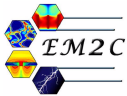

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Dimension reduction and surrogate-modelling for uncertain auto-igniting flame simulations

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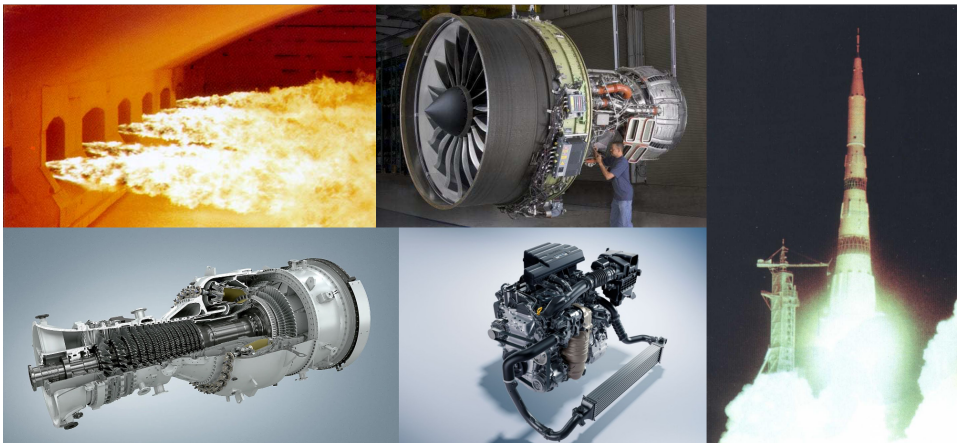
25/06/2020

A few words about combustion



Independance from fossil fuels

- Non-hydrocarbon fuels (e.g. Hydrogen-based)
- Bio-fuels

Risks and safety

- Extinction and ignition
- Transition towards detonation
- Wildfire propagation

Process improvement

- Pollutants prediction and reduction (Soot particules and NOx)
- Lean combustion
- Thermo-acoustic instabilities
- Plasma-assisted combustion

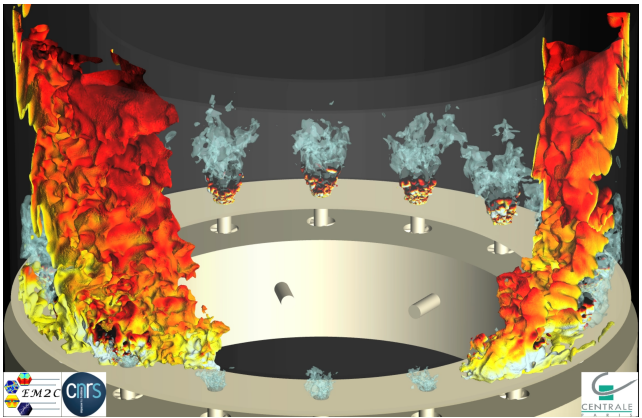
Transverse tools

- Experimental setups and diagnostics
- Simulation tools

An example of LES at EM2C

- Light-round ignition of the MICCA chamber[a]
- TFLES and subgrid-scale wrinkling model, 2-step global chemistry
- 2M CPU-hours on 10000 cores

[a] Philip et al. 2014.



For a typical jet flame simulation:

RANS

- $\sim$ 10k cells
- 1 CPU-hour
- Limited to steady states, models a lot of things

$\Rightarrow$ Cheap, but no very precise

DNS

- $\sim$ 10G cells
- 100M CPU-hour
- Resolves everything

$\Rightarrow$ Intractable for practical cases

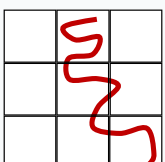
LES

- $\sim$ 10M cells
- 10k CPU-hour
- Captures unsteady phenomena and some details, models small scales

$\Rightarrow$ Sweet spot for combustion simulations

Resolution issue

Problem:
The flame front (~ 0.1 mm) is much thinner than the typical LES mesh cell (~ 1 mm)



Solution:
Subgrid-scale models

"Curse" of the chemistry

Problem:

- Fluid dynamics alone: 5 transport equations
- Fluid dynamics + CH_4 combustion: 57 transport equations +325 reaction source terms

Solution:
Chemistry reduction methods

We need approximate models to deal with combustion in LES

We pay for accuracy while uncertainties can be significant

Possible consequences of a deterministic approach

- Difficult comparison of simulations and experiment
- Poor pollution prediction
- Untimely ignition or extinction

Uncertainty sources

- Fuel composition (e.g. bio-fuels)
- Geometry (injector, swirler...)
- Operating point (Temperature, pressure, flow rate...)
- Combustion and turbulence models
- Chemical kinetic mechanism

Chemistry only

- [a]Sensitivity analysis on kinetic mechanisms
- [b]Consistency of a kinetic mechanism from a UQ standpoint, 102 Uncertain Parameters (UP)
- [cd]Uncertain H_2/O_2 mechanism

[a] Miller and Frenklach 1983.
[b] Frenklach, Packard, and Seiler 2002.
[c] Konnov 2008.
[d] Bell et al. 2019.

Reactive CFD

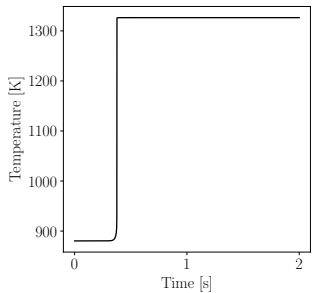
- [a]LES, 1UP (chemical kinetics)
- [b]LES, 3UP (turbulence model)
- [c]RANS, 7UP (operating conditions)
- [d]RANS, 21UP (chemical kinetics)

The way forward

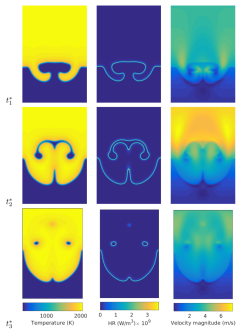
Complex UQ studies on LES

[a] Mueller, Iaccarino, and Pitsch 2013.
[b] Khalil et al. 2015.
[c] Constantine et al. 2015.
[d] Ji et al. 2019.

Nicolas DUMONT: Mostly theoretical work on 0D reactors, enables the use of chemistry tabulation for uncertain LES



Jan MATEU ARMENGOL: Parallel approach, up to 2D DNS



Goal of the study

Scaling up to handle 3D LES with uncertain chemistry

Contents

The case study

Configuration

- Lifted H_2 diffusion flame in a vitiated co-flow
- Quantity of interest: Lift-off height

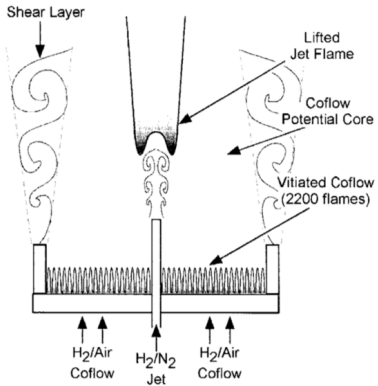
Why study this flame ?

- Simple flow configuration
- Flame stabilized in vitiated atmosphere
- Lift-off mainly piloted by auto-ignition delay[a b]

[a] Cao, Pope, and Masri 2005.

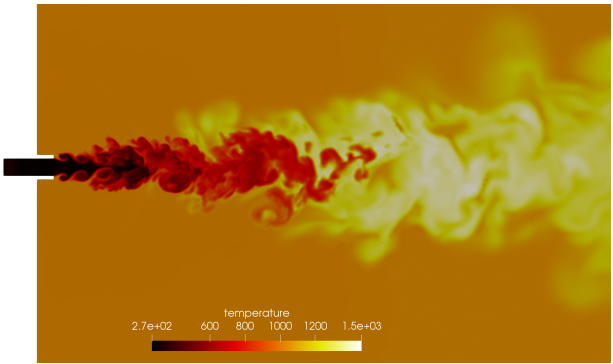
[b] Masri et al. 2004.

The Cabra[a] setup

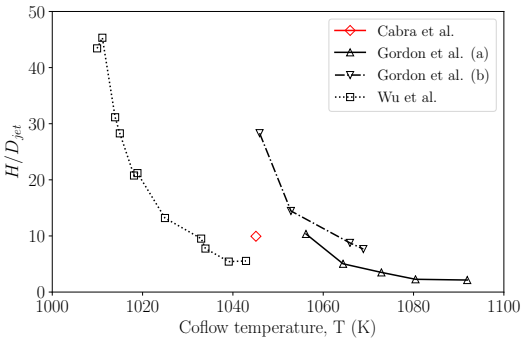


[a] Cabra et al. 2002.

