



Advanced Simulation of Turbulent Flows: UQ, Data Assimilation & Learning-based approaches

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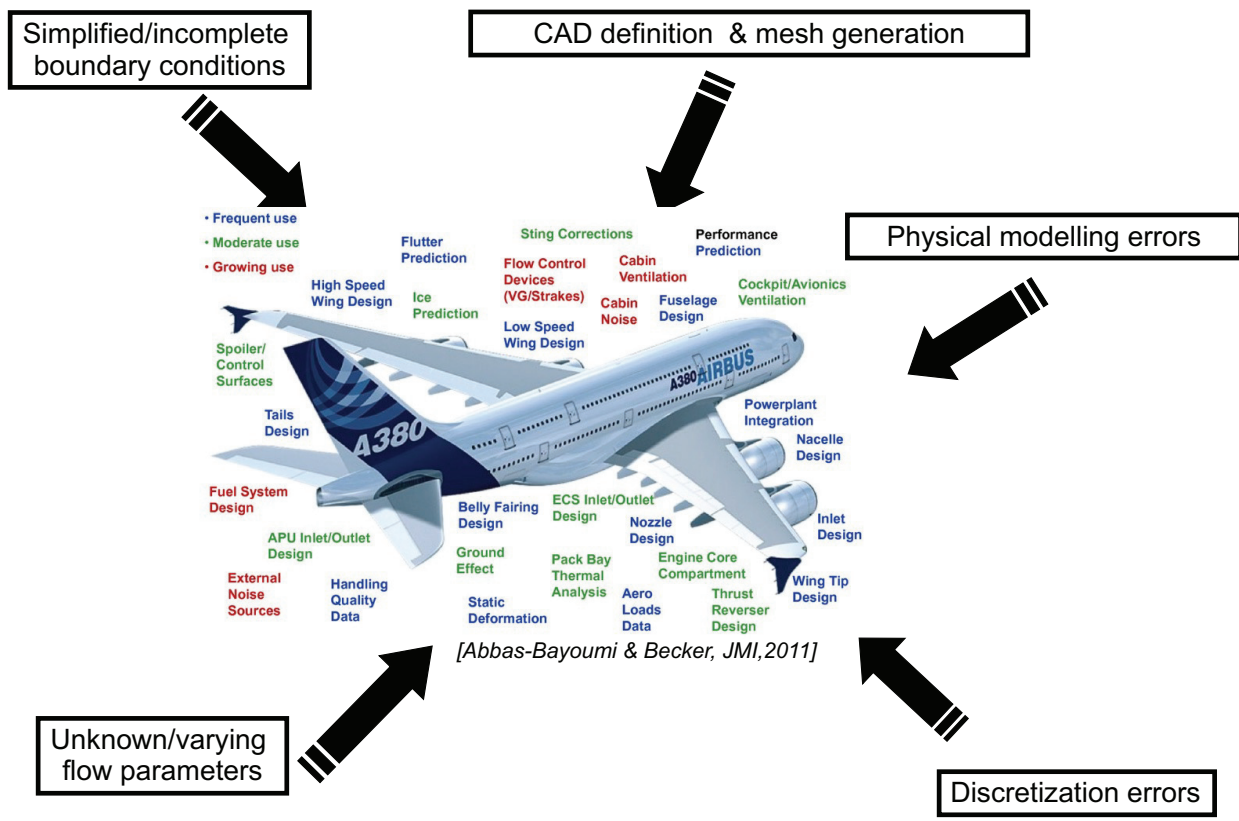
51th Fluid Dynamics Conference/37th Aerospace Numerical Simulation Symposium

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Simulation of complex systems



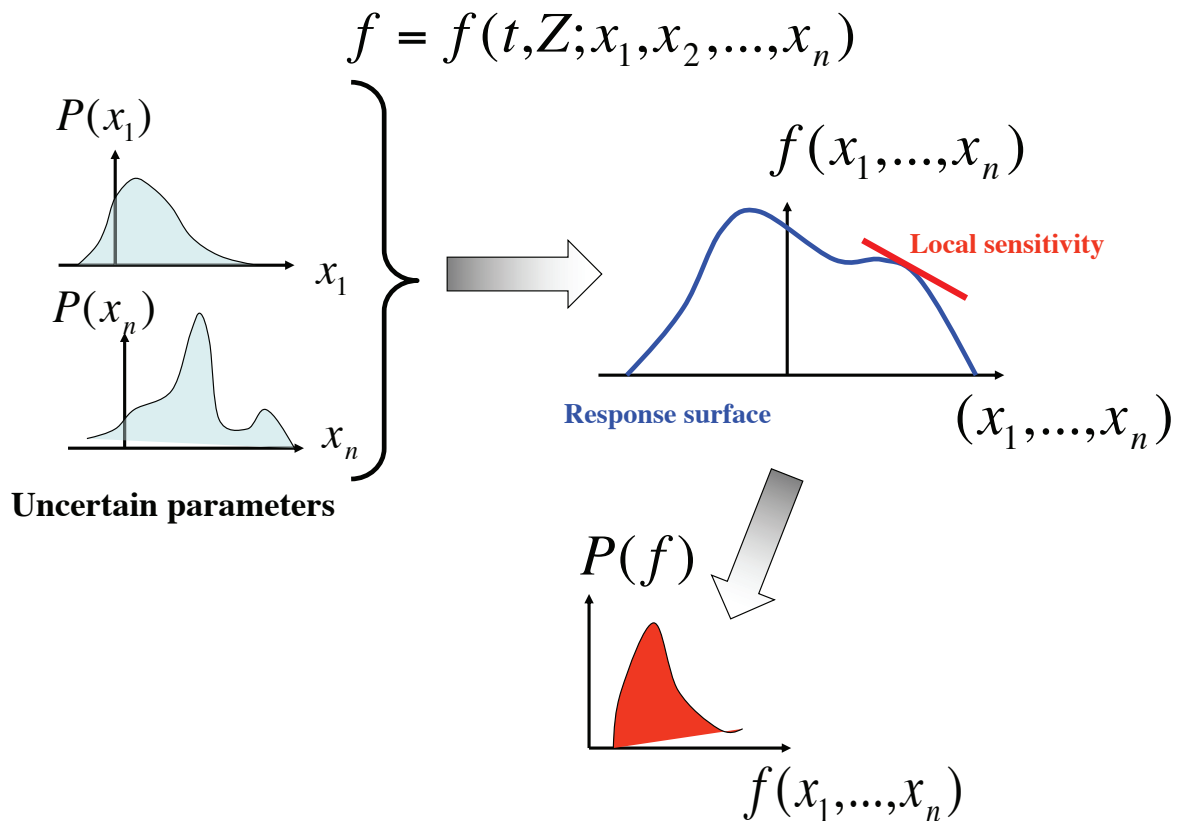
- Uncertainty Quantification and Propagation for turbulent flow simulations

→ Toward **Data-Augmented CFD**

- Data Assimilation: a way to reduce uncertainty
- Learning-based approaches: beyond classical CFD ?

- **Aleatoric uncertainties** (or irreducible uncertainties):
 - describe physical variations caused by intrinsic randomness in the system and its environment
 - can be characterized in terms of probability distributions and covariance matrices
- **Epistemic uncertainty**:
 - caused by a certain lack of knowledge (structural uncertainty in the model form or insufficient measurement data to quantify the value of an input parameter)
 - not probabilistic in nature
 - can better be described using intervals
 - can be reduced either by increasing model fidelity or by performing additional experiments
 - Data Assimilation can be used
- **Numerical errors**

Uncertain system description



Response Surface/Surrogate Model/ROM

Many works related to :

- *Surrogate models*
- *Response surfaces*
- *Reduced-order models*

For different purposes:

- *Sensitivity analysis*
- *Risk analysis*
- *Optimization (Goal-oriented modelling)*

Key features:

- *Each sample is a CFD run (expensive)*
- *Limited sampling (< 100-1000 samples in practice)*
- *Need for an accurate description of sensitivity*
- *Need for a prediction capability (new solutions)*
- *Monte Carlo too expensive for practical CFD*

- **Curse of dimensionality:**
1 uncertain parameter = 1 additional dimension
- **Curse of non-linearity**
Flow nonlinear dynamics couples all parameters
- **Curse of discontinuity**
Flow can exhibit bifurcation = « shocks » on response surface

Two main families of UQ/RS methods:

- *Intrusive methods* → *CFD solver modified*
- *Non-intrusive methods* → *CFD solver as a black box*

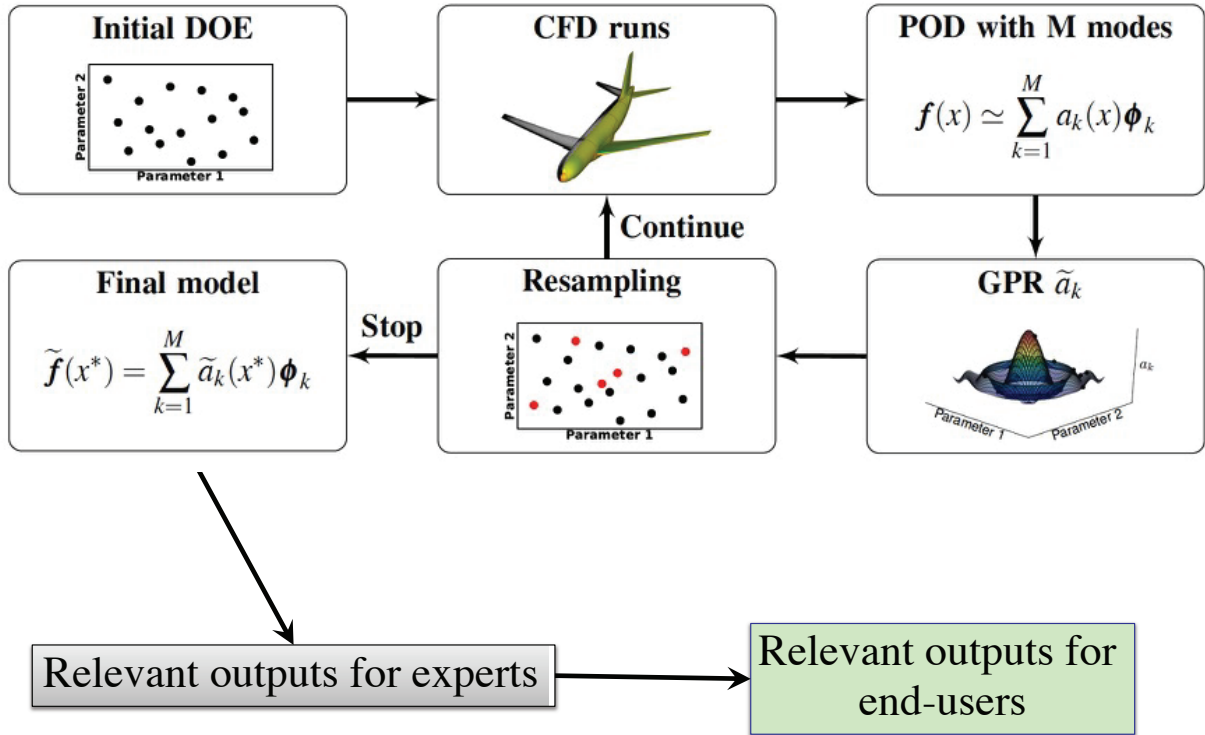
Huge number of existing methods:

- *Interpolant methods: ANOVA, Galerkin-type, gPC, ...*
- *Approximant methods: RBF, Kriging, POD, ANN ...*

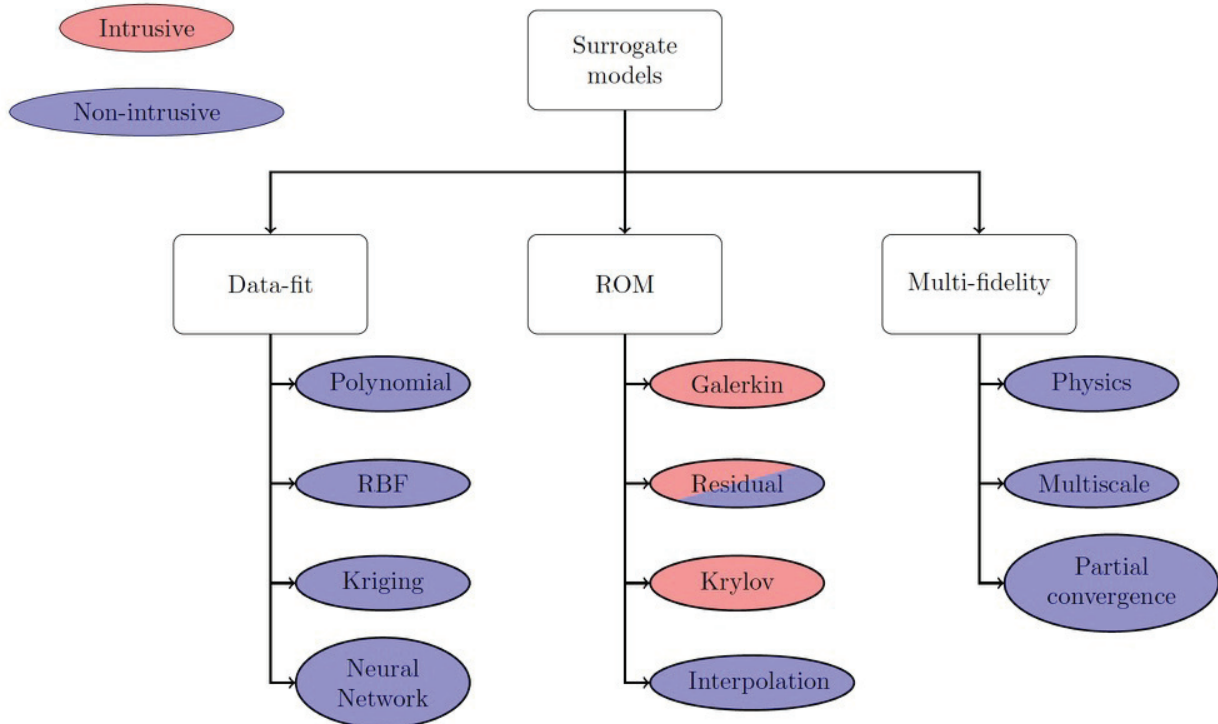
State-of-the-art:

- *Almost all applications done with non-intrusive methods*
- *Most works restricted to 3-5 uncertain parameters*
- *Most works related to smooth flows*
- *Most works related to steady flow solutions*
- *Kriging-based methods are very popular*

