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Uncertainty quantification and stochastic sensitivity analysis to assess and improve the reliability of large-eddy simulations

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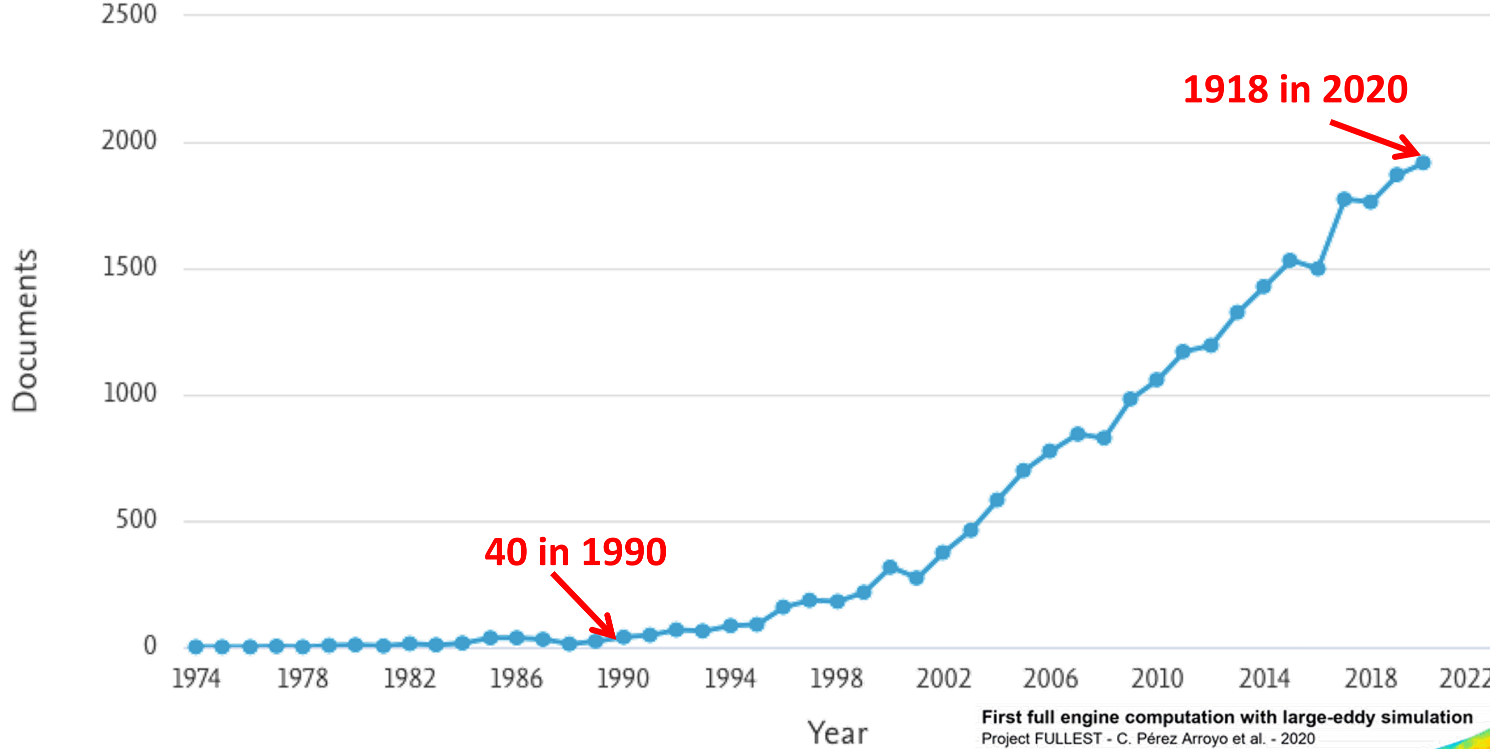
LES generalities

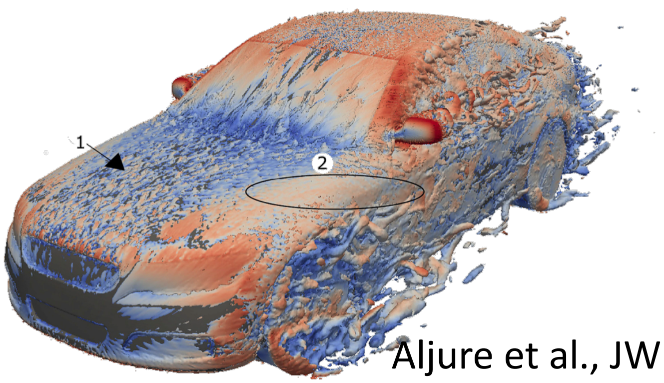
- ✓ Turbulence scales larger than a given dimension (typical the grid size) are directly simulated
- ✓ Only the effect of the non-resolved turbulence scales (SGS scales) on the motion of the large resolved scales is modeled → in most cases, this effect can be thought as mainly dissipative

LES is considered a *high-fidelity* approach compared with RANS/URANS, at the price of much larger computational requirements

LES nowadays

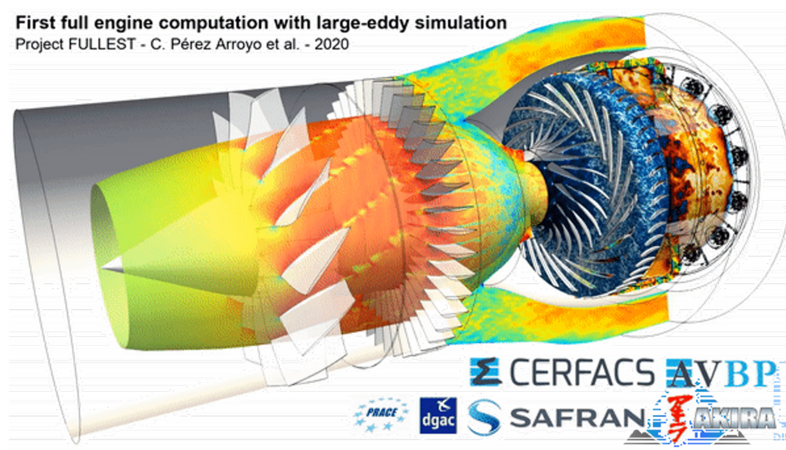
Number of papers in Scopus containing ‘Large-Eddy simulation(s)’ in title or abstract





Aljure et al., JWEIA (2018)

(b) $\omega^* \pm 50$



LES nowadays

- ✓ Number of applications of LES is *exponentially* increasing
- ✓ Variety and complexity of applications of LES has significantly increased
- ✓ LES available in most commercial and open-source CFD codes --> LES increasingly carried out by non expert users

Need for procedures or criteria to assess the accuracy and reliability of LES results

Although LES is considered a *high-fidelity* approach, validation is a complex task due to some peculiar problems, which are not present for instance with RANS/URANS

Sources of uncertainty/error in numerical simulations of turbulent flows

Grid resolution

Numerical accuracy

Discretization errors

Turbulence modeling

Modeling of other phenomena

Modeling errors

Simplifications/uncertainties in problem boundary conditions

Sources of uncertainty/error in numerical simulations of turbulent flows

Grid resolution → Discretization errors

Numerical accuracy → Discretization errors

Turbulence modeling → Modeling errors

Simplifications/uncertainties in problem boundary conditions

Sources of **uncertainty/error** in numerical simulations of turbulent flows

Grid resolution

Numerical accuracy

~~Discretization errors~~

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Sources of uncertainty/error in numerical simulations of turbulent flows

Grid resolution

Numerical accuracy

→ Discretization errors

Turbulence modeling

→ Modeling errors

Simplifications/uncertainties in problem boundary conditions

RANS/URANS

Sources of uncertainty/error in numerical simulations of turbulent flows

Grid resolution

Numerical accuracy

Turbulence modeling

Discretization errors

Modeling errors

In LES discretization and modeling errors can be of the same order and they may interact in a complex way

Simplifications/uncertainties in problem boundary conditions

LES

How to deal with discretization and modeling errors in LES?

Controversial ideas and approaches in the LES community

First approach: make the discretization errors negligible compared to the effects of a physically based SGS model

Grid resolution

Numerical accuracy

~~Discretization errors~~

Turbulence modeling

Modeling errors

How to deal with discretization and modeling errors in LES?

First approach (*extreme*): make the discretization errors negligible compared to the effects of a physically based SGS model

How to do that?