LES of the Cabra flame	
Mesh size	10M cells
CPU cost	10k hours
Turb. model	WALE
Comb. model	UFPV tabulation



In experiments[abc]

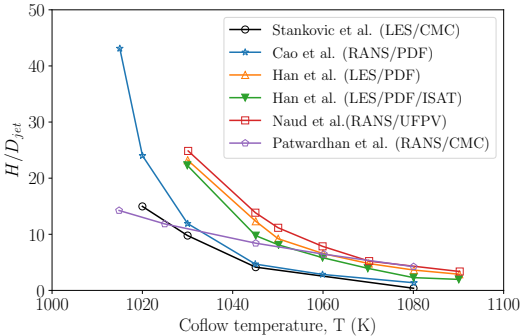


[a] Cabra et al. 2002.

[b] Gordon et al. 2007.

[c] Wu, Masri, and Bilger 2006.

In simulations[abcde]



[a] Stanković, Mastorakos, and Merci 2013.

[b] Cao, Pope, and Masri 2005.

[c] Han, Raman, and Chen 2016.

[d] Naud et al. 2015.

[e] Patwardhan et al. 2009.

Kinetic uncertainties

- Uncertain $H_2 - O_2$ kinetic mechanism: Konnov[a]
- Log normal distributions (eq. 2) of Arrhenius rate constants
- The other kinetic parameters are constant
- 33 uncertain variables

[a] Konnov 2008.

Arrhenius law:

$$k_j = A_j T^{\beta_j} exp\left(\frac{-Ea_j}{RT}\right) \quad (1)$$

$$\xi_j = \frac{ln(A_j/A_j^0)}{\frac{1}{3}ln(UF_j)} \sim \mathcal{N}(0,1),\ j = 1,...,33 \quad (2)$$

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Co-flow temperature uncertainty

- Cabra[a]: 3% ($\pm 30K$) uncertainty on co-flow temperature
- Must be taken into account to compare the simulation with the experimental results
- Uniform distribution (eq. 3) of co-flow temperature

$$T \sim \mathcal{U}(T_{Min}, T_{Max}) \qquad (3)$$

[a] Cabra et al. 2002.

Cost of the Monte-Carlo approach

- Unitary simulation cost: $\approx 10^4 h$
- Thumb-rule of the number of necessary runs with Monte-Carlo methods: 10^4
- Total cost of the "naive" approach: $10^8 h$

Cost-reduction levers

- Surrogate modelling:
  Building a surrogate model of the configuration with a few points and resample it to obtain the statistics
- Uncertain-dimension reduction
  $\Rightarrow$ Reduce the number of runs to build the surrogate

This study

Identifying a reduced set of uncertain variables and a surrogate modelling approach suitable for dealing with the case study.

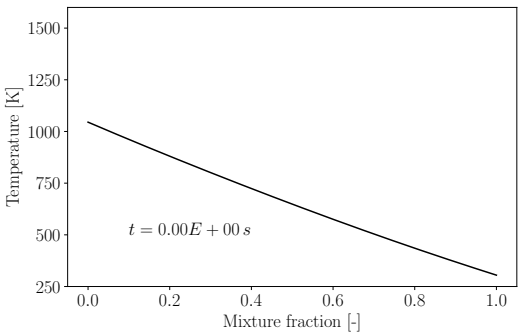
Reducing the physics

Auto-igniting diffusion flamelet - RP1

- Ihme et al.[a]: Chemistry in Cabra flame well emulated with UFPV tabulation
- UFPV = Auto-igniting diffusion flamelets
- A UQ study on unsteady diffusion flamelets should be representative for kinetic uncertainties
- Computation time / sample: $\sim$ 10 min

[a] Ihme and See 2010.

Auto-ignition of diffusion flamelet
Konnov[a] mechanism



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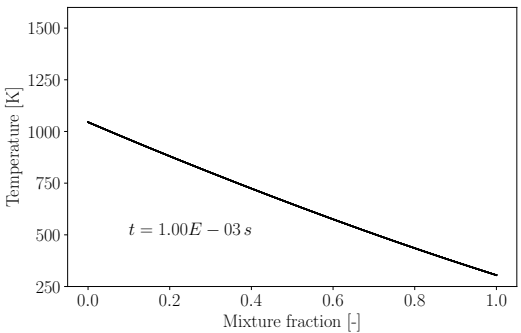

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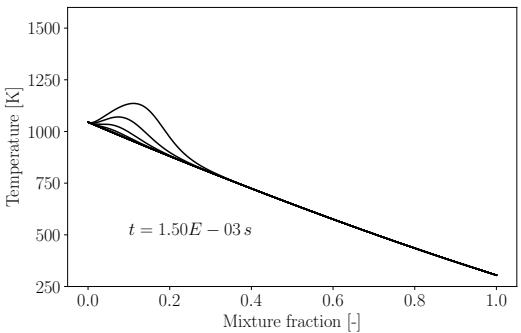

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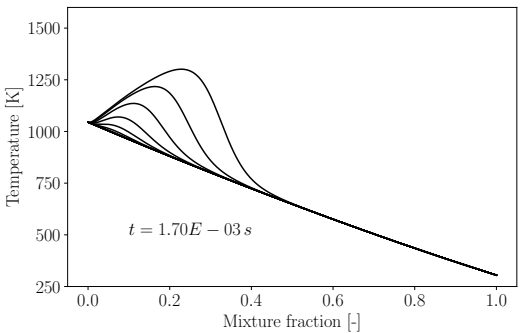

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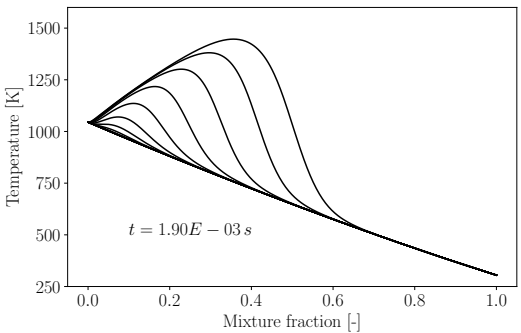

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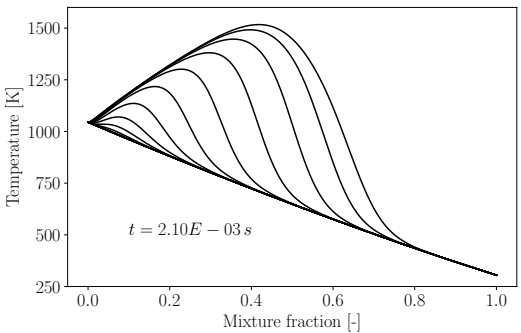

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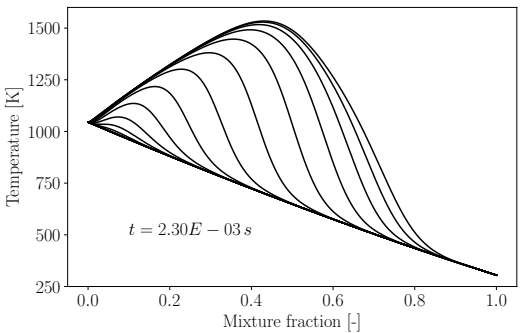

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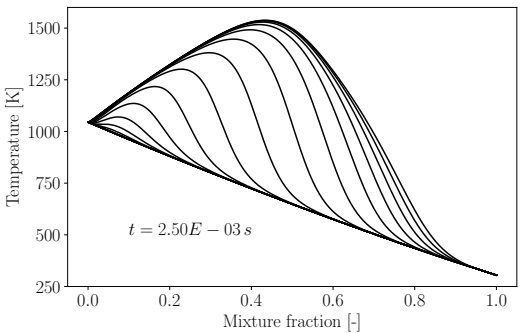

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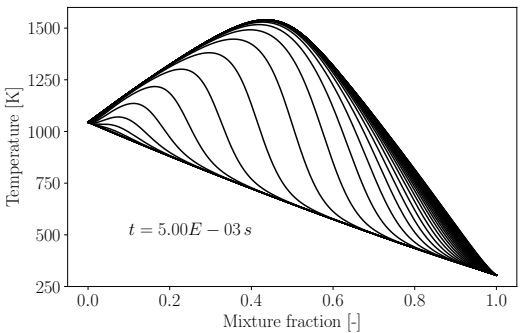

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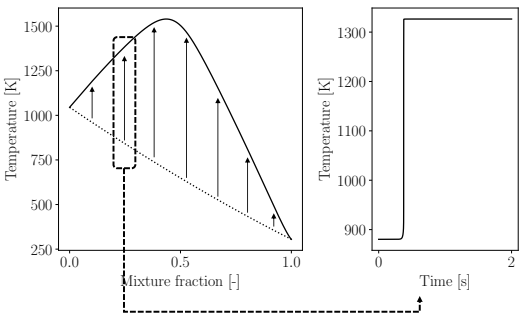
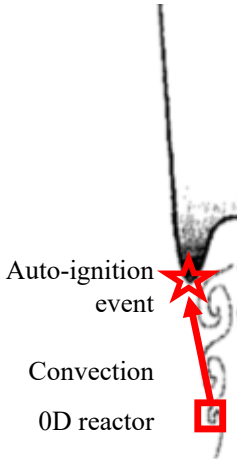


[a] Konnov 2008.