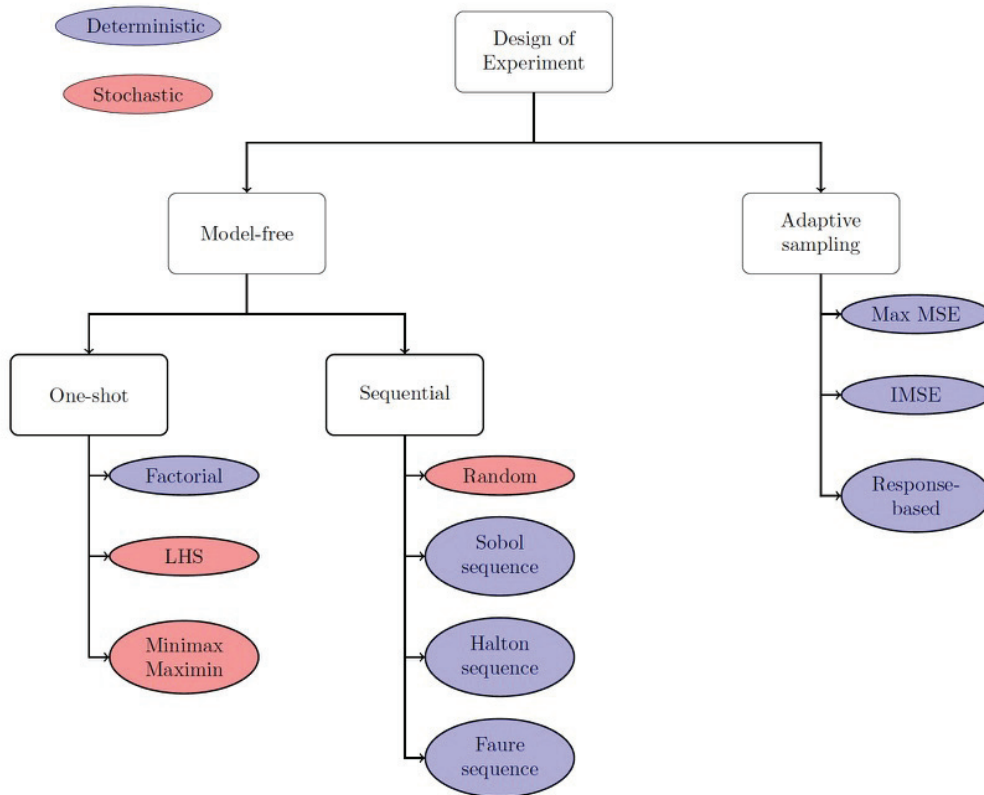
Typical loop for adaptive POD (non-intrusive method)



Most popular Surrogate Models in CFD



Design Of Experiments (DOE)



Uncertainty in turbulent flow simulations

- Operating and boundary conditions:
 - *Not always exactly known*
 - *Can be based on a (sub-)model*
- Parameters in turbulence/subgrid models:
 - *Rely on physical assumptions*
 - *Coupling with numerics*

Uncertainty in inflow BC

- Spatially developing shear flows very sensitive to inflow BC
- Dispersion in CFD results (jets, ...)
- Case study: 2D mixing layer with stochastic inflow BC

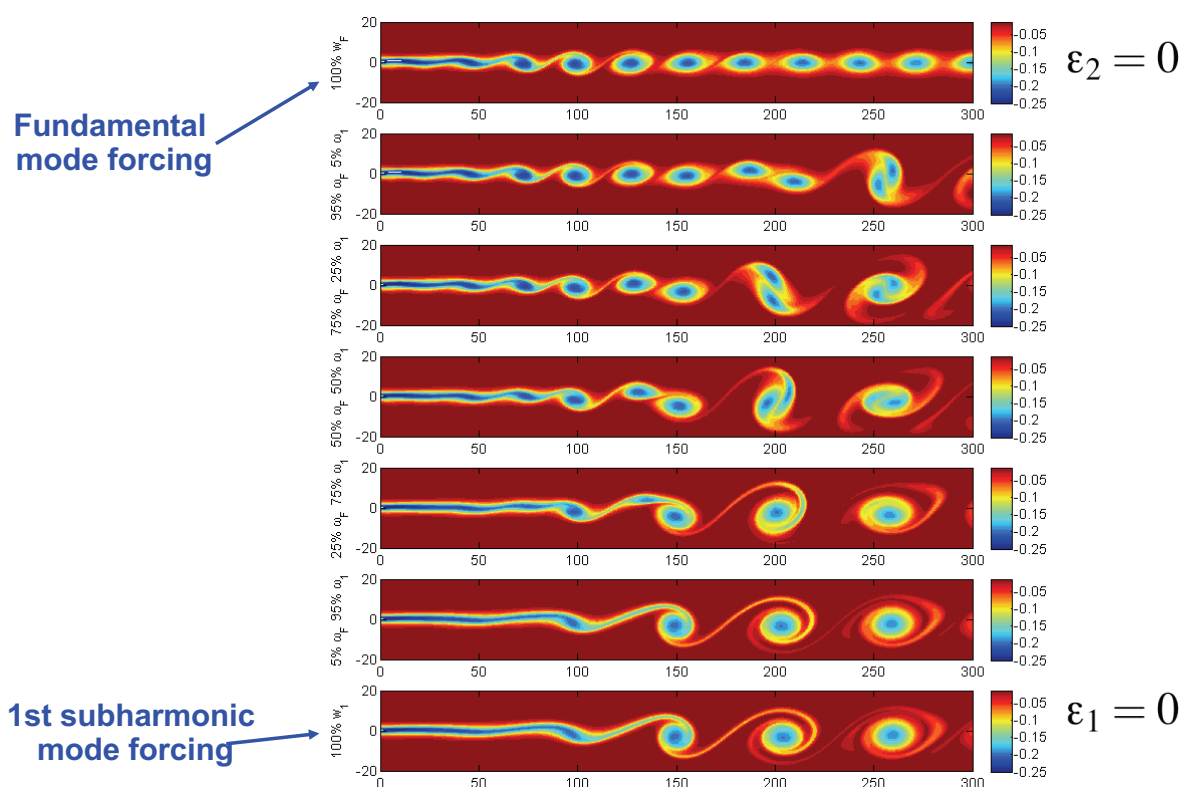
$$u_{in}(y, t) = \bar{u}_{in}(y) + \sum_{i=1}^N \epsilon_i [f(y) \sin(\omega_i t) + \gamma_i]$$

$$v_{in}(y, t) = \bar{v}_{in}(y) + \sum_{i=1}^N \frac{\epsilon_i}{i} [g(y) \sin(\omega_i t) + \gamma_i]$$

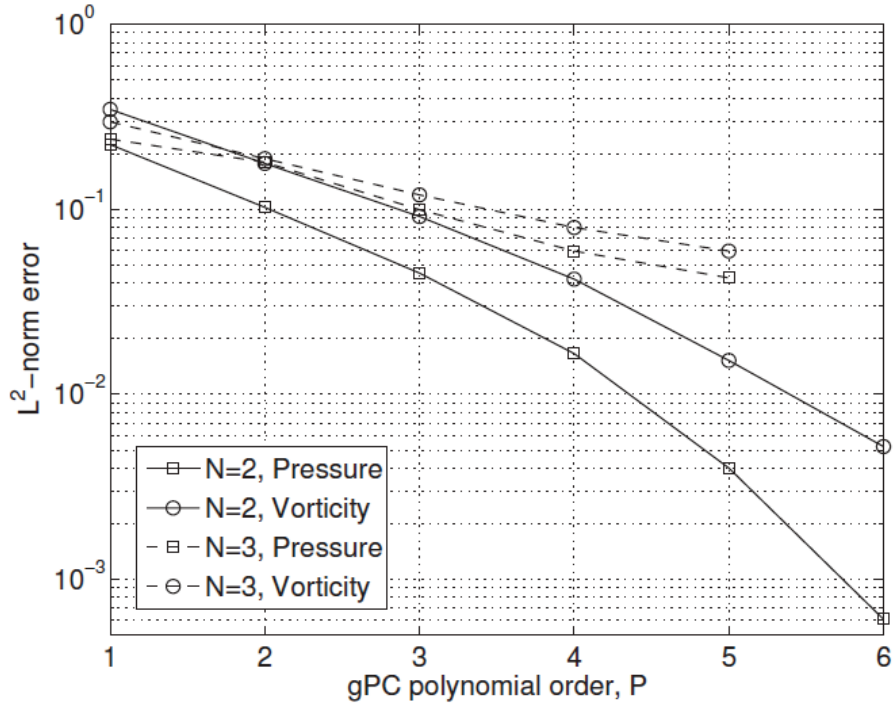
Present results: $N = 2 \quad \epsilon_1 + \epsilon_2 = U/10$

[Ko, Lucor, Sagaut, *Phys. Fluids*, 2008]

Deterministic solutions



NI-gPC expansion convergence

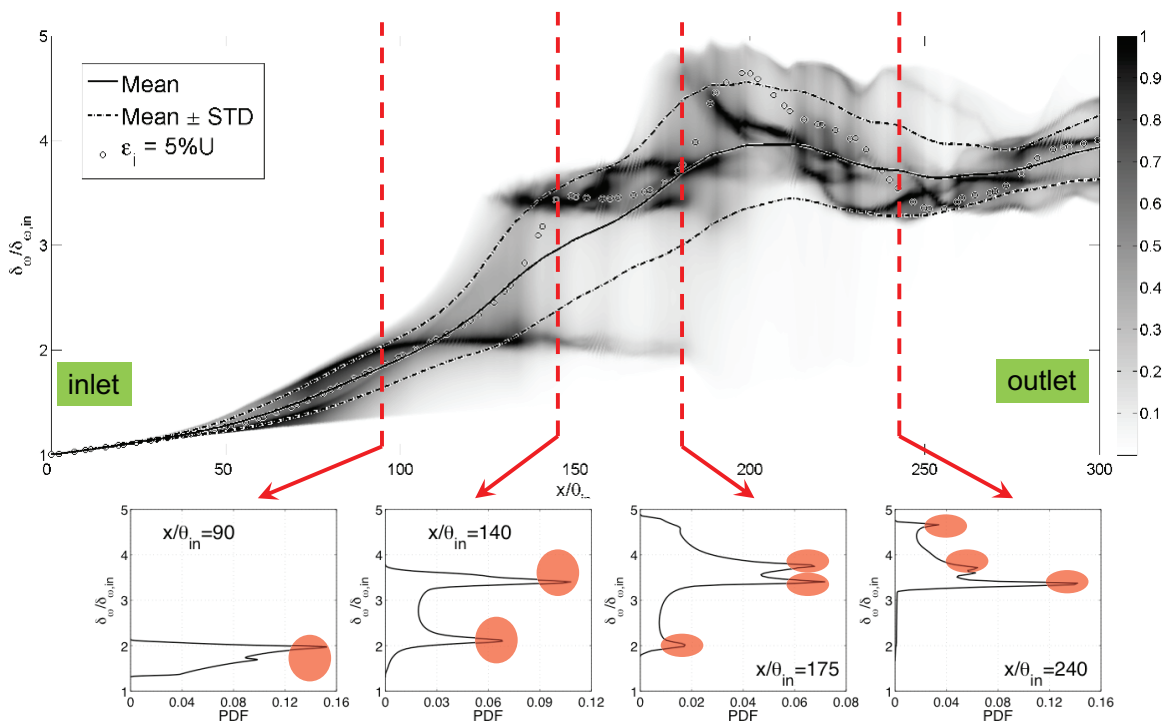


→ Pseudo-spectral convergence obtained

Stochastic analysis

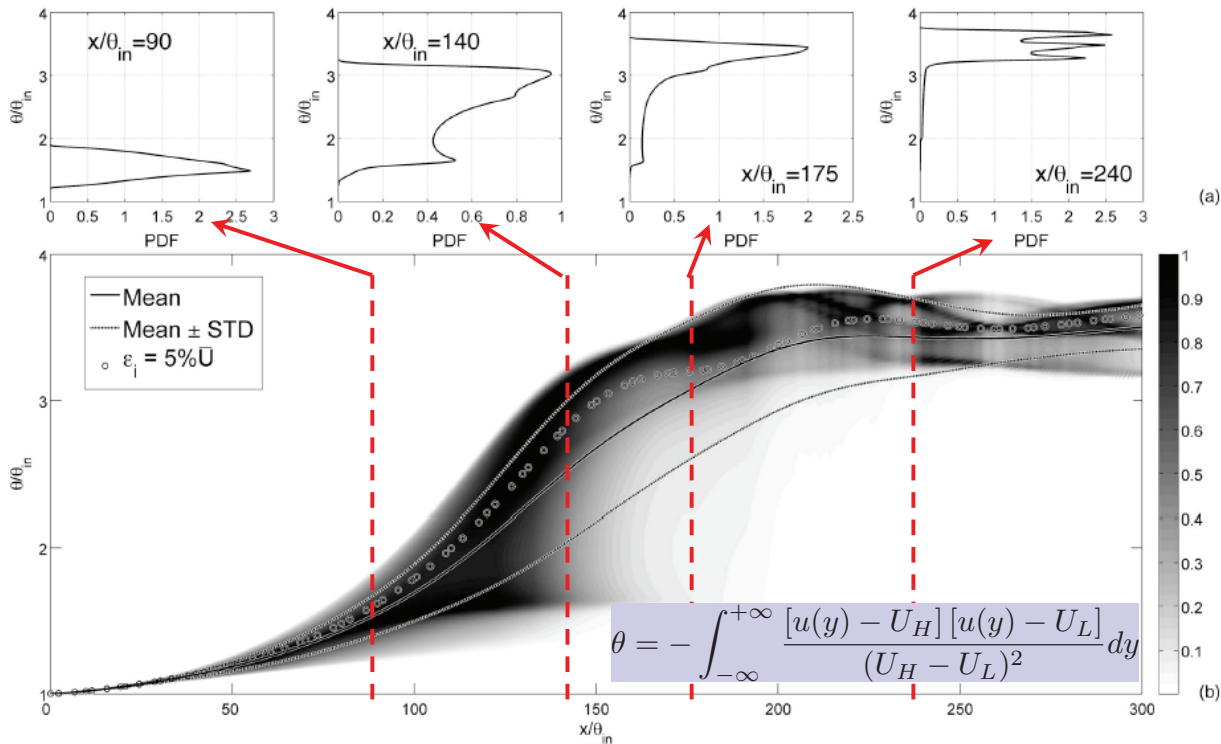
$$\delta_\omega = \frac{(U_H - UL)}{[\delta u(y)/\delta y]_{max}}$$

