Overview over some UQ activities in hypersonic flows

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Applied Modeling & Simulation Series
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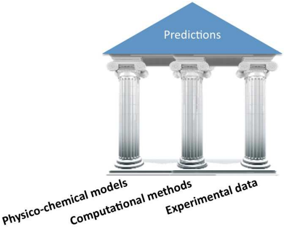
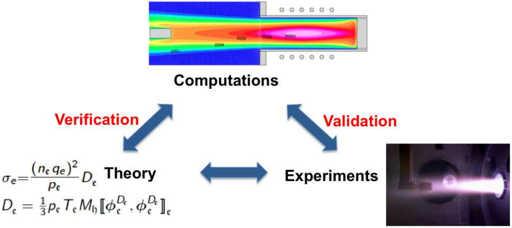
Outline

1. Brief introduction to UQ

2. UQ activities in hypersonic flows

Three pillars for predictive Computational Science

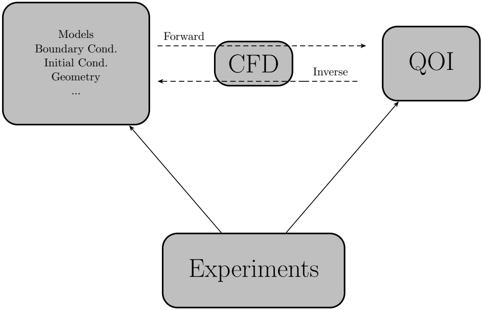




- Computation cannot be truly predictive without the coupling to theory and experiments. . .
- This coupling is precisely the verification and validation process!

$\Rightarrow$
- **Verification**: Is the computational method implemented correctly?
- **Validation** : Are we solving the right equations?

How experience can be taken into account in the numerical simulation ?



Uncertainty Quantification is the end-to-end study of the reliability of scientific predictions

FLUIDS MAKE THE UQ COMPLEX TO HANDLE → CHALLENGING !

Flows features unsteadiness, compressibility, discontinuities, turbulence, multiphase nature of the flow, and so on ...

- Measurements in fluid mechanics devices delicate and expensive
  - Complexity of measures
  - Sometimes scarce and inaccurate experimental data

  → increased amounts of uncertainties
- Complex Numerical simulation

The variability of a CFD numerical solution should be estimated taking into account every possible source of uncertainty (operating point, modeling,)

THE MATHEMATICAL SETTING OF THE PROBLEM

Let the output of interest $u(\mathbf{x}, t, \xi)$ be governed by the equation:

$$\mathcal{L}(\mathbf{x}, t, \boldsymbol{\xi}(\omega); u(\mathbf{x}, t, \boldsymbol{\xi}(\omega))) = \mathcal{S}(\mathbf{x}, t, \boldsymbol{\xi}(\omega)), \tag{1}$$

where $\mathcal{L}$ (algebraic or differential operator) and $\mathcal{S}$ are on $D \times T \times \Xi$, $\mathbf{x} \in D \subset \mathbb{R}^{n_d}$, with $n_d \in \{1, 2, 3\}$, $\boldsymbol{\xi}(\omega) = \{\xi_1(\omega_1), \ldots, \xi_d(\omega_d)\} \in \Xi$ with parameters space $\Xi \subset \mathbb{R}^d$

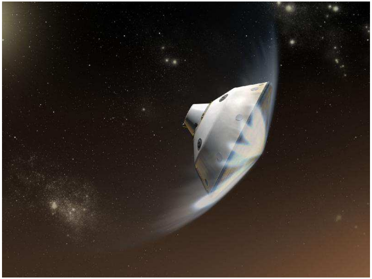
The objective of uncertainty propagation is to find the **probability distribution** of $u(\mathbf{y}, \boldsymbol{\xi})$ and its **statistical moments** $\mu_{\mathrm{u}_i}(\mathbf{y})$ given by

$$\mu_{\mathrm{u}_i}(\mathbf{y}) = \int_{\Xi} u(\mathbf{y}, \boldsymbol{\xi})^i f_{\xi}(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi}. \tag{2}$$

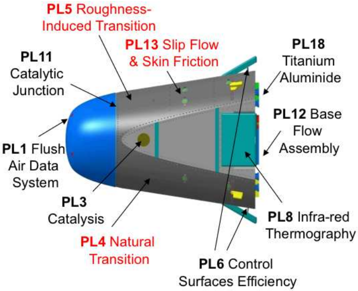
How compute this integral in an efficient way ?

Motivation: post-flight analysis of a space mission

- It requires an accurate determination of the free-stream conditions for the trajectory
- These quantities can be rebuilt from the heat flux and pressure measured on the spacecraft



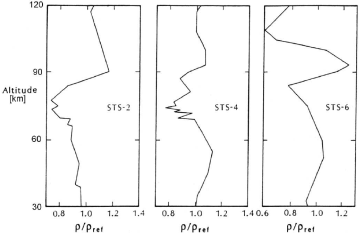
NASA Mars Science Laboratory



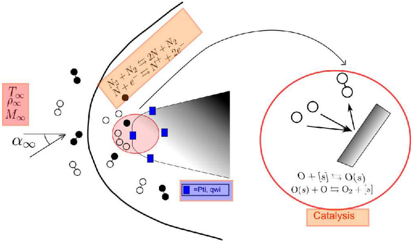
ESA European eXPErimental Re-entry Testbed

FLUSH AIR DATA SYSTEM (FADS) ON EXPERT

- ST measured densities can deviate up to 20% from the standard atmosphere model
- RAFLEX instrumentation: FADS comprising a set of sensors flush mounted in the TPS to measure static pressure (pressure taps) and heat flux (calorimeters)



Shuttle-derived densities compared to the 1962 U.S. standard atmosphere [Talay et al. 1985]



RAFLEX instrumentation on Expert

⇒ *Q1: What is the uncertainty on rebuilt free-stream conditions due to measurement uncertainties as well as of chemistry models?*

⇒ *Q2: What should be the sensor accuracy for a prescribed uncertainty on free stream conditions?*

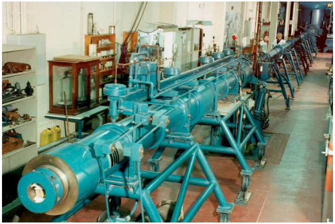
Rebuilding methodology

- Knowing that experimental data suffer from errors, the rebuilding methodology needs to integrate quantification of uncertainties
- Epistemic uncertainties on the chemistry models in the bulk and at the wall (surface catalysis) should also be taken into account

