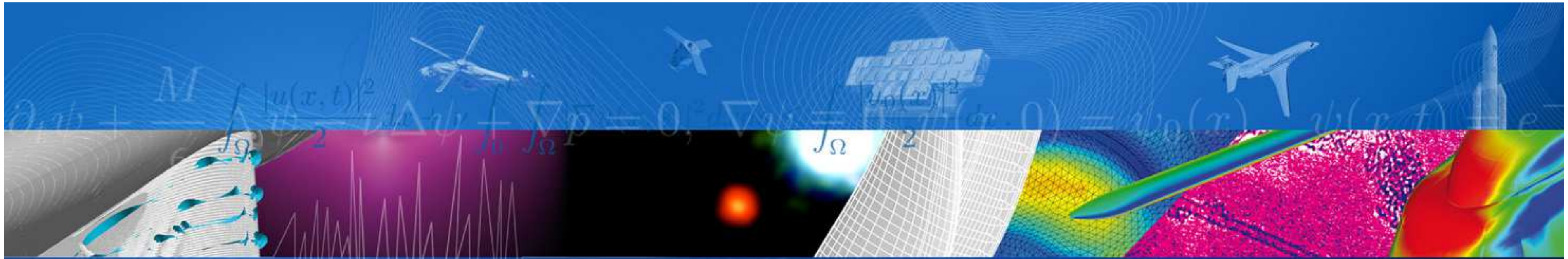


Modélisation de la turbulence et Intelligence Artificielle

Séminaire Aristote – En route vers l’Exascale
23 mai 2019

presenté par Vincent Couaillier

Fabbio Naddei, Marta de la Llave Plata, Marc Lazareff,
Florent Renac, Odile labbé, Lucas Franceschini,
Nicolo Fabbiane, Olivier Marquet, Benjamin Leclaire,
Julien Dandois, Denis Sipp

ONERA

THE FRENCH AEROSPACE LAB

return on innovation

PLAN

- ❑ Objectifs du projet HiFiTURB
- ❑ Contexte CFD et turbulence
- ❑ Résultats ONERA « turbulence et IA » préliminaires

CFD et Modélisation de la turbulence : Défi et opportunités

- **Le défi le plus important dans tous les domaines applicatifs de la mécanique des fluides numérique** (aérospatiale, énergie et propulsion, industries automobile, maritime, des procédés chimiques et bien d'autres encore) **reste lié à la modélisation de la turbulence et à la compréhension de la transition laminaire à turbulente** entrainant une mauvaise prédiction des caractéristiques dans les situations hors adaptation.

- **Les capacités des nouvelles plates-formes HPC** permettant des calculs à très grande échelle, combinées aux **développements récents des méthodes de résolution d'ordre élevé en CFD** ouvrent des opportunités sans précédent pour générer efficacement des bases de données LES / DNS pour des écoulements de plus en plus complexes et à grands nombres de Reynolds, du moins pour des configurations géométriques encore fondamentales.

- **Les progrès rapides en intelligence artificielle (IA),** utilisant en particulier les algorithmes de type Machine Learning (ML), fournissent des moyens entièrement nouveaux d'extraction d'information caractérisant les grandeurs physiques et leurs interactions à partir **de données massives générées par ces calculs LES / DNS**

- Objectif du projet européen HiFiTURB : associer ces méthodologies pour améliorer les modèles de turbulence des codes de calcul CFD utilisés dans le domaine industriel

Turbulence model, HPC & Maching learning
Conclusion

- The ability to *understand, model and predict turbulence and transition phenomena is the key requirement in the design of efficient and environmentally acceptable fluid-based energy transfer systems*

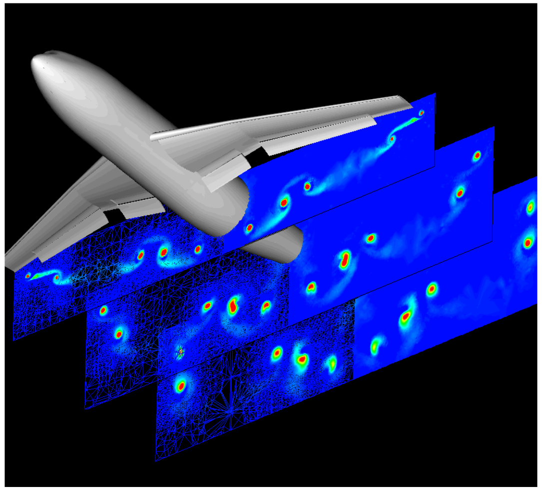
- Flow detachment (stall)
- Separation in high-load conditions and behind shocks
- Shock-boundary layer interactions, buffet, and transient loads causing substantial structural deformations due to strong gusts
- Atmospheric turbulence
- Extreme aircraft manoeuvres.
- Effectiveness of optimisation techniques
- …

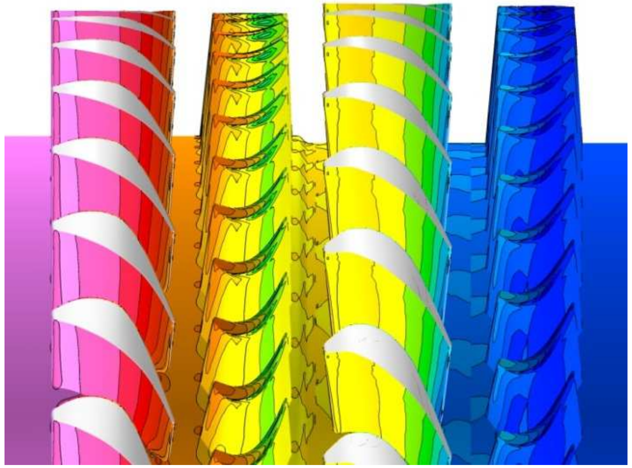
Current challenges for CFD accurate simulations
Courtesy : Airbus

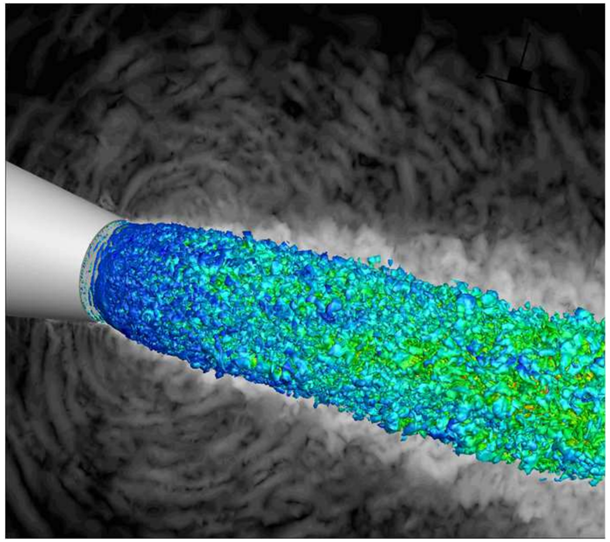
HIFITURB - Plan

- Objectifs du projet HiFiTURB
  - Simulations DNS et/ou LES (DNS sous-résolue ?) de référence
    - Méthodes de haute-fidélité avec schéma d'ordre élevé
    - Cas test représentatifs de problèmes CFD raides
  - Amélioration des modèles de turbulence RANS
    - Utilisation des bases de données générées
    - Méthodes Maching Learning

Processus de simulation numérique en mécanique des fluides







Définition du cas de calcul

Modèle physique et données opérationnelles avec incertitudes

- **Approche déterministe**
- **Approche stochastique**

→

Code de calcul

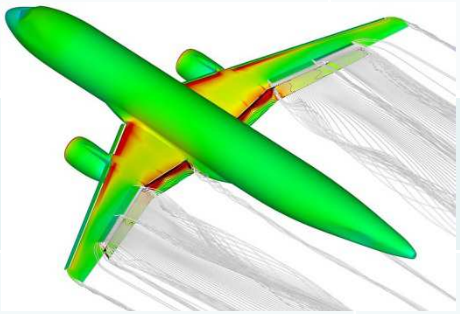
Méthodes de calcul CFD avec approximation du modèle continue et complétude des conditions aux limites ou conditions initiales (par ex.)

→

Analyse

Résultats de simulation avec propagation des incertitudes et des sensibilités numériques

CFD – Enjeux scientifiques et techniques



S6	**Maîtrise des systèmes complexes / Multiphysique précise**
S5	**Optimisation robuste avec incertitudes**
S4	**Optimisation de forme** — **Quantification des incertitudes opérationnelles** — **Contrôle des écoulements**
S3	**Analyse de sensibilités** - Paramètres du modèle - Paramètres opérationnels — **Multiphysique robuste**
S2	**Calcul direct (analyse) avec vérification et validation** - Solution analytique de (S1) - Méthodes numériques standard pour approximation de (S1) - Méthodes numériques de haute fidelité pour approximation de (S1) avec contrôle d'erreur
S1	**Modèle physique / mathématique CFD** (Euler, Navier-Stokes et sous-modèles associés) — **Modèles structure, thermique, …**

Accroissement des capacités de simulation numérique

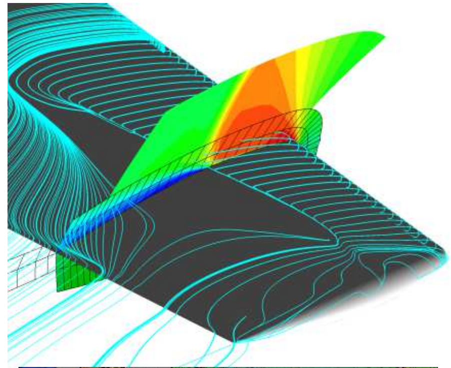
- Précision, efficacité et robustesse des algorithmes
- Optimisation méthodes de programmation / Architecture plateformes HPC
- Production de données massives (1 calcul DNS, des milliers de calcul RANS)

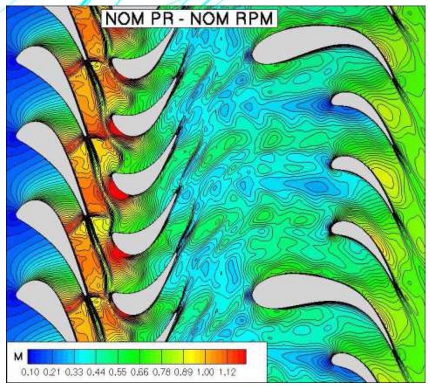
Some aspects of ONERA CFD

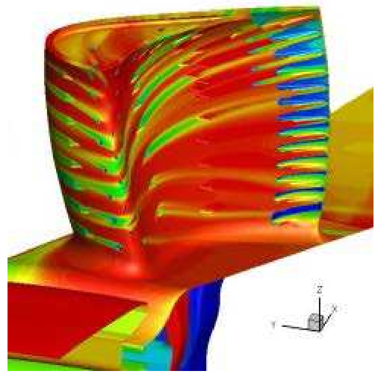
- **CFD considered mature technology for nominal flow configurations**
  - Many CFD codes and assessed models are daily used in industry
  - Main CFD codes at ONERA :
    - elsA for aerodynamics, aeroelasticity, aeroacoustics
    - CEDRE for energetics, aeroacoustics, mutiphysics
    - Used by industrial partners Airbus, Safran, EDF, CNES, EDF and ONERA CFD expertise used by Dassault
    - Under development CODA (ONERA, DLR, Airbus), ORION/Mosaic (ONERA, Safran)

