Bayesian Emulator Approach for Complex Dynamical Systems

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Outline

- Introduction
- Emulators
- Linear Structural Dynamics
- Applications
  - 3DOF example
  - Large (1200 DOF) simulation example
  - Experimental example
- Conclusions

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Introduction

- Complex engineering dynamical systems are often investigated running computer codes, also known as simulators (O'Hagan, 2006).
- A simulator is a function $\eta(\cdot)$ that, given an input **x**, it produces an output **y**.
- Sophisticated simulators can have a high cost of execution, measured in terms of:
  - CPU time employed
  - Floating point operations performed
  - Computer capability required

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Introduction

- A possible solution is to build an emulator of the expensive simulator.
- An emulator is a statistical approximation to the simulator, i.e., it provides a probability distribution for $\eta(\cdot)$.
- Emulators have already been implemented in a number of fields, which include:
  - Environmental science (Challenor et al., 2006)
  - Climate modeling (Rougier, 2007)
  - Medical science (Haylock and O'Hagan, 1996)

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Introduction

- In Structural Dynamics, an example of an expensive simulator is a high-resolution finite element model, which can be difficult to run even for obtaining a dynamic response at few frequency points.
- Emulation can thus be a useful computational tool to be implemented in a Structural Dynamics context.

Introduction

- To test the convenience of the use of emulators for studying engineering dynamical systems, the following problems will be addressed:

1. *Computational cost*. Can the output of a computer code be approximated using only a few trial runs?
2. *Efficiency.* Can the number of floating point operations in an expensive code be reduced but still produce a satisfactory output?
3. *Interpolation of experimental data.* Can experimental data be confidently interpolated to cope with the lack of a mathematical/computer model?

Emulators

- An emulator is built by first choosing n design points in the input domain of the simulator and obtaining the training set $\{\eta(\mathbf{x}_1), \ldots, \eta(\mathbf{x}_n)\}$.
- After that initial choice is made, an emulator should:
  - Reproduce the known output at any design point.
  - At any untried input, provide a distribution whose mean value constitutes a plausible interpolation of the training data. The probability distribution around this mean value should also express the uncertainty about how the emulator might interpolate.

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Emulators

- To illustrate what do the above criteria mean, an emulator was constructed to approximate the simple simulator $\mathbf{y} = cos(\mathbf{x})$.
- In the following figures, the solid line is the true output of the simulator. The circles represent the training runs, and the dots are the mean of the emulator, which provides the approximation.
- Note how the approximation improves when more design points are chosen.

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Emulators

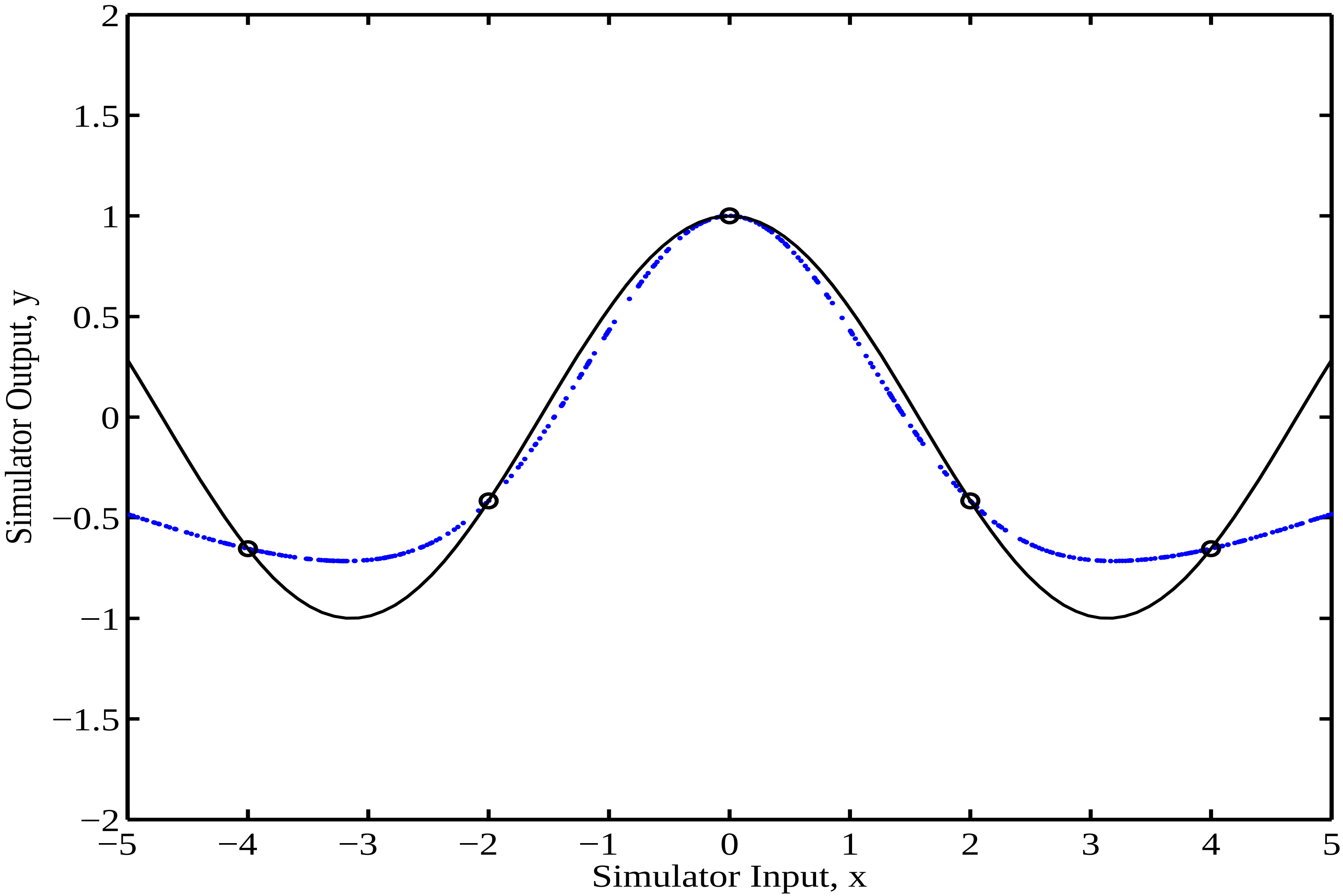

Figure 1: Approximation using 5 design points.

