Bayesian calibration with functional outputs with elastic partial matching

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Calibration of functional outputs

Experimental settings
x

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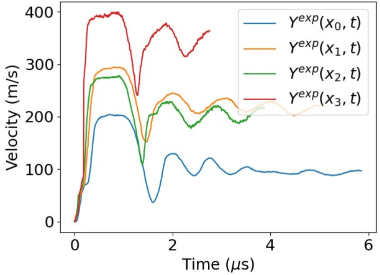
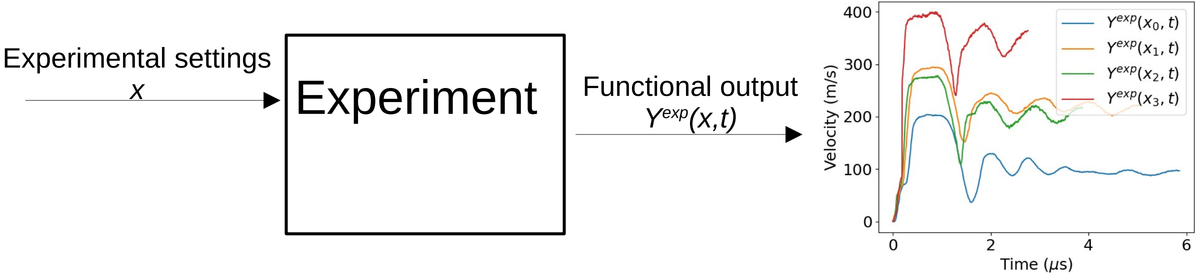
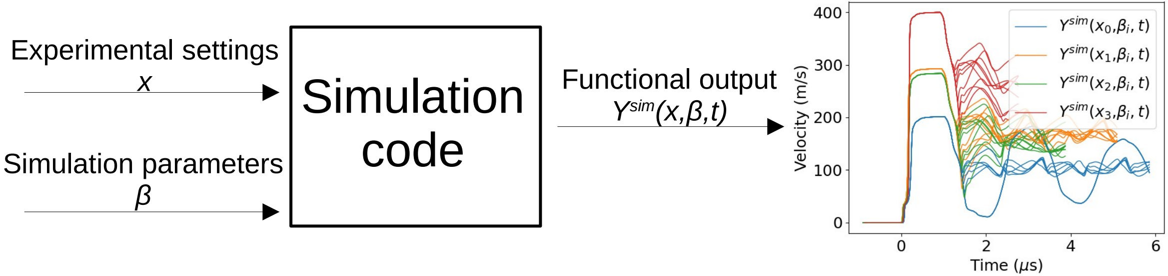
Functional output
$Y^{exp}(x,t)$



Calibration of functional outputs





How to estimate/calibrate the parameter β?

Bayesian calibration with functional outputs

Introduced by [Kennedy and O'Hagan, 2001] and extended to functional outputs by [Higdon et al., 2008].

Linking experiments, simulations, and the true model:

- Measurement error:

$$Y^{\text{exp}}(x,t) = Y^{\text{true}}(x,t) + \varepsilon^{\text{mes}}(x,t), \quad \varepsilon^{\text{mes}}(x,t) \sim \mathcal{N}(0, \sigma^2_{\text{mes}})$$

- Model discrepancy:

$$Y^{\text{true}}(x,t) = Y^{\text{sim}}(x,\beta,t) + \varepsilon^{\text{mod}}(x,t), \quad \varepsilon^{\text{mod}}(x,t) \sim \mathcal{GP}(0, k_\theta)$$

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$$\Rightarrow Y^{\text{exp}}(x,t) \mid \beta, \sigma^2_{\text{mes}}, \theta \sim \mathcal{GP}\left(Y^{\text{sim}}(x,\beta,t),\ k_\theta + \sigma^2_{\text{mes}} \delta_{(x,t)=(x',t')}\right)$$

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Bayesian inference: With priors $\pi(\beta)$, $\pi(\sigma^2_{\text{mes}})$, and $\pi(\theta)$:

$$\boxed{P(\beta, \sigma^2_{\text{mes}}, \theta \mid Y^{\text{exp}}) \propto P(Y^{\text{exp}} \mid \beta, \sigma^2_{\text{mes}}, \theta)\,\pi(\beta)\,\pi(\sigma^2_{\text{mes}})\,\pi(\theta)}$$

Surrogate modeling for functional outputs: GP with PCA

When simulations are expensive, we run the code N_{sim} times and build a surrogate model to replace it.[Perrin, 2020]

Inputs: $(\beta_j)_{j=1,\ldots,N_{\text{sim}}}$, **Outputs:** $(Y^{\text{sim}}(x_i, \beta_j, t_k))_{j=1,\ldots,N_{\text{sim}},k=1,\ldots,N_t}$

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Each component is treated independently: $\tilde{Y}_{Q,l}^{\text{sim}} \sim \mathcal{GP}\big(0,\ k_{\theta_l}^{\text{meta}}\big)$, where θ_l is learned by maximizing the likelihood. We can compute the posterior distribution:

$$\tilde{Y}_{Q,l}^{\text{sim}}(x_i, \beta) \mid (\beta_j, Y_{Q,l}^{\text{sim}}(x_i, \beta_j))_j \sim \mathcal{GP}(\mu_Q^{\text{post}},\ k_Q^{\text{post}})$$