- **But main key points have to be solved to put CFD a step further**
  - Expertise of end-users still needed to provide « correct results »
  - Error margins still not mastered
    - Computational errors (Verification process)
    - Uncertainties : physical model & boundary/initial conditions
  - Efficiency (cost) in particular for unsteady CFD dealing with scale-resolving problems for new computers architecture
  - CFD used in a multiphysics environment

- **Automatization and Accuracy Control challenge :**
  From End-users expertise to Expert CFD system

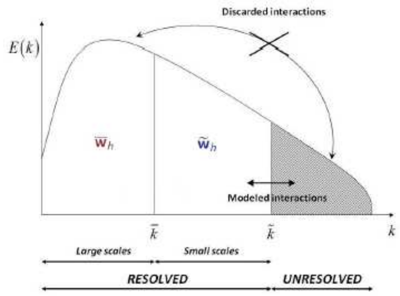






Turbulence : Scales constraints

- Laminar flows / Turbulent flows
- DNS / LES / RANS



$$Reynolds\ number: \ Re_L = \frac{\rho V L}{\mu}$$

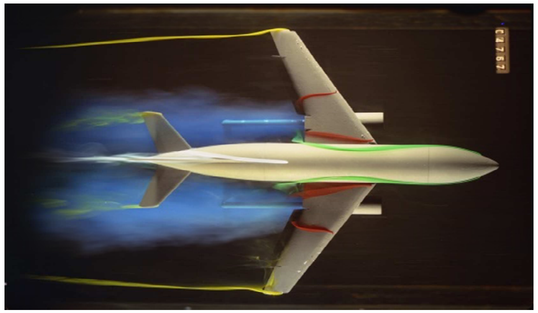
- DNS computations:
  - Kolmogorov scale = size of the smallest turbulent structure $\eta = L Re_L^{-3/4}$ per direction
  - With L integral scale representative of the larger turbulent structures
  - 1D computational domain with length N.h, N nomber of points, h mesh size, needs :

$$Nh \geq L$$

$$h \leq \eta$$

$$\eta N \geq NH \geq L$$

$$\Rightarrow N \geq L/\eta = \mathrm{Re}_L^{3/4}$$



- 3D DNS computation : $N_{3D} = Re_L^{9/4}$, $Re_L = 10^6 \rightarrow N_{3D} \approx 3.10^{13}$
- Constraints on time step for integration of the Navier-Stokes systems (explicit schemes)
  - Δt proportional to h for convective terms
  - Δt proportional to h^2 pour les termes de diffusion

Simulation of turbulence : DNS or turbulence modelling

- Direct Numerical Simulation : Necessitate a very fine mesh to take into account all the scales of turbulence

- Introduction of models to take into accout phenomena with scales not represented in the mesh
  - Large Eddy Simulation : LES
  - Reynolds Averaged Navier-Stokes equations : RANS
  - Hybrid RANS/LES methods

- LES methods : Filtered Navier-Stokes equations

  $u = \tilde{u} + u''$,

  $\tilde{u}$ filtered (or resolved) field

  u'' modelled field (or modelled scales) : $\widetilde{u''} \neq 0$

- RANS : Averaged Navier-Stokes equations

  $u = \bar{u} + u'$,

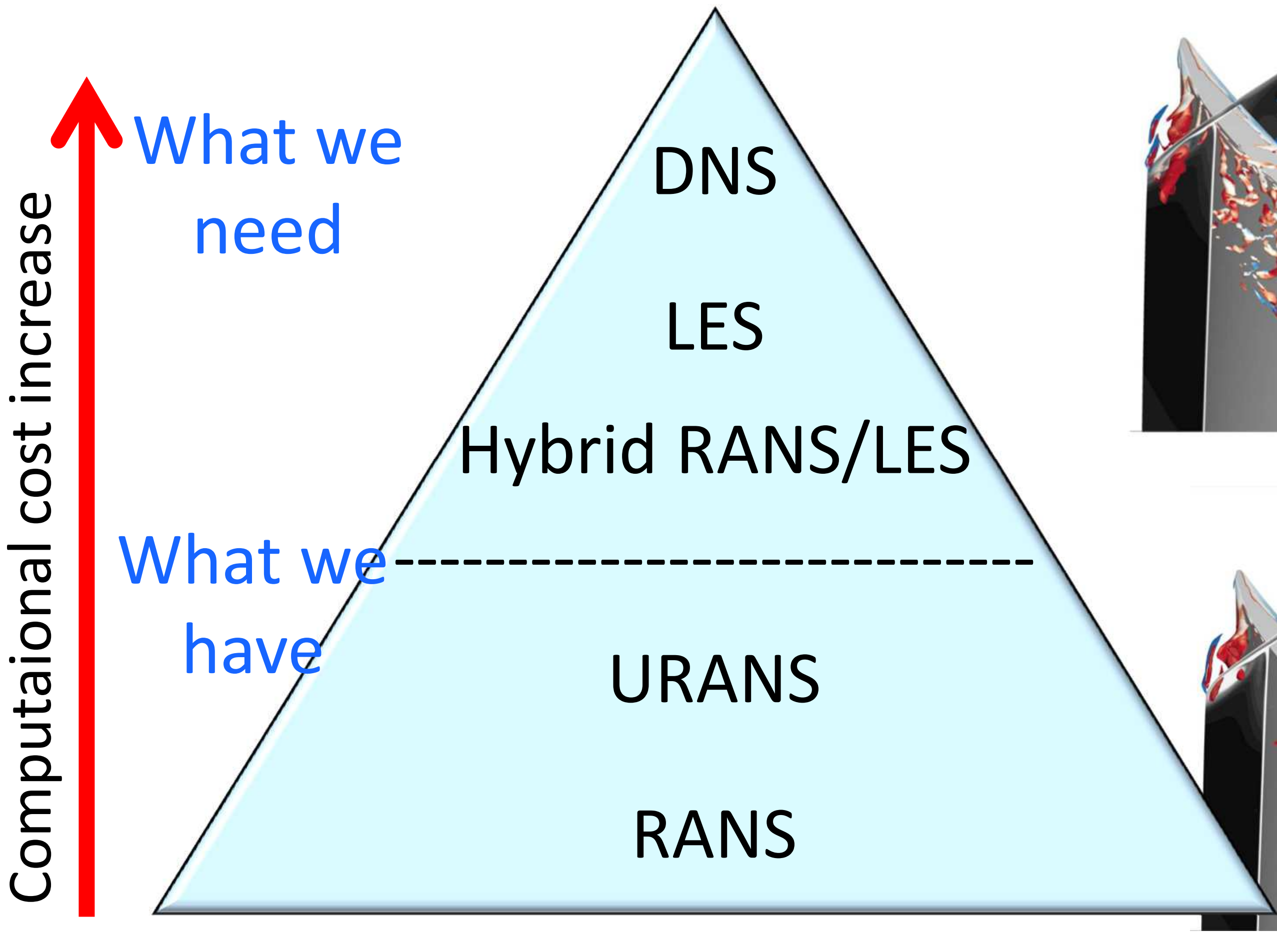
  $\bar{u}$ mean field

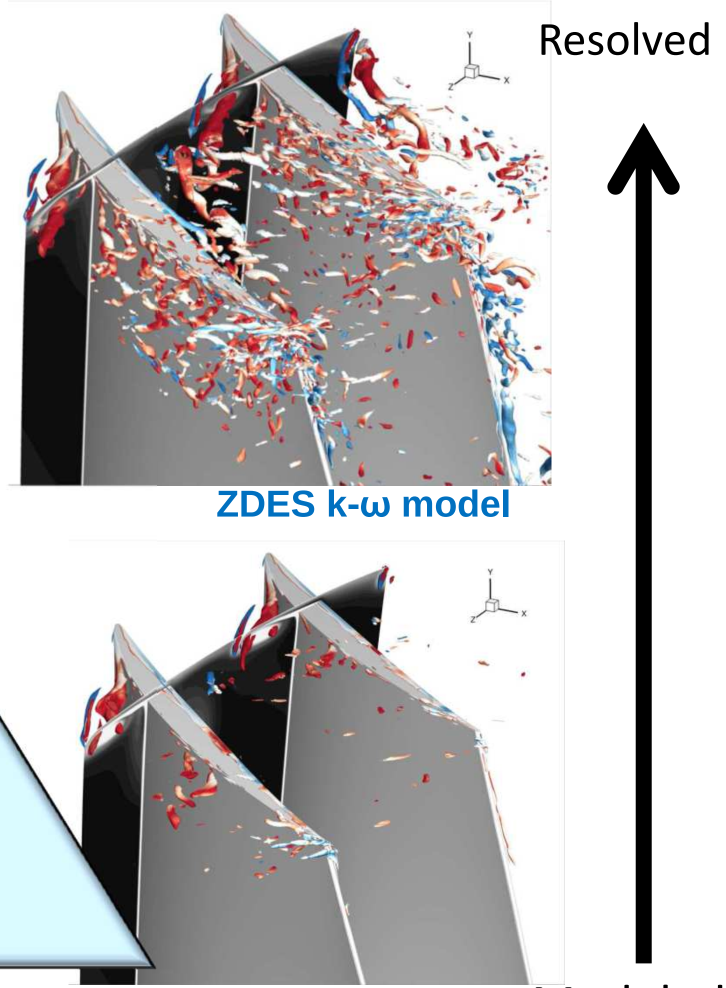
  u' fluctuations : $\overline{u'} = 0$

  All the turbulent scales are modeled (non resolved)

  $\bar{u}$ is the ensemble averaging (TBD)

Turbulence modelling





ZDES k-ω model

SAS Menter Model
Comparison on tip-leakage vortex

RANS : Reynolds Averaged Navier-Stokes system of equations

The RANS equations for compressible flows are (averaging notations removed)

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}.(\rho \vec{V}) = 0$$

$$\frac{\partial \rho \vec{V}}{\partial t} + \vec{\nabla} \cdot \left[\rho \vec{V} \otimes \vec{V} + p\bar{\bar{I}} - \bar{\bar{\tau}} - \bar{\bar{\tau}}_R\right] = 0$$

$$\frac{\partial \rho E}{\partial t} + \vec{\nabla} \cdot \left[\rho E \vec{V} + \left(p\bar{\bar{I}} - \bar{\bar{\tau}} - \bar{\bar{\tau}}_R\right) \cdot \vec{V} + \vec{q} + \vec{q}_R\right] = 0$$

