Sequential design of experiments on a stochastic multi-fidelity simulator

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MEASUREMENT AND STANDARDS

COMPETITIVENESS AND SAFETY VECTOR

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Outline

1. Introduction
2. Sequential design of experiments
3. Academic example

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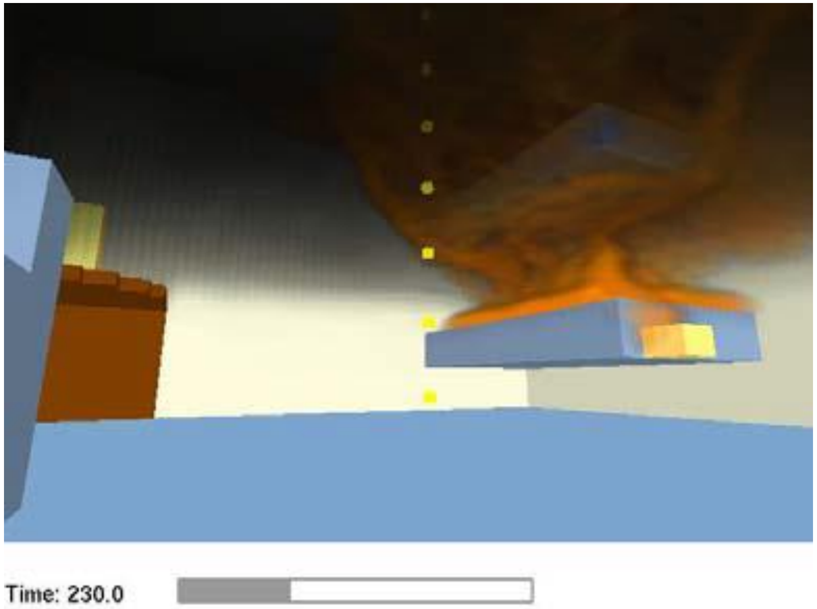
Context

- Fire safety: conformity of a smoke extraction system
  - Expensive experiments → use of numerical models

Real Experiment



Fire Dynamics Simulator (FDS)

- Images from [Kerber, 2005]

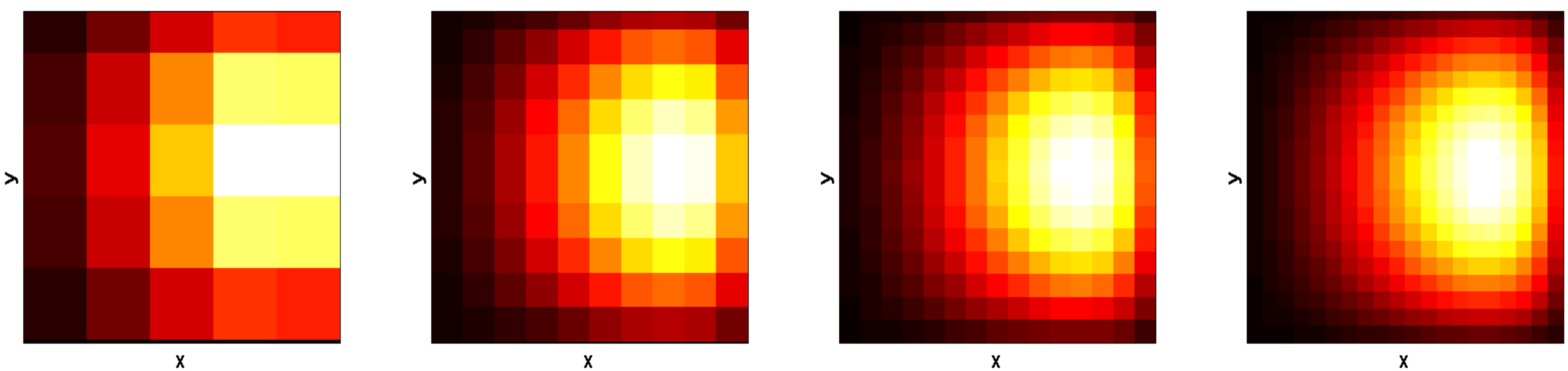
Properties of numerical models

- Main properties of the considered simulators:
  1. Multi-fidelity
  2. Tunable cost
  3. Stochastic outputs

Multi-fidelity

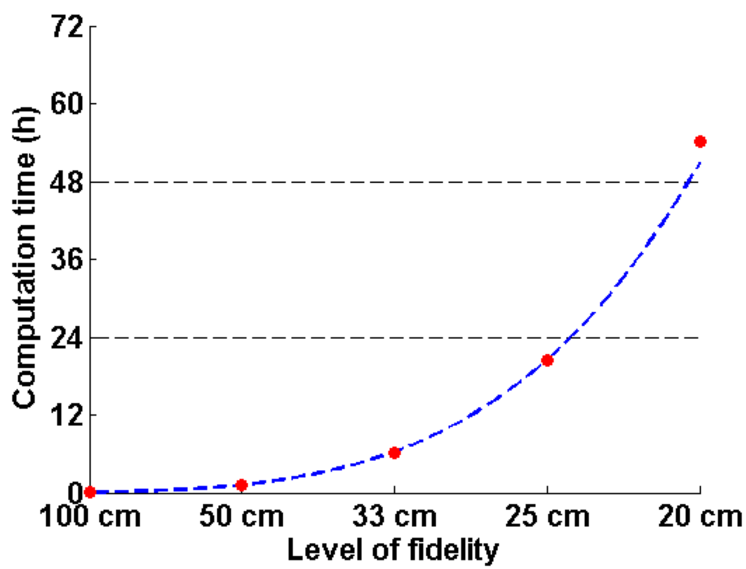
- Multi-fidelity: same physical phenomenon
  ➔ several models with various accuracy

