Design and analysis of multi-level numerical experiments, with application to fire safety

Rémi Stroh, Julien Bect, Séverine Demeyer, Nicolas Fischer, Emmanuel Vazquez

Design and analysis of multi-level numerical experiments, with application to fire safety

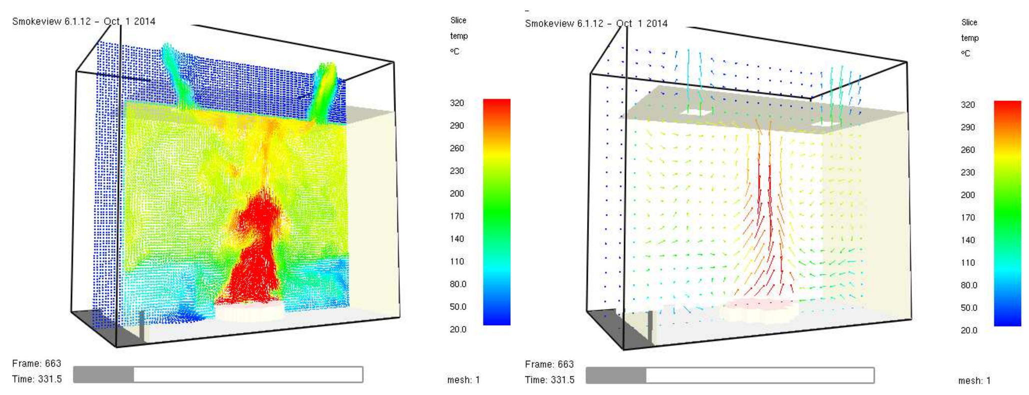
Rémi STROH[a, b], Julien BECT[a], Séverine DEMEYER[b], Nicolas FISCHER[b], Emmanuel VAZQUEZ[a]

[a] Laboratoire des Signaux & Systèmes (L2S), CentraleSupelec / Univ. Paris-Sud / CNRS, Université Paris-Saclay
[b] Laboratoire National de métrologie et d'Éssais (LNE)

Abstract

To assess the conformity of a building in case of fire, fire engineers use numerical simulations. A popular software for fire simulations is *Fire Dynamics Simulator* (FDS). It is based on a finite difference method that takes into account the random behavior of the fire. Thus, the response of FDS is stochastic. The mesh size used in the numerical scheme can be chosen by the user. When the mesh size decreases, the accuracy and the computation time of simulations increase. At low accuracy, one simulation takes a few minutes to run, whereas it can be several weeks at high accuracy.
We consider the problem of estimating the behavior of fine-mesh simulations (high-fidelity), using a combination of fine- and coarse-mesh simulations (low-fidelity). This approach is called multi-fidelity. We propose to extend the Bayesian multi-fidelity models proposed by Picheny and Ginsbourger [2013] and Tuo et al. [2014] to the case of stochastic simulators.

Fire Dynamics Simulator

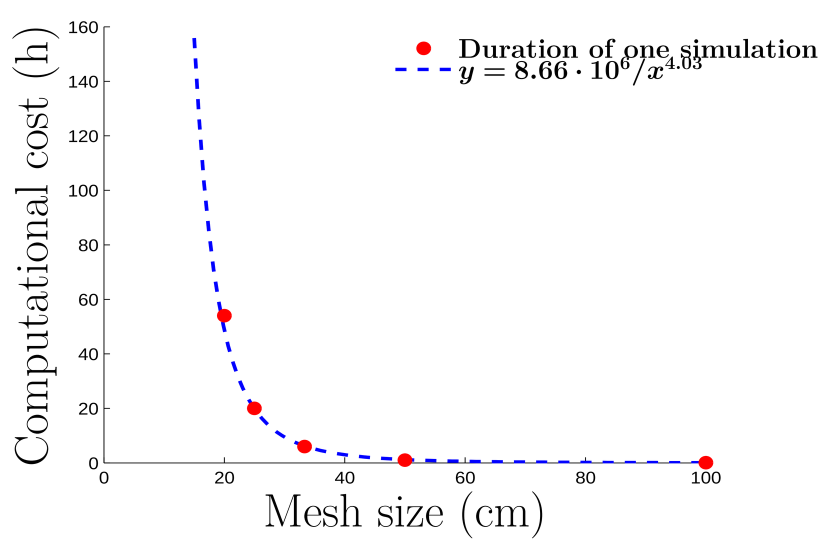


A FDS simulation at 20cm (left: high-fidelity) and 100cm (right: low-fidelity).