An even more reduced model: Homogeneous reactor - RP0

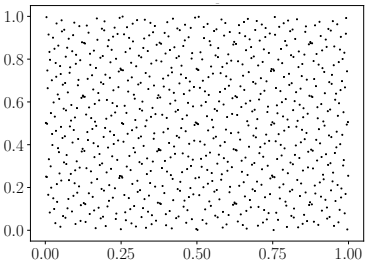
- Most reactive fuel/air ratio found in the flamelet model
- Very fuel lean, very hot
- The QoI becomes the auto-ignition delay time (τ)
- Computation time / sample: $\sim$ 0.1 s

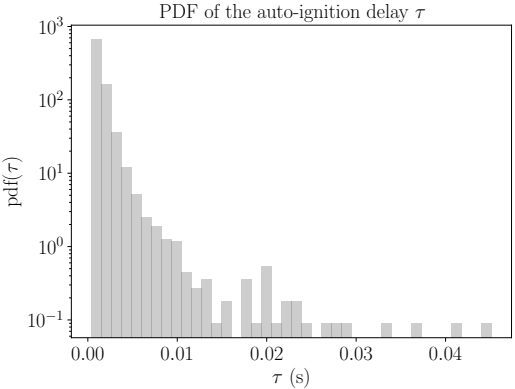


Quasi Monte-Carlo Sampling

10^5 samples drawn from the 34D Sobol sequence

Illustration of a 2D Sobol sequence





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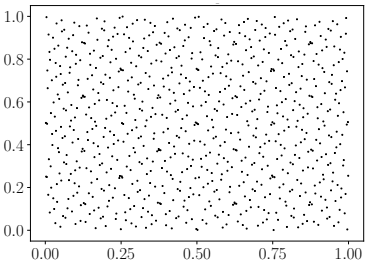

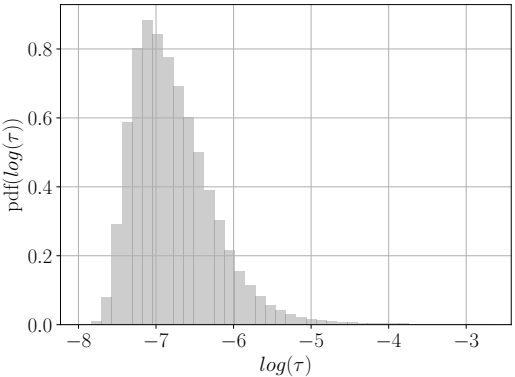

Useful statistics

- mean:
  1.40 ms
- Result of nominal simulation:
  1.02 ms
- 95% confidence interval:
  [0.54 ms, 4.1 ms]

A bit of perspective

- H_2/O_2 is one of the simplest/most studied mechanisms
- Here, CFD studies use kinetic mechanisms that are highly uncertain
- Depending on the case, confidence in CFD results should be carefully weighted

Reducing the uncertain dimension

Method 1: "Sobol" reduction

We use the Sobol' sensitivity indices (portions of the variance of the QoI explained by variables and groups of variables) to reduce the uncertain dimension.

Sobol-Hoeffding decomposition (hierarchical and orthogonal, unique):

$$F(\boldsymbol{\xi}) = \sum_{\iota \subseteq \mathcal{D}} F_\iota(\boldsymbol{\xi}_\iota) \tag{4}$$

Definition of Sobol indices:

$$\mathcal{S}_\iota = \frac{\mathbb{V}[F_\iota]}{\mathbb{V}[F]} \leq 1, \quad \sum_{\iota \subseteq \mathcal{D} \setminus \emptyset} \mathcal{S}_\iota = 1 \tag{5}$$

Method 1: "Sobol" reduction

We use the Sobol' sensitivity indices (portions of the variance of the QoI explained by variables and groups of variables) to reduce the uncertain dimension.

Sobol-Hoeffding decomposition for 2 variables:

$$F(\xi_1, \xi_2) = F_0 + F_1(\xi_1) + F_2(\xi_2) + F_{12}(\xi_1, \xi_2) \tag{4}$$

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Polynomial Chaos Expansion for 2 variables:

$$F(\xi_1, \xi_2) \approx \mathcal{P}(\xi_1, \xi_2) = \mathcal{P}_0 + \mathcal{P}_1(\xi_1) + \mathcal{P}_2(\xi_2) + \mathcal{P}_{12}(\xi_1, \xi_2) \tag{4}$$

Approximation of Sobol indices:

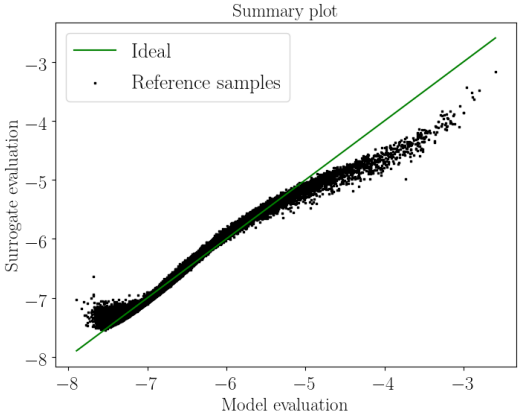
$$\mathcal{S}_\iota = \frac{\mathbb{V}[F_\iota]}{\mathbb{V}[F]} \approx \frac{\mathbb{V}[\mathcal{P}_\iota]}{\mathbb{V}[\mathcal{P}]} \leq 1 \tag{5}$$

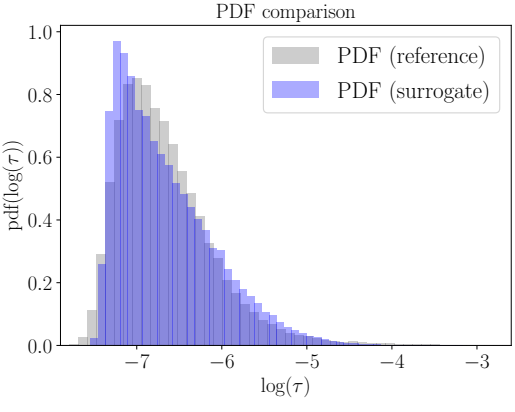
Obtaining the PCE of the auto-ignition delay

- We recycle the QMC samples already computed
- We generate a hybrid Legendre-Hermite polynomial basis of total order 2.
- We use a regression method to compute the PCE coefficients

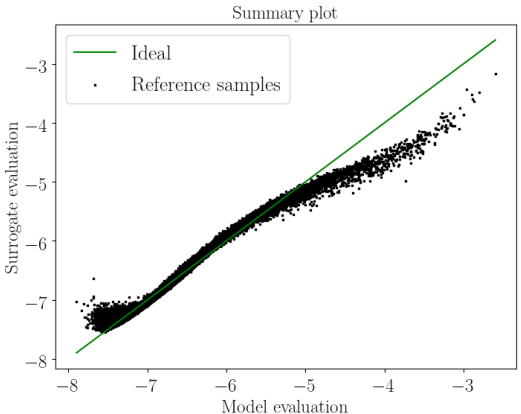
What about the quality of the PCE ?