It is necessary to model the following quantities in order to close the system

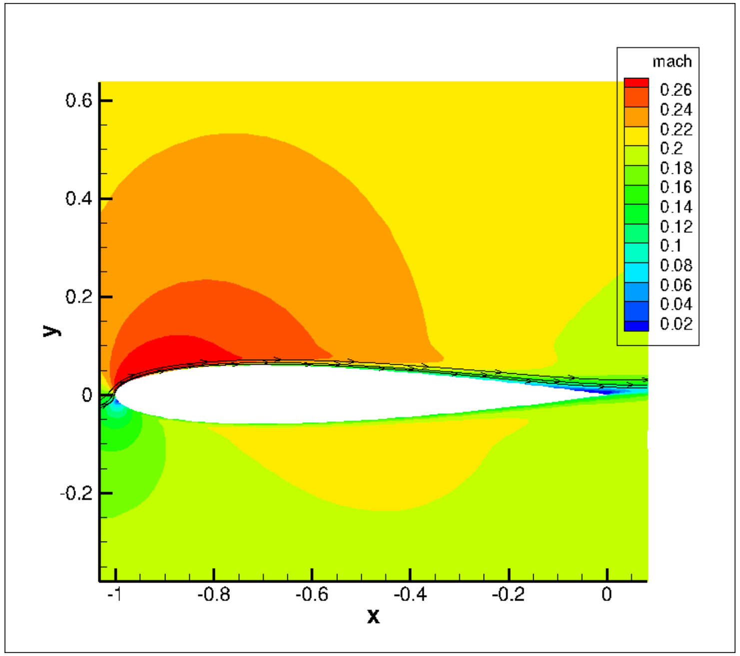
- Turbulent stress tensor (Reynolds tensor) : $\bar{\bar{\tau}}_R = -\overline{\rho \vec{V}' \otimes \vec{V}'}$
- Turbulent kinetic energy : $k = \frac{1}{2} \overline{\rho V'^2} / \bar{\rho}$ $\quad E = e + \frac{\vec{V}^2}{2} + k$
- Turbulent enthalpy flux : $\vec{q}_R = \frac{1}{2} \overline{\rho \vec{V}' h'}$

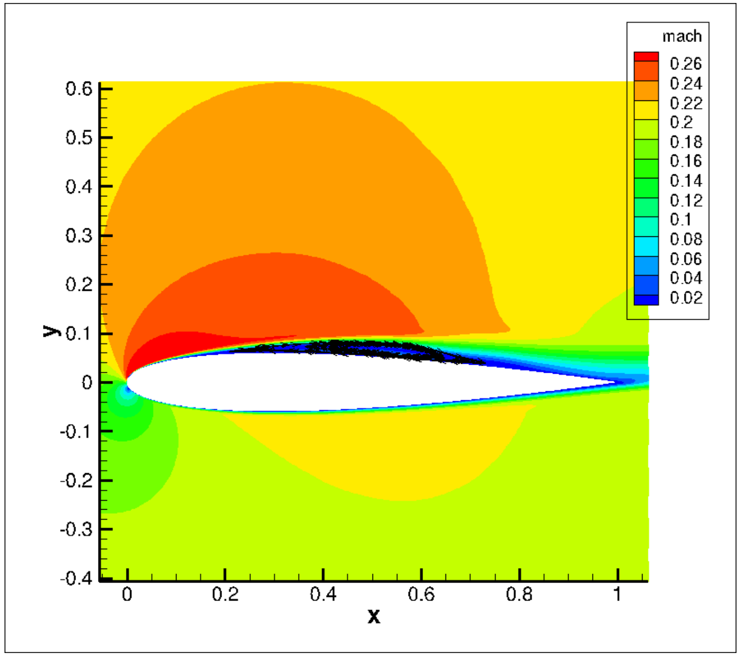
Turbulence model example : Wilcox K-ω model

$$\frac{\partial \rho k}{\partial t} + \vec{\nabla}.(\rho \overline{V} k) = \vec{\nabla}.\left[\left(\mu + \sigma^* \mu_t\right) \vec{\nabla} k\right] + \bar{\bar{\tau}}_t : \vec{\nabla} \overline{V} - \beta^* \rho k \omega$$

$$\frac{\partial \rho \omega}{\partial t} + \vec{\nabla}.(\rho \overline{V} \omega) = \vec{\nabla}.\left[\left(\mu + \sigma \mu_t\right) \vec{\nabla} \omega\right] + \alpha \frac{\omega}{k} \bar{\bar{\tau}}_t : \vec{\nabla} \overline{V} - \beta \rho \omega^2$$

Unsteady turbulent computations in non-matching meshes

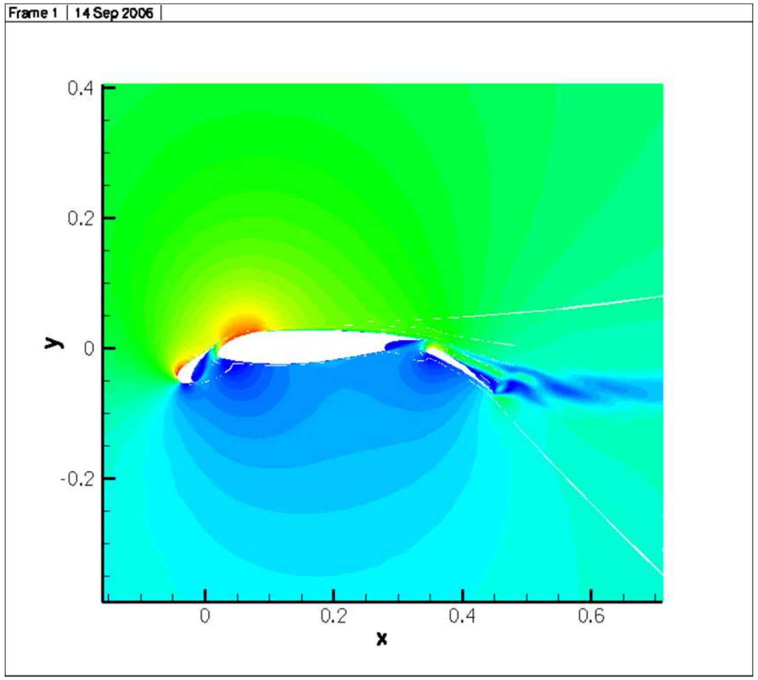


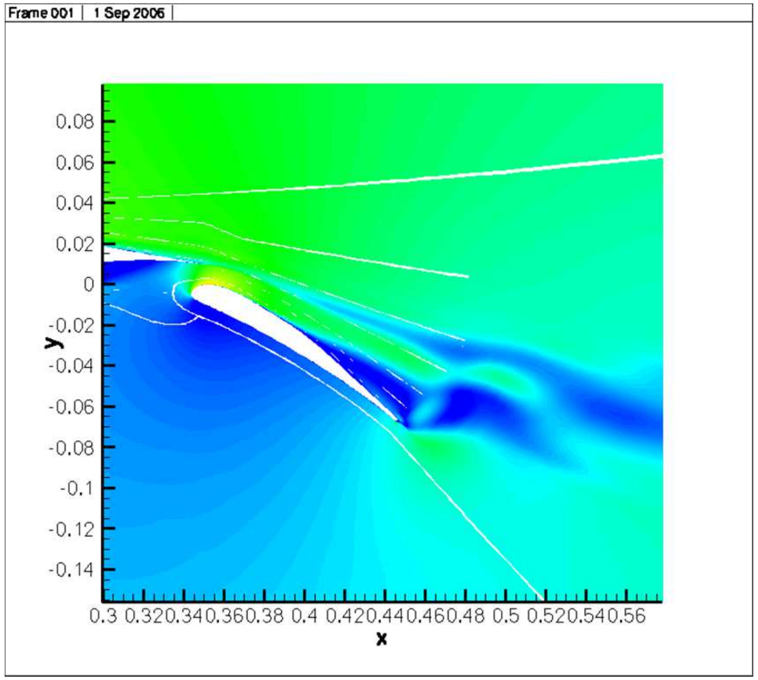


Calcul RANS/K-Omega sur maillage grossier 271 x 57

Calcul DNS "sous-résolu" sur maillage fin 1081 x 225

TC11 – URANS calculations – 12 Deg





SST Komega model – Unsteady computation
(the computation was first performed in a steady mode and did not converge; then it was performed in an unsteady mode using DTS)
K-Omega SST is in better agreement with the experiment than K-Omega Wilcox
Unsteady effects appear in the slat separation region

Estimation d'erreur

- Estimation de l'erreur : Définition de la référence
  - Calcul / expérience : Barre d'erreur de mesure
  - **Calcul / solution convergée (en DOFs) – Niveau de discrétisation espace/temps**
  - Convergence itérative
  - Précision machine
  - **Modélisation de la turbulence : LES (ref DNS filtrée ou DNS non filtrée) / filtrage explicite**
  - Prise en compte des incertitudes : méthodes NIPCM : comment définir les pdf d'entrée ?
  - NIPCM et PCM : Approches non intrusives en modélisation
    - PCM : intrusive dans le code CFD
    - NIPCM : non intrusive
  - Synergie calcul / expérience ou référence
    - Fusion de données : non intrusif dans le code
    - **Assimilation de données : intrusif dans le code pour prise en compte de données**
    - **IA pour modélisation de la turbulence**

Ordre élevé / Gain en précision

Mesure de l'erreur entre solution numérique et solution exacte : exemple sur une EDO d'ordre 1

$$\frac{du}{dx} = au \quad , \quad u(0) = 1$$

$$u_{exacte} = e^{ax} \quad , \quad u(0) = 1$$

$$D = [0,1] \quad , \quad h = \frac{1}{n}, \; n = (10, 20, \ldots, 7120)$$

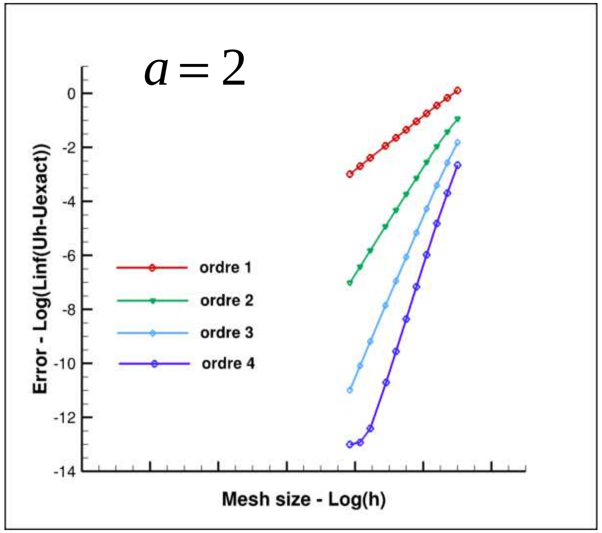
Branche asymptotique : $\underset{h \to 0}{u_{exacte} = u_h + Ch^p}$

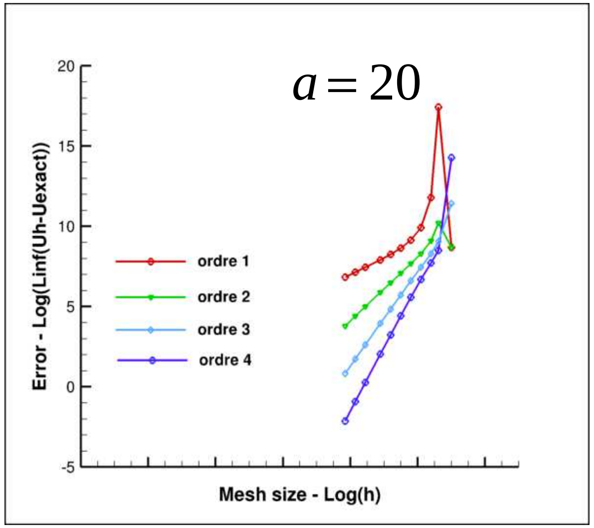
$$O1: \quad u_{h,i} = \frac{u_{h,i-1}}{1 - ah}$$

$$O2: \quad u_{h,i} = \frac{-u_{h,i-2} + 4u_{h,i-1}}{3 - 2ah}$$

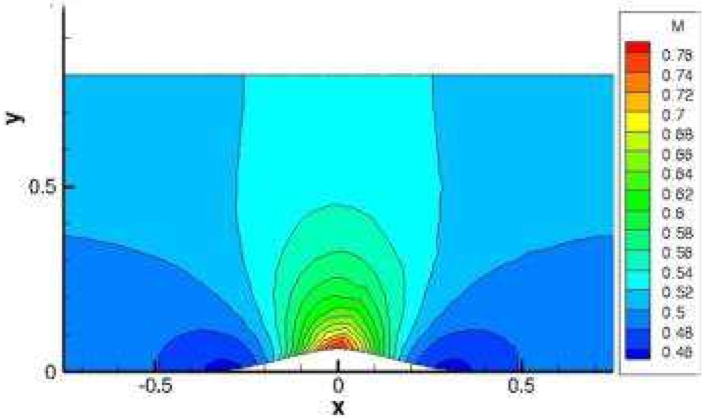
$$O3: \quad u_{h,i} = \frac{2u_{h,i-3} - 9u_{h,i-2} + 18u_{h,i-1}}{11 - 6ah}$$

$$O4: \quad u_{h,i} = \frac{-3u_{h,i-4} + 16u_{h,i-3} - 36u_{h,i-2} + 48u_{h,i-1}}{25 - 12ah}$$