- High-order methods on fine (structured) grids
- No numerical dissipation

see e.g. Ghosal (1996), Kravchenko and Moin (1997)

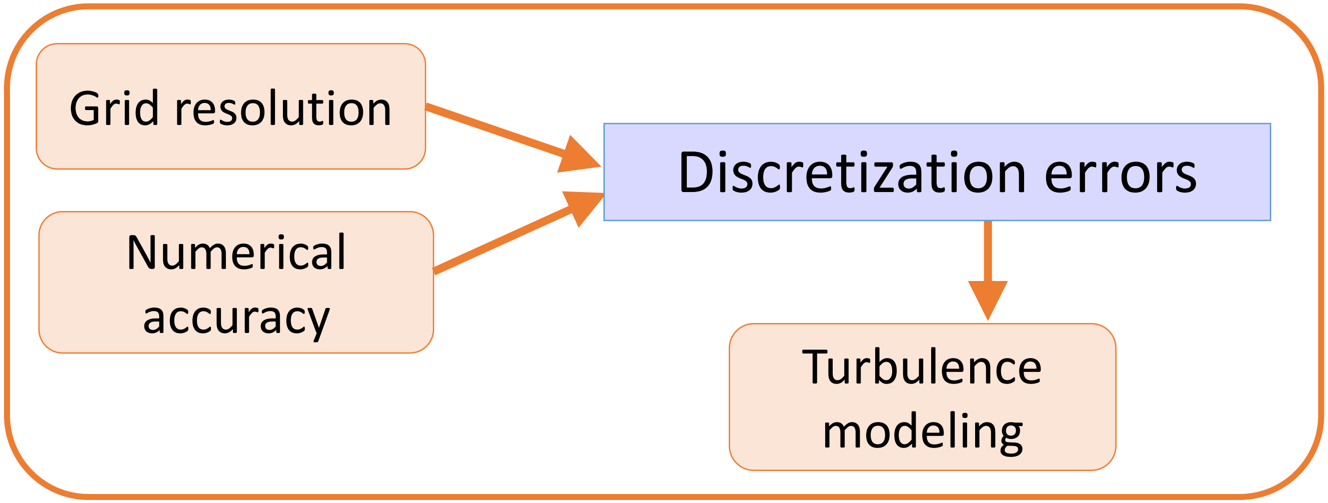
Grid independence through explicit filtering of width significantly larger than the grid size

see e.g. Geurts and van der Bos (1995), Bose et al. (2010))

Both solutions are unpractical for complex engineering/industrial flows

How to deal with discretization and modeling errors in LES?

Second approach (*extreme*): get rid of *physically based* SGS models and use numerical dissipation to provide a *SGS-like* dissipation

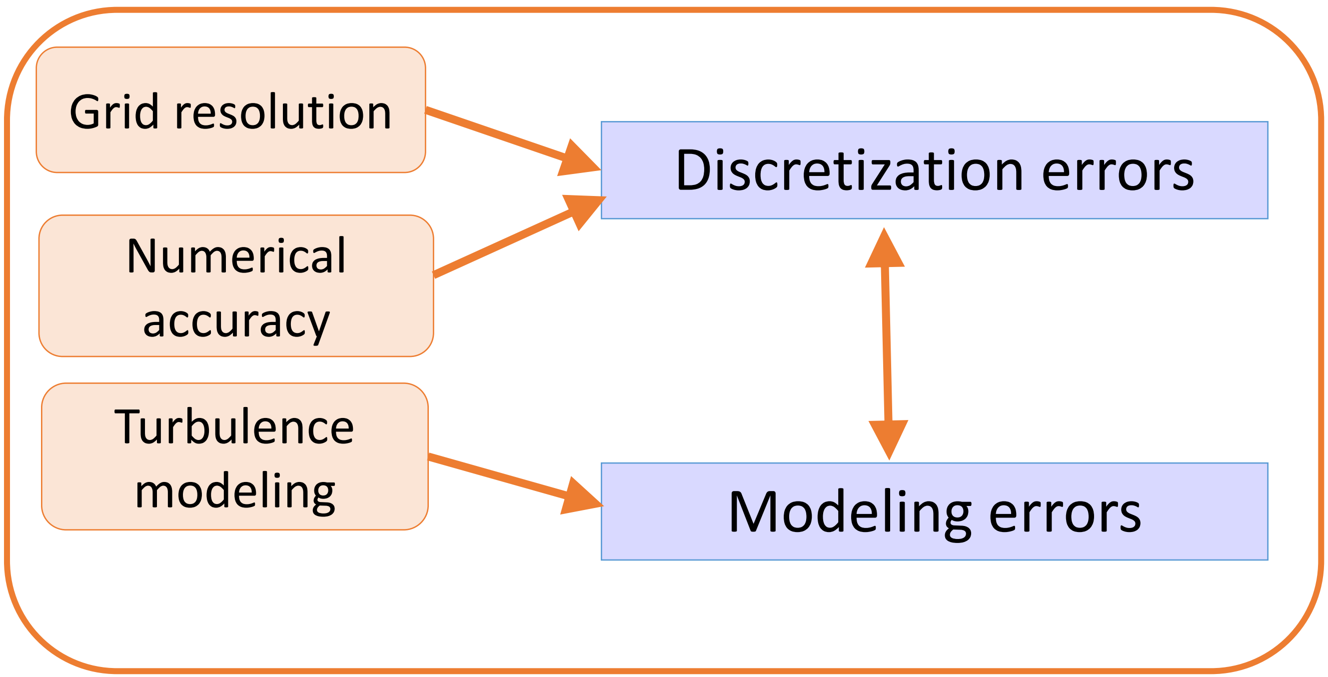


ILES (e.g. Uranga et al. (2011), Bassi et al. (2015), de Wiart et al. (2015)); MILES (e.g. Boris et al., 1992); SVV (e.g. Karamanos & Karniadakis (2000))….

Since SGS modeling is provided by numerical dissipation there is again a tricky coupling between grid resolution, numerics and turbulence modeling

How to deal with discretization and modeling errors in LES?

Third approach (compromise): keep a *physically based* SGS model and a *not perfect* numerical discretization



Discretization and modeling errors may interact in a complex way

Difficulties in the assessment of LES accuracy and reliability

Difficulties in assessment of accuracy and reliability of LES

Error compensation

Unexpected behaviors in classical validation (benchmarking against reference experimental and numerical data) mainly due to compensation of errors

- for given numerical scheme and SGS model, accuracy deteriorating with grid refinement,
- for given grid and SGS modeling, lower-order schemes giving better results than higher-order ones,
- SGS models having completely different behaviors if used with different numerical methods or grids.

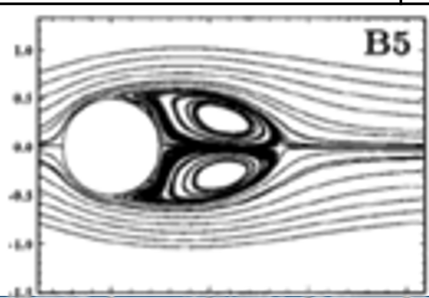
Difficulties in assessment of accuracy and reliability of LES

Example of error compensation: flow around a circular cylinder at Re=3900
Second-order compressible flow solver introducing a small amount of numerical viscosity (designed for LES) on two different grids and with different SGS models (Ouvrard et al, C&F (2010))

Prediction of the length of the mean recirculation length behind the cylinder
Reference experimental value: Lr=1.51D±0.15D

Coarse grid	
SGS modeling	**Lr**
No model	1.24D
Vreman	0.97D
Smagorinsky	0.81D
WALE	0.75D

SGS viscosity



On the coarse grid, the no-model simulation gives the *best* results . However, this is due to error compensation:

- grid coarseness leads to an underestimation of Lr (see Kravchenko & Moin (1999))
- reducing SGS viscosity results in longer recirculation lengths

Difficulties in assessment of accuracy and reliability of LES

Example of error compensation: flow around a circular cylinder at Re=3900
Second-order compressible flow solver introducing a small amount of numerical viscosity (designed for LES) on two different grids and with different SGS models (Ouvrard et al, C&F (2010))

Prediction of the length of the mean recirculation length behind the cylinder
Reference experimental value: Lr=1.51D±0.15D

Fine grid	
SGS modeling	**Lr**
No model	1.85D
Vreman	1.83D
Smagorinsky	1.54D
WALE	1.22D

SGS viscosity

On the fine grid the effect of grid resolution has become negligible → the no model simulation overestimate the recirculation bubble length and the Smagorinsky model gives the *best* prediction.

Which is the optimal amount of total dissipation to be introduced?

Difficulties in assessment of accuracy and reliability of LES

Classical validation: benchmarking against reference experimental and numerical data

Another difficulty, which is related to the reliability of LES, is to quantify the variability of the results with simulation and modeling parameters. This is due to the large computational costs of each single simulation, especially for complex cases.

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How much the accuracy of the results is sensitive to the modeling and computational set-up?

Error-landscape methodology: a full response surface of the LES error behavior is built from a systematic variation of the parameters influencing the discretization and modeling errors, as, e.g., model constants and grid resolution.

This approach provides a framework to characterize the combined effects of modeling and discretization, but at the cost of a large number of simulations → not affordable for complex flow configurations and for a large number of parameters.
Applied only to simple academic cases (see e.g. Meyers et al. (2003, 2006, 2010), Kempf et al. (2011), Geurts (2009)).

Verification&validation methods: adaptation to LES of classical V&V procedures (e.g., Oberkampf and Trucano, 2002)

- ✓ Quality indexes which measure the 'distance' between LES and DNS (see e.g., Celik et al. (2009))
- ✓ Extrapolations of different errors from systematic model and grid resolution variations (e.g., Freitag and Klein (2005), Xing (2015)).

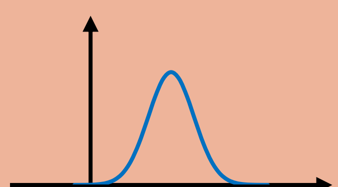
These approaches rely on some 'empirical' assumptions, whose general validity has not been proven.

Assessment of accuracy and reliability of LES

Uncertainty quantification and stochastic sensitivity analysis: the idea is to consider some of the modeling and simulation parameters as uncertain random variables, described by a given PDF, and to propagate these uncertainties through the computational model to quantify statistically the variability of the results.