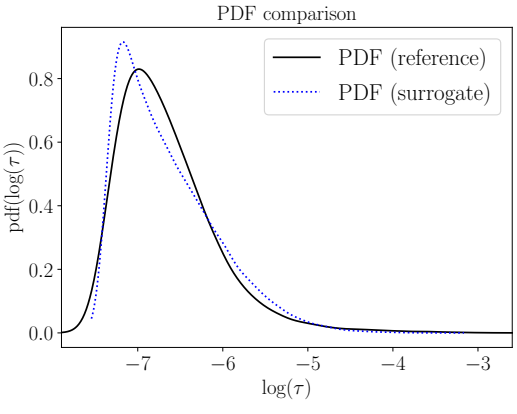
- The QoI may not be adequately emulated
- We need a proper validation of the PCE





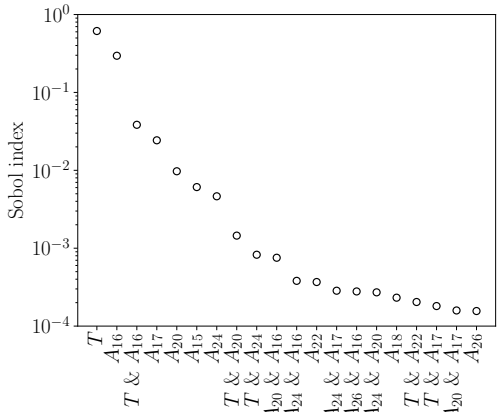
The surrogate is not ideal but it still captures the main feature of the distribution. Further validation will be necessary when reducing the uncertain dimension.





The surrogate is not ideal but it still captures the main feature of the distribution. Further validation will be necessary when reducing the uncertain dimension.

We plot the first- and second-order Sobol indices of the QoI in decreasing order:



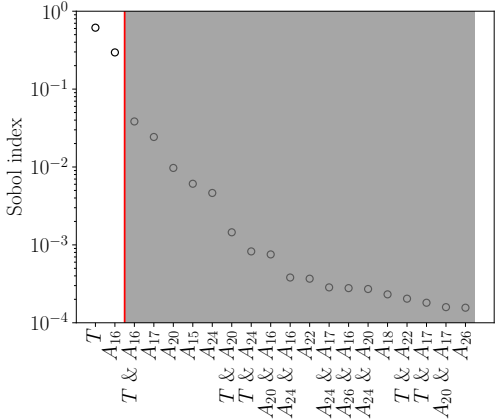
- **Temperature** uncertainty is predominant
- The uncertainty on the 16th reaction is next
  - $H + O_2 = OH + O$
  - Explained by very high sensitivity despite low uncertainty factor[a]
  - Consistent with the literature[b]

[a] Masten, Hanson, and Bowman 1990.

[b] Ji et al. 2019.

Selection of relevant uncertainties

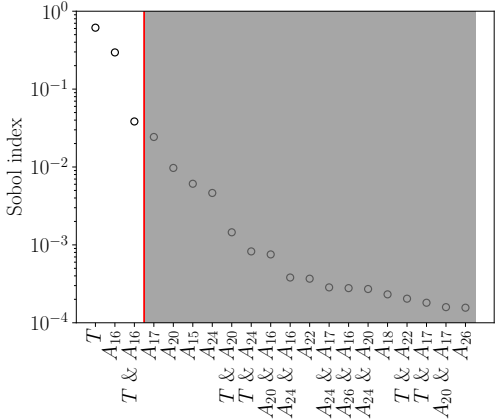
- $\mathcal{S}_T \sim \mathcal{S}_{A_{16}}$
- Every other sobol indices are at least one order of magnitude lower



Selection of relevant uncertainties

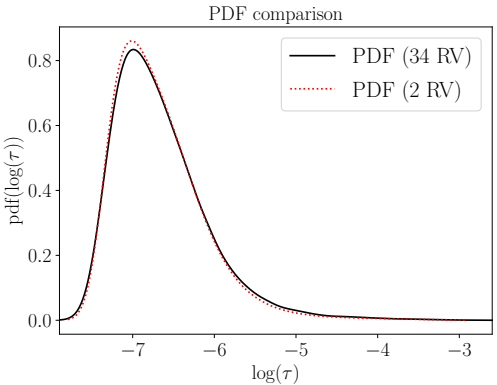
- $\mathcal{S}_T \sim \mathcal{S}_{A_{16}}$
- Every other sobol indices are at least one order of magnitude lower

$\Rightarrow$ Over 95% of the variance should be explained in a 2D uncertain space



Validation

- We sample again RP0 in the reduced uncertain space
- We compare the PDF of the QoI for 34 and 2 input random variables (RV)
- The PDF nearly collapse
  $\Rightarrow$ The dimension reduction is validated



Method 2: Active direction detection

We sort the directions $\boldsymbol{w}_i$ in which the QoI F encounters the steepest gradients, and then retain only the most important direction.

Assumptions:

- F is monotonous with each ξ_i
- An Active Direction (AD) can be discovered
- On the AD, F is not too far from a linear function

We can then determine the AD $\boldsymbol{w}_1$ with a linear regression of F:

$$F(\boldsymbol{\xi}) = \boldsymbol{b}^T \boldsymbol{\xi} + b_0 + \tilde{F}(\boldsymbol{\xi}) \tag{6}$$

And:

$$\boldsymbol{w}_1 = \boldsymbol{b}^T / \|\boldsymbol{b}\|_2 \tag{7}$$

Expectations

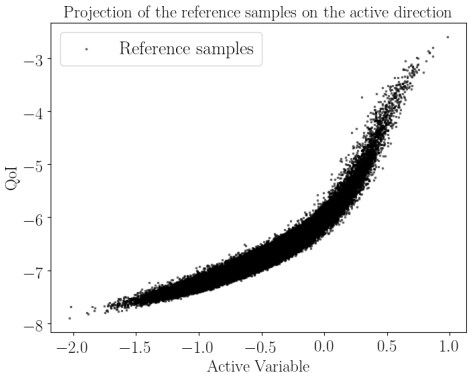
- Most of the variability should be retained on the AD
- A surrogate built on the AD should also be a good approximation of F

Warning

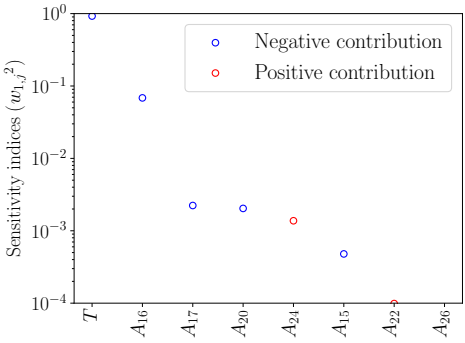
There is no a priori quantitative guarantee of the quality of the active direction

Application to the Full chemistry + Temperature (34D)

We obtain a "noisy" 1D dataset

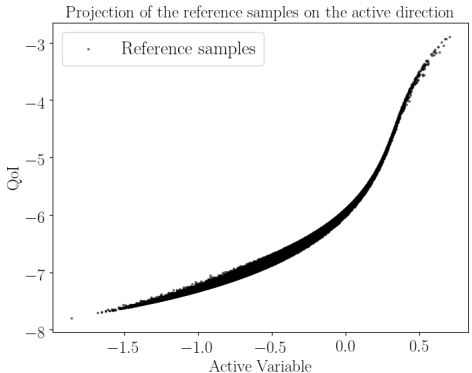


We can extract sensitivity indices from the AD coordinates

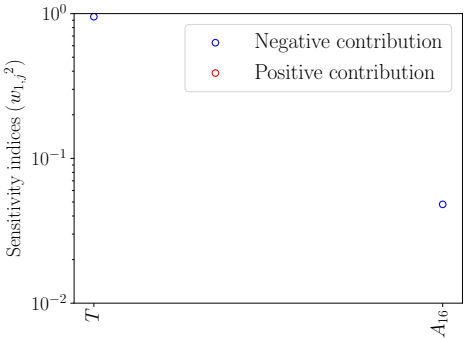


Combining the two methods: Application to the Sobol-reduced dataset (2D)

We obtain a much less noisy 1D dataset



We can extract sensitivity indices from the AD coefficients



Design of experiment for the unmitigated problem

Roadmap

1. Identify several surrogate modelling methods
2. Benchmark them on the RP0
   $\Rightarrow$ Representative of the performance on the unmitigated physical problem (LES)
3. Validation tests of the best method on different problems
4. If conclusive, keep on with the method for the uncertain LES