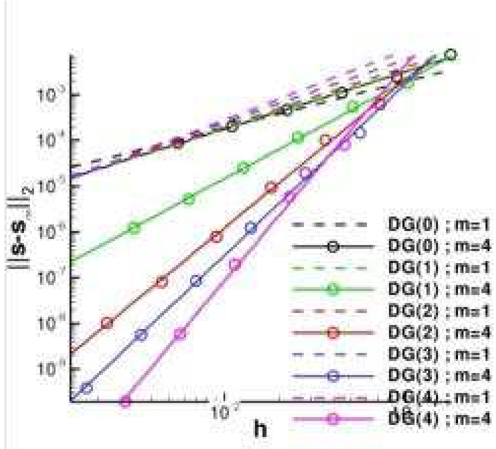




Aghora – Verification of method accuracy : scheme / geometry

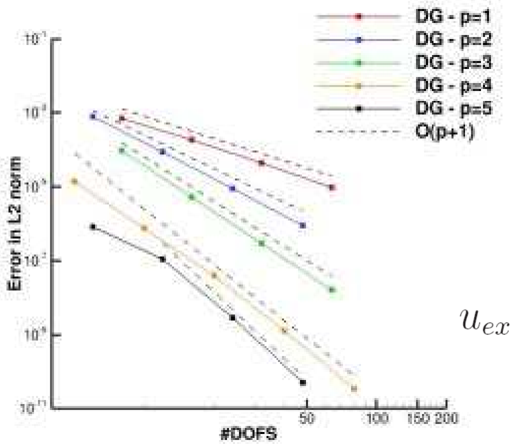


Subsonic Euler flow



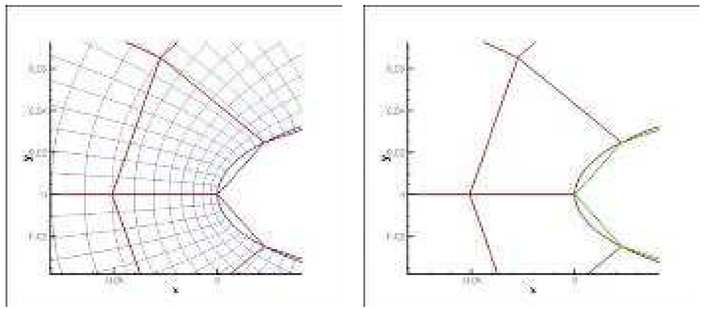
Entropy error vs. Mesh refinement

High-order scheme/geometry for accuracy of HO spectral type schemes (Aghora – HOCFD 2012)



$$u_{ex}\left(y\right) = u_c\left(1 - \frac{y^2}{h^2}\right)$$

Strong demand on of High-Order meshes

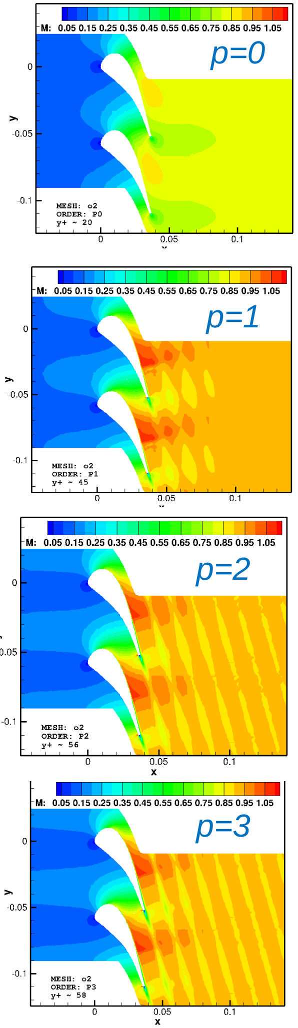


Sophie Gerald, Jean-Baptiste Chapelier

Manufactured solution for Navier-Stokes : Poiseuille flow

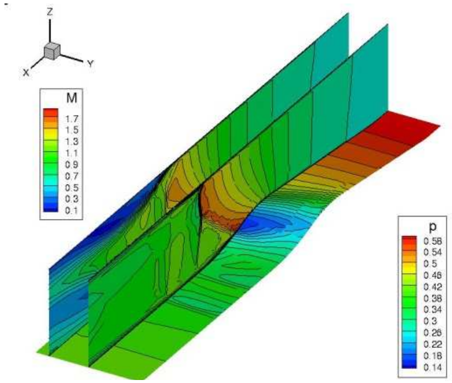
Error numerical solution / exact solution

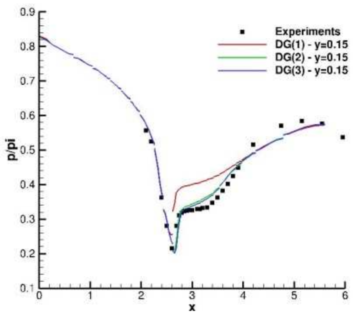
Aghora – Turbine transsonique VKI LS89
Calculs DG avec modèle RANS/SA et LES

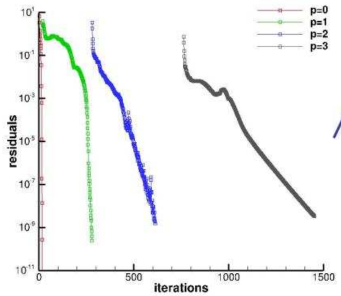


Transonic VKI turbine
at iso-Mesh : from p=0 to p=3

O. Labbé

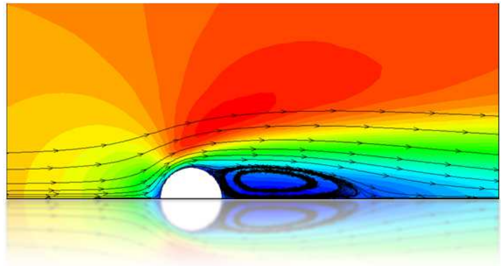


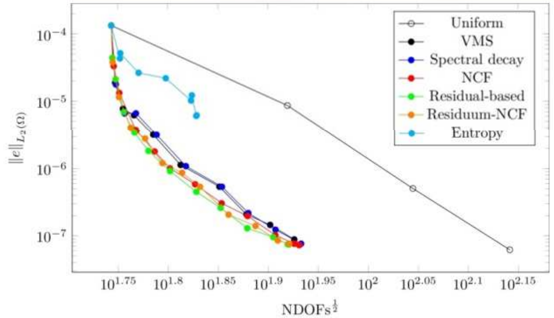


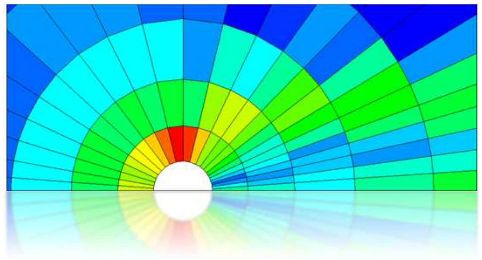


ONERA 3D swept Bump (Exp. J. Délery)
Efficient implicit method for HO-DG

F. Renac



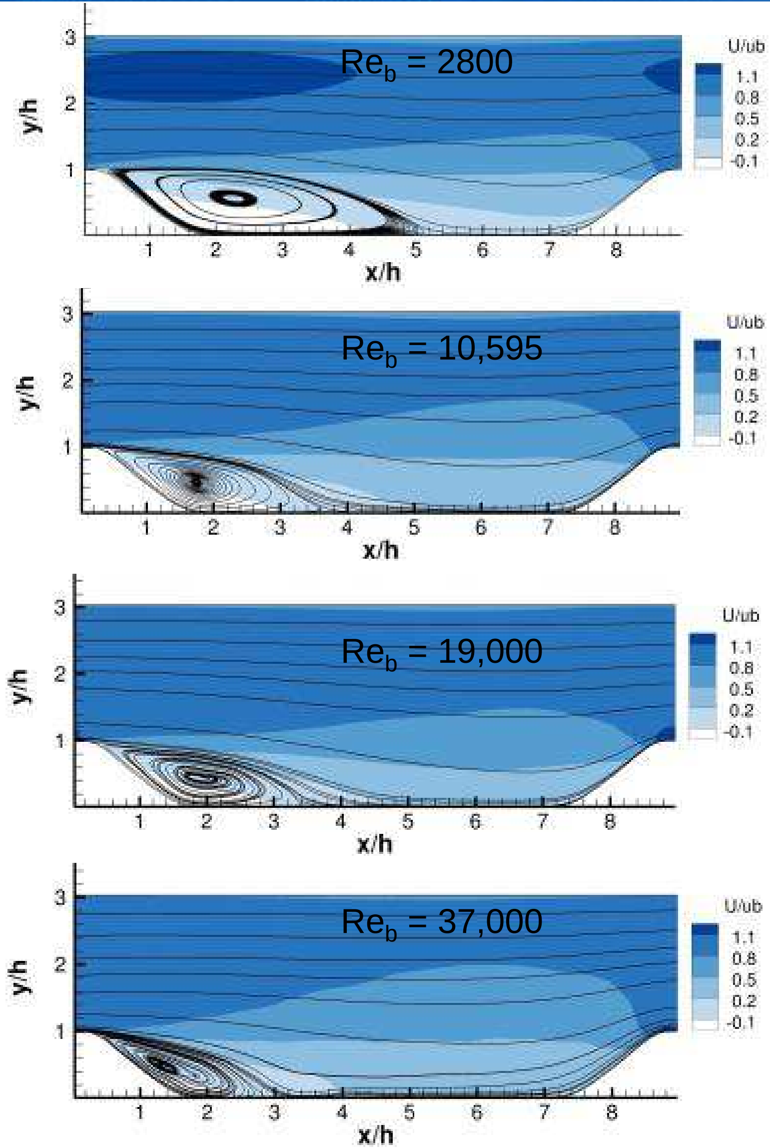




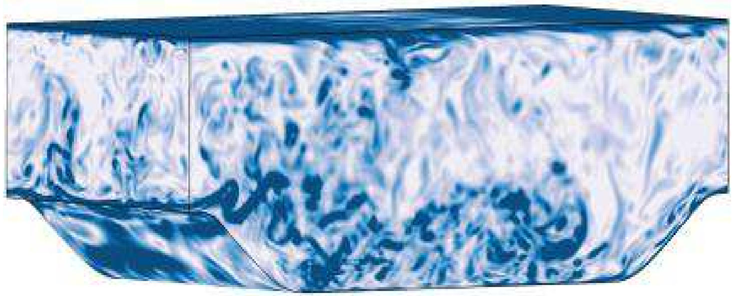
FD-09. CFD Solver Techniques
AIAA-2018-0368.
Fabio Naddei et al.