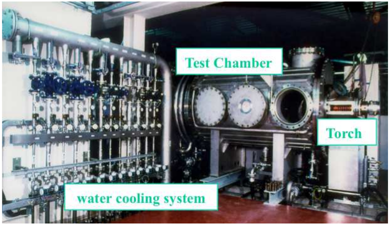
$\Rightarrow$ Rebuilding the free stream conditions from the FADS data amounts to solving a stochastic inverse problem

Validation and prediction

- Validation
  - Experimental databases of ground facilities will be used to validate the simulation tools and improve our understanding of physical phenomena
- Prediction
  - Prediction of the free stream properties in flight with their associated uncertainty



VKI Longshot M14 free piston tunnel



VKI Plasmatron facility

Strong collaboration between INRIA (P.M. Congedo) and VKI (T. Magin) and several other people

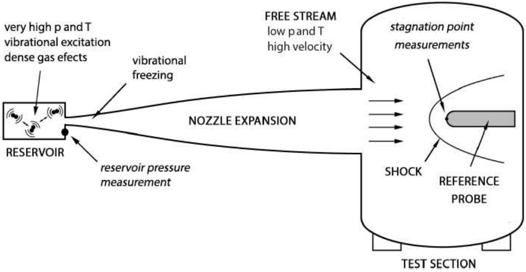
- Characterization of the free stream conditions in the VKI Longshot facility (Bart Van Hove, J. Tryoen, M. Duvernet)
- Uncertainty Analysis of Carbon Ablation in the VKI Plasmatron (A. Turchi, F. Sanson, F. Panerai)
- Sensitivity analysis concerning the chemical reaction uncertainties during an atmospheric reentry (K. Tang, M. Panesi)

- Sensitivity analysis and characterization of the uncertain input data for the EXPERT vehicle (J. Tryoen, N. Villedieu)

Characterization of the free stream conditions in the VKI Longshot facility

Characterization of the free stream conditions in the VKI Longshot facility

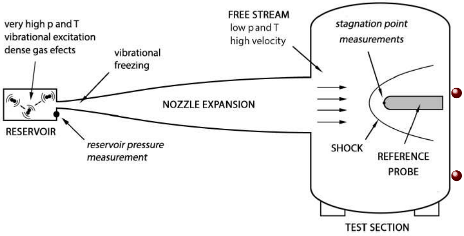
Mach14 Hypersonic Wind Tunnel with either nitrogen or carbon dioxide



- No chemical thermo-reactive effects
- Rebuilding of free stream conditions: p_1, T_1, v_1
- Epistemic uncertainty on T_{v1}

Characterization of the free stream conditions in the VKI Longshot facility

Forward Problem



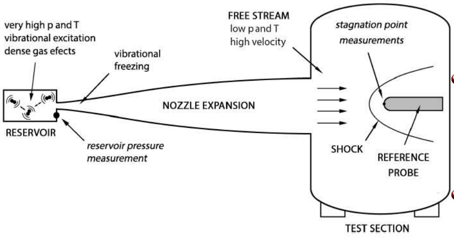
- **Input data**
  - Freestream pressure p_1, temperature T_1 and shock speed v_1
  - Vibrational temperature T_{v1}
- **Output data**
  - Stagnation-point pressure p_{st} and heat flux q_{st}
  - Reservoir pressure p_0

- **1D code** :
  - perfect gas equation of state in the reservoir / non-equilibrium flow model in the nozzle expansion
  - Keyes'/Lemmon/Jacobsen/Sutherland viscosity models for freestream conditions/post-shock/stagnation point
  - Fay-Riddel model to compute the stagnation heat flux
  - Rankine-Hugoniot relations applied through the shock / flow assumed incompressible after the shock

$\Rightarrow$ **Sources of uncertainties**
  - Unknown: $p_1 \sim \mathcal{U}(190, 230)$, $T_1 \sim \mathcal{U}(45, 60)$ and $v_1 \sim \mathcal{U}(1500, 1800)$
  - Epistemic uniform uncertainty on $T_{v1} \sim \mathcal{U}(1000, 1500)$

Characterization of the free stream conditions in the VKI Longshot facility

Inverse Problem



- Measurements
  - Stagnation-point pressure p_{st} and heat flux q_{st}
  - Reservoir pressure p_0
- Uncertainties
  - Experimental data
  - vibrational temperature

- Validation of a new inverse method for determining uncertainties on free stream conditions p_1, T_1 and v_1 from measurements

⇒ Proposed approach relying on a Bayesian Inference setting

Characterization of the free stream conditions in the VKI Longshot facility
Bayesian inference for stochastic inverse method

- Forward model : $\mathbf{d} = F(\mathbf{m}, T_{v1})$, $\mathbf{d} = (p_{\mathrm{st}}, q_{\mathrm{st}}, p_0)$, $\mathbf{m} = (p_1, T_1, v_1)$
- "*prior* pdf + set of experimental data = *posterior* pdf fitting data"
- Bayes' rule

$$p(\mathbf{m}|\mathbf{d}^1, \ldots, \mathbf{d}^n) = \frac{p(\mathbf{d}^1, \ldots, \mathbf{d}^n|\mathbf{m}, T_{v1}) p_{\mathbf{m}}(\mathbf{m}) p_{T_{v1}}(T_{v1})}{\int p(\mathbf{d}^1, \ldots, \mathbf{d}^n|\mathbf{m}, T_{v1}) p_{\mathbf{m}}(\mathbf{m}) p_{T_{v1}}(T_{v1}) \mathrm{d}\mathbf{m}\mathrm{d}T_{v1}}$$

  - Experimental data : $\{\mathbf{d}^1, \ldots, \mathbf{d}^n\}$
    Hypothesis: $\mathbf{d}^j = F(\mathbf{m}, T_{v1}) + \mathbf{e}^j, \mathbf{e}^j \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma})$, $j = 1, \ldots, n$,
    $\mathbf{\Gamma} = \mathrm{diag}(\sigma^2_{p_{\mathrm{st}}}, \sigma^2_{q_{\mathrm{st}}}, \sigma^2_{p_0})$

$$\rightarrow p(\mathbf{d}^1, \ldots, \mathbf{d}^m|\mathbf{m}, T_{v1}) = \prod_{j=1}^{n} p_{\mathbf{d}^j}(\mathbf{d}^j|\mathbf{m}, T_{v1}) = \prod_{j=1}^{n} p_{\mathbf{e}}(\mathbf{d}^j - F(\mathbf{m}, T_{v1}), \mathbf{\Gamma})$$