Low fidelity → High fidelity



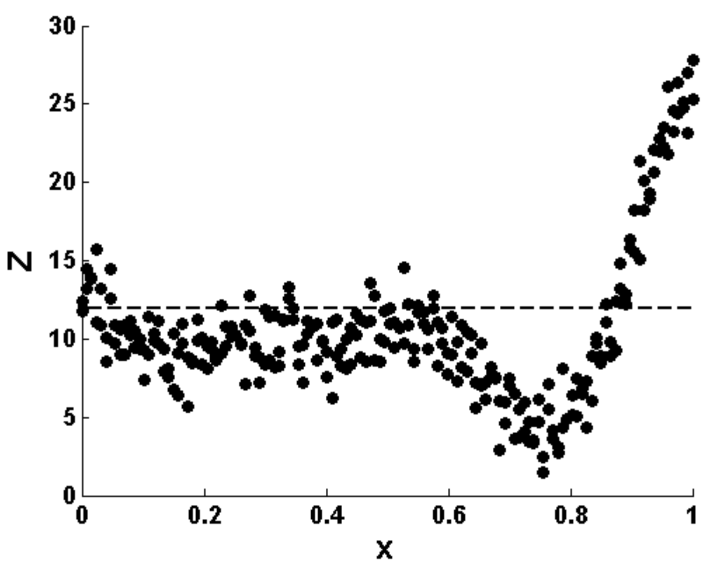
Tunable cost

- Cost of observation: function of the fidelity $C(t)$
  - Cheap simulation, but low fidelity
  - High fidelity simulation, but time-consuming



Stochastic outputs

- Stochastic: same input ➔ different outputs



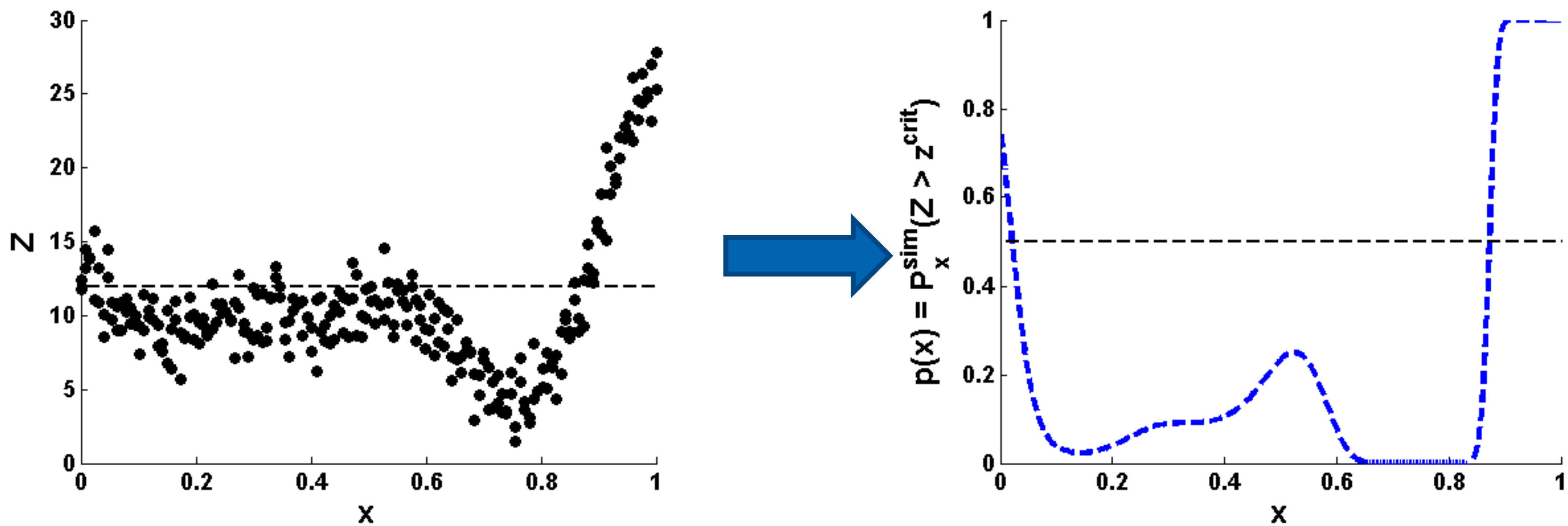
Quantity of Interest

$(x,t) \longrightarrow$ **Simulator** $\longrightarrow Z \longrightarrow \mathbb{P}^{\text{sim}}_{x,t^{HF}}\left(Z > z^{crit}\right)$

- Probability of exceeding a critical threshold z^{crit}

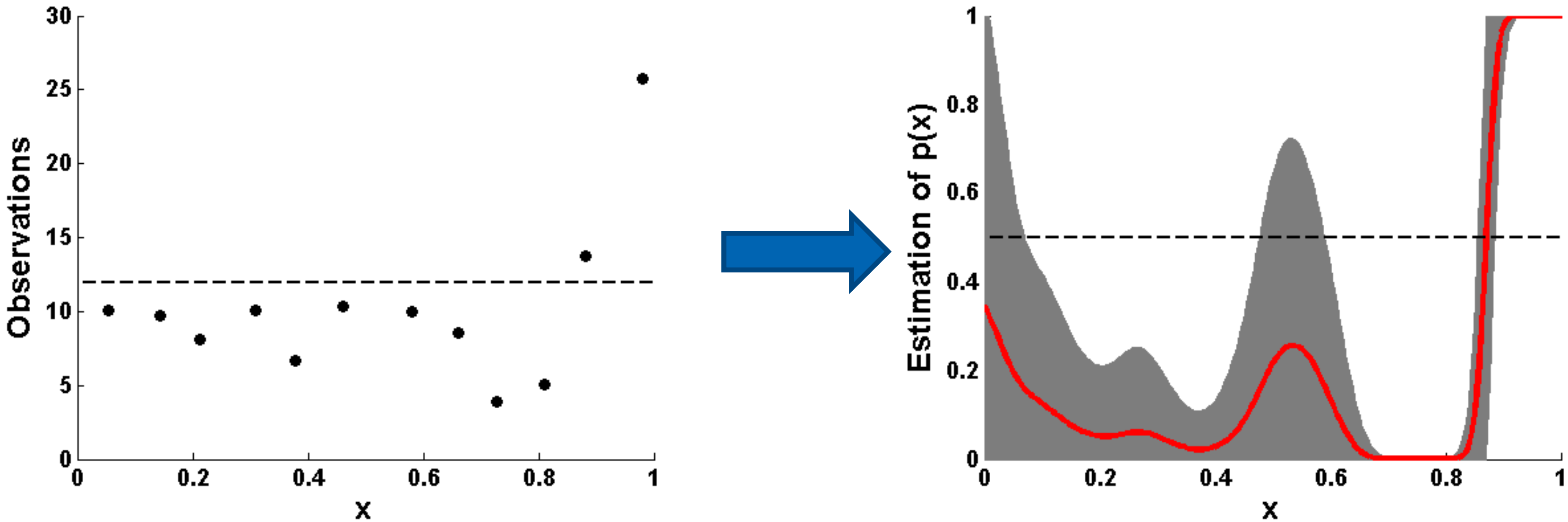
$$p(x, t^{HF}) = \mathbb{P}^{sim}_{x,t^{HF}}\left(Z > z^{crit}\right)$$