Emulators

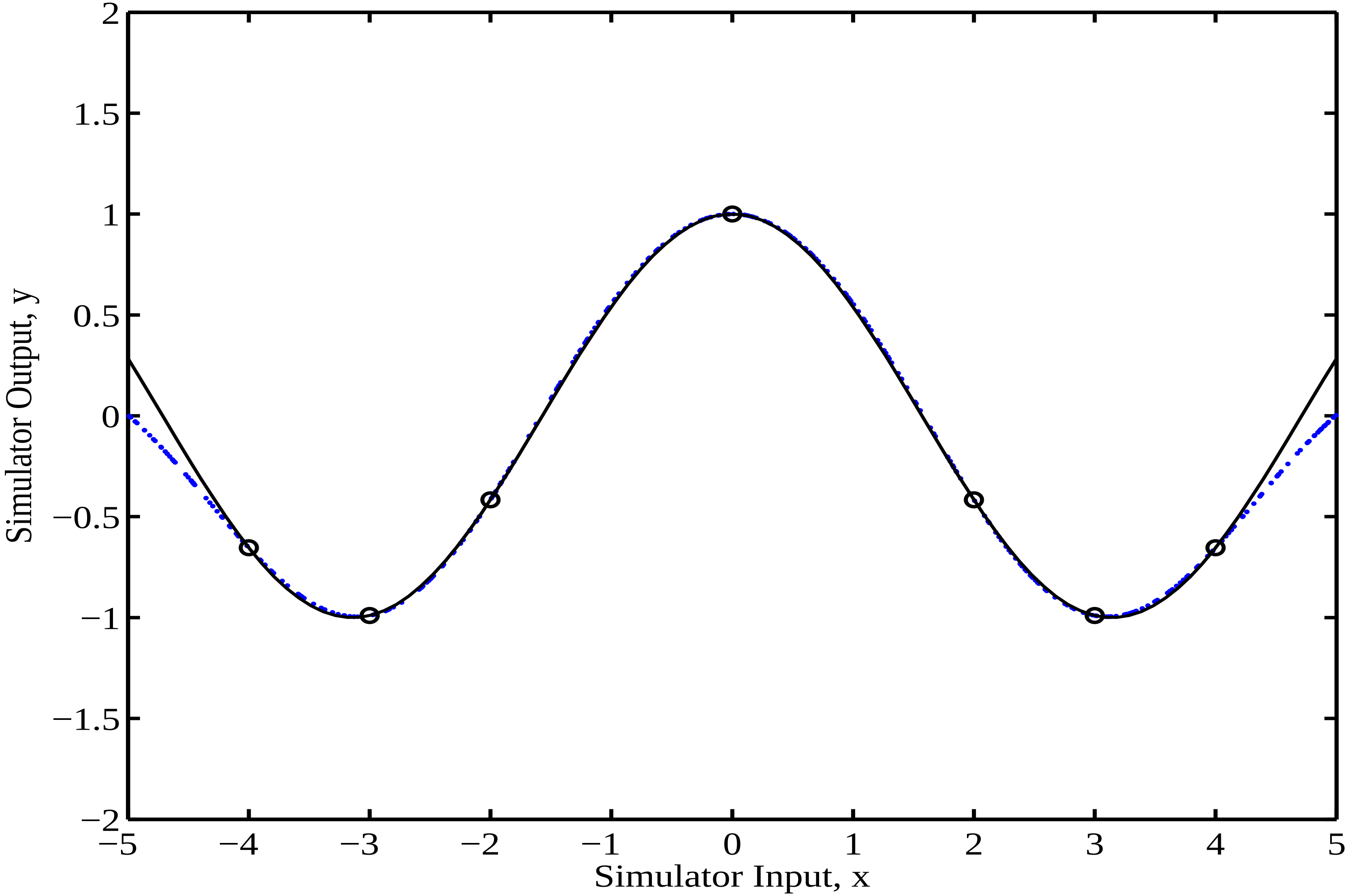

Figure 2: Approximation using 7 design points.

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Emulators

- In the same way, the following figures show upper and lower probability bounds of two standard deviations for the mean of the emulator. The solid line is the true output of the simulator. The circles represent the training runs, and the dots are the bounds.
- Note how the uncertainty about the approximation is reduces as more design points are chosen.

Emulators

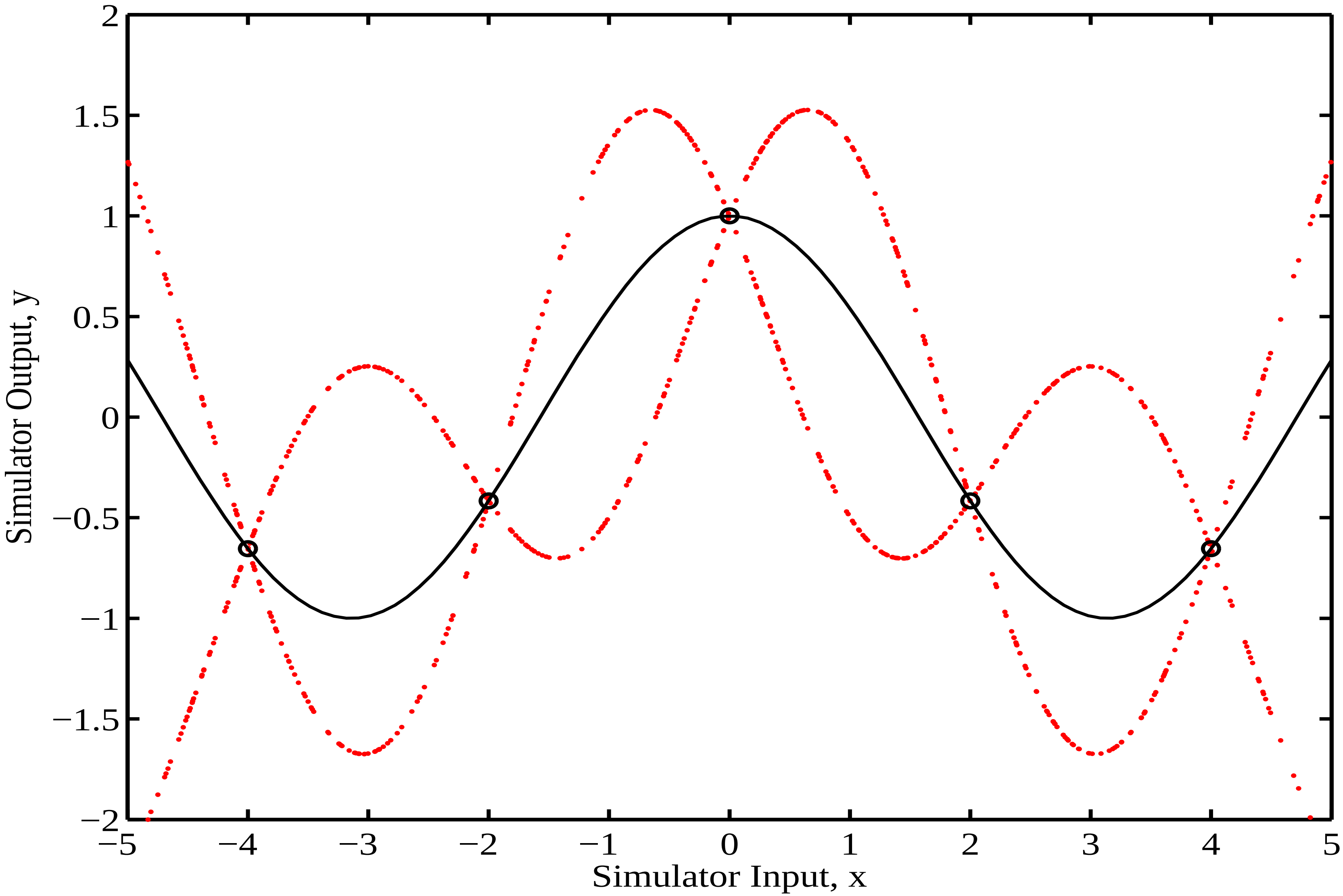

Figure 3: Uncertainty using 5 design points.

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Emulators

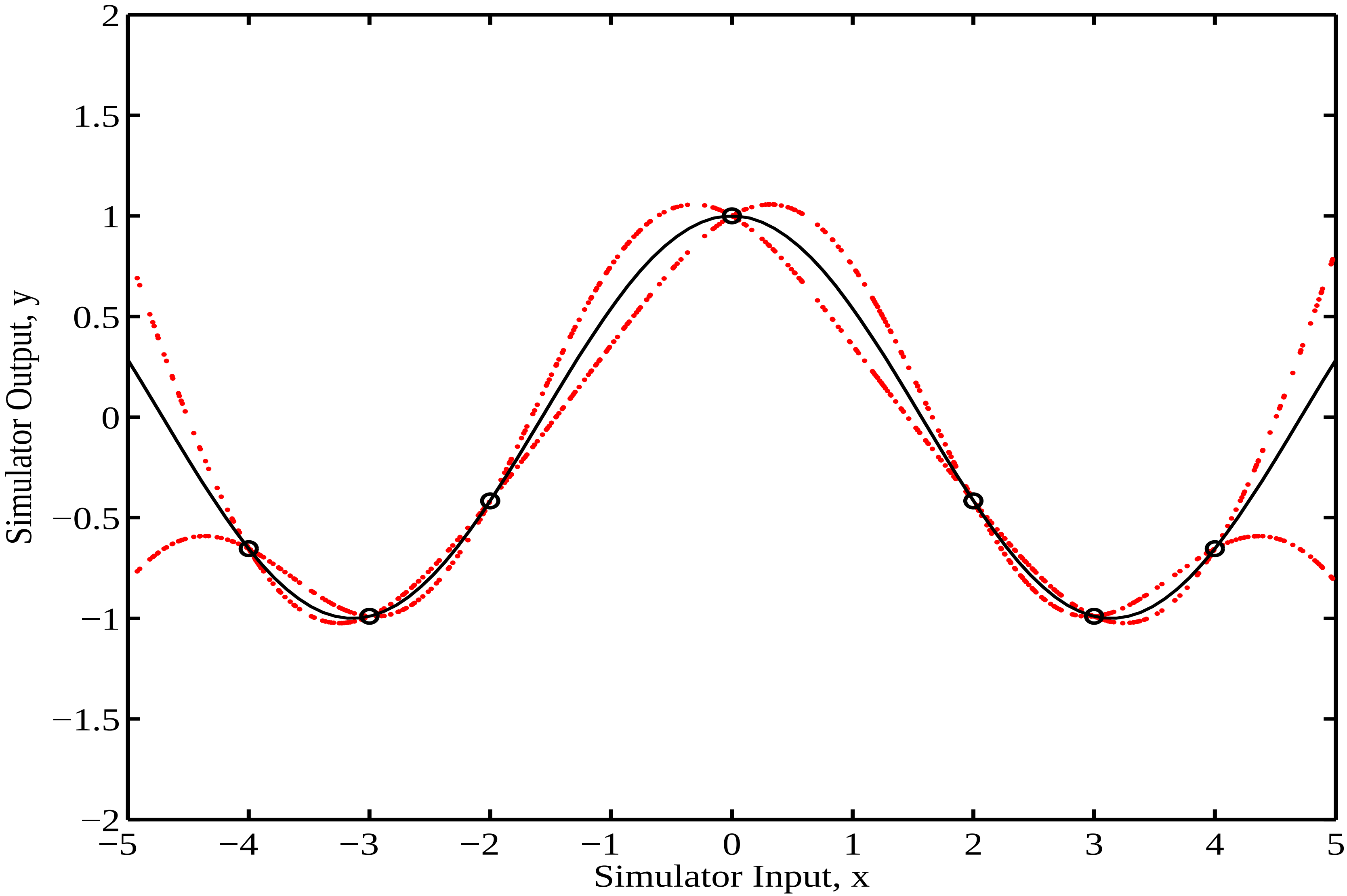

Figure 4: Uncertainty using 7 design points.