  - *prior* pdf $p_{\mathbf{m}} \propto 1_{p_1 \in [190,230]} 1_{T_1 \in [45,60]} 1_{v_1 \in [1500,1800]}$
  - uniform pdf $p_{T_{v1}} \propto 1_{T_{v1} \in [1000,1500]}$
- measurement errors $\boldsymbol{\sigma}_{\mathrm{obs}} = (\sigma_{p_{\mathrm{st}}}, \sigma_{q_{\mathrm{st}}}, \sigma_{p_0})$ supposed known

IN PRACTICE

- Samples of the normalized posterior
$$p(\mathbf{m}|\mathbf{d}^1,\dots,\mathbf{d}^n) \propto p(\mathbf{d}^1,\dots,\mathbf{d}^n|\mathbf{m},T_{v1})p_{\mathbf{m}}(\mathbf{m})p_{T_{v1}}(T_{v1})$$
obtained with Markov Chain Monte Carlo methods

- Let $(\mathbf{m}^k)_{k=t_b}^{K}$ such a sample (t_b "burning" time),
$$\mathbb{E}(f(\mathbf{m})|\mathbf{d}^1,\dots,\mathbf{d}^n) \approx \frac{1}{K-t_b+1}\sum_{k=t_b}^{K} f(\mathbf{m}^k)$$

  $\rightarrow$ computation of *posterior* statistics (mean, standard deviation, densities, error bars, . . .)

Characterization of the free stream conditions in the VKI Longshot facility
Numerical Results

A noisy data vector $\{\mathbf{d}^1, \ldots, \mathbf{d}^{10}\}$ is generated
$\rightarrow$ solving the forward model for a true vector of input parameters
$(\mathbf{m}^{\text{true}}, T_v^{\text{true}}) = (200, 50, 1621, 1245)$
$\rightarrow$ perturbing the true output value $\mathbf{d}^{\text{true}} = (p_0^{\text{true}}, p_{\text{st}}^{\text{true}}, q_{\text{st}}^{\text{true}})$ (Gaussian noise)

CHARACTERIZATION OF THE FREE STREAM CONDITIONS IN THE VKI LONGSHOT FACILITY
NUMERICAL RESULTS

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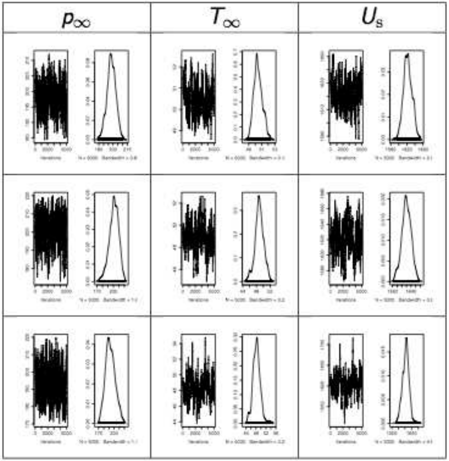
Various cases are considered :

1. a 5% observation error ($\sigma_i/\mathbf{d}_i^{\text{true}} = 0.05$) with known T_v,
2. a 10% observation error ($\sigma_i/\mathbf{d}_i^{\text{true}} = 0.10$) with known T_v, and
3. a 10% observation error ($\sigma_i/\mathbf{d}_i^{\text{true}} = 0.10$) with uncertainty on T_v ($T_v \sim \mathcal{U}(1000, 1500)$).
4. Experimental observations

Results (5% and 10% error with known T_v, 10% with unknown T_v)



- Spread of supports of PDF between (i) and (ii) $\rightarrow$ increase of measurement errors
- AND between (ii) and (iii) $\rightarrow$ adding uncertainty on the vibrational temperature
- Propating PDFin a numerical code and estimating output variability

Characterization of the free stream conditions in the VKI Longshot facility

Numerical Results (1)

		$\sigma_i/\mathbf{d}_i^{\text{true}} = 0.05$ T_v known	$\sigma_i/\mathbf{d}_i^{\text{true}} = 0.10$ T_v known	$\sigma_i/\mathbf{d}_i^{\text{true}} = 0.10$ T_v unknown
mean	p_∞	198.2	200.9	192.9
	T_∞	50.44	48.87	48.25
	U_s	1622	1620	1606
std	p_∞	4.632	8.544	9.260
	T_∞	0.6514	1.271	1.526
	U_s	10.66	19.87	25.76
std/mean	p_∞	2.337×10^{-2}	4.523×10^{-2}	4.80×10^{-2}
	T_∞	1.291×10^{-2}	2.601×10^{-2}	3.163×10^{-2}
	U_s	0.657×10^{-2}	1.226×10^{-2}	1.604×10^{-2}
90% confidence intervals	p_∞	[190.1,205.8]	[185.2,213.8]	[177.9,209.5]
	T_∞	[49.47,51.61]	[46.60,51.03]	[45.82,50.63]
	U_s	[1605,1640]	[1585,1653]	[1562,1645]

- Uncertainty of p_∞ is the most important: std/mean nearly two and four times more with respect to that ones related to T_∞, and U_s, when T_v is known.
- Large variation of pressure mean (4%) observed when T_v is unknown or known
- Smaller variations observed for mean of T_∞ (3.2%) and for mean of U_s (1.60%) w.r.t. p_∞ when T_v is unknown
- For a given observation, p_∞ most difficult parameter to predict, more than T_∞
- Importance of free-stream pressure

Characterization of the free stream conditions in the VKI Longshot facility
Application of bayesian-strategy to experimental measurements

- Some experimental points chosen by considering the sensors acquisition in the Longshot facility
- Five points are selected on the experimental curves, at different time-steps equal to 0.5, 5, 10, 15, 20 ms
- Uncertainties on error measurements are considered
- Uncertainty on the heat flux at the stagnation point is much more elevated with respect to the pressure uncertainty

temps (ms)	0.5	5	10	15	20
p0 [Pa]	2.75*10^8	1.42*10^8	0.98*10^8	0.65*10^8	0.45*10^8
p_stagn [Pa]	1.5*10^5	0.85*10^5	0.58*10^5	0.42*10^5	0.3*10^5
q_stagn [W/m^2]	2.5*10^6	0.82*10^6	0.55*10^6	0.45*10^6	0.3*10^6

p0	± 2%
p_stagn	± 2%
q_stagn	± 8%

Characterization of the free stream conditions in the VKI Longshot facility
Application of bayesian-strategy to experimental measurements