  - t^{HF}: the highest-fidelity level



Design of experiments

- Goal: selecting $(x_1, t_1), \ldots, (x_n, t_n)$ to estimate the function p with a minimal cost $C(t_1) + \cdots + C(t_n)$
  - Observations $(x_i, t_i; z_i)_{1 \le i \le n}$ ➔ Estimation $\hat{p}_n$ of p



Sequential design of experiments

- Goal: selecting $(x_1, t_1), \dots, (x_n, t_n)$ to estimate the function p with a minimal cost $C(t_1) + \cdots + C(t_n)$

- Sequential design
  - use the n first observations to select the $(n+1)^{th}$ observation

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Model of the simulator

- Prior distribution:
  - Output Z at x, t follows a normal distribution
    $$Z|\xi \sim \mathcal{N}\big(\xi(x,t), \lambda(x,t)\big)$$
  - Mean function ξ: Gaussian process
    $$\xi \sim \mathcal{GP}(m, k)$$
- Posterior distribution: kriging
  - Mean function $\xi|\chi_n$
    $$\xi|\chi_n \sim \mathcal{GP}(m_n, k_n)$$

Auto-regressive multi-fidelity covariance

- Mean function

$$\xi(x,t) = \begin{cases} \xi_{LF}(x) & \text{if } t = 1 \\ \rho\xi_{LF}(x) + \delta(x) & \text{if } t = 2 \end{cases}$$

  - ξ_{LF}: low-fidelity simulator
  - $\xi_{HF} = \rho\xi_{LF} + \delta$: high-fidelity simulator, linked to the low-fidelity by a linear relationship

➔ Covariance function

$$k\big((x,t),(x',t')\big) = \begin{cases} k_{LF}(x,x') & if\ t = t' = 1 \\ \rho k_{LF}(x,x') & if\ t \neq t' \\ \rho^2 k_{LF}(x,x') + k_\delta(x,x') & if\ t = t' = 2 \end{cases}$$

  - k_{LF}: covariance of the low-fidelity simulator
  - k_δ: covariance of the difference between high- and low-fidelity levels
  - ρ: correlation between the low- and high-fidelity levels

[Kennedy and O'Hagan, 2000], [Le Gratiet and Cannamela, 2015]

Non-stationary multi-fidelity covariance

- Mean function

$$\xi(x,t) = \xi_0(x) + \epsilon(x,t)$$

  - ξ_0: ideal simulator (Ex: mesh size = 0)
  - ϵ: system error between ideal and real simulators at t

➔ Covariance function

$$k\big((x,t),(x',t')\big) = k_0(x,x') + r(t,t') \cdot k_\epsilon(x,x')$$

  - k_0: covariance of ξ_0
  - k_ϵ: covariance of ϵ according to x
  - r: rules the decrease of the error
- [Picheny and Ginsbourger, 2013], [Tuo et al., 2014]

Probability of exceeding the critical threshold

- Probability of exceeding the critical threshold:

$$p(x,t) = \mathbb{P}^{sim}_{x,t}\left(Z > z^{\text{crit}} \middle| \chi_n\right) = \Phi\left(\frac{\xi(x,t) - z^{crit}}{\sqrt{\lambda(x,t)}}\right)$$

- First and second moments
  - Expectation: $\mathbb{E}_n[p(x,t)] = \Phi(u_n(x,t)) = \hat{p}_n(x,t)$
    Variance: $\mathbb{V}ar_n[p(x,t)] = \Phi_2(u_n(x,t), u_n(x,t); r_n(x,t)) - \Phi^2(u_n(x,t))$
  - $u_n(x,t) = \frac{m_n(x,t) - z^{crit}}{\sqrt{\sigma_n^2(x,t) + \lambda(x,t)}}$ $\quad r_n(x,t) = \frac{\sigma_n^2(x,t)}{\sigma_n^2(x,t) + \lambda(x,t)}$
  - $\sigma_n^2(x,t) = k_n\big((x,t),(x,t)\big)$
  - Φ: cumulative distribution function (cdf) of the normal distribution
    Φ_2: cdf of the bivariate normal distribution

Measure of uncertainty

- Measure of uncertainty

$$H_n = \mathbb{E}_n[\|\hat{p}_n(\cdot, t^{HF}) - p(\cdot, t^{HF})\|^2] = \int_{\mathbb{X}} \mathbb{V}ar_n[p(x, t^{HF})]dx$$

  - $\mathbb{L}^2$-norm of the error of the estimator at the highest level of fidelity

Stepwise Uncertainty Reduction

- Measure of uncertainty

$$H_n = \mathbb{E}_n[\|\hat{p}_n(\cdot, t^{HF}) - p(\cdot, t^{HF})\|^2] = \int_{\mathbb{X}} \mathbb{V}ar_n[p(x, t^{HF})]dx$$

- Stepwise uncertainty reduction algorithm

$$(x_{n+1}, t_{n+1}) = \underset{x,t}{\operatorname{argmin}}\{\mathbb{E}_n[H_{n+1} | X_{n+1} = x, T_{n+1} = t]\}$$

- [Vazquez and Bect, 2009]

