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# Optimal Uncertainty Quantification of a Risk Measurement from a Computer Code
# A PhD born in Barcelonnette (ETICS'1)

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& Merlin Keller (EDF) & Bertrand Iooss(EDF)

ETICS'10, Evian les bains, octobre 2025

# NAISSANCE DU SUJET

# BARCELONNETTE !!

Petite ville de la vallée de l'Ubaye (Alpes de Haute Provence), célèbre pour :

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- → Ses activités d'eau vive ;
- → Ses belles montagnes ;
- → ses sept cols, dont la Bonnette $(2\,715m)$ ;
- → …


# PETIT QUIZZ UBAYEN

Qu'est-ce qu'un "Choucas" ? (cochez la bonne réponse)

- ☐ Un bar karaoke
- ☐ Une boisson alcoolisée
- ☐ Un oiseau de la famille des corvidés

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# PROGRAMME SCIENTIFIQUE D'ETICS 2016

Lecturers (source **https://uq.math.cnrs.fr/etics**) :

→ François Bachoc (Université Paul Sabatier) : Calibration of computer experiments

→ Sébastien Da Veiga (SafranTech) : Advanced methods in sensitivity analysis

→ Stéphane Gaïffas (Ecole Polytechnique) : Methods for covariance matrix estimation -

→ Tim Sullivan (Free University of Berlin / Zuse Institute Berlin) : Optimal distributionally robust uncertainty quantification

# INTRODUCTION

# INDUSTRIAL CONTEXT

We study a mock-up of a water pressured nuclear reactor during an intermediate break loss of coolant accident in the primary loop.

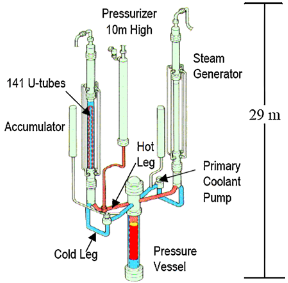



**Figure :** The replica of a water pressured reactor, with the hot and cold leg.

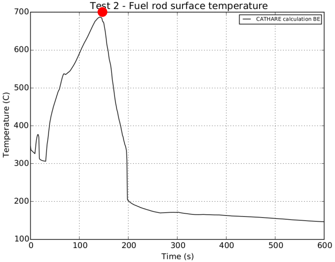
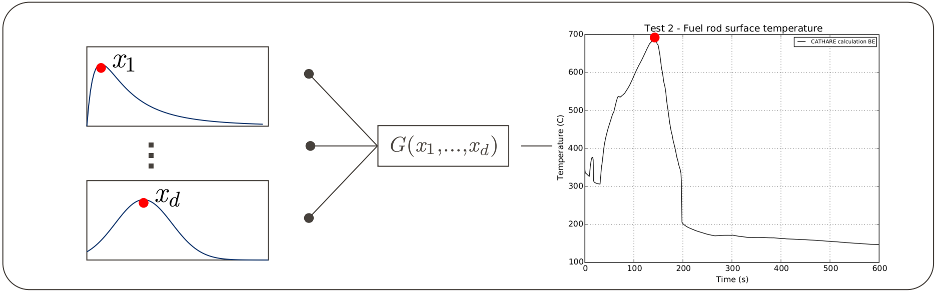



**Figure :** CATHARE code temperature output for nominal parameters.

# DETERMINISTIC METHOD

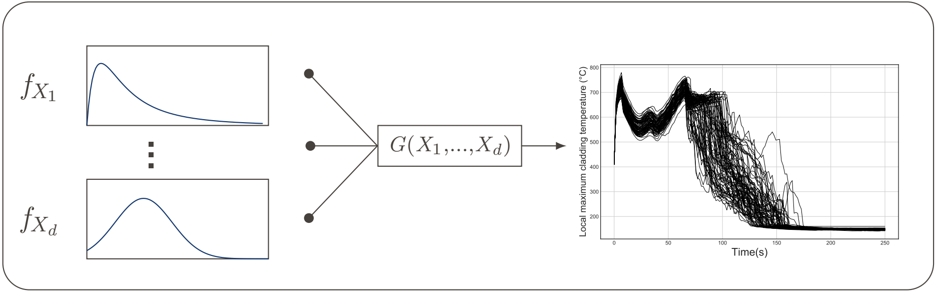
$$\underbrace{(x_1, \ldots, x_d)}_{\text{uncertain input parameters}} \rightsquigarrow \boxed{\texttt{COMPUTER MODEL}} \rightsquigarrow y$$




Our use-case is a thermal-hydraulic computer code (CATHARE), which simulates a intermediate break loss of coolant accident. The variable of interest is the peak cladding temperature.

# PROBABILISTIC MODELIZATION

$$\underbrace{(X_1, \dots, X_d)}_{\boldsymbol{\mu}} \rightsquigarrow \boxed{\texttt{COMPUTER MODEL}} \rightsquigarrow Y$$




Let $G$ be our computer code, the output distribution writes $F_{\boldsymbol{\mu}}(h) = \mathbb{P}_{\boldsymbol{\mu}}(G(X) \leq h)$.

