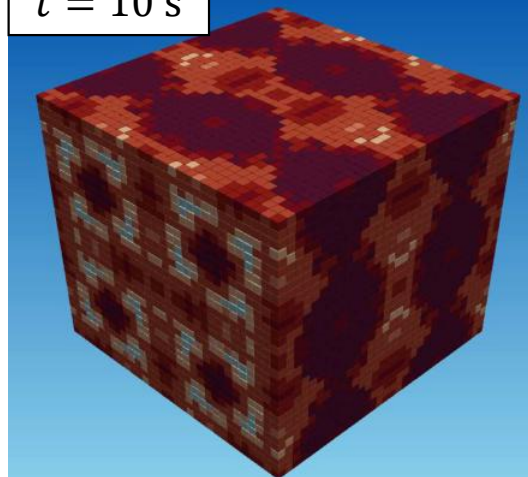
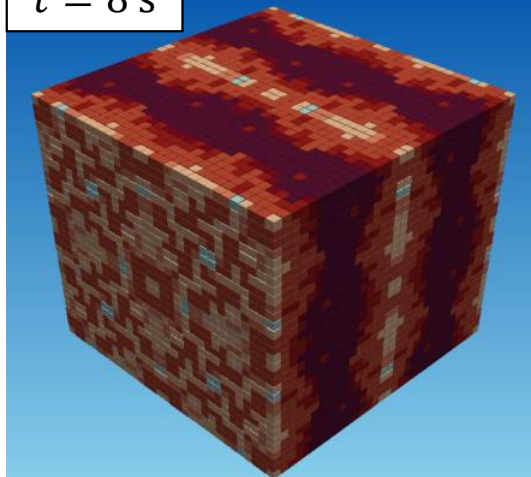


