



LEARNING AND UNCERTAINTY QUANTIFICATION FROM COMPLEX SIMULATIONS

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Division of Digital Sciences and Technologies, Department of Applied Mathematics

April 28, 2026



LEARNING AND UNCERTAINTY QUANTIFICATION FROM/WITH SDE MODELS AND COMPLEX SIMULATIONS

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April 28, 2026
UCC Cork, Ireland

IFPEN AT A GLANCE

Public sector
R&I institution

Training
center

Industrial
Group

INTERNATIONAL SCOPE in the field of
ENERGY, MOBILITY and THE ENVIRONMENT



1,523 employees

incl. **1,074** R&I engineers & technicians

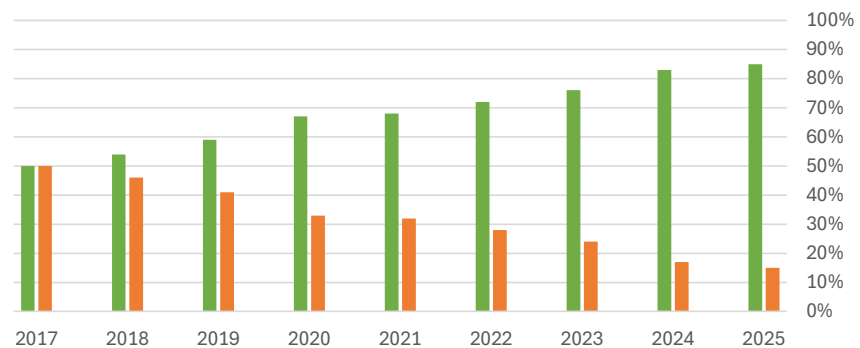
€117,6 M Budget allocation in 2025

€162,1 M Own resources in 2025

Research & Innovation activities

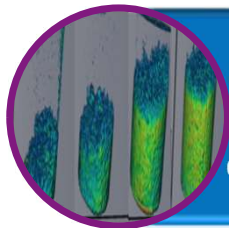
Green technologies

**Responsible & profitable
Oil & Gas**

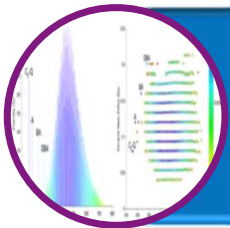


FUNDAMENTAL RESEARCH AROUND 9 SCIENTIFIC CHALLENGES

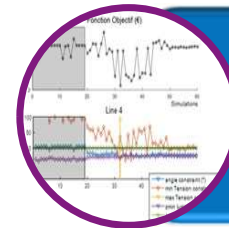
From the understanding of physical phenomena to the evaluation of a complete system, via numerical modeling of these phenomena



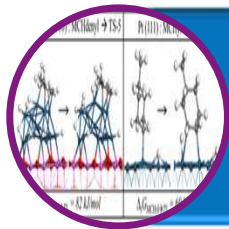
Material and fluid characterization



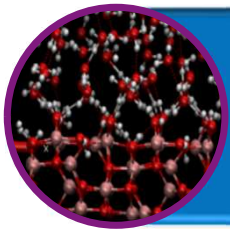
Massive data flows



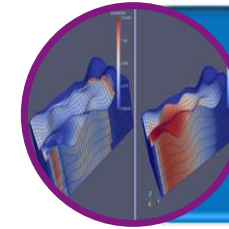
Command and optimization



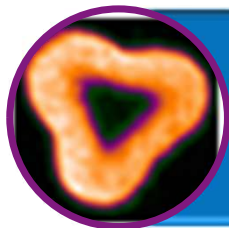
Reaction mechanisms



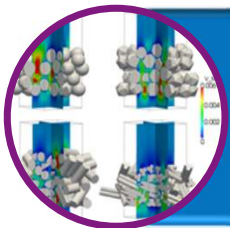
Descriptors



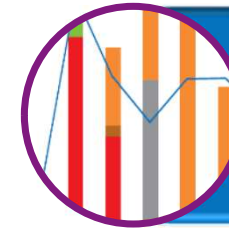
Code performance



Containment effect



Modeling of coupled phenomena



Economic and environmental evaluations

OUR FIELDS OF COMPETENCE

Earth sciences

Geology – Sedimentology
 Geochemistry
 Geostatistics – Geological modeling
 Geomechanics
 Petrophysics and transfers in porous media

Chemical Sciences

Catalysis and reaction kinetics
 Organic and mineral synthesis
 Separation and adsorption techniques
 Theoretical chemistry

Analysis and Characterization

Chemical analysis
 Structural analysis and imaging
 Mechanical testing
 Microfluidics
 High throughput experimentation (HTE)

Physical Sciences

Transfer and transport physics
 Rheology and behavior of materials
 Thermodynamics / Molecular modeling

Physical chemistry

Complex fluids, colloids and condensed matter
 Surface, interface and materials science
 Electrochemistry and corrosion

Biosciences and Biotechnology

Microbiology
 Genomics
 Biocatalysis
 Fermentation

Engineering Sciences

Solid mechanics
 Fluid mechanics
 Chemical and process engineering
 Combustion and engine technologies
 Electrical and electronic engineering
 Automation and control systems
 Systems modeling and simulation

Mathematics And Computer Sciences

Numerical Methods, UQ and optimization
 Signal processing – Data science
 Meshing and visualization
 Software design
 Real-time systems
 High performance computing
 Bio-informatics

Economics

Microeconomics and econometrics
 Macroeconomics
 Economic modeling
 Forecasting and scenario modeling
 Technical and economic evaluation
 Environmental impact evaluation and life-cycle assessment

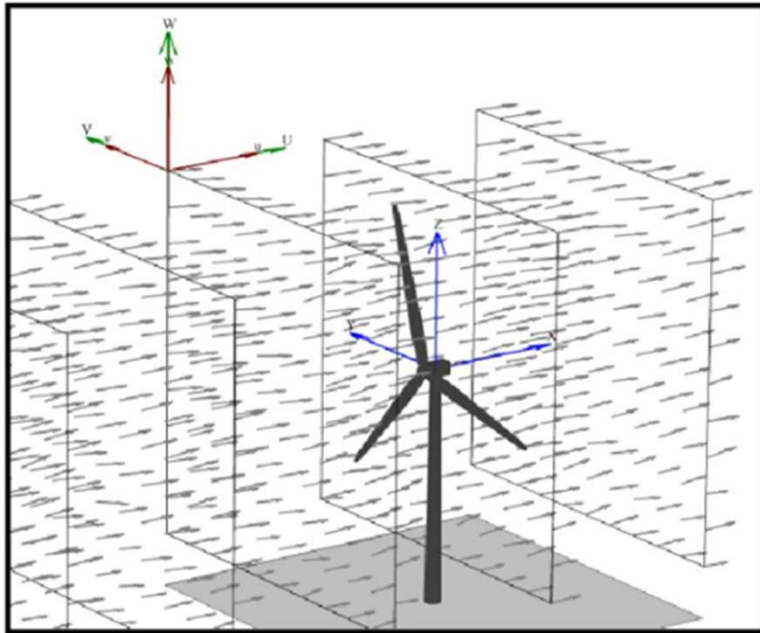
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- Wind field generation
 - Stochastic wind from SDE?
 - Non-linear stochastic frequency-domain simulators?
 - Towards Machine-learned non-stationary wind generator (PhD)
 - UQ of complex simulators, the Black-box framework
 - Active learning and Poincaré-Malliavin-Nualart inequalities
 - Metamodelling of complex simulator with functional inputs, bridging Gaussian processes and SDE
- } Part I
- } Part II
- } Opening

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WIND VELOCITY AS A STATIONARY GAUSSIAN PROCESS



The rotor-plane wind field is modelled as a **vector stochastic process**:

$$\mathbf{U}(x, y, t) = (u(x, y, t), v(x, y, t), w(x, y, t))$$

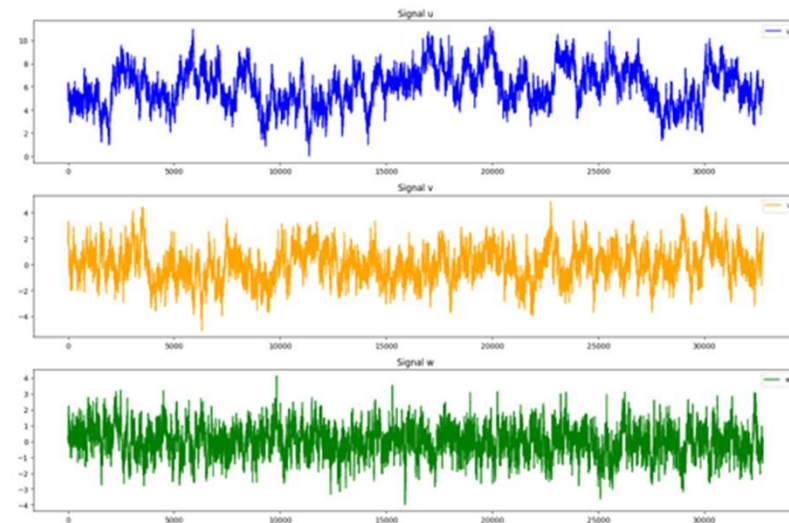
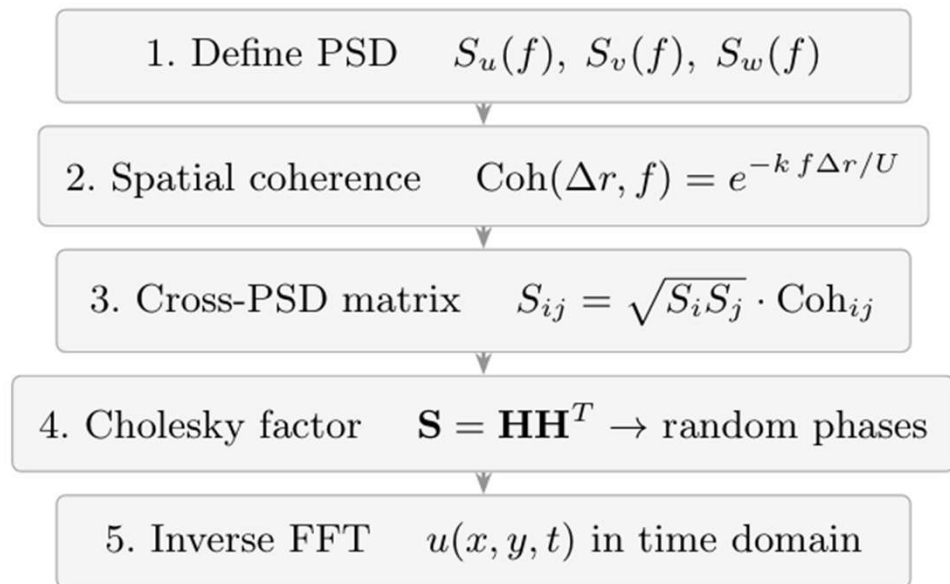
Under the **stationary hypothesis**, all statistical moments are constant:

- ▶ mean U_{hub} ,
- ▶ variance σ_u^2 ,
- ▶ Kaimal one-sided PSD (Power Spectral Density)

$$S_u(f) = \sigma_u^2 \frac{4L_u/U_{\text{hub}}}{(1 + 6fL_u/U_{\text{hub}})^{5/3}}$$

IEC 61400-1 Ed.3 Eq.(A.10); Kaimal et al. (1972)

DIRECT PIPELINE USING TURBSIM LIKE GENERATOR

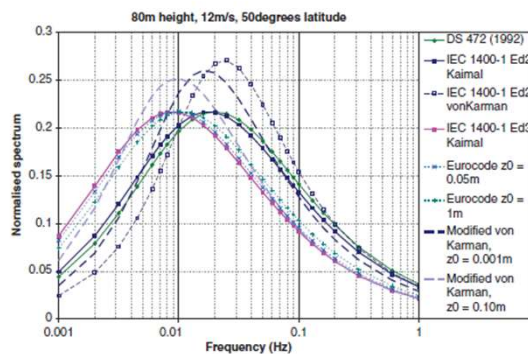


$u(x_0, y_0, t), v(x_0, y_0, t), w(x_0, y_0, t)$ for (x_0, y_0) at the hub center.