Stepwise Uncertainty Reduction

- Measure of uncertainty

$$H_n = \mathbb{E}_n[\|\hat{p}_n(\cdot, t^{HF}) - p(\cdot, t^{HF})\|^2] = \int_{\mathbb{X}} \mathbb{V}ar_n[p(x, t^{HF})]dx$$

- Stepwise uncertainty reduction algorithm

$$(x_{n+1}, t_{n+1}) = \underset{x,t}{\operatorname{argmin}}\{\mathbb{E}_n[H_{n+1} | X_{n+1} = x, T_{n+1} = t]\}$$

- Analytical expression

$$\mathbb{E}_n[H_{n+1} | X_{n+1} = x, T_{n+1} = t]$$
$$= \int_{\mathbb{X}} \left[\Phi_2(u_n(y, t^{HF}), u_n(y, t^{HF}); r_n(y, t^{HF})) - \Phi_2\left(u_n(y, t^{HF}), u_n(y, t^{HF}); \tilde{r}_n\left((\boldsymbol{x}, \boldsymbol{t}), (y, t^{HF})\right)\right)\right] dy$$

- $$\tilde{r}_n\left((x, t), (y, t^{HF})\right) = \frac{k\left((x,t),(y,t^{HF})\right)^2}{\left(\sigma_n^2(x,t)+\lambda(x,t)\right)\cdot\left(\sigma_n^2(y,t^{HF})+\lambda(y,t^{HF})\right)}$$

Cost of observation

- Different costs $C(x,t)$ of observations
  ➔ Trade-off between H_n reduction and cost $C(x,t)$

- [Huang et al. 2006], [Le Gratiet and Cannamela, 2015]: comparison between benefit and cost

Maximum Speed of Uncertainty Reduction

- Maximum Speed of Uncertainty Reduction (MSUR)

$$(x_{n+1}, t_{n+1}) = \underset{x,t}{\operatorname{argmax}} \left\{ \frac{H_n - \mathbb{E}_n[H_{n+1} | X_{n+1} = x, T_{n+1} = t]}{C(x,t)} \right\}$$

  - MSUR = Benefit/Cost
  - Adaptable for any measure of uncertainty H_n
  - If C is constant ➔ equivalent to SUR algorithm

Simplification

- If the cost depends only on the level $C(x,t) = C(t)$

➔ Algorithm: separate optimization of the point x and the level t

1. $x^\star(t) = \underset{x}{\mathrm{argmin}}\{\mathbb{E}_n[H_{n+1}|X_{n+1} = x, T_{n+1} = t]\}$
2. $t_{n+1} = \underset{t}{\mathrm{argmax}}\left\{\frac{H_n - \mathbb{E}_n[H_{n+1}|X_{n+1}=x^\star(t), T_{n+1}=t]}{C(t)}\right\}$
3. $x_{n+1} = x^\star(t_{n+1})$

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   a. Presentation of the example
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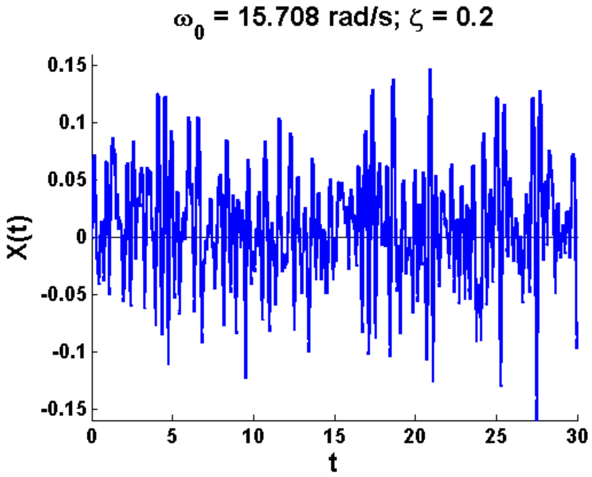
Stochastic damped harmonic oscillator

- Consider a damped harmonic simulator with random drive

$$\ddot{X}(t) + 2\zeta\omega_0\dot{X}(t) + \omega_0^2 X(t) = W(t)$$

  - ω_0: the undamped angular frequency
  - ζ: the damping ratio
  - W: a Brownian motion, with spectral density $S = 1$
  - Initial conditions: $X(t=0) = 0$, $\dot{X}(t=0) = 0$



- [Au and Beck, 2001]