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Step 3: Reconstruction in the original space

$$\tilde{Y}^{\text{sim}}(x_i, \beta) \sim \mathcal{GP}\Big(D_Q(\mu_Q^{\text{post}}),\, D_Q^T \text{diag}(k_Q^{\text{post}})\, D_Q\Big)$$

Bayesian calibration and time warping

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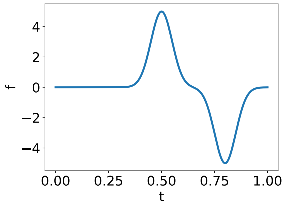
[Francom et al., 2025] suggests calibrating in a new space to compare

- **Amplitudes:** aligned versions of the functions,
- **Phases:** time warping required for alignment.

2. Elastic calibration with partial alignment

Distances between functions

Which function is the closest to f ?



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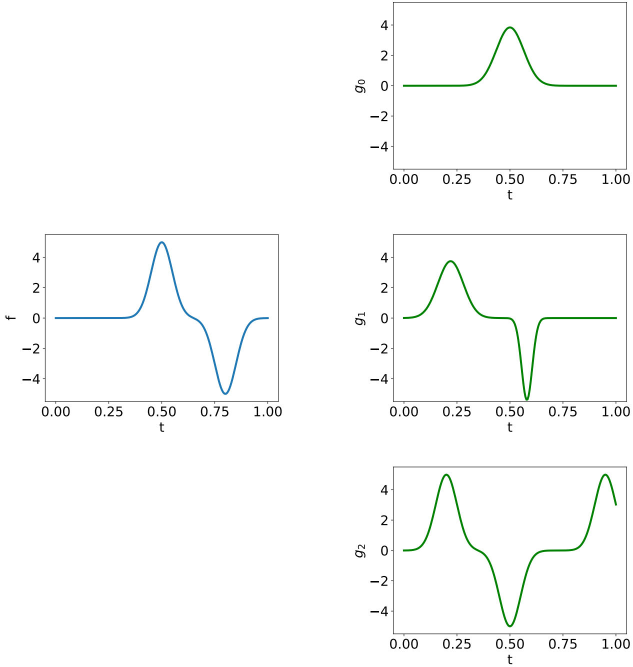

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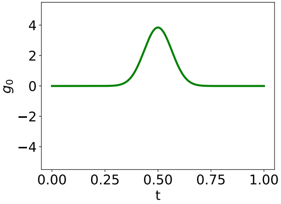
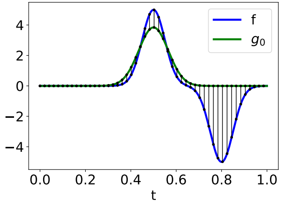
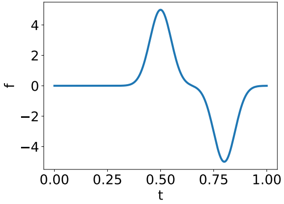
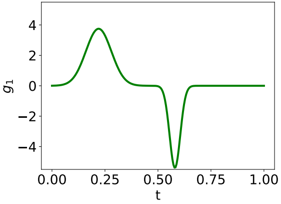
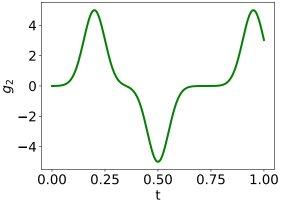


L2 distance →









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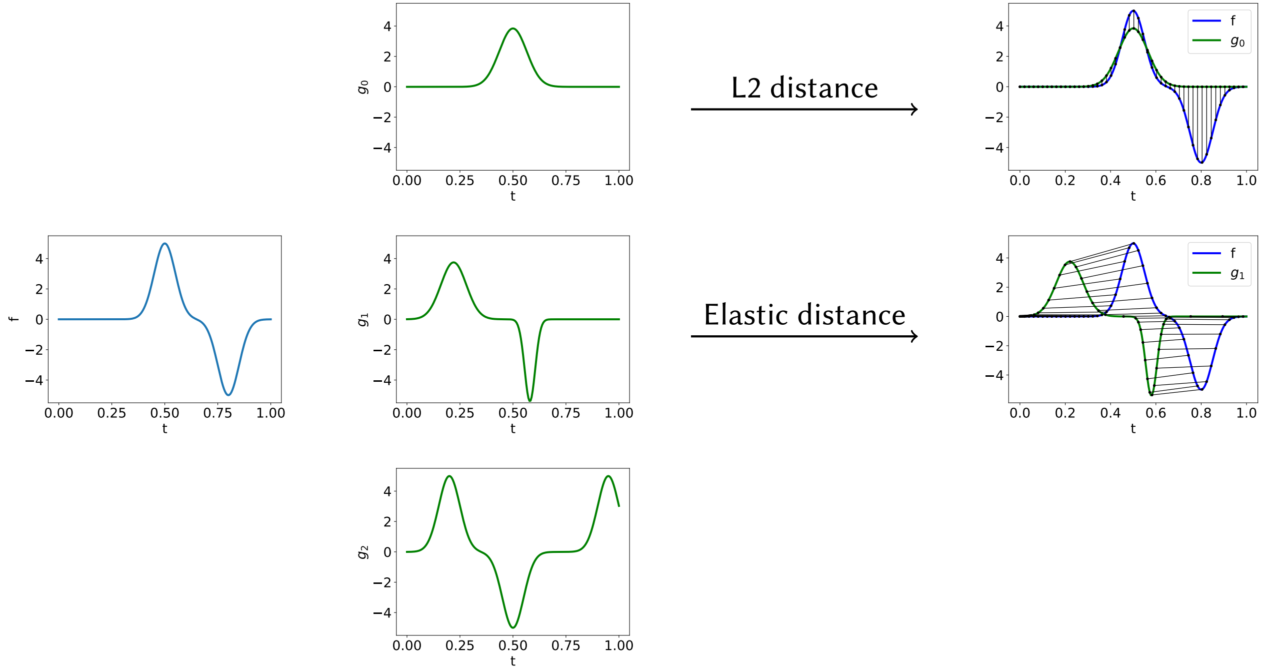