$t = 10 \text{ s}$



$t = 12 \text{ s}$

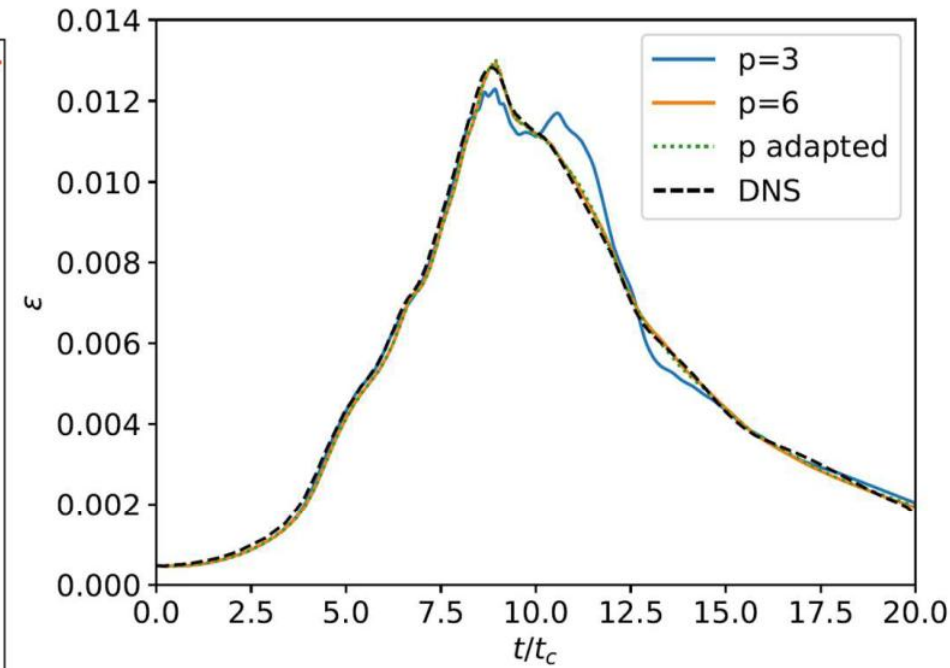
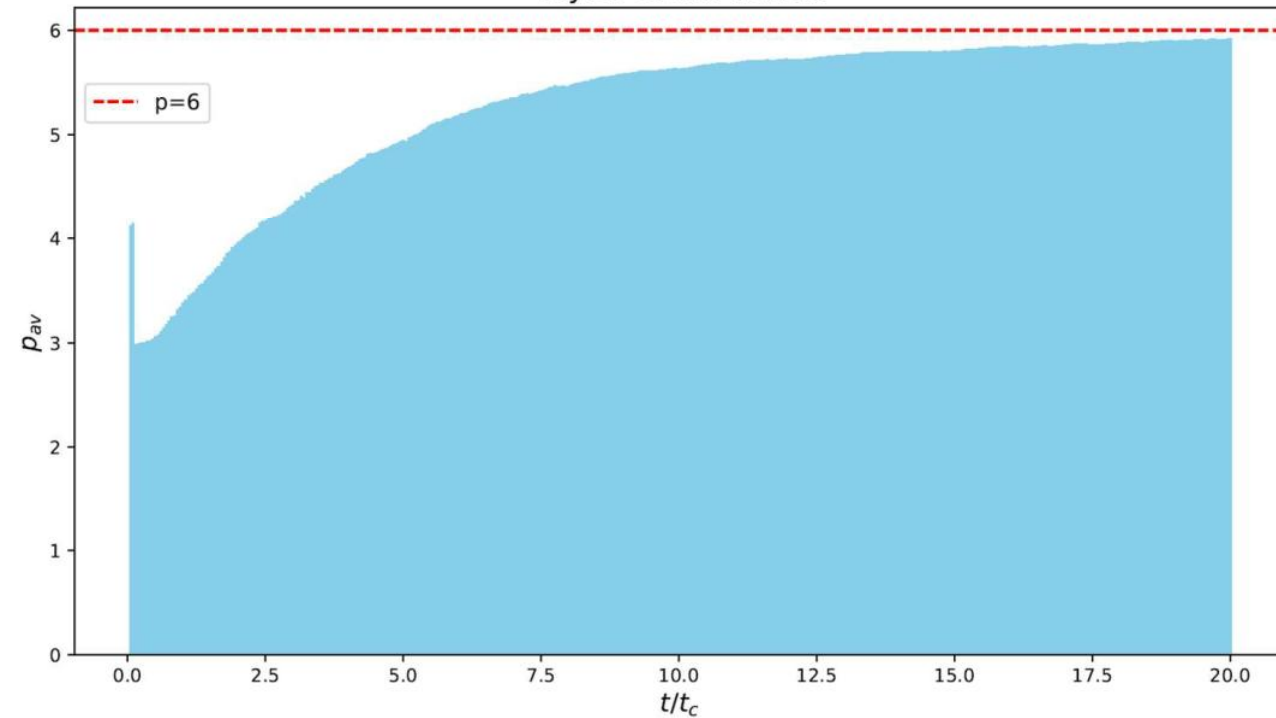
Velocity  
magnitude