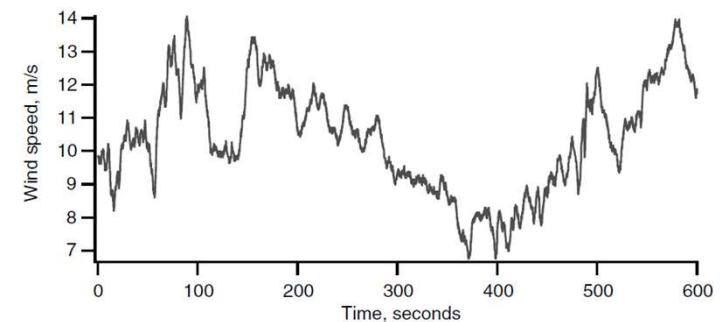
STOCHASTIC WIND FROM EDS?

Jean-Lou PFISTER (IFPEN)

- Usual engineering approach: define parametrized temporal and spatial correlations from a spectrum, then compute the vector-valued 3D wind speed timeseries^{1,2}
 - Pros: temporal/spatial correlations are experimentally measurable
 - Cons: timeseries generated once and for all (memory/cpu issues for long timeseries)

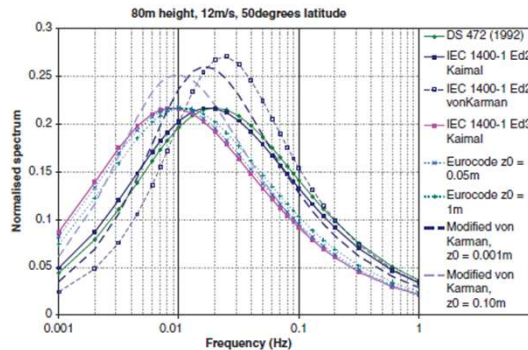


Stochastic wind generator
(TurbSim, pyConTurb, Hipersim...)

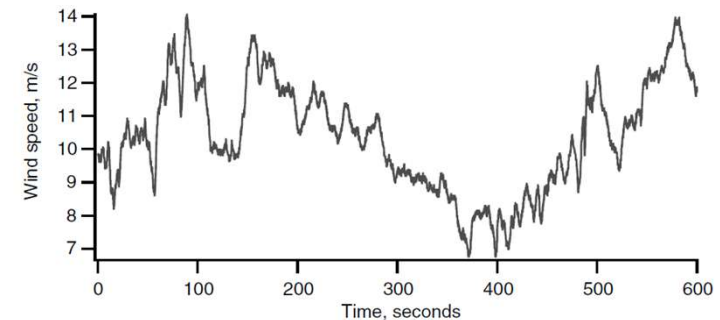


STOCHASTIC WIND FROM SDE?

Jean-Lou PFISTER (IFPEN)



Stochastic wind generator
(TurbSim, pyConTurb, Hipersim...)



- **Alternative approach(?):** define parametrized temporal and spatial correlations, find a SDE whose solutions would match these statistics, and solve it on-the-fly
 - Could solve computational issues
 - Possibility to add richer dynamics (transients, extreme events, etc.)
 - Easier to compute derivative based sensitivities (for instance impact of TI on output loads)

NON-LINEAR STOCHASTIC FREQUENCY-DOMAIN SIMULATORS?

Jean-Lou PFISTER (IFPEN)

- Usual engineering approach:
 - Frequency-domain
 - Define parametrized temporal and spatial correlations from a spectrum,
 - then compute the vector-valued 3D wind speed timeseries,
 - **Time-domain**
 - **Solve a non-linear aero-servo-hydro-elastic wind turbine time-domain simulator,**
 - Frequency-domain
 - Extract spectral properties (vibration frequencies & amplitudes)
- **Can we stay in the frequency domain?**
 - May speed-up dramatically the calculations – e.g. assuming an almost-periodic behaviour of the turbine (non-linear periodic motion + random linear fluctuations)
 - May enable an efficient calculation of the sensitivities of outputs wrt input wind temporal/spatial correlations

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 - Towards Machine-learned **non-stationary** wind generator (PhD)
- SDE for molecular dynamics (PhD)
- UQ of complex simulators, the Black-box framework
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SOURCE OF NON-STATIONARITY

PhD Simon QUERNE (Nov. 2024 – Nov. 2027)

Supervision: Laurent DUMAS (UVSQ), Charles Tillier (UVSQ), **Jean-François LECOMTE (IFPEN)**

Slowly varying mean

Synoptic-scale pressure gradients change U_{hub} on minute-to-hour time scales.
Deterministic trend or slow AR process.

Wind veer

Direction changes with height introduce cross-correlation between u and v . Ignored in the IEC simplified model.

Intermittent turbulence

ABL transitions (stable \rightarrow convective) modify σ_u and L_u non-smoothly.
Regime-switching Markov models apply.

Gusts and frontal passages

Deterministic transients (EOG, EWS) superimposed on background turbulence.
Duration $\mathcal{O}(10\text{ s})$.

Wind shear variations

Thermal stratification (Monin–Obukhov) alters $\alpha(t)$. Relevant for large rotors where top/bottom speed ratio $> 20\%$.

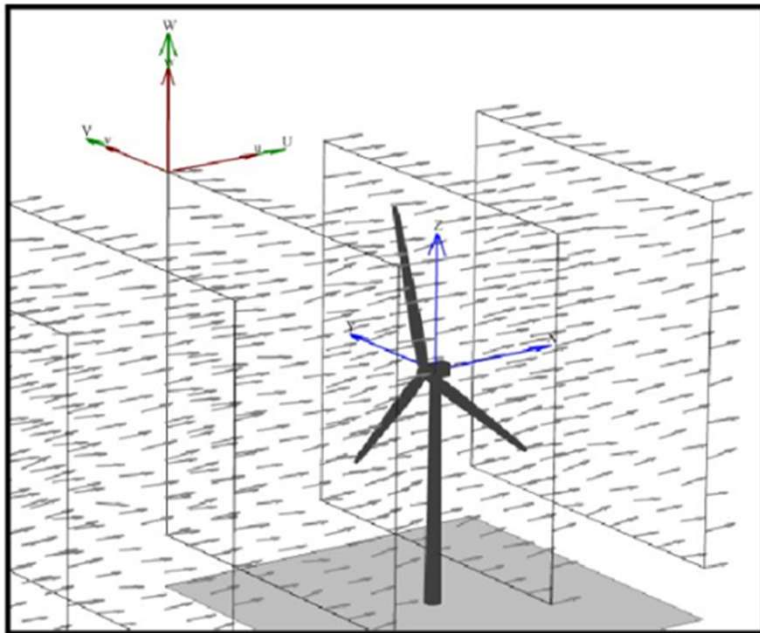
Wake effects

Upstream turbine wakes: added turbulence and velocity deficit — modelled as modified inlet statistics.

WIND VELOCITY AS A STATIONARY GAUSSIAN PROCESS

PhD Simon QUERNE (Nov. 2024 – Nov. 2027)

Supervision: Laurent DUMAS (UVSQ), Charles Tillier (UVSQ), **Jean-François LECOMTE (IFPEN)**



The rotor-plane wind field is modelled as a **vector stochastic process**:

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- ▶ mean U_{hub} ,
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$$S_u(f) = \sigma_u^2 \frac{4L_u/U_{\text{hub}}}{(1 + 6fL_u/U_{\text{hub}})^{5/3}}$$

IEC 61400-1 Ed.3 Eq.(A.10); Kaimal et al. (1972)

UNCERTAIN INPUT PARAMETERS

PhD Simon QUERNE (Nov. 2024 – Nov. 2027)

Supervision: Laurent DUMAS (UVSQ), Charles Tillier (UVSQ), **Jean-François LECOMTE (IFPEN)**

The stationary model maps a parameter vector θ to a wind field realisation.
Non-stationarity is introduced by letting θ vary in time or carry uncertainty:

$$\mathbf{U}(x, y, t; \theta(t)), \quad \theta(t) = [U_{\text{hub}}(t), \sigma_u(t), L_u(t), \alpha(t), \varepsilon_{\text{EOG}}(t)]$$

| $U_{\text{hub}}(t)$ | $\sigma_u(t)$ | $L_u(t)$ | $\alpha(t)$ | $\varepsilon_{\text{EOG}}(t)$ |
|--|--|---|---|---|
| Time-varying mean speed. Weibull distribution or slow AR(1) drift. | Turbulence std dev ($I_u = \sigma_u/U_{\text{hub}}$). IEC class A/B/C or log-normal. | Integral length scale. Controls spectral peak. Uncertain from measurements. | Shear exponent (power law). Varies with atmospheric stability (Obukhov L). | Extreme-event indicator. Binary or Poisson arrival for EOG, ECD, etc. |

Key remark

$\theta(t)$ can be treated as a **random variable** (uncertainty analysis) or as a **stochastic process** itself (non-stationary model).

TOWARDS A LEARNED WIND FIELD GENERATOR (1)

PhD Simon QUERNE (Nov. 2024 – Nov. 2027)

Supervision: Laurent DUMAS (UVSQ), Charles Tillier (UVSQ), **Jean-François LECOMTE (IFPEN)**

Non-stationary **TurbSim** pipeline relies on hand crafted physical priors (θ) and remains costly for large MC ensembles.

A **data-driven generator** trained on realistic wind fields could replace or complement it.

Denoising Diffusion Probabilistic Model (DDPM)

A DDPM learns to reverse a Markov diffusion process:

$$p_{\phi}(\mathbf{U}^{(0)}) = \int p(\mathbf{U}^{(T)}) \prod_{t=1}^T p_{\phi}(\mathbf{U}^{(t-1)} | \mathbf{U}^{(t)}) d\mathbf{U}^{(1:T)}$$

The reverse step is parametrised by a neural network $\epsilon_{\phi}(\mathbf{U}^{(t)}, t)$ trained to denoise a Gaussian-corrupted wind field.

Physical constraints

The generation is **conditioned** on θ (mean speed, turbulence class, shear...) to enforce IEC-compatible statistics while capturing non-stationary structure beyond the Kaimal model.

DDPM WIND GENERATOR: PROPOSED WORKFLOW (1)

PhD Simon QUERNE (Nov. 2024 – Nov. 2027)

Supervision: Laurent DUMAS (UVSQ), Charles Tillier (UVSQ), **Jean-François LECOMTE (IFPEN)**

Training phase (offline, once)

1. Collect a dataset of wind fields $\{\mathbf{U}_i^{(0)}, \boldsymbol{\theta}_i\}$ from TurbSim runs or measurements.
2. Train the conditional DDPM $\epsilon_\phi(\cdot, t, \boldsymbol{\theta})$ to minimise $\mathcal{L}(\phi)$.
3. Validate generated spectra against Kaimal PSD and spatial coherence targets.

Inference phase (online, per realisation)

1. Specify $\boldsymbol{\theta}$ (possibly non-stationary: $\boldsymbol{\theta}(t)$).
2. Sample $\mathbf{U}^{(T)} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$.
3. Run T reverse denoising steps conditioned on $\boldsymbol{\theta}$.
4. Output: one realisation $\mathbf{U}(x, y, t; \boldsymbol{\theta})$.