Uncertainty in Input Data

Input Data probability density function (PDF)



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Propagation

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Uncertainty Quantification/Sensitivity analysis

- Output quantities = errors →quantification of errors and of their variability
- Output quantities = results →sensitivity analysis to different parameters (reliability)

Input Data Optimization/Calibration

How to propagate uncertainties?

Difficulties in assessment of accuracy and reliability of LES

Uncertainty quantification and stochastic sensitivity analysis

The oldest and simplest method to propagate uncertainties is Direct Monte Carlo (and its variants) → it requires an enormous number of deterministic simulations → not viable for complex applications and for a large number of uncertain parameters

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Techniques allowing to build continuous response surfaces of the output quantities of interest starting from a few deterministic simulations (surrogate models).

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Polynomial chaos expansion, stochastic collocation, Kriging and its variants…

Generalized polynomial chaos

- A set of uncertain input parameters are considered as random quantities, ξ(ω)
- The output quantities, R(ω), also considered as a random field, can be approximated through their Galerkin projection over a polynomial orthogonal basis:

$$R(\omega) = \sum_{j=0}^{+\infty} \beta_j \Psi_j(\xi(\omega)) \Longrightarrow R_{gPC}(\omega) = \sum_{j=0}^{T} \beta_j \Psi_j(\xi(\omega))$$

- The polynomials of the basis, Ψ_j, must be a priori selected.
- The polynomial expansion is truncated to a finite (small) number, T, which depends on the order of retained polynomials, P, and on the number of the input parameter, M. One of these two criteria is usually followed:

$$T = \frac{(M+P)!}{M!P!} - 1$$

Total order criterion

$$T = \prod_{j=1}^{M} (P+1) - 1$$

Tensor-product expansion

Generalized polynomial chaos

- The coefficients of the gPC expansion, β_j, can be computed as follows:

$$\beta_j = \frac{\langle R, \Psi_j \rangle}{\langle \Psi_j, \Psi_j \rangle} \Longrightarrow \beta_j = \frac{1}{\psi_j^2} \int_\Omega w(\xi) R(\xi) \Psi_j(\xi) d\xi$$

weight function

- For a given PDF of the input parameters, the *optimal* polynomial family for the gPC expansion is the one which is orthogonal respect to a weighting function similar to the PDF of the input random variable.

- The integrals in the expression of the coefficients may be computed through quadrature formulas, as e.g. Gaussian quadrature.

- For a given accuracy, this determines the number and the location in the parameter space of the quadrature points.

Deterministic simulations must be carried out for input parameter values corresponding to each quadrature point.

Generalized polynomial chaos

Summary

- Input uncertain parameters
- Variation Ranges
- PDF

Order of polynomials retained in the truncated expansion

Quadrature formula used in the computation of the expansion coefficients

Polynomial family

Deterministic simulations to be carried out

Curse of dimensionality: for large numbers of parameters and increasing the truncation order, the number of required deterministic simulations rapidly increases (for Gaussian quadrature it is $(P+1)^M$) → this approach can become unaffordable especially if deterministic simulations are LES

Stochastic collocation

- A set of uncertain input parameters are considered as random quantities, $\xi(\omega)$
- The output quantities, $R(\omega)$, also considered as a random field, is approximated by the Lagrangian interpolant polynomial passing through a suitable number, N_c, of collocation points in the parameter space:

$$R_{SC}(\omega) = \sum_{k=1}^{N_c} R_k L_k(\xi)$$

Value of R in the k^{th} collocation point

- Given N_c, the key issue is to select the *optimal* set of collocation points. Once again, this is related to the PDF of the input parameters.
- Stochastic collocation is well suited to the use of Smolyak sparse grids, which allows the number of collocation points, and thus of deterministic simulations, to be reduced while preserving a good accuracy of the response surface.

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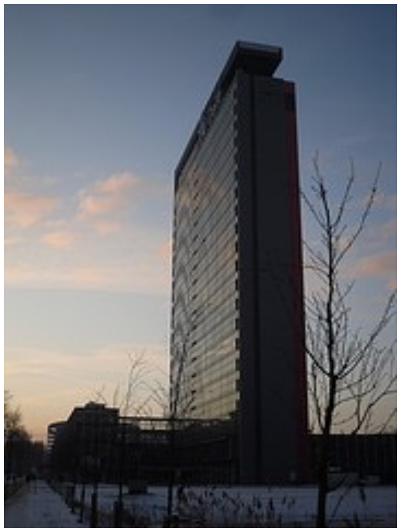
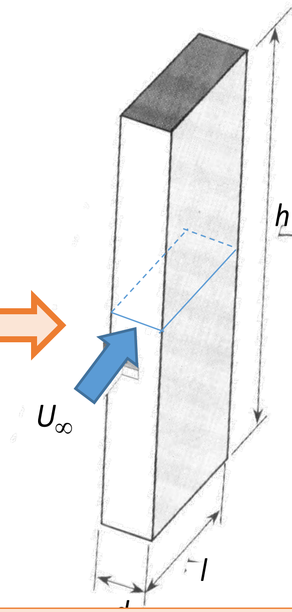
Uncertainty quantification and stochastic sensitivity analysis

- Stochastic approaches are increasingly used for uncertainty quantification and sensitivity analysis in CFD (see e.g., Xiao and Cinnella, PAS (2018) for a review paper on applications to RANS/URANS).
- Not so many applications to LES. Some examples:
  - Uncertainties in boundary/inflow conditions: pipe flow (Congedo et al., IJNMF (2013)), duct with pin fins (Carnevale et al., J. Turbomach (2015)), dispersion in urban area (Margheri and Sagaut, JCP (2016)), mixing layers (Meldi et al., JFM (2020)), elongated rectangular cylinder (BARC) (Rocchio et al., JWEIA (2020))…
  - Uncertainties in SGS modeling together with grid refinement/numerics: isotropic turbulence (Lucor et al., JFM (2007), Meldi et al., PF (2011)), spatially-evolving mixing layers (Meldi et al., PF (2012)), elongated rectangular cylinder (BARC) (Mariotti et al., EJM (2017)), channel flow (Safta et al., IJNMF (2017), Rezaeiravesh and Liefvendhal, PF(2018), Jofre et al., FTC (2018)), Rezaeiravesh et al., CaF (2021)…

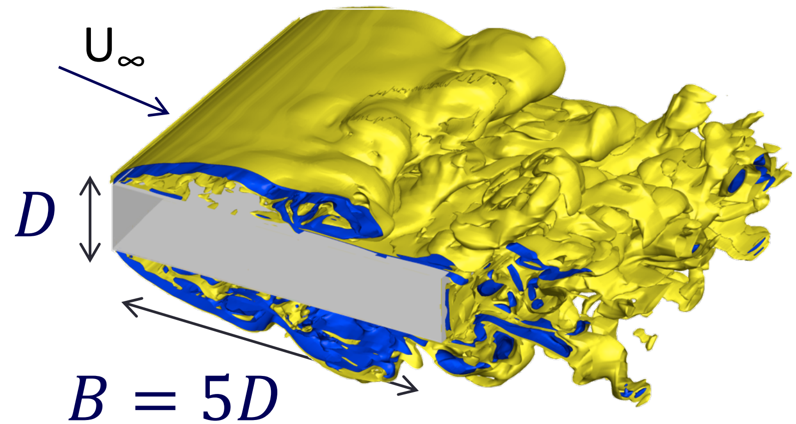
Benchmark on the aerodynamics of a 5:1 rectangular cylinder

The rectangular cylinder is an archetypal geometry for tall buildings, towers and bridges.

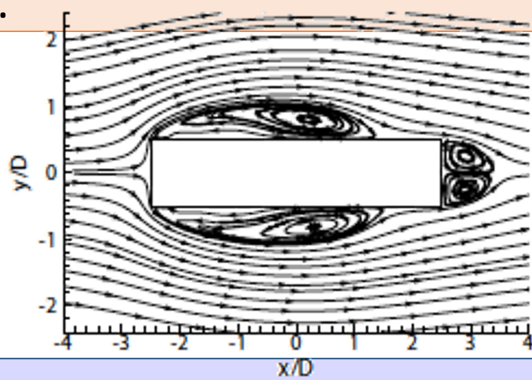




BARC benchmark: flow around a 5:1 infinite cylinder (Bruno et al., IJWEIA 126, 2014; also on the ERCOFTAC Wiki database) at rather large Re ($2x10^4$-$4x10^4$)



In spite of the simple geometry, the flow is complex: flow separation at the upstream corners, unsteady reattachment on the cylinder side, vortex shedding from the downstream corners.