$p_{av}$

# 3.4. Taylor Green Vortex

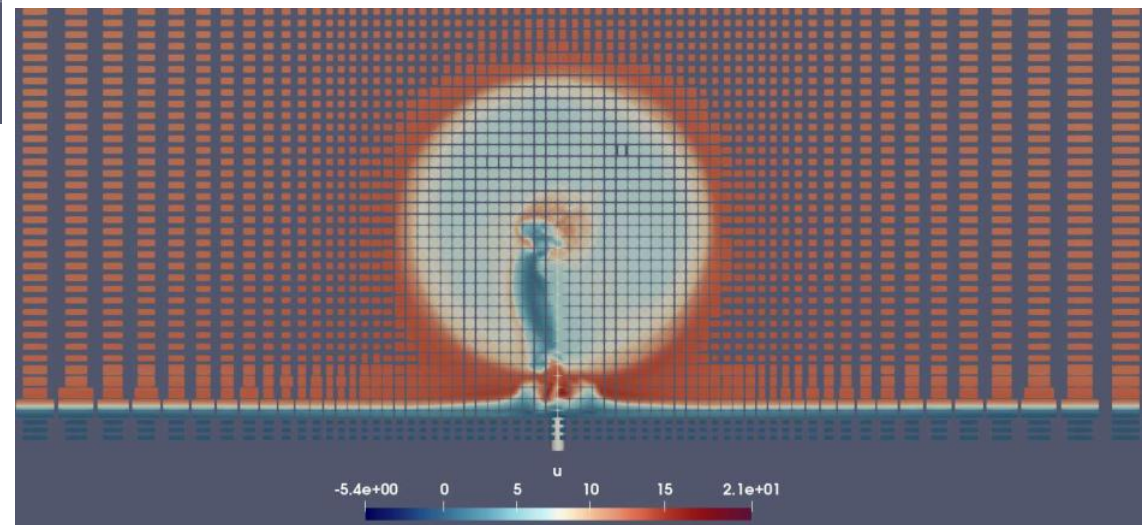
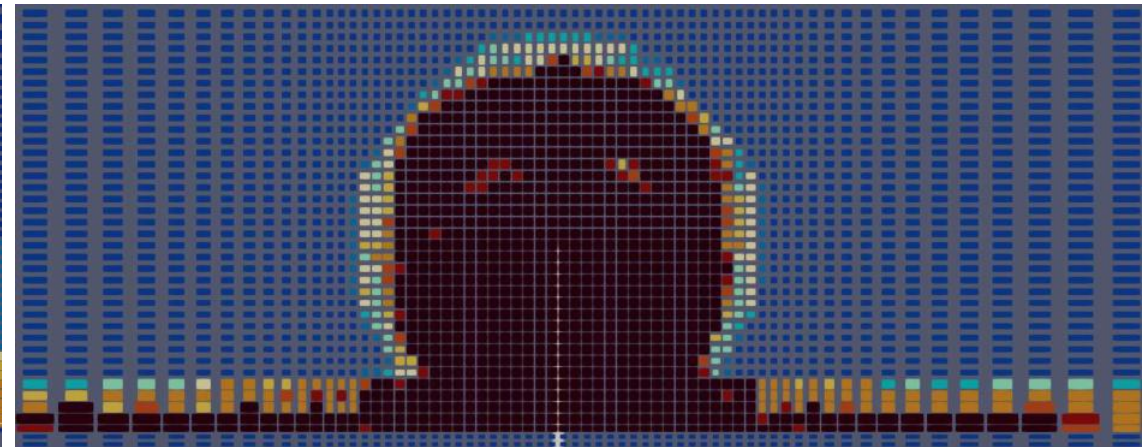
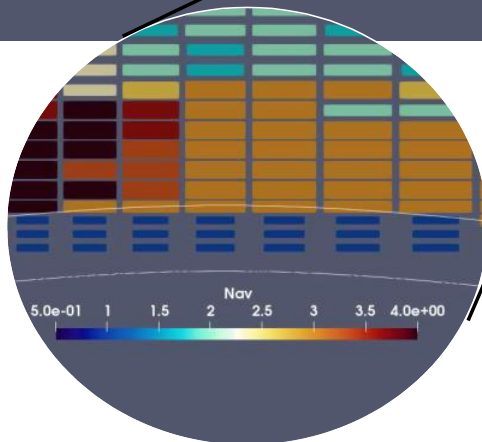
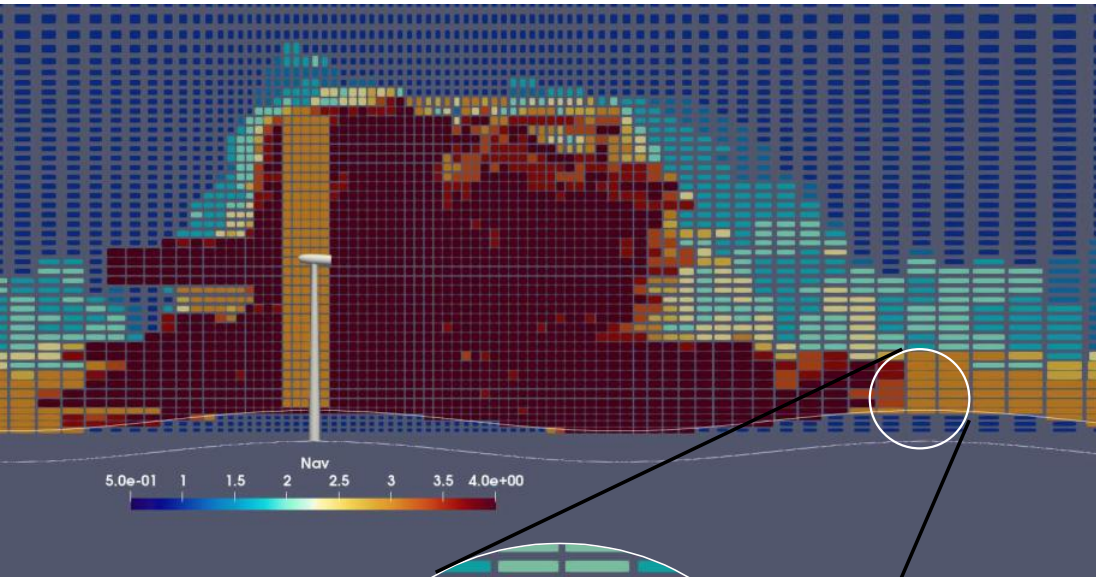
Taylor Green Vortex