Laminar cylinder - Efficiency of local p-refinement with various error indicators

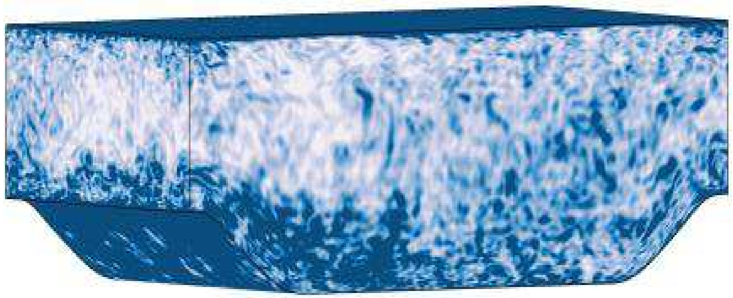
Periodic hill – instantaneous field and mean flow



Ecoulements instantanés



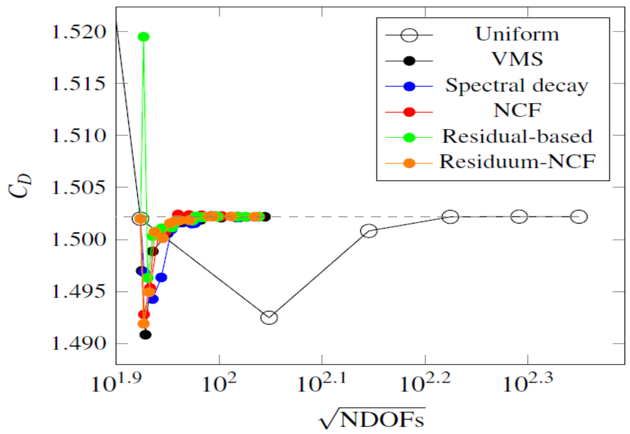
Re_b = 2800



M. De la Lllave Plata

Re_b = 10,595

Convergence analysis for steady laminar flow

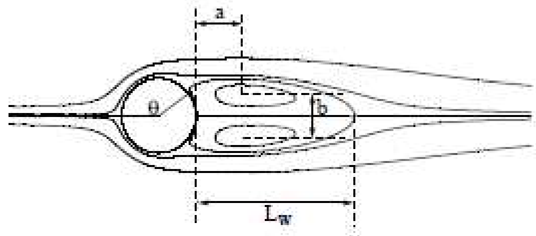


Aghora.

Same Cd with margin error of 10^{-4}
obtained with DG code Aghora, FV codes elsA and CANARI with h and/or p refinement and artificial external boundary extension

Table 1: Physical parameters of the flow pattern around a circular cylinder at $Re = 40$: Drag coefficient C_D, separation angle θ_s, wake length L_w/D and location of recirculation centre (a, b).

	C_D	θ_s	L_w/D	a/D	b/D
Tritton [1]	1.48				
Dennis & Chang [2]	1.52	126.2°	2.35		
Coutanceau & Bouard [3]		126.2°	2.13	0.76	0.59
Fornberg [4]	1.50	124.4°	2.24		
He & Doolen [5]	1.50	127.2°	2.25		
Ye et al. [6]	1.52		2.27		
Calhoun [7]	1.62	125.8°	2.18		
Russel & Wang [8]	1.60		2.29		
Tseng & Ferziger [9]	1.53		2.21		
Linnick & Fasel [10]	1.54	126.4°	2.28	0.72	0.60
Chung [11]	1.54		2.30		
Le et al. [12]	1.56		2.22		
Ding et al. [13]	1.58	127.2°	2.35		
Taira & Colonius [14]	1.54	126.3°	2.30	0.73	0.60
Posdziec & R. Grundmann [15]	1.49				
Patil & Lakshisha [16]	1.56	127.3°	2.14		
Bouchon et al. [17]	1.50	126.6°	2.26	0.71	0.60
Present reference solution	1.49	126.4°	2.24	0.71	0.59



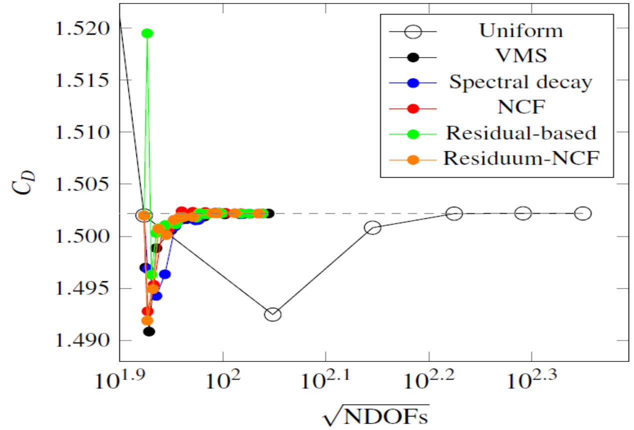
R. Gautier, D. Biau, E. Lamballais : A reference solution of the flow around a circular cylinder at Rey = 40
https://hal.archives-ouvertes.fr/hal-00876327

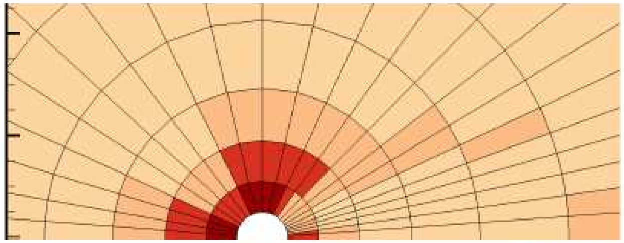
Error estimator and p-adaptation

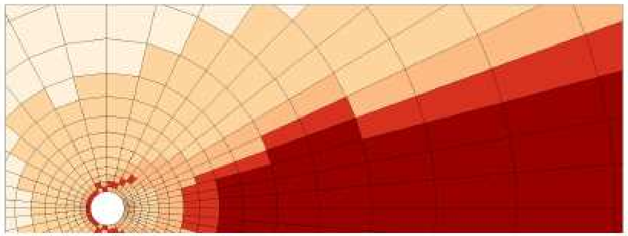
'A comparison of refinement indicators for p-adaptive simulations of steady and unsteady flows using discontinuous Galerkin methods', F. Naddei, M. de la Llave Plata, V. Couaillier, JCP 2019

Error estimators considered

- Small-scale energy density (SSED) (Kuru *et al.* , 2016)
- Spectral decay (SD) (Tumolo *et al.* , 2013)
- Non-conformity (NCF) (Gassner *et al.* , 2009)
- Residual-based (RB) (Hartmann & Houston, 2002)
- Residuum-NCF (RNCF) (Dolejší *et al.* , 2013)







Considered test cases

- **Euler steady**:
  Gaussian bump $M = 0.5$, Cylinder $M = 0.3$
- **Laminar steady**:
  Joukowski airfoil M= 0.5 Re= 1000,
  Cylinder M= 0.1 Re= 40
- **Laminar unsteady**:
  Cylinder M= 0.1 Re= 100

Aghora.

Propagation of uncertainties : Non Intrusive Polynomial Chaos Methods

ξ Input Random variable : Geometry, boundary conditions, initial conditions for unsteady problems
Scalar parameter in a RANS turbulence model

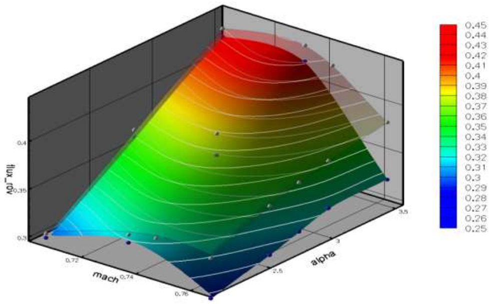
$\xi \to D(\xi)$ Probability Density Function in a set Γ known or defined a priori

Evaluation of the moments of an output fonction *U* defined in F

- Could be a space-time function as a velocity component of an unsteady CFD computation
- Practically in CFD *U* is often a scalar integral quantity : Drag or lift coefficient for aircraft flows, Pressure ratio for turbo-engines, …
- The deterministic CFD computations are performed only for a finite number of ξ values in Γ leading to a discrete representation of (ξ ,U) in the space $\Gamma \otimes$F
- Need to use a surrogate model to reconstruct U on the full space

$$u(x,t,\xi) = \sum_{i=0}^{p} u^i(x,t)\psi_i(\xi) \qquad (1)$$

ψ_i A set of polynomial consistent with the pdf D in order to get an orthogonal basis



Airfoil RAE2822 : Surrogate models using Kω or Kω-SST turbulence model

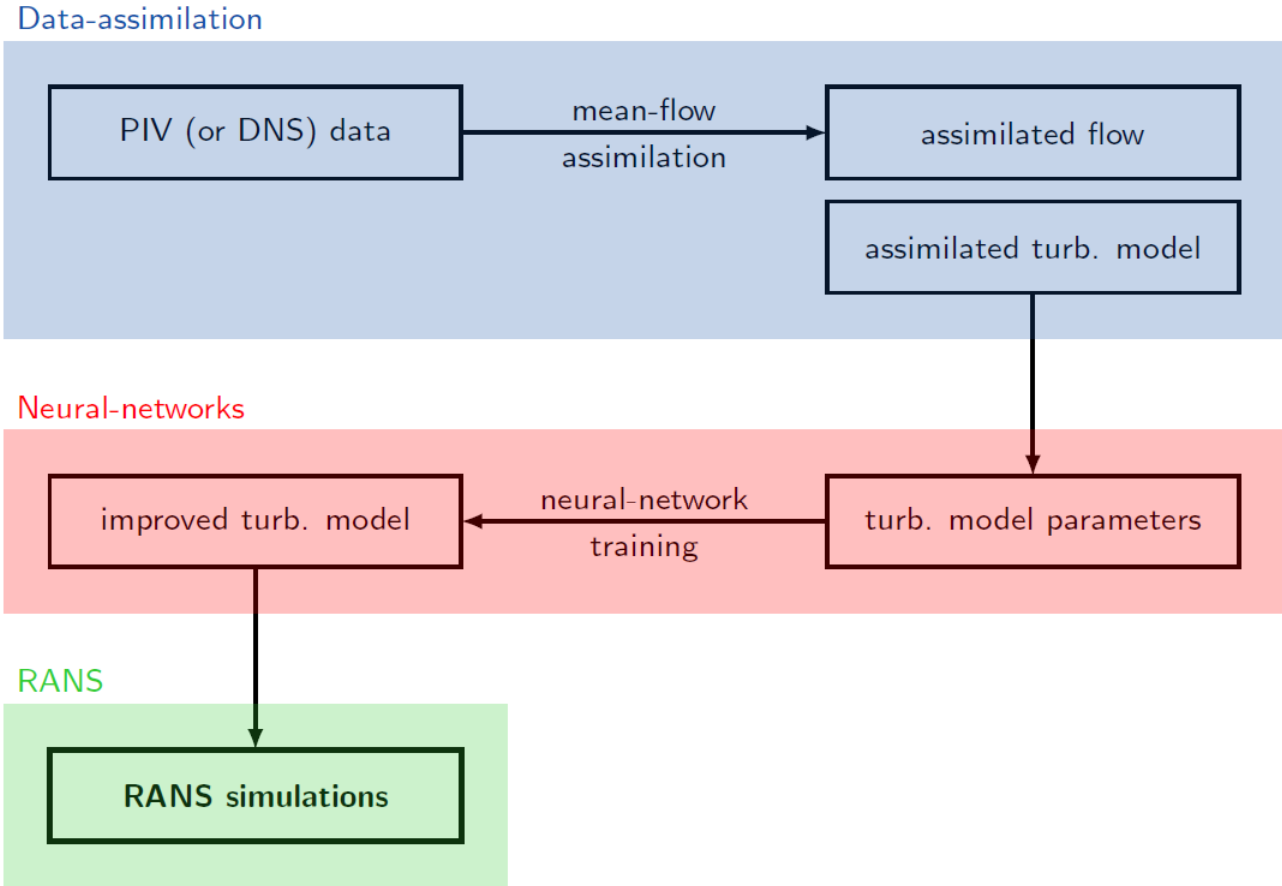
Turbulence model & Maching learning

- Improvement of RANS turbulence modeling to get as much as possible the quality of DNS/LES modelling
  - On mean flow quantities, integral/global quantities
- Use of reference data
  - Well-resolved DNS/LES computations of « simple flow configurations »
  - Experimental data : at ONERA project on synergy CFD/Experiments
  - Flight data
  - …
- Based on Data Assimilation methods
- Based on Machine learning, …
- Apply Improved turbulence models on advanced / complex flow configurations