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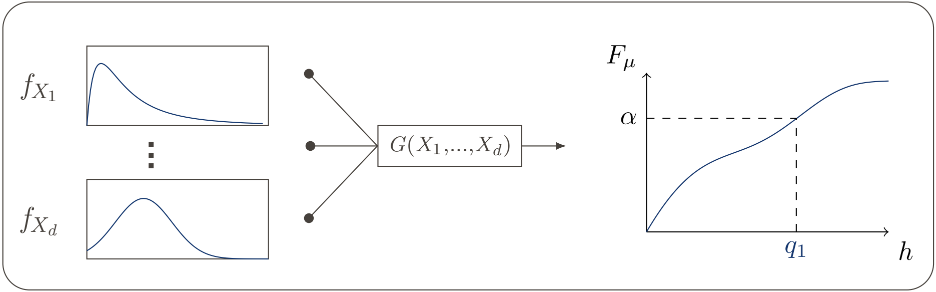


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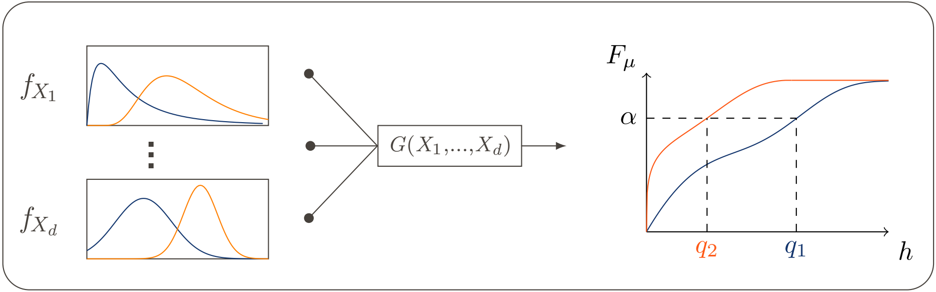
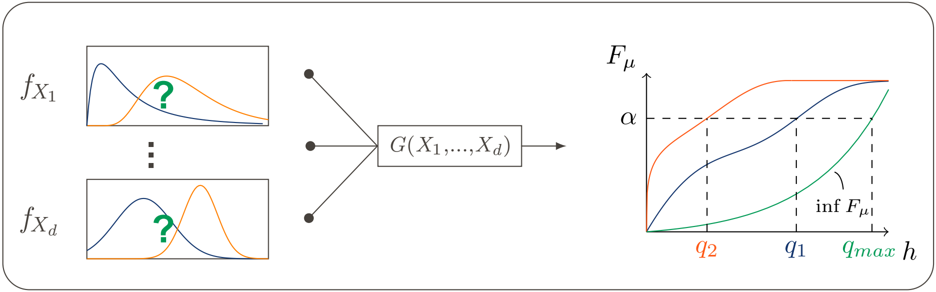



The quantity of interest (here a quantile) depends on the input distributions $\mu$.

# PROBABILISTIC MODELIZATION

$$\underbrace{(X_1, \ldots, X_d)}_{\mu} \rightsquigarrow \texttt{COMPUTER MODEL} \rightsquigarrow Y$$




OUQ consists in finding the optimum of the quantity of interest over a set of input distribution $\mu \in \mathcal{A}$.

# UNCERTAINTY MODELIZATION

We consider robustness by finding bounds on a quantity of interest $\phi$

$$\boldsymbol{\mu} \in \mathcal{P}(X) \mapsto \phi(\boldsymbol{\mu})$$

→ We optimize the quantity of interest over a measure space $\mathcal{A}$

$$\sup_{\boldsymbol{\mu} \in \mathcal{A}} \phi(\boldsymbol{\mu})$$

→ The measure space $\mathcal{A}$ should be compatible with the data, it should effectively represent the uncertainty on the distribution.

# THE MOMENT CLASS

In this work we will focus on two different optimization space.

→ The moment class :

$$\mathcal{A}^* = \left\{ (\mu_1, \ldots, \mu_d) \in \prod_{i=1}^{d} \mathcal{P}([l_i, u_i]) \mid \mathbb{E}_{\mu_i}[X^j] \leqq c_i^{(j)} \ , \ j = 1, \ldots, N_i \right\} \ ,$$

→ and the unimodal moment class

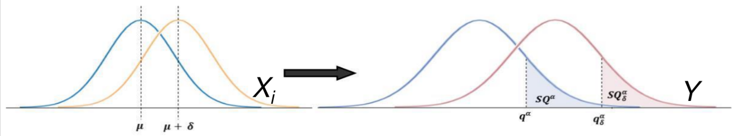
$$\mathcal{A}^\dagger = \left\{ \text{Unimodal } \boldsymbol{\mu} \in \prod_{i=1}^{d} \mathcal{P}([l_i, u_i]) \mid \mathbb{E}_{\mu_i}[X^j] \leqq c_i^{(j)} \ , \ j = 1, \ldots, N_i \right\} \ ,$$

**Problem** : this is an optimization over an infinite non parametric space...

# OTHER "DISTRIBUTION ROBUSTNESS" METHODS (1/2)

**Perturbed Law indices (see Lemaitre et al. 2015)**

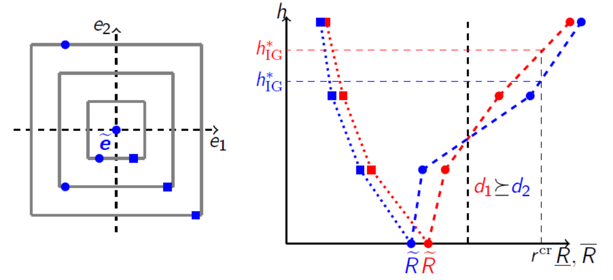
PLI is a reliability sensitivity index, quantifying the robustness of a QOI to uncertain input law assumptions, typically moments