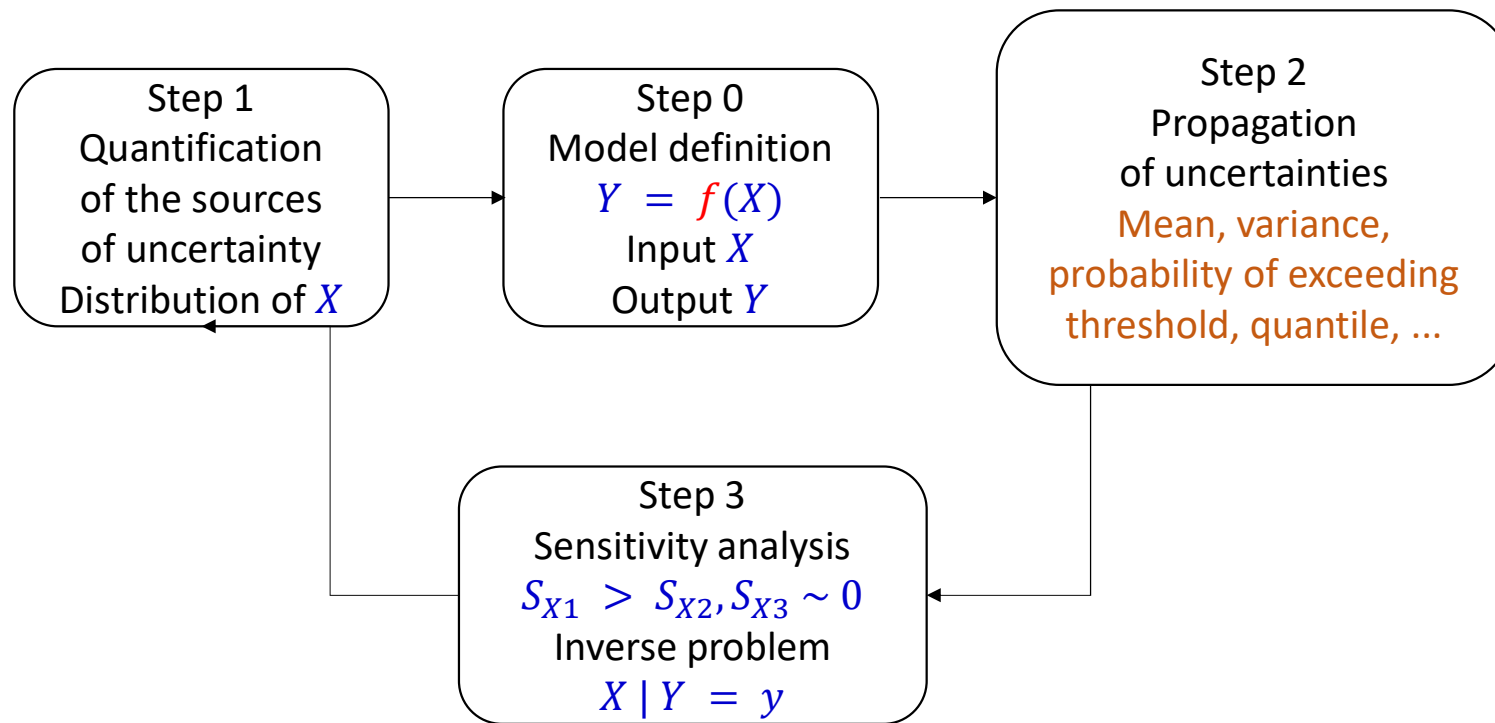
NON-STATIONARY WIND FIELD GENERATION

Can we do the same or better with dedicated and taylored SDEs ?

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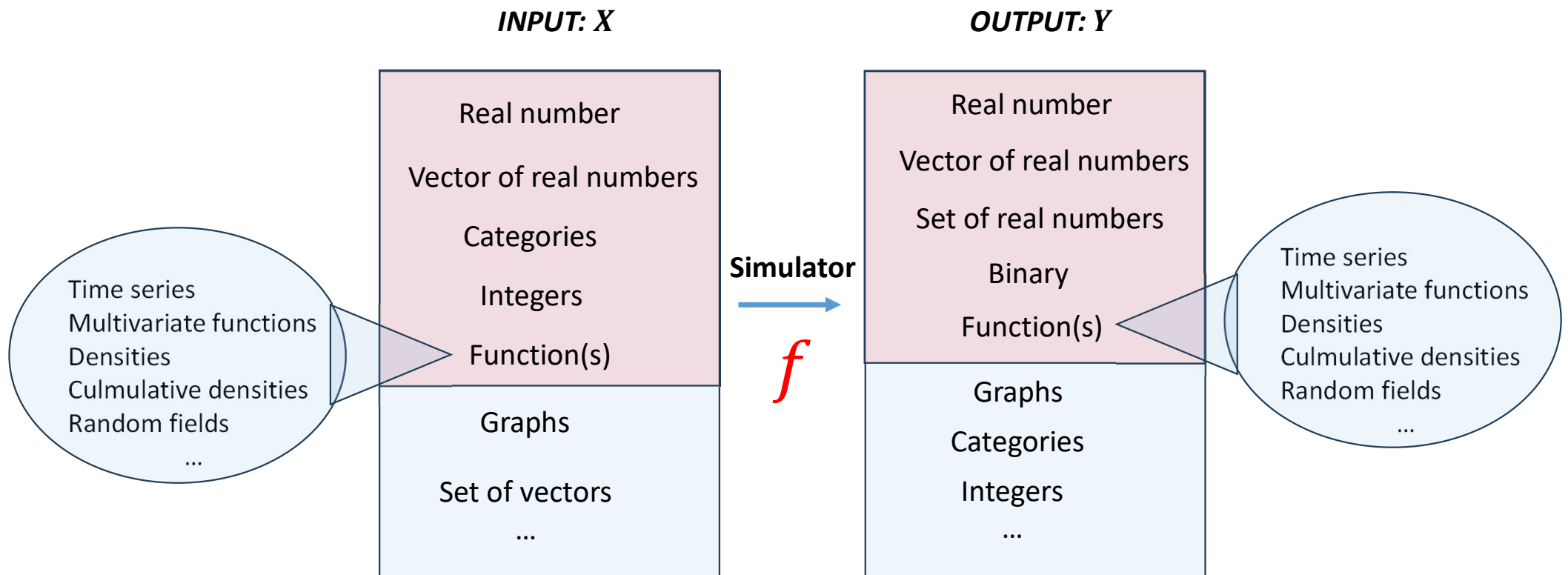
UNCERTAINTY QUANTIFICATION PIPELINE



Extract from a lecture, An introduction to Uncertainty Quantification, by Josselin Garnier.

RT-UQ workshop 12 and 13 November 2025 at Institut Henri Poincaré, Paris, France. <https://uq.math.cnrs.fr/>

UNCERTAINTY QUANTIFICATION – INPUTS AND OUTPUTS

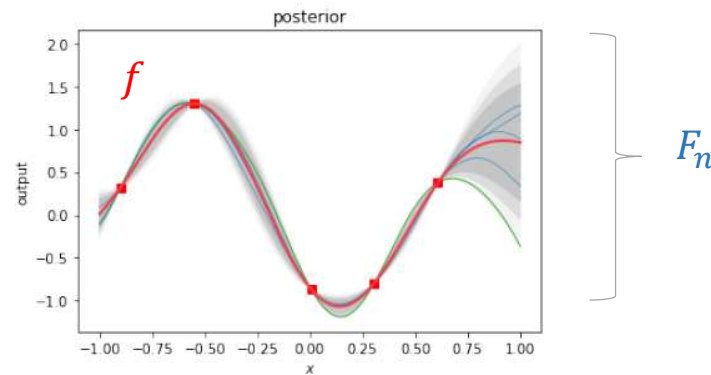


FRUGAL LEARNING

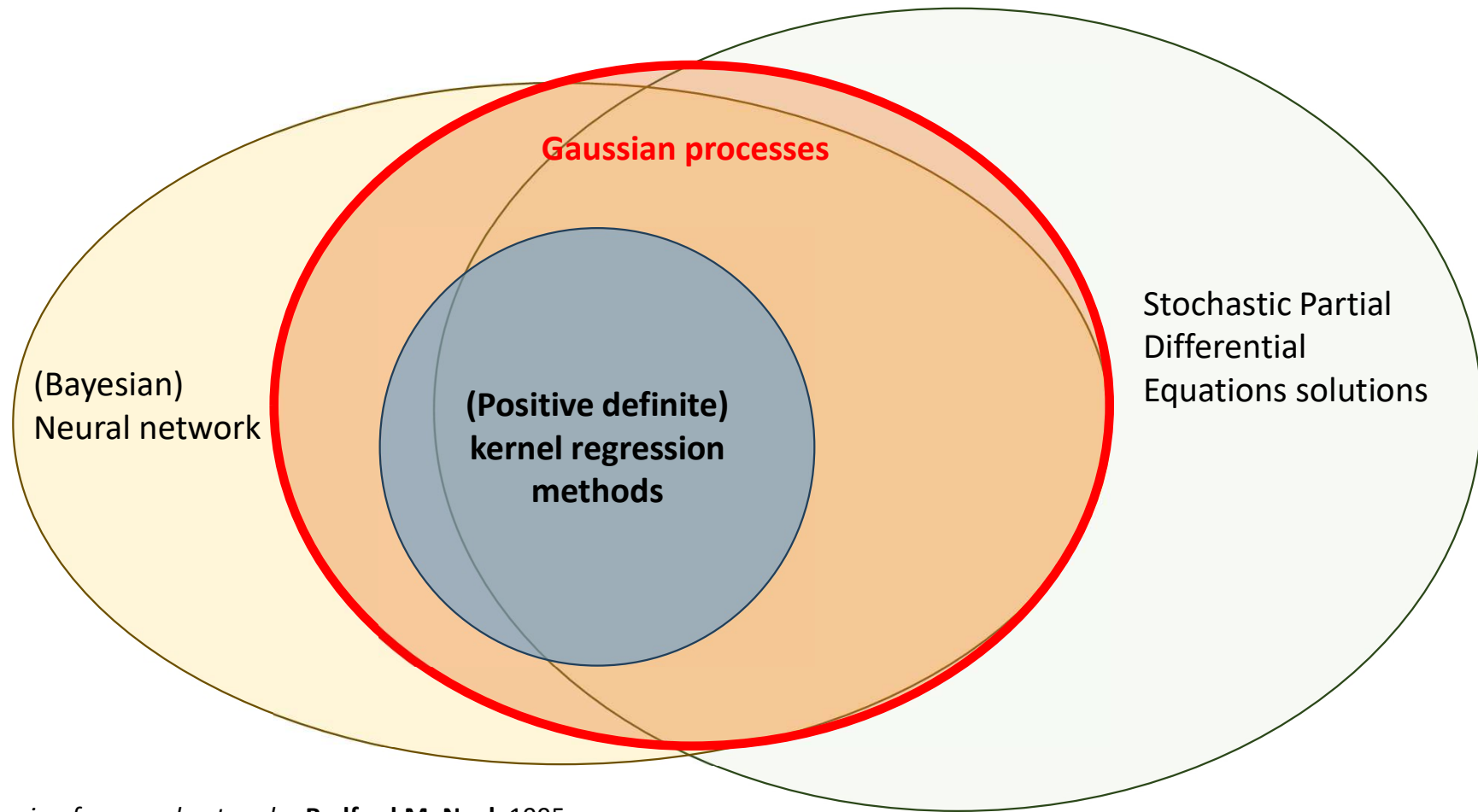
- **Complex numerical model** representing a physical phenomena with high fidelity
- Computational time constraint imposes an access to a **reduced number of simulation**
- **UQ analysis are costly in simulations**
- Introduction of a **surrogate model: Gaussian processes** →

Probabilistic model
ease uncertainty modelling and
quantification

$f \xleftrightarrow{\sim} F_n$ Gaussian process, f is a realization of F_n
built on n data points



MACHINE LEARNING AND STOCHASTIC MODELLING - SKETCH



Bayesian learning for neural networks, Radford M. Neal, 1995.