- Different behavior with respect to the synthetic test-case
- Temperature variability (in terms of standard deviation to mean ratio) is greater than the pressure one for each time-step
- Velocity variability of the same order of magnitude than pressure, that is quite different with respect to the previous results

		5ms	10ms	15ms
mean	p_∞	333.8	227.9	166.2
	T_∞	28.2	24.67	24.9
	U_s	1520.0	1422	1413
std	p_∞	5.29	7.12	5.63
	T_∞	0.719	1.45	1.21
	U_s	20.2	45.25	36.5
std/mean	p_∞	1.586×10^{-2}	3.12×10^{-2}	3.39×10^{-2}
	T_∞	2.553×10^{-2}	5.90×10^{-2}	4.84×10^{-2}
	U_s	1.327×10^{-2}	3.18×10^{-2}	2.58×10^{-2}
90% confidence intervals	p_∞	[325.5,342.3]	[216.8,239.5]	[157.3,175.1]
	T_∞	[26.9,29.22]	[21.95,26.75]	[22.98,26.97]
	U_s	[1482.6,1548.09]	[1397.3,1487.15]	[1354.5,1472.2]

Characterization of the free stream conditions in the VKI Longshot facility

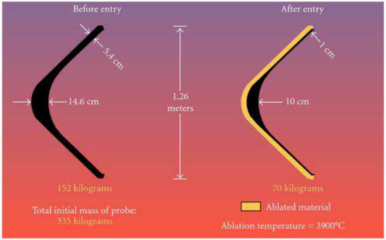
Conclusion

- Setting up of a rigorous framework to take into account measurement and model uncertainties in the resolution of the inverse problem
- Detailed probability characterization from MCMC sampling
- Some notions concerning the physics of the phenomenon are provided, *i.e.* the variability of the free-stream pressure
- Stagnation measurement error needed for a prescribed level of accuracy on the free-stream conditions
- The importance of modelling some unknown variables, such as for example the vibrational temperature, can be assessed.

Uncertainty Analysis of Carbon Ablation in the VKI Plasmatron

Motivations

- **To understand** the operational behavior of the TPS materials
- **To study** the gas/surface interaction physics occurring during reentry
- **To improve** the prediction capacity and **reduce** the design margins



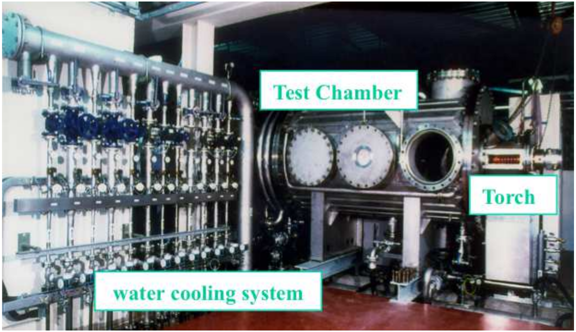
GALILEO MISSION
Destination: Jupiter
Date: 1989–2003

...THE BEST RACE CAR IS THE ONE THAT FALLS APART RIGHT AFTER THE FINISH LINE...

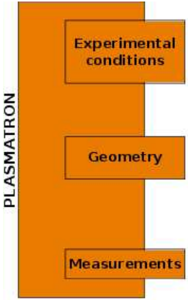
Plasmatron facility (The most powerful induction-coupled plasma wind tunnel in the world)

Role: performing reusable/ablative TPS tests

- Gas: Air, N_2, CO_2, Ar
- Power: 1.2 MW – most powerful ICP in the world –
- Heat-flux: up to 16 MW/m^2 (superorbital re-entry)
- Pressure: 10 – 800 mbar



Put the players together



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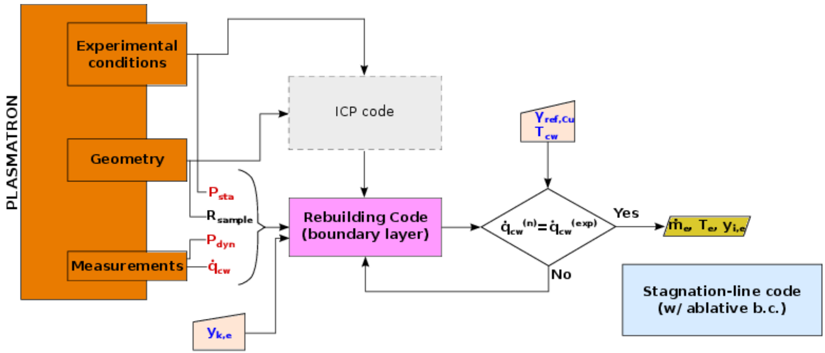

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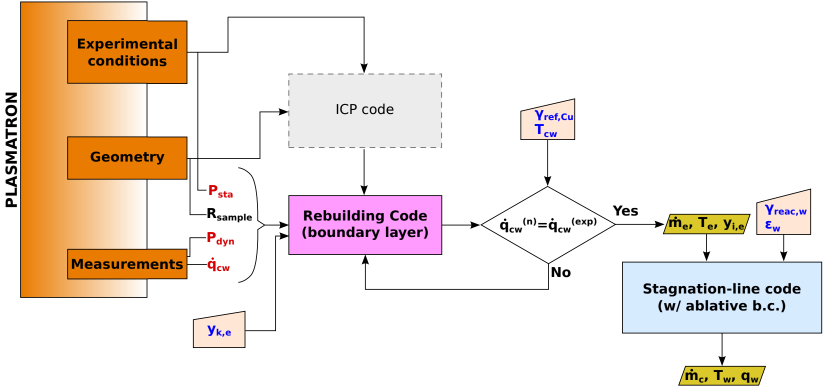
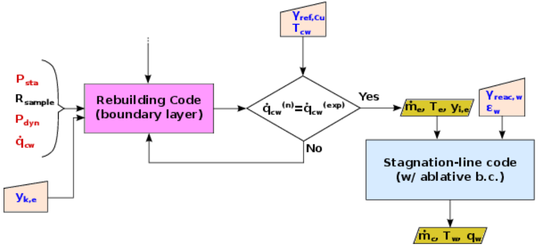


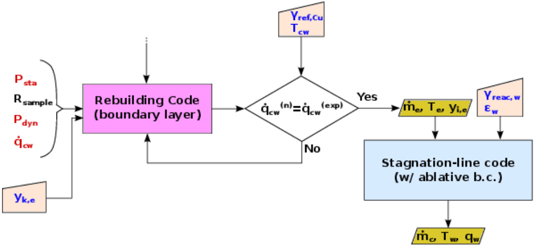
Uncertain inputs generate...uncertain outputs!!!