# OTHER "DISTRIBUTION ROBUSTNESS" METHODS (2/2)

## Info-gap theory (see Ajenjo et al. 2022)

Info-gap is a none probablistic theory, quantifying the robustness of a QOI when uncertain inputs lie in *nested convex sets*

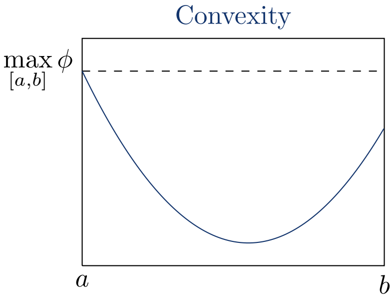


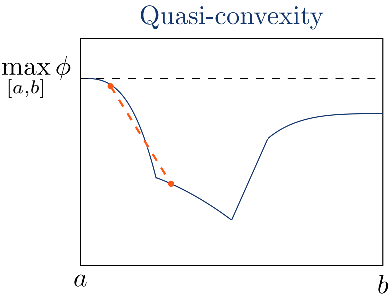
# REDUCTION THEOREM

# QUASI-CONVEX FUNCTION

A function $\phi$ is said to be quasi-convex if

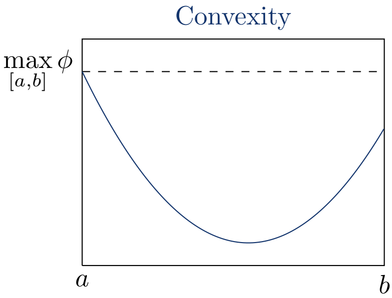
$$\phi(\lambda x + (1-\lambda) y) \leq \max \{\phi(x); \phi(y)\}$$

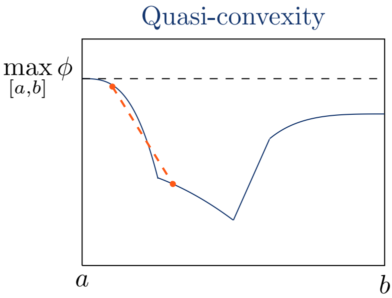


# QUASI-CONVEX FUNCTION

From the Bauer maximum principle, a convex function on a compact convex set reaches its maximum on the extreme points




⇝ The Bauer maximum principle remains true for quasi-convex function.

# REDUCTION THEOREM

**Reduction theorem**

→ The (unimodal) moment class is compact convex.

→ The quantity of interest $\phi$ is a quasi-convex lower semicontinuous function of the measure $\mu \in \mathcal{A}$

Then,

$$\sup_{\mu \in \mathcal{A}} \phi(\mu) = \sup_{\mu \in \Delta} \phi(\mu) \ ,$$

where $\Delta$ is the set of extreme points of $\mathcal{A}$.

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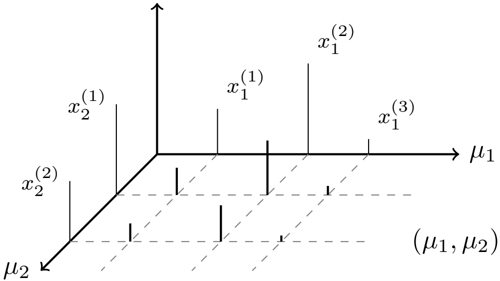
# EXTREME POINTS CHARACTERIZATION (1/2)

## Extreme points of the moment class

If you have $N_i$ constraints on $\mu_i$, then $\mu_i$ can be specified as a convex combination of at most $N_i + 1$ Dirac masses

$$\Delta^* = \left\{ \mu \in \mathcal{A}^* \mid \mu_i = \sum_{k=1}^{N_i+1} \omega_k \delta_{x_k},\ x_k \in [l_i, u_i] \right\}$$

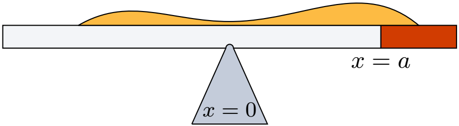


# PHYSICAL ILLUSTRATION

## First approach

You are given 1kg of sand to arrange however you wish on a seesaw balanced around $x = 0$.

→ How much mass can you pur on **the region $x \geq a$?**



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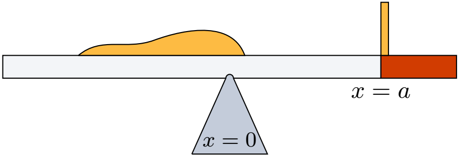

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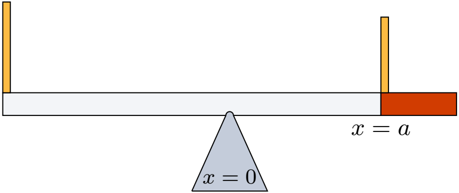


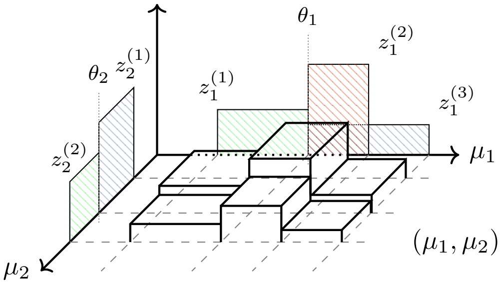
# EXTREME POINTS CHARACTERIZATION (2/2)

## Extreme points of the unimodal moment class

If you have $N_i$ constraints on $\mu_i$, then $\mu_i$ can be specified as a convex combination of at most $N_i + 1$ uniform distributions

$$\Delta^{\dagger} = \left\{ \mu \in \mathcal{A}^{\dagger} \mid \mu_i = \sum_{k=1}^{N_i+1} \omega_k \mathcal{U}(\theta_i, z_k),\ z_k \in [l_i, u_i] \right\}$$

where $\theta_i$ denotes the mode of $\mu_i$.