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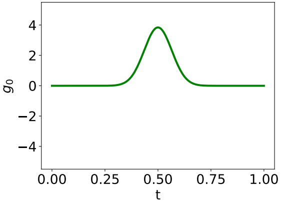

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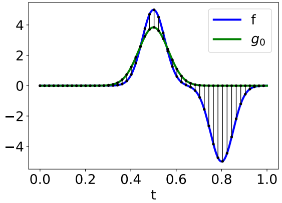
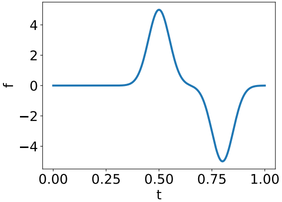
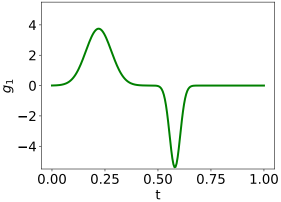
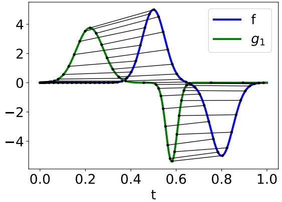
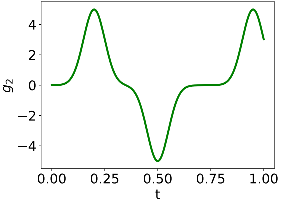




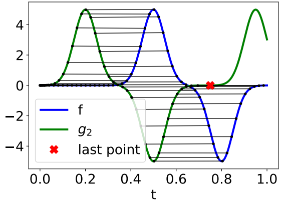


Elastic distance →





Partial elastic distance →



Elastic distance

We call a **phase** a function γ belonging to:

$$\Gamma = \left\{ \gamma : [0,1] \to [0,1] \;\middle|\; \begin{array}{l} \gamma(0) = 0, \quad \gamma(1) = 1, \\ \gamma, \gamma^{-1} \text{increasing and differentiable} \end{array} \right\}$$

$$\boxed{d(f, g_1) = \inf_{\gamma \in \Gamma} E(f, g_1 \circ \gamma)}$$

where

$$E(f_1, f_2) = \|Q(f_1) - Q(f_2)\|_2^2 \text{ and } Q(f)(t) = \text{sgn}(\dot{f}(t))\sqrt{|\dot{f}(t)|}$$

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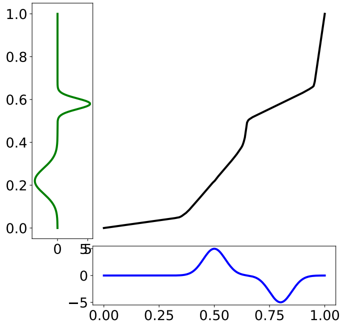

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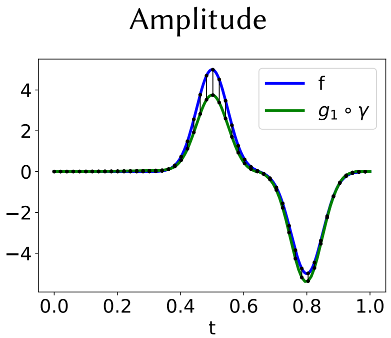

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[Srivastava and Klassen, 2016] introduces two important properties for E:

- **Invariance to simultaneous warping:** For $\gamma \in \Gamma$, $E(f_1, f_2) = E(f_1 \circ \gamma, f_2 \circ \gamma)$.
- **Inverse symmetry:** If $\gamma = \arg\inf_{\gamma \in \Gamma} E(f_1, f_2 \circ \gamma)$, then $\gamma^{-1} = \arg\inf_{\gamma \in \Gamma} E(f_1 \circ \gamma, f_2)$.

[Srivastava et al., 2011] shows that E satisfies these properties.