Neural networks and quantum field theory, J. Halverson, A. Maiti and K. Stoner, 2020

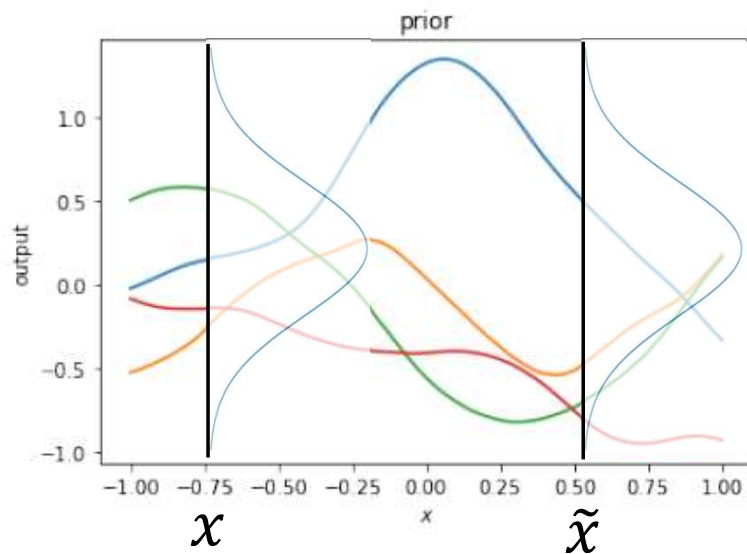
GAUSSIAN PROCESS MODEL FROM PRIOR TO POSTERIOR

Design of experiments

$$\mathcal{F}_n = \{F(x_1) = f(x_1), \dots, F(x_n) = f(x_n)\}$$

Prior model

$$F \sim N(\mu, k)$$



$$\text{Cov}(F(x), F(\tilde{x})) = k(x - \tilde{x})$$

Posterior model

$$F_n = F | \mathcal{F}_n \sim N(\mu_n, k_n)$$

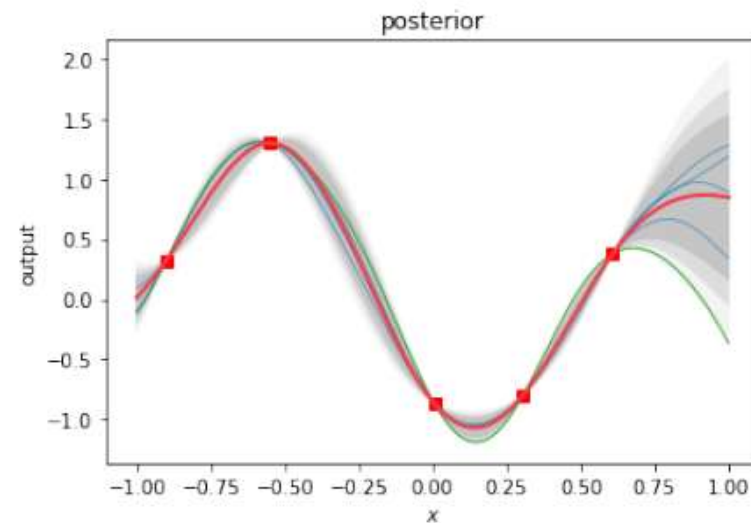


Figure: $\text{TwoBumps}(x) = -(0.7x + \sin(5x + 1) + 0.1 \sin(10x))$.

$$A|B \Leftrightarrow A \text{ knowing } B$$

QUANTITIES OF INTEREST

$$Y = f(X) \quad \begin{array}{l} (\Omega, \mathbb{P}) \rightarrow (\mathbb{H}, \mathbb{P}_X) \\ \omega \rightarrow Y(\omega) \end{array}$$

Interesting question, fully informative
What is the distribution of Y ?

But often we are interested in a specific
quantity of interest function of Y

$$\mathcal{O}(Y) \rightarrow \mathcal{O}_f$$

“If you possess a restricted amount of information for solving some problem, try to solve the problem directly and never solve a more general problem as an intermediate step. It is possible that the available information is sufficient for a direct solution but is insufficient for solving a more general intermediate problem.”

V.N. Vapnik, Statistical Learning Theory, p-12, Wiley, 1998

QUANTITIES OF INTEREST

$$Y = f(X) \quad (\Omega, \mathbb{P}) \rightarrow (\mathbb{H}, \mathbb{P}_X)$$

$$\omega \rightarrow Y(\omega)$$

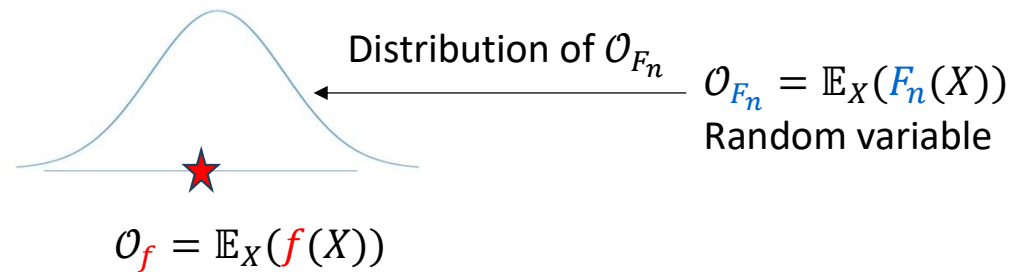
Interesting question, fully informative
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Step 2
Propagation
of uncertainties
Mean, variance,
probability of exceeding
threshold, quantile,
Sensitivity analysis
Inverse problem
 $\mathcal{O}_f \rightarrow \mathcal{O}_{F_n}$

$$\mathbb{E}_X(f(X)) = \mathcal{O}_f \rightarrow \mathcal{O}_{F_n} = \mathbb{E}_X(F_n(X))$$



SEQUENTIAL UNCERTAINTY REDUCTION PIPELINE

My goal: \mathcal{O}_f

Current DoE: \mathcal{X}_n used to build the stochastic model \mathcal{O}_{F_n}

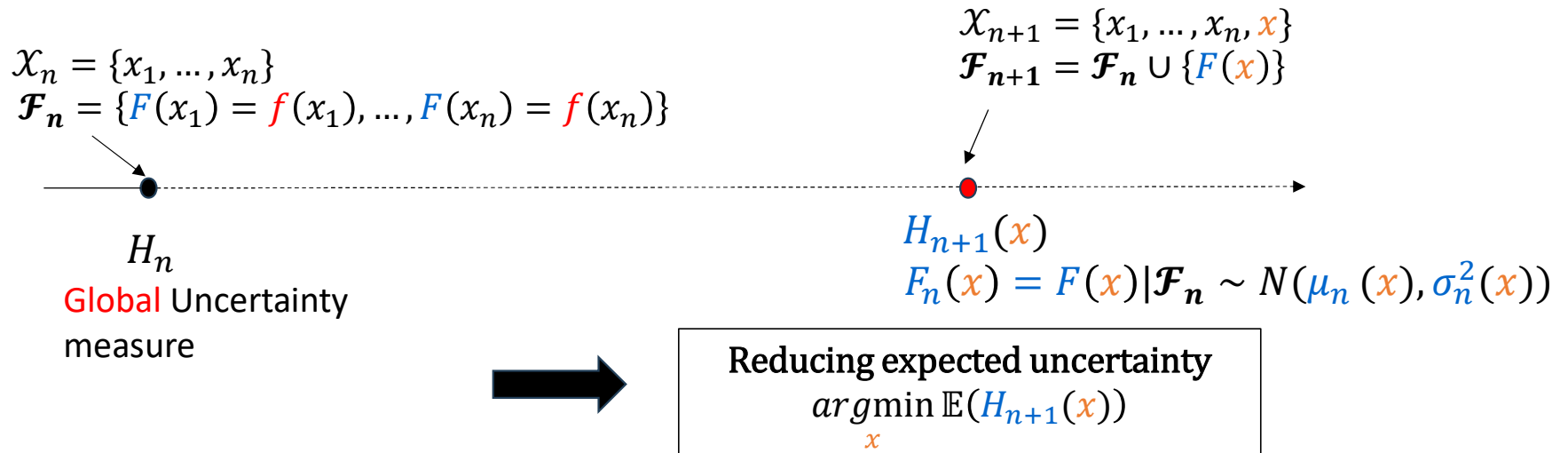
Define (global) uncertainty measure \mathcal{H}_n

Go from \mathcal{X}_n to $\mathcal{X}_n \cup \{x\}$ such that the expected uncertainty \mathcal{H}_{n+1} is minimal i.e.

$$\operatorname{argmin}_x \mathcal{H}_{n+1}(x)$$



STEPWISE UNCERTAINTY APPROACH: SUR



Advantages of SUR strategies

- Present « smoother » criteria to optimize
- Show **better performances than “classical”** strategies (Bect [2012])

Obstacles linked to SUR strategies

- If not analytical, criteria can be expensive to estimate requiring GP conditional simulations.
Few solutions:
 - quadrature methods
 - simplifying approximation

QUANTITIES OF INTEREST

$$Y = f(X) \quad (\Omega, \mathbb{P}) \rightarrow (\mathbb{H}, \mathbb{P}_X)$$

$$\omega \rightarrow Y(\omega)$$

Interesting question, fully informative
What is the distribution of Y ?

But often we are interested in a specific
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$$\mathcal{O}(Y) \rightarrow \mathcal{O}_f$$

Standard strategies

Add sequentially points to the learning design:

- for improving F_n as a model of f
- For improving a goal oriented heuristic criteria
- **For reducing the « real » uncertainty on the sought quantity**

Set estimation

Output: sets

$$\{x, f(x) < s\}$$

$$\forall i, \{x, f_i(x) < s_i\}$$

C. Duhamel PhD

$$\{u, \mathbb{E}_X(f(u, X)) < s\}$$

R. El Amri PhD

$$\{x, \mathbb{I}(x) = NaN\}$$

M. Menz PostDoc

Bayesian inversion, calibration

Output: distribution, Random Var

$$X|Y_{real,m}Y_m \text{ or } p(X|Y_{real,m}, Y_m)$$

$$C_f(\mathcal{X}_m) = p_f(X|\mathcal{X}_m) \text{ or } X|\mathcal{X}_m$$

A. Hirvoas, A. Barry PhD

Chance constraint optimization

Output: number, function

$$\min_u C(u)$$

$$\text{s.t } c(u) = \mathbb{P}_X(g \circ f(u, X) > 0) > 1 - \epsilon$$

A. Cousin PhD

$$\mathbb{E}_X(g \circ f(X))$$

Moment, probability estimation

Output: number

$$\mathbb{P}_X(g \circ f(X) > 0)$$

A. Murangira, V. Breaz PostDoc

Sensitivity analysis

Output: vector

$$S^f(X)$$

E. Bartok PhD



Metamodelling

Output: function



E. Rondeaux PhD



Space-filling design

Output: finite set of functions

$$\mathcal{X}_n$$

L. Calzolari PhD



QUANTITIES OF INTEREST

$$Y = f(X) \quad (\Omega, \mathbb{P}) \rightarrow (\mathbb{H}, \mathbb{P}_X)$$

$$\omega \rightarrow Y(\omega)$$

Interesting question, fully informative
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$$\mathcal{O}(Y) \rightarrow \mathcal{O}_f$$

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A. Murangira, V. Breaz PostDoc

Sensitivity analysis

Output: vector

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E. Bartok PhD



Metamodelling

Output: function



E. Rondeaux PhD



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Output: finite set of functions

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L. Calzolari PhD



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$$\omega \rightarrow Y(\omega)$$

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2.

Set estimation

Output: sets

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M. Menz PostDoc

Bayesian inversion, calibration

Output: distribution, Random Var

$$X|Y_{real,m}Y_m \text{ or } p(X|Y_{real,m}, Y_m)$$

$$C_f(\mathcal{X}_m) = p_f(X|\mathcal{X}_m) \text{ or } X|\mathcal{X}_m$$

A. Hirvoas, A. Barry PhD

1.

