Quelques applications de la quantification d'incertitude en CFD appliquée à l'énergie

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Bacchus / MoST (INRIA - LEGI) UQ for CFD applied to energy

Sources d'incertitudes variées dans la simulation d'écoulements :

- conditions aux limites ou conditions initiales mal connues,
- incertitudes de modélisation
 - fermetures thermodynamiques
 - ou modèles de turbulence aux paramètres incertains

Outils disponibles pour propager ces incertitudes :

- chaos polynomial non-intrusif
- techniques semi-intrusives originales (équipe Bacchus INRIA)

Applications récentes de ces méthodes de propagation d'incertitude à la simulation d'écoulements en lien avec la production d'énergie

Simulation d'écoulements incertains en lien avec la production d'énergie :

- impact des incertitudes d'entrées sur la prédiction de l'écoulement dans des turbines hydrauliques (partie I)
- optimisation des performances de turbines utilisant des gaz denses (partie II)
- extraction d'énergie d'un écoulement par un profil animé d'un mouvement oscillant incertain (partie III)



Partie I : Optimisation de la position du tourillon d'une directrice de turbine Francis en prenant en compte les incertitudes sur les conditions d'entrée dans le distributeur









Context and motivation

Typical 2D simulation of Francis turbine's distributor



Context and motivation

Experimental observation :

• Variability of torque distributions depending on the selected guide vanes around the distributor



Is it possible to compare a mean numerical value and its associated variance with the mean experimental data and its associated variance ?

Context and motivation

Proposed numerical strategy :

Inlet boundary conditions :

Mean flow rate Q and mean incidence angle θ with their associated variance ΔQ and $\Delta \theta$



How to propagate the uncertainty of inlet boundary conditions in order to obtain the mean torque of the guide vane and its variance ?



The problem at hand is no longer the computation of a turbulent flow with prescribed inlet boundary conditions : one must take into account the influence of the uncertain inlet conditions on the flow solution.

Specific Uncertainty Quantification (UQ) tools are needed to propagate the inlet uncertainties throughout the flow simulation in order to obtain a statistical description of the flow in the distributor.

Mean flow solution = mean values of the guide vane torque when the 2 uncertain parameters ΔQ and $\Delta \theta$ vary in the interval, respectively, [0,95 x Q ; 1,05 x Q] and $[\theta - 10^\circ; \theta + 10^\circ]$ following a uniform probability density function (pdf).

Flow variance = variance of the guide vane torque when the 2 uncertain parameters ΔQ and $\Delta \theta$ vary in the interval, respectively, [0,95 x Q ; 1,05 x Q] and $[\theta - 10^\circ; \theta + 10^\circ]$ with a uniform pdf.

UQ: Non-Intrusive Polynomial Chaos

Principles :

• Expansion of the stochastic solution into a truncated series

$$y(x,t,\xi) = \sum_{\gamma=1}^{n_o} y_{\gamma}(x,t) \Psi_{\gamma}(\xi)$$

- ξ = random variable
- $\Psi_\gamma(\xi)$ = polynomial of degree γ depending on the choice of ξ
- ξ = uniform variable $\Rightarrow \Psi_{\gamma}(\xi)$ = Legendre polynomial

UQ: Non-Intrusive Polynomial Chaos

Principles (cont'd) :

- polynomial functions $\, \Psi_{_{\gamma}} \,$ orthogonal with respect to the pdf of $\, \xi \,$
- PC coefficients computed from a set of points and weights (ξ_i, ω_i)

$$y_{\gamma}(x,t) = \left\|\Psi_{\gamma}\right\|^{-2} \sum_{i=1}^{n} y(x,t,\xi_i) \Psi_{\gamma}(\xi_i) \omega_i$$

UQ : Non-Intrusive Polynomial Chaos

Implementation :

- available library providing $\xi_i, \omega_i, \Psi_\gamma(\xi_i)$: NISP (available in Scilab e.g.)
- deterministic computations to be performed $\rightarrow y(x,t,\xi_i)$
- mean E and variance $\,\sigma\,$ of the random process :

$$E(y(x,t,\xi)) = y_1(x,t)$$

$$\sigma(y(x,t,\xi)) = \sum_{\gamma} y_{\gamma}^2(x,t)$$

UQ: Non-Intrusive Polynomial Chaos

Implementation :

• multiple random variables (e.g. : ΔQ and $\Delta \theta$)

→ tensorization of the previous formula

- If the highest degree of the PC is p and the number of random variables is m, the number of deterministic flow computations to perform in order to compute the mean and variance of the stochastic flow solution is $(p+1)^m$
- In the present study *p=2* and *m=2* so that 9 distributor simulations must be performed to obtain the mean velocity distributions with their associated error bars. 72 simulations are performed since 8 opening angles are considered.