Reduction method	**Short form**
Sobol indices (2D)	Sob
Active direction (1D)	AD

Surrogate method	**Short form**
PCE (Projection)	PCE-P
PCE (Regression)	PCE-R
Kriging	Kr
Spline	Sp

Methodology example: Sob+PCE-P

The projection method

- Based on the computation of integrals
- Accesible with advanced quadrature rules
- Should not need many sample points to build a decent surrogate

To compute the PCE coefficients, we project the QoI on each basis polynomial. With:

$$F(\boldsymbol{\xi}) \approx \mathcal{P}^p(\boldsymbol{\xi}) = \sum_{k=0}^{P} f_k \cdot \psi_k(\boldsymbol{\xi})$$

We have:

$$f_k = \frac{\langle F, \psi_k \rangle}{\langle \psi_k, \psi_k \rangle} \tag{8}$$

The projection method

- Based on the computation of integrals
- Accesible with advanced quadrature rules
- Should not need many sample points to build a decent surrogate

To compute the PCE coefficients, we project the QoI on each basis polynomial. With:

$$F(\boldsymbol{\xi}) \approx \mathcal{P}^p(\boldsymbol{\xi}) = \sum_{k=0}^{P} f_k \cdot \psi_k(\boldsymbol{\xi})$$

We have:

$$f_k = \frac{1}{\langle \psi_k, \psi_k \rangle} \int_{\Xi} F(\boldsymbol{x}) \psi_k(\boldsymbol{x}) \pi_{\boldsymbol{\xi}}(\boldsymbol{x}) d\boldsymbol{x} \qquad (9)$$

The projection method

- Based on the computation of integrals
- Accesible with advanced quadrature rules
- Should not need many sample points to build a decent surrogate

To compute the PCE coefficients, we project the QoI on each basis polynomial. With:

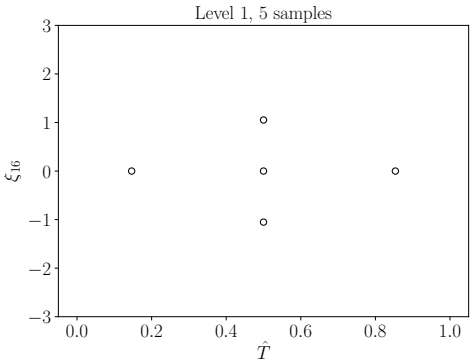
$$F(\boldsymbol{\xi}) \approx \mathcal{P}^p(\boldsymbol{\xi}) = \sum_{k=0}^{P} f_k \cdot \psi_k(\boldsymbol{\xi})$$

We have:

$$f_k \approx \frac{1}{\langle \psi_k, \psi_k \rangle} \sum_{i=1}^{N} w^{(i)} F(\boldsymbol{\xi}^{(i)}) \psi_k(\boldsymbol{\xi}^{(i)}) \qquad (10)$$

Sampling method

- Nested quadrature method: Fejer of the second kind
- ~~Tensorisation~~
- Sparse "Smolyak" tensorisation
- Easy addition of new dimensions if necessary



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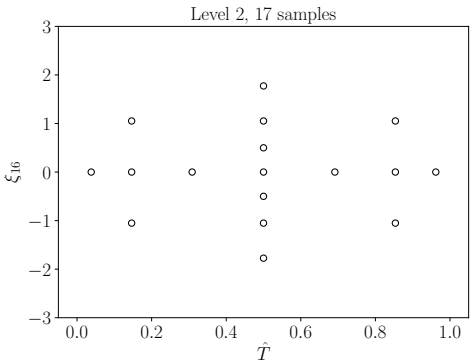

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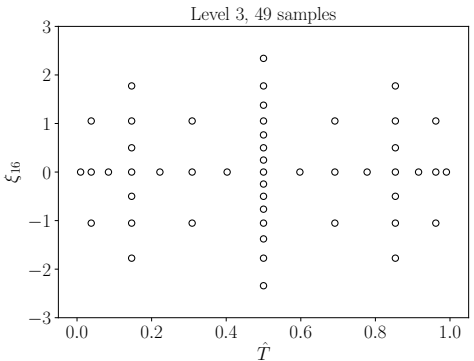

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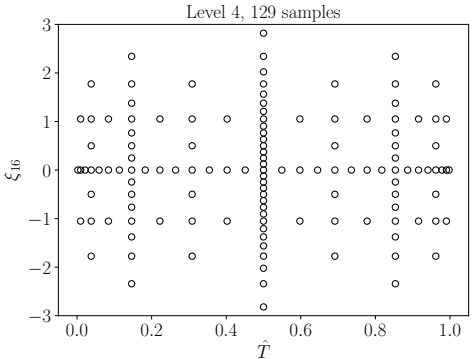

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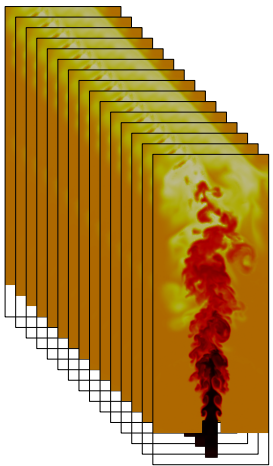
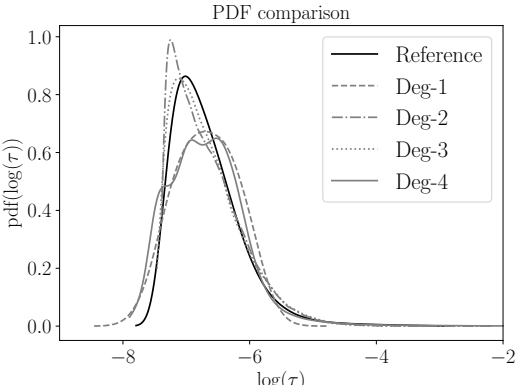
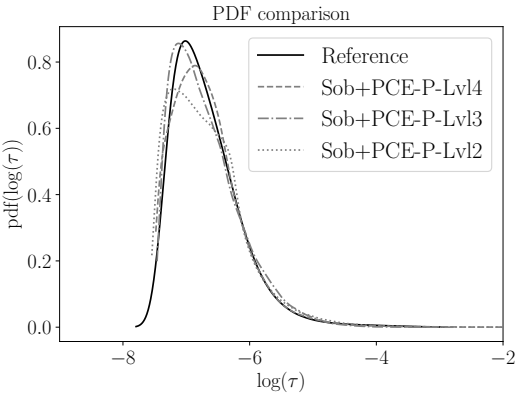
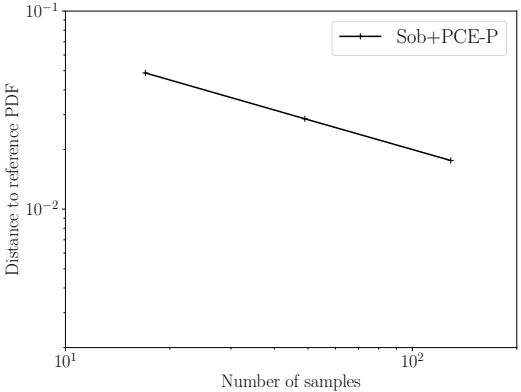


Selection of the best PCE for a level 3 quadrature (49 samples)



Based on the Wasserstein distance to the reference, the PCE of total order 3 is the best performing for 49 samples with the projection method


PDF comparison
Reference
Sob+PCE-P-Lvl4
Sob+PCE-P-Lvl3
Sob+PCE-P-Lvl2
pdf(log(τ))
log(τ)
0.0
0.2
0.4
0.6
0.8
−8
−6
−4
−2


Sob+PCE-P
Distance to reference PDF
Number of samples
10^{-1}
10^{-2}
10^{1}
10^{2}

Sampling method

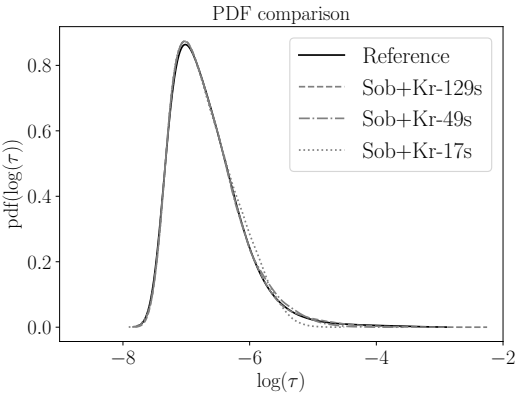
Quasi Monte-Carlo method: Sobol sequence
Because very few points and:

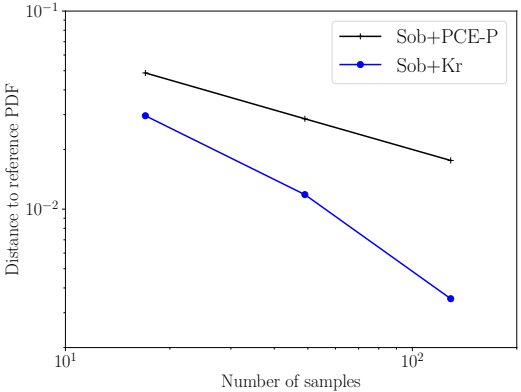
- Not really interested in randomization
- Very interested in filling the uncertain space

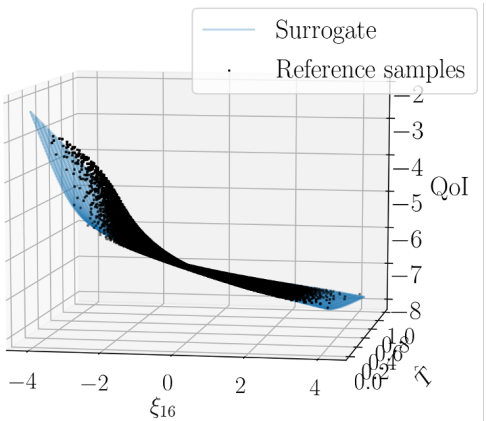
Kriging settings

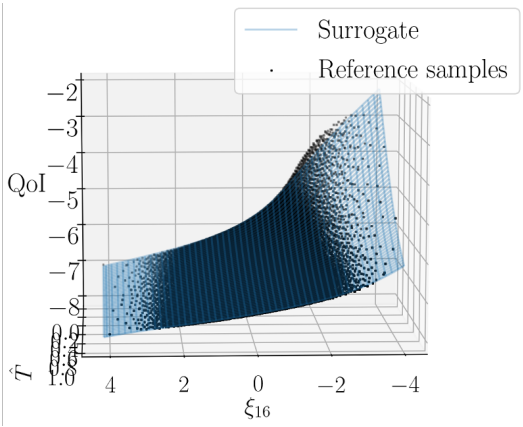
Beginner's choice:

- Matérn covariance kernel
- Linear trend


PDF comparison
Reference
Sob+Kr-129s
Sob+Kr-49s
Sob+Kr-17s
pdf(log(τ))
log(τ)
0.0
0.2
0.4
0.6
0.8
−8
−6
−4
−2


Sob+PCE-P
Sob+Kr
Distance to reference PDF
Number of samples
10^{-1}
10^{-2}
10^{1}
10^{2}


Surrogate
Reference samples
QoI
ξ_{16}
$\hat{T}$


Surrogate
Reference samples
QoI
$\hat{T}$
ξ_{16}

Global fit $\Rightarrow$ more relevant for non-polynomial QoI

Sampling method

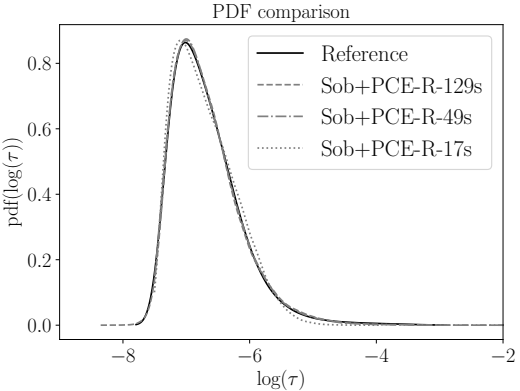
Quasi Monte-Carlo method: Sobol sequence

Because very few points and:

- Not really interested in randomization
- Very interested in filling the uncertain space

PCE-R settings

- Parametric study on total degree (Fixed basis)
- Least-square optimisation to find the coefficients, K-fold cross validation


PDF comparison
Reference
Sob+PCE-R-129s
Sob+PCE-R-49s
Sob+PCE-R-17s
pdf(log(τ))
log(τ)
0.0
0.2
0.4
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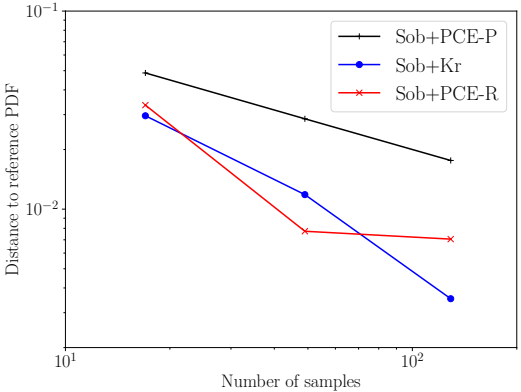

Sob+PCE-P
Sob+Kr
Sob+PCE-R
Distance to reference PDF
Number of samples
10^{-1}
10^{-2}
10^{1}
10^{2}

There is no guarantee the AD stays strictly the same when we change the physical model
$\Rightarrow$ We need to determine a new AD for each physical problem.

Situation 1: Direct AD

- The original uncertain space has 34D
- We consider sampling a few tens of realisations

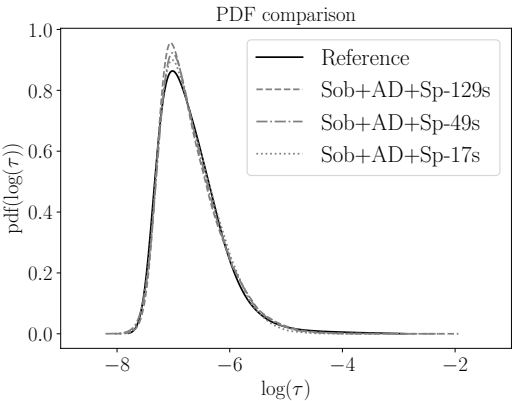
$\Rightarrow$ The direct determination of an AD on the original uncertain space (linear regression) is not over-determined enough

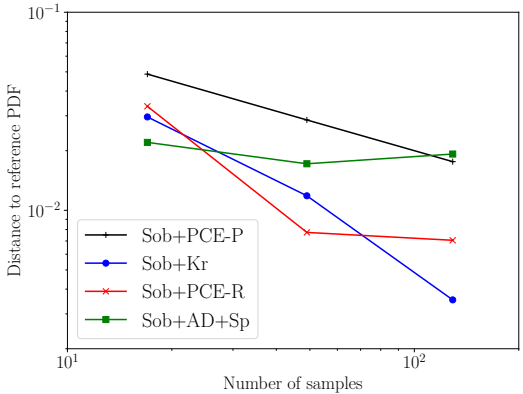
Situation 2: Sob+AD

- The reduced uncertain space has only 2D
- We consider sampling a few tens of realisations

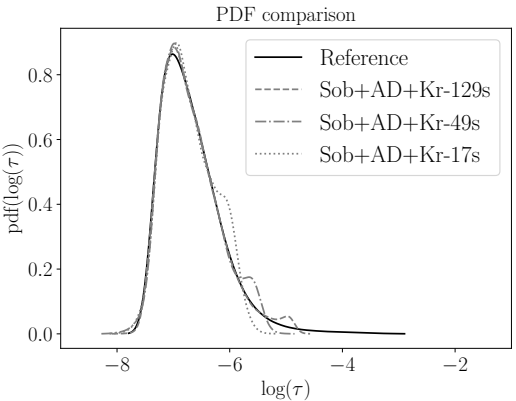
$\Rightarrow$ The direct AD is well over-determined

