Offline data assimilation for uncertainty-aware degradation prognostics in systems with sparse data

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Outline

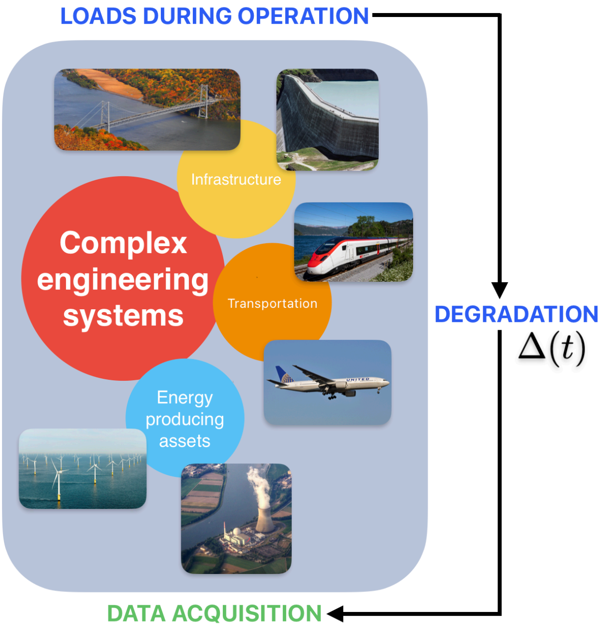

Complex engineering systems
Infrastructure
Transportation
Energy producing assets

LOADS DURING OPERATION

LOADS DURING OPERATION

DEGRADATION

$$\Delta(t)$$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DEGRADATION
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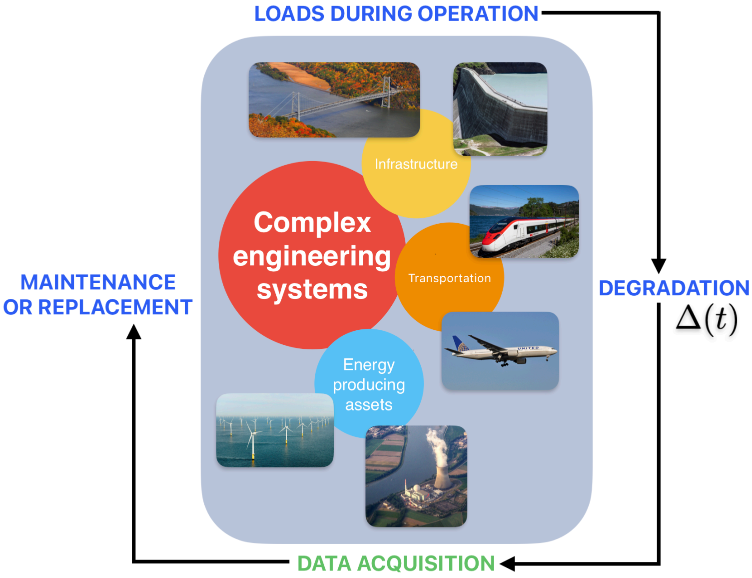
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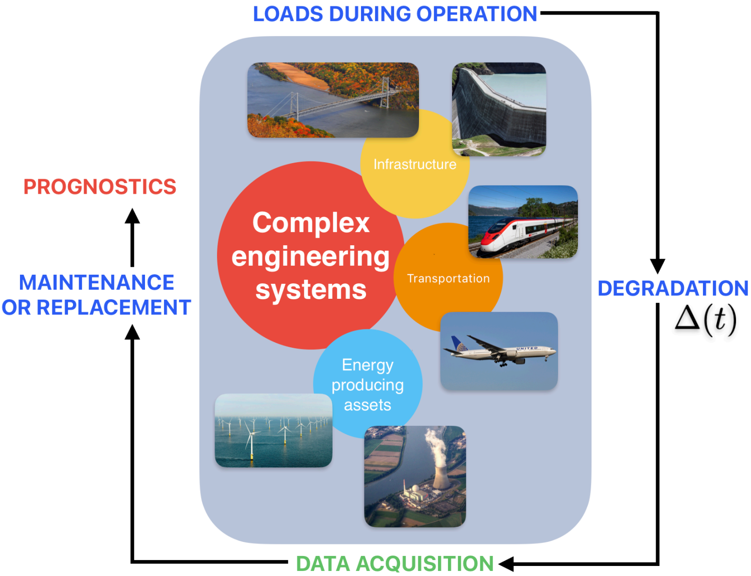
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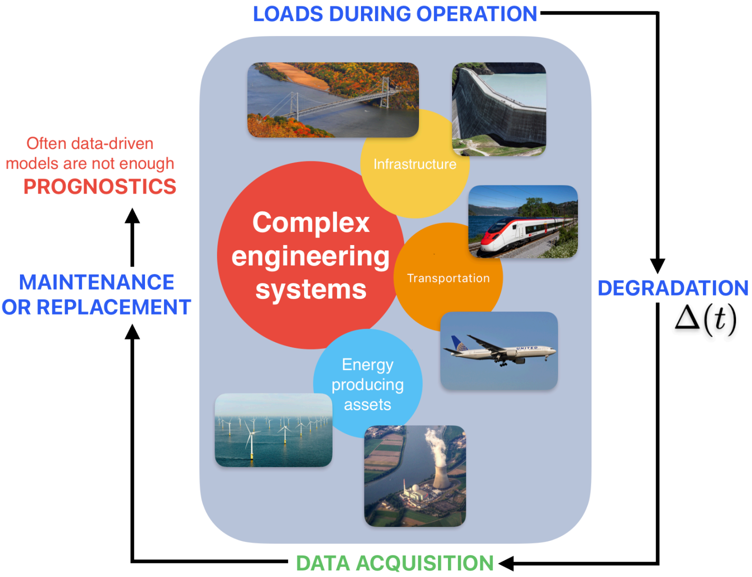