PDF of vorticity thickness of time-averaged flow



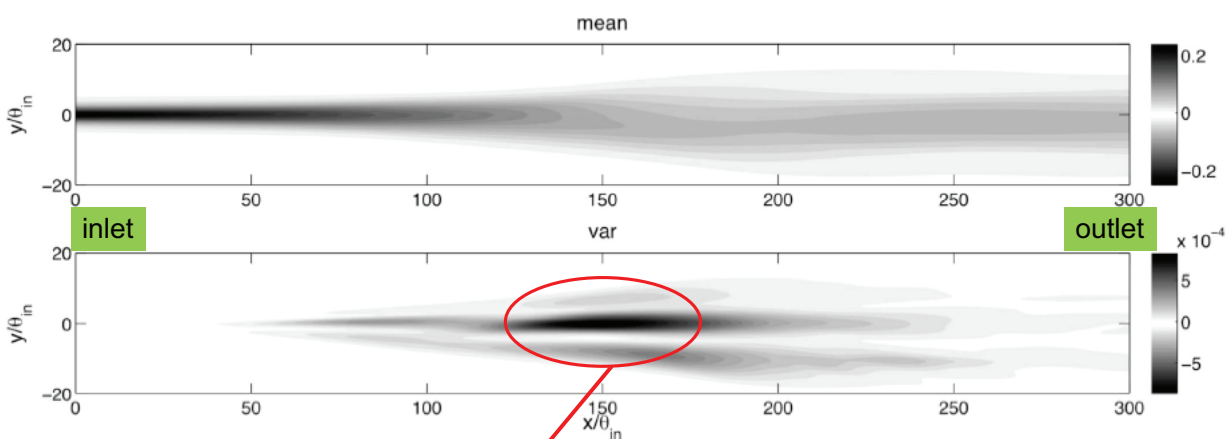
Stochastic analysis

PDF of momentum thickness of time-averaged flow



Stochastic analysis

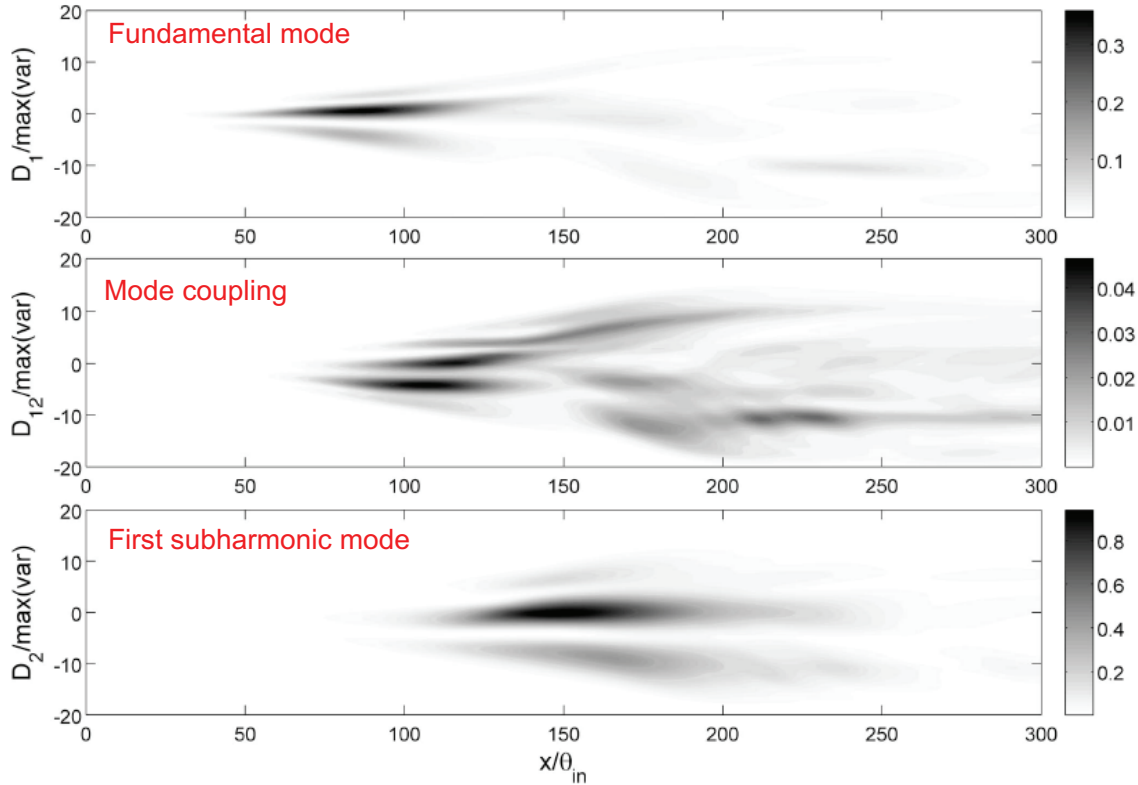
Mean vorticity and variance of mean vorticity



Strong variability due to vortex pairing mechanism

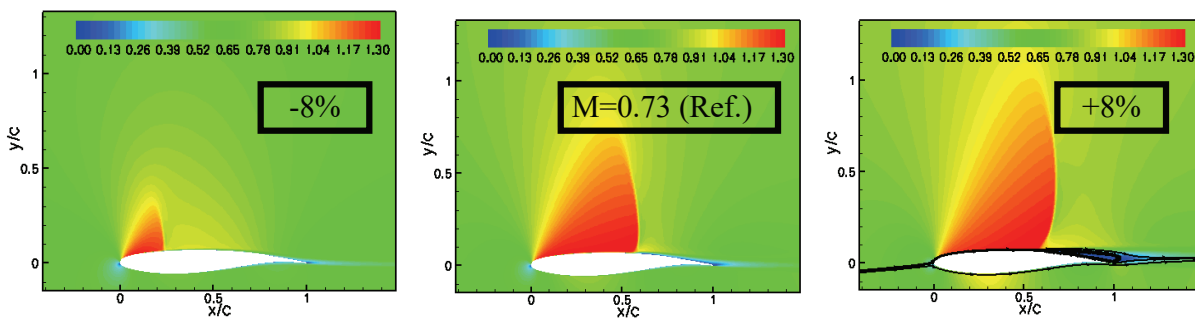
Stochastic analysis

Partial variance of mean vorticity



Stochastic flow around OAT15A airfoil

Deterministic solutions



Case study:

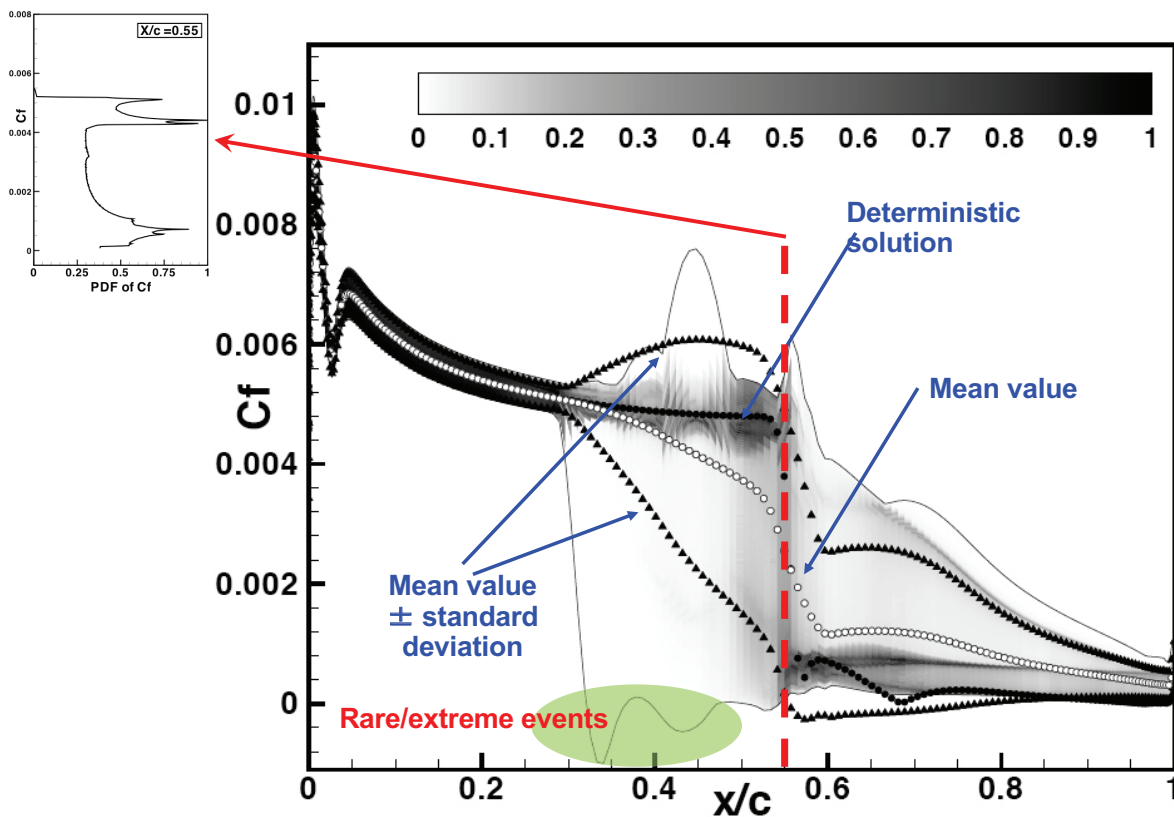
- Mach = $0.73 \pm 5\%$
- angle of attack = $2.5^\circ \pm 20\%$

Key physical mechanisms:

- $M_\infty < 0.73$: shock displacement
- $M_\infty > 0.73$ boundary layer separation

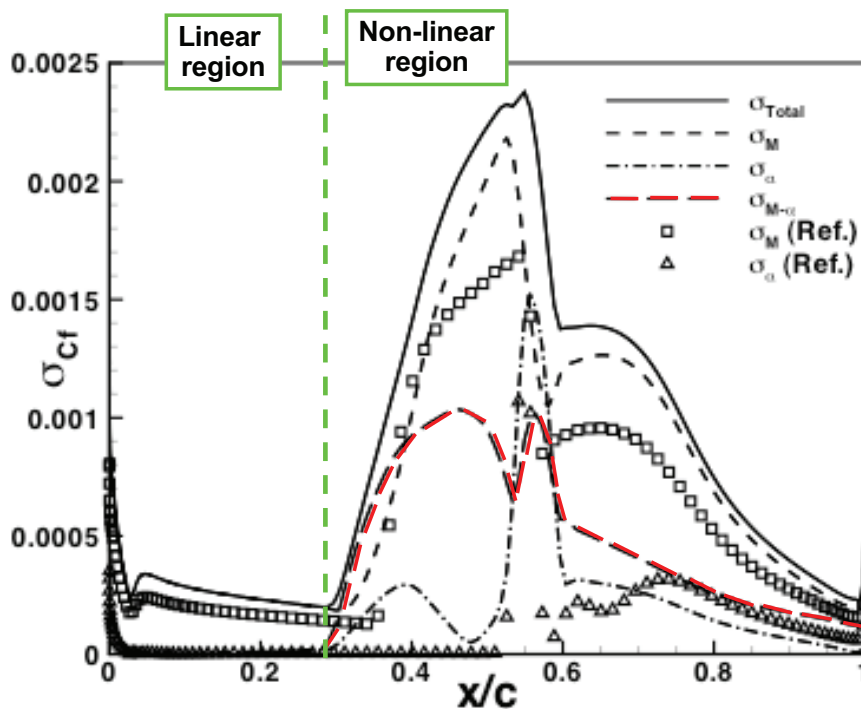
[Simon et al., CMAME, 2010]

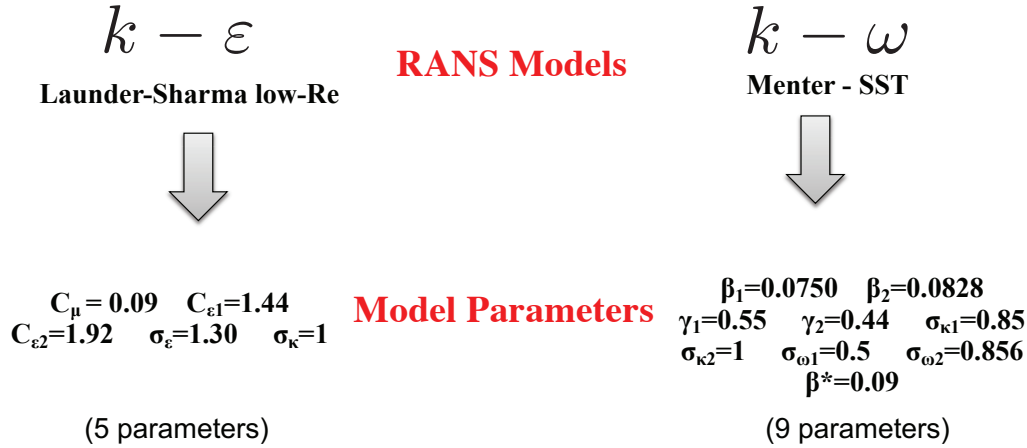
PDF of skin friction



Stochastic non-linearities

Non-linear sensitivity/coupling analysis via Sobol coefficients





Classical set of 3 canonical turbulent flows

- freely decaying homogeneous isotropic turbulence
- homogeneous shear flow in the asymptotic regime
- boundary layer in the logarithmic region

[Margheri et al., C&F, 2014]

K-ε Launder-Sharma		Menter K-ω SST	
$C_\mu \left(\frac{\kappa_{log}}{u_\tau^2} \right)$	$C_\mu = \left(\frac{\kappa_{log}}{u_\tau^2} \right)^{-2}$	$\beta^* \left(\frac{\kappa_{log}}{u_\tau^2} \right)$	$\beta^* = \left(\frac{\kappa_{log}}{u_\tau^2} \right)^{-2}$
$C_{\varepsilon 1} \left(n, \frac{P}{\varepsilon} \right)$	$C_{\varepsilon 1} = \frac{C_{\varepsilon 2} - 1}{\frac{P}{\varepsilon}} + 1$	$a_1 \left(\frac{\kappa_{log}}{u_\tau^2} \right)$	$a_1 = \left(\frac{\kappa_{log}}{u_\tau^2} \right)^{-1}$
$C_{\varepsilon 2} (n)$	$C_{\varepsilon 2} = 1 - \frac{1}{n}$	$\beta_1 \left(n, \frac{\kappa_{log}}{u_\tau^2} \right)$	$\beta_1 = -\frac{\beta^*}{n}$
$\sigma_\varepsilon \left(n, \frac{P}{\varepsilon}, \kappa_{VK}, \frac{\kappa_{log}}{u_\tau^2} \right)$	$\sigma_\varepsilon = \frac{\kappa_{VK}^2}{\sqrt{C_\mu} (C_{\varepsilon 2} - C_{\varepsilon 1})}$	$\gamma_1 \left(n, \frac{P}{\varepsilon}, \frac{\kappa_{log}}{u_\tau^2} \right)$	$\gamma_1 = \frac{\beta_1}{\beta^* \frac{P}{\varepsilon}}$
σ_κ	$\sigma_\kappa = 1$	$\sigma_{\omega 1} \left(n, \frac{P}{\varepsilon}, \kappa_{VK}, \frac{\kappa_{log}}{u_\tau^2} \right)$	$\sigma_{\omega 1} = \frac{\sqrt{\beta^*} \left(\frac{\beta_1}{\beta^*} - \gamma_1 \right)}{\kappa_{VK}^2}$
		$\sigma_{\kappa 1} \left(n, \frac{P}{\varepsilon}, \kappa_{VK}, \frac{\kappa_{log}}{u_\tau^2} \right)$	$\sigma_{\kappa 1} = \frac{\beta^* \sigma_{\omega 1}}{\beta_1}$
		$\beta_2 \left(n, \frac{\kappa_{log}}{u_\tau^2} \right)$	$\beta_2 = -\frac{\beta^*}{n}$
		$\gamma_2 \left(n, \frac{P}{\varepsilon}, \frac{\kappa_{log}}{u_\tau^2} \right)$	$\gamma_2 = \frac{\beta_2}{\beta^* \frac{P}{\varepsilon}}$
		$\sigma_{\omega 2} \left(n, \frac{P}{\varepsilon}, \kappa_{VK}, \frac{\kappa_{log}}{u_\tau^2} \right)$	$\sigma_{\omega 2} = \frac{\sqrt{\beta^*} \left(\frac{\beta_2}{\beta^*} - \gamma_2 \right)}{\kappa_{VK}^2}$
		$\sigma_{\kappa 2}$	$\sigma_{\kappa 2} = 1$