Results :

9 deterministic computations per opening angles (stochastic DOE)



Differences remain between experiment and simulation at small opening angles which cannot be entirely explained by fluctuating / uncertain inlet conditions

Another factor to investigate = turbulence modeling strategy

Influence of the turbulence model : RANS / LES comparison



• Satisfactory agreement between LES results and experiment with uncertain inlet conditions taken into account

Outcome : ANalysis Of VAriance (ANOVA)

Polynomial Chaos expansion coefficients yield the respective contribution to the variance of each uncertain variable



- At small opening angle (less than 20 deg) the torque variance is mainly due to flow rate fluctuation
- At large opening angle (more than 25 deg) the torque variance is mainly induced by inflow angle fluctuation



- Impact of inflow incidence variation limited to th stay vane region (as designed)
- Impact of flow rate variation on the guide vane region (hence on the torque) due to confinement effect between neighboring vanes

Guide vane optimization

Usual optimization problem :

e = -5 mm

Single design parameter : position of the guide vane axis along the vane's chord

e = 5 mm

e = 0 mm



- Eccentricity : distance between the actual axis position and the guide vane original location. Variation between 5 and 5 mm
- Three sets of simulations : one for each extremum and one for the original position
- Creation of a (polynomial) surrogate model for C(e;γ)

Guide vane optimization

Usual optimization problem (cont'd)

Definition of objectives and constraints for optimisation



$$\underbrace{Objectives:}_{J_1 = \min_e} \left(\max_{\gamma} (C(e;\gamma)) + 2 \times C(e;\gamma = 0^\circ) \right) \\
 J_2 = \min_e \left(\max_{\gamma} (C(e;\gamma)) - |C(e;\gamma_{\max})| \right) \\
 \underbrace{Constraints:}_{\gamma} \\
 \max_{\gamma} (C(e;\gamma)) > 0 \\
 C(e;\gamma = 0^\circ) < 0 \\
 C(e;\gamma_{\max}) < 0$$

Constrained bi-objective optimization problem solved using a non dominated sorting genetic algorithm (NSGA) with penalty method

Robust guide vane optimization



Robust guide vane optimization

Robust optimization problem : Results



Partie II :

Optimisation en présence d'incertitudes des performances de turbines utilisant des gaz denses

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Dense gases: definition & thermodynamic description

 Single phase vapours, characterized by complex molecules& moderate to large molecular weights

Example : $dodecamethylcyclohexasiloxane C_{12}H_{36}Si_6O_6$ also known under the commercial name of D6

 Need for a complex equation of state (Peng-Robinson, Span-Wagner,) in order to accurately describe the thermodynamic behavior of these gases **Dense gases:** Peng-Robinson-Strijek-Vera (PRSV) cubic EoS

• <u>Thermal EoS</u>:

pressure as a function of temperature and specific volume

$$p = \frac{RT}{v-b} - \frac{a(T;\omega)}{v^2 + 2bv - b^2}$$

- *R*, *b* : gas constants
- ω : acentric factor
- <u>Caloric EoS</u> : internal energy as a function of temperature

$$e(T) = e_c + \int_{T_c}^T C_{v,\infty}(T) dT$$

with $C_{v,\infty}(T) = C_{v,\infty}(T_c) (T/T_c)^n$ and φ_c = value of variable φ at the critical point

Dense gases:

- Lack of experimental data for dense gases properties
 - the thermal and caloric EoS depend on stochastic variables described by their respective pdf

$$p = \frac{RT}{v-b} - \frac{a(T;\omega)}{v^2 + 2bv - b^2}$$
 Acentric factor



When inserted in the conservation laws governing the gas flow, these uncertainties propagate to yield a stochastic flow solution.