LOADS DURING OPERATION
Often data-driven
models are not enough
PROGNOSTICS
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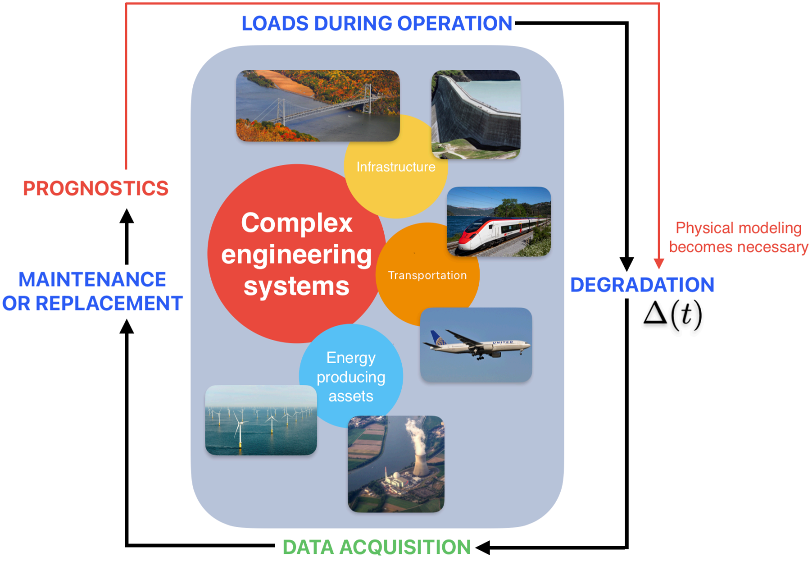
DEGRADATION
$\Delta(t)$
Energy producing assets
DATA ACQUISITION


LOADS DURING OPERATION
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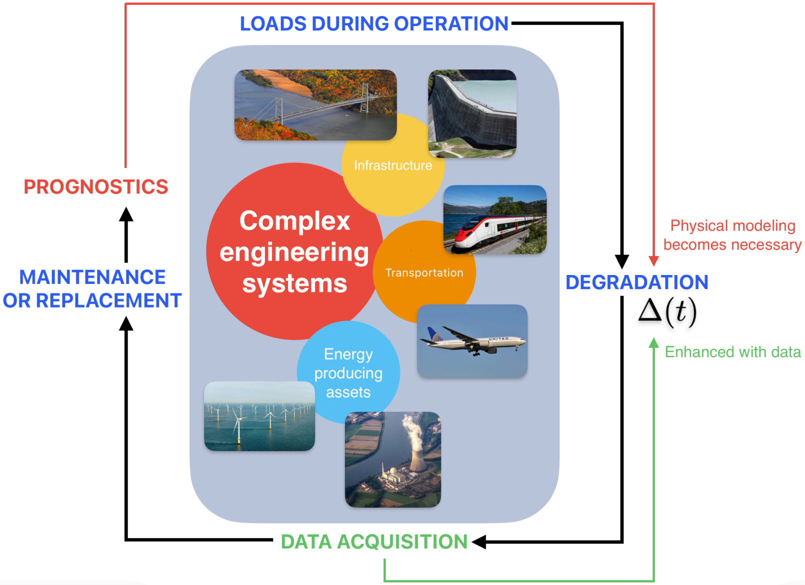
Physical modeling becomes necessary
DEGRADATION
$\Delta(t)$
DATA ACQUISITION


LOADS DURING OPERATION
Infrastructure
Complex engineering systems
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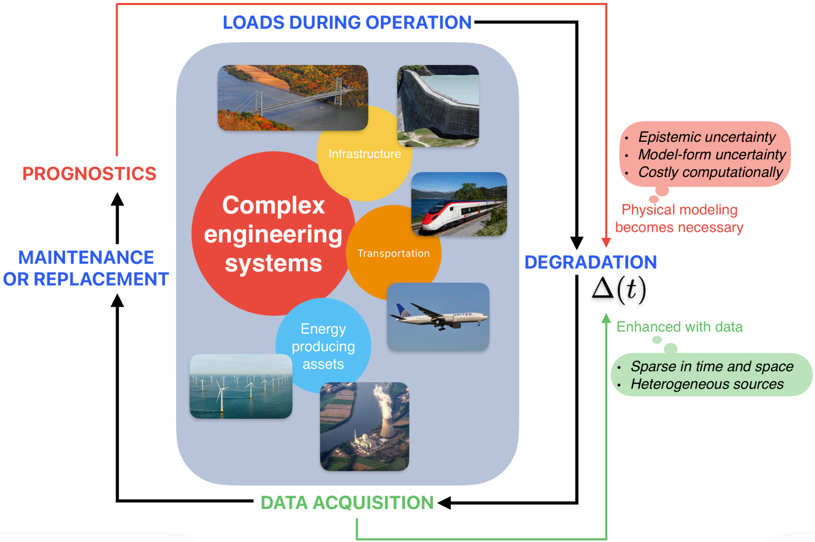
Energy producing assets
PROGNOSTICS
MAINTENANCE OR REPLACEMENT
Physical modeling becomes necessary
DEGRADATION
$\Delta(t)$
Enhanced with data
DATA ACQUISITION

What challenges?