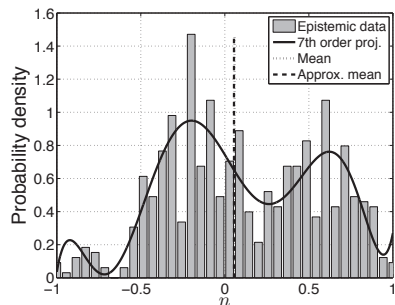
Analytical expressions depending on 4 physical parameters



Physical parameters: dispersion of reference data

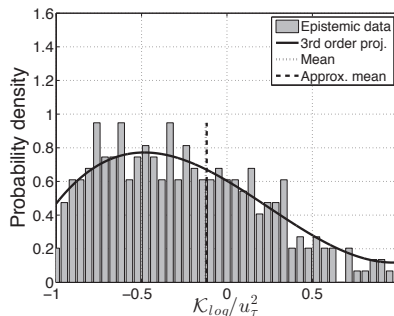
Isotropic turbulence

n



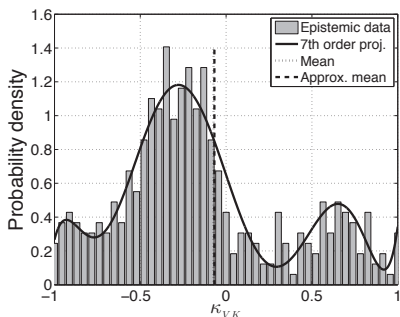
TBL

κ_{log}/u_τ^2



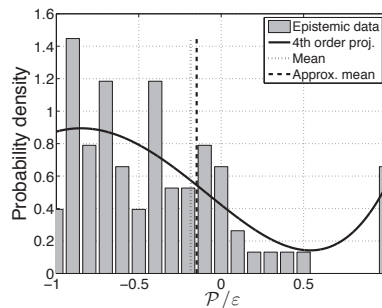
TBL

κ_{VK}



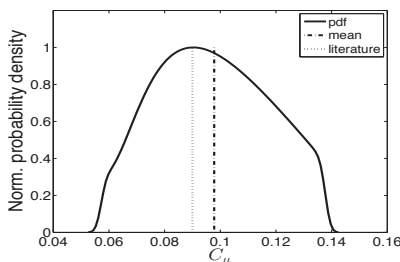
Homogeneous shear

P/ϵ

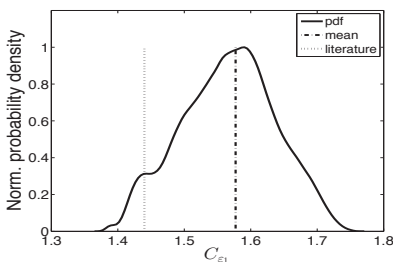


Uncertainty propagation via gPC: Launder-Sharma k-epsilon model

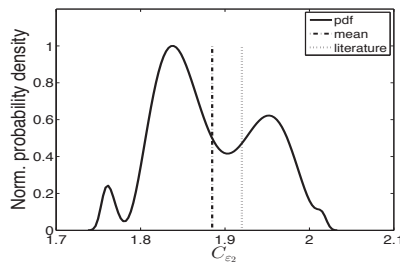
C_μ



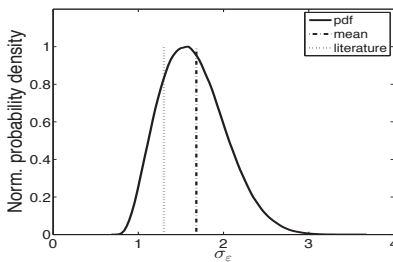
$C_{\epsilon 1}$



$C_{\epsilon 2}$



σ_ϵ

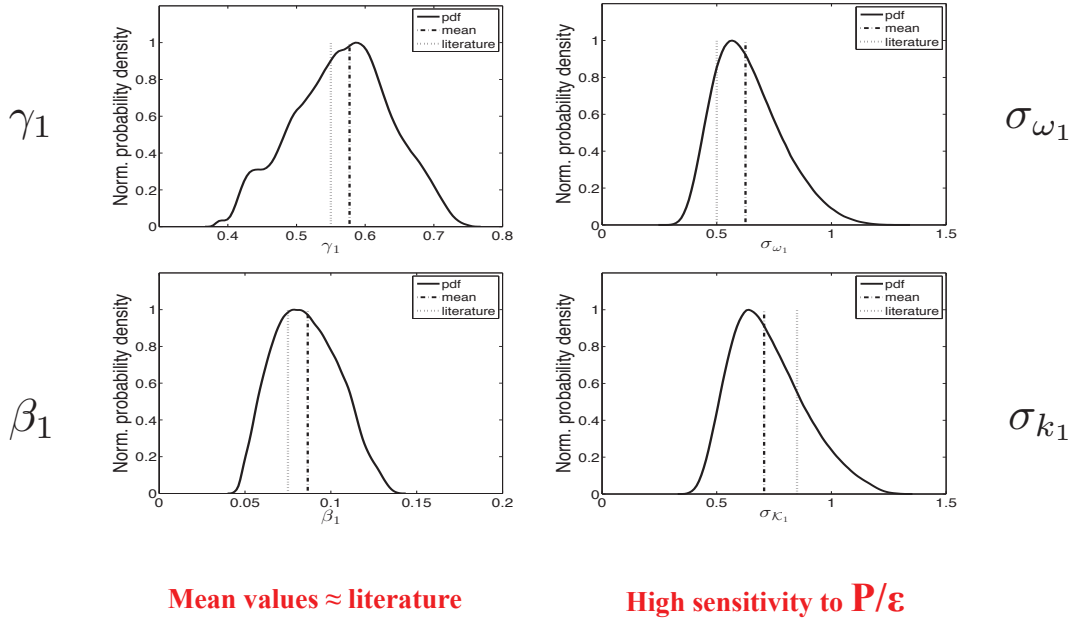


Mean value for $C_\mu \approx 0.09$

High sensitivity to P/ϵ

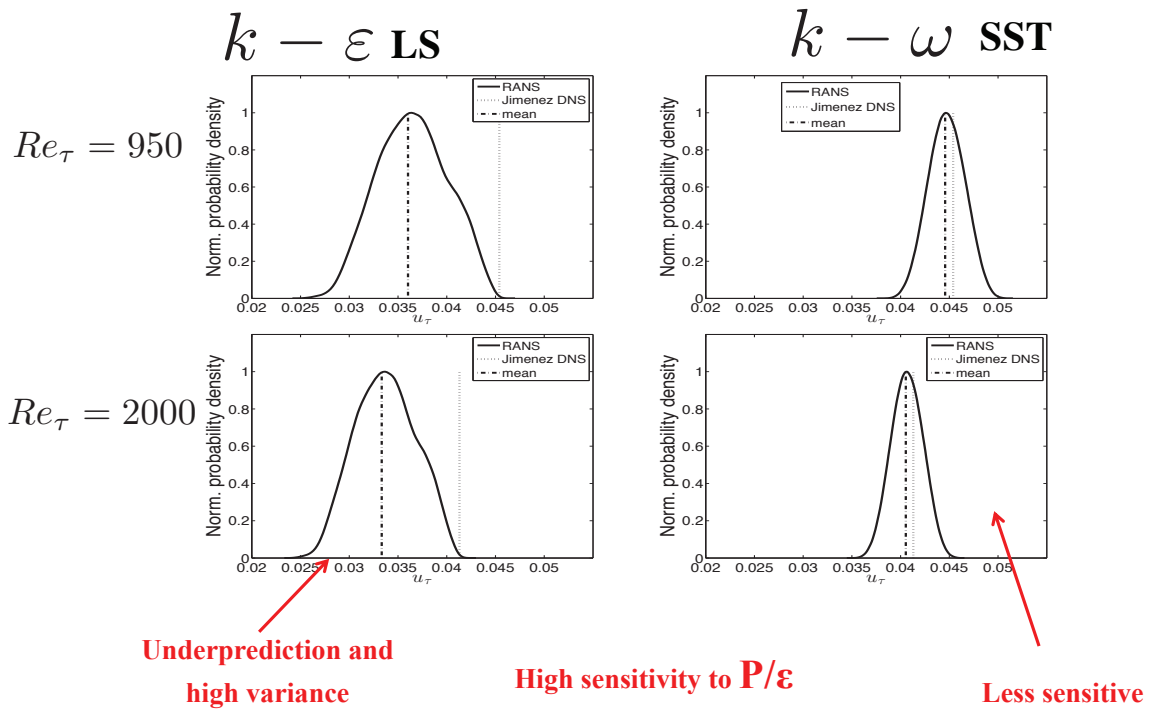


Uncertainty propagation via gPC: k- ω SST model



Simulation with uncertain RANS models

Friction velocity in turbulent plane channel

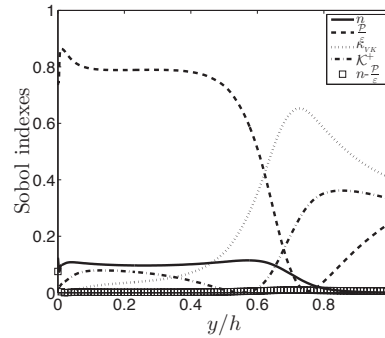
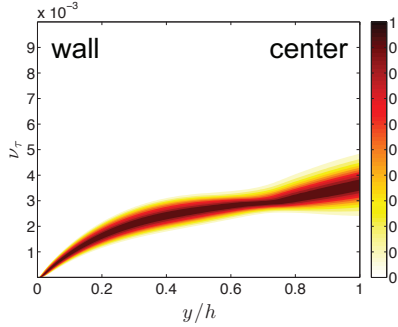




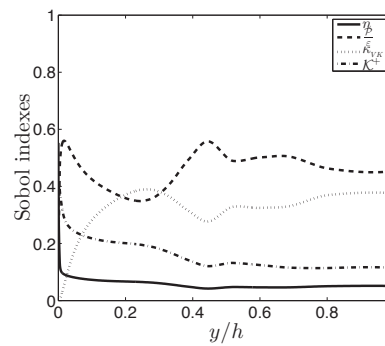
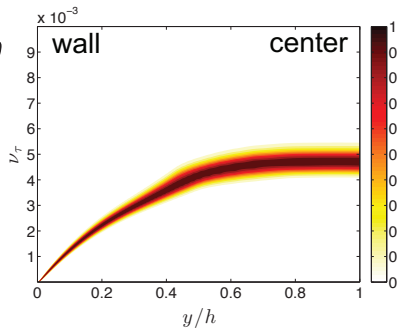
Simulation with uncertain RANS models

Eddy-viscosity profile and Sobol index profiles in a turbulent plane channel

$k - \epsilon$
LS
 $Re_\tau = 2000$



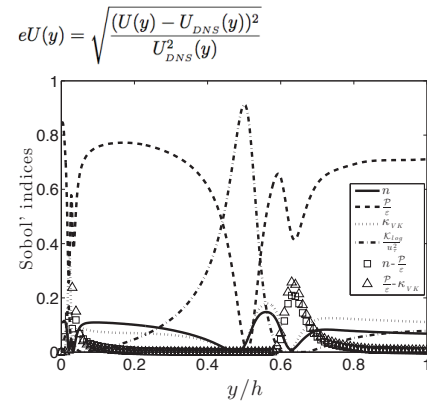
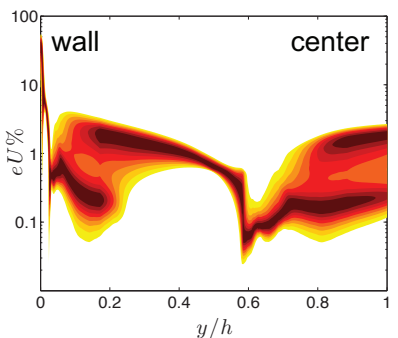
$k - \omega$
SST
 $Re_\tau = 2000$



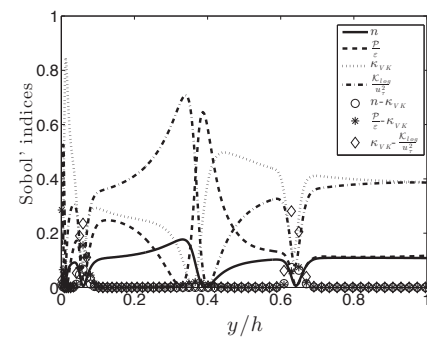
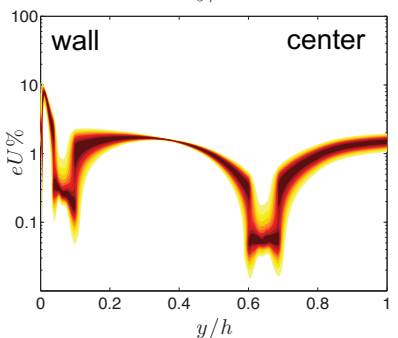
Simulation with uncertain RANS models