Emulators

- From the perspective of Bayesian Statistics, $\eta(\cdot)$ is a random variable in the sense that it is unknown until the simulator is run.
- Assume that $\eta(\cdot)$ deviates from the mean of its distribution in the following way

$$\eta(\mathbf{x}) = \sum_{j=1}^{n} \beta_j h_j(\mathbf{x}) + Z(\mathbf{x}) \tag{1}$$

where for all j, $h_j(\mathbf{x})$ is a known function and β_j is an unknown coefficient.

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Emulators

- The function $Z(\cdot)$ in Eq.(1) is assumed to be a Gaussian stochastic process (GP) with mean zero and covariance given by

$$Cov(\eta(\mathbf{x}), \eta(\mathbf{x}')) = \sigma^2 e^{-(\mathbf{x}-\mathbf{x}')^T \mathbf{B}(\mathbf{x}-\mathbf{x}')} \qquad (2)$$

  where **B** is a positive definite diagonal matrix that contains smoothness parameters.

- If the mean of $\eta(\cdot)$ is of the form $m(\cdot) = \mathbf{h}(\cdot)^T\boldsymbol{\beta}$ then $\eta(\cdot)$ has a GP distribution with mean $m(\cdot)$ and covariance given by Eq.(2).

Emulators

- The latter is symbolized as

$$\eta(\cdot)|\boldsymbol{\beta}, \sigma^2 \sim N(\mathbf{h}(\cdot)^T \boldsymbol{\beta}, \sigma^2 C(\cdot, \cdot)) \tag{3}$$

- This prior distribution contains subjective information about the relation of the input and the unknown output . The next step is to update this belief by adding objective information, represented by the vector of observations $\mathbf{y} = [\mathbf{y}_1 = \eta(\mathbf{x}_1), \ldots, \mathbf{y}_n = \eta(\mathbf{x}_n)]^T$.

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Emulators

- Using standard integration techniques, it can be shown (Haylock and O'Hagan, 1996) that such update is

$$\eta(\cdot)|\mathbf{y},\sigma^2 \sim N(m^{**}(\cdot),\sigma^2 C^{**}(\cdot,\cdot)) \tag{4}$$

  where $m^{**}(\cdot)$ constitutes the fast approximation of $\eta(\mathbf{x})$ for any $\mathbf{x}$ in the input domain.

- Moreover, it can be shown that

$$\frac{\eta(\mathbf{x}) - m^{**}(\mathbf{x})}{\widehat{\sigma}\sqrt{\frac{(n-q-2)C^{**}(\mathbf{x})}{n-q}}} \sim t_{n-q} \tag{5}$$

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Structural Dynamics

- Consider the problem of modeling the response of a structural system to different frequency ranges of vibration.
- To obtain the corresponding Frequency Response Function (FRF), the following equation of motion must be solved:

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{C}\dot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{f}(t) \qquad (6)$$

where **K**, **C** and **M** $\in \mathrm{R}^{N\times N}$ are respectively the stiffness, damping and mass matrices, $\mathbf{f}(t)$ is the forcing vector and $\mathbf{q}(t)$ the response vector.

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Structural Dynamics

- Equation(6) can be solved in terms of the excitation frequency level, $\omega \in [0, ..., \infty)$, as

$$\overline{\mathbf{q}}(\omega) = [-\omega^2\mathbf{M} + i\omega\mathbf{C} + \mathbf{K}]^{-1}\bar{\mathbf{f}}(\omega) \qquad (7)$$

where $\overline{\mathbf{q}}(\omega)$ and $\bar{\mathbf{f}}(\omega)$ are the Fourier transforms of $\mathbf{q}(t)$ and $\mathbf{f}(t)$. Since it is a complex-valued function, the relevant simulator becomes:

$$\eta(\omega) = \left| [-\omega^2\mathbf{M} + i\omega\mathbf{C} + \mathbf{K}]^{-1}\bar{\mathbf{f}}(\omega) \right| \qquad (8)$$

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Structural Dynamics

- To emulate the FRF expressed in Eq.(8), the following algorithm is proposed.
  1. Select n initial frequency values $\omega_1, \ldots, \omega_n$.
  2. Obtain the vector of observations $\mathbf{y} = [\mathbf{y}_1 = \eta(\omega_1), \ldots, \mathbf{y}_n = \eta(\omega_n)]^T$.
  3. Update the prior distribution (3), which contains subjective information, by adding the objective information $\mathbf{y}$. This will enable the calculation of $m^{**}(\cdot)$, the mean of the updated posterior distribution (4) given the data $\mathbf{y}$. As already mentioned, such mean constitutes an approximation of $\eta(\omega)$ for any ω.

Structural Dynamics

- For a damped three-degree-of-freedom spring-mass system, it can be shown that the FRF for k fixed is

$$\eta(\omega) = \sum_{j=1}^{3} \frac{\widetilde{\mathbf{x}}_j^T \bar{\mathbf{f}}(i\omega)}{\sqrt{(\omega_j^2 - \omega_j)^2 + (2\omega\omega_j\zeta_j)^2}} \widetilde{x}_{kj} \qquad (9)$$

where $k = 1, \ldots, 3$ and for all j, ω_j are the natural frequencies, $\widetilde{\mathbf{x}}_j$ are the normal modes and ζ_j are the damping ratios.

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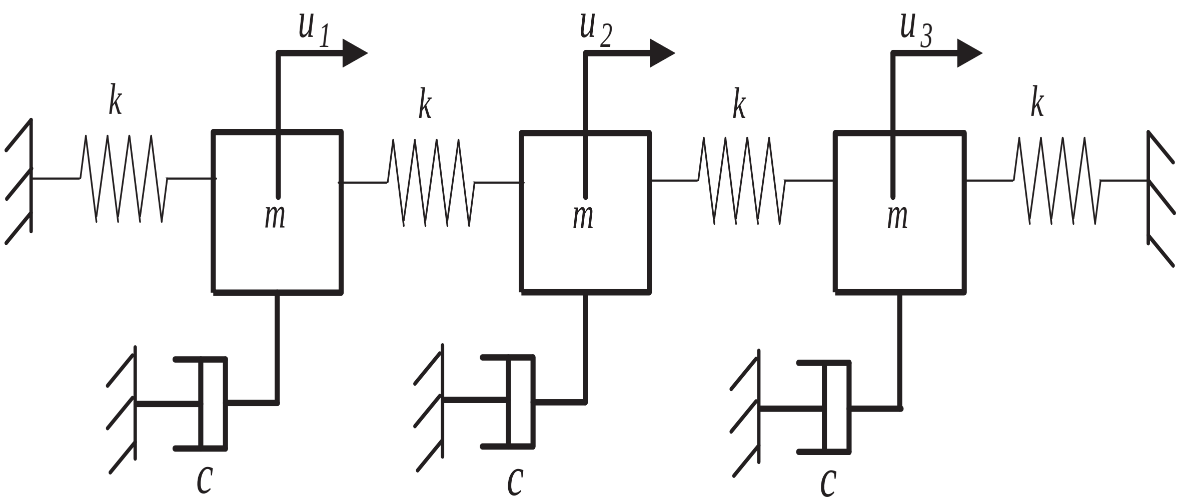
Applications

- In the figure below, the mass of each block is 1 kg and the stiffness of each spring is 1 N/m. The viscous damping constant of the damper associated with each block is 0.2 Ns/m. Suppose he dynamic response when only the first mass is subjected to unit initial displacement is to be obtained.



Applications

- Twenty-one equally-spaced design points were selected and the smoothness parameters calculated. The above algorithm was then applied to construct the corresponding emulator for the FRF.
- The results for $k = 1$ are shown below. As before, the circles represent the training runs, the dots represent the mean emulator and the uncertainty bounds respectively, and the solid line is the true value of the simulator.