The topology of the flow (also mean flow) on the cylinder side is deeply related to the prediction of quantities of interest, such as pressure distribution, oscillating load amplitude…

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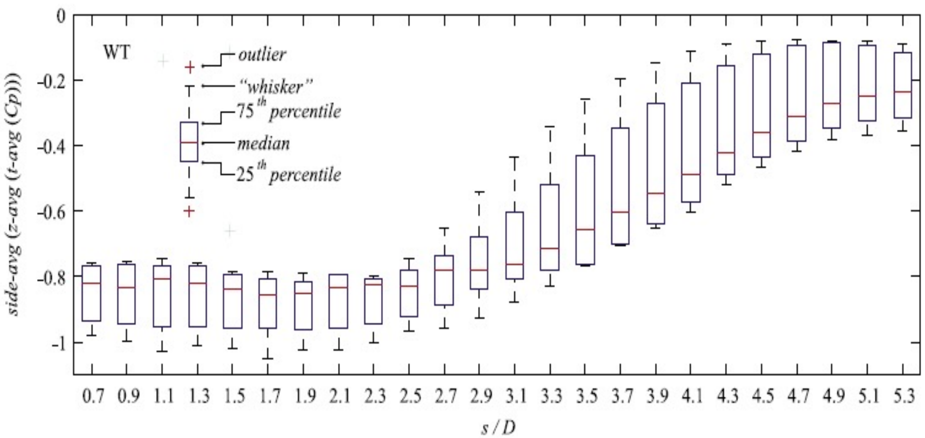
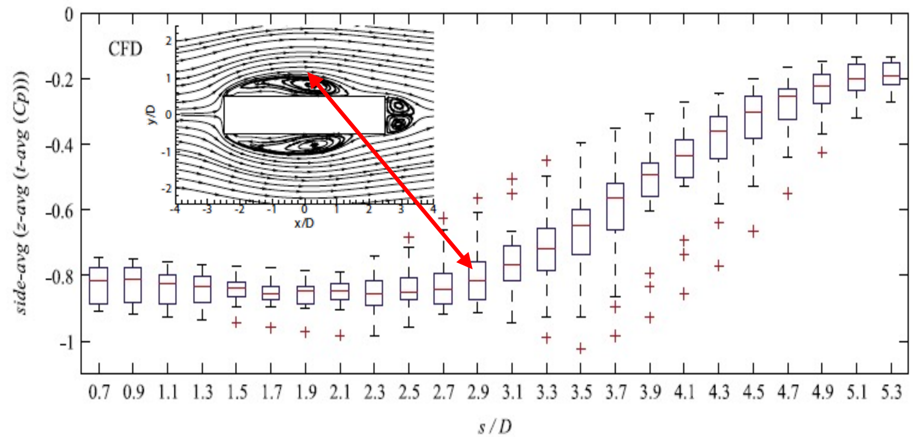
Benchmark on the aerodynamics of a 5:1 rectangular cylinder

- ✓ Up to 70 numerical and experimental realizations of the BARC flow configuration have been collected. (Bruno, Salvetti, Ricciardelli, JWEIA 2014); 51% of the numerical contributions were LES.
- ✓ No reference experiments (different experiments in different facilities).



Experiments



Simulations

- ✓ Embarrassing dispersion (unacceptable for engineers and designers) of some flow quantities of interest, as e.g. the mean pressure distribution on the cylinder side, also in experiments.
- ✓ Different mean flow topology on the cylinder side: shorter and longer mean recirculation zones

Which are the 'correct' results?

Benchmark on the aerodynamics of a 5:1 rectangular cylinder

Which are the 'correct' results?

👍 A recent experimental work (Mannini et al., JWEIA (2017)) indicated that the dispersion of the experimental data can be explained by differences in freestream turbulence → the mean recirculation zone on the cylinder side becomes shorter as the freestream turbulence intensity increases.

👎 As for numerical simulations, deterministic sensitivity analyses to some parameters were not conclusive and gave unexpected results

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👎 A priori more reliable simulations giving results which significantly deviate from the ensemble average of BARC contributions and also from the experiments.

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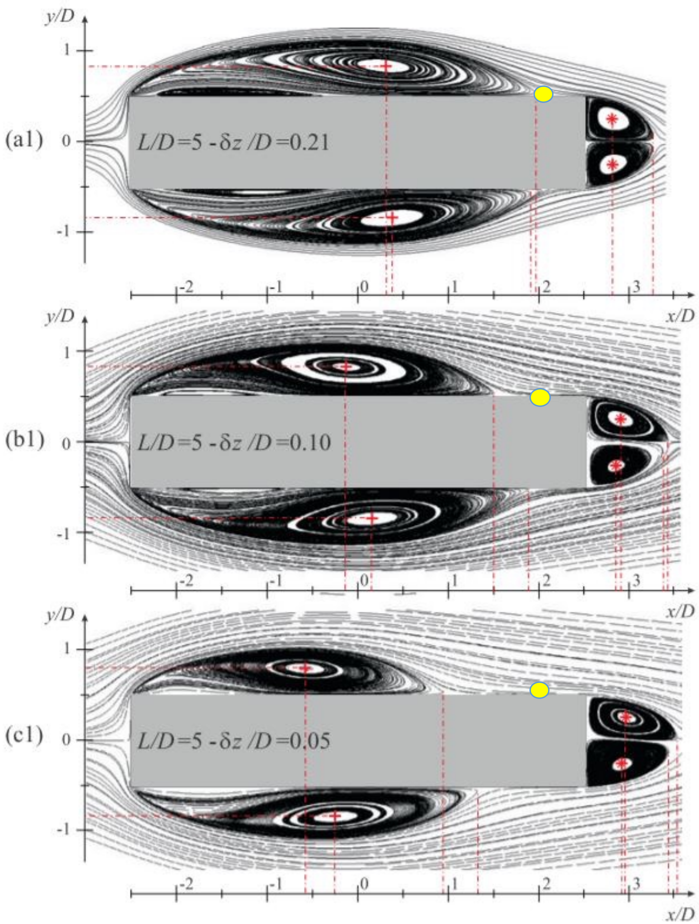
Benchmark on the aerodynamics of a 5:1 rectangular cylinder

Large-eddy simulations of Bruno et al (JWEIA, 2012)



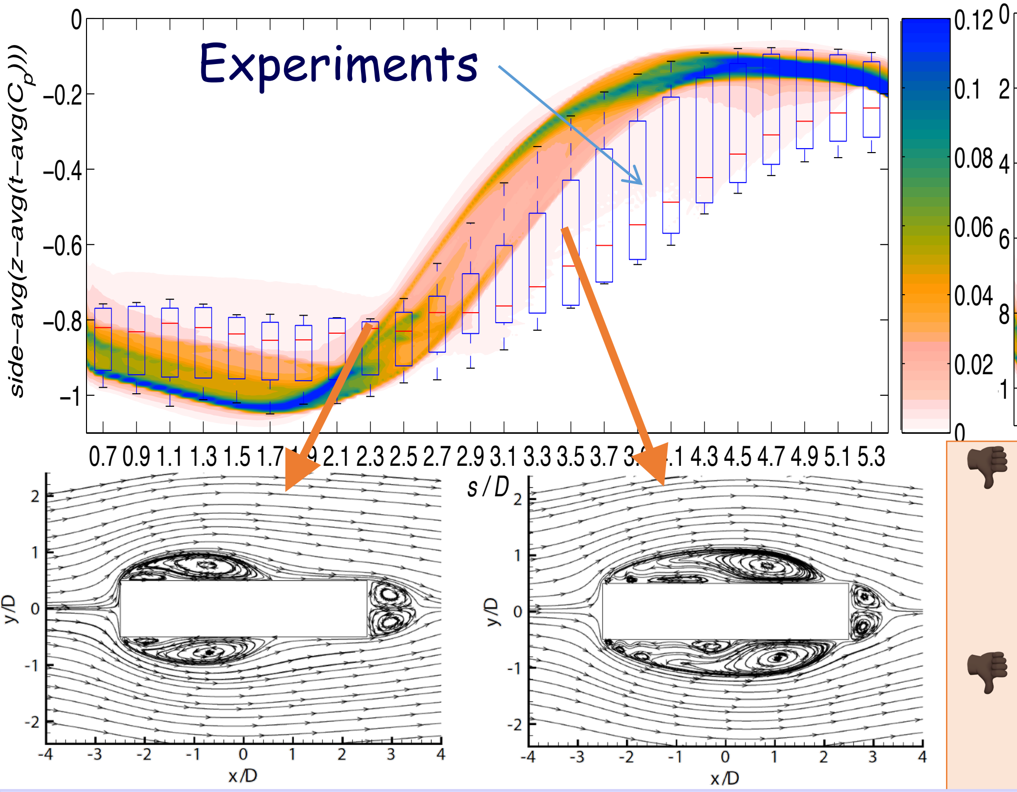
Increasing spanwise grid resolution

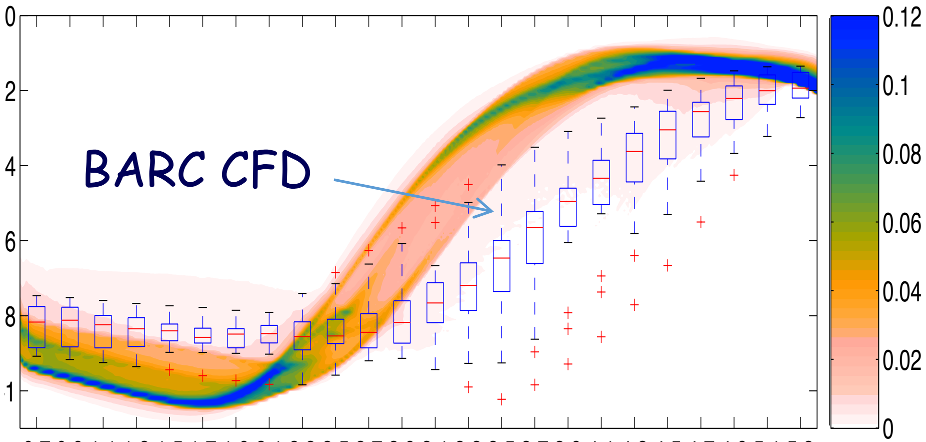
- ✓ Strong impact of the spanwise grid resolution.
- ✓ The mean recirculation zone on the cylinder side becomes shorter as the spanwise grid resolution increases.
- ✓ The results on the finest grid significantly deviate from the ensemble average of BARC contributions and also from the experiments (too short mean recirculation zone).
- ✓ No inlet turbulence in LES → simulations should give a recirculation zone longer than in experiments.