Velocity error profile and Sobol index profiles

$k - \epsilon$
LS
 $Re_\tau = 2000$

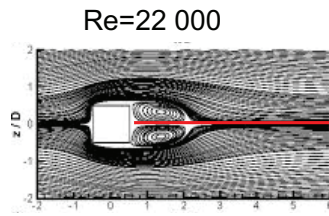


$k - \omega$
SST
 $Re_\tau = 2000$

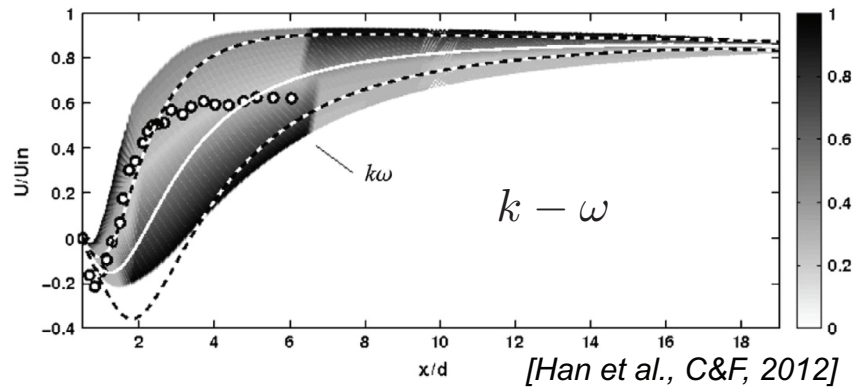
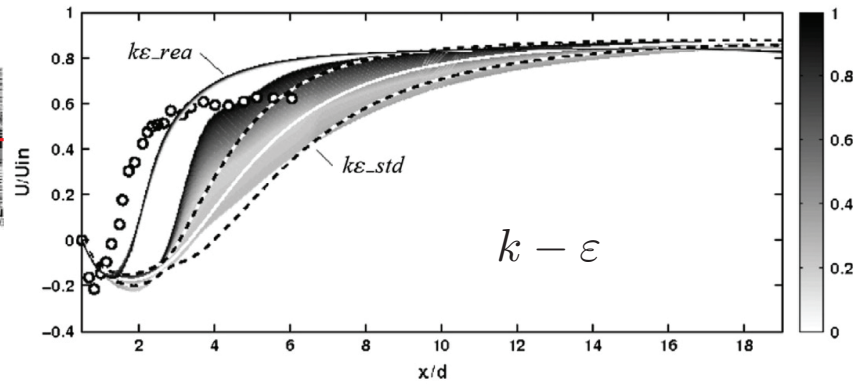


Uncertainty to inlet conditions

Uncertainty in inlet turbulence in RANS simulations

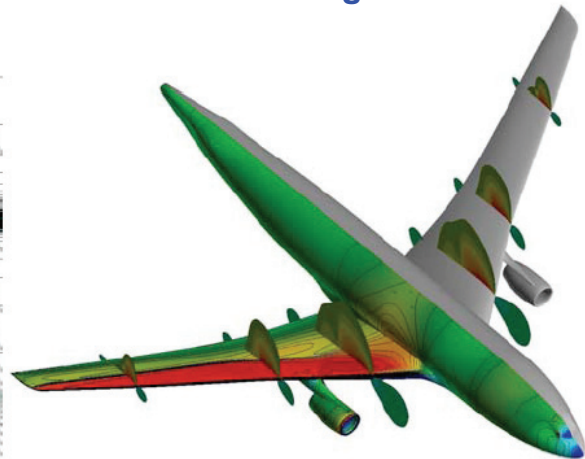
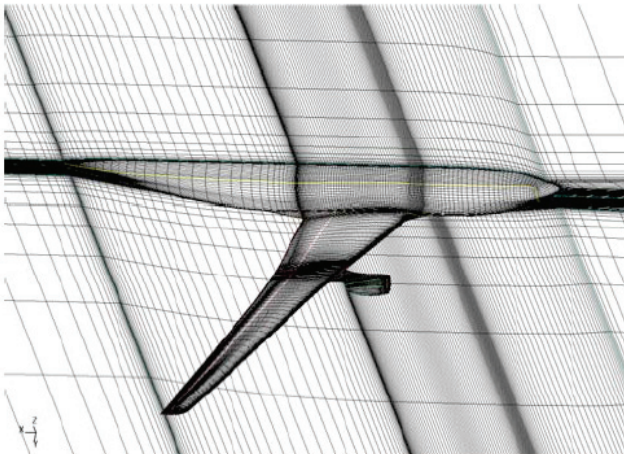


Mean velocity along wake centerline



Kriging-based shape optimization

Goal-oriented response surface building



AS28 full aircraft configuration
RANS simulation of transonic flow

48 design (uncertain) variables
Search for minimal Drag solution

[Laurenceau, PhD, 2008]

Results of optimization

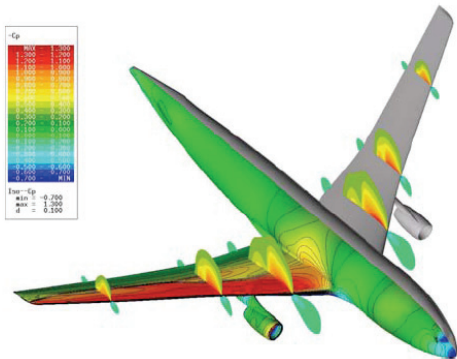
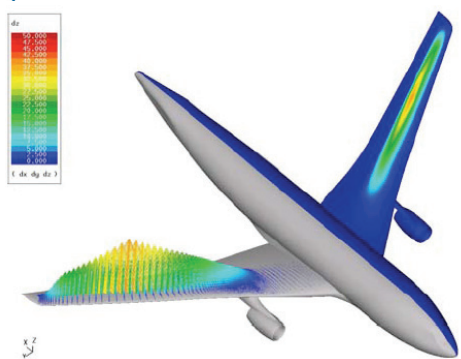
Classical optimization:
 • Adjoint-based
 • BFGS algorithm

Surrogate-based optimization:
 • Kriging-based
 • Adaptive DOE

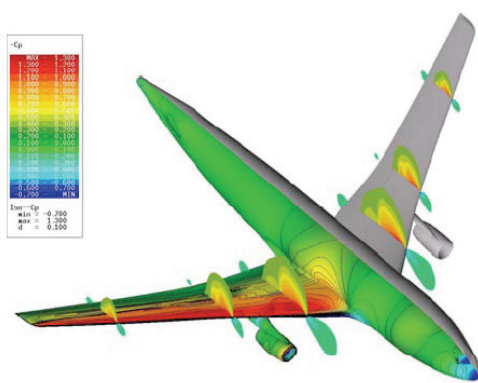
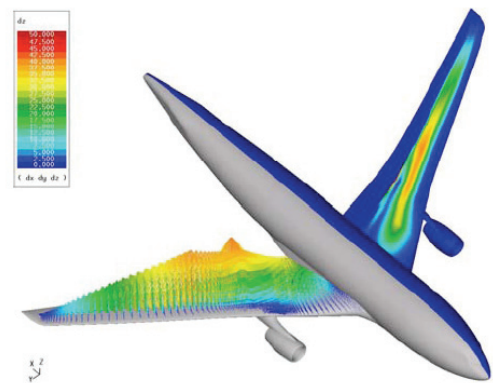
	Reference	DOT-BFGS	RS Kriging	RS Cokriging
$Cd = F$	100	96,2 (-3,8%)	97,8 (-2,2%)	95,8 (-4,2%)
Cdf	36,5	36,6	36,6	36,5
Cdp	63,5	59,6	61,5	59,3
Cdw	7,2	2,9	3,8	1,9
Cd_{vp}	19,4	19,2	21,8	22,9
Cd_i	36,9	37,5	35,9	34,6
Cl	100	101,7	99,2	96,1
$O(\Delta Cd_i)$ d� au ΔCl	0	-1	+0.5	+2.5

Surrogate-based optimization:
 • Co-Kriging-based (gradient)
 • Adaptive DOE

Optimized solutions

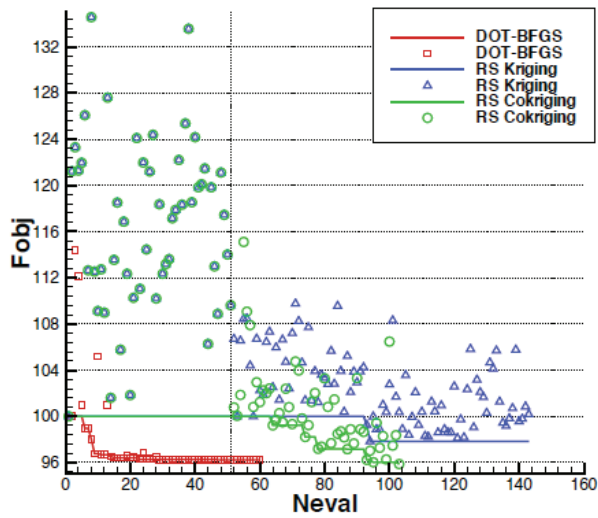


DOT-BFGS solution

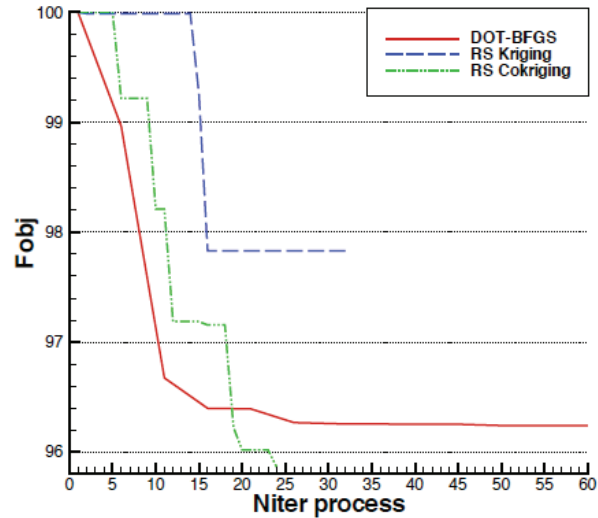


RS-CoKriging solution

Aix-Marseille universit  Convergence of optimization procedure



Cost function versus Number of evaluations



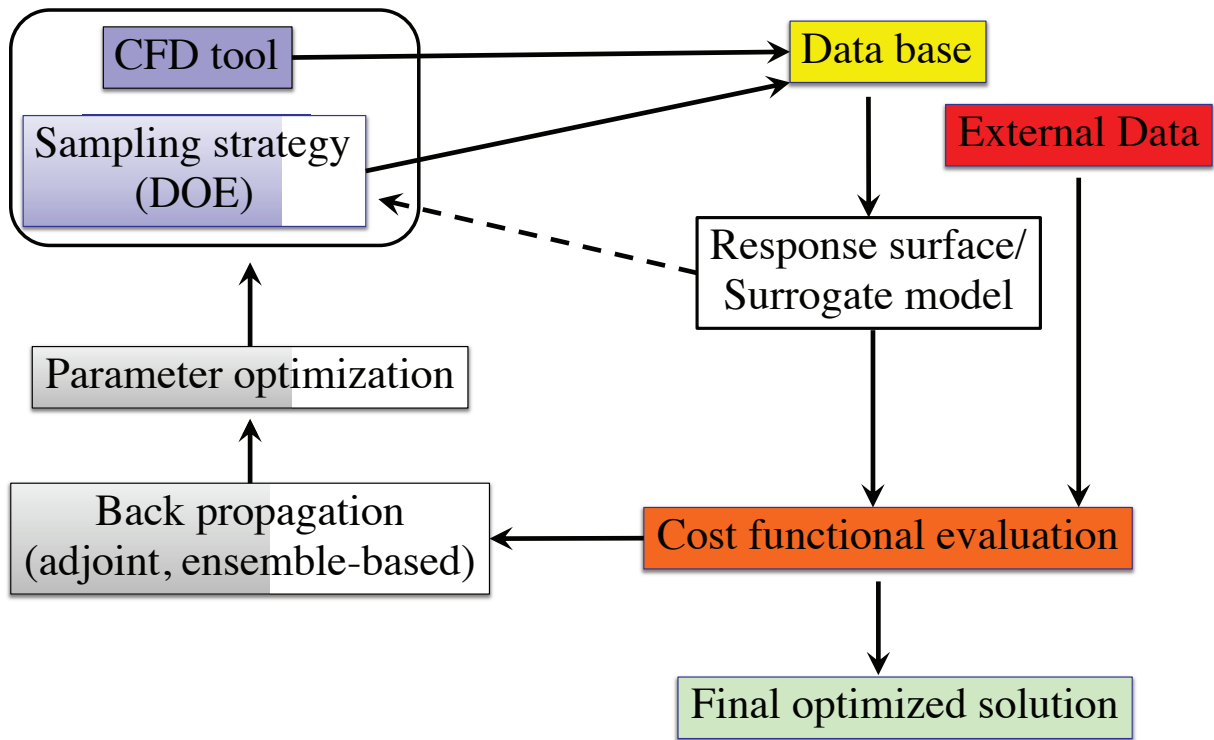
Cost function versus Number of iterations

	DOT-BFGS	RS Kriging	RS Cokriging
F^{ref}	96,2 (-3,8%)	97,8 (-2,2%)	95,8 (-4,2%)
$n_{iter} ; n_{eval} + n_{grad}; n_s^{ini}$	60 ; 60+11 ; 0	32 ; 143+0 ; 51	24 ; 103+10 ; 51

Aix-Marseille universit  Data Assimilation in turbulent flow simulations

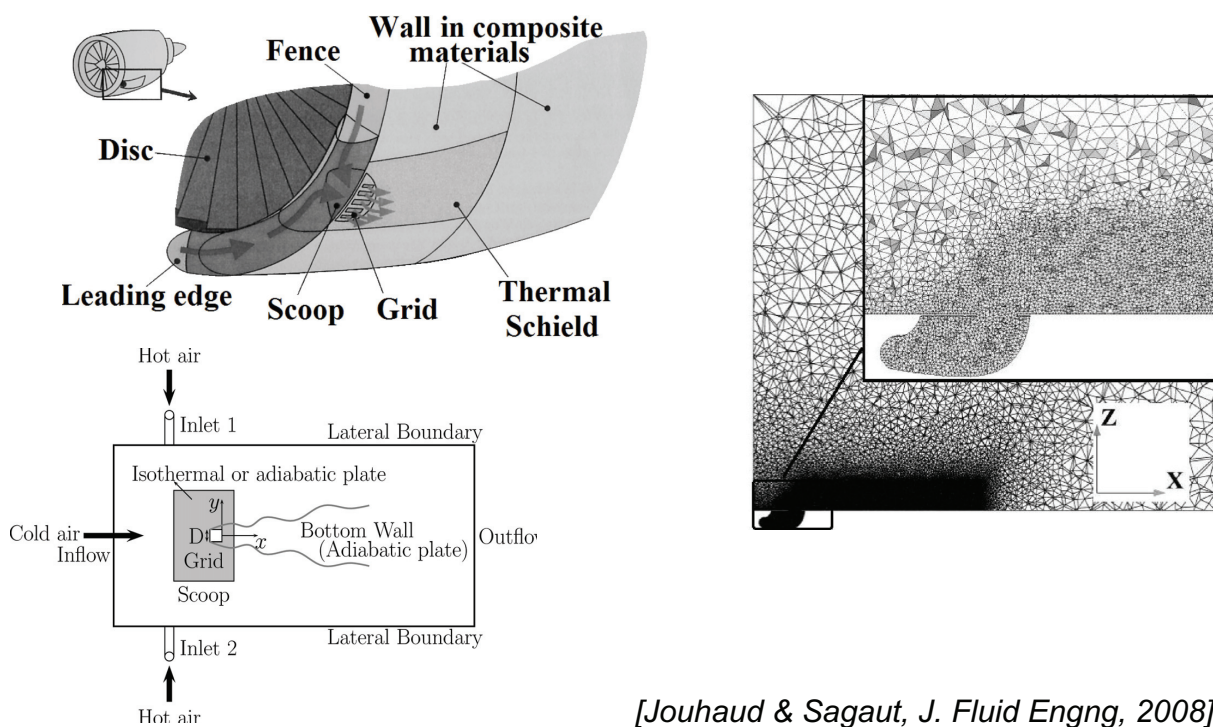
- Main types of use
 - *Calibration of free parameters*
 - *Reconstruction of initial/boundary conditions*
 - *CFD as optimal high resolution reconstruction of experiments (« CFD interpolation »)*
- Main families:
 - *Stochastic approaches: Bayesian inference, ...*
 - *Variational optimization*