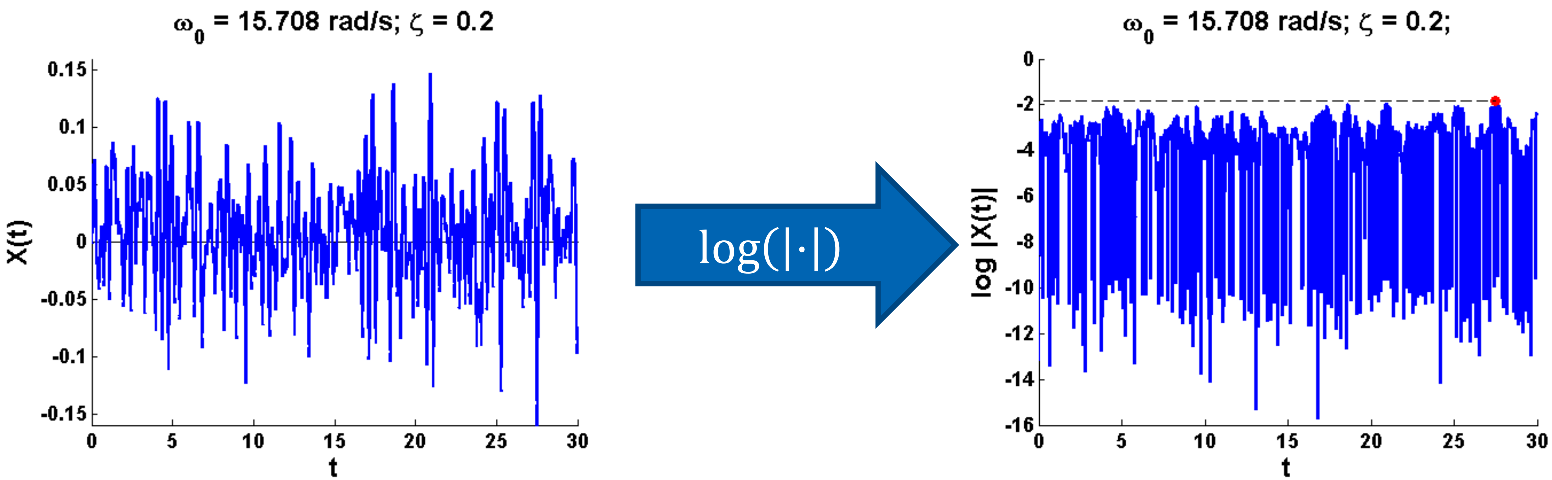
Simulator

- Consider a damped harmonic simulator with random drive

$$\ddot{X}(t) + 2\zeta\omega_0\dot{X}(t) + \omega_0^2 X(t) = W(t)$$

- Ideal simulator

$$F: (\omega_0, \zeta) \mapsto \max_{0 \leq t \leq t^{\mathrm{end}} = 30} \{\log|X(t)|\}$$



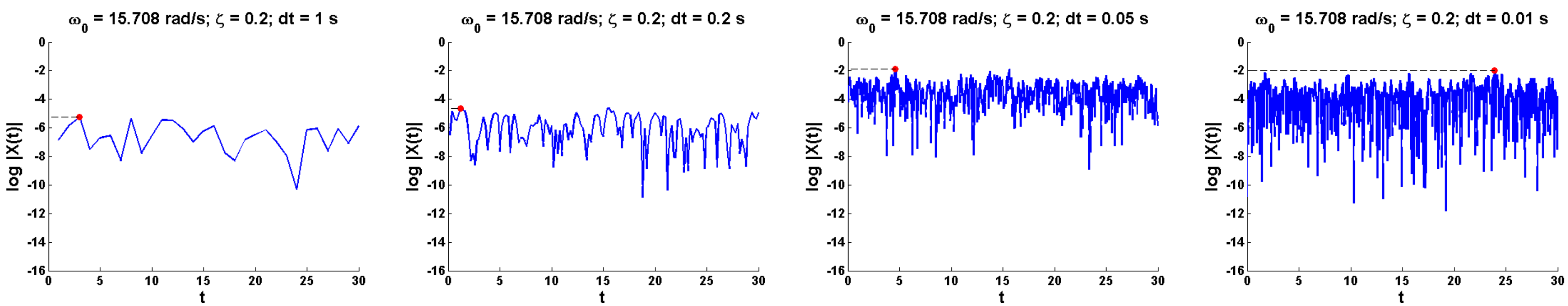
Academic multi-fidelity simulator

- Approximation by an *explicit Exponential Euler Scheme*

$$X(n \cdot dt) \approx \tilde{X}_n$$

- Multi-fidelity simulator

$$f : (\omega_0, \zeta, dt) \mapsto \max_{0 \leq n \leq \left\lceil \frac{t^{\mathrm{end}}}{dt} \right\rceil} \left\{ \log \left| \tilde{X}_n \right| \right\}$$

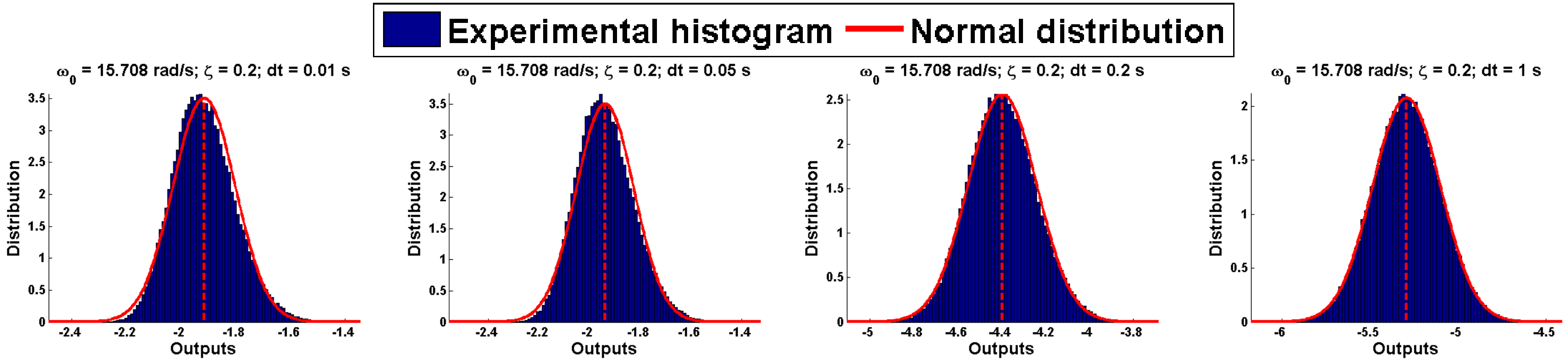


$dt = 1$ s $\quad dt = 0.2$ s $\quad dt = 0.05$ s $\quad dt = 0.01$ s

- [Jentzen and Kloeden, 2009]

Output distributions at a fixed input

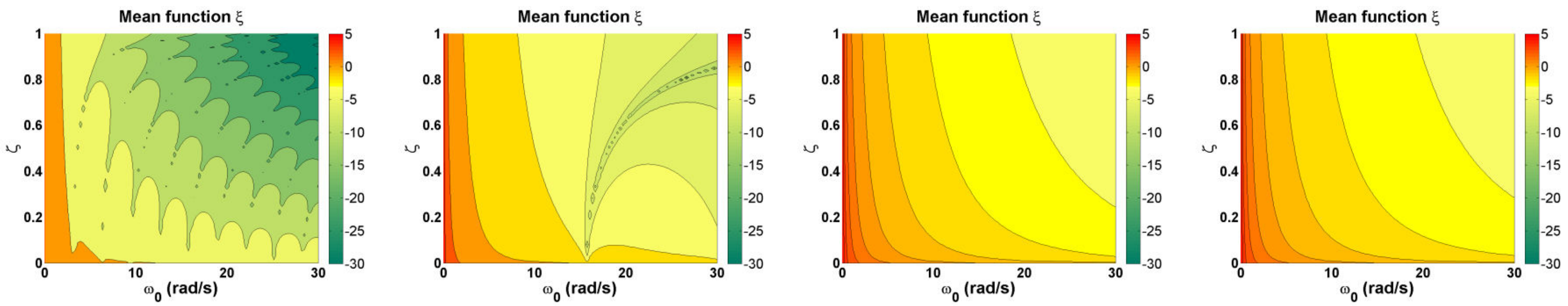
- The output distribution at (ω_0, ζ, dt) can be approximated by a normal distribution
  - 10^5 simulations at $\omega_0 = 15.708\ \mathrm{rad}/s$ and $\zeta = 0.2$