Data-driven turbulence modeling applied to separated flows

Data-driven turbulence modeling applied to separated flows

Lucas Franceschini, **Nicolo Fabbiane**, Olivier Marquet, Benjamin Leclaire, Julien Dandois and Denis Sipp



A correction of Spalart-Allmaras model

Incompressible Reynolds-Averaged Navier-Stokes (RANS) with Spalart-Allmaras (SA) model:

$$\boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \nabla \cdot \left((\nu + \nu_t(\tilde{\nu})) \left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T \right) \right)$$

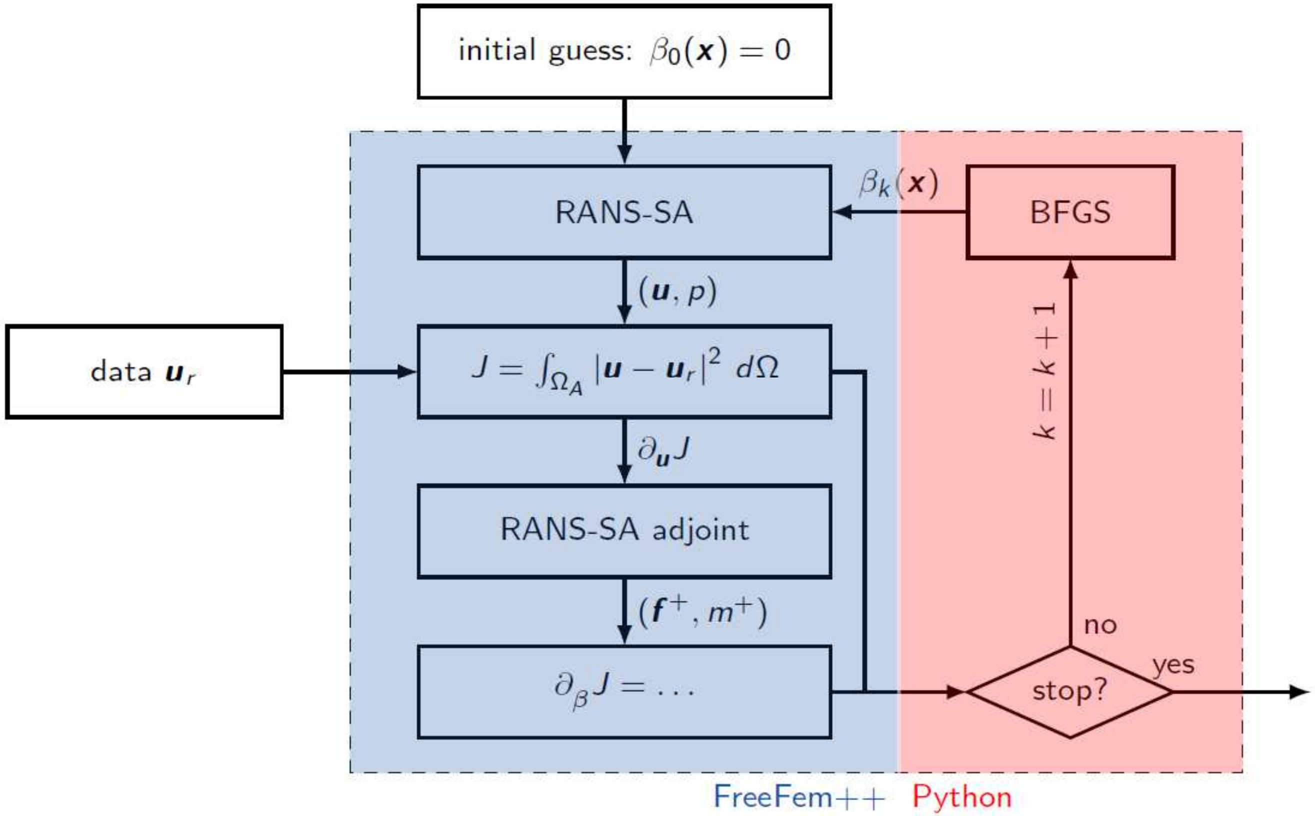
$$\nabla \cdot \boldsymbol{u} = 0$$

$$\boldsymbol{u} \cdot \nabla \tilde{\nu} = \beta(\boldsymbol{x}) \underbrace{c_{b1}\, \tilde{S}(\boldsymbol{u}, \tilde{\nu})\, \tilde{\nu}}_{P(\boldsymbol{u},\tilde{\nu}) \text{ production}} + \underbrace{\frac{1}{\sigma} \nabla \cdot ((\nu + \tilde{\nu})\nabla \tilde{\nu})}_{D(\tilde{\nu}) \text{ dissipation}} - \underbrace{c_{w1}\, f_w(\boldsymbol{u}, \tilde{\nu}) \left(\frac{\tilde{\nu}}{d} \right)^2}_{W(\boldsymbol{u},\tilde{\nu}) \text{ destruction}}$$

Duraisamy and Singh (2016): use $\beta(\boldsymbol{x})$ to correct the production term $P(\boldsymbol{u}, \tilde{\nu})$.

Adjoint-based optim. . . assimilation

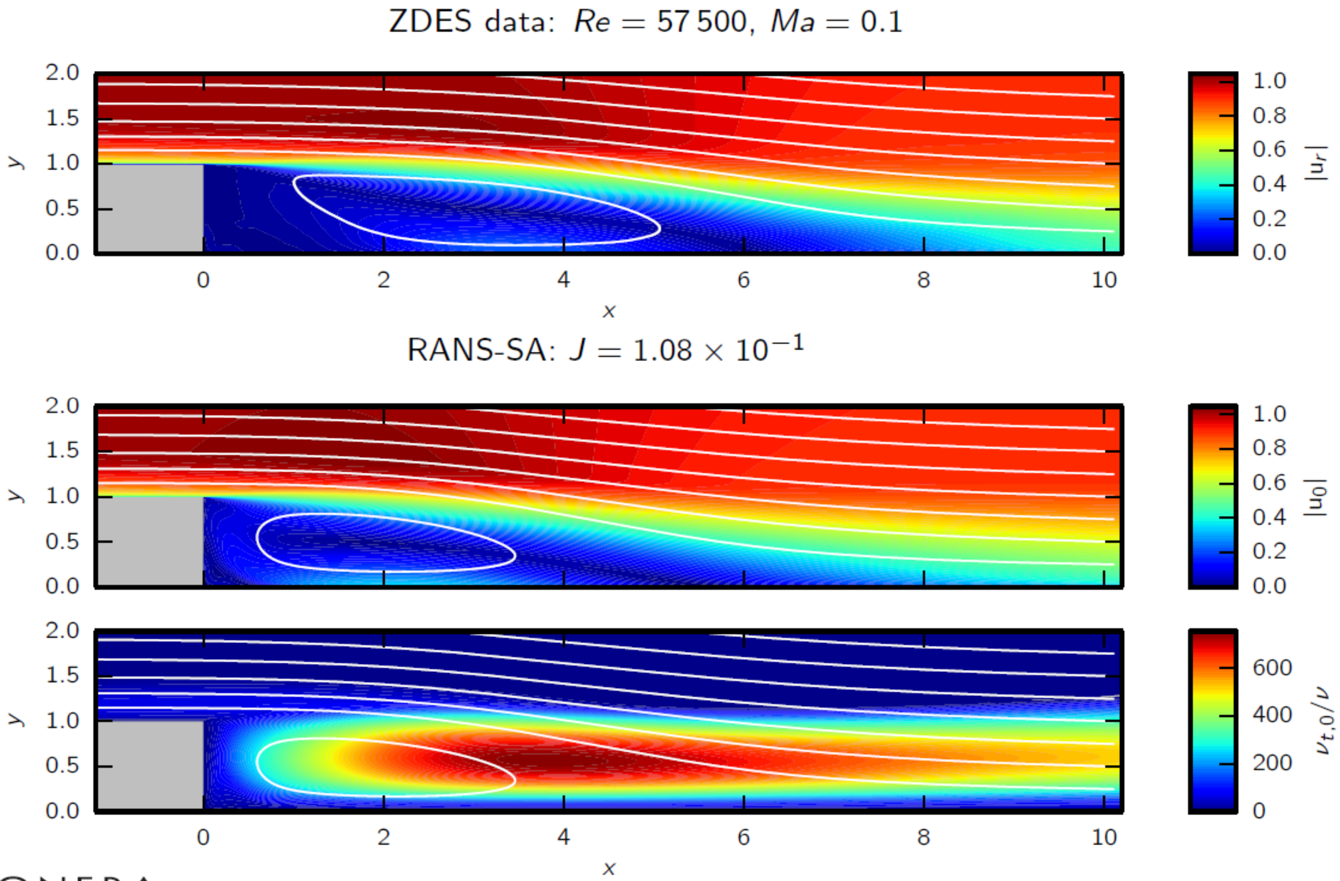
Adjust the production mask $\beta(\boldsymbol{x})$ to match the data $\boldsymbol{u}_r$, i.e. minimize the cost function J.