Aix*Marseille universit  Typical loop for non-intrusive DA methods



Aix*Marseille universit  Optimization of LES parameters

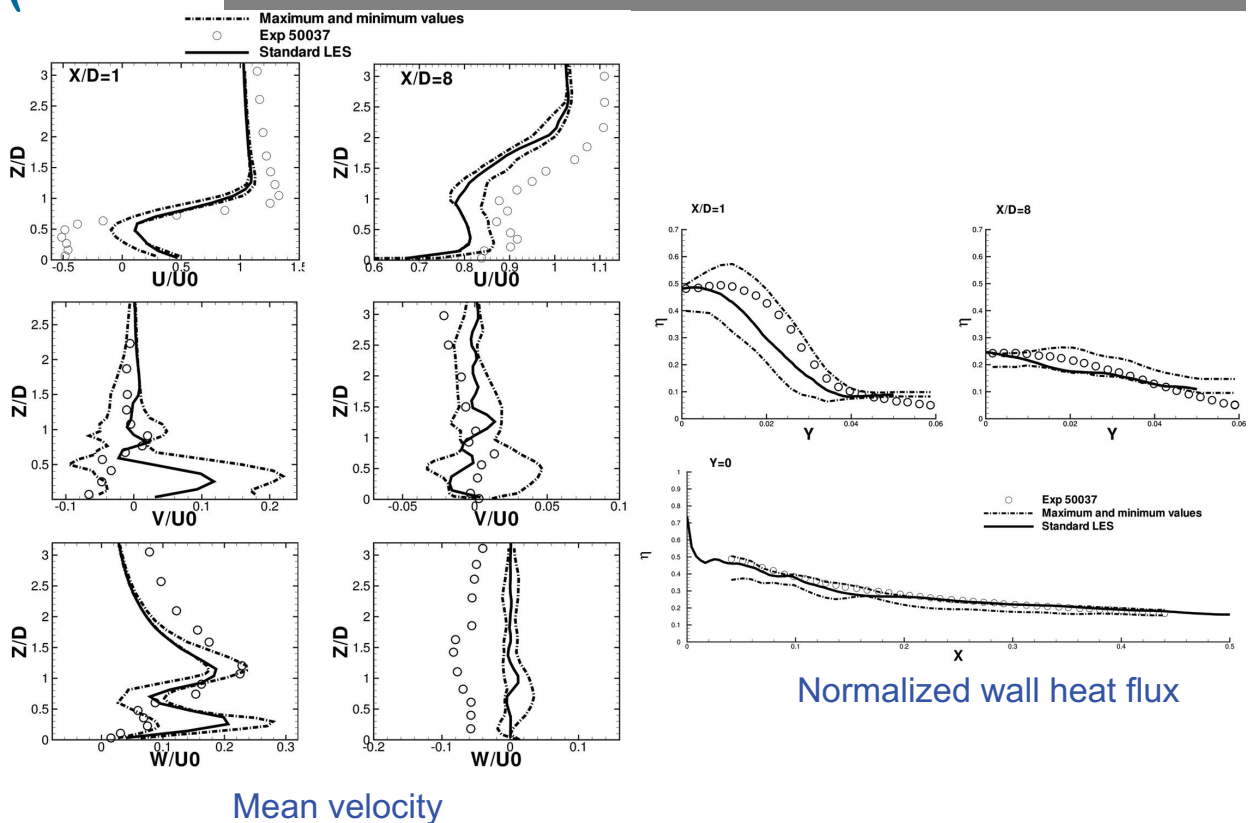
Hot jet exhaust in aircraft engine



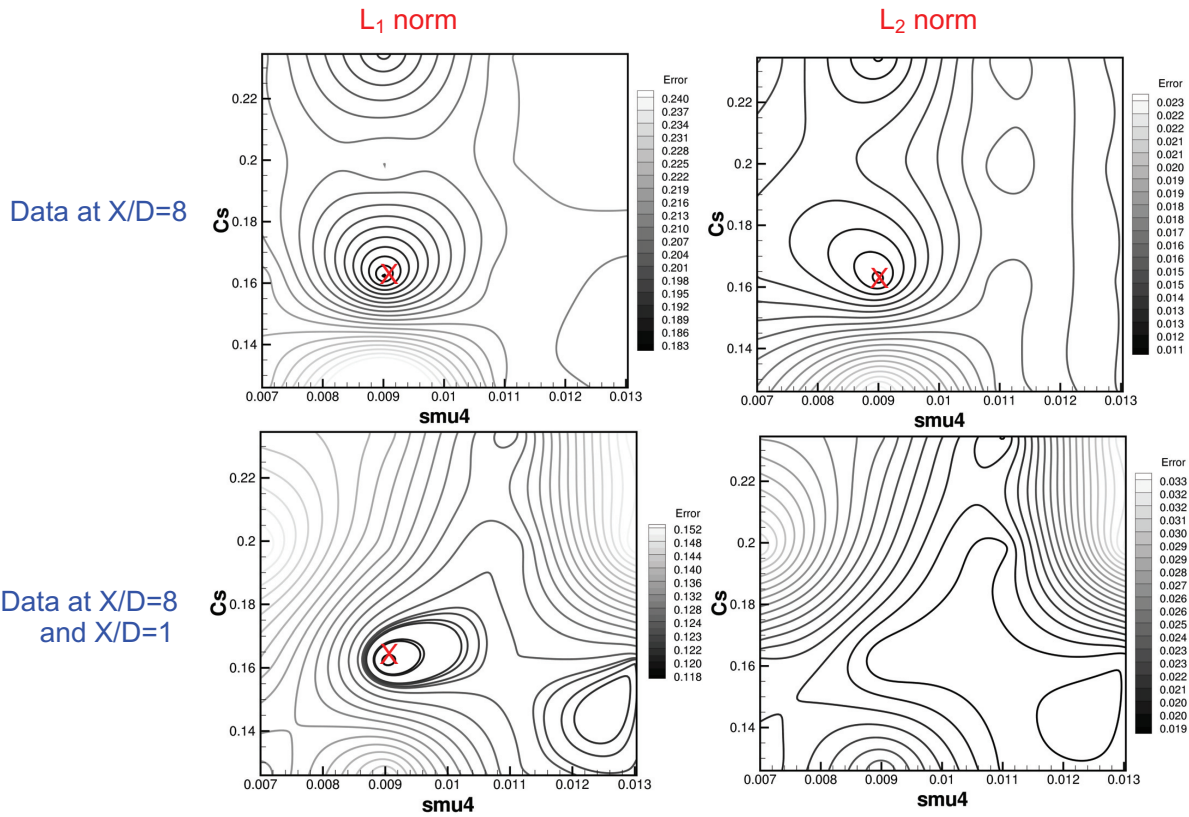
[Jouhaud & Sagaut, J. Fluid Engng, 2008]

- Implicit coupling between numerical errors and subgrid model
 - *Non-monotonous convergence vs. Grid refinement*
 - *Case-dependent optimal parameters*
- Present work:
 - *Single-grid dual optimization of:*
 - *Numerical diffusion (Jameson scheme)*
 - *Subgrid diffusion (Smagorinsky model)*
 - *Kriging-based response surface & optimization*
 - *Assimilation of experimental data:*
 - *Velocity and heat flux measurements*
 - *Variants of cost function*

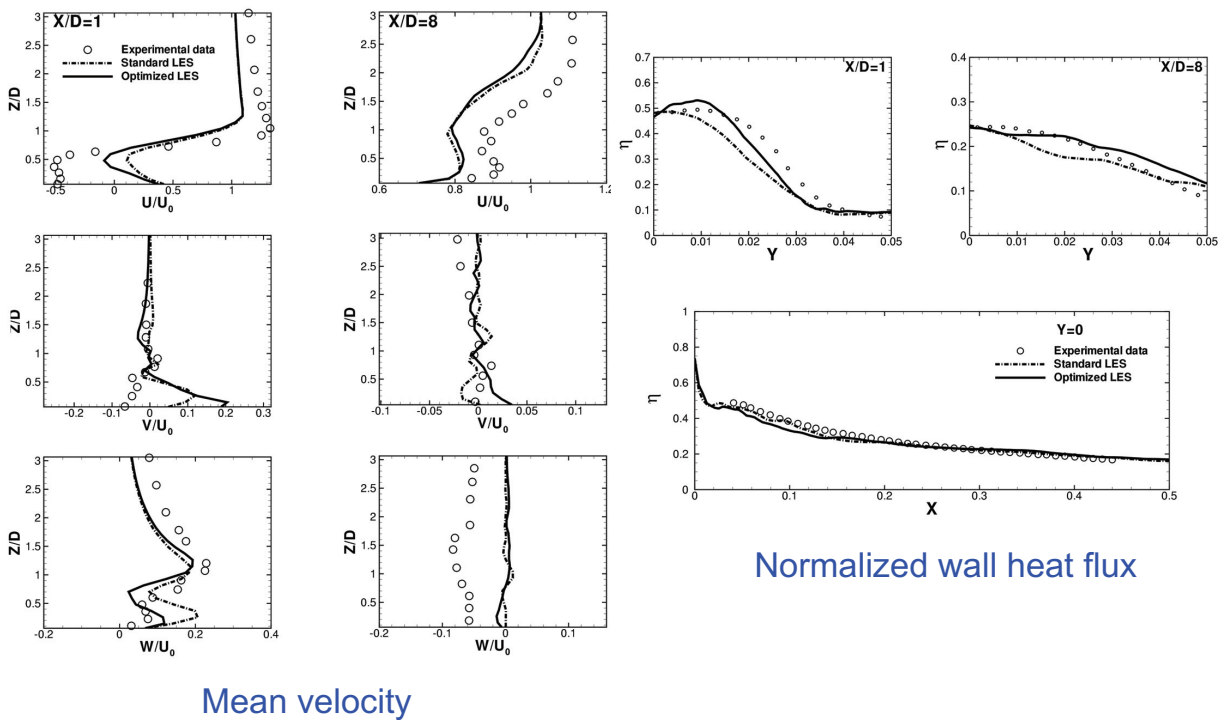
Mean flow predicted by LES



Kriging-based error map



Optimized LES



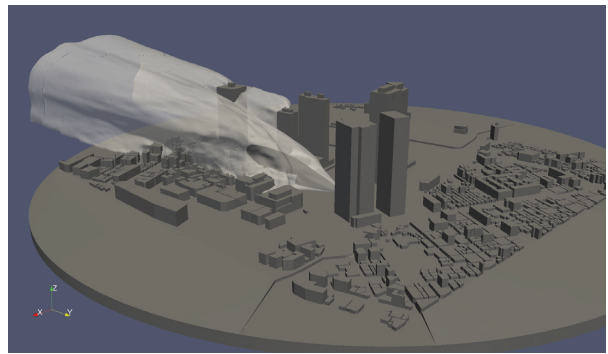
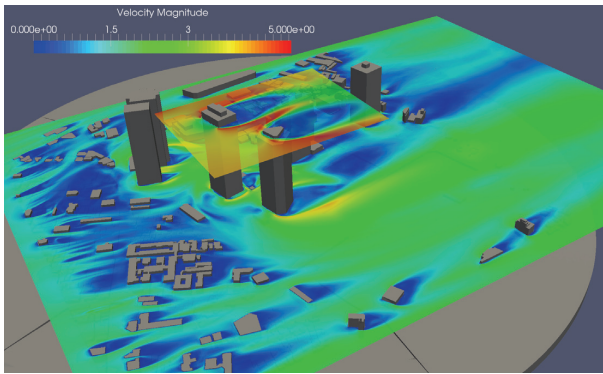
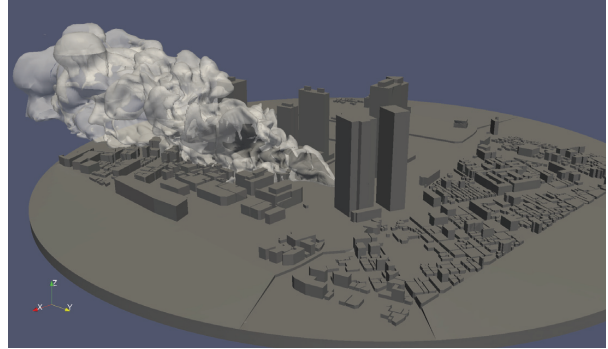
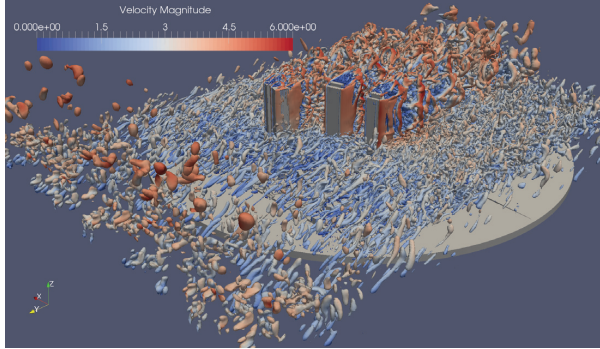
Normalized wall heat flux