?

Benchmark on the aerodynamics of a 5:1 rectangular cylinder

- ✓ This motivated a stochastic sensitivity analysis to spanwise grid resolution and SGS dissipation (Mariotti et al., EJM/FLUIDS (2017)).
- ✓ LES carried out by NEK5000 (spectral element code).
- ✓ Uncertain input parameters: grid resolution in the spanwise direction and to the weight of a modal filter (SGS dissipation).
- ✓ Uniform input parameter PDF → gPC expansion with Legendre polynomials
- ✓ gPC expansion truncated at order 3→16 deterministic LES simulation



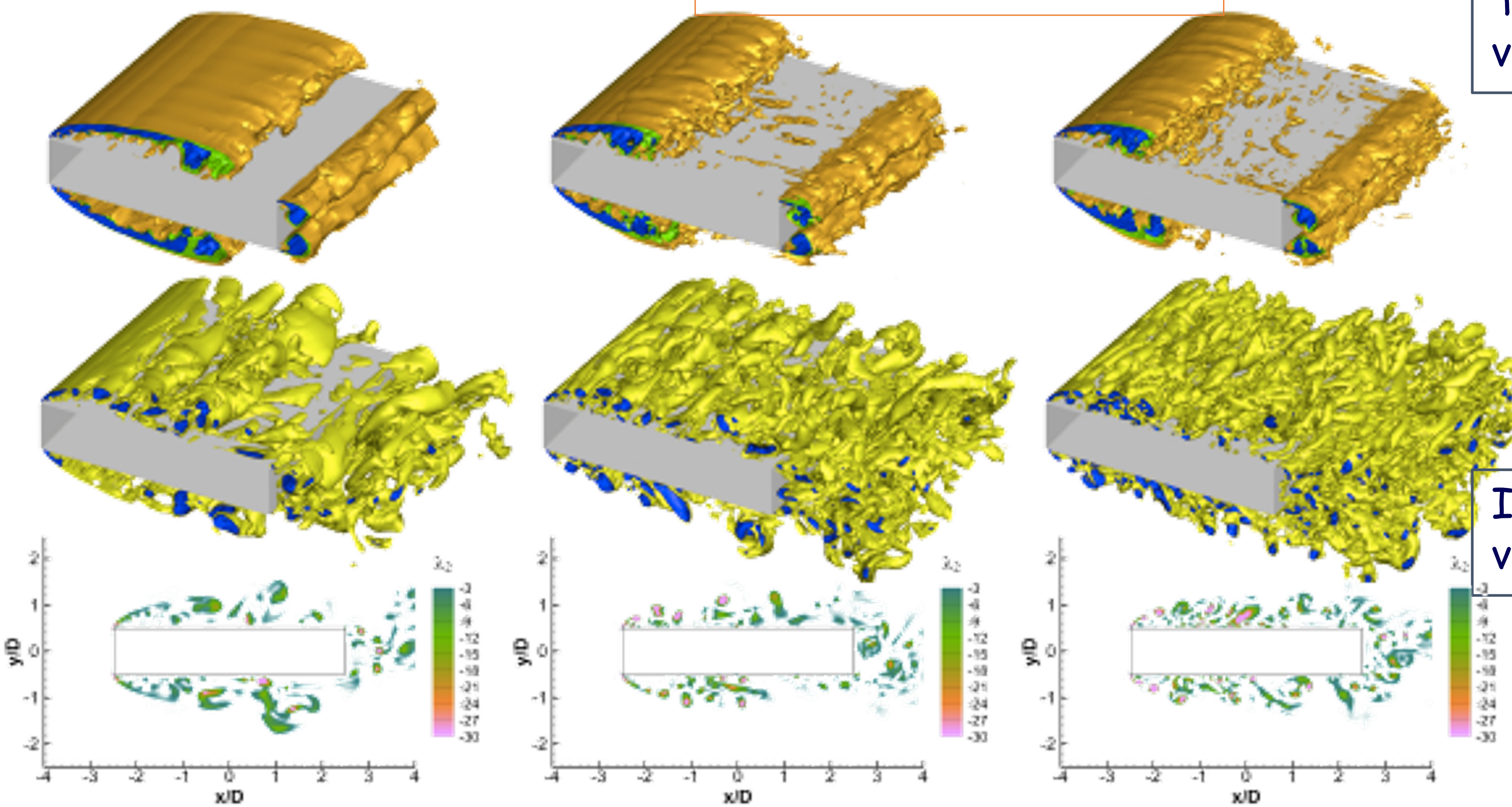


- 👎 Significantly different mean flow topology can be obtained by varying the spanwise grid resolution and SGS dissipation (short and long mean recirculation zones).
- 👎 The short mean recirculation zones are the 'most probable' configuration (in agreement with Bruno et al. (2002)).

Benchmark on the aerodynamics of a 5:1 rectangular cylinder

Fixed SGS dissipation

Time-averaged vortex indicator



Instantaneous vortex indicator

Increasing spanwise resolution

- Increasing the spanwise resolution the shear layers detaching from the front corners loose coherence upstream →shorter mean recirculation zone. In agreement with Bruno et al. (2012) with a different numerical approach and SGS modeling.
- Same behavior when decreasing the SGS dissipation for fixed grid resolution.

Benchmark on the aerodynamics of a 5:1 rectangular cylinder

Best results (fine resolution and small SGS dissipation) tend to deviate from the ensemble of the numerical contributions to BARC. This can be understood since almost all the other contributions have coarser resolutions or larger eddy viscosities (hybrid RANS/LES).

…but…

best results also deviate from experimental data.

Sources of uncertainty/error

Discretization errors

Modeling errors

Simplifications/uncertainties in problem boundary conditions

Benchmark on the aerodynamics of a 5:1 rectangular cylinder

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...but...

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Uncertainties/mismatch in boundary conditions?

~~Inlet turbulence~~

The highly-refined LES have no inlet turbulence → they should give longer recirculation zones than in experiments instead of shorter ones

~~Periodic boundary conditions~~

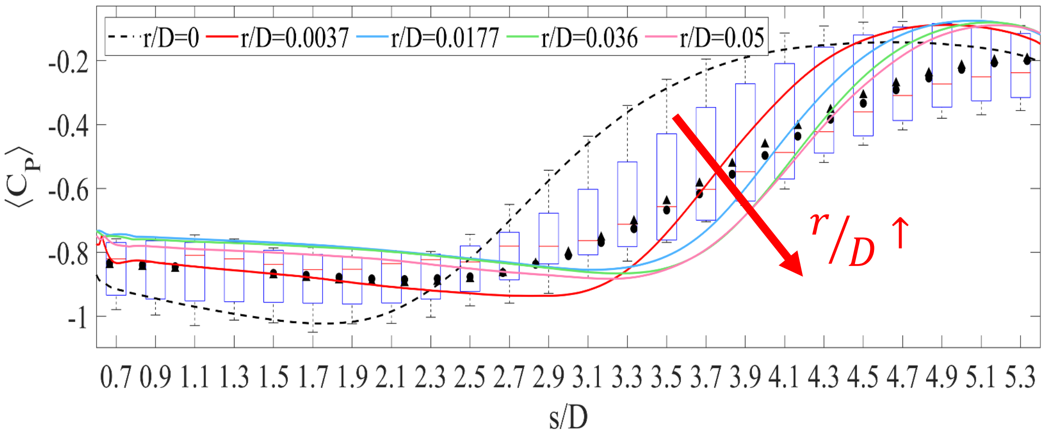
Possible effects of the spanwise length together with periodic boundary conditions? Previous studies (also Bruno et al. 2012) indicate that they are small

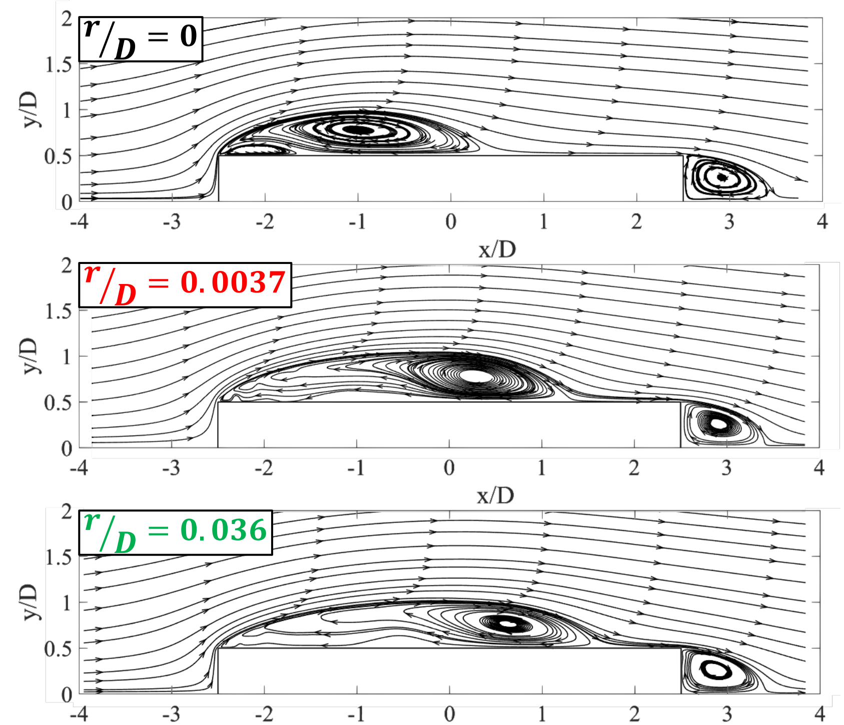
Perfectly sharp corners

Possible effect of perfectly sharp upstream corners in the numerical simulations while they have a certain degree of roundness in experiments