Uncertainty Quantification

- Two distinct methods are used for UQ in order to cross validate the results obtained with low-order polynomials
 - Non Intrusive Polynomial Chaos (NIPC) (as implemented in the NISP package)
 - Probabilistic Collocation Method (PCM) as developed by Loeven et al (AIAA Paper 2007-317)

Putting it all together :

optimization of an ORC turbine using a dense gas

Baseline configuration : VKI LS-59 cascade

Uncertainties in the flow description coming from :

- the EoS
- the operating conditions, subject to fluctuations
- the geometric tolerances



Putting it all together :

optimization of an ORC turbine using a dense gas



ORC turbine : CFD (deterministic) solution

Main features of the flow solver :

- cell-centered third-order finite volume formulation
- accommodating an arbitrary EoS (here PRSV)
- non-reflecting (characteristic-based) inlet & outlet boundaries
- wall slip condition using multi-D linear extrapolation from interior points to calculate the wall pressure
- applied on a 192 x 16 structured grid
- unit cost of a CFD calculation : about 7 minutes

ORC turbine : CFD solution for the baseline configuration



Optimization problem : objective function

• Power output :

$$PO = \Delta h \cdot \dot{m}$$

where Δh is the static enthalpy variation between the turbine inlet and outlet,

 \dot{m} is the mass flow

Setting the optimization under uncertainty

• The fluid is fixed (D6)

... but its properties are not known with certainty

➔ 3 of the PRSV EoS are described as stochastic variables following a uniform pdf defined by the mean value and the variance

	n	$c_{v\infty}$	ω
Mean	0.5729	105.86	0.7361
Range	0.5385 - 0.6073	99.50-112.20	0.7214 - 0.7508
	Power-law Is exponent	at Acentric factor	

Setting the optimization under uncertainty

- The inlet / outlet flow conditions are fixed ... but these conditions are not known with certainty
- described by 3 stochastic variables following a uniform pdf defined by the mean value and the variance

& pressure					
	Inlet total t	Outlet pressure			
Range	0.9972-1.080	0.8736-0.9464	0.576 - 0.624		
Mean	1.039	0.910	0.600		
	T_{in}/T_c	p_{in}/p_c	p_{out}/p_c		

• The incidence and stagger angles are design parameters, varying in the design space : $\beta \in [25^{\circ}, 35^{\circ}]$

$$\beta \in [25^\circ, 35^\circ]$$
$$\theta \in [-5^\circ, 5^\circ]$$

Optimization problem : the brute force approach

8 uncertain parameters : 2 design parameters 6 operating point parameters

> CFD + UQ tools + NSGA

Uniform pdf for each parameter

NIPC & PCM are applied with a second-order polynomial expansion for each stochastic variable : size of the DOE = 6571

1 objective function statistically described by its mean and variance

Optimization problem : a better strategy

Use the analysis of variance (ANOVA) to determine which parameters contribute most significantly to the variance of the objective functions

a reduction of the stochastic space is expected hence a reduced computational cost for each design



The ANOVA analysis is performed *a priori*, for a reference configuration :

	T_{in}/T_c	p_{in}/p_c	p_{out}/p_c	eta	θ
Mean	1.039	0.910	0.600	30.0	0.0
Range	0.9972 - 1.080	0.8736 - 0.9464	0.576 - 0.624	29.7 - 30.3	-0.3-0.3

ANOVA

Contribution (%) of the uncertain parameters to the variance of the merit functions (baseline configuration)



<u>ANOVA</u>

The most influential parameters are :

- the inlet total temperature
- the inlet total pressure
- the exit pressure

These conclusions are confirmed when the same analysis is performed using statistics derived from a higher-order stochastic polynomial representation but with approximate Sparse Grid quadrature formulae

3rd order Full tensorization : DOE of size 65536 Sparse grid : DOE of size 701

4th order Full tensorization : DOE of size 390 625 Sparse grid : DOE of size 5421

Optimization problem :

3 uncertain operating conditions 2 (deterministic) design parameters Deterministic EoS



2nd order polynomial Full tensorization DOE of size 27 PCM or NIPC <u>Computational results</u>: computed Pareto front(s) after 20 generations containing 20 individuals 2 runs using PCM and NIPC for UQ



Computational results

Contours of the Mach number variance



LV design

HM design

Optimization problem : an improved strategy (in the long run)