$dt = 1$ s | $dt = 0.2$ s | $dt = 0.05$ s | $dt = 0.01$ s

Mean function

- Mean function ξ
  - 10^5 simulations
  - $0 \leq \omega_0 \leq 30\ \mathrm{rad/s},\ 0 \leq \zeta \leq 1$ - Grid: 100×100



$dt = 1$ s

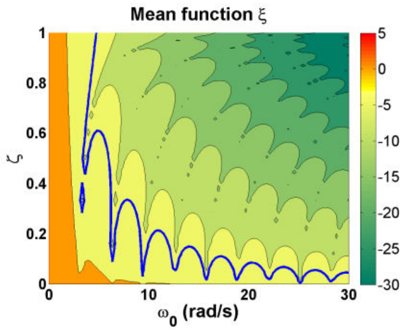
$dt = 0.2$ s

$dt = 0.05$ s

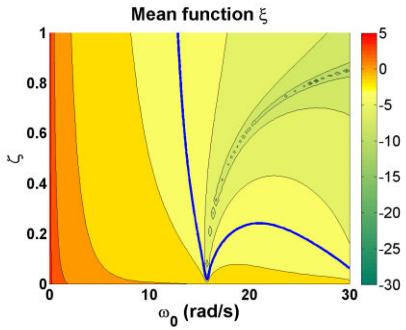
$dt = 0.01$ s

Threshold

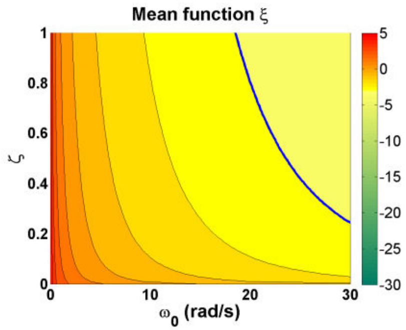
- Critical threshold $z^{crit} = -3$



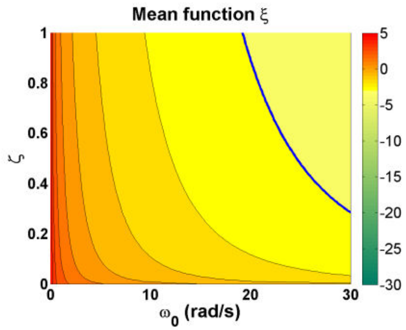
$dt = 1$ s



$dt = 0.2$ s



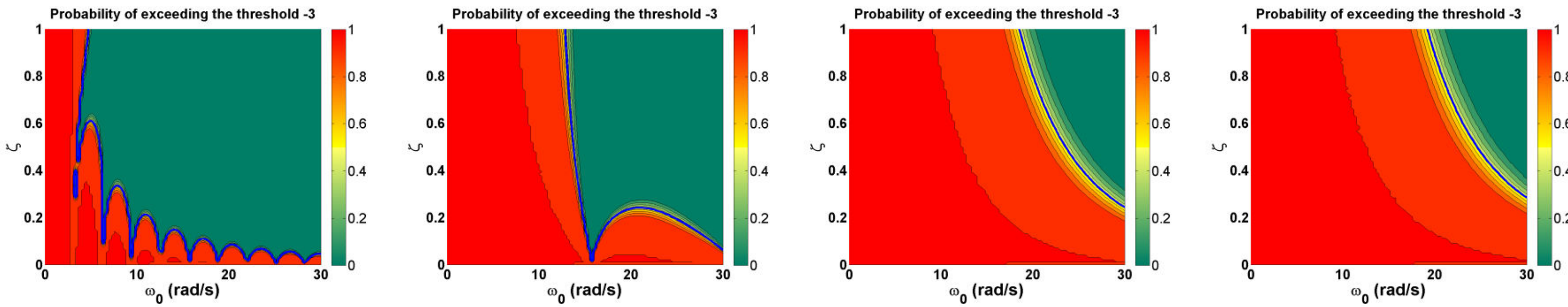
$dt = 0.05$ s



$dt = 0.01$ s

Probability of exceeding the threshold

- True probability of exceeding the threshold $p(\omega_0, \zeta; dt)$

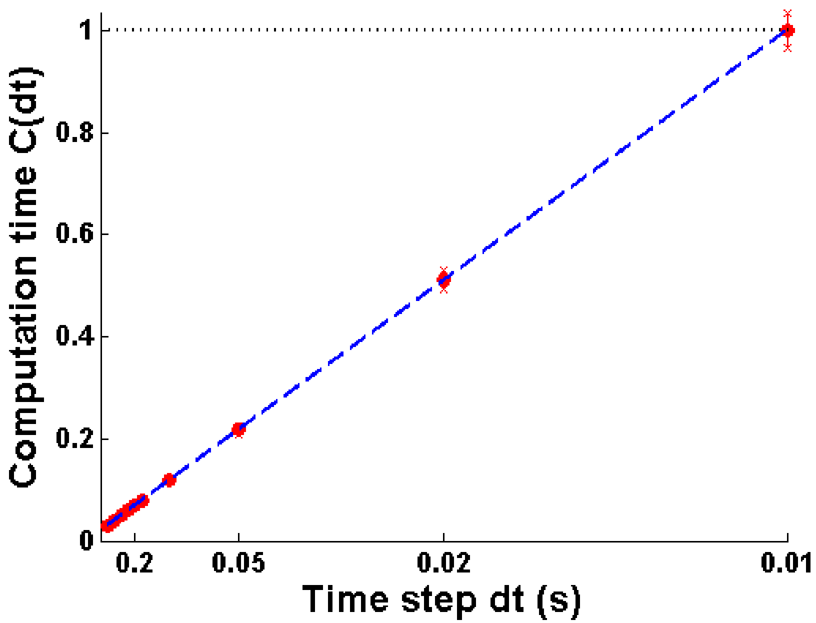


$dt = 1$ s $dt = 0.2$ s $dt = 0.05$ s $dt = 0.01$ s

Computation time

- Computation time $C(dt)$: linear in $1/dt$.