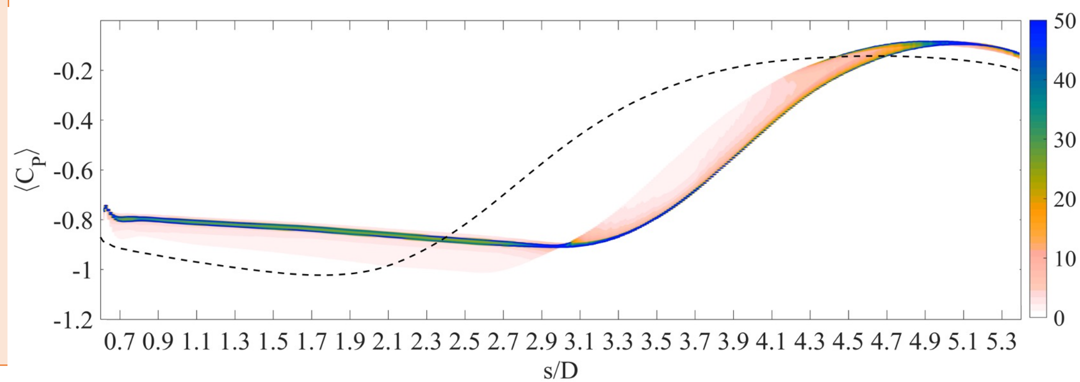
Benchmark on the aerodynamics of a 5:1 rectangular cylinder

Additional LES with a grid resolution and SGS dissipation giving a short recirculation region for sharp corners for corners having a small rounding, with two different values of the curvature radius: r/D=0.01 and 0.05 (Rocchio et al. , JWEIA (2020))



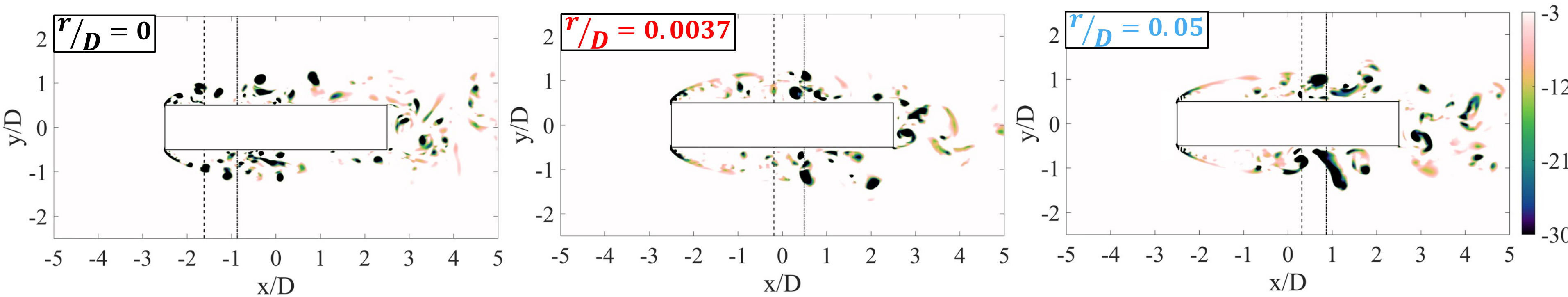


- The rounding of the upstream corners has a strong impact on the length of the mean recirculation region and, thus, on the pressure distribution over the cylinder side.
- Increasing the curvature radius the length of the mean recirculation region increases
- The largest difference is between the sharp corner and the smallest curvature radius.



Benchmark on the aerodynamics of a 5:1 rectangular cylinder

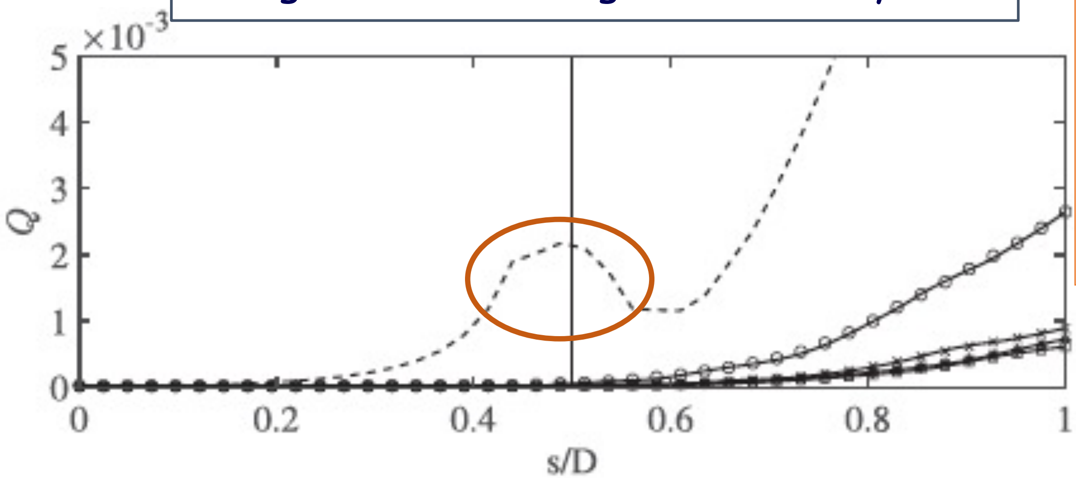
Instantaneous vortex indicator



Increasing corner curvature radius

- ✓ The effect of the corner curvature radius on the mean recirculation length is once again related with differences in the behavior of the detaching shear layers. Increasing r/D → the shear layers loose coherence more downstream → longer mean recirculation region.

Integral of TKE along the shear layer



The sharp edge introduces too-high velocity fluctuations → if not damped (SGS dissipation or grid coarseness), they lead to a too early roll up of the shear layer → too short mean recirculation region

Lessons learned

👍 A paradox explained: the discrepancy between experiments and the results of *high-fidelity* simulations may be due to the perfectly sharpness of the upstream corners in the simulations.

👍 With rounded edges, the sensitivity to SGS dissipation and spanwise grid refinement is reduced (talk by Rocchio et al., *Numerical Methods for Turbulent Flows*)

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Is the strong impact of upstream-edge rounding physical or numerical?

Experiments in the wind tunnel of University of Pisa with different carefully-measured rounding of the upstream edges → for small roundings (same range considered in the numerical analysis), the sensitivity of experimental measurements is very low → the effect observed in LES is numerical

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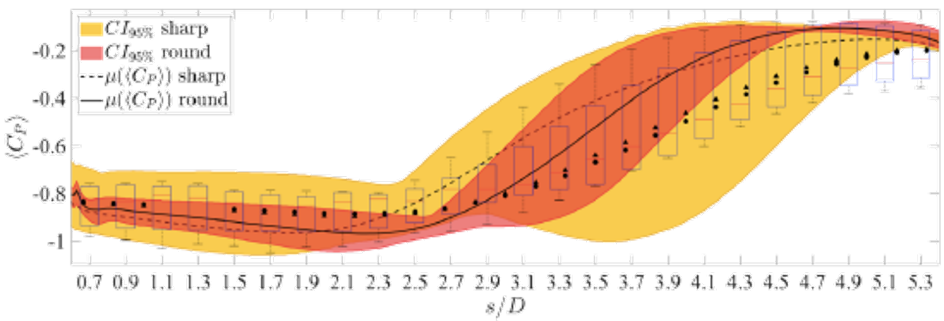
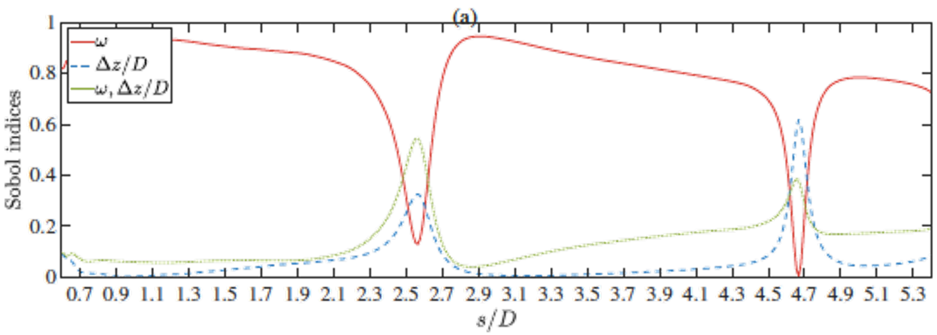
Practical implications for this kind of flows (flow separation at the upstream corners and reattachment on the cylinder side) → treatment of the upstream edges is critical