Oscillating Airfoil/Hydrofoil in Power-Extracting Regime



• Pitching and heaving motion :

$$\begin{cases} \theta(t) = \theta_0 \sin(\omega t) \\ y(t) = H_0 \sin(\omega t + \pi/2) \end{cases}$$

(T. Kinsey, G. Dumas, AIAA Journal 2008)

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Oscillating Airfoil/Hydrofoil in Power-Extracting Regime



 Optimal motion parameters

 (θ₀, f^{*}) found for a fixed heaving amplitude H₀ = 1

Oscillating Airfoil /Hydrofoil and Uncertain Motion

- Usual deterministic case : θ_0, H_0, ω take fixed values
- In practice, parameters displaying some random variations $\Rightarrow \theta_0, H_0, \omega$ described by their probability density function
- resulting airfoil behavior (e.g. efficiency of the power-extraction device) statistically described (mean and variance)

Position of the problem

• available solver :

time-marching incompressible flow solver based on Artificial Compressibility formulation extended in a Arbitrary Lagrangian Eulerian framework

- Question #1 : how to extend this solver to obtain the first moments of a quantity of interest, such as $C_X(t)$, $C_Y(t)$ over a flow period or the airfoil power-extracting efficiency ?
- Question #2 : how to make the computation of $\overline{C_X}(t)$, $\sigma(C_X)(t)$, $\overline{C_Y}(t)$, $\sigma(C_Y)(t)$ **CPU efficient** and **flexible** (accommodating any type of pdf for the input random variables) ?

Possible strategies

- straightforward extension : coupling the time-marching CFD solver with a non-intrusive UQ strategy
- CFD improvement (efficiency) : switching from time-marching to the **Time Spectral Method (TSM)**
- UQ improvement (flexibility) : implementing a **Semi-Intrusive UQ strategy** within the TSM solver
- Preliminary application to the oscillating airfoil in uncertain motion

General framework : space discretization

• Finite Volume formulation for the ALE-AC system :

$$\frac{\partial \mathbf{w}_i}{\partial \tau} + \mathbf{K} \frac{\partial \mathbf{w}_i}{\partial t} + \mathcal{R}_i^E(\mathbf{w}, \mathbf{x}, \mathbf{s}) = \mathcal{R}_i^V(\mathbf{w}, \mathbf{x})$$

• inviscid residual (balance of numerical inviscid fluxes computed on each face $\Gamma_{i,k}$ of grid cell i):

$$\mathcal{R}_{i}^{E}(\mathbf{w}, \mathbf{x}, \mathbf{s}) = \frac{1}{|C_{i}|} \sum_{k} \mathcal{H}_{i,k}^{E} |\Gamma_{i,k}|$$

• viscous residual :

$$\mathcal{R}_i^V(\mathbf{w}, \mathbf{x}) = \frac{1}{|C_i|} \sum_k \mathcal{H}_{i,k}^V |\Gamma_{i,k}|$$

Time discretization : conventional BDF formulation

• BDF-ALE-AC system :

$$\frac{\mathbf{w}_i^{n,m+1} - \mathbf{w}_i^{n,m}}{\Delta \tau_i^{n,m}} + \mathbf{K} \frac{\left(\frac{3}{2} \mathbf{w}_i^{n,m} - 2 \mathbf{w}_i^n + \frac{1}{2} \mathbf{w}_i^{n-1}\right)}{\Delta t} + \mathcal{R}_i(\mathbf{w}^{n,m}) = 0$$

• convergence to the steady-state with respect to τ at each physical time-step $n\Delta t$ using an implicit formulation :

$$\Delta \mathbf{w}_{i}^{n,m} = -\Delta \tau_{i}^{n,m} \mathcal{R}_{i}^{t}(\mathbf{w}^{n,m+1})$$

$$\Downarrow$$

$$\mathcal{I}(\Delta \mathbf{w}_{i}^{n,m}) = -\Delta \tau_{i}^{n,m} \mathcal{R}_{i}^{t}(\mathbf{w}^{n,m})$$

Application of the deterministic BDF solver



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Taking into account the uncertain motion

Stochastic solution

- $\mathbf{w}(\mathbf{x}, t, \xi) \Rightarrow C_X(t, \xi), C_Y(t, \xi)$
- ξ = set of n_{ξ} independent random variables $\xi = (\xi_1, \dots, \xi_{n_{\xi}})$
- *e.g.* $n_{\xi} = 1$ and $\xi_1 = H_0$
- H_0 described by a uniform pdf over the interval [0.95, 1.05]
- how to obtain $\overline{C_X}(t)$, $\sigma(C_X)(t)$, $\overline{C_Y}(t)$, $\sigma(C_Y)(t)$?