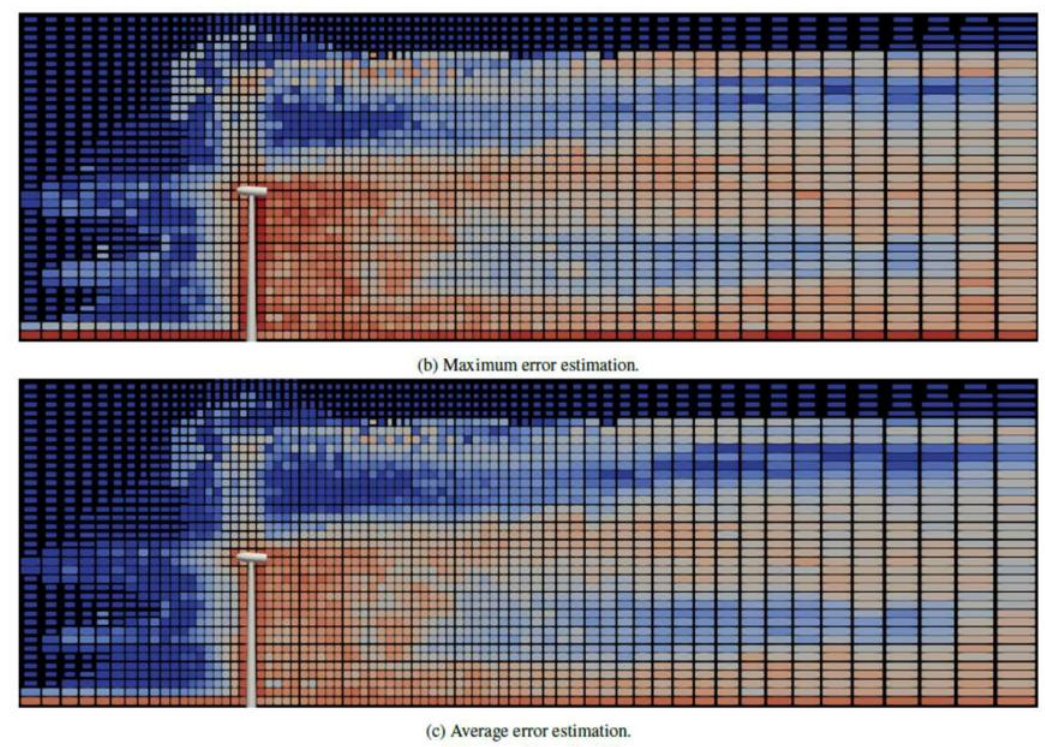
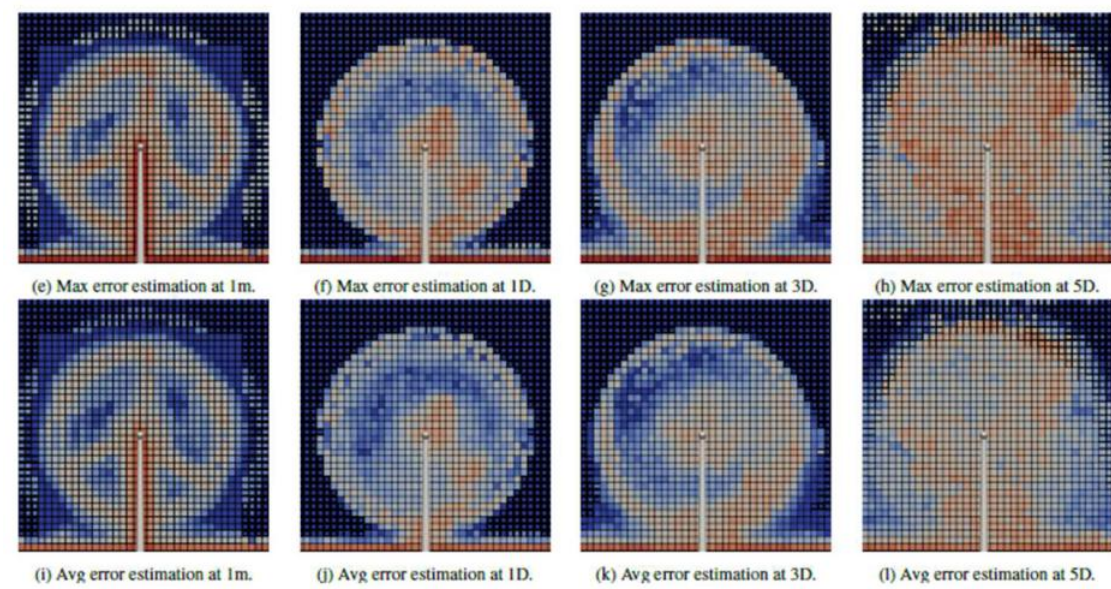
	$p = 6$	$p_{adapted}$
Computational cost (h)	102	41