Data-driven turbulence modeling applied to separated flows

Flow assimilation (I)

Data: back-facing step simulations by Beneddine et al. (2016)



Data-driven turbulence modeling applied to separated flows

Flow assimilation (I)

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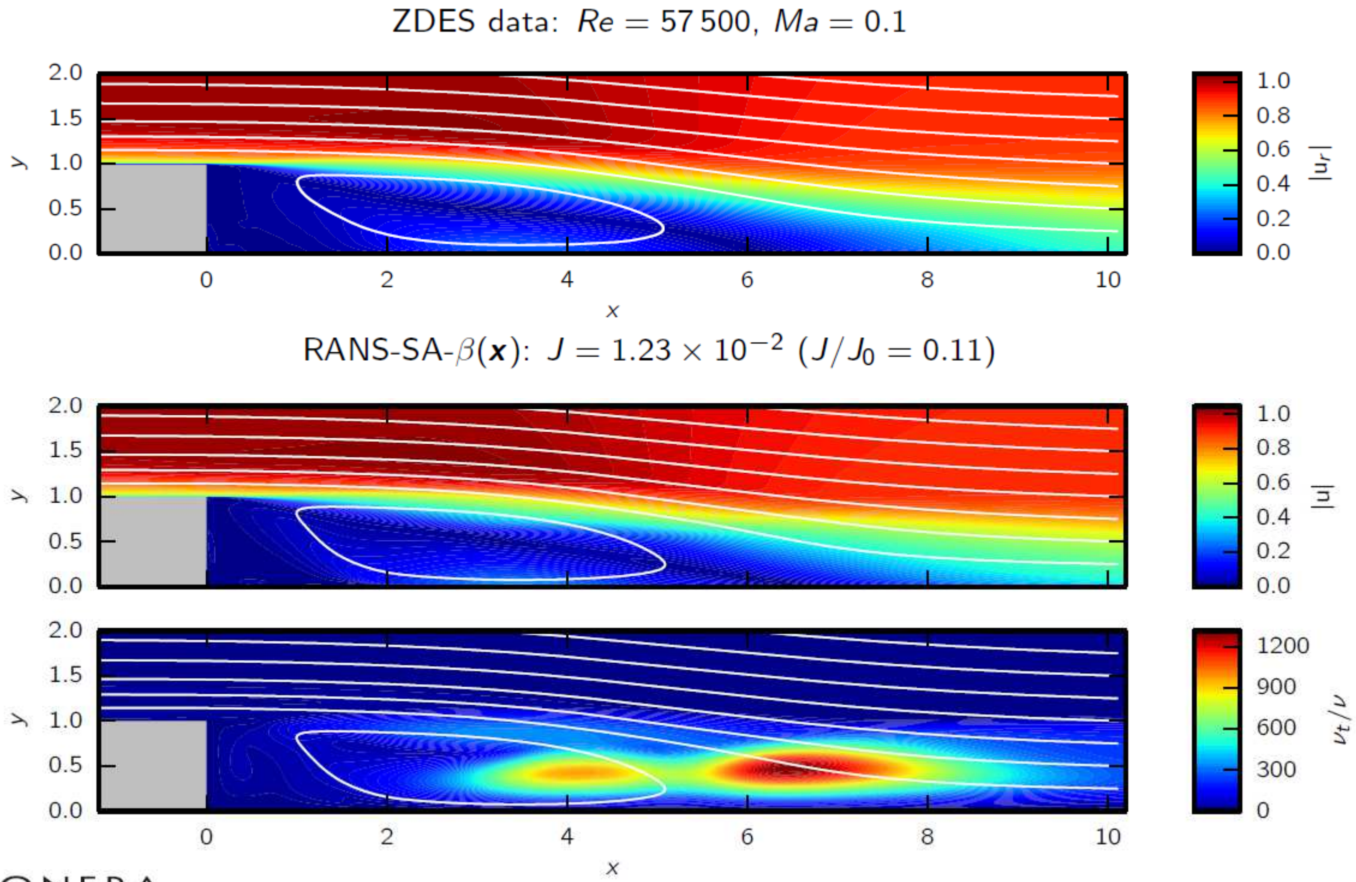

Flow assimilation (I)

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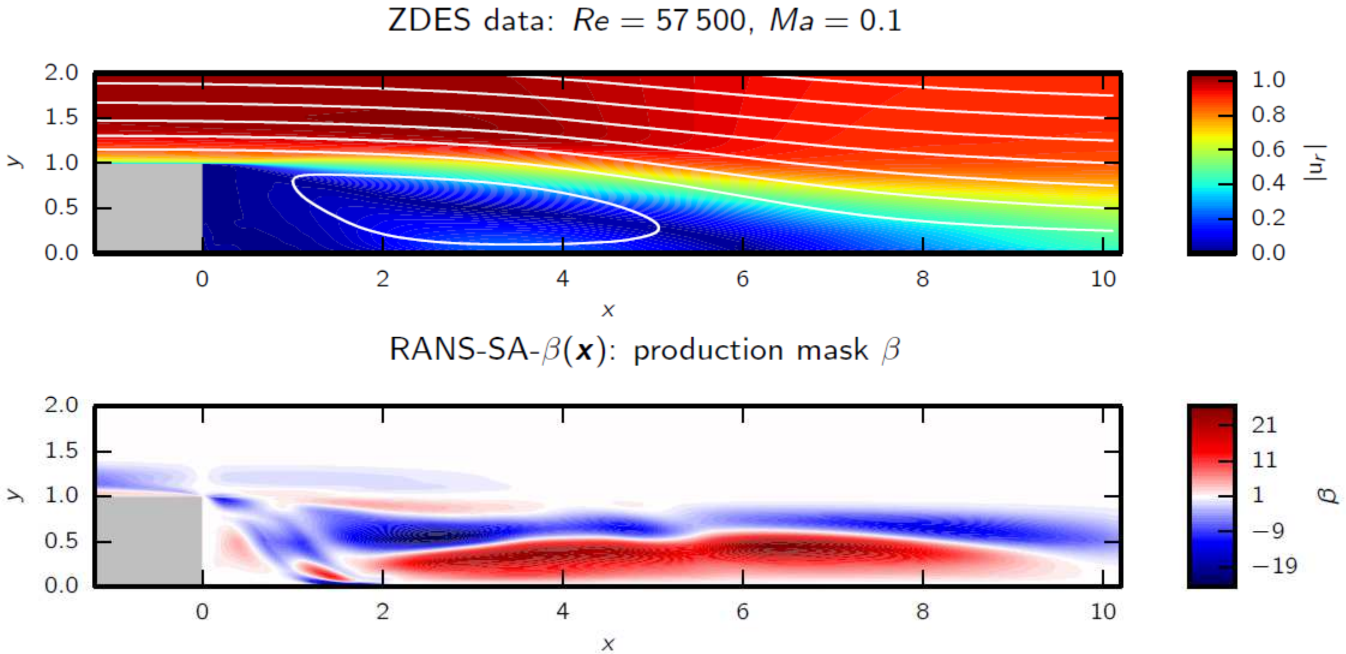


$|\beta| \approx 20$ ▶ not a *small* correction of Spalart-Allmaras anymore!

Data-driven turbulence modeling applied to separated flows

Neural network

Produce a general input/output (I/O) function that reproduces the SA correction.

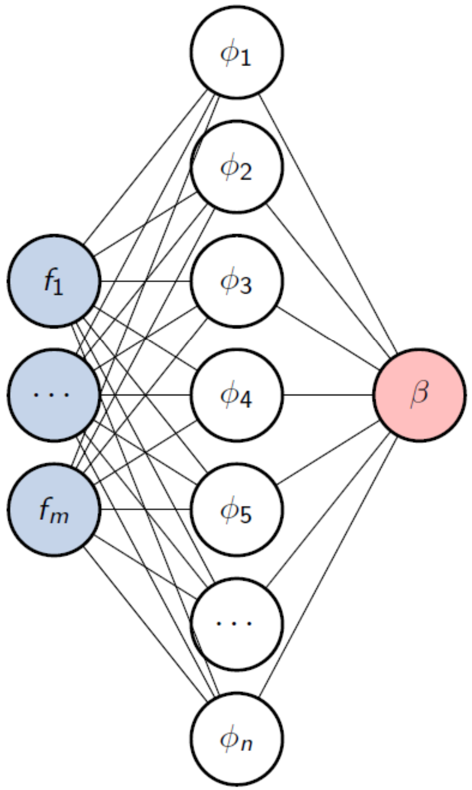
$$\boxed{\beta(\boldsymbol{x}) \rightarrow \beta(\boldsymbol{u}, \tilde{\nu}) \rightarrow \beta(\{f_j(\boldsymbol{u}, \tilde{\nu})\})}$$

- Not directly function of the state $(\boldsymbol{u}, \tilde{\nu})$ but on a set of observables $\{f_j(\boldsymbol{u}, \tilde{\nu})\}$
- Neural network (`scikit-learn` package): 1 layer of n=100 neurons.

$$\phi_i = \max\left(0, b_i + \sum_{j=1}^{m} a_{ij}\, f_j(\boldsymbol{u}, \tilde{\nu})\right)$$

$$\beta = \beta_0 + \sum_{i=1}^{n} w_i \phi_i$$

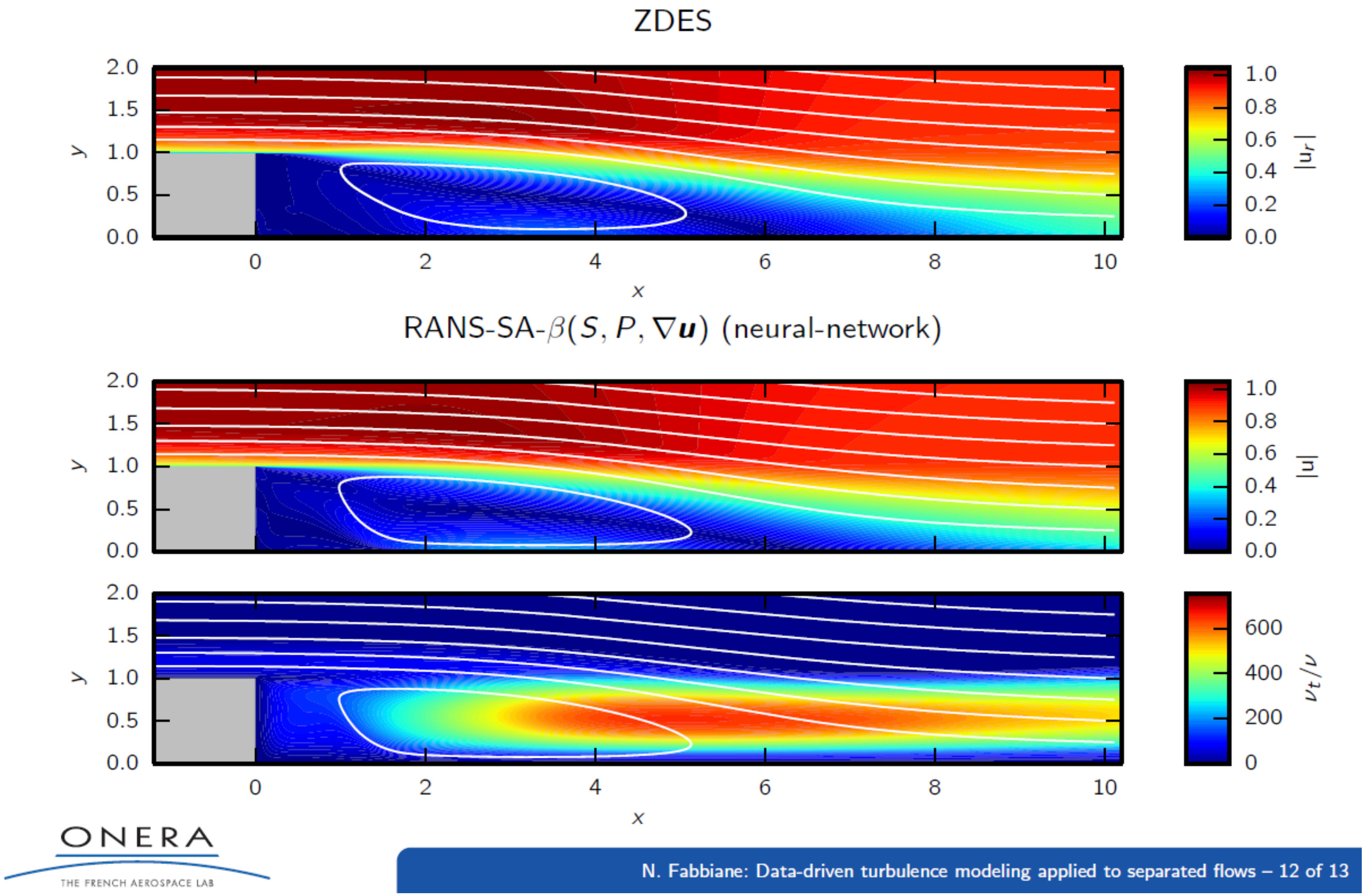
- Which observables $f_j(\boldsymbol{u}, \tilde{\nu})$?
  First attempt: $\boxed{\{f_j\} = \{\ln(S), P, \nabla \boldsymbol{u}\}}$