# REDUCTION THEOREM FOR A PROBABILITY OF FAILURE

Consider the quantity of interest to be a probability of failure (PoF).

$\rightsquigarrow$ it is a linear function of the input measure, thus is quasi-convex.

Over the moment class $\mathcal{A}^*$, the optimal PoF can be computed on the set of discrete finite input distributions :

$$\sup_{\boldsymbol{\mu}\in\mathcal{A}^*} \phi(\boldsymbol{\mu}) = \sup_{\boldsymbol{\mu}\in\mathcal{A}^*} F_{\boldsymbol{\mu}}(h) \ ,$$

$$= \sup_{\boldsymbol{\mu}\in\Delta^*} \mathbb{P}_{\boldsymbol{\mu}}\big(G(X_1,\dots,X_d) \le h\big) \ ,$$

$$= \sup_{\boldsymbol{\mu}\in\Delta^*} \sum_{i_1=1}^{N_1+1} \dots \sum_{i_d=1}^{N_d+1} \omega_{i_1}^{(1)} \dots \omega_{i_d}^{(d)} \ \mathbb{1}_{\{G(x_{i_1}^{(1)},\dots,x_{ip}^{(p)})\le h\}} \ .$$

# DISCRETE MEASURES

Let enforce $N$ moment constraints on a measure $\mathbb{E}_\mu[X^j] = c_j$ .
OUQ theorem guaranties the optimal measure to be supported on at most $N+1$ points :

$$\mu = \sum_{i=1}^{N+1} \omega_i \delta_{x_i}$$

We have the following system of constraint equations :

$$\begin{cases} \omega_1 + \dots + \omega_{N+1} = 1 \\ \omega_1 x_1 + \dots + \omega_{N+1} x_{N+1} = c_1 \\ \quad \vdots \qquad\qquad \vdots \qquad \vdots \\ \omega_1 {x_1}^N + \dots + \omega_{N+1} {x_{N+1}}^N = c_N \end{cases}$$

$\leadsto$ The weights are uniquely determined by the positions.

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# GEOMETRICAL INTERPRETATION

**Example :** Let $\mu$ be supported on $[0,1]$ such that $\mathbb{E}_\mu[X] = 0.5$ and $\mathbb{E}_\mu[X^2] = 0.3$.

$$\Delta^* = \left\{ \mu = \sum_{i=1}^{3} \omega_i \delta_{x_i} \in \mathcal{P}([0,1]) \mid \mathbb{E}_\mu[X] = 0.5,\ \mathbb{E}_\mu[X^2] = 0.3 \right\} ,$$

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✓ $\mathbf{x} = (0.1, 0.4, 0.9)$ gives weights $\boldsymbol{\omega} = (0.05, 0.73, 0.22)$

✗ $\mathbf{x} = (0.1, 0.3, 0.9)$ gives weights $\boldsymbol{\omega} = (-0.19, 0.92, 0.27)$

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× $\mathbf{x} = (0.1, 0.3, 0.9)$ gives weights $\boldsymbol{\omega} = (-0.19, 0.92, 0.27)$

$$\mathcal{V}_{\Delta^*} = \left\{ \mathbf{x} = (x_1, x_2, x_3) \in [0,1]^3 \mid \mu = \sum_{i=1}^{3} \omega_i \delta_{x_i} \in \Delta^* \right\}$$

**How to optimize over and explore the manifold $\mathcal{V}_\Delta$ ?**

# POSSIBLE WAYS OF OPTIMIZING

→ Optimization under constraints : the position and the weight must satisfy the Vandermonde system.

→ Optimization by rewriting the objective function : changing the parameterization of the problem so that the constraint are naturally enforced in the objective function.

↳ Canonical moments allows to efficiently explore the set of optimization $\Delta^*$.

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# CANONICAL MOMENTS PARAMETERIZATION

# CLASSICAL MOMENTS PROBLEM

$$\left(\frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \ldots\right)$$

$\rightsquigarrow$ Moment sequence of $\mathcal{U}[0,1]$

$$\left(1, \frac{4}{3}, 2, \ldots\right)$$

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Conclusion : there is no relation between the classical moments and the intrinsic structure of the distribution.

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Conclusion : there is no relation between the classical moments and the intrinsic structure of the distribution.