Expectation estimation for Chance constraint optimization

$$\min_u C(u)$$

$$\text{s.t } c(u) = \mathbb{P}_X(g \circ F_n(u, X) > 0) > 1 - \epsilon$$

A. Cousin PhD

$$\mathbb{E}_X(g \circ F_n(X))$$

Moment, probability estimation

Output: number

$$\mathbb{P}_X(g \circ F_n(X) > 0)$$

A. Murangira, V. Breaz PostDoc

Sensitivity analysis

Output: vector

$$S^{F_n}(X)$$

E. Bartok PhD



Metamodelling

Output: function



E. Rondeaux PhD



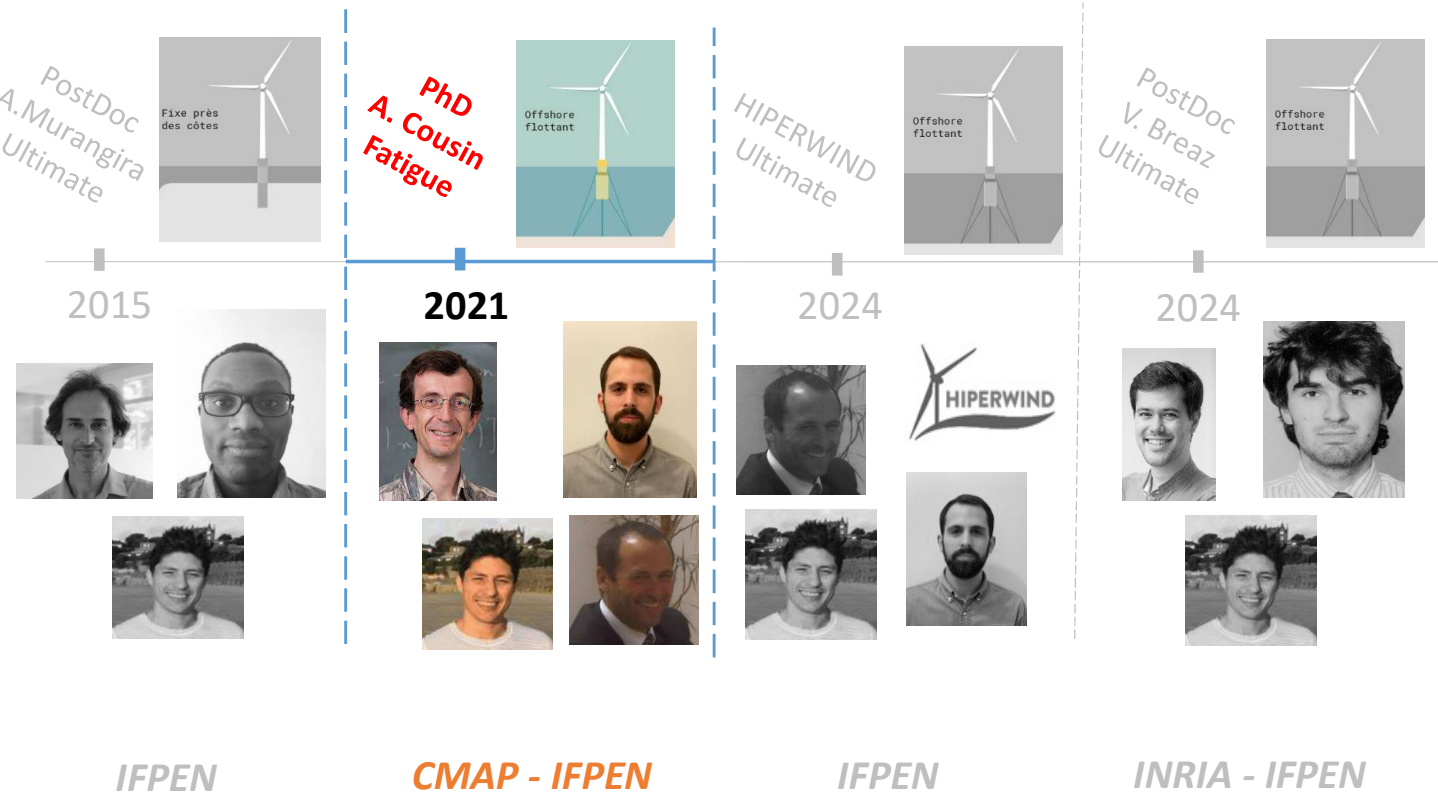
Space-filling design

Output: finite set of functions

$$\mathcal{X}_n \quad \text{L. Calzolari PhD}$$



ROBUST DESIGN AND RELIABILITY ANALYSIS



Chance constraint optimization
Output : number, function

$$\min_u C(u)$$

$$\text{s.t } c(u) = \mathbb{P}_X(g \circ f(u, X) > 0) > 1 - \epsilon$$

A. Cousin PhD $\mathbb{E}_X(g \circ f(X))$

Moment, probability estimation
Output : number

$$\mathbb{P}_X(g \circ f(X) > 0)$$

A. Murangira, V. Breaz PostDoc

CHANCE CONSTRAINT OPTIMIZATION - A. COUSIN PHD

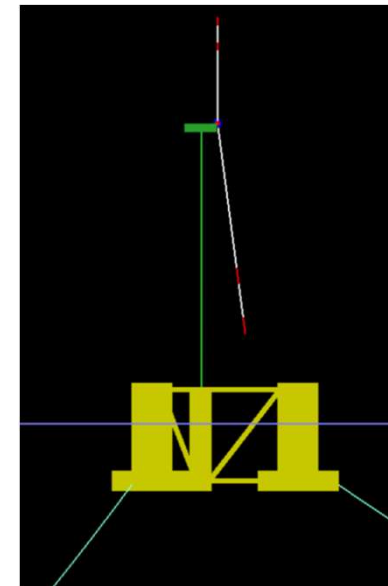
Optimize the cost of mooring system under fatigue and feasibility constraints

$$\begin{aligned} & \min_{d \in \Omega_d} \text{cost}(d) \quad \text{such that} \\ & \mathbb{P}_{X_p, \eta} \left(\max_{t \in [0, T]} |\mathcal{S}(d, X_p; t)| > \mathcal{S}_{\max} \right) < 10^{-4} \\ & \mathbb{P}_{X_p, \eta} \left(\min_{t \in [0, T]} \mathcal{T}^l(d, X_p; t) < 0 \right) < 10^{-4}, \quad l = 1, 2, 3 \\ & \mathbb{P}_{X_{d_2}, X_p, X_R, \eta} \left(\int_0^T \mathcal{D}^l(d, X_{d_2}, X_p; t) dt > X_R \right) < 10^{-4}, \quad l = 1, 2, 3. \end{aligned}$$

d : length to the mooring, mass per unit, position of lines to columns

Uncertainties: Azimuth, damping and fatigue law coefficients

NREL 5MW turbine on DeepCWind floater



DEEPLINES™

The sea elevation **stationary Gaussian process** defined by its **spectral density** (JONSWAP)

CHANCE CONSTRAINT OPTIMIZATION - A. COUSIN PHD

Optimize the cost of morning system under fatigue and feasibility constraints

$$\begin{aligned}
 & \min_{d \in \Omega_d} \text{cost}(d) \quad \text{such that} \\
 & \mathbb{P}_{X_p, \eta} \left(\max_{t \in [0, T]} |\mathcal{S}(d, X_p; t)| > \mathcal{S}_{\max} \right) < 10^{-4} \\
 & \mathbb{P}_{X_p, \eta} \left(\min_{t \in [0, T]} \mathcal{T}^l(d, X_p; t) < 0 \right) < 10^{-4}, \quad l = 1, 2, 3 \\
 & \mathbb{P}_{X_{d_2}, X_p, X_R, \eta} \left(\int_0^T \mathcal{D}^l(d, X_{d_2}, X_p; t) dt > X_R \right) < 10^{-4}, \quad l = 1, 2, 3.
 \end{aligned}$$

Extreme value theory
(linearization of the equation of motion) \downarrow

$$\begin{aligned}
 & \min_{d \in \Omega_d} \text{cost}(d) \quad \text{such that} \\
 & \mathbb{E}_{X_p} \left[F_\epsilon \left(\sum_{j=1}^7 \exp \left(a_{T p^j}(d, X_p, s^j)^2 - \frac{a_{T p^j}(d, X_p, s^j) (\mathcal{S}_{\max} + \mu_{\mathcal{S}}(d, X_p, s^j))}{\sqrt{m_{\mathcal{S}, 0}(d, X_p, s^j)}} \right) \right) \right] < 10^{-4} \\
 & \mathbb{E}_{X_p} \left[F_\epsilon \left(\sum_{j=1}^7 \exp \left(b_{T p^j}^l(d, X_p, s^j)^2 - \frac{b_{T p^j}^l(d, X_p, s^j) \mu_{\mathcal{T}^l}(d, X_p, s^j)}{\sqrt{m_{\mathcal{T}^l, 0}(d, X_p, s^j)}} \right) \right) \right] < 10^{-4}, \quad l = 1, 2, 3 \\
 & \mathbb{E}_{X_p} \left[\Phi \left(\frac{\log(T \sum_{j=1}^7 p^j E_{\mathcal{T}^l}(d, X_p, s^j)) - (\mu_R + \mu_{d_2})}{\sqrt{\sigma_R^2 + \sigma_{d_2}^2}} \right) \right] < 10^{-4}, \quad l = 1, 2, 3.
 \end{aligned} \tag{5.6}$$

- New quantity of interest:

$$\mathbb{E}_X(g \circ F_n(X))$$

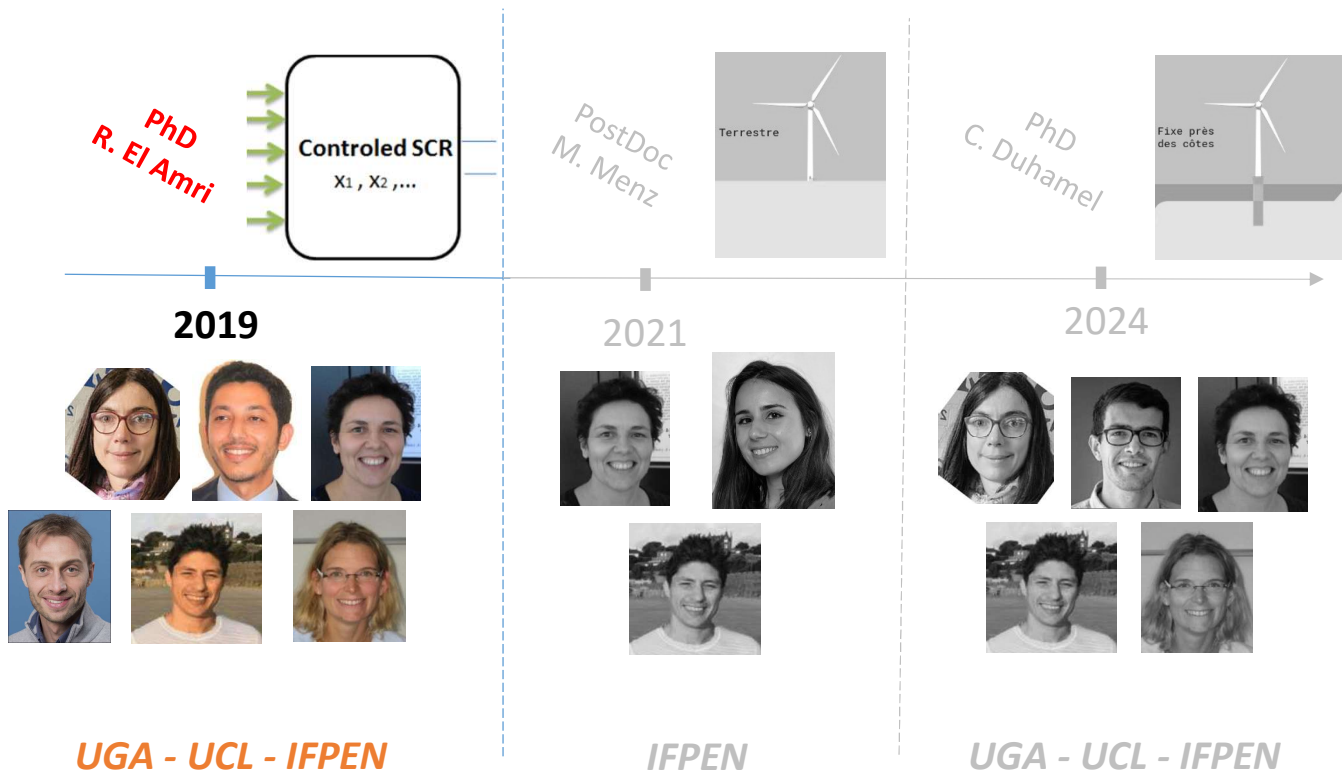
- Improving a goal oriented heuristic criteria:

$$\operatorname{argmax}_x p_X(x) [g(\mu_n^+(x)) - g(\mu_n^-(x))]$$

$$\text{with } \mu_n^\pm = \mu_n \pm 2\sigma_n$$

$$\operatorname{argmax}_{\substack{u \in \mathcal{U} \\ v \in \{v_i, i=1, \dots, K\}}} p_U(u) \left[g_1 \left(\mu^+(u, v) + \sum_{v_i \neq v} \mu(u, v_i) \right) - g_1 \left(\mu^-(u, v) + \sum_{v_i \neq v} \mu(u, v_i) \right) \right]$$