- Degradation level of the system $(t \mapsto \Delta(t))$ → predict the remaining useful life (RUL) [Vachtsevanos et al., 2006] for a fixed threshold $\Delta_* \in \mathbb{R}_+$:

$$\text{RUL}(\Delta_*) = \underset{t > t_P}{\text{argmin}}\{\Delta(t) \geq \Delta_*\} \quad (1)$$

where t_P is the present time.

  → Relies usually on physics-based simulation codes, and/or data driven methods

- Idea: build a hybrid framework for evaluating the SG clogging RUL using the physics-based model and the data-driven models

→ *Data assimilation*, but not straightforward!

Available tools

- *Physics-based computer simulation model* $g : \mathcal{X} \subset \mathbb{R}^d \to \mathbb{R}^N$ with prior uncertainty on input variables $\boldsymbol{X}$, one input $\boldsymbol{x}_0$ gives a full degradation trajectory:

$$g(\boldsymbol{x}_0) = (g(t_1, \boldsymbol{x}_0), \ldots, g(t_N, \boldsymbol{x}_0)) \tag{2}$$

and $\mathrm{pr}_\ell \circ g(\boldsymbol{X}) := g(t_\ell, \boldsymbol{X})$ models $\Delta(t_\ell)$ → grey-box, physics known with non-intrusive surrogate modeling strategy $\widehat{g}$

- q *heterogeneous degradation data groups* (from different sensors, statistical models,...) $\mathcal{D} = (\boldsymbol{y}^1, \ldots, \boldsymbol{y}^q)$ with different sizes $\boldsymbol{y}^i \in \mathbb{R}^{m_i}$ → corresponding to different time indices in $\mathcal{J}_i$ so that $\mathcal{J} = \cup_{i=1}^q \mathcal{J}_i$ and $|\mathcal{J}| = m_1 + \ldots + m_q$, such that:

$$y^i(t_\ell) = \Delta(t_\ell) + \eta_\ell^i \tag{3}$$

with $\eta_\ell^i \sim \mathcal{N}(0, R^i)$ → homoskedastic noise for each data group

Outline

Offline data assimilation

- Perform offline sequential data assimilation over time windows [Geir Evensen, 2022] using ensemble methods
- Let $\boldsymbol{Z} = (\boldsymbol{X}, \boldsymbol{Y})$ where $\boldsymbol{Y} = g(\boldsymbol{X}) + \epsilon = \widehat{g}(\boldsymbol{X})$ are the computer model emulator outputs on a prescribed time window and $\boldsymbol{X}$ are uncertain parameters that do not vary over time
- The goal of assimilation is to estimate the distribution $p(\boldsymbol{Z} \mid \mathcal{D})$
- Use *modular* approach on each time window:
  1. Tailored Bayesian model updating (BMU) to obtain a posterior distribution $p_{\boldsymbol{X}|\mathcal{D}}$ for the input parameters: $(\boldsymbol{X}|\mathcal{D}) \sim p_{\boldsymbol{X}|\mathcal{D}}$.
  2. Apply smoothing to estimate $p(\boldsymbol{Y}|\boldsymbol{X} \sim p_{\boldsymbol{X}|\mathcal{D}}, \mathcal{D})$, yielding the assimilated posterior approximation:

$$p(\boldsymbol{Z}|\mathcal{D}) \approx p(\boldsymbol{Y}|\boldsymbol{X} \sim p_{\boldsymbol{X}|\mathcal{D}}, \mathcal{D}) p_{\boldsymbol{X}|\mathcal{D}}. \tag{4}$$