- DNS-like grid refinement (unpractical for high Reynolds numbers)
- Include a rounding with a given curvature radius (data on tolerances of experimental models would be useful);
- Ad-hoc numerical/analytical treatment of the corners

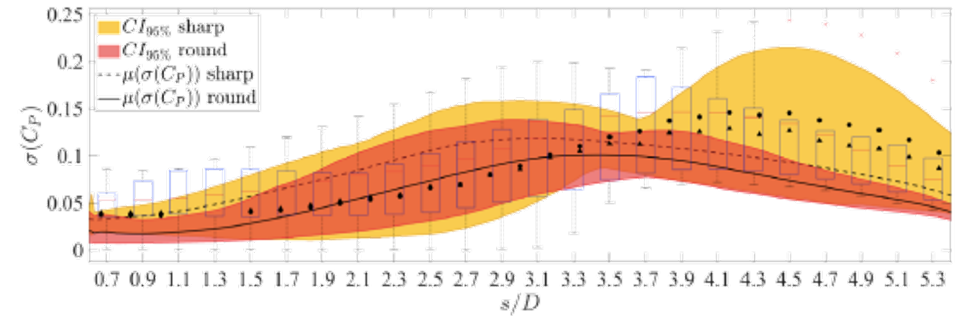
Stochastic sensitivity analysis to spanwise grid resolution and SGS dissipation for r/D=0.0037

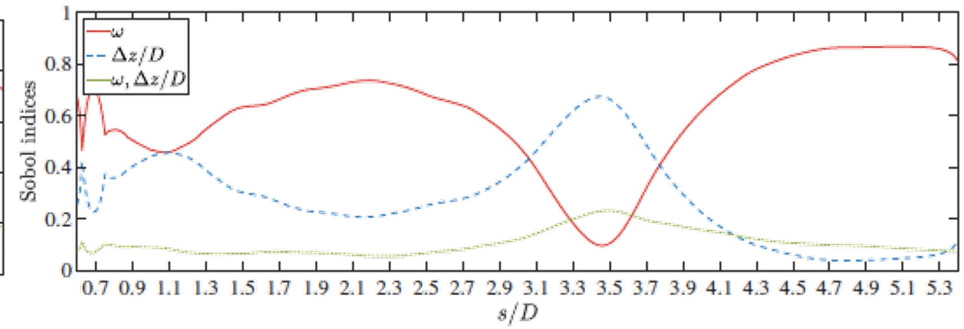
Mean pressure coefficient





Pressure coefficient standard deviation



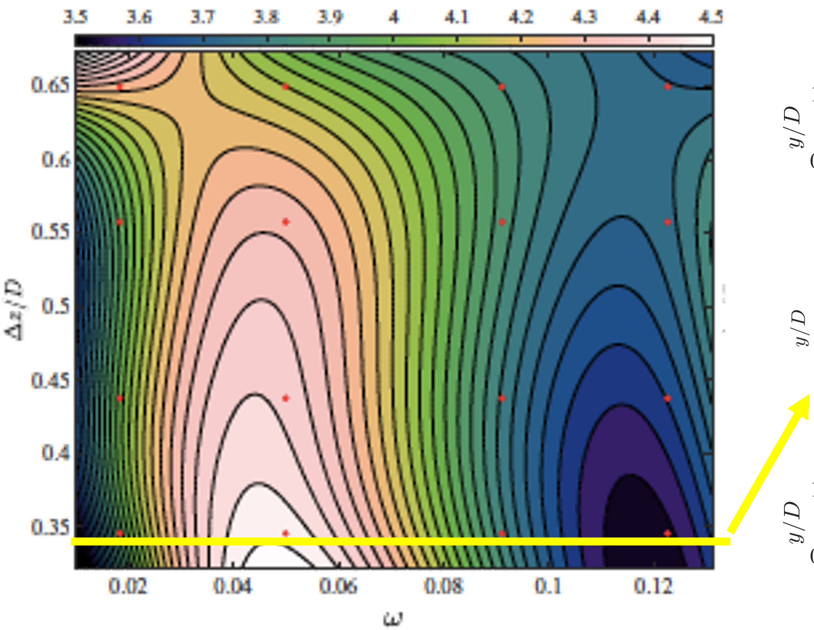


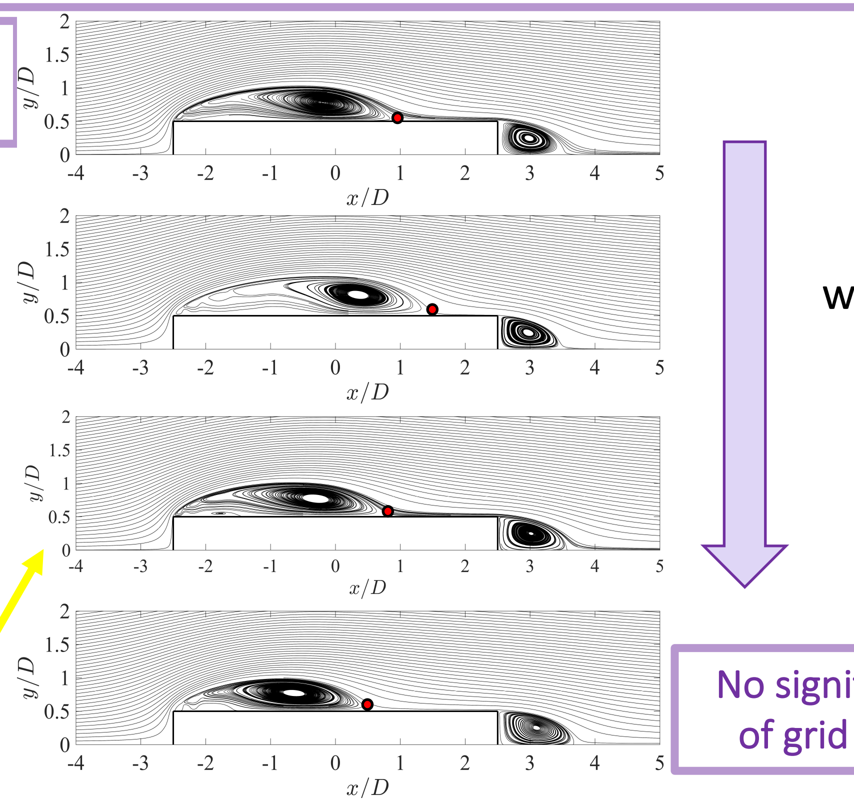
- ✓ The variability of the pressure distribution on the cylinder side s is considerably reduced passing from the sharp-edge case to the round-edge one
- ✓ The variation range for the round-edge case falls inside the range of the experimental data (Bruno et al., 2014)
- ✓ For the round-edge case, the mean and fluctuating pressure distributions are mostly sensitive to the filter weight (SGS dissipation), while for sharp edges the dominating parameter was the spanwise grid refinement

How the mean flow reattachment location depends on the considered parameters?

- ✓ Sharp edges: a clear trend is observed. The mean flow reattachment point moves upstream when the grid resolution is increased and when the SGS dissipation (w) is decreased.
- ✓ Rounded edges?

Response surface of the location of the mean flow reattachment point





No significant effects of grid refinement

- ✓ The reattachment location moves downstream with increasing w up to w=0.05 and then it moves upstream.
- ✓ Values of w around 0.05 give largest lengths of the mean recirculation region → best agreement with experiments. Slight increase of the recirculation length by increasing grid refinement.

Further lessons learned

- 👍 In LES simulations with rounded corners the variability of the results with spanwise grid refinement and SGS dissipation is reduced compared with the sharp-edge case.
- 👍 The results are independent of spanwise grid resolution.
- 👍 However, a significant impact of the modal filter weight is still present. Values around w=0.05 seem to be 'optimal' in terms of agreement with the experiments.

Concluding Remarks

Assessment of quality and reliability of LES results is a complex task due to some peculiar problems:

- Interaction/compensation of errors
- Difficulty in systematic sensitivity analysis to computational and modeling parameters

Stochastic techniques allowing continuous response surfaces in the parameter space to be built starting from a *few* simulations can be useful to:

- Analyze/quantify errors
- Assess the sensitivity to parameters and possibly calibrate them

but

they are currently limited in the number of input uncertain parameters, especially if the single deterministic simulations imply large costs

Further developments of these approaches

Other approaches. Supervised AI?

Thank you for the attention!

Thanks to:

Alessandro Mariotti, Benedetto Rocchio, Lorenzo Siconolfi

Uncertainty quantification and stochastic sensitivity analysis

Spatially-evolving mixing-layer (Meldi et al., Phys. Fluids 24, 2012)

- A highly-resolved LES is used as a reference.
- The sensitivity of the errors on the predictions obtained by LES on coarser grids to grid features and SGS modeling is investigated through gPC expansion.
- Input parameters: grid stretching ratio in the streamwise and lateral directions, strX and strY, Smagorinsky model constant, C_S. Uniform PDF → Legnedre polynomials.
- gPC expansion truncated to 3rd order + Gaussian quadrature: 64 LES on *coarse* grids
- Errors on mean streamwise velocity, momentum thickness, shear stress.
- Sensitivity analysis carried out separately in the *inlet-dependent* upstream region and in the *fully-turbulent* downstream region.