SET ESTIMATION



Set estimation

Output: sets

$$\{x, f(x) < s\}$$

$$\forall i, \{x, f_i(x) < s_i\}$$

C. Duhamel PhD

$$\{u, \mathbb{E}_X(f(u, X)) < s\}$$

R. El Amri PhD

$$\{x, \mathbb{I}^f(x) = NaN\}$$

M. Menz PostDoc

ROBUST SET ESTIMATION

$$\mathcal{O}_{\mathcal{L} \circ F_n} = \{u, \mathbb{E}_X(F_n(u, X)) < s\} = \{u, [\mathcal{L} \circ F_n](u) < s\}$$

- Uncertainty measure: Vorob'ev deviation ([Molchanov, 2006])

$$d_V(\mathcal{O}_{[\mathcal{L} \circ F_n]}) = \mathbb{E}_{[\mathcal{L} \circ F_n]} \left(\lambda(\mathcal{O}_{[\mathcal{L} \circ F_n]} \Delta \mathcal{Q}_{n, \alpha_n^*}) \right)$$

$$\mathbb{E}_{F_n} \left(\lambda(\mathcal{O}_{F_n} \Delta \mathcal{Q}_{n, \alpha_n^*}) \right) = \int_{\mathcal{Q}_{n, \alpha_n^*}^c} \pi_n(u) du + \int_{\mathcal{Q}_{n, \alpha_n^*}} 1 - \pi_n(u) du$$

- SUR criteria on Vorob'ev deviation:

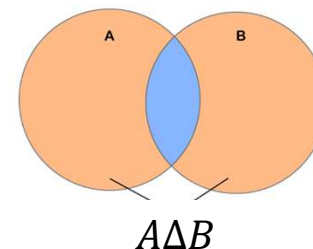
$$\operatorname{argmin}_u \mathbb{E}_{[\mathcal{L} \circ F](u) | \mathcal{F}_n} [d_V(\mathcal{O}_{[\mathcal{L} \circ F]_{n+1}})]$$

$$\operatorname{argmin}_x \operatorname{Var} [[\mathcal{L} \circ F]_{n+1}(u_{n+1})]$$

$$[\mathcal{L} \circ F_n](u) = \mathbb{E}_X(F_n(u, X))$$

Is a known Gaussian process $\mathcal{GP}(\mu_n^\mathcal{L}, \sigma_n^\mathcal{L})$

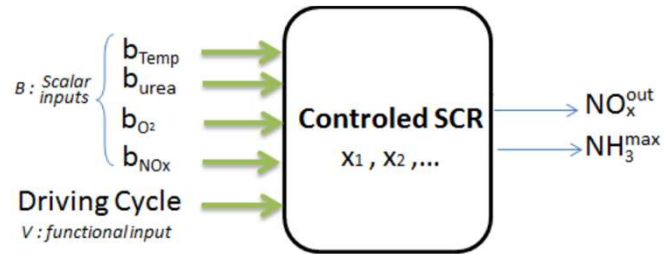
$$\pi_n(u) = \mathbb{P}([\mathcal{L} \circ F_n](u) < s)$$



$$\begin{aligned} \mathcal{Q}_{n, \alpha_n^*} &= \mathbb{P}(\pi_n(u) > \alpha_n^*) \\ &= \{u, \mu_n^\mathcal{L}(u) + \Phi^{-1}(\alpha_n^*) \sigma_n^\mathcal{L}(u) \leq s\} \end{aligned}$$

$$\alpha_n^* \text{ such that } \lambda(\mathcal{Q}_{n, \alpha_n^*}) = \mathbb{E}_{F_n} \left(\lambda(\mathcal{O}_{\mathcal{L} \circ F_n}) \right)$$

ROBUST SET ESTIMATION FOR SYSTEMS CONTROLE



$$f : \begin{cases} \mathbb{X} \times \mathcal{V} & \rightarrow \mathbb{R} \\ (x, V) & \mapsto f(x, V) = \max_{t \in I} NH_3(t) \end{cases}$$

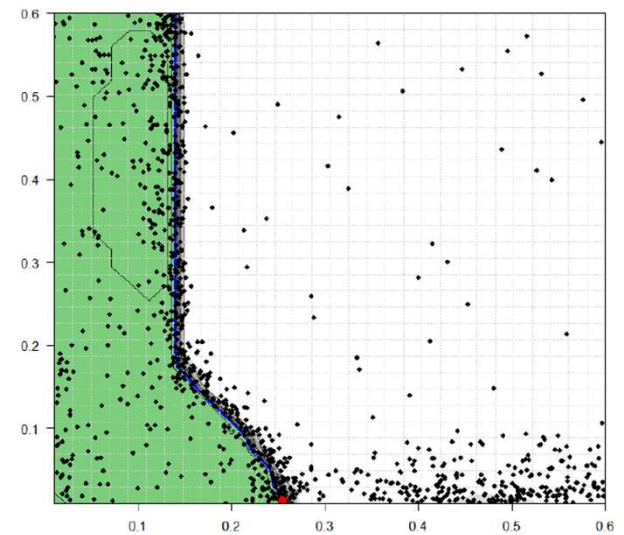
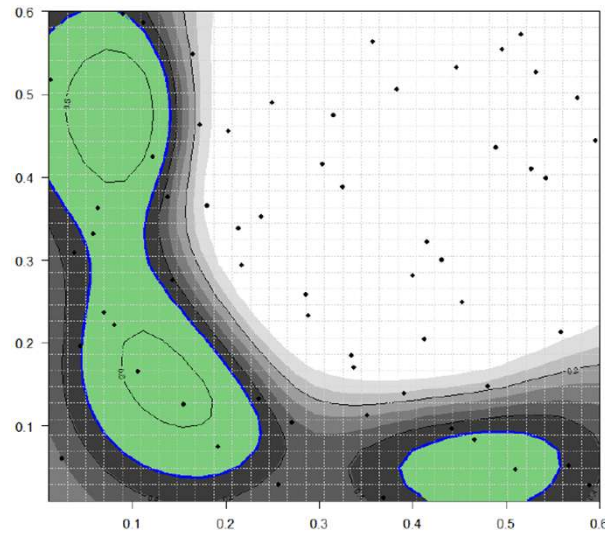
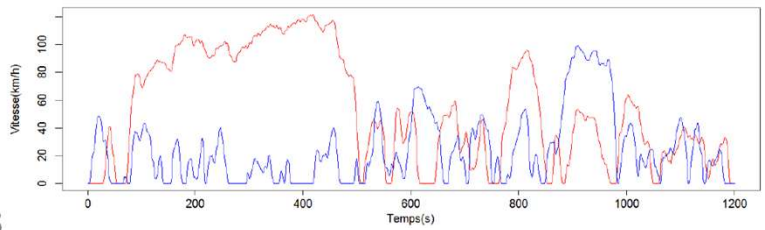
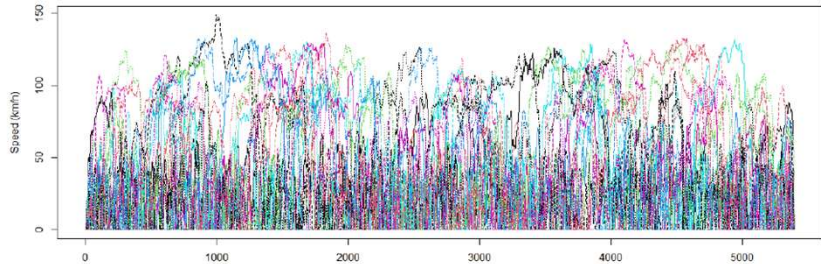
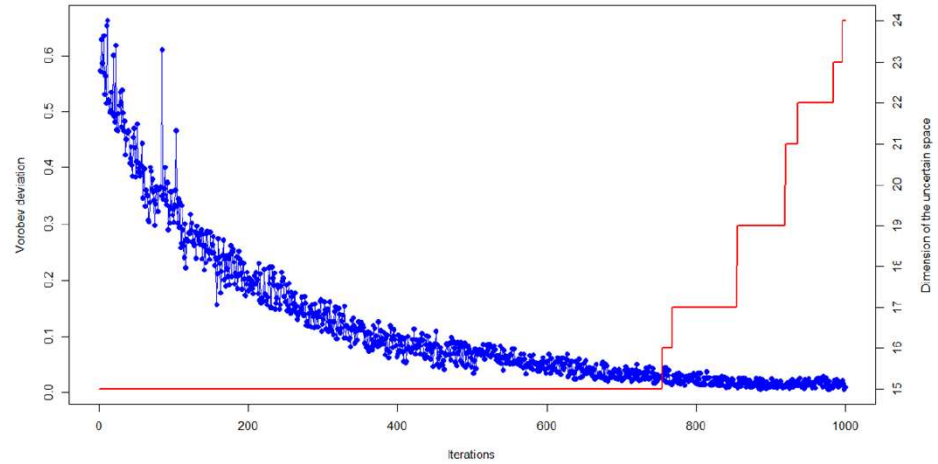
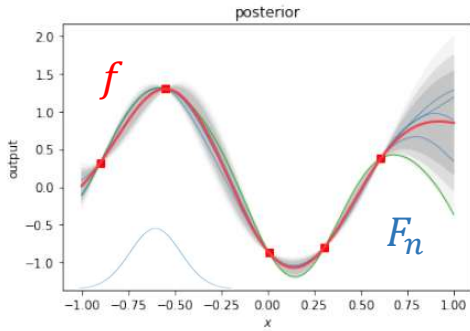


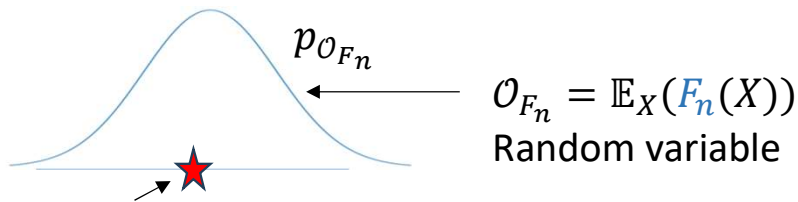
TABLE OF CONTENTS

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- **Active learning and Poincaré-Malliavin-Nualart inequalities**
- Metamodelling of complex simulator with functional inputs, bridging Gaussian processes and SDE

GOAL ORIENTED UNCERTAINTY REDUCTION



$$\mathcal{O}: L_2(\mathbb{R}^d, \Omega) \rightarrow \mathbb{R}$$



$$\mathcal{O}_f = \mathbb{E}_X(f(X))$$

reduction of the variance: $Var(\mathcal{O}_{F_n})$

stepwise uncertainty reduction (**SUR**) approach:

$$x_{n+1} = \underset{x}{\operatorname{argmin}} \mathbb{E}_{Y(x)|Y_n} [Var(\mathcal{O}_{F_{n+1}})]$$

$$\mathcal{O}: L_2(\Omega; L_2(D)) \rightarrow L_2(\Omega, \mathbb{R})$$

What about

$$\mathcal{O}_{F_n} = \mathbb{E}_X(F_n(X)^k)$$

$$\mathcal{O}_{F_n} = \mathbb{E}_X(g \circ F_n(X))$$

$$\mathcal{O}_{F_n} = \mathbb{P}_X(g \circ F_n(X) > 0)$$

$$\mathcal{O}_{F_n} = q_{g \circ F_n(X)}(\alpha)$$

$$\mathcal{O}: L_2(\mathbb{R}^d, \Omega) \rightarrow L_2(\Omega, \mathbb{R}^d)$$

What about

$$\mathcal{O}_{F_n} = (S_1, S_2, S_{12}, \dots)$$

$$\mathcal{O}: L_2(\Omega; L_2(D)) \rightarrow (\Omega, \mathbb{S})$$

What about

$$\mathcal{O}_{F_n} = \{x, g \circ F_n(x) < s\}$$

$$\mathcal{O}_{F_n} = \{u, \mathbb{E}_X(g \circ F_n(u, X)) < s\}$$

$$\mathcal{O}_{F_n} = \{u, \mathbb{P}_X(g \circ F_n(u, X) > 0) < \epsilon\}$$

$$\mathcal{O}: L_2(\mathbb{R}^d, \Omega) \rightarrow L_2(\Omega, \mathbb{H})$$

What about

$$\mathcal{O}_{F_n} = G(\cdot, F_n)$$

...