FDS has two main characteristics:

- finite difference methods $\Rightarrow$ mesh size can tuned;
- random behavior of fire $\Rightarrow$ stochastic simulator.

Fine mesh	Coarse mesh
Accurate	Imprecise
Expensive	Cheap



Calculation cost (in h) along mesh size (in cm).

Objective: build a (meta-)model of FDS at high-fidelity from low-fidelity results:

- combining results from different levels of accuracy $\Rightarrow$ multi-fidelity;
- using Gaussian process $\Rightarrow$ Bayesian framework.

Proposed model

Data:

- inputs: $(x_i, t_i) \in (\mathbb{X} \times \mathbb{T}) \subset (\mathbb{R}^d \times \mathbb{R}^+)$, where t stands for the mesh size;
- outputs $(z_i) \in \mathbb{R}$.

Likelihood:
stochastic code + independent observations:

$$(z_i)_{1 \le i \le n} \sim \mathcal{N}\left(\xi(x_i, t_i); \operatorname{diag}(\lambda(x_i, t_i))\right). \quad (1)$$

Prior:

1. ξ is a Gaussian process:

$$\xi(x,t) \sim GP\left(m(x,t); k((x,t),(x',t'))\right); \quad (2)$$

2. ξ converges when t tends to 0:

$$\xi_0(x) = \lim_{t \xrightarrow{L^2} 0} \xi(x,t). \quad (3)$$

3. Denote $\varepsilon(x,t) = \xi(x,t) - \xi_0(x)$.
$\left.\begin{array}{l}\xi_0 = \text{ideal level } (t = 0 \text{ cm}) \\ \varepsilon = \text{numerical error}\end{array}\right\}$ independent [Picheny and Ginsbourger, 2013, Tuo et al., 2014],

$$\Rightarrow k((x,t),(x',t')) = k_0(x,x') + k_\varepsilon((x,t),(x',t')). \quad (4)$$

4. the variations of ε along $\mathbb{T}$ are independent:

$$t \ge s \ge r \ge 0 \Rightarrow \varepsilon(x,t) - \varepsilon(x,s) \perp\!\!\!\perp \varepsilon(x,s) - \varepsilon(x,r)$$

$$\Rightarrow k_\varepsilon((x,t),(x',t')) = k_\varepsilon(x,x'; \min\{t,t'\}). \quad (5)$$

5. ξ is stationary along $\mathbb{X}$:

$$\begin{aligned} m(x,t) &= m(t); \\ k_0(x,x') &= k_0(x-x'); \\ k_\varepsilon(x,x'; \min\{t,t'\}) &= k_\varepsilon(x-x'; \min\{t,t'\}); \\ \lambda(x,t) &= \lambda(t); \end{aligned} \quad (6)$$

6. Gaussian prior on $\ln(\lambda(t))_{t\in\mathbb{T}}$:

$$\ln(\lambda(t))_{t\in\mathbb{T}} \sim \mathcal{N}\left(\ln(\lambda_0); s^2 + \varsigma^2 \mathbb{1}_{t=t'}\right), \quad (7)$$

independent of ξ, with $s^2 \gg \varsigma^2$.

Other hypotheses:

- constant mean $m(t) = m \sim \mathcal{U}_{\mathbb{R}}$;
- Matérn covariance for ξ_0: $k_0(x-x') = \mathcal{M}_\nu(x-x')$;
- Separable and Matérn covariance for ε:

$$k_\varepsilon(x-x'; \min\{t,t'\}) = \min\{t,t'\}^L \cdot \mathcal{M}_\nu(x-x');$$

- Parameters λ_0, s^2 and ς^2 are fixed.