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Applications

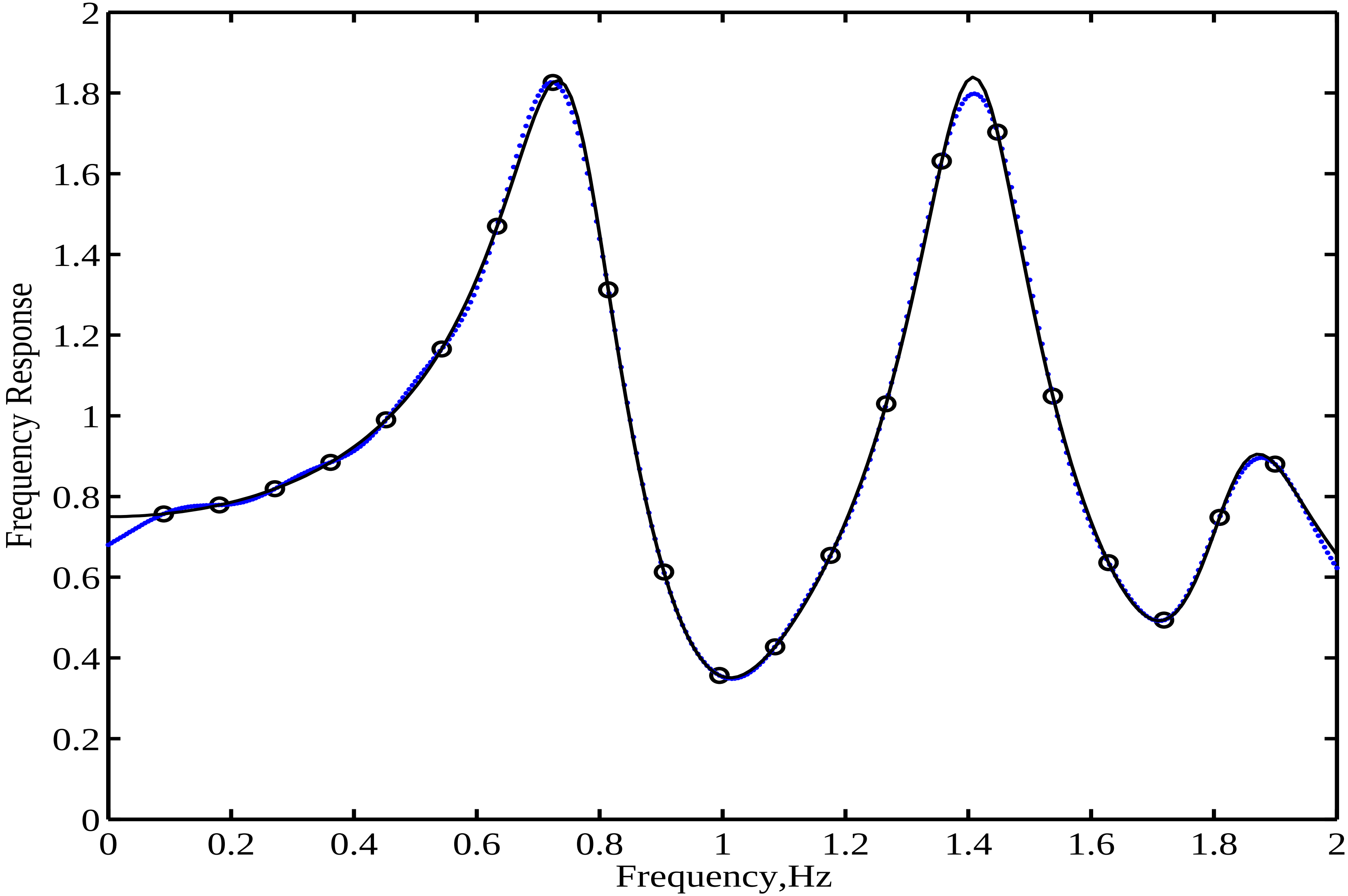

Figure 5: Approximation using 21 design points.

Applications

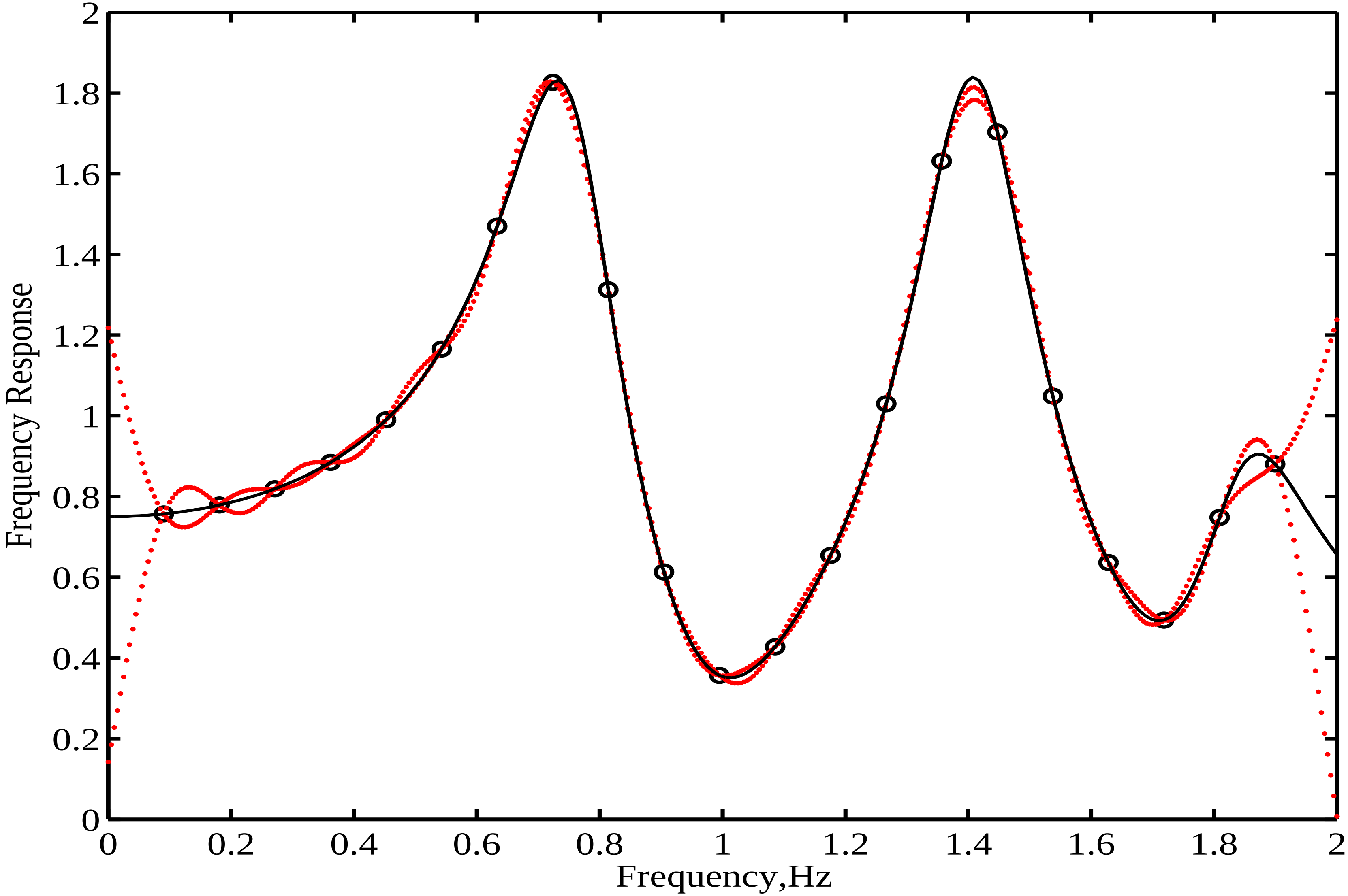

Figure 6: Uncertainty using 21 design points.

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Applications

- Unfortunately, Eq.(8) cannot always be solved analytically. Furthermore, a simulator can be very expensive to run for real-life engineering applications, v.g., modeling the response of an aircraft, or parts of it, to vibration.
- The potential use of intensive computation is a suitable scenario to apply emulators.
- The following figures refer to a realization of a simulator (Adhikari et al., 2007) of the frequency response of a steel plate with a fixed edge.