INTRODUCTION TO POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

$\mathcal{O}: L_2(\Omega; L_2(D)) \rightarrow L_2(\Omega; \mathbb{R})$, If $\mathcal{O}_{F_n} \in \mathbb{D}^{1,2}(\gamma_n)$ then

$$\text{Var}(\mathcal{O}_{F_n}) \leq \mathbb{E}_{F_n} \left(\|\mathcal{D}\mathcal{O}_{F_n}\|_{\mathbb{H}_n}^2 \right)$$

- \mathbb{H}_n : Cameron-Martin space (RKHS associated to the covariance kernel) of F_n
 - γ_n : posterior probability measure of the process, defined over an infinite-dimensional space of functional paths
 - $\mathbb{D}^{1,2}(\gamma_n)$: completion of the set of smooth cylindrical random variables $\{\psi[F_n(x_1), \dots, F_n(x_k)]\}$ w.r.t. the norm $\|S\|_{1,2} = \mathbb{E}_{\gamma_n}(S^2) + \mathbb{E}_{\gamma_n}(\|\mathcal{D}S\|_{\mathbb{H}_n}^2)$ named the « Sobolev-Watanabe » space.
 - $\mathcal{D}: \mathbb{D}^{1,2}(\gamma_n) \rightarrow L^2(B, \gamma_n; \mathbb{H}_n)$ is the Malliavin derivative we apply to the random variable \mathcal{O}_{F_n}
 - $\mathcal{D}\mathcal{O}_{F_n}$ is random variable with realization in \mathbb{H}_n
 - \mathcal{O}_{F_n} has to belong to the « Sobolev-Watanabe » space $\mathbb{D}^{1,2}(\gamma_n)$
-
- **We can generalize this type of results to the case of non-smooth operators** (for instance involving indicator functions) by using the notion of Watanabe distributions (in L. Schwartz sense) and isoperimetric inequalities.

POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to active learning of expectations

$$\mathcal{O}_{g \circ F_n} = \mathbb{E}_X(g \circ F_n(X))$$

First approach: reduce uncertainty on the **integrand** term $g \circ F_n(X)$

- **Heuristic** criteria

$$\operatorname{argmax}_x p_X(x) [g(\mu_n^+(x)) - g(\mu_n^-(x))] \text{ with } \mu_n^\pm = \mu_n \pm 2\sigma_n$$

Example:

See *[thesis Alexis Cousin, 2021]*

- **Variance** based criteria

$$\operatorname{argmax}_x \operatorname{Var}(g \circ F_n(x))$$

Example:

$$\operatorname{Var}(\exp[F_n(x)]) = \exp(2\mu_n(x) + \sigma_n(x))(\exp(\sigma_n(x)) + 1)$$

POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to active learning of expectations

$$\mathcal{O}_{g \circ F_n} = \mathbb{E}_X(g \circ F_n(X))$$

Second approach: reduce uncertainty on the real objective $\mathcal{O}_{g \circ F_n}$

$$\boxed{\text{Var}(\mathcal{O}_{g \circ F_n}) \leq \mathbb{E}_{F_n} \left(\|\mathcal{D}\mathcal{O}_{g \circ F_n}\|_{\mathbb{H}_n}^2 \right)}$$

Global uncertainty measure

SUR criteria:

$$\mathbb{E}_{F(x)|\mathcal{F}_n} \left(\mathbb{E}_{F_{n+1}} \left(\|\mathcal{D}\mathcal{O}_{g \circ F_{n+1}}\|_{\mathbb{H}_{n+1}}^2 \right) \right) = \sigma_n(x)^{-2} \mathbb{E}_{X, X'} [k_n(X, x) k_n(X', x) A_{n+1}(X, X')]$$

$$A_{n+1}(X, X') = \mathbb{E}_{F(x)|\mathcal{F}_n} \left(\mathbb{E}_{F_{n+1}} [g'(F_{n+1}(X)) g'(F_{n+1}(X'))] \right)$$

POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to active learning of expectations

For example: $g = Id$

$$\mathcal{O}_{F_n} = \mathbb{E}_X(F_n(X))$$

Second approach: reduce uncertainty on the real objective \mathcal{O}_{F_n}

$$\text{Var}(\mathcal{O}_{F_n}) = \mathbb{E}_{F_n} \left(\|\mathcal{D}\mathcal{O}_{F_n}\|_{\mathbb{H}_n}^2 \right)$$

- SUR criteria:

$$\mathbb{E}_{F(x)|\mathcal{F}_n}[\text{Var}(\mathcal{O}_{F_{n+1}})] = \text{Var}(\mathcal{O}_{F_{n+1}}) = \mathbb{E}_{F_{n+1}} \left(\|\mathcal{D}\mathcal{O}_{F_{n+1}}\|_{\mathbb{H}_{n+1}}^2 \right) = \sigma_n(x)^{-2} \mathbb{E}_X [k_n(X, x)]^2$$

[Cousin et al, 2024]

POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to active learning of expectations

For example: $g = \exp$

$$\mathcal{O}_{\exp \circ F_n} = \mathbb{E}_X(\exp \circ F_n(X))$$

Second approach: reduce uncertainty on the real objective $\mathcal{O}_{\exp \circ F_n}$

$$\text{Var}(\mathcal{O}_{\exp \circ F_n}) \leq \mathbb{E}_{F_n} \left(\left\| \mathcal{D} \mathcal{O}_{\exp \circ F_n} \right\|_{\mathbb{H}_n}^2 \right)$$

- SUR criteria - one point:

$$\underset{x}{\operatorname{argmin}} \mathbb{E}_{F(x)|\mathcal{F}_n} \left[\mathbb{E}_{F_{n+1}} \left(\left\| \mathcal{D} \mathcal{O}_{\exp \circ F_{n+1}} \right\|_{\mathbb{H}_{n+1}}^2 \right) \right] = \underset{x}{\operatorname{argmax}} \sigma_n(x)^{-2} \mathbb{E}_{X, X'} [k_n(X, x) k_n(X', x) A_n(X, X')]$$

$$A_n(X, X') = \exp \left[\mu_n(X) + \mu_n(X') + \frac{1}{2} (\sigma_n(X) + \sigma_n(X') + 2k_n(X, X')) \right]$$

POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to active learning of expectations

- Non-stationarity issues

$$\begin{aligned} \mathcal{O}_f &= \mathbb{E}_X(f(X)) \\ &= \mathbb{E}_X(\exp \circ \underbrace{\log[f(X)]}_{\tilde{f}}) \end{aligned} \quad \longrightarrow \quad \mathcal{O}_{F_n} = \mathbb{E}_X(\exp \circ F_n(X))$$

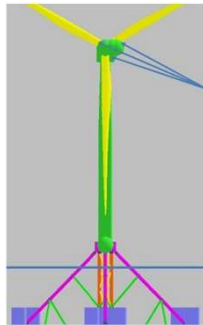
POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to active learning of expectations

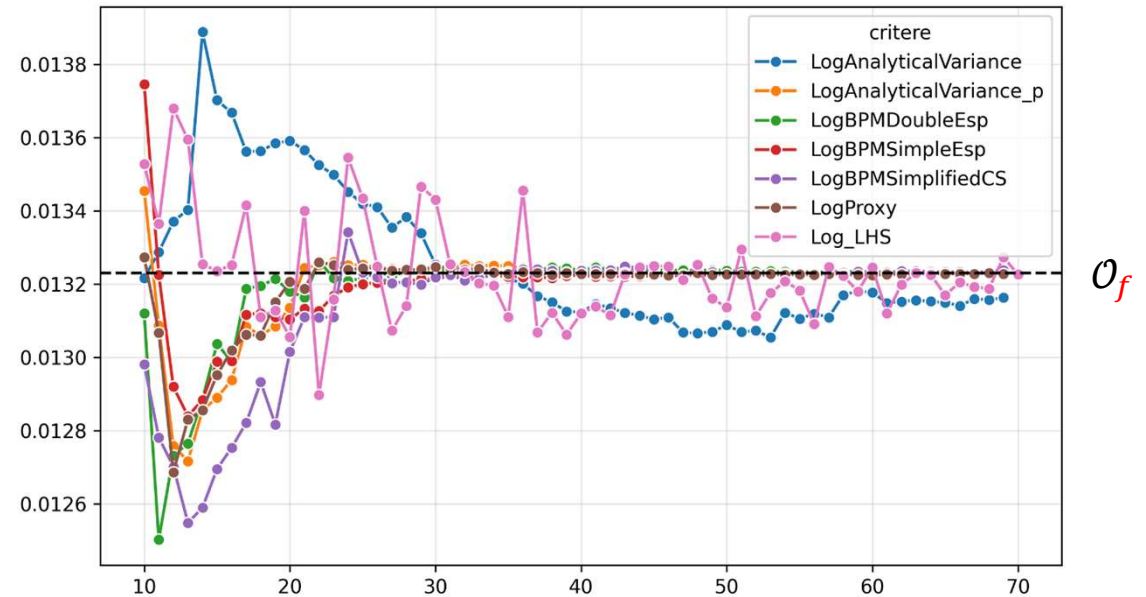
$$\mathcal{O}_{F_n} = \mathbb{E}_X(\exp \circ F_n(X))$$

- Estimation mean annual damage at the top of a mooring line.
- 6MW tension leg platform (TLP) wind turbine model.

- **2D input case: (U, σ_U)**
- Initialization: 20 points
- Monte Carlo: 50000 points
- Iteration: 30, one point at the time



| | |
|---|---------------------|
| $\operatorname{argmax}_x p_X(x) [g(\mu_n^+(x)) - g(\mu_n^-(x))]$ | Proxy |
| $\operatorname{argmax}_x p_X(x)^2 \exp(2\mu_n(x) + \sigma_n(x)) (\exp(\sigma_n(x)) + 1)$ | Analytical variance |
| $\operatorname{argmax}_x \sigma_n(x)^{-1} \mathbb{E}_X \left[k_n(X, x) \exp \left(\mu_n(X) + \frac{1}{2} \sigma_n^2(X) \right) \right]$ | Simple Exp |
| $\operatorname{argmax}_x \sigma_n(x)^{-2} \mathbb{E}_X [k_n(X, x)^2]$ | Simplified |



Double Exp. $\operatorname{argmax}_x \sigma_n(x)^{-2} \mathbb{E}_{X, X'} \left[k_n(X, x) k_n(X', x) \exp \left[\mu_n(X) + \mu_n(X') + \frac{1}{2} (\sigma_n(X) + \sigma_n(X') + 2k_n(X, X')) \right] \right]$

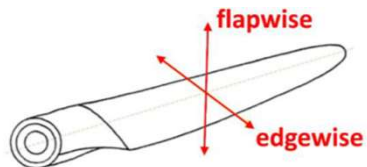
POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to active learning of expectations

$$\mathcal{O}_{F_n} = \mathbb{E}_X(\exp \circ F_n(X))$$

- Estimation mean annual **flapwise** and **edgewise** blade root damage
- 6MW tension leg platform (TLP) wind turbine model.