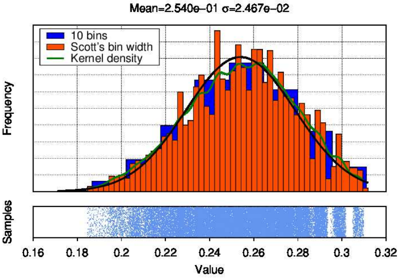


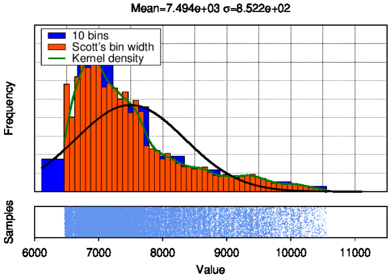
	variable
	Dynamic Pressure
	Static Pressure
STEP 1: BOUNDARY-LAYER CODE	Cold Wall Heat Flux
	Cold Wall Temperature
	Catalycity
	Nitrogen/Oxygen ratio

	variable
	$C_s + O \rightarrow CO$
	$2C_s + O_2 \rightarrow 2CO$
STEP 2: STAGNATION-LINE CODE	$C_s + N \rightarrow CN$
	$3C_s \rightarrow C_3$
	$N + N \rightarrow N_2$
	TPS wall emissivity

Coupled analysis: input uncertainty distributions



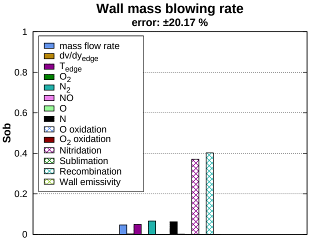


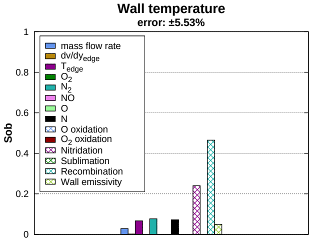


Coupled analysis w/ nitridation

ABLATION QOI

VARIABLE	MEAN	VARIANCE	$\Delta_{stoch-nom}$	$\varepsilon_{\text{old}}\,(\pm)$
mass blowing rate	0.029 [kg / m^2s]	3.48e-5	–28.4%	16.72%
temperature	2661 [K]	2.17e+4	+5.0%	4.56%



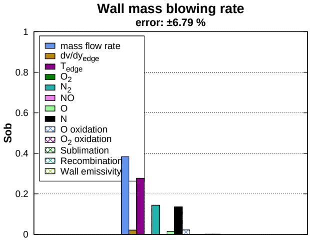


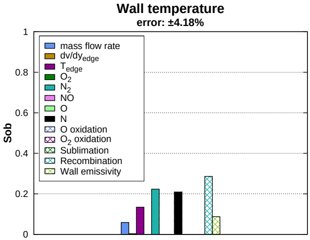
CONSIDERING ALL THE UNCERTAINTIES SLIGHTLY AFFECT THE ERROR!

Coupled analysis w/o nitridation

ABLATION QOI

VARIABLE	MEAN	VARIANCE	$\Delta_{stoch-nom}$	$\varepsilon_{\text{old}}(\pm)$
mass blowing rate	0.020 [kg / m^{2}s]	1.94e-6	−2.9%	1.15%
temperature	2818 [K]	1.39e+4	+0.8%	1.80%





REBUILDING UNCERTAINTIES AFFECT THE MASS BLOWING RATE!

Conclusions

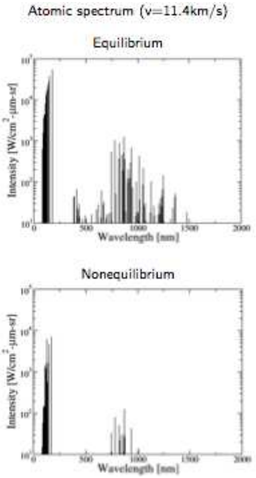
- decoupled analyisis
  - Strong impact on the QOIs of a questionable phenomenon such as the surface nitridation when considered
  - Small variations of the QOIs uncertainties when nitridation is neglected: consequence of the analyzed ablation regime
- coupled analyisis
  - The influence of the nitridation uncertainties remains the bigger
  - Measurement and model uncertainties from the rebuilding procedure cause the error to grow when nitridation is neglected

Perspectives

- Assess more plausible ranges for the most influential parameters
- Analyze different ablation regimes
- Compare the obtained results with the experimental measurements

Sensitivity analysis concerning the chemical reaction uncertainties during an atmospheric reentry

Sensitivity analysis concerning the chemical reaction uncertainties during an atmospheric reentry



- Understanding kinetic and radiative processes is crucial during the reentry
- Physico-chemical models are complex and prone to many uncertainties
  - Rates for kinetic and energy relaxation are usually the most uncertain since they are difficult to messure experimentally

⇒ Q1: Which elementary reactions are important in chemical mechanisms?
⇒ Q2: What is the influence of the uncertainty of their rate coefficients on heat flux prediction?

Sensitivity analysis concerning the chemical reaction uncertainties during an atmospheric reentry

Reactions for which the rate coefficients are considered uncertain

Trajectory points	Time [s]	u_∞ [km/s]	p_∞ [Pa]	T_∞ [K]	Mach
Point 1	22.4	11.711	13.19	243.29	37.45

- Quantity of interest: Radiative heat flux at a distance corresponding to the stand-off distance for the ERC capsule