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Applications

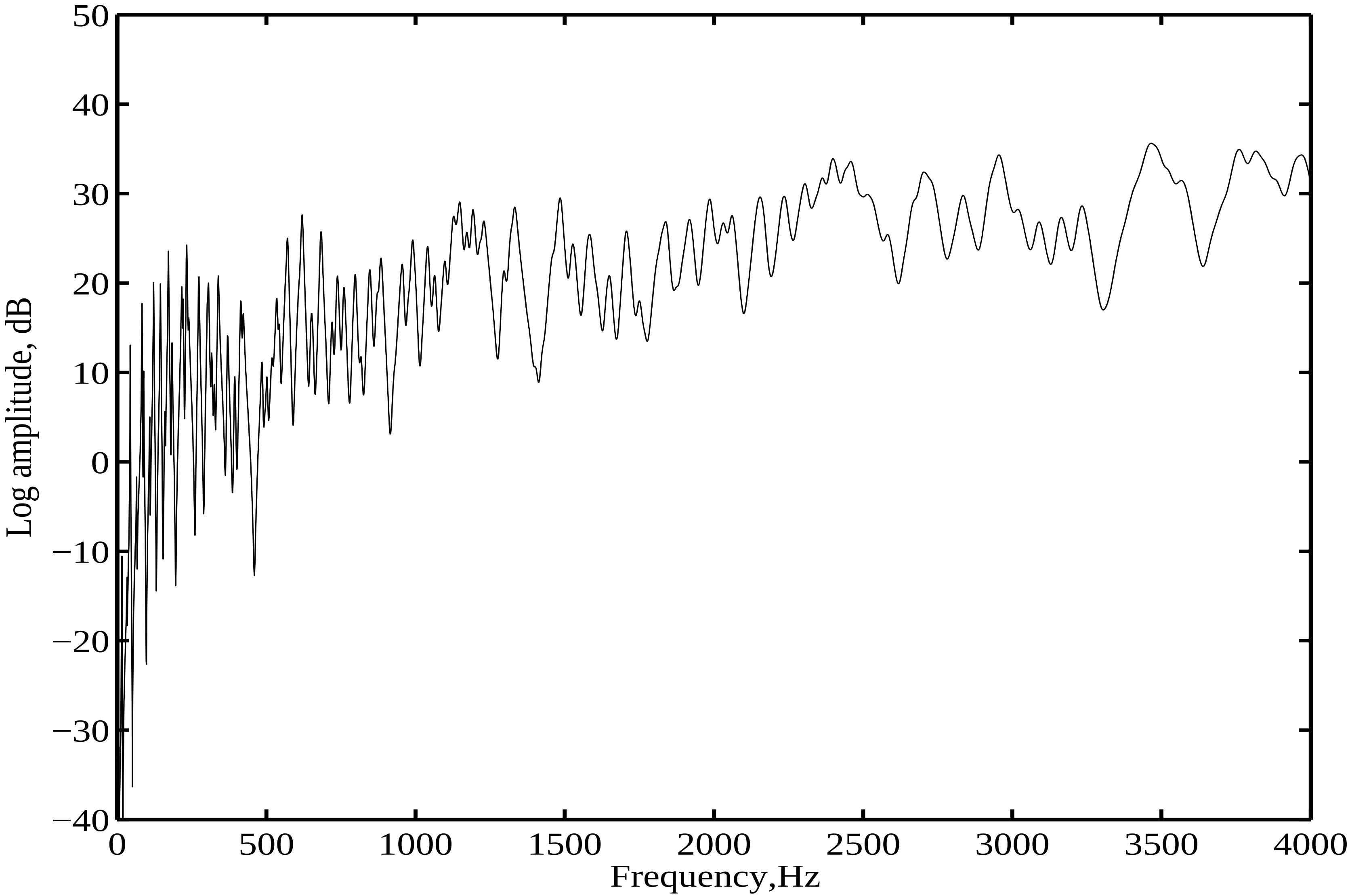

Figure 7: Simulator of the FRF of a steel plate subject to vibration.

Applications

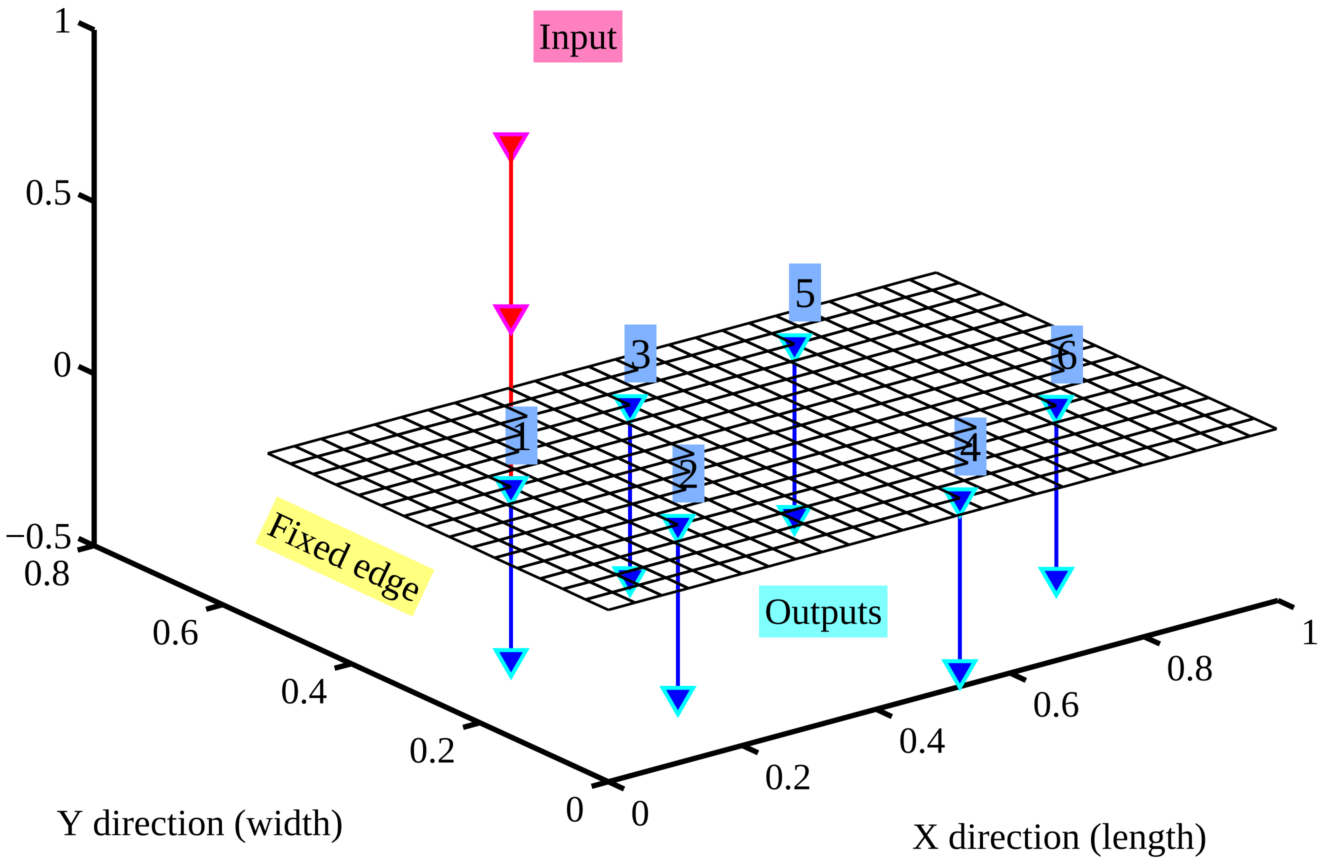

Figure 8: The plate is divided into 25 × 15 elements, resulting in 1200 DOF.

Applications

- To test the potential application of emulation to engineering dynamical systems, the input domain of the previously shown simulator was divided in low (0-1 kHz), medium (1-2.5 kHz) and high (2.5-4 kHz) frequency ranges.
- The following figure shows a comparison between selecting a different number of design points to approximate the response of node 1 to vibration in the medium-frequency range. Note how the approximation is improved, the more design points are used.