Data-driven turbulence modeling applied to separated flows

- Data assimilation : $\beta(x)$ for a given geometrical and physical configuration
- Machine learning using Neural network : Define $\beta^*(u,\tilde{\vartheta})$ to be used for various flow configurations
- $\beta^*(u,\tilde{\vartheta})$ define using $\{f_j(u,\tilde{\vartheta})\} = \{\ln(S)\,, P, \nabla u\}$ at the training points
- Minimize a norm of $[\beta^*(\{f_j(u,\tilde{\vartheta})\}) - \beta(x)]$ at the training points using back propagation
- Variables in blue (previous slide) are the quantities to be defined by the training process
- Activation fonction : Max (0, entry)
- Back-facing step :
  - 30,000 points for RANS computation
  - 7,500 for training with NN

Validation


ZDES
RANS-SA-β(S, P, ∇u) (neural-network)
2.0
1.5
1.0
0.5
0.0
y
0
2
4
6
8
10
x
1.0
0.8
0.6
0.4
0.2
0.0
|u_r|
|u|
600
400
200
0
ν_t/ν
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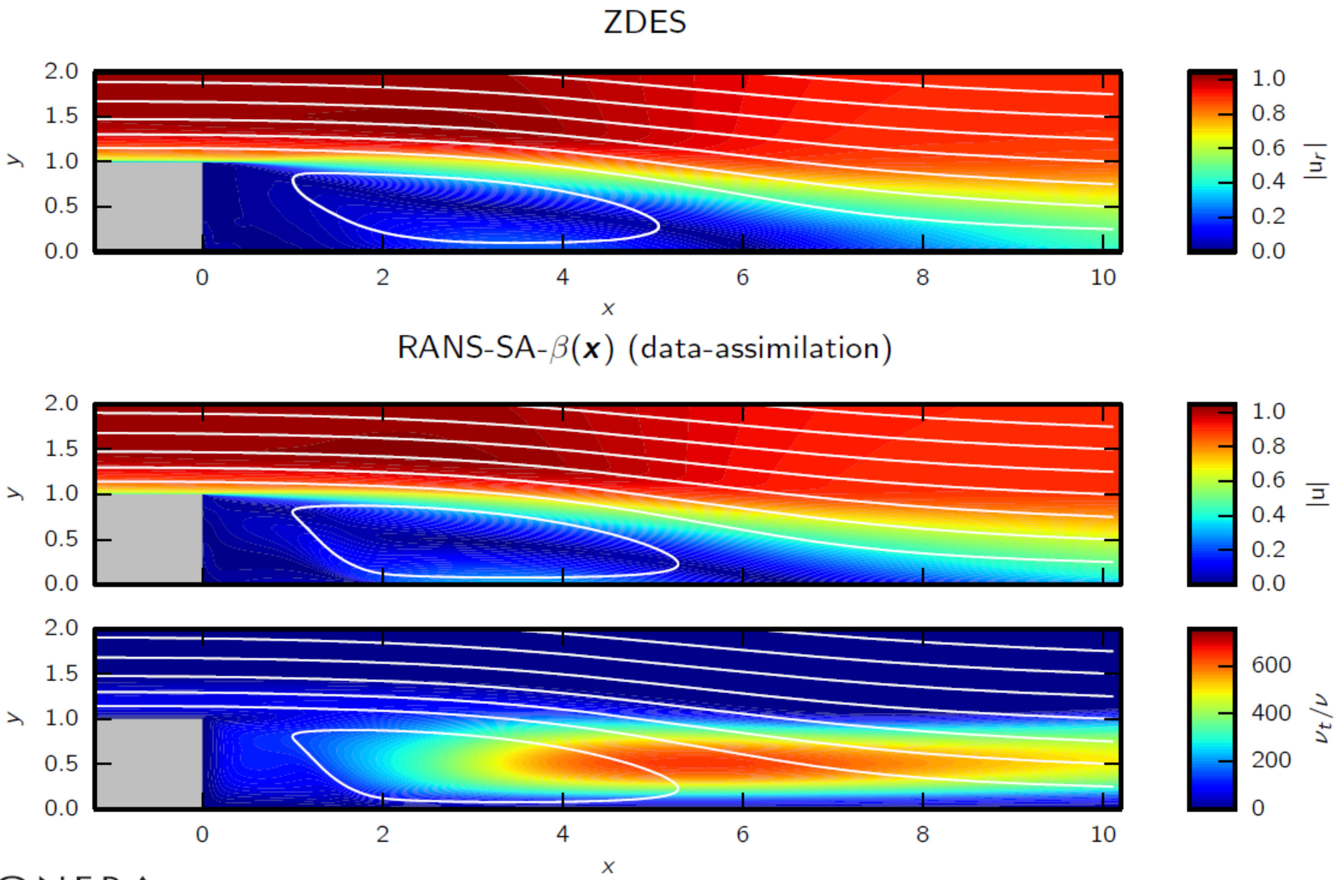
N. Fabbiane: Data-driven turbulence modeling applied to separated flows – 12 of 13

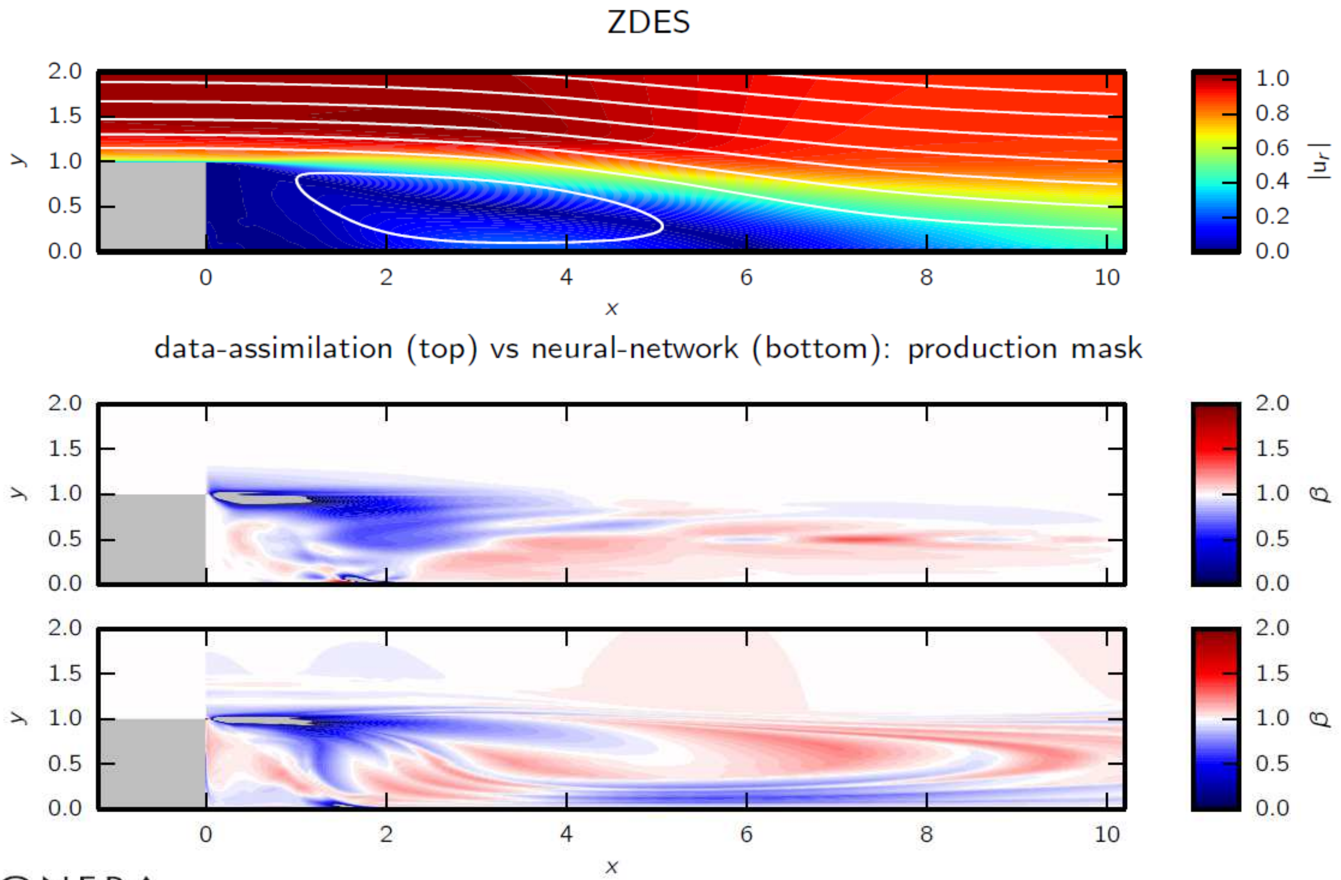
Validation



ZDES
RANS-SA-$\beta(\boldsymbol{x})$ (data-assimilation)
y
x
2.0
1.5
1.0
0.5
0.0
0
2
4
6
8
10
$|u_r|$
$|u|$
ν_t/ν
0.2
0.4
0.6
0.8
200
400
600

Data-driven turbulence modeling applied to separated flows

Validation



N. Fabbiane: Data-driven turbulence modeling applied to separated flows – 12 of 13

Conclusion

- A correction of Spalart-Allmaras is fitted to ZDES data.
  - Adjoint-based assimilation algorithm.
  - No appriciable difference between balanced and unbalanced c_{w1}.
- A neural network is trained to generalize the identified correction. . .
- . . . and tested on the *training* flow-case.
- The algorithm can be (is already) generalised for different cost functions:
  - pressure matching,
  - skin friction matching
  - . . .

  and different measuments techniques, i.e. include a measurment operator in the procedure.

Next step(s):

- Explore different input variables for the neural-network model.
- Blind-test on a *different-but-similar* flow case.

Turbulence model, HPC & Maching learning
Conclusion

- Turbulence with DNS at high Reynolds numbers (Scale-Resolved simulation) needs
  - Compute : More than exascale computing resources
  - Huge memory storage
  - Algorithms breakthrough (accuracy, efficiency)
  - Can be mitigated by LES and hybrid RANS/LES

- Turbulence with RANS needs
  - Major improvements in turbulence models
  - Artificial Intelligence combined with increasing capacity of memory storage should allow to make significant steps forward
  - ONERA is developing stronger synergy between CFD, experiments & data

- ***European project HiFi-TURB on AI for turbulence modelling starting mid-2019***