Partial elastic distance [Bryner and Srivastava, 2021]

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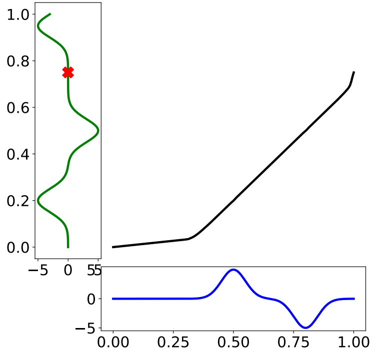

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Alignment of set of functions

For a set of functions f_i:

- We choose one function f_{ref} from the dataset
- For each function we compute, $\gamma_i = \arg\min_{\gamma \in \Gamma} E(f_{\text{ref}}, f_i \circ \gamma)$

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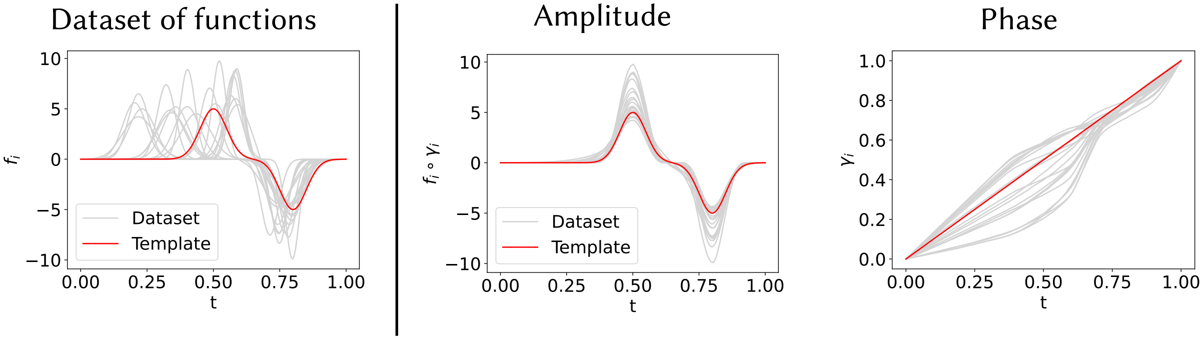

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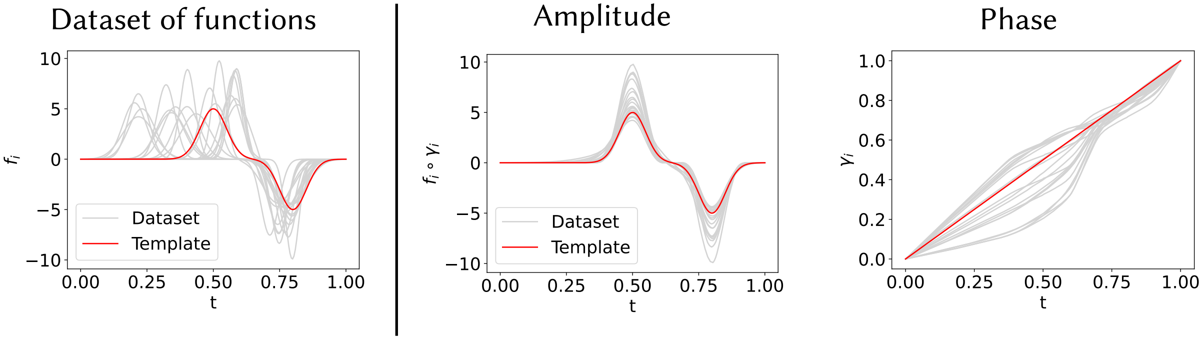

[Francom et al., 2025] proposed performing the calibration in the Amplitude/Phase space rather than in the original space. We propose to adapt their method for partial elastic alignment.

The model [Francom et al., 2025] with final time

Step 1: Alignment on y_{ref} between functions with final time [Bryner and Srivastava, 2021]

$$(\gamma_i, t_f) = \arg\min_{\gamma \in \Gamma, t_f \in \mathbb{R}} E(y_{\text{ref}}, y_i \circ \gamma)\Big|_{[0,t_f]} + \text{pen}(t_f)$$

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$$\psi = \sqrt{\dot{\gamma}} \text{ and } v = \exp^{-1}_{\psi_{\text{id}}}(\psi)$$

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Step 3: Surrogate modeling (GPR) of v^{sim}, $f^{\text{sim}} = y_i^{\text{sim}} \circ \gamma_i$, and t^{sim}, denoted $\tilde{v}^{\text{sim}}$, $\tilde{f}^{\text{sim}}$, and $\tilde{t}^{\text{sim}}$.