Illustration of the methodology

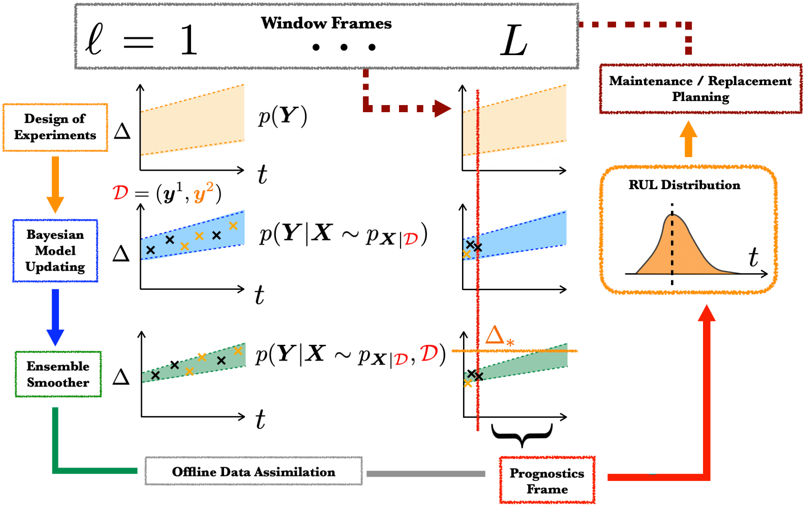


Figure 1: A sketch of the offline data assimilation methodology

On the prognostics window

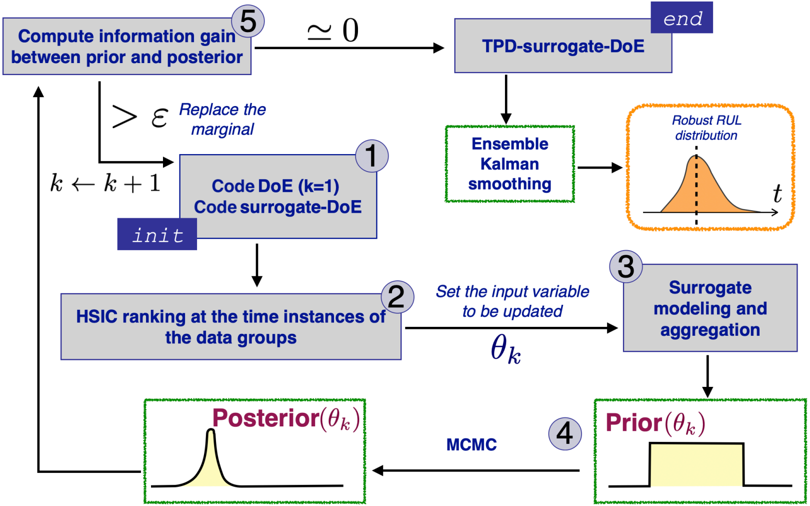
- Assimilation is performed offline until the prognostics window $\ell = L$ is reached, then the RUL distribution can be computed:

$$\mathbb{P}(\mathrm{RUL}(\Delta_*) \leq t_j \mid \mathcal{D}) = \int_{\mathbb{R}} \mathbf{1}\{\mathrm{pr}_{j+1}(\boldsymbol{y}) \geq \Delta_*\} p(\boldsymbol{y}|\mathcal{D}, \boldsymbol{X} \sim p_{\boldsymbol{X}|\mathcal{D}}) d\boldsymbol{y}, \tag{5}$$

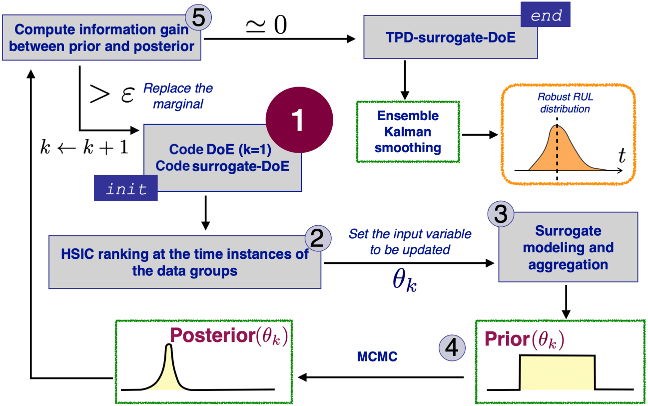
- In practice this probability is estimated using a Monte Carlo ensemble $\{(\boldsymbol{X}^{(i)}, \widehat{g}(\boldsymbol{X}^{(i)}))\}_{i=1}^{n} \sim p_{\boldsymbol{X}|\mathcal{D}} \otimes \widehat{g}\# p_{\boldsymbol{X}|\mathcal{D}}$:

$$\mathbb{P}(\mathrm{RUL}(\Delta_*) \leq t_j \mid \mathcal{D}) \approx \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\{\mathrm{pr}_{j+1} \circ \widehat{g}(\boldsymbol{X}^{(i)}) \geq \Delta_*\} \tag{6}$$

The BMU algorithm



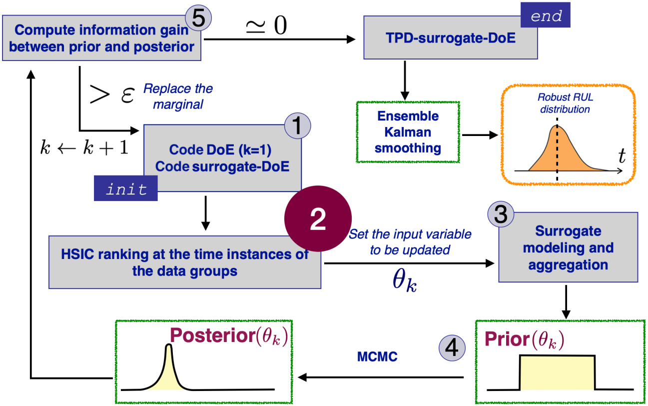
Step (1)



Perform k iterations where $1 \leq k \leq d$:

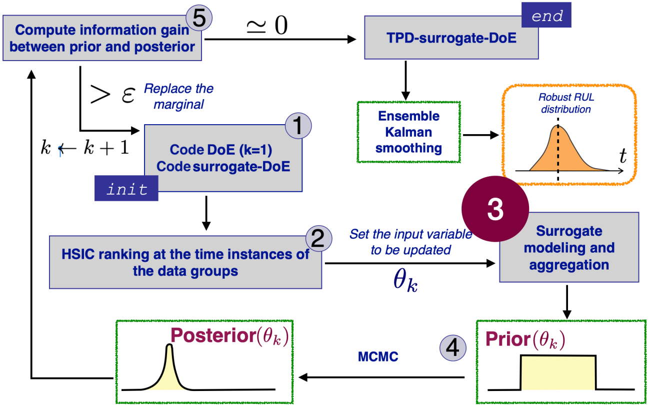
1. If $k = 0$, assume uniform independent priors $\mu_{\boldsymbol{X},k} \simeq \mathcal{U}[-1, 1]^{\otimes d} \to$ generate a design of experiments $\text{DoE}_g^{\mu_{\boldsymbol{X},k}} = \{(\boldsymbol{X}^{(j)}, g(\boldsymbol{X}^{(j)}))\}_{1 \leq j \leq n}$

Step 2



2. Compute **HSIC indices** [Gretton et al., 2005] between input variables and outputs at data time instances → **given data** sensitivity analysis method to assess *individual* input variable influence on the output

Step 3



3. If g is time-costly, build and validate p metamodels $\widehat{\boldsymbol{g}} = (\widehat{g}^{(1)}, \ldots, \widehat{g}^{(p)})$ with chosen strategy $\rightarrow$ avoid metamodeling bias with *convex aggregation* on the unit-simplex chosing $\boldsymbol{w} \in \Delta^{p-1} := \{\boldsymbol{w} \in [0,1]^p, \ \|\boldsymbol{w}\|_1 = 1\}$, fix nominal value of $\boldsymbol{U}_{0,k} = \boldsymbol{u}_{0,k}$ by taking the mean

Metamodeling step 3

The metamodeling process involves:

- *Data generation:* Using the DoE of g at n input samples $\{\boldsymbol{X}^{(i)}\}_{i=1}^{n} \sim \mu_{\boldsymbol{X}}$, assemble the data matrix:

$$\boldsymbol{Y} = \left[g(\boldsymbol{X}^{(1)}), \ldots, g(\boldsymbol{X}^{(n)})\right] \in \mathbb{R}^{N \times n} \tag{7}$$

- *Dimensionality reduction:* Apply a Karhunen–Loève (KL) decomposition [Sullivan, 2015] using the empirical covariance matrix $\widehat{C} = \frac{1}{n}\boldsymbol{Y}\boldsymbol{Y}^{\top}$. Perform singular value decomposition (SVD):

$$\boldsymbol{Y} = \boldsymbol{V}\boldsymbol{\Sigma}\boldsymbol{W}^{\top}, \tag{8}$$

  where $\boldsymbol{V}$ contains the KL modes $\{\boldsymbol{\Phi}_k\}_{k=1}^{m}$, and $\boldsymbol{\Sigma}$ holds the singular values.

- *Mode selection:* Retain m modes to capture a prescribed variance (e.g., 99%). Project trajectories onto the retained modes:

$$\xi_k(\boldsymbol{X}^{(i)}) = g(\boldsymbol{X}^{(i)})^{\top}\boldsymbol{\Phi}_k, \quad k = 1, \ldots, m \tag{9}$$

Metamodeling step 3

- *Surrogate modeling:* For each mode k, construct a surrogate model $\widehat{\xi}_k(\boldsymbol{X})$ using a Gaussian process [Rasmussen and Williams, 2006] with identical prior mean and kernel for all modes
- *Reconstruction:* Reconstruct the full trajectory using the surrogate models:

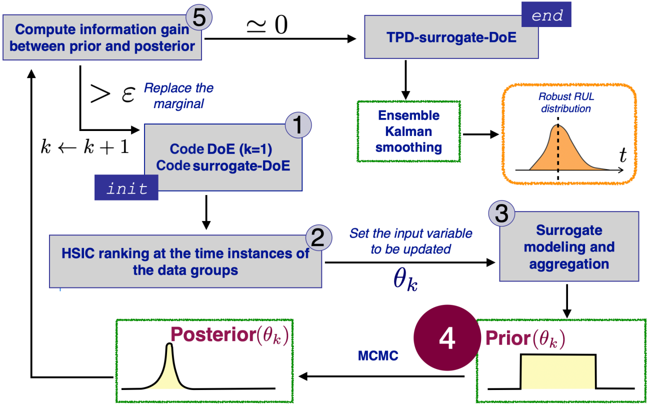
$$\widehat{g}(\boldsymbol{X}) = \sum_{k=1}^{m} \widehat{\xi}_k(\boldsymbol{X}) \boldsymbol{\Phi}_k \tag{10}$$

- *Aggregation:* Combine multiple surrogate models $\{\widehat{g}^{(i)}\}_{i=1}^{p}$ using convex aggregation weights $\boldsymbol{w} \in \boldsymbol{\Delta}^{p-1}$ to form the aggregated surrogate model:

$$\widehat{g}^{\text{agg}}(\boldsymbol{X}) = \sum_{i=1}^{p} w_i \widehat{g}^{(i)}(\boldsymbol{X}) \tag{11}$$