# 3.5. Offshore Wind Turbine DTU 10MW



# 3.5. Offshore Wind Turbine DTU 10MW



The error is higher:

- Near the **Actuator Line**.
- On the **no-slip wall boundary condition**.
- Inside the **Immersed Boundaries (tower and nacelle)**.
- Inside the **wake**.

# Ongoing Work

---

# 4. Ongoing work



- RL p-adaptation for moving **Immersed Boundaries**.
- RL p-adaptation for **acoustics**.
- **Comparison** with different state-of-the-art p-adaptation algorithms.
- Dynamic **load balancing** to improve MPI parallelization for evolving meshes.

Results in Engineering  
Volume 21, March 2024, 101693

ELSEVIER

Full Length Article

### A reinforcement learning strategy for p-adaptation in high order solvers

David Huergo <sup>a</sup>, Gonzalo Rubio <sup>a, b</sup>, Esteban Ferrer <sup>a, b</sup>

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arXiv:2407.19000v1 [physics.flu-dyn] 26 Jul 2024



### Reinforcement learning for anisotropic p-adaptation and error estimation in high-order solvers

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# Conclusions

---

# 5. Conclusions



- RL for **p-adaptation** leads to a general approach to **improve the accuracy** and **reduce the computational time** of CFD simulations.
- The proposed methodology can be potentially applied for **any PDE and computational mesh**.
- The RL agent **has to be trained only once for 1D** cases, but provides an **accurate adaptation in 3D turbulent simulations**.
- The proposed methodology provides a cheap **estimation of the spatial error in each element** of the computational mesh.

**Reinforcement Learning** can be applied to **minimize manual intervention**, to **improve the accuracy** of numerical simulations and to **speed-up** a CFD code.



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# Thank you!

## Funding



This research has been co-funded by the European Union (ERC, Off-coustics, project number 101086075). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.