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Step 4: Bayesian calibration

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$$t_f^{\text{exp}}(x) = \tilde{t}^{\text{sim}}(x,\beta) + \varepsilon_t(x)$$

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If we denote, θ_f, θ_v and θ_t the hyperparameters of ε_f, ε_v and ε_t and $\pi(\theta)$ their priors :

$$\boxed{P(\beta, \theta_y, \theta_v, \theta_t | y^{\text{exp}}) \propto P(f^{\text{exp}}|\beta, \theta_f) P(v^{\text{exp}}|\beta, \theta_v) P(t_f^{\text{exp}}|\beta, \theta_t) \pi(\beta) \pi(\theta_f) \pi(\theta_v) \pi(\theta_t)}$$

3. Anharmonic oscillator

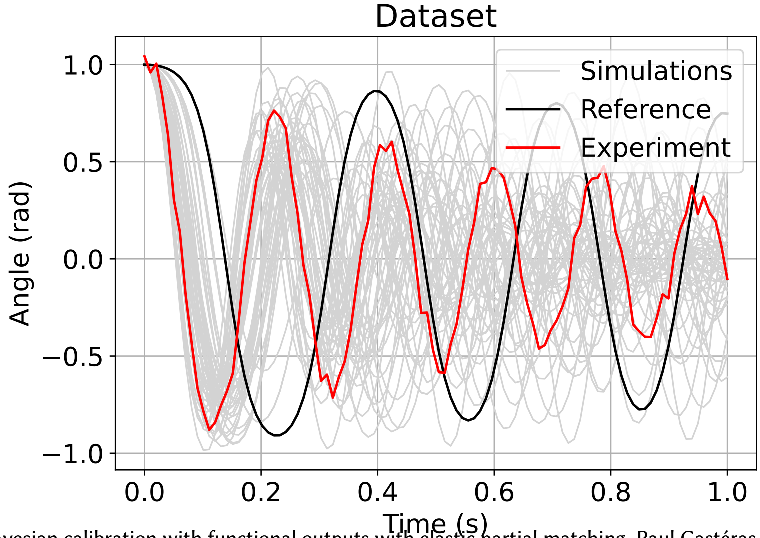
Anharmonic oscillator

Equation :

$$\frac{d^2\theta}{dt^2} + \alpha_1 \frac{d\theta}{dt} + \alpha_2(\theta - \alpha_0\theta^3) = 0.$$

Calibration of

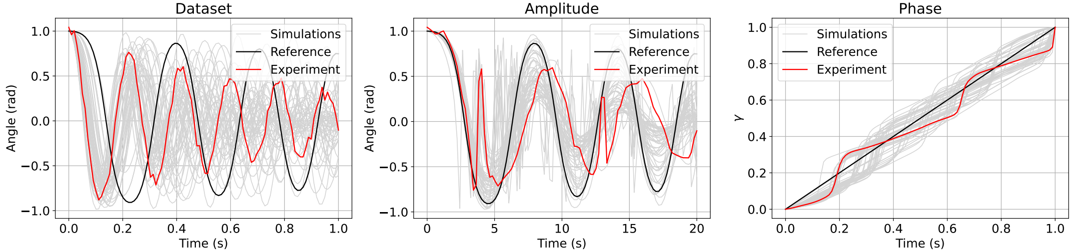
$$\beta \in [0,1]^3 \text{ where } \alpha_0 = 0.48\beta_0 + 0.5, \alpha_1 = 0.3\beta_1, \alpha_2 = 2\beta_2 + 2$$



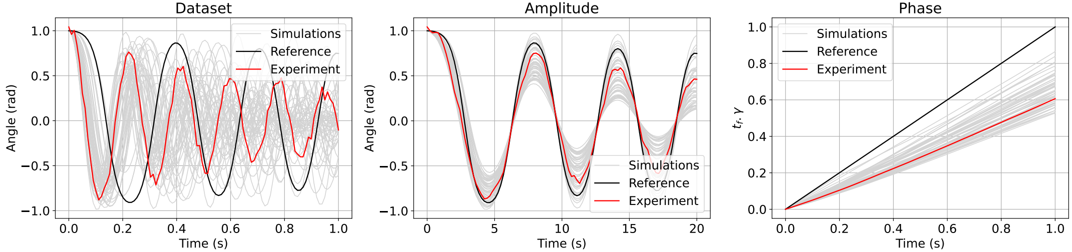
$$\beta_{exp} = [0.5, 0.3, 0.8],$$
$$\sigma^2_{exp} = 0.05^2,$$
$$N_{\text{sim}} = 50,$$
$$N_t = 100.$$

Anharmonic oscillator: Amplitude/Phase decomposition

Elastic decomposition



Partial elastic decomposition



Anharmonic oscillator : surrogate models

Prediction of the model :

$$Q^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}$$

$\rightarrow$ close to 1 = good prediction.

Credible intervals of the model :

IAE_α evaluates the quality of the quantiles of level α for different values α [Marrel and Iooss, 2024]

$\rightarrow$ close to 0 = good credible intervals.