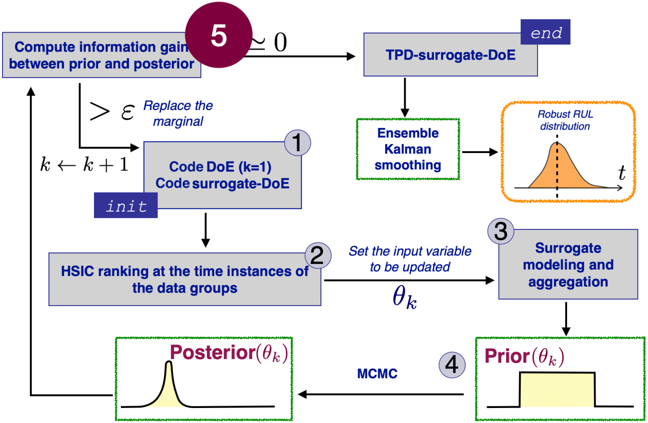
This ensures robustness by leveraging multiple models while minimizing bias

Step 4



4. Estimate the posterior distribution $\widehat{p}(\theta_k | \boldsymbol{y}^1, \ldots, \boldsymbol{y}^q, \boldsymbol{u}_{0,k})$ with an MCMC sampling procedure

Step (5)



5. Compute the Kullback-Leibler divergence d_{KL} between prior distribution $\mathcal{U}(\theta_k)$ and the estimated density:
   - If $d_{KL} > \varepsilon$, update the prior $\mu_{\mathbf{x},k}$ by replacing marginal $\mathcal{U}(\theta_k)$ with $\widehat{p}(\theta_k|\mathbf{y}^1, \ldots, \mathbf{y}^q, \mathbf{u}_{0,k})$ and continue $k \leftarrow k+1$
   - Otherwise, stop and obtain an *updated* RUL prediction by computing $g\#\mu_{\mathbf{x},k^*}$

Bayesian updating step 4

Proposition

Assume $\lambda := 1/\sigma_{\boldsymbol{\eta}}^2 \sim \mathcal{G}(\frac{m}{2}, \frac{1}{2}\|\mathbf{y} - f(\theta)\|^2)$ *(Gamma distribution), where* m *is the number of data points in* $\mathbf{y}$; $\theta \sim \mathcal{U}(\theta)$, *and* $p(\theta, \lambda) \propto \lambda^{-1}$. *Then:*

$$p(\theta|\mathbf{y}) \propto \|\mathbf{y} - f(\theta)\|^{-m} \tag{12}$$

Moreover, if multiple groups of data at different time-instances are considered, $\mathbf{y}^1, \ldots, \mathbf{y}^q$, *with respective priors on the inverse of their standard deviations* $\lambda_i \sim \mathcal{G}(\frac{m_i}{2}, \frac{1}{2}\|\mathbf{y}^i - f(\theta)\|^2)$, *then the generalization is:*

$$p(\theta|\mathbf{y}^1, \ldots, \mathbf{y}^q) \propto \prod_{i=1}^{q} \|\mathbf{y}^i - f(\theta)\|^{-m_i} \tag{13}$$

Proof. Bayes' theorem and simplifications.

Bayesian updating step 4

$$p(\theta_k|\mathbf{y}^1,\ldots,\mathbf{y}^q,\mathbf{u}_{0,k}) \propto \frac{1}{M}\sum_{r=1}^{M}\prod_{i=1}^{q}\|\mathbf{y}^i - \langle \mathbf{w}^{(r)}, \widehat{\mathbf{g}}(\mathbf{u}_{0,k},\theta_k)\rangle\|^{-m_i} \qquad (14)$$

- Use Random Walk Metropolis-Hastings (RWMH) MCMC algorithm [Sullivan, 2015] to sample from (14)
- Monte-Carlo integration using sample $\{\mathbf{w}^{(r)}\}_{r=1}^{M}$ from the Dirichlet-$\mathbb{1}_p$ distribution on the simplex $\rightarrow$ integrate hyperparameter
- Test convergence of RWMH chains with Gelman-Rubin test [Gelman and Rubin, 1992]
- Updated densities are conditioned on nominal values $\mathbf{u}_{0,k}$ of *other* $d-1$ *input variables* $\rightarrow$ future work on how to integrate uncertainty
- Use log-sum-exp trick for numerical computation

- We don't need sequential updating at each time-step $p(g(t_k, \boldsymbol{X})|\mathcal{D})$ (which is the goal of filtering), but to assimilate the data on the entire window frame
- Indeed the data is *unavailable* at each time-step, so we need to account of all the information on a window
- The good paradigm for this is smoothing, i.e getting estimates from the full-posterior distribution $p(g(t_1, \boldsymbol{X}), \dots, g(t_k, \boldsymbol{X})|\mathcal{D}) \rightarrow$ Ensemble Kalman smoothing (EnKS) [Evensen and van Leeuwen, 2000]