Straightforward approach

- coupling the time-marching CFD solver with a **non-intrusive** UQ strategy
- computational cost directly related to the cost of a deterministic CFD run (for a fixed ξ_i)
 - \Rightarrow cost reduction by using Time Spectral Method instead of BDF

TSM for incompressible flow

TSM design principles

• Periodic flow solution described by a truncated Fourier series :

$$\mathbf{w} = \sum_{k=-N}^{N} \widehat{\mathbf{w}_k}(x) e^{\underline{i}k\omega t}$$

- Nyquist-Shannon theorem $\Rightarrow \widehat{\mathbf{w}_k}(x) = \frac{1}{2N+1} \sum_{n=0}^{2N} \mathbf{w}_n e^{-\underline{i}k\omega n\Delta t}$ with $\mathbf{w}_n \equiv \mathbf{w}(t_n = n\Delta t)$ and $\Delta t = T/(2N+1)$
- after transformation, the new (steady) system to solve is :

$$\mathbf{K}D_t(\mathbf{w}_n) + \mathcal{R}(\mathbf{w}_n, \mathbf{x}_n, \mathbf{s}_n) = 0, \qquad 0 \le n < 2N + 1$$

with D_t the spectral time operator : $D_t(\mathbf{w}_n) = \sum d_p \mathbf{w}_{n+p}$.

TSM vs Time Marching (BDF)

Convergence to steady-state ($\theta_0 = 60^\circ$, $H_0 = 1$ and $f^* = 0.18$)

TSM / BDF : same level of accuracy using ${\cal N}=8~(17~{\rm TSM}~{\rm modes})$



TSM modes obtained for a CPU cost about 1/5 of the BDF overall CPU cost (Antheaume & Corre, AIAA J. 2011)

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UQ for CFD applied to energy



Taking into account the uncertain motion

Efficiency improvement

• coupling the TSM solver with NIPC

Flexibility improvement

• insert a Semi-Intrusive (SI) UQ strategy (Abgrall & al, 2011) into the TSM solver

SI UQ strategy : design principles

- tessellation of the random space as in finite volume methods for the space variables
- probabilistic solution numerically described by the conditional expectancies of point values or cell averages
- evaluation of these conditional expectancies constructed from the deterministic scheme

Principles

• conditional expectancy of the TSM-ALE-AC system

$$\mathbf{K}D_t(\mathbf{w}_{i,n,j}) + E(\mathcal{R}_{i,n}(\mathbf{w}, \mathbf{x}, \mathbf{s}) | \Omega_j) = 0,$$

with $\mathbf{w}_{i,n,j} = E(\mathbf{w}_{i,n}|\Omega_j)$

• conditional expectancy of the residual :

$$E(\mathcal{R}_{i,n}(\mathbf{w})|\Omega_j) = \frac{1}{|C_i|} \sum_k \left[E(\mathcal{H}^E_{(i,k),n}|\Omega_j) - E(\mathcal{H}^V_{(i,k),n}|\Omega_j) \right] |\Gamma_{i,k}|$$

• conditional expectancy of numerical fluxes :

$$E(\mathcal{H}_{(i,k),n}^{E/V}|\Omega_j) = \frac{1}{\mu(\Omega_j)} \int_{\Omega_j} \mathcal{H}_{(i,k),n}^{E/V}(\omega) \,\mu(\omega) d\omega$$