# MOMENT SPACE

We define the moment space $M_n = \{\mathbf{c}_n(\mu) = (c_1, \ldots, c_n) \mid \mu \in \mathcal{P}([0,1])\}$

Given $\mathbf{c}_n \in \operatorname{int} M_n$, we define the extreme values

$$c_{n+1}^+ = \max\{c : (c_1, \ldots, c_n, c) \in M_{n+1}\}$$
$$c_{n+1}^- = \min\{c : (c_1, \ldots, c_n, c) \in M_{n+1}\}$$

They represent the maximum and minimum value of the $(n+1)$th moment a measure can have, when its moments up to order $n$ equal to $c_n$.

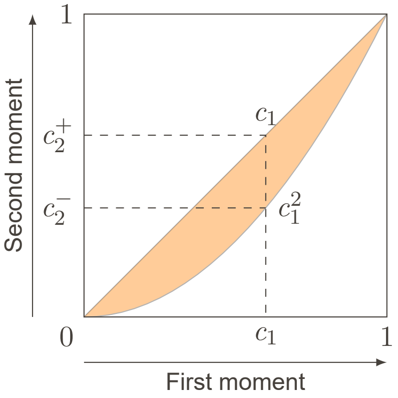


Figure : representation of $M_2$

# CANONICAL MOMENTS

The $n$th canonical moment is defined as

$$p_n = p_n(\mathbf{c}) = \frac{c_n - c_n^-}{c_n^+ - c_n^-}$$

## Properties of canonical moments

→ $p_n \in [0, 1]$,

→ The canonical moments are invariants by affine transformation. Which means we can always transform a measure supported on $[a, b]$ to $[0, 1]$

# LINK BETWEEN SUPPORT AND CANONICAL MOMENTS

Given a measure $\mu = \sum_{i=1}^{n+1} \omega_i \delta_{x_i}$, we have two representations of the same polynomial $P^*_{n+1}$ :

→ Its roots are the measure support points :

$$P^*_{n+1}(z) = \prod_{i=1}^{n+1} (z - x_i) .$$

→ Its coefficients are function of a sequence of the measure canonical moments $\mathbf{p} = (p_1, \dots, p_{2n+1})$ :

$$P^*_{n+1}(z) = \varphi_0(\mathbf{p}) + \varphi_1(\mathbf{p}) z + \cdots + \varphi_{n+1}(\mathbf{p}) z^{n+1} .$$

# LINK BETWEEN SUPPORT AND CANONICAL MOMENTS

Given a measure $\mu = \sum_{i=1}^{n+1} \omega_i \delta_{x_i}$, we have two representations of the same polynomial $P_{n+1}^*$ :

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# EFFECTIVE PARAMETERIZATION

Let $\mu \in \Delta^* = \left\{ \sum_{i=1}^{n+1} \omega_i \delta_{x_i} \in \mathcal{P}([a,b]) \mid \mathbb{E}_\mu[X^j] = c_j,\ 1 \leq j \leq n \right\}$

# EFFECTIVE PARAMETERIZATION

$\mu \in \Delta^*$

$\downarrow$

The support of $\mu$ is the roots of a polynomial

$P^*_{n+1} = \prod_{i=1}^{n+1}(x - x_i)$

$P^*_{n+1}$

# EFFECTIVE PARAMETERIZATION

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$$P_{n+1}^* = \prod_{i=1}^{n+1}(x - x_i)$$

$$P_{n+1}^*$$

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$$P_{n+1}^* = \varphi_0(\mathbf{p}) + \varphi_1(\mathbf{p})z + \cdots + \varphi_{n+1}(\mathbf{p})z^{n+1}$$

$$\mathbf{p} = (p_1, \ldots, p_n, p_{n+1}, \ldots, p_{2n+1})$$

# EFFECTIVE PARAMETERIZATION

$$\mu \in \Delta^*$$

↓ The support of $\mu$ is the roots of a polynomial

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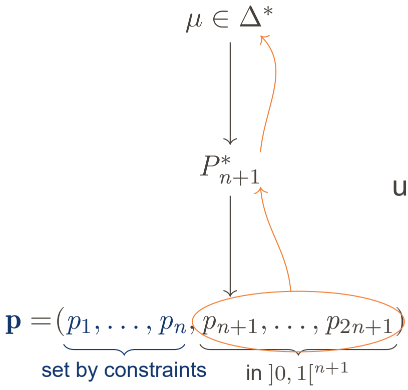
$$P^*_{n+1} = \varphi_0(\mathbf{p}) + \varphi_1(\mathbf{p})z + \cdots + \varphi_{n+1}(\mathbf{p})z^{n+1}$$

$$\mathbf{p} = (\underbrace{p_1, \ldots, p_n}_{\text{set by constraints}}, \underbrace{p_{n+1}, \ldots, p_{2n+1}}_{\text{in } ]0,1[^{n+1}})$$

# EFFECTIVE PARAMETERIZATION




We can explore the whole set $\Delta^*$ using a parameterization in $]0,1[^{n+1}$.