Reaction	Reaction ID	Min	Nominal	Max
$N(1) + e^- \rightleftharpoons N(2) + e^-$	1	$1.4470 \cdot 10^{15}$	$1.4470 \cdot 10^{16}$	$1.4470 \cdot 10^{17}$
$N(1) + e^- \rightleftharpoons N(3) + e^-$	2	$3.8673 \cdot 10^{14}$	$3.8673 \cdot 10^{15}$	$3.8673 \cdot 10^{16}$
$N(2) + e^- \rightleftharpoons N(3) + e^-$	3	$3.6169 \cdot 10^{14}$	$3.6169 \cdot 10^{15}$	$3.6169 \cdot 10^{16}$
$O(1) + e^- \rightleftharpoons O(2) + e^-$	4	$8.2744 \cdot 10^{11}$	$8.2744 \cdot 10^{12}$	$8.2744 \cdot 10^{13}$
$O(1) + e^- \rightleftharpoons O(3) + e^-$	5	$5.6319 \cdot 10^{10}$	$5.6319 \cdot 10^{11}$	$5.6319 \cdot 10^{12}$
$O(2) + e^- \rightleftharpoons O(3) + e^-$	6	$2.7049 \cdot 10^{13}$	$2.7049 \cdot 10^{14}$	$2.7049 \cdot 10^{14}$
$N(1) + e^- \rightleftharpoons N^+ + e^- + e^-$	7	$5.1688 \cdot 10^{13}$	$5.1688 \cdot 10^{14}$	$5.1688 \cdot 10^{15}$
$N(2) + e^- \rightleftharpoons N^+ + e^- + e^-$	8	$4.6563 \cdot 10^{11}$	$4.6563 \cdot 10^{12}$	$4.6563 \cdot 10^{13}$
$O(1) + e^- \rightleftharpoons O^+ + e^- + e^-$	9	$3.2477 \cdot 10^{11}$	$3.2477 \cdot 10^{12}$	$3.2477 \cdot 10^{13}$
$O(2) + e^- \rightleftharpoons O^+ + e^- + e^-$	10	$5.1616 \cdot 10^{11}$	$5.1616 \cdot 10^{12}$	$5.1616 \cdot 10^{13}$

Sensitivity analysis concerning the chemical reaction uncertainties during an atmospheric reentry
ANOVA analysis of the Heat Flux

Coefficient of variation =0.099%

- Uncertain excitation reactions for the two species only involve the ground electronic level and the metastable levels
- The radiating levels are high-lying energy levels above the metastable states.
- How computing efficiently the ranking of most predominant uncertainties ?

Radiative heat flux	Value
Mean value μ	$1964.378[kW/m^2]$
Deviation σ	$1.936[kW/m^2]$

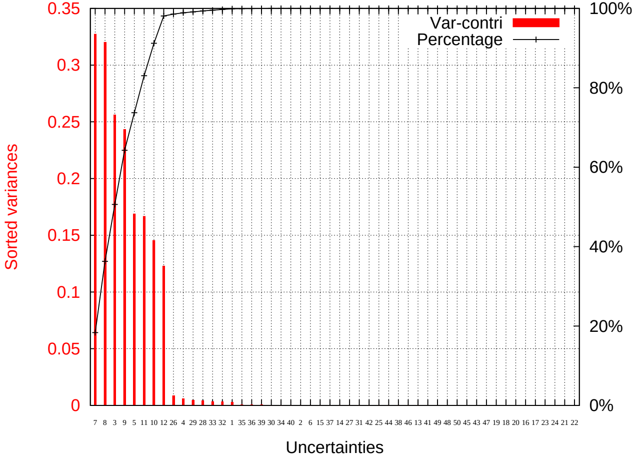
Sensitivity analysis concerning the chemical reaction uncertainties during an atmospheric reentry

Anchored ANOVA analysis (IJNME 2014, K. Tang, P.M. Congedo) applied to 50 uncertainties problem

- Compared to standard ANOVA, **anchored ANOVA**, with arbitrary anchor point, loses orthogonality if employing the same measure
  $\Rightarrow$ Reduced number of deterministic computations
- Covariance decomposition of output variance + adaptivity
- Some variables can be inactive for certain order of interactions
- The active dimension is determined by means of a threshold

Sensitivity analysis concerning the chemical reaction uncertainties during an atmospheric reentry

Anchored ANOVA analysis (IJNME 2014, K. Tang, P.M. Congedo) applied to 50 uncertainties problem



Sensitivity analysis concerning the chemical reaction uncertainties during an atmospheric reentry

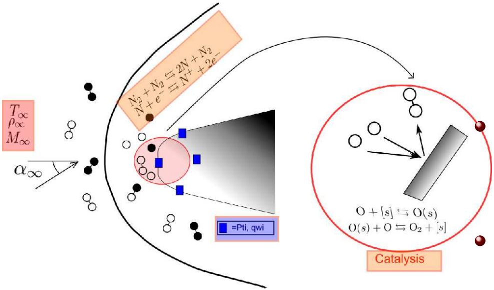
Major reactions among 50 reactions for which the rate coefficients are considered uncertain

Reaction	Reaction ID
N(2)+e=N(4)+e	7
N(2)+e=N(5)+e	8
N(1)+e=N(4)+e	3
N(2)+e=N(6)+e	9
N(12)+e=N(13)+e	22
N(1)+e=N(6)+e	5
N(3)+e=N(5)+e	11
N(3)+e=N(4)+e	10
N(3)+e=N(6)+e	12
N(1)+e=N(2)+e	1
O(13)+e=O(14)+e	48
O(7)+e=O(8)+e	42
O(1)+e=O(4)+e	28
O(1)+e=O(2)+e	26
O(2)+e=O(5)+e	33
...	...

$\Rightarrow$ Low order interactions of input variables have the main impact on QOI
$\Rightarrow$ The anchored ANOVA analysis allow us to retrieve the reactions that are significant to the QOI

Sensitivity analysis and characterization of the uncertain input data for the EXPERT vehicle

Characterization of the uncertain input data for the EXPERT vehicle
Forward problem

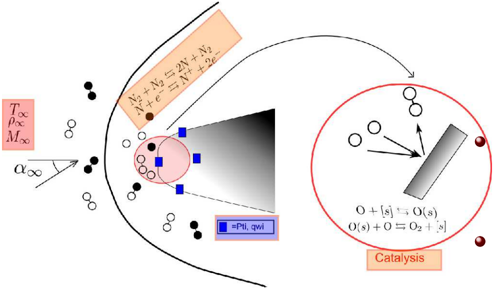


- **Input data**
  - Freestream pressure p_∞ and Mach number M_∞
  - Catalytic recombination coefficient γ and gas reaction rate coefficients $k_r, \quad r \in \{1, \ldots, n_R\}$
- **Output data**
  - Stagnation-point pressure p_{st} and heat flux q_{st}

- **COSMIC code** [Barbante 2001]: Axisymmetric NS eqs, high temperature reacting flows with gas/surface interaction
- **MUTATION library**: 5 species air $(\mathrm{N}, \mathrm{O}, \mathrm{N}_2, \mathrm{O}_2, \mathrm{NO})$ Park 2001 chemical mechanism, assuming thermal eq.