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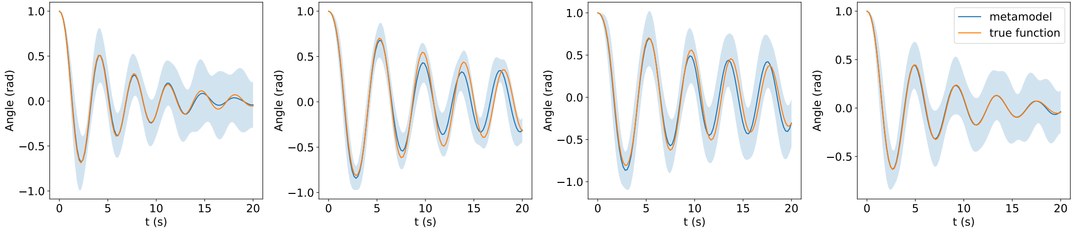
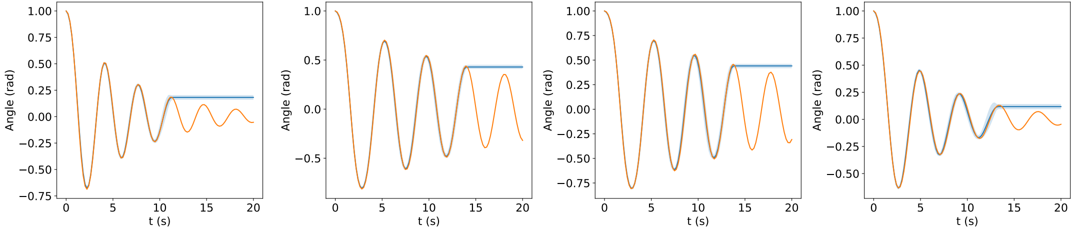
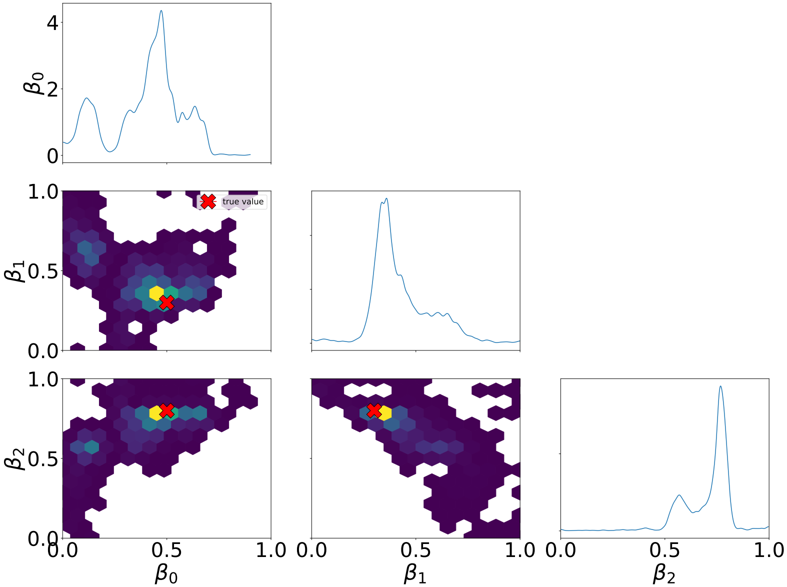
Without elastic decomposition: $Q^2 = 0.85$, $\text{IAE}_\alpha = 0.17$



With partial elastic decomposition $Q^2 = 0.97$, $\text{IAE}_\alpha = 0.02$



Anharmonic oscillator : Functional calibration



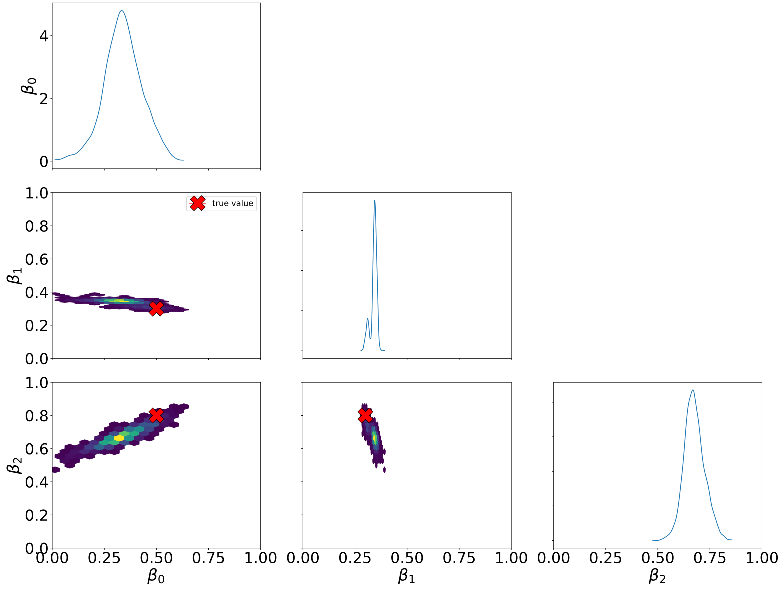
$$Y^{\text{exp}}(t) = \tilde{Y}^{\text{sim}}(\beta, t) + \epsilon^{\text{mes}}(t)$$

$$\epsilon^{\text{mes}}(t) \sim \mathcal{N}(0, \sigma^2_{\text{mes}})$$

$$\beta \sim \mathcal{U}([0,1]^3)$$

Sampling with Sequential Monte Carlo

Anharmonic oscillator : Partial elastic calibration



$$
\begin{aligned}
f^{\text{exp}}(t) &= \tilde{f}^{\text{sim}}(t,\beta) + \varepsilon^{\text{mes}}(t)\\
v^{\text{exp}}(t) &= \tilde{v}^{\text{sim}}(t,\beta) + \varepsilon^{\text{mod}}(t)\\
t_f^{\text{exp}} &= \tilde{t}^{\text{sim}}(\beta)
\end{aligned}
$$