# GENERATION OF ADMISSIBLE MEASURES

**Theorem**

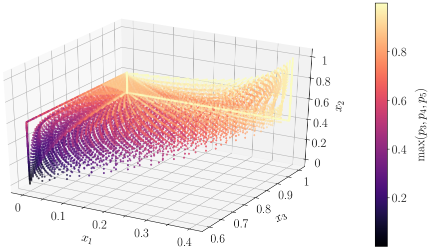
The manifold

$$\mathcal{V}_{\Delta^*} = \Big\{ \mathbf{x} = (x_1, \ldots, x_{n+1}) \in [0,1]^{n+1} \text{ s.t.}$$
$$\mu = \sum_{i=1}^{n+1} \omega_i \delta_{x_i} \textit{ satisfies the constraints} \Big\}$$

is an algebraic variety, it is the zero locus of the set of polynomials

$$\left\{ P^*_{n+1} \mid (p_{n+1}, \ldots, p_{2n+1}) \in [0,1]^{n+1} \right\}$$

# SET OF ADMISSIBLE MEASURES




- → Consider $\mu$ in $[0,1]$ and two moment constraints : $c_1 = 0.5$ and $c_2 = 0.3$ equivalent to $p_1 = 0.5$ and $p_2 = 0.2$.
- → We generate randomly $(p_3, p_4, p_5) \in [0,1]^3$ and compute for every sequence $P_3^*$ whose roots constitute the coordinates of the points.
- → The point coordinates correspond to the support of a discrete measure in $\mathcal{A}$.

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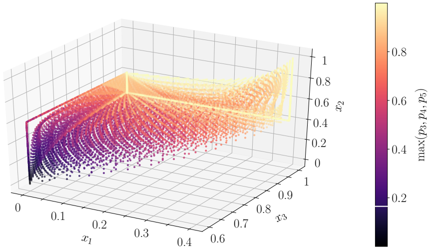


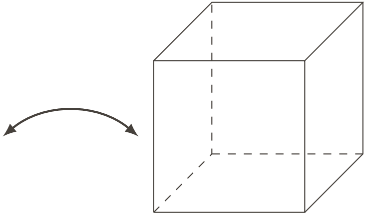

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# ALGORITHM

**Algorithm 1 :** P.O.F COMPUTATION

**Inputs :** - lower bounds, $\mathbf{l} = (l_1, \dots, l_d)$
- upper bounds, $\mathbf{u} = (u_1, \dots, u_d)$
- constraints sequences of moments, $\mathbf{c}_i = (c_i^{(1)}, \dots, c_i^{(N_i)})$ and its corresponding sequences of canonical moments, $\mathbf{p}_i = (p_i^{(1)}, \dots, p_i^{(N_i)})$ for $1 \le i \le d$.

**function** *P.O.F*($p_1^{(N_1+1)}, \dots, p_1^{(2N_1+1)}, \dots, p_d^{(N_d+1)}, \dots, p_d^{(2N_d+1)}$)

  **for** $i = 1, \dots, d$ **do**

    **for** $k = 1, \dots, N_i$ **do**

      $P_{i*}^{(k+1)} = (X - l_i - (u_i - l_i)(\zeta_i^{2k} + \zeta_i^{(2k+1)}))P_{i*}^{(k)} - (u_i - l_i)^2 \zeta_i^{(2k-1)} \zeta_i^{(2k)} P_{i*}^{(k-1)}$ ;

    $x_i^{(1)}, \dots, x_i^{(N_i+1)} =$ roots$(P_i^{*(N_i+1)})$ ;

    $\omega_i^{(1)}, \dots, \omega_1^{(N_i+1)} =$ weight$(x_i^{(1)}, \dots, x_1^{(N_i+1)}, \mathbf{c}_i)$ ;

  **return** $\sum_{i_1=1}^{N_1+1} \dots \sum_{i_d=1}^{N_d+1} \omega_1^{(i_1)} \dots \omega_d^{(i_d)} \mathbb{1}_{\{G(x_1^{(i_1)}, \dots, x_d^{(i_d)}) \le h\}}$ ;

ILLUSTRATION

# INDUSTRIAL CONTEXT

Our use-case is a thermal-hydraulic computer code (CATHARE), which simulates a intermediate break loss Of coolant accident. The variable of interest is the peak cladding temperature.