$\Rightarrow$ **Sources of uncertainties**
  - Unknown: $p_\infty \sim \mathcal{U}(16.3, 24.3)$ and $M_\infty \sim \mathcal{U}(13.7, 17.3)$
  - Arrhenius gas reaction rate coefficients: $\log_{10}(A_r) \sim \mathcal{N}(\mu_{r,0}, \sigma_r^2)$
  - Epistemic uniform uncertainty on $\gamma \sim \mathcal{U}(0.001, 0.002)$

CHARACTERIZATION OF THE UNCERTAIN INPUT DATA FOR THE EXPERT VEHICLE
INVERSE PROBLEM



- FADS measurements
  - Stagnation-point pressure p_{st} and heat flux q_{st}
- Uncertainties
  - Experimental data + chemical model parameters

- Investigation of one point of the trajectory of the EXPERT vehicle where chemical non-equilibrium effects are important

$$(p_\infty = 20.3, T_\infty = 245.5, M_\infty = 15.5)$$

$\Rightarrow$ **Objective**: determine uncertainties on freestream conditions p_∞ and M_∞ from the FADS data

Characterization of the uncertain input data for the EXPERT vehicle
Numerical difficulties

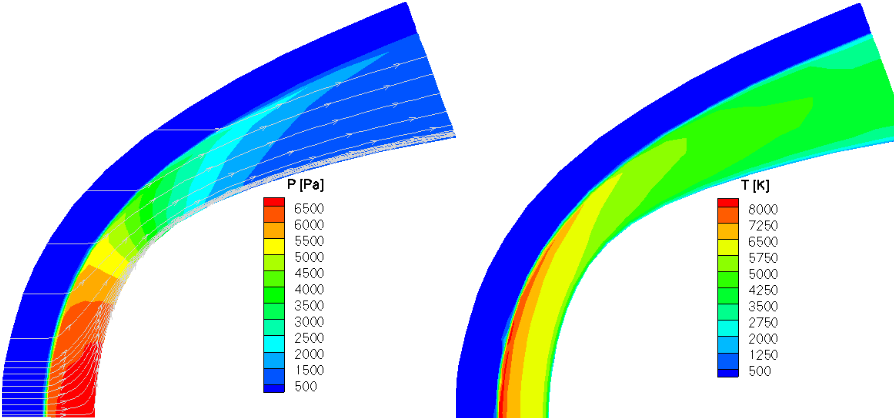
- Large number of uncertainties
- Time consuming CFD computation
  ($\approx$ 1h for one deterministic calculation!)
- Definition of efficient numerical techniques for Uncertainty Quantification (UQ)

Characterization of the uncertain input data for the EXPERT vehicle
Proposed approach

1. Study of the forward problem
   - *prior* uniform uncertainty on p_∞ and M_∞
   - use of NISP methods to compute PC expansions of p_{st} and q_{st}
   - sensitivity analysis from PC expansions
   - compute PC metamodels with uncertainties that have the most impact
2. Resolution of the stochastic inverse problem
   - Bayesian Inference methods
   - use of PC metamodels to accelerate the Bayesian algorithm

Characterization of the uncertain input data for the EXPERT vehicle
Deterministic Code

COSMIC [Barbante 01]



Pressure and temperature iso-contours of the flow around EXPERT obtained with input data mean values

Very short digression on PC

Polynomial Chaos (PC) expansions

[Wiener 38; Cameron & Martin 47; Ghanem & Spanos 91]
Every QOI u can be expanded in a convergent series of the form

$$u(\boldsymbol{\xi}) \approx u^{\mathrm{PC}}(\boldsymbol{\xi}) = \sum_{\alpha=0}^{\mathrm{P}} u_\alpha \Psi_\alpha(\boldsymbol{\xi}),$$

- $\mathrm{P} = (n_{\boldsymbol{\xi}} + \mathrm{No})!/n_{\boldsymbol{\xi}}!\mathrm{No}!$, No: expansion degree
- $\{\Psi_\alpha\}_{\alpha=0,\dots,\mathrm{P}}$ polynomial functions orthogonal w.r.t $p_{\boldsymbol{\xi}}$
- correspondence between $p_{\boldsymbol{\xi}}$ and $\{\Psi_\alpha\}$
- $\{u_\alpha\}_{\alpha=0,\dots,\mathrm{P}}$: deterministic spectral coefficients

Determination of $\{u_\alpha\}$ by a non-intrusive spectral method (NISP)

$$u_\alpha = \|\Psi_\alpha\|^{-2} \int u(\boldsymbol{\xi})\Psi_\alpha(\boldsymbol{\xi}) \approx \|\Psi_\alpha\|^{-2} \sum_{i=1}^{n} u(\mathbf{x}, t, \boldsymbol{\xi}_i)\Psi_\alpha(\xi_i)\omega_i$$

$(\boldsymbol{\xi}_i, \omega_i)$ quadrature formulae points and weigths $\rightarrow$ deterministic code used as a black box

Characterization of the uncertain input data for the EXPERT vehicle

Uncertainty Quantification

- PC forward expansions obtained from NISP methods
  $p_{\mathrm{st}}^{\mathrm{PC}}(p_\infty, M_\infty, \gamma, k_1, k_2, k_3, k_4) = \sum_\alpha (p_{\mathrm{st}})_\alpha \Psi_\alpha(p_\infty, M_\infty, \gamma, k_1, k_2, k_3, k_4)$
  $q_{\mathrm{st}}^{\mathrm{PC}}(p_\infty, M_\infty, \gamma, k_1, k_2, k_3, k_4) = \sum_\alpha (q_{\mathrm{st}})_\alpha \Psi_\alpha(p_\infty, M_\infty, \gamma, k_1, k_2, k_3, k_4)$
- Estimation of means, variances, and sensitivity information

	p_{st}			q_{st}		
	$\mathrm{No}=2$	$\mathrm{No}=3$	$\mathrm{No}=4$	$\mathrm{No}=2$	$\mathrm{No}=3$	$\mathrm{No}=4$
μ	$6.49 \cdot 10^3$	$6.49 \cdot 10^3$	$6.49 \cdot 10^3$	$2.75 \cdot 10^5$	$2.75 \cdot 10^5$	$2.75 \cdot 10^5$
σ^2	$1.36 \cdot 10^6$	$1.37 \cdot 10^6$	$1.39 \cdot 10^6$	$9.73 \cdot 10^9$	$2.01 \cdot 10^{10}$	$6.18 \cdot 10^{10}$

Table : Means (μ) and variances (σ^2) of p_{st} and q_{st} for $\mathrm{No} = 2, 3, 4$

Coefficients of variation (σ/μ) : 18% for p_{st}, 52% for q_{st}!