Time step dt	1 s	0.2 s	0.05 s	0.01 s
CPU Time (ms)	0.799 ms	1.85 ms	5.78 ms	26.7 ms
Cost function $C(dt)$	0.030 ¤	0.069 ¤	0.217 ¤	1.00 ¤



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Definition of the problem

- Target: probability of exceeding the threshold at the highest level of fidelity $dt = 0.01$ s

- Initial design: Nested LHS on 5 levels

dt (s)	1.00	0.50	0.33	0.25	0.20	0.17	0.10	0.05	0.02	0.01
Nb. points	180	60	20	10	5	0	0	0	0	0

- [Qian, 2009]

- Initial budget: 9.87 ¤
  1 ¤ = cost for 1 observation at the level $dt = 0.01$ s
  = cost for 1.96 observations at the level $dt = 0.02$ s
  = cost for 33.4 observations at the level $dt = 1$ s
  = …

Comparison between designs of experiments

- Initial budget: 9.87 ¤
  Supplementary budget: 10 ¤
- 6 designs of experiments (DoE)
  - 5 Single level DoE
  - Multi-level DoE

Sequential design	Criterion	Nb. Points Initial design	Nb. Points Final design
Single level ($dt = 0.17\ s$)	SUR	275	275+145 = 420
Single level ($dt = 0.10\ s$)	SUR	275	275 + 85 = 360
Single level ($dt = 0.05\ s$)	SUR	275	275 + 46 = 321
Single level ($dt = 0.02\ s$)	SUR	275	275 + 19 = 294
Single level ($dt = 0.01\ s$)	SUR	275	275 + 10 = 285
Multi-level	MSUR	275	275 + ? = ?

Comparison between designs of experiments

- Initial budget: 9.87 ¤
  Supplementary budget: 10 ¤
- 6 designs of experiments (DoE)
  - 5 Single level DoE
  - Multi-level DoE

- Same model:
  - Same covariance function
  - Hyper-parameters estimated on a large design
  - Fixed hyper-parameters during the sequential designs
- Each DoE: 12 repetitions

Criteria of comparison

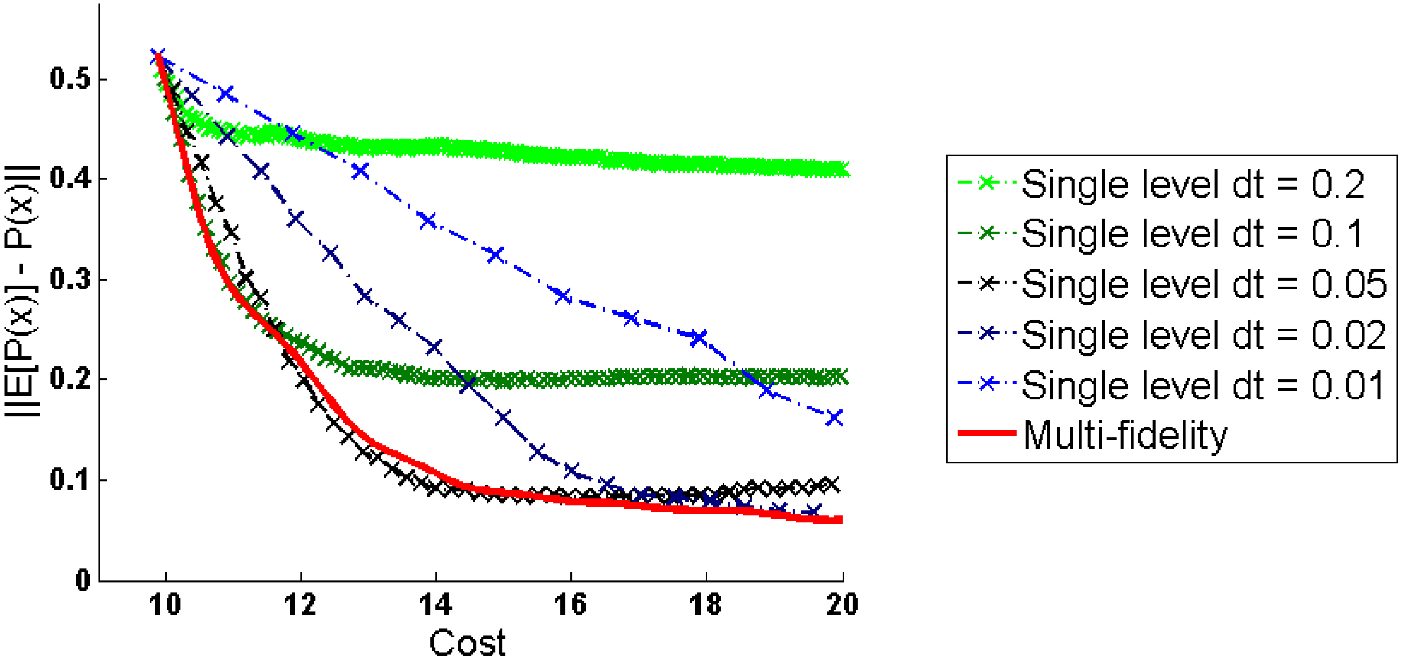
$\mathbb{L}^2$-error on the probability function

$$\sqrt{\int_{[0;30]\times[0;1]} (\hat{p}_n(x,t^{HF}) - p(x,t^{HF}))^2 dx}$$

$$t^{HF} = 0.01\ s$$

Multi-fidelity is better

$\mathbb{L}^2$-error on the probability function



- Low-fidelity levels are biased
  High-fidelity levels are slow
- In this example, multi-fidelity finds the best trade-off

Conclusion

- Goal: sequential design of experiments to estimate probability on stochastic multi-fidelity numerical models

- New SUR criteria to estimate probability of exceeding a threshold on stochastic simulator

- Adaptation to multi-fidelity model ➔ Maximum Speed of Uncertainty Reduction (MSUR)
  - MSUR = (Uncertainty Reduction)/Cost

- Results on an academic example ➔ automatic trade-off between cost and fidelity

Do you have any questions?