Mean velocity



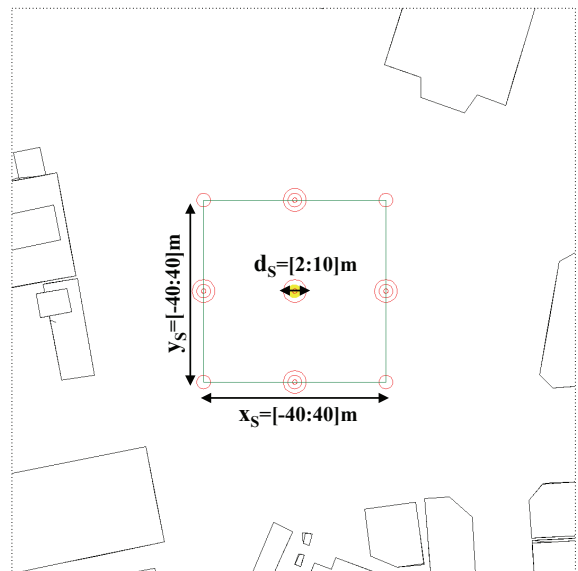
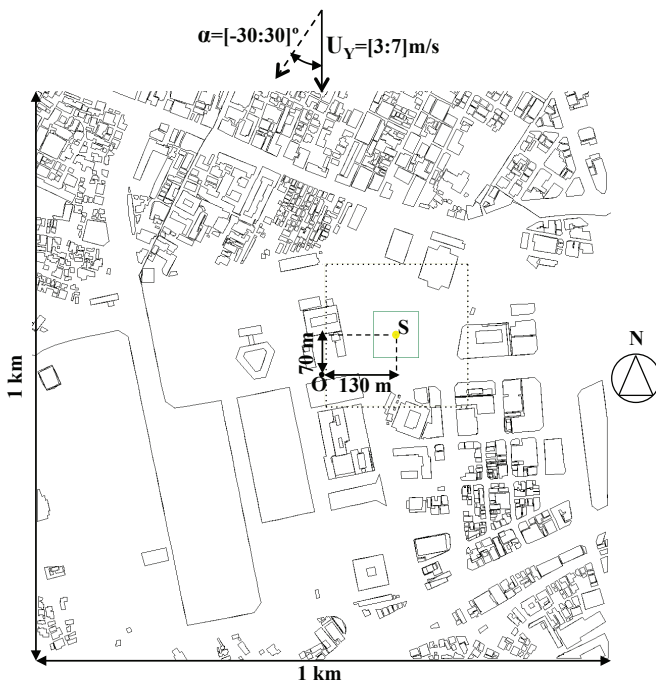
Reconstruction of physical parameters Pollutant dispersion in Shinjuku (AIJ database)

Steady scalar source on the ground



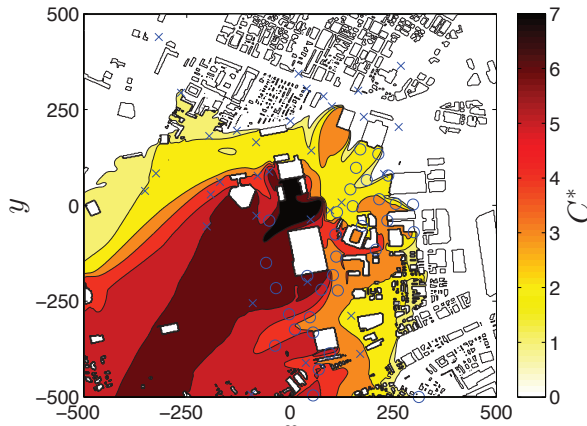
Uncertain/unknown parameters

Pollutant source : uncertain location & diameter \rightarrow 3 parameters
Wind speed and wind direction \rightarrow 2 parameters

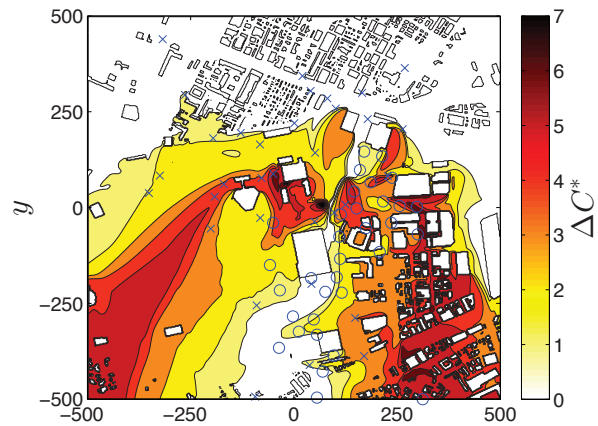


[Mons et al., JWE&IA, 2017]

DA-based reconstruction of 5 parameters



Initial guess solution



Associated error

Non-intrusive (adjoint-free) EnVar-type approach:

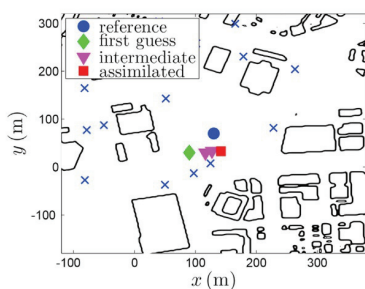
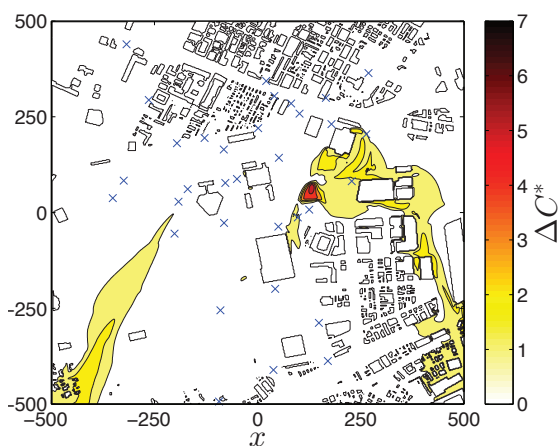
- Variational optimization
- Ensemble-based evaluation of gradient
- Direct propagation
- Optimized generation of new realizations at each iteration

[Mons et al., JCP, 2016]

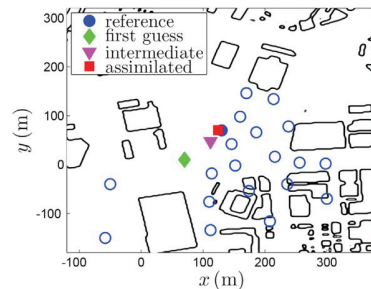
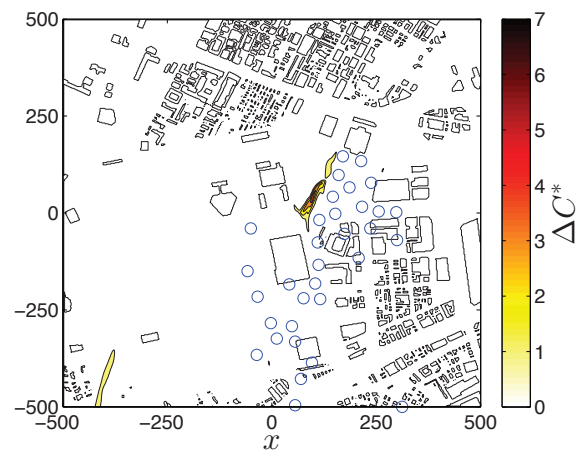
[Mons et al., JFM, 2017]

Optimized solution: error on concentration

Fixed sensor location



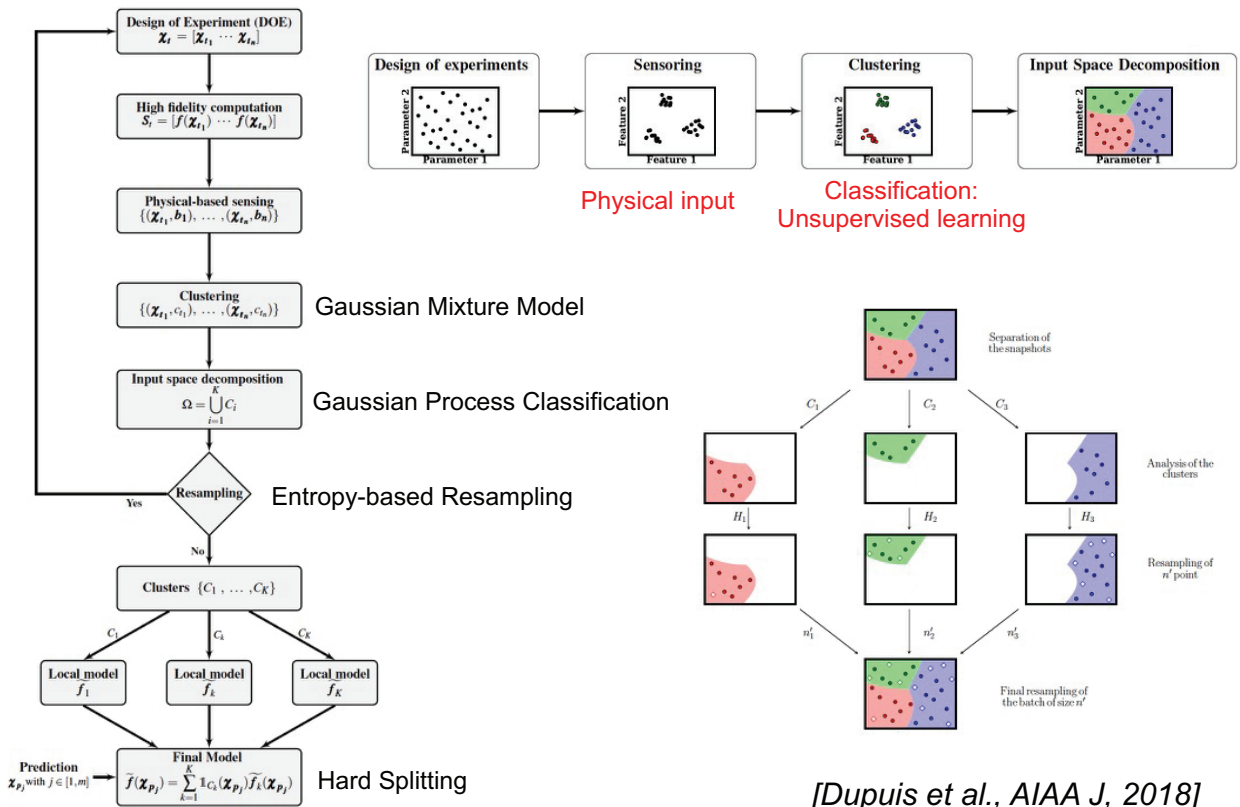
Optimal sensor location



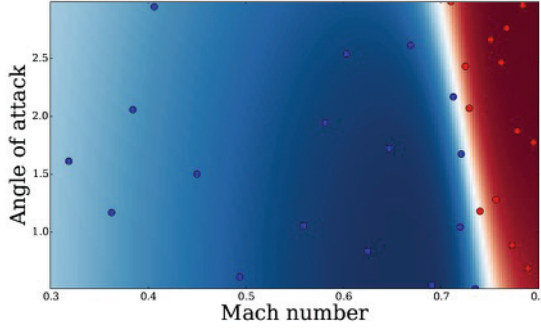
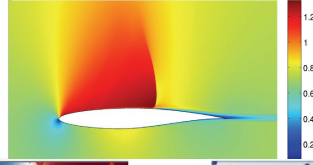
Learning-based methods for CFD

- Main types of use
 - *Improvement of classical CFD methods*
 - *Surrogate Models*
 - *Physical submodels (turbulence ...)*
 - *Physical analysis (very rare)*
 - *Direct prediction without CFD*
- Main families:
 - *Supervised learning methods*
 - *Unsupervised learning methods*

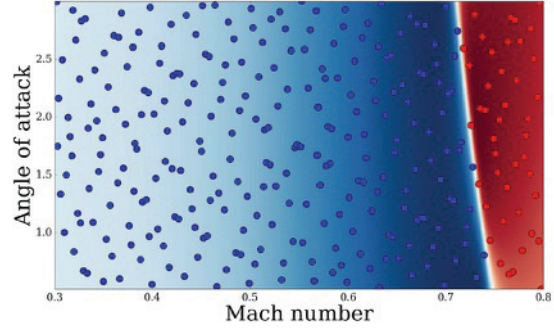
Local Decomposition Method



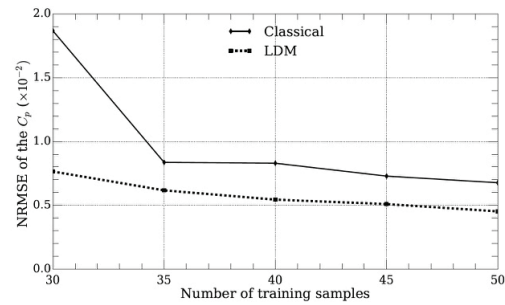
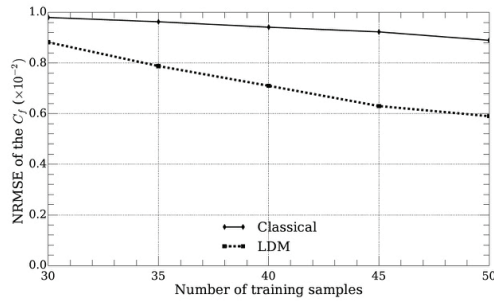
LDM for 2D transonic airfoil RAE2822



(a) Training set

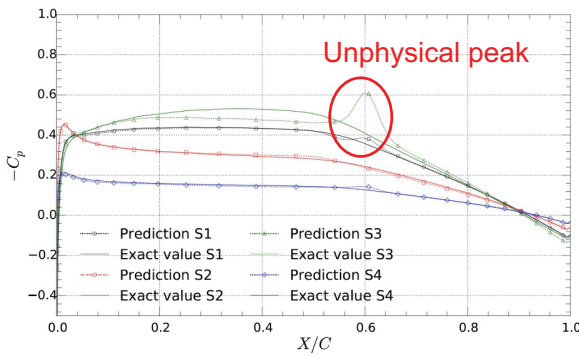


(b) Test set

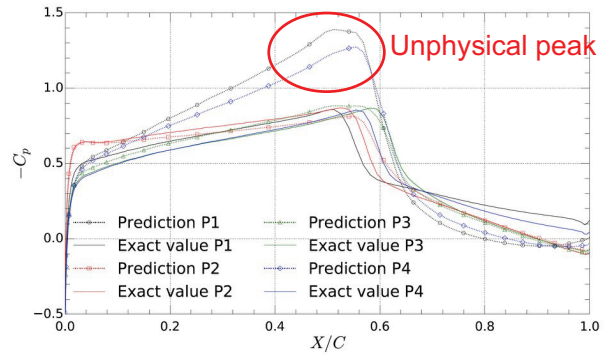


LDM for RAE2822 airfoil

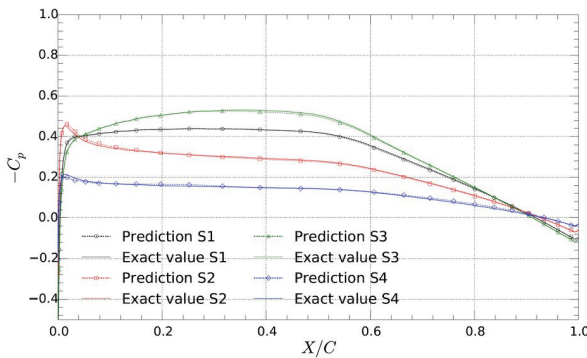
Prediction of C_p by global POD, $M < 1$



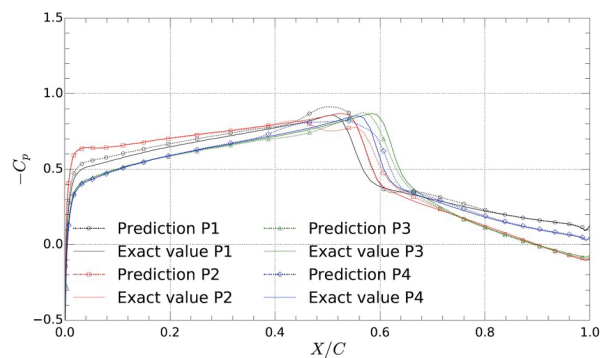
Prediction of C_p by global POD, $M > 1$