CHARACTERIZATION OF THE UNCERTAIN INPUT DATA FOR THE EXPERT VEHICLE
UNCERTAINTY QUANTIFICATION

		p_{st}	q_{st}
p_∞	S_1	$3.99 \cdot 10^{-1}$	$1.07 \cdot 10^{-2}$
	$S_{T,1}$	$4.07 \cdot 10^{-1}$	$6.18 \cdot 10^{-2}$
M_∞	S_2	$5.87 \cdot 10^{-1}$	$2.52 \cdot 10^{-1}$
	$S_{T,2}$	$5.99 \cdot 10^{-1}$	$7.14 \cdot 10^{-1}$
γ	S_3	$6.76 \cdot 10^{-4}$	$9.40 \cdot 10^{-2}$
	$S_{T,3}$	$2.30 \cdot 10^{-3}$	$3.03 \cdot 10^{-1}$
$\mathrm{O_2 + N_2 \rightarrow 2O + N_2}$	S_4	$4.54 \cdot 10^{-6}$	$9.31 \cdot 10^{-4}$
	$S_{T,4}$	$1.65 \cdot 10^{-4}$	$2.70 \cdot 10^{-2}$
$\mathrm{O_2 + O \rightarrow 2O + O}$	S_5	$3.90 \cdot 10^{-6}$	$6.35 \cdot 10^{-4}$
	$S_{T,5}$	$1.17 \cdot 10^{-4}$	$2.23 \cdot 10^{-2}$
$\mathrm{NO + O \rightarrow N + O + O}$	S_6	$2.21 \cdot 10^{-4}$	$3.01 \cdot 10^{-2}$
	$S_{T,6}$	$7.56 \cdot 10^{-4}$	$1.02 \cdot 10^{-1}$
$\mathrm{NO + N \rightarrow N + O + N}$	S_7	$6.58 \cdot 10^{-4}$	$8.86 \cdot 10^{-2}$
	$S_{T,7}$	$2.28 \cdot 10^{-3}$	$3.00 \cdot 10^{-1}$

TABLE : Sobol first order (S_i) and total order indices ($S_{T,i}$) for No $= 3$

Characterization of the uncertain input data for the EXPERT vehicle
Bayesian inference for the stochastic inverse problem

- Forward model : $\mathbf{d} = F(\mathbf{m}, \mathbf{c})$, $\mathbf{d} = (p_{\mathrm{st}}, q_{\mathrm{st}})$, $\mathbf{m} = (p_\infty, M_\infty)$, $\mathbf{c} = (\gamma, k_1, k_2, k_3, k_4)$
- "*prior* pdf + set of experimental data = *posterior* pdf fitting data"
- Bayes' rule
- measurement errors parameters $\boldsymbol{\sigma}_{\mathrm{st}} = (\sigma_{p_{\mathrm{st}}}, \sigma_{q_{\mathrm{st}}})$ supposed known
- metamodel $p_{\mathrm{st}}^{\mathrm{PC}}$ convergent, negligible dependence on chemical parameters $\rightarrow$ use of $p_{\mathrm{st}}^{\mathrm{PC}}(p_\infty, M_\infty, \gamma_0, k_{1,0}, k_{2,0}, k_{3,0}, k_{4,0})$ as a reduced PC metamodel in the Bayesian setting

Characterization of the uncertain input data for the EXPERT vehicle
Bayesian inference for the stochastic inverse problem

- metamodel $p_{\mathrm{st}}^{\mathrm{PC}}$ convergent, negligible dependence on chemical parameters
  $\rightarrow$ use of $p_{\mathrm{st}}^{\mathrm{PC}}(p_\infty, M_\infty, \gamma_0, k_{1,0}, k_{2,0}, k_{3,0}, k_{4,0})$ as a reduced PC metamodel in the Bayesian setting (chemical parameters fixed at their mean values)
- metamodel $q_{\mathrm{st}}^{\mathrm{PC}}$ non-convergent, important dependence on all parameters
  $\rightarrow$ can not be used as a metamodel in the Bayesian setting
- idea : solve first the stochastic inverse problem considering only $\{p_{\mathrm{st}}^1, \ldots, p_{\mathrm{st}}^n\}$ and using $p_{\mathrm{st}}^{\mathrm{PC}}$ in order to modify prior distribution of (p_∞, M_∞)

CHARACTERIZATION OF THE UNCERTAIN INPUT DATA FOR THE EXPERT VEHICLE

NUMERICAL RESULTS

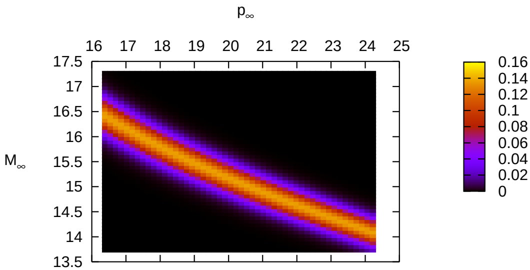
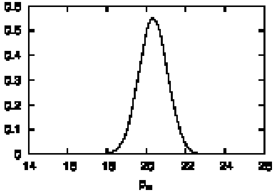


FIGURE : Joint posterior density relying on $p_{\mathrm{st}}^{\mathrm{PC}}$

- Prior distribution of (p_∞, M_∞) modified through Bayesian algorithm using metamodel for p_{st}
- A set of couples (p_∞, M_∞) plausible w.r.t measurements of p_{st}

Characterization of the uncertain input data for the EXPERT vehicle
Numerical Results

If M_∞ known: $M_\infty = 15$, uniform prior distribution $p_\infty \in [16.3, 24.3]$ + pseudo-measurements of $p_{\rm st}$ = posterior distribution for p_∞



- $\mu = 20.35$, $\sigma^2 = 0.48$, 90% confidence interval $[18.97, 21.71]$
- posterior approx. Gaussian because $p_{\rm st}$ roughly linear w.r.t. (p_∞, M_∞)
  It is not the case when considering $q_{\rm st}$ measurements!

Characterization of the uncertain input data for the EXPERT vehicle

- Setting up of a rigorous framework to take into account uncertainties in the resolution of the inverse problem
- Preliminary results obtained on the reconstruction from heat flux measurements
- Fast evaluation of a new prior distribution for (p_∞, M_∞) relying on p_{st} measurements and Bayesian algorithms
- Future validation based on the VKI Longshot and Plasmatron facilities by exploiting previous analysis

A cooperative work with some funding

Collaborative work VKI/INRIA

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- INRIA : P.M. Congedo, J. Tryoen, K. Tang, F. Sanson, M. Duvernet
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