Thank you for your attention!

References (1/5): SUR-algorithm

1. Stephen I. N. Kerber. Evaluation of the Ability of Fire Dynamic Simulator to Simulate Positive Pressure Ventilation in the Laboratory and Practical Scenarios. *PhD thesis, University of Maryland*, December 2005. http://hdl.handle.net/1903/3243

2. Emmanuel Vazquez and Julien Bect. A sequential Bayesian algorithm to estimate a probability of failure. *IFAC Proceedings* Volumes, 42(10):546–550, 2009.

3. Clément Chevalier, Julien Bect, David Ginsbourger, Emmanuel Vazquez, Victor Picheny, and Yann Richet. Fast parallel kriging-based stepwise uncertainty reduction with application to the identification of an excursion set. *Technometrics*, 56(4):455–465, 2014. http://dx.doi.org/10.1080/00401706.2013.860918

References (2/5): auto-regressive multi-fidelity

4. Marc C. Kennedy and Antony O'Hagan. Predicting the output from a complex computer code when fast approximations are available. *Biometrika*, 87(1):1–13, 2000. http://biomet.oxfordjournals.org/content/87/1/1.abstract

5. Loïc Le Gratiet and Claire Cannamela. Cokriging-based sequential design strategies using fast cross-validation techniques for multi-fidelity computer codes. *Technometrics*, 57(3):418–427, 2015. http://dx.doi.org/10.1080/00401706.2014.928233

References (3/5): non-stationary multi-fidelity

6. Victor Picheny and David Ginsbourger. A nonstationary space-time Gaussian process model for partially converged simulations. *SIAM/ASA Journal on Uncertainty Quantification*, 1(1):57–78, 2013. http://dx.doi.org/10.1137/120882834

7. Rui Tuo, C. F. Jeff Wu, and Dan Yu. Surrogate modeling of computer experiments with different mesh densities. *Technometrics*, 56(3):372–380, 2014. http://dx.doi.org/10.1080/00401706.2013.842935

References (4/5): multi-fidelity sequential design

8. Deng Huang, Theodore T. Allen, William I. Notz, and R. A. Miller. Sequential kriging optimization using multiple-fidelity evaluations. *Structural and Multidisciplinary Optimization*, 32(5):369–382, 2006. http://dx.doi.org/10.1007/s00158-005-0587-0

9. Loïc Le Gratiet and Claire Cannamela. Cokriging-based sequential design strategies using fast cross-validation techniques for multi-fidelity computer codes. *Technometrics*, 57(3):418–427, 2015. http://dx.doi.org/10.1080/00401706.2014.928233

10. Lawrence D. Phillips and Carlos A. Bana e Costa. Transparent prioritisation, budgeting and resource allocation with multi-criteria decision analysis and decision conferencing. *Annals of Operations Research*, 54(1):51-68, 2007. http://dx.doi.org/10.1007/s10479-007-0183-3

References (5/5): academic example

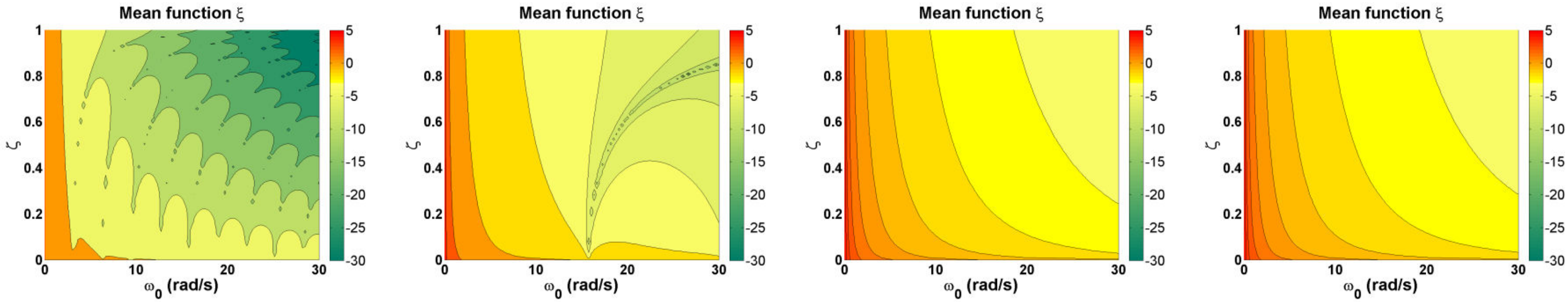
11. Siu-Kui Au and James L. Beck. Estimation of small failure probabilities in high dimensions by subset simulation. *Probabilistic Engineering Mechanics*, 16(4):263–277, 2001. http://www.sciencedirect.com/science/article/pii/S0266892001000194

12. Arnulf Jentzen and Peter E. Kloeden. Overcoming the order barrier in the numerical approximation of stochastic partial differential equations with additive space–time noise. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 465(2102): 649–667, 2009. http://rspa.royalsocietypublishing.org/content/465/2102/649

13. Peter Z. G. Qian. Nested latin hypercube designs. *Biometrika*, 96(4):957–970, 2009. http://biomet.oxfordjournals.org/content/early/2009/09/22/biomet.asp045.abstract

Mean and variance functions

- Mean function ξ and variance function λ



$dt = 1$ s $dt = 0.2$ s $dt = 0.05$ s $dt = 0.01$ s