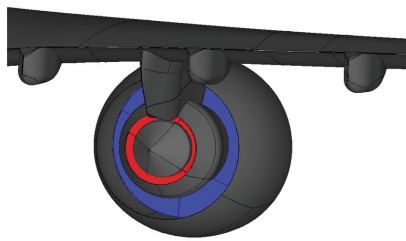
Prediction of C_p by LDM, $M < 1$



Prediction of C_p by LDM, $M > 1$



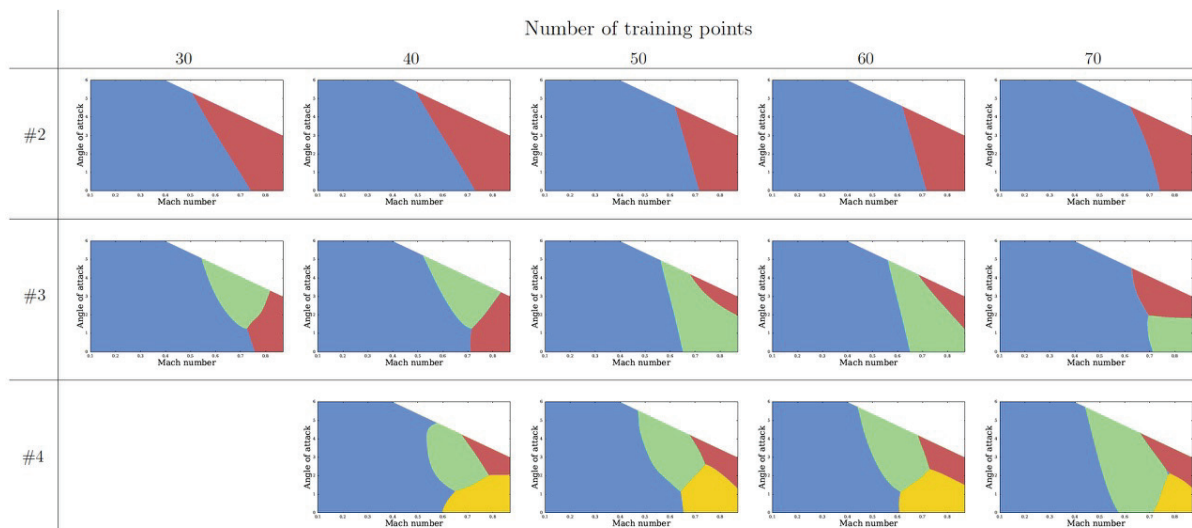
LDM for XRF1 aircraft



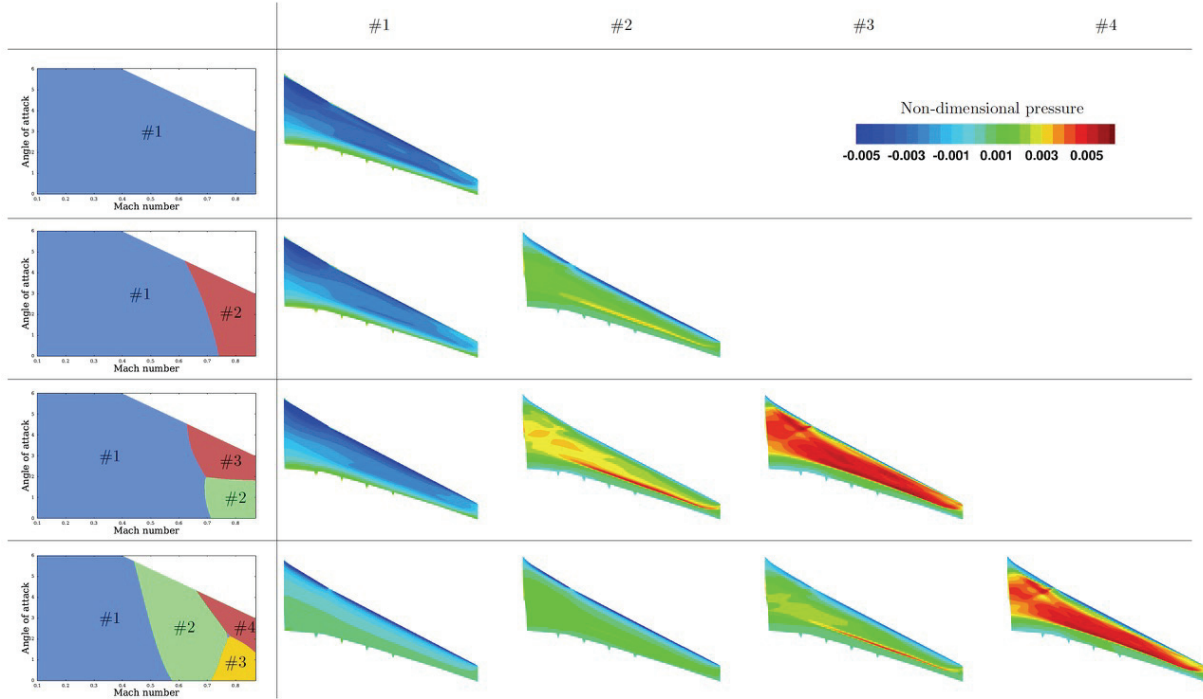
Freestream variable	Amplitude of variation
Mach number	0.1 - 0.87
Angle of attack ($^\circ$)	0.0 - 6.0
Reynolds number	$2.0 \times 10^6 - 9.5 \times 10^7$
T_t core	2.4 - 3.2
P_t core	1.0 - 1.5
T_t fan	1.0 - 1.3
P_t fan	1.0 - 1.6

LDM for XRF1 aircraft

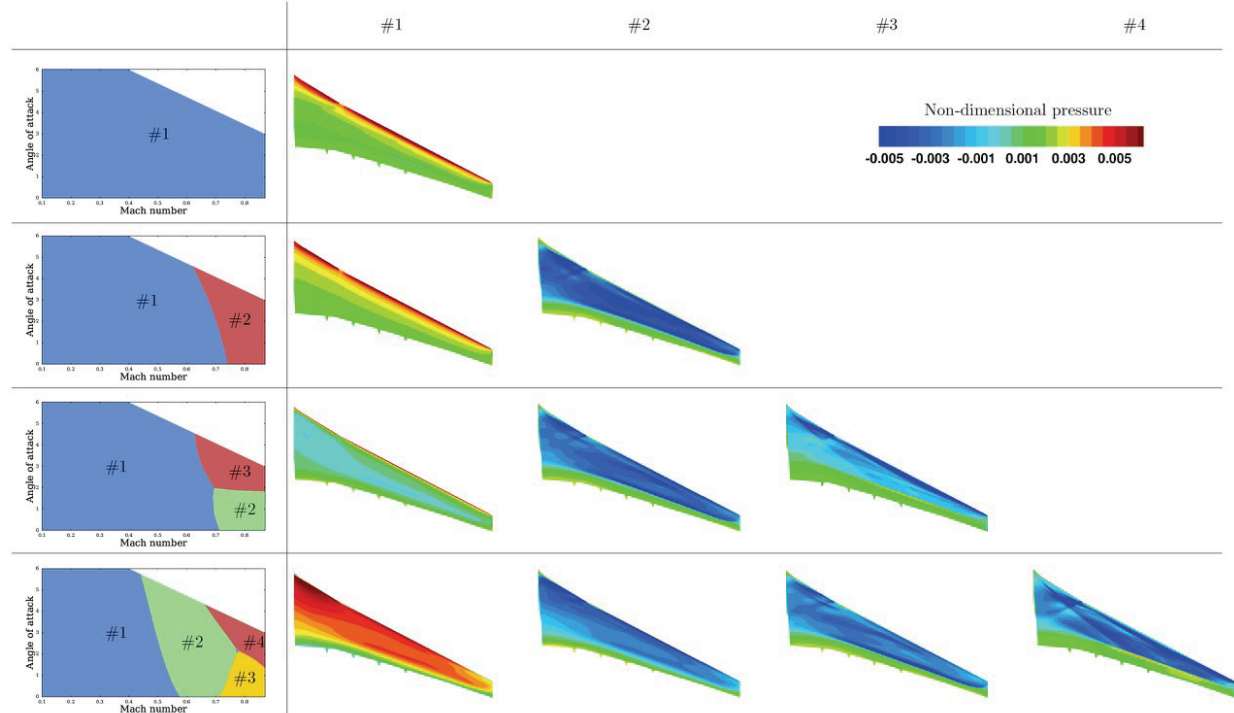
Clustering of the solution space via LDM



First pressure mode



Second pressure mode



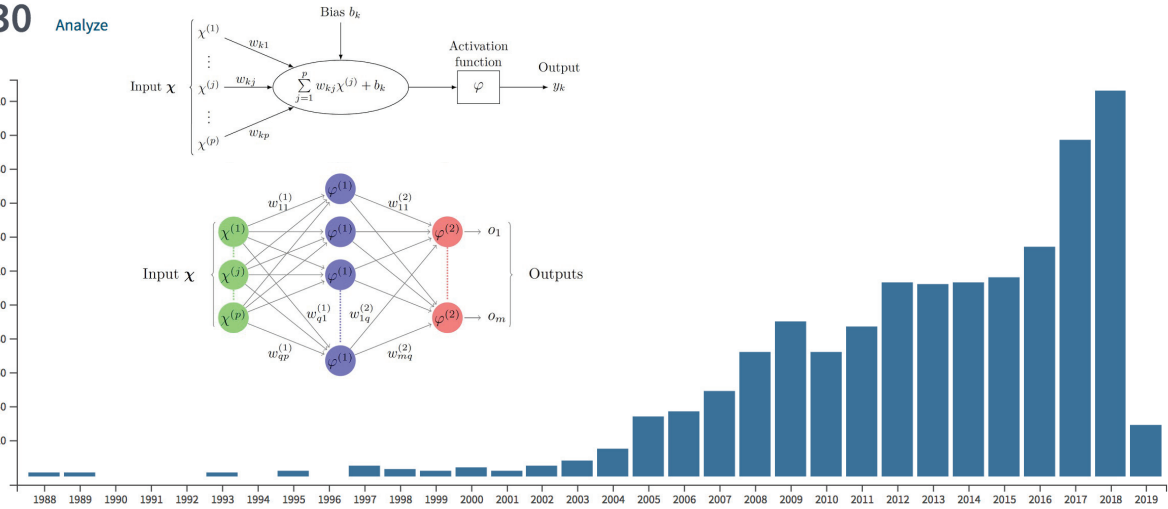


Neural Networks for CFD

Web of Science search: Fluid Mechanics + Neural Network

Total Publications

1530 Analyze



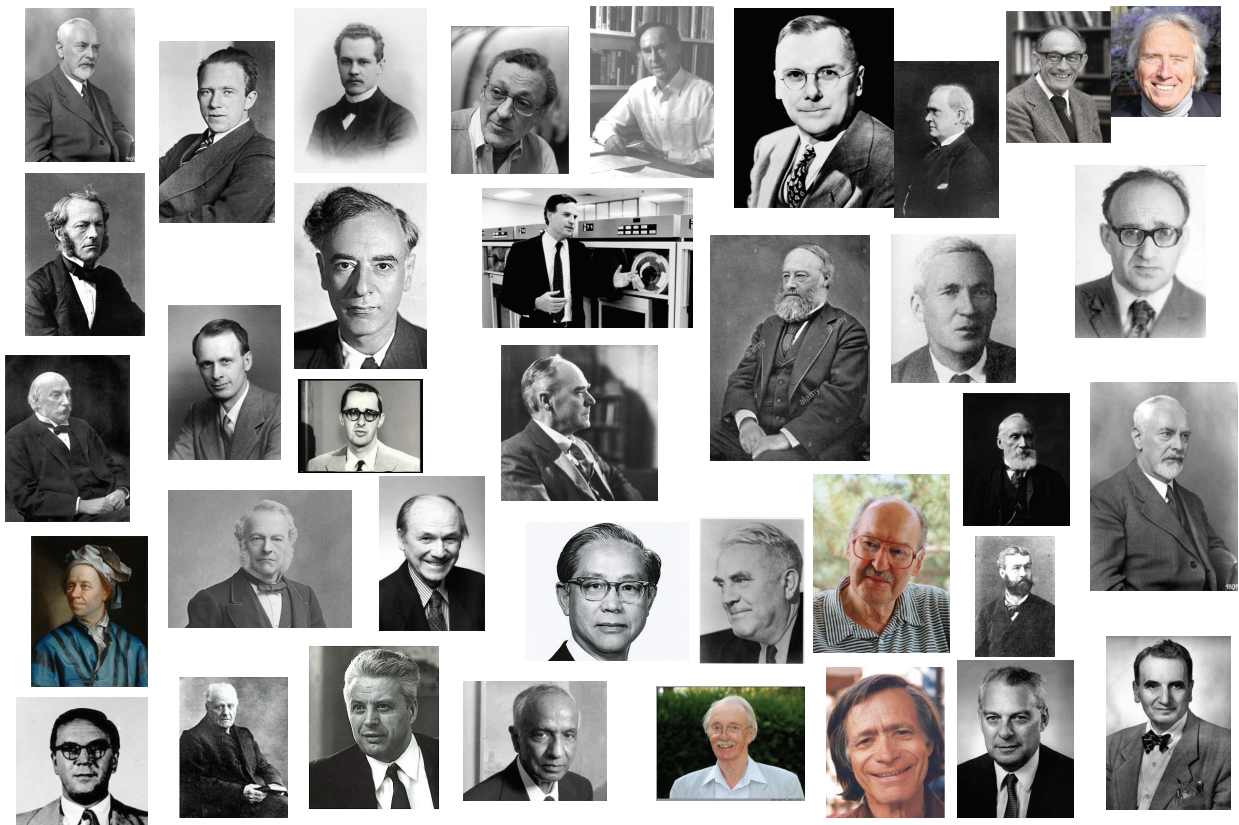
No « Deep Blue effect » in the field of turbulence research yet (*first win in 1996*)

Mostly:

- Re-tuning of existing turbulence model
- Surrogate for eddy viscosity or terms in transport equations



The historical Neural Network in turbulence research



- Uncertainty Quantification for CFD
 - *Methods already exist*
 - *Curse of Dimensionality = main problem (DOE/cost)*
 - *Foreknowledge about input uncertainties*

- Data-based Augmented CFD:
 - *Case-by-case improvement of CFD*
 - *No new turbulence model up to now*
 - *Direct prediction ? Not ready yet, e.g. Airbus' requirements :*
 - Total Drag : 2% max error on full aircraft (O(10) Drag Counts)
 - Total Lift: 1% max error on full aircraft
 - Noise : 1 dB max error (OASPL)
 - Heat transfer: 10° max error

Thank you very much for your attention