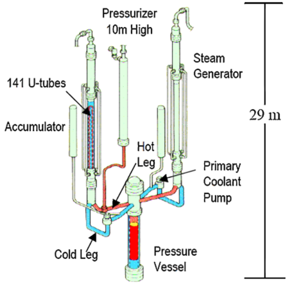



**Figure :** The replica of a water pressured reactor, with the hot and cold leg.

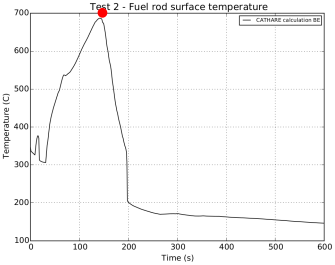



**Figure :** CATHARE code temperature output for nominal parameters.

# MOMENT CONSTRAINTS FOR CATHARE

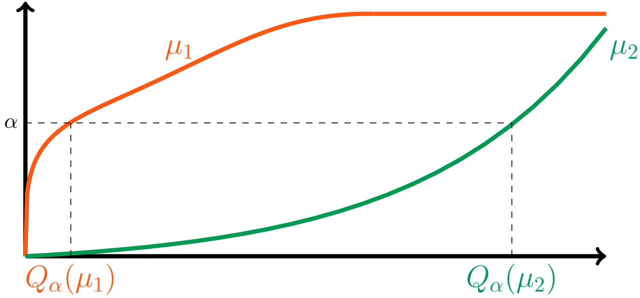
| Variable | Bounds | Initial distribution (truncated) | Mean | Second order moment |
|---|---|---|---|---|
| $n°10$ | $[0.1, 10]$ | $LogNormal(0, 0.76)$ | $1.33$ | $3.02$ |
| $n°22$ | $[0, 12.8]$ | $Normal(6.4, 4.27)$ | $6.4$ | $45.39$ |
| $n°25$ | $[11.1, 16.57]$ | $Normal(13.79$ | $13.83$ | $192.22$ |
| $n°2$ | $[-44.9, 63.5]$ | $Uniform(-44.9, 63.5)$ | $9.3$ | $1065$ |
| $n°12$ | $[0.1, 10]$ | $LogNormal(0, 0.76)$ | $1.33$ | $3.02$ |
| $n°9$ | $[0.1, 10]$ | $LogNormal(0, 0.76)$ | $1.33$ | $3.02$ |
| $n°14$ | $[0.235, 3.45]$ | $LogNormal(-0.1, 0.45)$ | $0.99$ | $1.19$ |
| $n°15$ | $[0.1, 3]$ | $LogNormal(-0.6, 0.57)$ | $0.64$ | $0.55$ |
| $n°13$ | $[0.1, 10]$ | $LogNormal(0, 0.76)$ | $1.33$ | $3.02$ |

**Table :** Corresponding moment constraints of the 9 most influential inputs of the CATHARE model. Two moment constraints are enforced, that correspond to the mean and the variance of each input distribution.

# QUASI-CONVEXITY OF THE QUANTILE (HEURISTIC)

Why is the quantile a quasi-convex function of the measure ?

Let denote $Q_p(\mu)$ the quantile of order $p$ of a distribution $\mu$.



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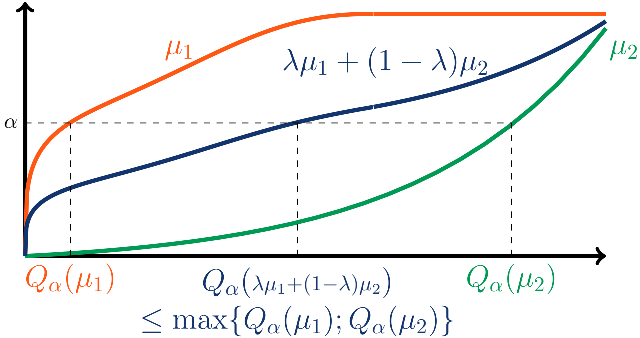

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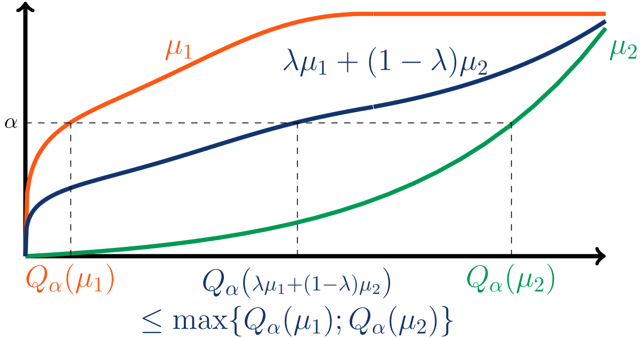
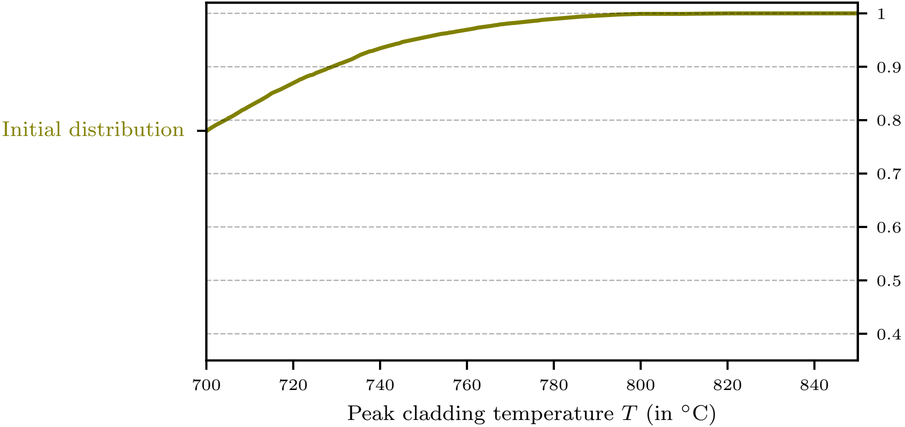


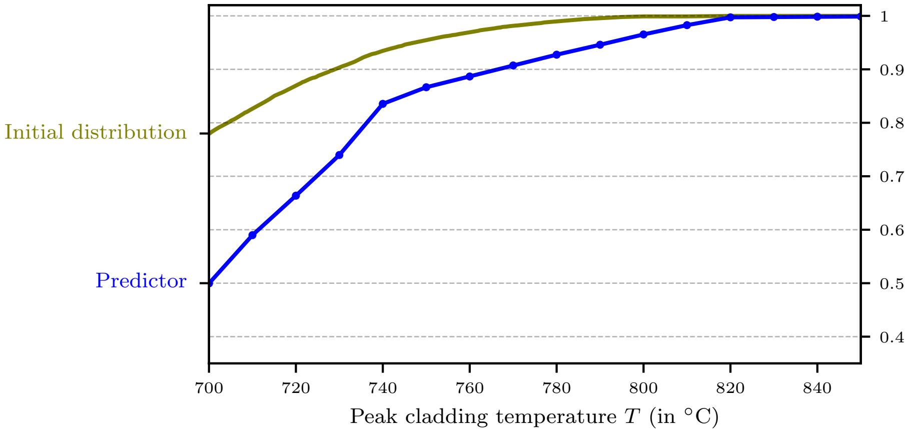

$\rightsquigarrow$ For the same reason, the superquantile is a quasi-convex function of the measure.