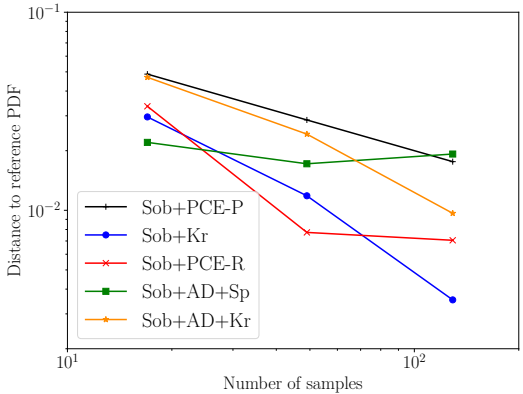
With spline surrogates

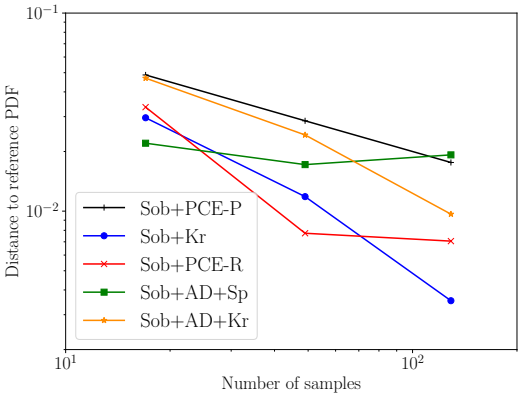




With kriging surrogates





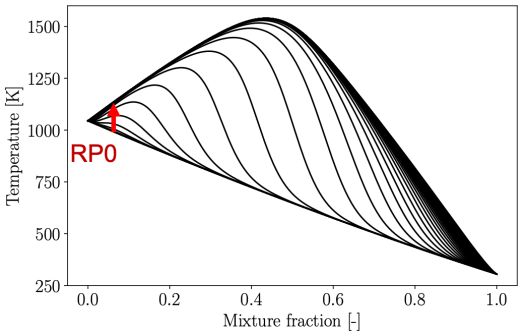


Remarks

- The global fit provided by PCE-R is always better than PCE-P in this case
- The surrogates built on active directions are not performing as well as expected
- Kriging and PCE-R are performing better than the other methods for nearly every dataset size

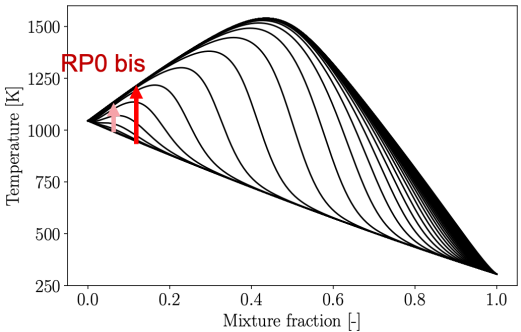
Check #1: RP0 bis

-



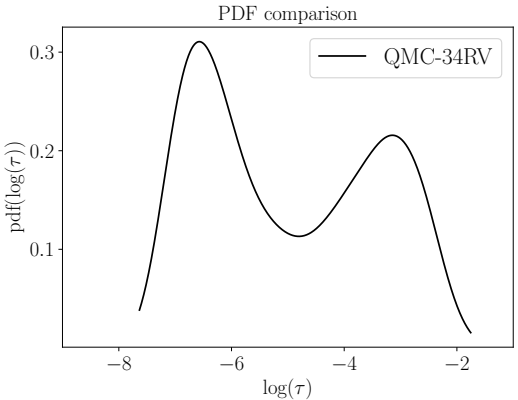
Check #1: RP0 bis

- We change the fuel-air ratio of the reactor



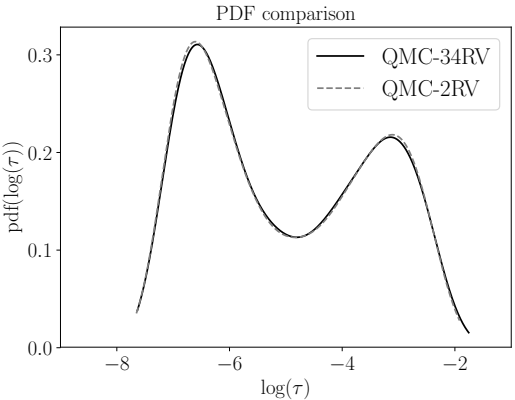
Check #1: RP0 bis

- We change the fuel-air ratio of the reactor
- The distribution of the QoI becomes bimodal



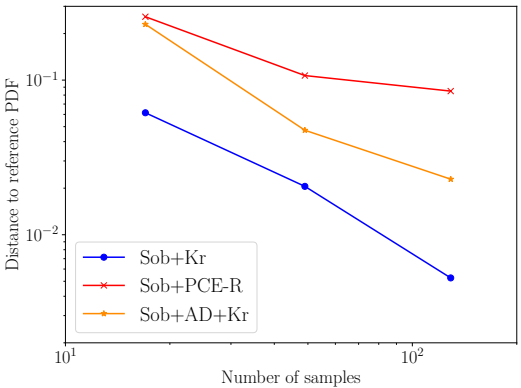
Check #1: RP0 bis

- We change the fuel-air ratio of the reactor
- The distribution of the QoI becomes bimodal
- The uncertain dimension reduction still holds



Check #1: RP0 bis

- We change the fuel-air ratio of the reactor
- The distribution of the QoI becomes bimodal
- The uncertain dimension reduction still holds
- Kriging on the 2D space is still the best performing method
- Regression PCE is not robust enough for this configuration



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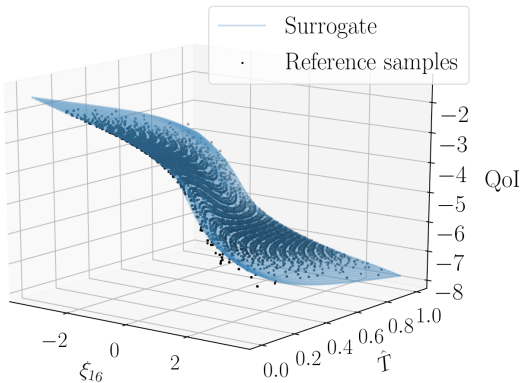
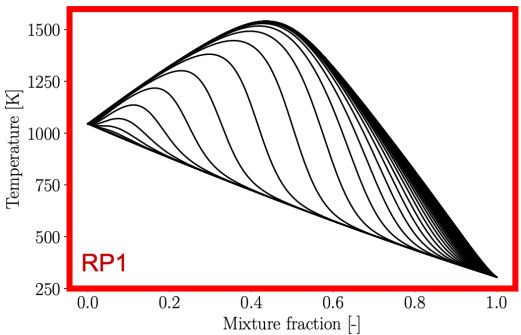
Kriging response surface



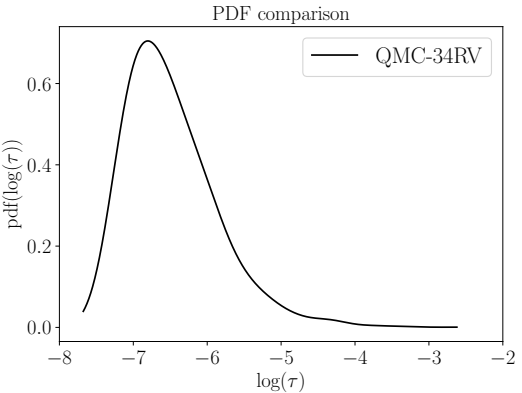
Check #2: RP1

- Now we look at the whole flamelet model (RP1)



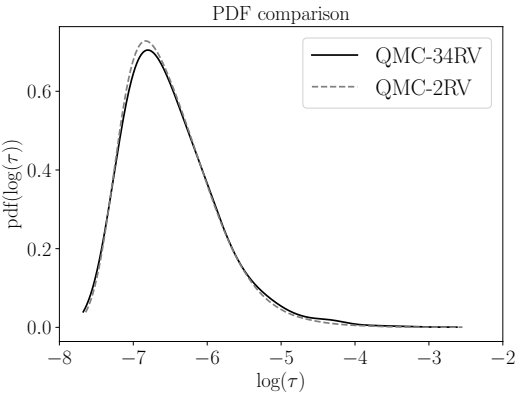
Check #2: RP1

- Now we look at the whole flamelet model (RP1)



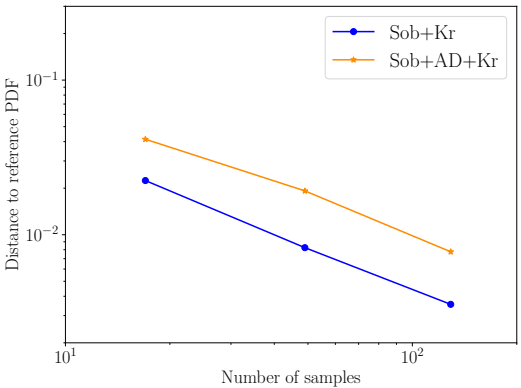
Check #2: RP1

- Now we look at the whole flamelet model (RP1)
- The uncertain dimension reduction still holds



Check #2: RP1

- Now we look at the whole flamelet model (RP1)
- The uncertain dimension reduction still holds
- Kriging on the 2D space is still the best performing method



Conclusion

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Dimension reduction

- We used a representative reduced problem to perform sensitivity analysis
- A 2D uncertain space has been found in which most of the variance is reproduced
- When such preliminary study is not doable for some variables, one can still try to reduce the uncertain dimension with active directions

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- Quadrature sampling can be ruled out in this case as PCE-P is performing worse than every other method
- Kriging seems to be the best candidate for efficient surrogate modelling on very reduced dataset
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Conclusion

- For the uncertain LES, a limited Sobol-sequence sampling will be performed on the 2D uncertain space
- On this small dataset, Kriging will be performed to obtain a surrogate of the lift-off height of the Cabra flame

Perspectives

Now we "only" need to compute a few tens of LES !