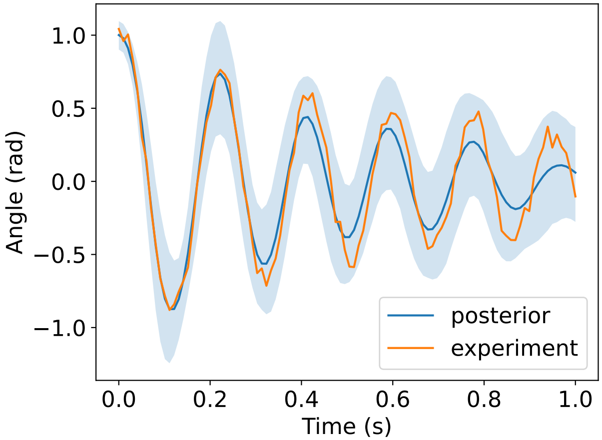
$$
\begin{aligned}
\varepsilon^{\text{mes}}(x,t) &\sim \mathcal{N}(0,\sigma^2_{\text{mes}})\\
\varepsilon^{\text{mod}}(x,t) &\sim \mathcal{GP}(0,\sigma^2_{\text{mod}}k_l)
\end{aligned}
$$

$$
\begin{aligned}
\sigma^2_{\text{mod}} &\sim \mathcal{N}(0,1)\mathbf{1}_{\sigma^2_{\text{mod}}>0}\\
l &\sim \Gamma(1,1)\\
\beta &\sim \mathcal{U}([0,1]^3)
\end{aligned}
$$

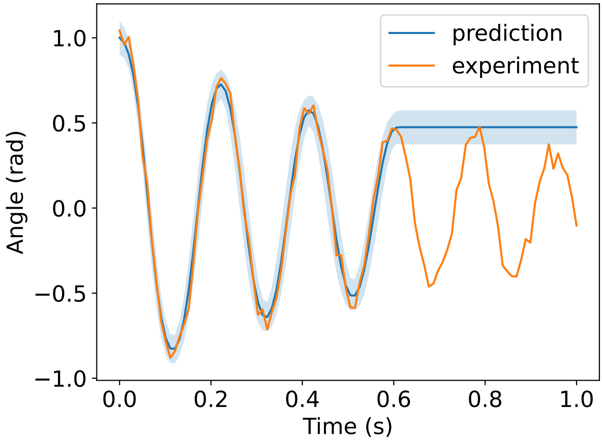
Sampling with Sequential Monte Carlo

Anharmonic oscillator : Comparison of the predictions

Without elastic decomposition



With partial elastic decomposition



Conclusion

We introduced a new calibration method based on the Bayesian elastic calibration framework [Francom et al., 2025] and on partial elastic matching [Bryner and Srivastava, 2021]. It enables:

- Comparison of patterns that do not occur at the same time,
- Model discrepancy in phase,
- Partial elastic surrogate model.

Conclusion

We introduced a new calibration method based on the Bayesian elastic calibration framework [Francom et al., 2025] and on partial elastic matching [Bryner and Srivastava, 2021]. It enables:

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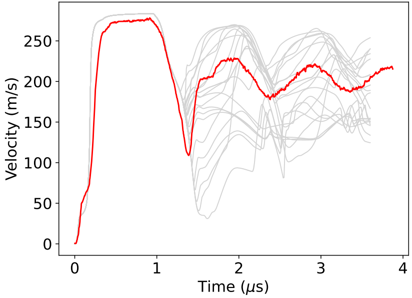
Future work



- The alignment transform is not continuous. How to build surrogate models in those cases ?
- Investigate other representation that combine phases and final times.

THANK YOU

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4. References

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Transformation of the phase space

$$\gamma \in \Gamma = \left\{ \gamma : [0,1] \to [0,1] \;\middle|\; \begin{array}{l} \gamma(0) = 0, \gamma(1) = 1 \\ \gamma, \gamma^{-1} \text{ increasing and differentiable} \end{array} \right\}$$

First transformation: $\psi = Q(\gamma) = \sqrt{\dot{\gamma}} \in \Psi$
$\Rightarrow ||\psi||_2^2 = \int_0^1 \psi(t)^2 = 1 \Rightarrow \Psi \subset S_\infty$

Second transformation:

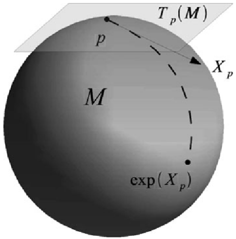
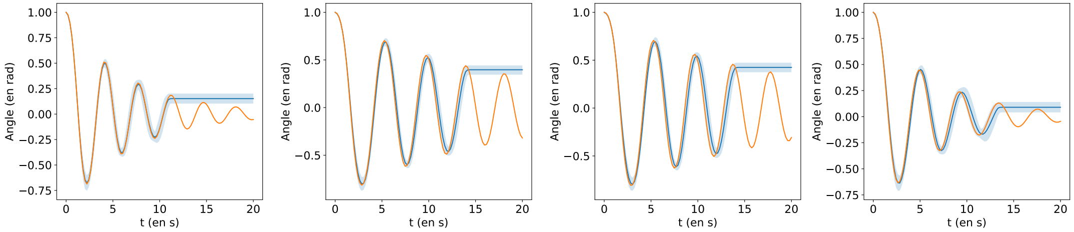