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Applications

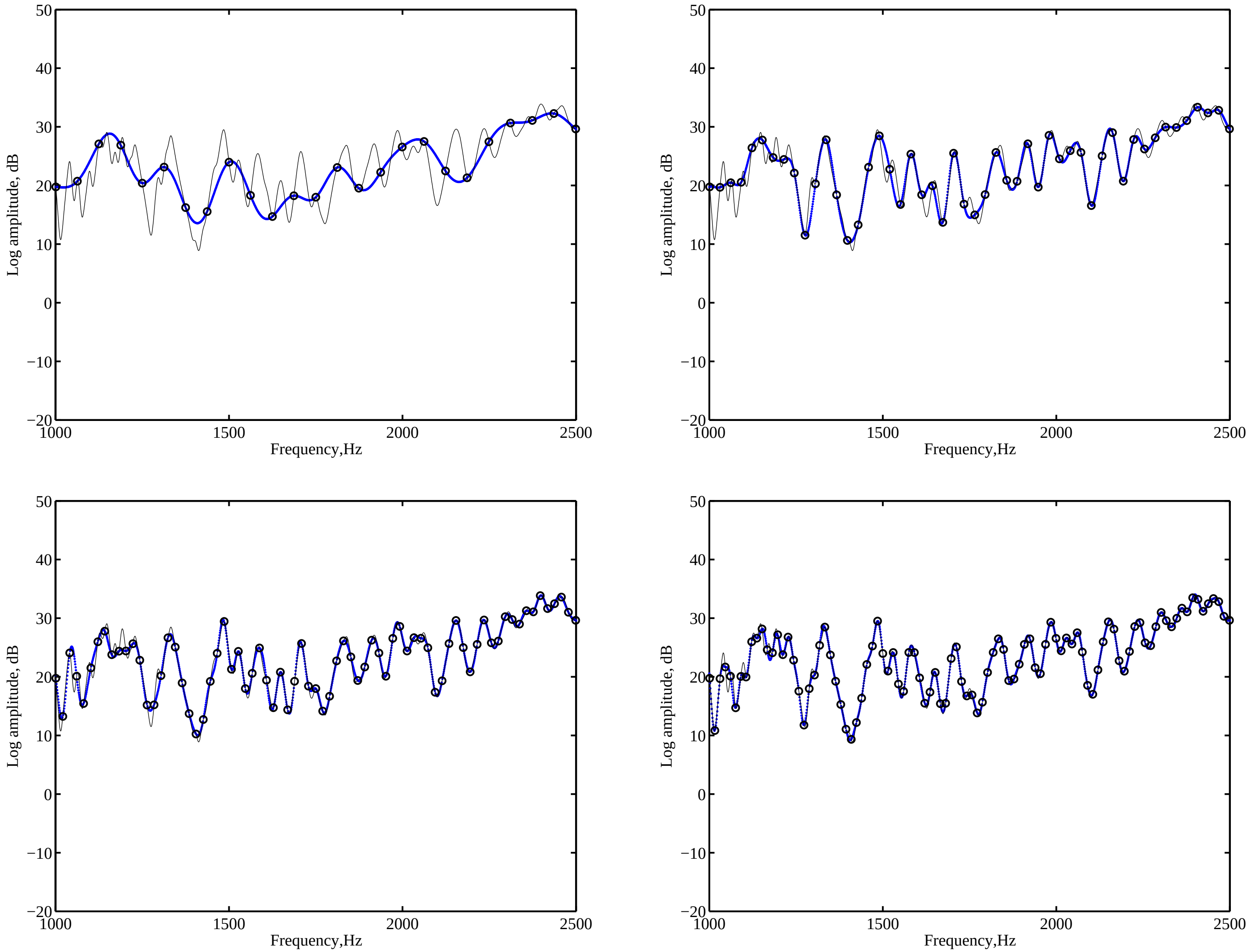

Figure 9: Emulation with 25, 50, 75 and 100 design points, mid-freq range.

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Applications

- One hundred equally-spaced design points were selected in each range, upon which an emulator was constructed to infer the value of the output at untried inputs. The results for the mean of the emulator in the different frequency ranges and the corresponding probability bounds are shown in the following figures.

Applications

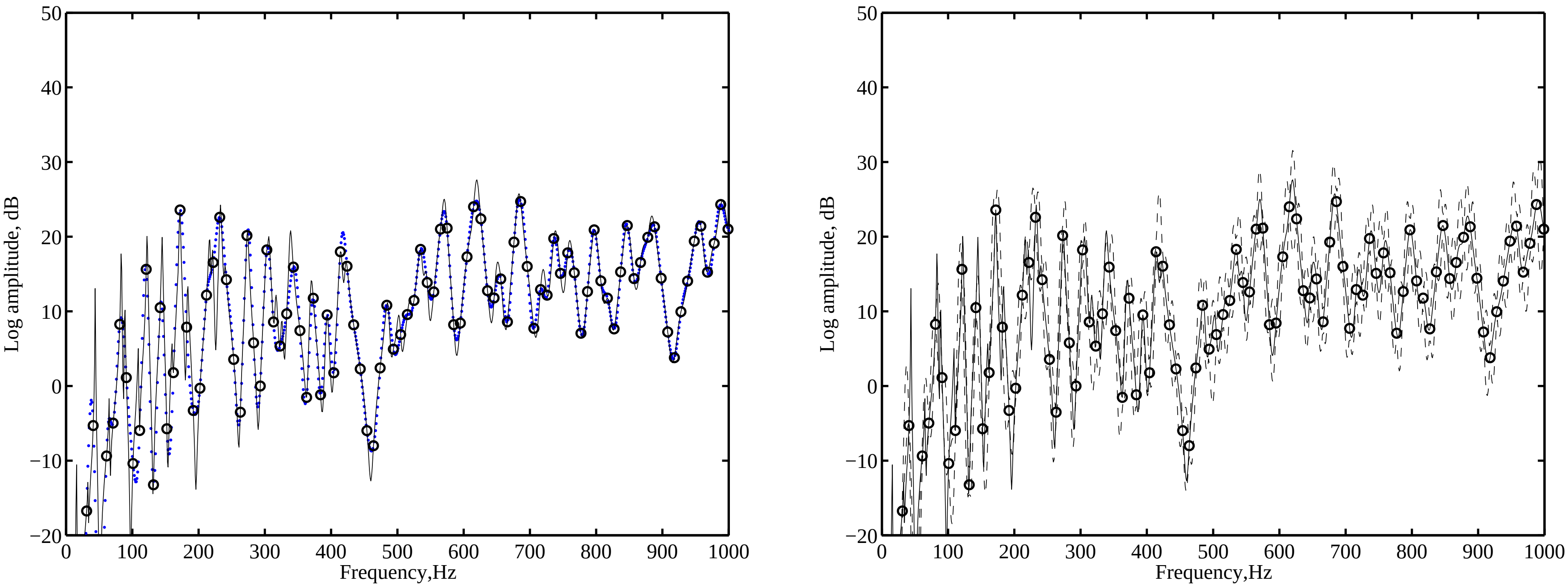

Figure 10: Emulation of the response of node 1, low-frequency range.

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Applications

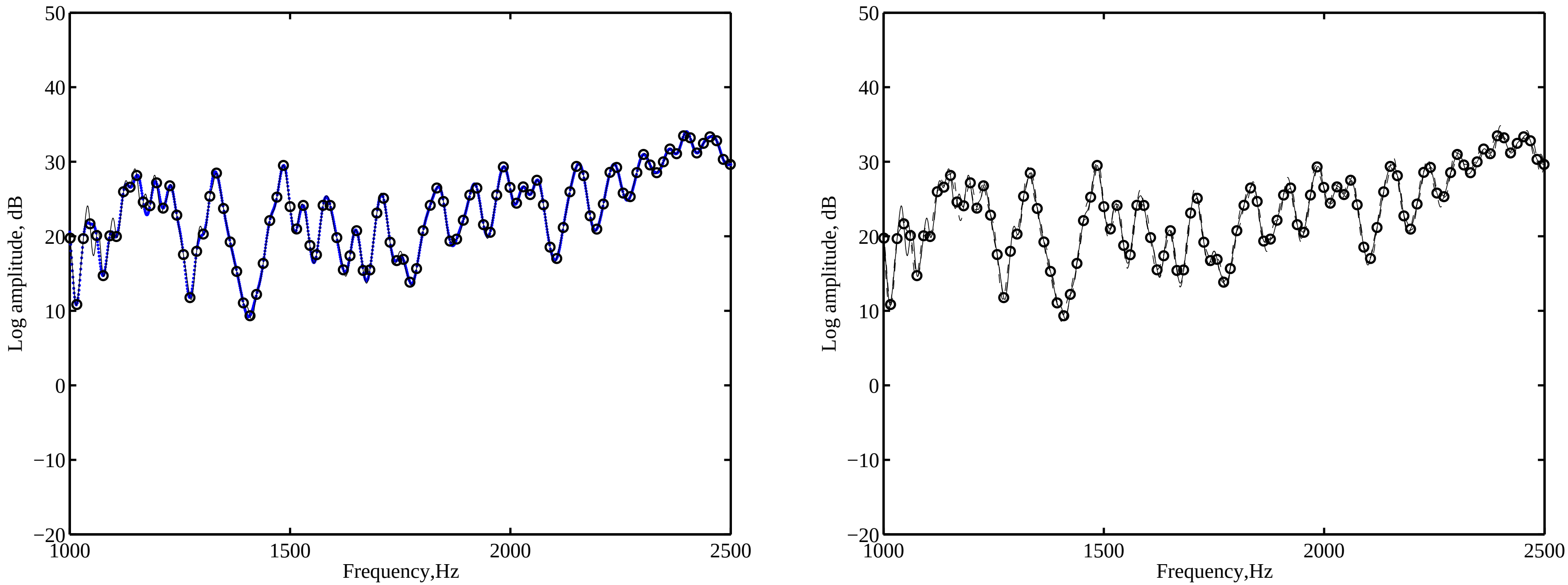

Figure 11: Emulation of the response of node 1, medium-frequency range.