• 6D case ($U, \sigma_U, \theta_{wind}, H_s, T_p, \theta_{wave}$)



Results coming soon

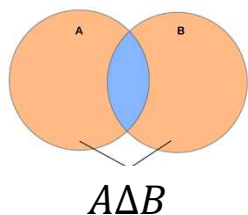
POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to robust active learning of sets

$$\mathcal{O}_{F_n} = \{u, \mathbb{E}_X(F_n(u, X)) < s\} \quad \text{or} \quad \mathcal{O}_{F_n} = \{u, \mathbb{P}_X(F_n(u, X) > 0) < s\}$$

$$\boxed{\mathcal{O}_{\mathcal{L}_{F_n}} = \{u, \mathcal{L}_{F_n}(u) < s\}} \quad \text{where } \mathcal{L}_{F_n}(u) = \mathbb{E}_X(F_n(u, X)) \quad \text{or} \quad \mathbb{P}_X(F_n(u, X) > 0)$$

- Uncertainty measure : Vorob'ev deviation $d_V(\mathcal{O}_{\mathcal{L}_{F_n}})$



$$\boxed{d_V(\mathcal{O}_{\mathcal{L}_{F_n}}) = \mathbb{E}_{\mathcal{L}_{F_n}} \left(\lambda \left(\mathcal{O}_{\mathcal{L}_{F_n}} \Delta \mathcal{Q}_{n, \alpha_n^*} \right) \right)}$$

$$\begin{aligned} \forall u \mathcal{L}_{F_n}(u) &\sim \text{Law} \left(\mu_n^{\mathcal{L}}(u), \sigma_n^{\mathcal{L}}(u) \right) \\ \mathcal{Q}_{n, \alpha_n^*} &= \{ u, \mu_n^{\mathcal{L}}(u) + \Phi_{\mathcal{L}}^{-1}(\alpha_n^*) \sigma_n^{\mathcal{L}}(u) \leq s \} \\ \alpha_n^* &\text{ such that } \lambda(\mathcal{Q}_{n, \alpha_n^*}) = \mathbb{E}_{F_n} \left(\lambda(\mathcal{O}_{F_n}) \right) \end{aligned}$$

- SUR criteria on Vorob'ev deviation

$$\boxed{\underset{x}{\operatorname{argmin}} \mathbb{E}_{\mathcal{L}_F(x) | \mathcal{F}_n} \left[d_V \left(\mathcal{O}_{\mathcal{L}_{F_{n+1}}} \right) \right]}$$

POINCARÉ-MALLIAVIN-NUALART INEQUALITIES

Application to robust active learning of sets

$$\text{where } \mathcal{L}_{F_n}(u) = \begin{cases} \mathbb{E}_X(F_n(u, X)) \\ \text{or} \\ \mathbb{P}_X(F_n(u, X) > 0) \end{cases}$$

- Inequality on Vorob'ev deviation $d_V(\mathcal{O}_{F_n})$:

$$V_{int} = \int \text{Var}(H_u(F_n)) du = \int \pi_n(u)(1 - \pi_n(u)) du$$

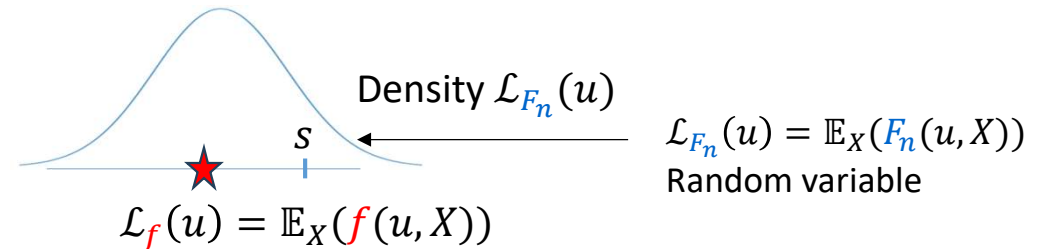
$$\begin{cases} H_u(F_n) = \mathbb{I}_{\mathcal{L}_{F_n}(u) < s} \\ \pi_n(u) = \mathbb{P}_{F_n}(\mathcal{L}_{F_n}(u) < s) \end{cases}$$

$$V_{int} \leq d_V(\mathcal{O}_{F_n}) \leq \frac{V_{int}}{\min(\alpha_n^*, 1 - \alpha_n^*)}$$

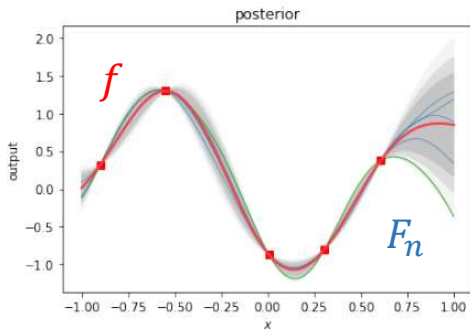
- Possible local uncertainty measure

$$\text{Var}(H_u(F_n)) \leq \mathbb{E}_{F_n} \left(\left\| \mathcal{D}H_u(F_n) \right\|_{TV} \right) = C_{F_n}(u) p_{\mathcal{L}_{F_n}(u)}(s)$$

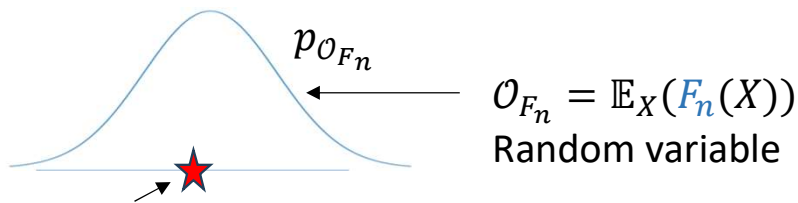
$$V_{int} \leq \int C_{F_n}(u) p_{\mathcal{L}_{F_n}(u)}(s) du$$



DOORS ARE WIDE OPEN



$$\mathcal{O}: L_2(\mathbb{R}^d, \Omega) \rightarrow \mathbb{R}$$



$\mathcal{O}_{F_n} = \mathbb{E}_X(F_n(X))$
Random variable

$$\mathcal{O}_f = \mathbb{E}_X(f(X))$$

reduction of the variance $\text{Var}(\mathcal{O}_{F_n})$

stepwise uncertainty reduction (**SUR**) approach

$$x_{n+1} = \underset{x}{\operatorname{argmin}} \mathbb{E}_{Y(x)|Y_n} [\text{Var}(\mathcal{O}_{F_{n+1}})]$$

$$\mathcal{O}: L_2(\mathbb{R}^d, \Omega) \rightarrow L_2(\Omega, \mathbb{R})$$

What about

$$\mathcal{O}_{F_n} = \mathbb{E}_X(F_n(X)^k)$$

$$\mathcal{O}_{F_n} = \mathbb{E}_X(g \circ F_n(X))$$

$$\mathcal{O}_{F_n} = \mathbb{P}_X(g \circ F_n(X) > 0)$$

$$\mathcal{O}_{F_n} = q_{g \circ F_n(X)}(\alpha)$$

$$\mathcal{O}: L_2(\mathbb{R}^d, \Omega) \rightarrow L_2(\Omega, \mathbb{R}^d)$$

What about

$$\mathcal{O}_{F_n} = (S_1, S_2, S_{12}, \dots)$$

...

$$\mathcal{O}: L_2(\mathbb{R}^d, \Omega) \rightarrow L_2(\Omega, \mathbb{S})$$

What about

$$\mathcal{O}_{F_n} = \{x, g \circ F_n(x) < s\}$$

$$\mathcal{O}_{F_n} = \{u, \mathbb{E}_X(g \circ F_n(u, X)) < s\}$$

$$\mathcal{O}_{F_n} = \{u, \mathbb{P}_X(g \circ F_n(u, X) > 0) < \epsilon\}$$

$$\mathcal{O}: L_2(\mathbb{R}^d, \Omega) \rightarrow L_2(\Omega, \mathbb{H})$$

What about

$$\mathcal{O}_{F_n} = G(\cdot, F_n)$$

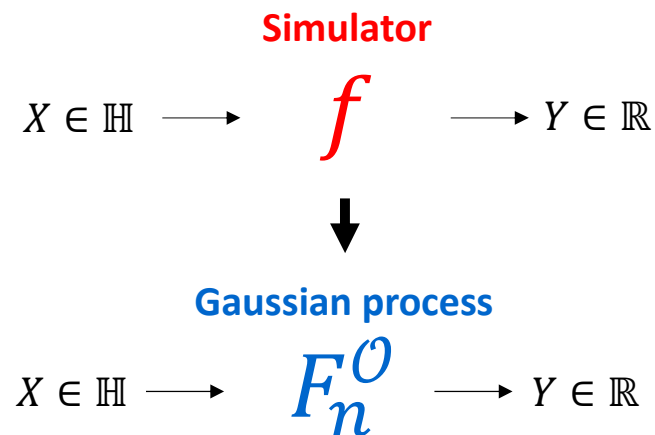
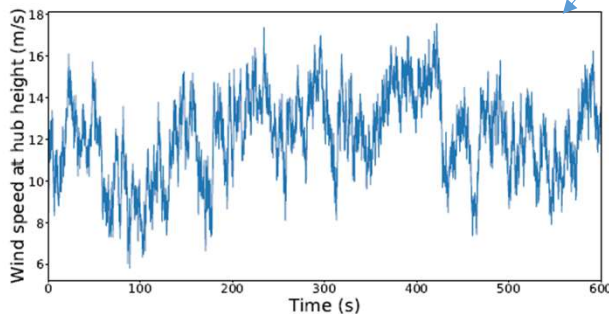
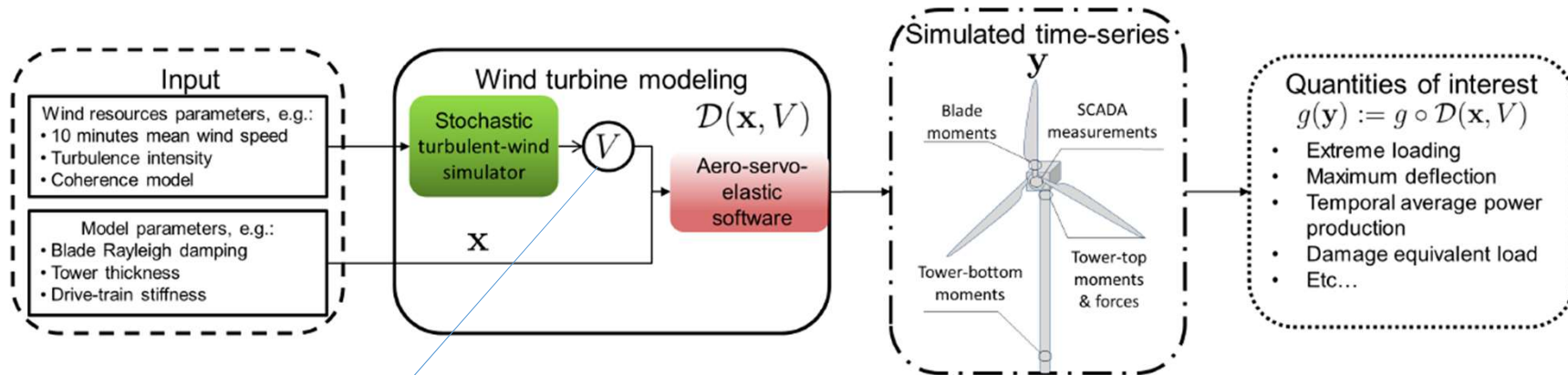
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- **Metamodelling of complex simulator with functional inputs, bridging Gaussian processes and SDE**

FUNCTIONAL METAMODELLING MOTIVATION



How do we define the Gaussian process with functional inputs: F_n^O ?

GAUSSIAN PROCESS INDEXED BY FUNCTIONAL INPUTS

- Bounded or unbounded linear GP model such that for $X \in \mathbb{H}$

$$F_n^{\mathcal{O}}(X) = \sum_{i>1} \xi_i \langle X, \mathcal{O}\phi_i \rangle_{\mathbb{H}}$$

- $\mathcal{O}: \mathbb{V} \rightarrow \mathbb{H}$
- (ϕ_i) orthonormal basis of \mathbb{V}
- (ξ_i) standard normal random variables

TOWARDS OPERATOR BASED FUNCTIONAL-RELIABILITY

$$\mathbb{P}_{F_{in}} \left(\max_{t \in [0, T]} F_n^O(t; F_{in}) > g_{max} \right) \sim 10^{-4}$$

- Space-filling design for functional inputs: \mathcal{X}_0 [*Thesis Calzolari, Nov. 2024 - Nov. 2027*]
- Building a GP model with functional inputs associated to scalar or time dependent output
- Probability estimation with active learning ...

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