Figure of [Srivastava and Klassen, 2016]

$$T_\psi(\Psi) = \left\{ v \in L^2 \;\middle|\; \int_0^1 v(t)\,\psi(t)\,dt = 0 \right\}$$
$$\exp_\psi^{-1}(\psi_1) = \frac{\kappa}{\sin(\kappa)}(\psi_1 - \cos(\kappa)\psi)$$
$$\text{where } \kappa = d_p(\psi, \psi_1) = \cos^{-1}\left(\int_0^1 \psi\psi_1\right)$$

Anharmonic oscillator : surrogate models

Final time but no elasticity: $Q^2 = 0.95$, $\mathrm{IAE}_\alpha = 0.06$



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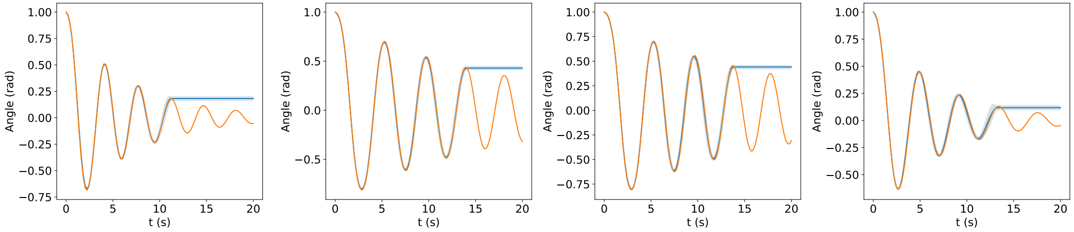
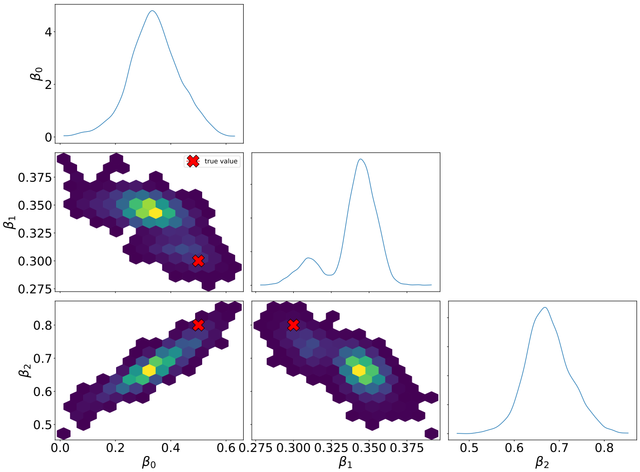
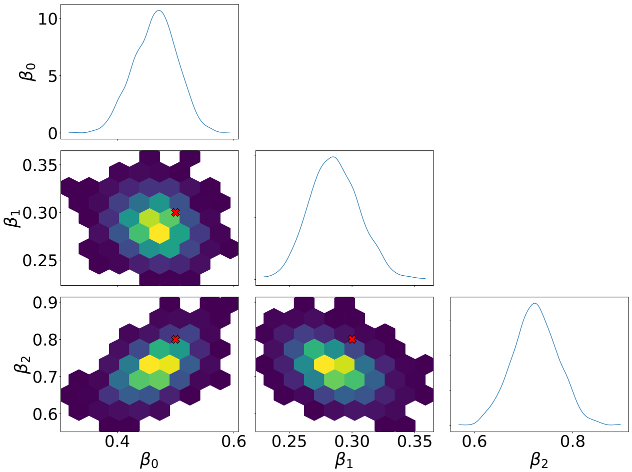


Anharmonic oscillator : Calibration

With partial elastic decomposition:

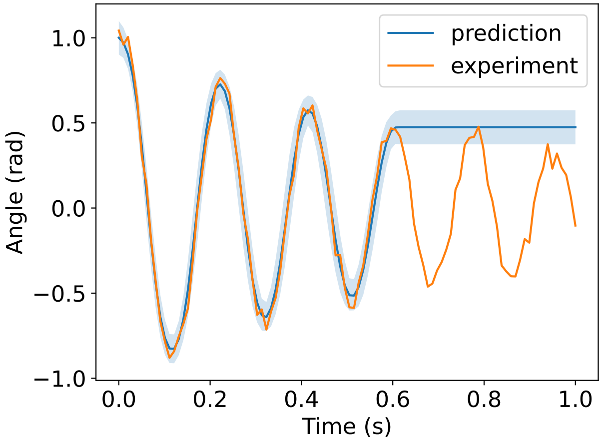


Final time but no elasticity:



Anharmonic oscillator : Comparison of the predictions

With partial elastic decomposition



Final time but no elasticity