Questions ?

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Backup slides

Let $(F : \boldsymbol{\xi} \in \Xi) \in \mathbb{R}^d \to \mathbb{R}$ be the physical model where $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_d)$ are independent real valuded random variables of joint-PDF $p_{\boldsymbol{\xi}}$
Let $\{\psi_\alpha\}$ be the set of d-variate orthogonal polynomials

$$\psi_\alpha(\boldsymbol{\xi}) = \prod_{i=1}^{d} \psi_{\alpha_i}^{(i)}(\xi_i) \tag{11}$$

If $F \in \mathcal{L}_2(\Xi, p_{\boldsymbol{\xi}})$, it has a (spectrally) convergent PC expansion:

$$F(\xi) = \lim_{N \to \infty} \sum_{\|\alpha\| \leq N} \psi_\alpha(\boldsymbol{\xi}) F_\alpha, \quad \|\alpha\| = \sum_{i=1}^{d} |\alpha_i| \tag{12}$$

With the Sobol-Hoeffding decomposition written as:

$$F(\boldsymbol{\xi}) = \sum_{\iota \subseteq \mathcal{D}} F_\iota(\boldsymbol{\xi}_\iota) \tag{13}$$

We get the approximate S-H functionals as truncated PC terms:

$$F\iota(\boldsymbol{\xi}_\iota) \approx \sum_{\|\alpha\| \in \mathcal{A}_\iota} \psi_\alpha(\boldsymbol{\xi}_\iota) F_\alpha \tag{14}$$

With $\mathcal{A}_\iota = \{\alpha \in \mathcal{A},\, \alpha_i > 0 \text{ for } i \in \iota, \alpha_i = 0 \text{ for } i \notin \iota\} \subsetneq \mathcal{A}$ Then:

$$\mathcal{S}_\iota(F) \approx \frac{\sum_{\alpha \in \mathcal{A}_\iota} F_\alpha^2 \langle \psi_\alpha, \psi_\alpha \rangle}{\sum_{\alpha \in \mathcal{A}} F_\alpha^2 \langle \psi_\alpha, \psi_\alpha \rangle} \tag{15}$$

Finding an active subspace (AS) starts with performing a base change on the uncertain space:

$$\boldsymbol{C}_F = \int_{\Xi} (\nabla_{\boldsymbol{\xi}} F(\boldsymbol{x})) (\nabla_{\boldsymbol{\xi}} F(\boldsymbol{x}))^T \pi_{\boldsymbol{\xi}}(\boldsymbol{x}) d\boldsymbol{x} = \boldsymbol{W} \Lambda \boldsymbol{W}^{\boldsymbol{T}} \tag{16}$$

Where $\boldsymbol{W} = (\boldsymbol{w}_1, ..., \boldsymbol{w}_d)$ is a unitary matrix and :

$$\Lambda = \boldsymbol{Diag}(\lambda_1, ..., \lambda_d), \backslash \forall i \in [\![1, d-1]\!], \lambda_i > \lambda_{i-1}$$

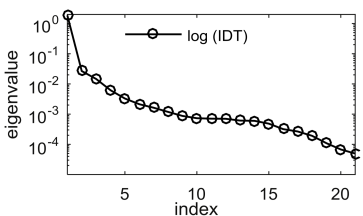
Goal of the operation

Sort the directions $\boldsymbol{w}_i$ in which the QoI F encounters the greatest gradients

Basis truncature

Truncature possible at rank r whenever $\lambda_r \gg \lambda r + 1$
$Span(\boldsymbol{w}_1, ..., \boldsymbol{w}_r)$ is called the active subspace

Illustration of AS eigenvalues[a]



[a] Ji et al. 2019.

Expectations

- Most of the variability should be retained on the AS
- A surrogate built on the AS should also be a good approximation of F

Warning

There is no a priori quantitative guarantee of the adequacy of the reduced space

Practical obtention of the active subspace

M is the necessary number of samples, d the initial dimension of the problem, α an over-sampling factor, β the largest dimension acceptable for the AS

1^{st} Scenario

Gradient obtained "for free" with each sample (adjoint simulation)

$M = \alpha \cdot \beta \cdot log(d)$

2^{nd} Scenario

Gradient information computed with finite differences

$M = \alpha \cdot \beta \cdot d \cdot log(d)$

3^{rd} Scenario

Assumptions:

- F is monotonous with each ξ_i
- A 1D AS can be discovered (Active Direction)
- On the AD, F is not too far from a linear function

We can then determine the AD with a linear regression of F:

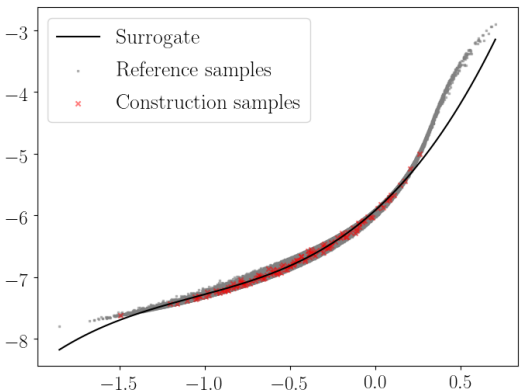
$$F(\boldsymbol{\xi}) = \boldsymbol{b}^T \boldsymbol{\xi} + b_0 + \tilde{F}(\boldsymbol{\xi}) \tag{17}$$

And:

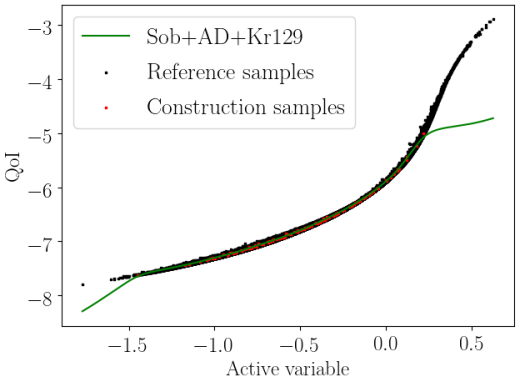
$$\boldsymbol{w}_1 = \boldsymbol{b}^T / \|\boldsymbol{b}\|_2 \tag{18}$$

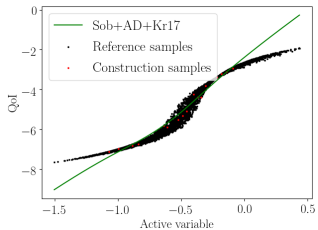
With the cost: $M = \alpha \cdot d$

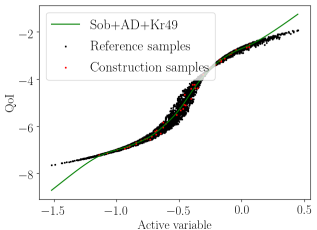
Spline, 129 samples

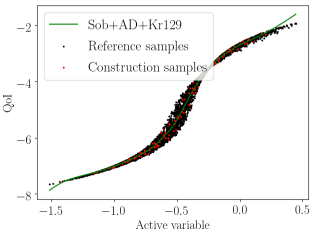


Kriging, 129 samples




Sob+AD+Kr17
Reference samples
Construction samples
QoI
Active variable


Sob+AD+Kr49
Reference samples
Construction samples
QoI
Active variable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