# OPTIMIZATION FOR CATHARE




$$q_{init}^{0.95} = 760^\circ C$$

# OPTIMIZATION FOR CATHARE




$$q_{init}^{0.95} = 760°\,C \quad \rightsquigarrow \quad q_{optim}^{0.95} = 788°\,C$$

# UNCERTAINTY TAINTING THE METAMODEL (1/2)

We recall the probability of failure $F_\mu(h)$ is computed as

$$\inf_{\mu \in \mathcal{A}} F_\mu(h) = \inf_{\mu \in \mathcal{A}} \mathbb{P}_\mu\Big(G(X_1, \ldots, X_d) \leq h\Big) ,$$

$$= \inf_{\mu \in \Delta} \sum_{i_1=1}^{N_1+1} \cdots \sum_{i_d=1}^{N_d+1} \omega_{i_1}^{(1)} \ldots \omega_{i_d}^{(d)} \mathbb{1}_{\{G(x_{i_1}^{(1)}, \ldots, x_{i_p}^{(p)}) \leq h\}} .$$

$\rightsquigarrow$ The simple approach replaces uncertain $G(\mathbf{x})$ by the predictor of the kriging metamodel $\mathscr{G}(\mathbf{x}, \boldsymbol{\theta})$, that is, the GP expectation.

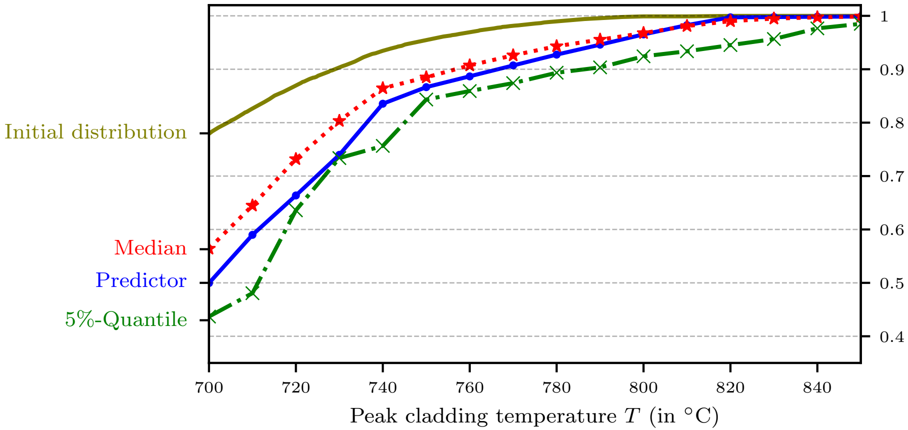
# UNCERTAINTY TAINTING THE METAMODEL (2/2)

$\rightsquigarrow$ We propose to compute $F_\mu(h)$ for several trajectories of the metamodel, and minimize a *quantile* of the resulting sample, rather than the *expectation*.

$$\inf_{\mu \in \mathcal{A}} F_\mu(h, \boldsymbol{\theta}) = \inf_{\mu \in \mathcal{A}} \mathbb{P}_\mu\Big(\mathscr{G}(X_1, \dots, X_d, \boldsymbol{\theta}) \leq h\Big) ,$$

$$= \underbrace{\inf_{\mu \in \Delta} \sum_{i_1=1}^{N_1+1} \dots \sum_{i_d=1}^{N_d+1} \omega_{i_1}^{(1)} \dots \omega_{i_d}^{(d)}}_{\text{get a sample for different realization of the gaussian process}} \mathbb{1}_{\{\mathscr{G}(x_{i_1}^{(1)}, \dots, x_{i_p}^{(p)}, \boldsymbol{\theta}) \leq h\}} .$$

# OPTIMIZATION FOR CATHARE




$$q_{init}^{0.95} = 760^\circ C \quad \rightsquigarrow \quad q_{optim}^{0.95} = 788^\circ C \quad \rightsquigarrow \quad q_{\substack{optim \\ robust}}^{0.95} = 830^\circ C$$

# CONCLUSION AND PERSPECTIVES

- → The reduction theorem gives the basis for numerical optimization of the quantity of interest.
- → The moment class and unimodal moment class have very interesting topological structure.
- → The canonical moment parameterization is well suited for exploring the extreme points, thus fastening the global optimization.
- → Inequality moment constraints can also be enforced.

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→ The canonical moment parameterization is well suited for exploring the extreme points, thus fastening the global optimization.
→ Inequality moment constraints can also be enforced.

→ Limited to *classical* moment constraints.
→ Possible extension to quantile classes.
→ Need to account for metamodel uncertainty
→ Raw global optimization to be refined by computing gradient of the quantity of interest.
→ Computation subject to curse of dimensionality : reducing the input dimension is a mandatory first step.

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THANK YOU FOR YOUR ATTENTION！