Semi-Intrusive UQ strategy

Principles

- conditional expectancy of the inviscid numerical flux :
 - standard third-order Gaussian quadrature to compute the integral
 - polynomial reconstruction of the stochastic solution

$$E(\mathcal{H}_{(i,k),n}^{E}|\Omega_{j}) = \beta_{j_{1}}\mathcal{H}^{E}(\mathbf{P}_{i,n,j}(\omega_{j_{1}});\mathbf{P}_{o(i,k),n,j}(\omega_{j_{1}})) + \beta_{j_{2}}\mathcal{H}^{E}(\mathbf{P}_{i,n,j}(\omega_{j_{2}});\mathbf{P}_{o(i,k),n,j}(\omega_{j_{2}}))$$

with
$$\beta_{j_{(1,2)}} = \frac{\mu(\omega_{j_{(1,2)}})p_{j_{(1,2)}}}{\mu(\Omega_j)}$$

• similar formulation for the conditional expectancy of the viscous numerical flux

$$E(\mathcal{H}_{(i,k),n}^{V}|\Omega_{j}) = \beta_{j_{1}}\mathcal{H}^{V}(\nabla \mathbf{P}_{N_{(i,k)}^{1},n,j}(\omega_{j_{1}}); \nabla \mathbf{P}_{N_{i,k}^{2},n,j}(\omega_{j_{1}})) + \beta_{j_{2}}\mathcal{H}^{V}(\nabla \mathbf{P}_{N_{i,k}^{1},n,j}(\omega_{j_{2}}); \nabla \mathbf{P}_{N_{i,k}^{2},n,j}(\omega_{j_{2}}))$$

Polynomial reconstruction of the stochastic solution

• second-order accuracy \Rightarrow quadratic reconstruction in cell Ω_j :

$$\mathbf{P}_{i,n,j} = \mathbf{a} + \mathbf{b} \left(\omega - \omega_j \right) + \mathbf{c} \left(\omega - \omega_j \right)^2$$

 \bullet coefficients ${\bf a},\,{\bf b}$ and ${\bf c}$ determined by requiring

$$E(\mathbf{P}_{i,n,l}|\Omega_l) = \mathbf{w}_{i,n,l}$$
 for $l = j - 1, j, j + 1$

• final form of the polynomial reconstruction :

$$\mathbf{P}_{i,n,j}(\omega) = \alpha_j^{-}(\omega) \, \mathbf{w}_{i,n,j-1} + \alpha_j^0(\omega) \, \mathbf{w}_{i,n,j} + \alpha_j^+(\omega) \, \mathbf{w}_{i,n,j+1}$$

with coefficients $\alpha_j^{-/0/+}(\omega)$ computed once for all and depending on the pdf of the random variable

Practical implementation

- structure of the solution algorithm basically unchanged w.r.t the baseline deterministic TSM solver
- stochastic solution $\mathbf{w}_{i,j}$ or its polynomial reconstruction $\mathbf{P}_{i,j}$ replacing the purely deterministic physical state \mathbf{w}_i
- extra evaluations (quadrature formula on Ω_j) of the (otherwise unchanged) inviscid and viscous numerical flux formulae on each face of the physical cell C_i
- computation of the solution first moments from the conditional expectancies :

$$\overline{w}_{i,n} = \sum_{j} \mathbf{w}_{i,n,j} \quad , \quad \sigma(\mathbf{w})_{i,n} = \sum_{j} \int_{\Omega_j} (\overline{w}_{i,n} - \mathbf{w}_{i,n,j})^2 d\mu$$

Oscillating NACA0015 airfoil with uncertain motion

- $\theta_0 = 60^\circ$, $f^* = 0.18$ and H_0 described by a uniform pdf over [0.95, 1.05]
- SI-TSM with a 5-point grid to discretize the random space
- to be compared with the fourth-order NIPC making use of a 5-element DOE
- 17 modes are used for the TSM approach (both for SI-TSM and NIPC-TSM)

SI-TSM vs NIPC-TSM

Convergence to steady-state for SI-TSM



SI-TSM vs NIPC-TSM





Conclusions générales & Perspectives

Quantification d'incertitudes et CFD

- prise en compte d'incertitudes en CFD : une démarche en voie de "routinisation"
- forte attractivité court / moyen terme des méthodes non-intrusives
- avec cependant nécessité d'un savoir-faire en matière de modèles substituts indispensables à la réduction des coûts
- voie prometteuse : méthodes semi-intrusives recyclant le savoir-faire "CFD déterministe"
- forte attractivité en termes de flexibilité (choix des pdfs) et d'efficacité
- perspective moyen terme car nécessité du développement de version "stochastique" des solveurs existants