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Applications

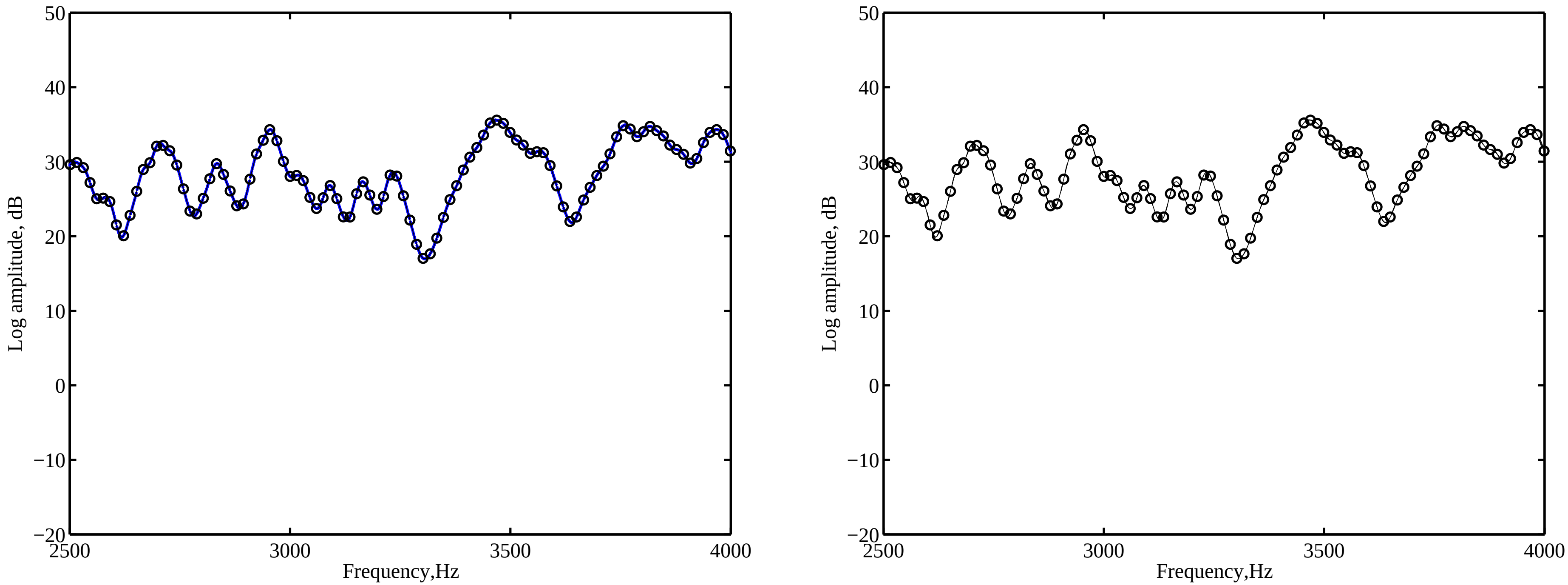

Figure 12: Emulation of the response of node 1, high-frequency range.

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Applications

- A setup in which there is no simulator available, due perhaps to the lack of knowledge of the physics of the system, was also considered.
- To approximate the response function of a plate subject to vibration, an experiment (Adhikari et al., 2007) was performed.
- The physical and geometrical properties of the plate are shown in the following table.

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Applications

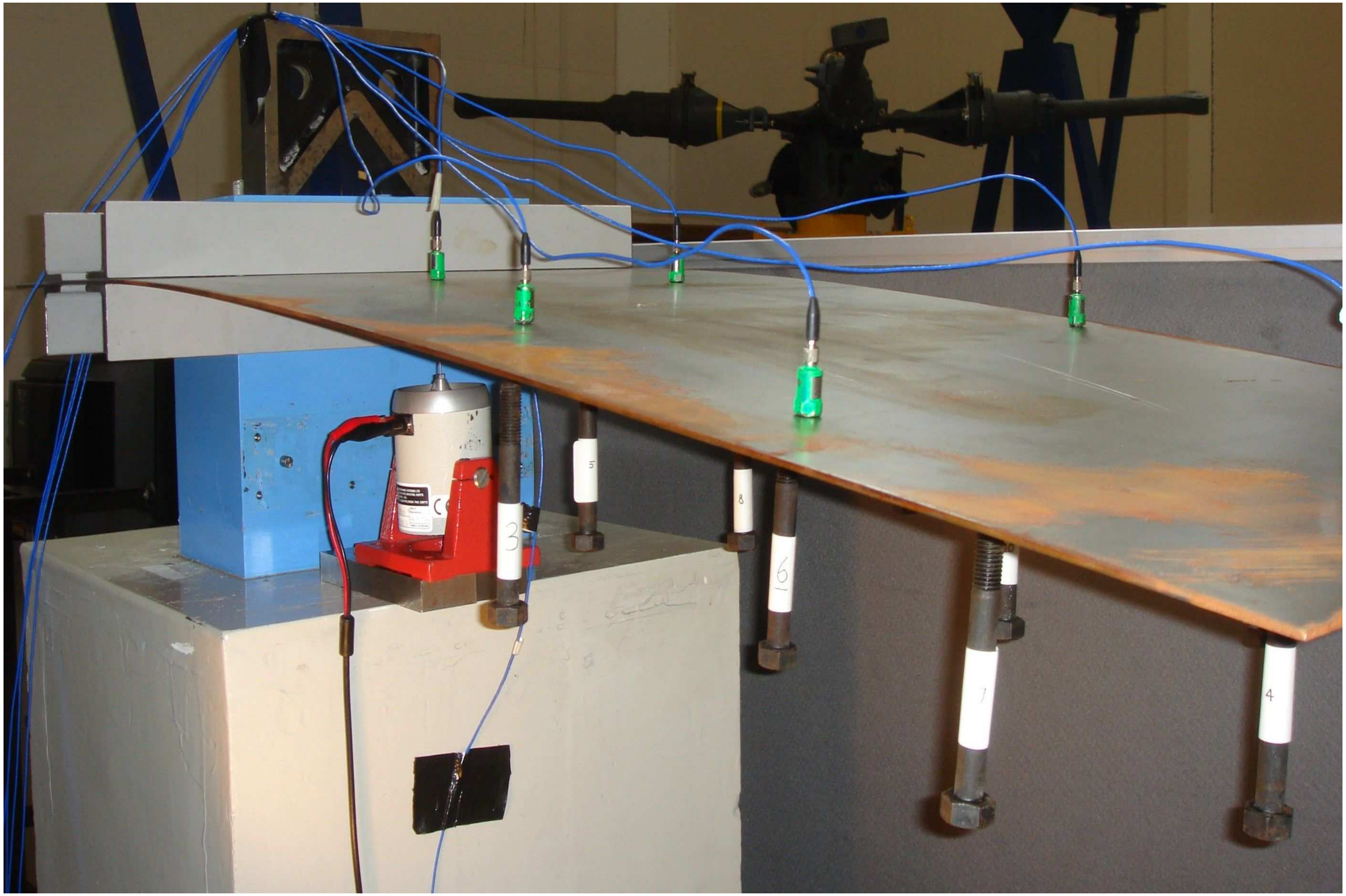

Figure 13: Experimental setup

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Applications

Plate Properties	Numerical values
Length	998 mm
Width	530 mm
Thickness	3.0 mm
Mass density	7860 kg/m^3
Young's modulus	2.0×10^5 MPa
Poisson's ratio	0.3
Total weight	12.47 kg

Table 1: Material and geometric properties of the plate considered for the experiment.

Applications

- In an experimental context like the one described, there would only be real measurements available.
- These measurements would act as the training runs and emulation should be applied the same way as in the previous cases. This would reduce the number of experimental runs necessary to obtain an empirical FRF.
- The results of doing so for the referred experiment are shown below, for every frequency range.

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Applications

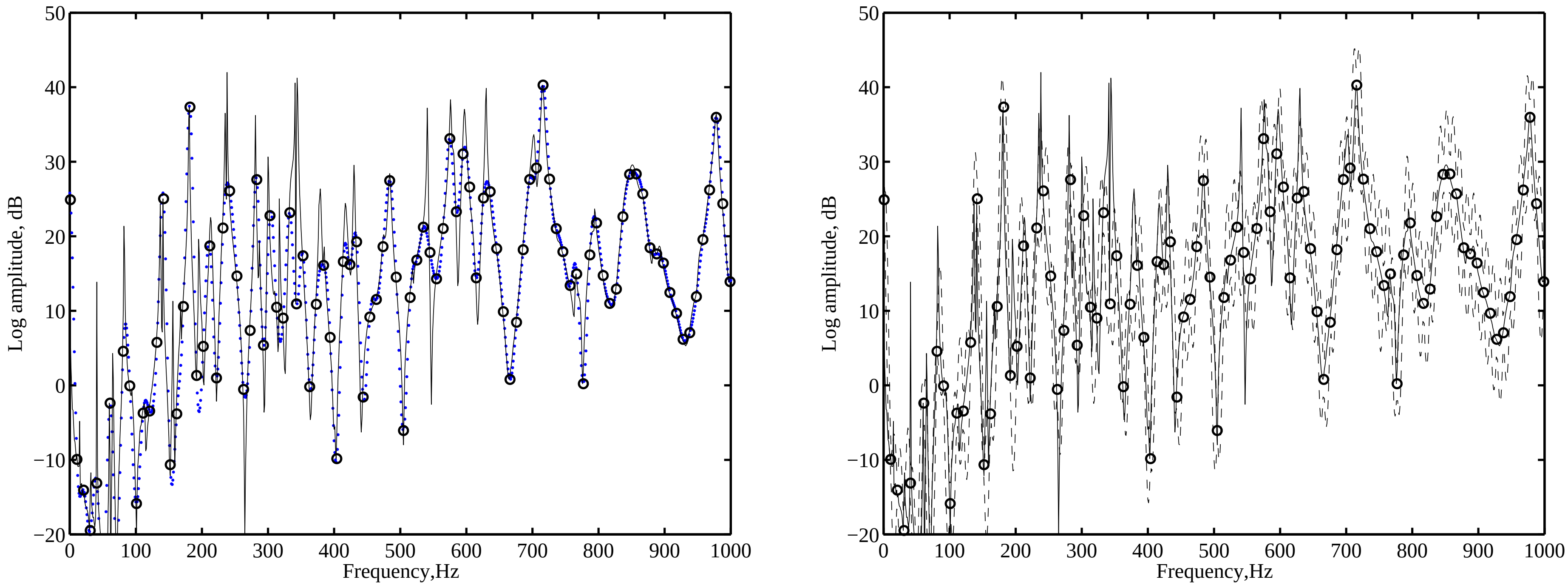

Figure 14: Emulation of the response of node 1, low-frequency range. The initial design is based on experimental measurements.