- Build an ensemble $\{g(\boldsymbol{X}^{(k)})\}_{k=1}^{n} \sim g\#h_{\boldsymbol{X}|\mathcal{D}}$, suppose for each data-group $i = 1, \ldots, q$:

$$y^i(t_\ell^i) = g(t_\ell^i, \boldsymbol{X}) + \eta_i, \tag{15}$$

where the variance R^i of the noise *is known*

- Define the ensemble mean and anomalies:

$$\overline{g}(t) = \frac{1}{n}\sum_{k=1}^{n} g(t, \boldsymbol{X}^{(k)}), \quad A^{(k)}(t) = g(t, \boldsymbol{X}^{(k)}) - \overline{g}(t) \tag{16}$$

- The cross-covariance between ensemble states at any time t and the observation times t_ℓ^i are approximated empirically:

$$\widehat{C}(t, t_\ell^i) = \frac{1}{n-1}\sum_{k=1}^{n} A^{(k)}(t) A^{(k)}(t_\ell^i) \tag{17}$$

- We define the Kalman gain for each t in the time-window:

$$K_t = \frac{\widehat{C}(t, t_\ell^i)}{\widehat{C}(t, t_\ell^i) + R^i} \tag{18}$$

- And defining the innovation term as $d_\ell^{(k)} = y^i(t_\ell^i) - g(t_\ell^i, \boldsymbol{X}^{(k)})$, we update all the ensembles following:

$$g(\boldsymbol{X}^{(k)}) \leftarrow g(\boldsymbol{X}^{(k)}) - K_t \cdot d_\ell^{(k)} \tag{19}$$

- This process is repeated *sequentially* across all observation times t_ℓ^i, for all data groups $i \in \{1, \ldots, q\}$

Outline

- Clogging of SGs is a complex multiphysics phenomenon that occurs following long operational periods in pressurized-water reactors (PWR) of the French nuclear fleet $\rightarrow$ undermines performance & weakens the structures $\rightarrow$ *may require chemical cleanings*

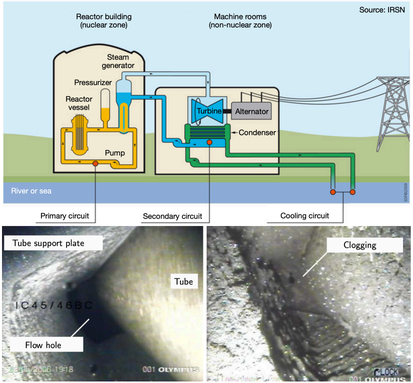
- 

Figure 2: PWR scheme, and example of video examination during a PWR outage (© IRSN, EDF)

- No state-of-the-art model allowing for ground insights on diagnostics and prognostics of clogging rate τ_c $\rightarrow$ very hard to model $\&$ challenging to create reproducible lab experiment for model validation $+$ not a lot of literature [Srikantiah and Chappidi, 2000; Prusek et al., 2013; Girard, 2014; Yang et al., 2017]
- Available scarce video field data as well as indirect measurements $\rightarrow$ allow to construct data-driven regression algorithms [Pinciroli et al., 2021] $\approx$ not enough data to have robust predictive models
- Another tool is the physical clogging model developed by [Prusek et al., 2013] $\rightarrow$ subsequent numerical model THYC-Puffer-DEPO [Feng et al., 2023] $\approx$ lack of enough trustworthy field data for precise V&V
- Necessary decision-making on chemical cleaning planning under uncertainty $\rightarrow$ ***how to make use of the available knowledge and models for achieving reliable predictions?***

- Computer code THYC-Puffer-DEPO, complex multiphysics [Jaber et al., 2024b] , chaining of 3 codes $\rightarrow$ allows to simulate SG clogging on entire lifespan of the asset integrating past chemical cleanings and predicting future τ_c levels
- Two data groups $q = 2$, corresponding to field data and regression data

Input variable	Distribution
α	$\mathcal{U}(100, 103)$
β	$\mathcal{U}(0.02, 0.025)$
ϵ_e	$\mathcal{U}(0.2, 0.5)$
ϵ_c	$\mathcal{U}(0.01, 0.3)$
d_p	$\mathcal{U}(0.5, 10.0) \times 10^{-6}$
$\Gamma_p(0)$	$\mathcal{U}(1.0, 8.0) \times 10^{-9}$
a_v	$\mathcal{U}(0, 15) \times 10^{-4}$

Table 1: Probabilistic modeling of uncertain input variables

- $L = 3$ time windows, 5 MCMC chains are launched for GR convergence test, use uniform proposal distributions
- Computing time around 40 min $\rightarrow 5/7$ distributions are informed by the data, distinct modes for a_v