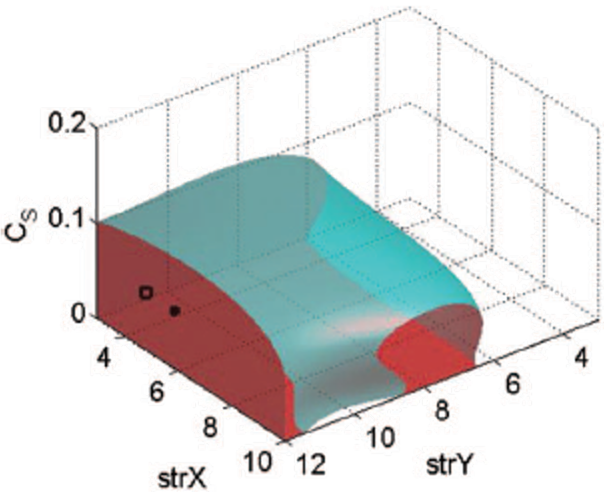
⇩

✓ Quantification of errors and of their dependence on the uncertain parameters (the Smagorinsky constant was found to have the largest impact on the results).

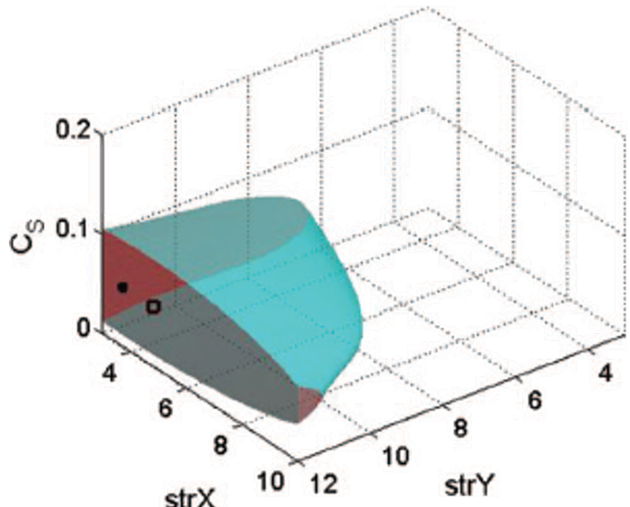
✓ Identification of low-error regions in the parameter space and possible *optimization* of the input parameters.

Spatially-evolving mixing-layer (Meldi et al., Phys. Fluids 24, 2012)

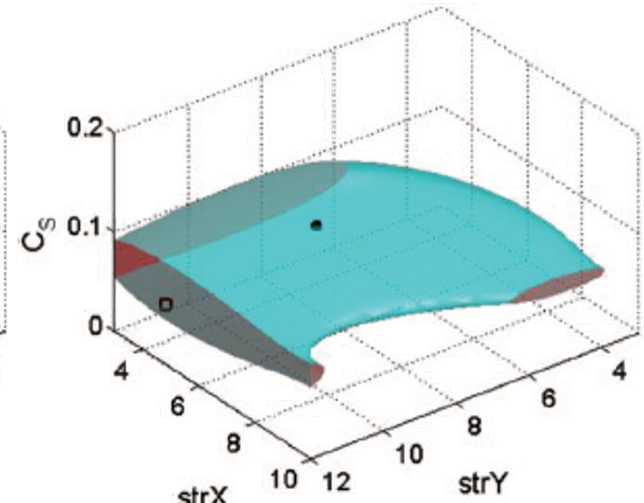
Parameter *optimization*: parameter space regions where the error on the different considered quantities <1.2 the minimum one -- Inlet-dependent region



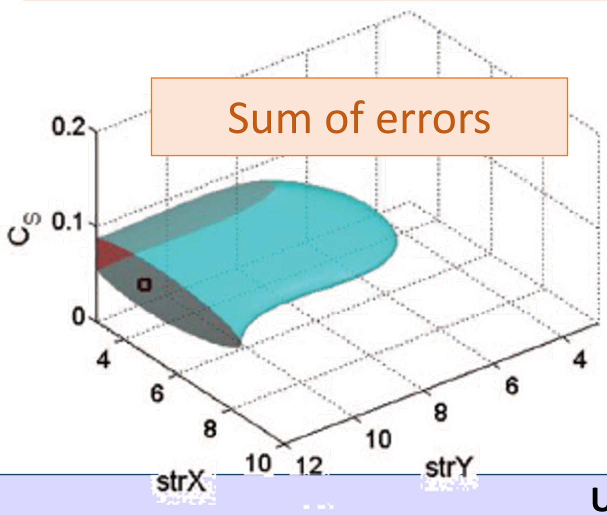
Mean streamwise velocity



Momentum thickness



Shear stress

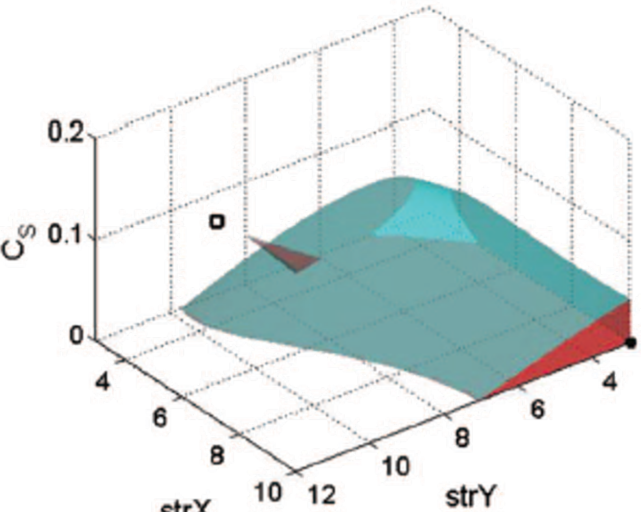


Sum of errors

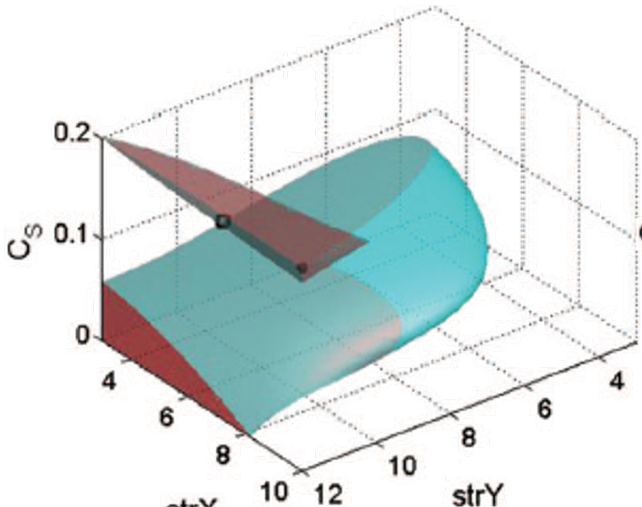
- ✓ The low-error regions for the single variables overlap.
- ✓ A significant part of the uncertainty space at low error for all the physical quantities is recoverable → robust optimum parameter choice.

Spatially-evolving mixing-layer (Meldi et al., Phys. Fluids 24, 2012)

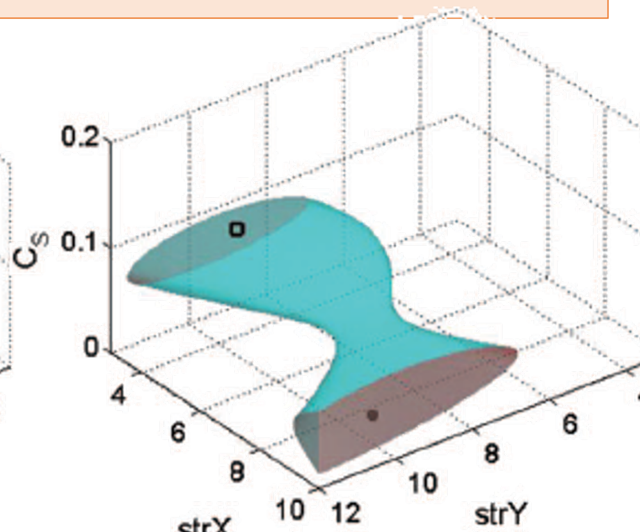
Parameter optimization: parameter space regions where theerror different considered quantities <1.75 the minimum one – Fully-turbulent region



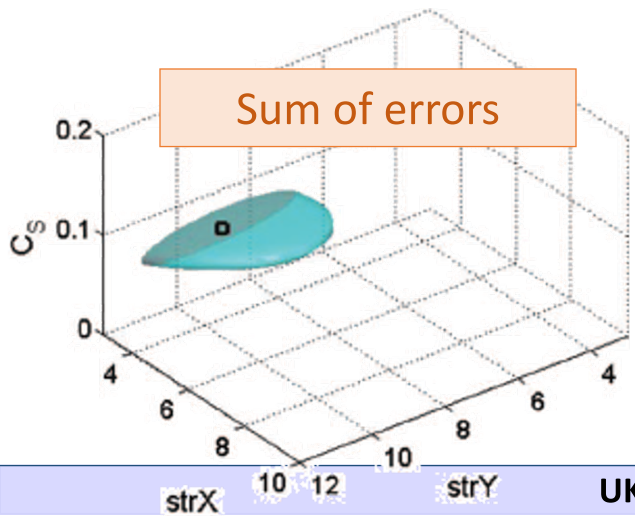
Mean streamwise velocity



Momentum thickness



Shear stress



Sum of errors

- ✓ The low-order regions for the single variables do not overlap.
- ✓ More complex shape of the optimal regions → more difficult optimization of the simulation parameters.