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Applications

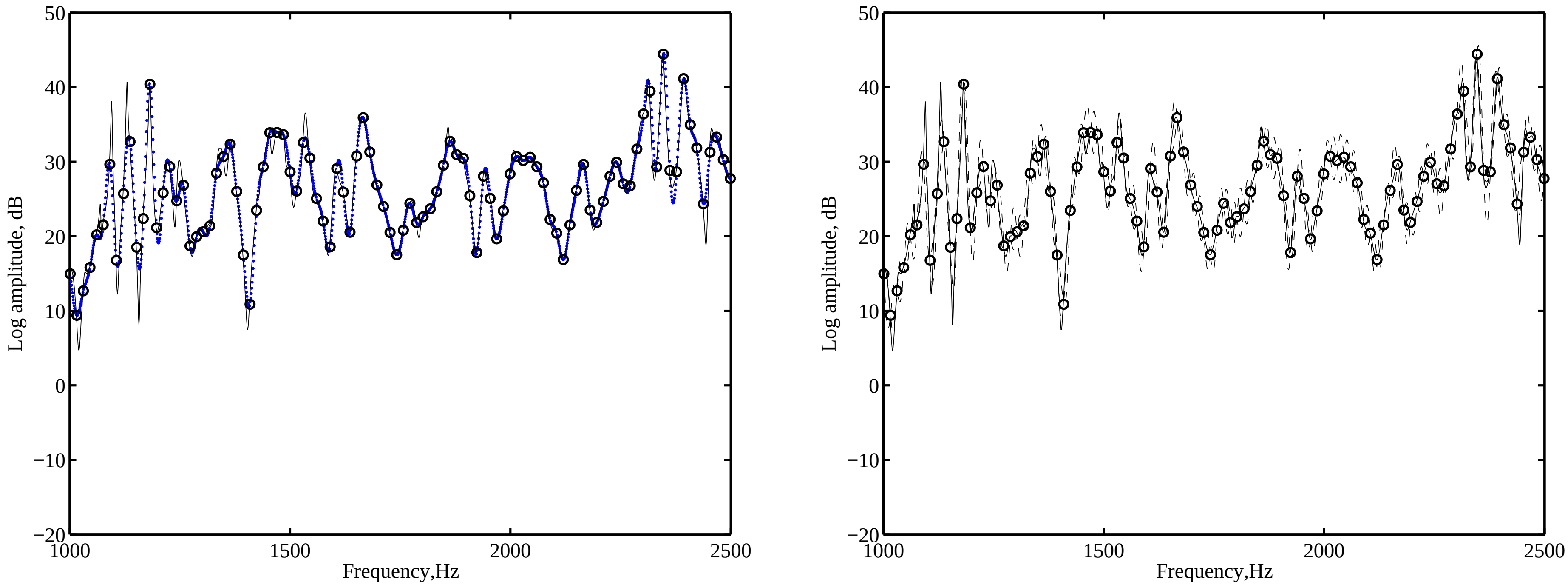

Figure 15: Emulation of the response of node 1, medium-frequency range. The initial design is based on experimental measurements.

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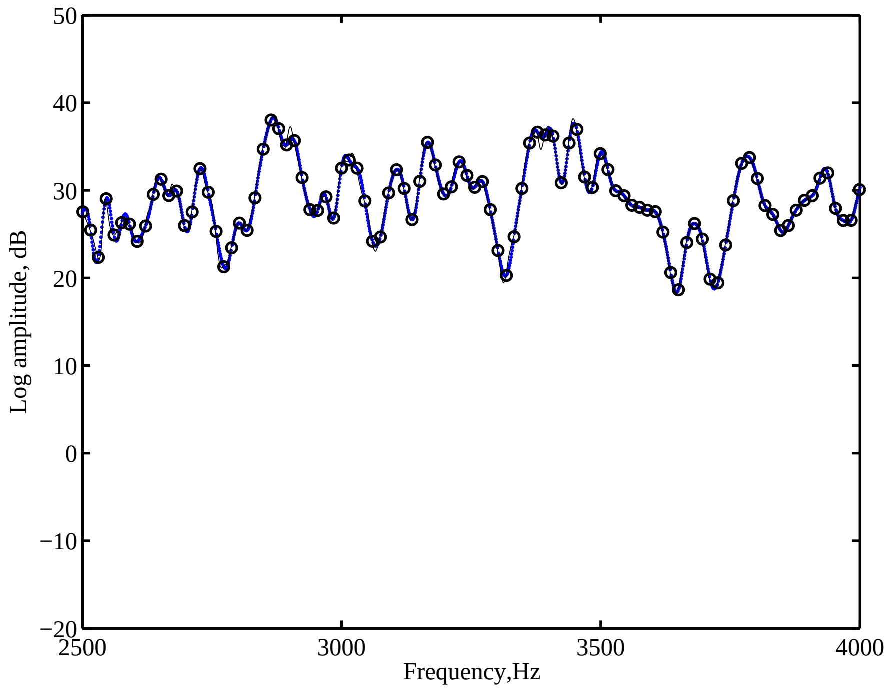
Applications



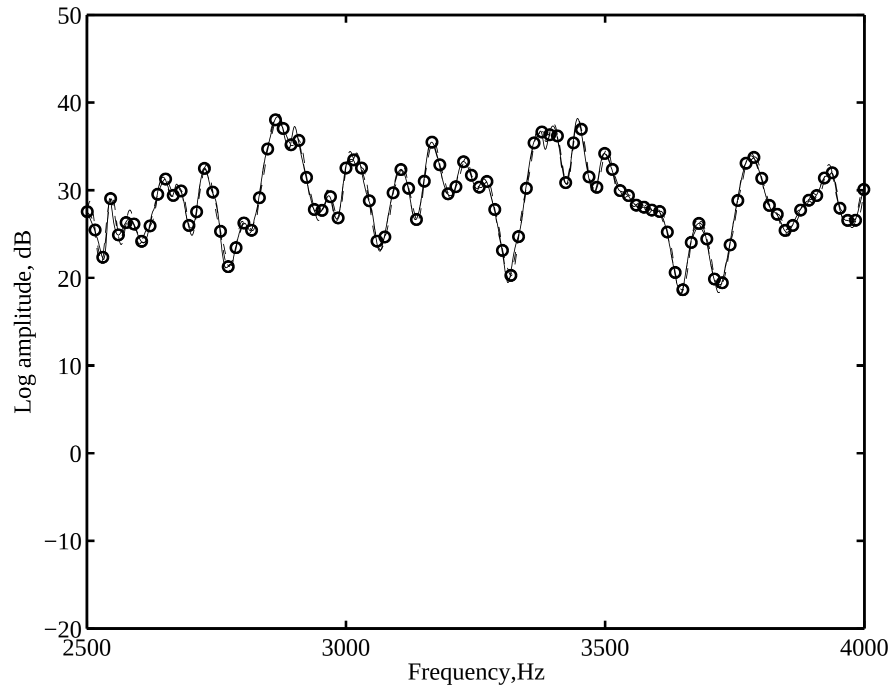


Figure 16: Emulation of the response of node 1, high-frequency range. The initial design is based on experimental measurements.

Conclusions

- Computer codes for structural dynamics can become very expensive to run, as the number of degrees of freedom in the system increases.
- The use of emulators has been proposed, since they provide a fast approximation to the output of the original code using in only a few training runs.
- With regards to computational cost, an emulator for a simple spring-mass system with three degrees of freedom was constructed to illustrate how the mean of the emulator approximates the FRF.

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Conclusions

- Regarding efficiency, the dynamic response of a system with 1200 degrees of freedom was emulated using only 300 training runs, thus reducing the number of necessary floating point operations. The results were particularly appealing for the medium and high-frequency ranges.
- To interpolate experimental data, real measurements were used as the set of training runs necessary to construct an emulator and the real experimental output was compared with the corresponding approximation.

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