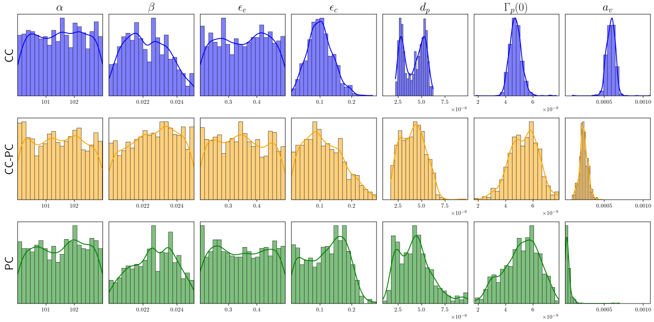


Figure 3: Posterior distributions of TPD clogging simulation code

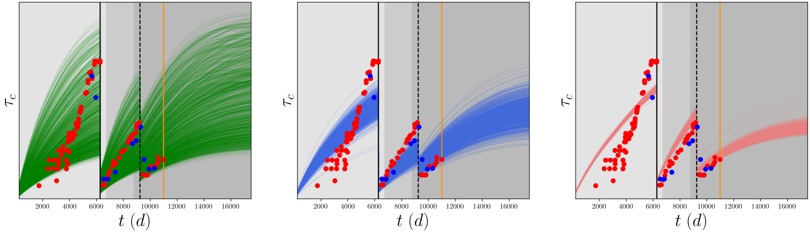
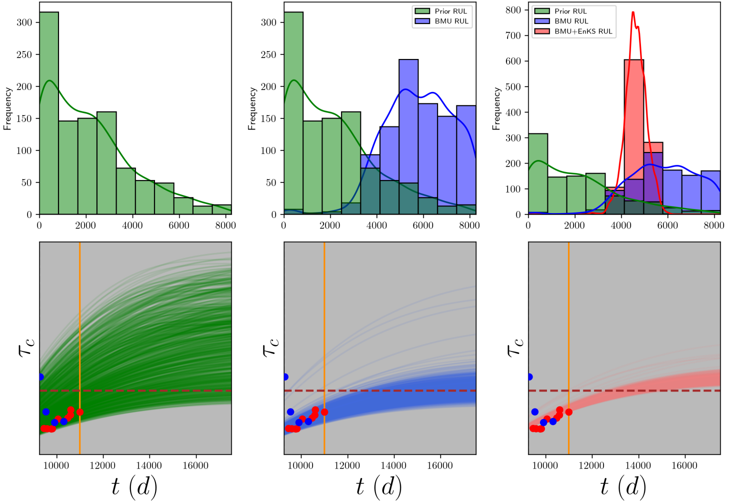


Figure 4: Prior/posterior and smoothed TPD emulations with Karhunen-Loève expansion surrogate

Results: posterior RUL



- RUL prediction uncertainty substantially reduced and mean of the distribution is shifted compared to the prior $\rightarrow$ positive impact for maintenance planning

Outline

Summary

Take-home messages:

- Offline data assimilation generic modular approach involving iterative BMU, non-intrusive emulators, heterogeneous data groups and ensemble Kalman smoothing
- Reduces parametric uncertainty of a computer simulation code that outputs future trajectories and RUL estimation, more informed decision making
- Demonstrated the approach on nuclear SG clogging use-case, showing reduced RUL uncertainty

Contributions:

- Paper published in **Reliability Engineering & System Safety** [Jaber et al., 2026]
- Reproducible code in `GitHub repository`

- How to integrate uncertainty in nominal parameters $\boldsymbol{u}_k$?
- Prior work on adaptive conformal prediction for GP surrogate models validation [Jaber et al., 2024a] (available GitHub repository)
- We define the cross-conformal estimator at a new point $\boldsymbol{X}^{(n+1)}$ using the posterior mean of the GP $\widetilde{g}$ and the posterior variance $\widetilde{\gamma}$:

$$\widehat{C}_{n,\alpha}^{J+GP}(\boldsymbol{X}^{(n+1)}) = \left[\widehat{q}_{n,\alpha}^{\pm}\left\{\widetilde{g}_{-i}(\boldsymbol{X}^{(n+1)}) \pm R_i^{LOO\gamma} \times \widetilde{\gamma}_{-i}(\boldsymbol{X}^{(n+1)})\right\}\right]$$

where $R_i^{LOO\gamma}$ is the Leave-One-Out error normalized by $\widetilde{\gamma}$

- Since the intervals are adaptive, can we use it as a proxy for metamodel accuracy for some step in the methodology? Surrogate refinement, or active learning?

Thank you for your attention!

Figure 5: Paper

Figure 6: GitHub

Let's connect: `edgar.jaber@ens-paris-saclay.fr`

Outline

- Hilbert-Schmidt Independence Criterion (HSIC) [Gretton et al., 2005], kernel method $\rightarrow$ evaluates sensitivity of a single-input in a given-data context, no need for surrogate models
- Theoretical result for all $i \in \{1, \ldots, d\}, k \in \{1, \ldots, N\}$:

$$\mathrm{HSIC}(X_i, g(\boldsymbol{X}, t_k)) = 0 \iff X_i \perp g(\boldsymbol{X}, t_k) \tag{20}$$

- The index disposes of U-stat and V-stat estimators $+$ hypothesis testing with corresponding p-value $\rightarrow$ implemented in the OpenTURNS
- The normalized R^2_{HSIC} index is better suited for interpretation:

$$R^2_{\mathrm{HSIC}}(X_i, g(\boldsymbol{X}, t_k)) = \frac{\mathrm{HSIC}(X_i, g(\boldsymbol{X}, t_k))}{\sqrt{(\mathrm{HSIC}(X_i, X_i)\mathrm{HSIC}(g(\boldsymbol{X}, t_k), g(\boldsymbol{X}, t_k)))}} \in [0, 1]$$

- Empirical evidence suggests that R^2_{HSIC} can be used confidently for variable ranking $\rightarrow$ HSIC-ANOVA decompositions also exist *but* only pathological cases create stark differences (see [Sarazin et al., 2022])

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