Parameter estimation

- maximization of the joint posterior density (MAP) w.r.t. $(\lambda(t))_{t\in\{t_i\}}$, L and all covariance parameters.

Numerical experiments

One numerical experiment on FDS:

- $d = 8$ inputs + the tuning parameter;
- 1 output: maximal temperature at 1,8 m, T^c_{20cm}.

To check efficiency of our model, 4 models are compared:

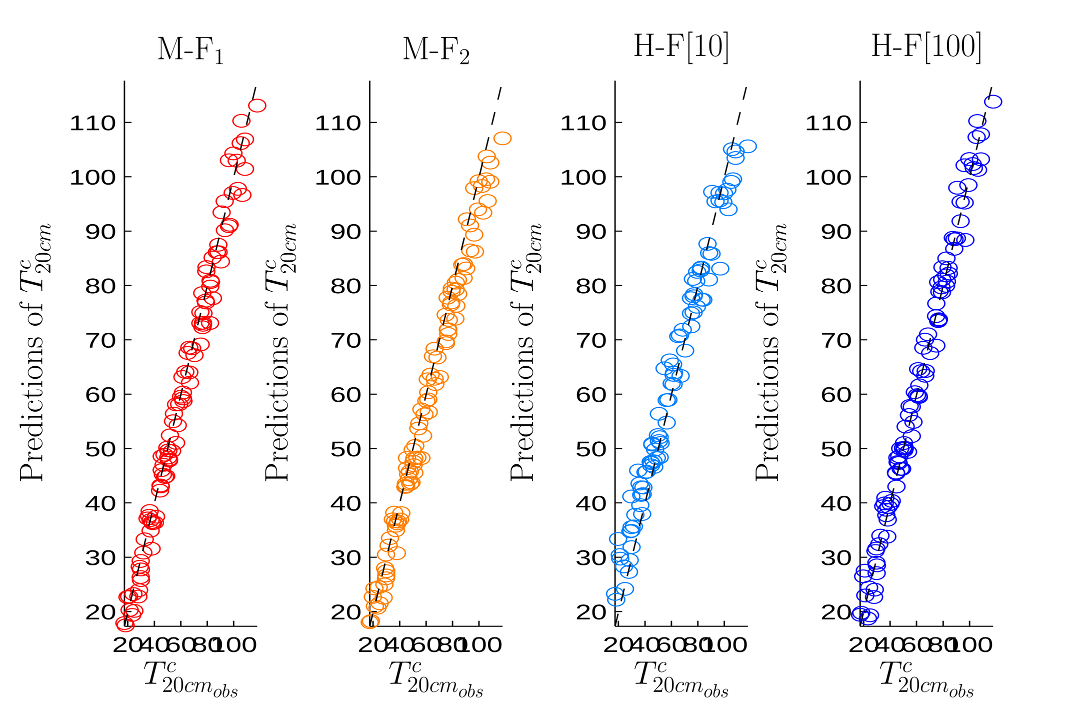
- M-F$_1$: our model (see above);
- M-F$_2$: same as M-F$_1$, but, instead of assumptions 3, 4, and 5, covariance k is a stationary Matérn covariance on $\mathbb{X} \times \mathbb{T}$;
- H-F[10]: a high-fidelity model. Constant mean, Matérn covariance on $\mathbb{X}$, homoscedastic noise;
- H-F[100]: same as H-F[10], but with more points. This model serves us as reference.

The following designs are used:

		Learning data					Validation
Model	Cost	100cm	50cm	33cm	25cm	20cm	20cm
M-F$_1$/M-F$_2$	1	270	90	30	10	0	100
H-F[10]	≈ 1.1	0	0	0	0	10	90
H-F[100]	≈ 11	0	0	0	0	100	LOO

(LOO = Leave One Out)

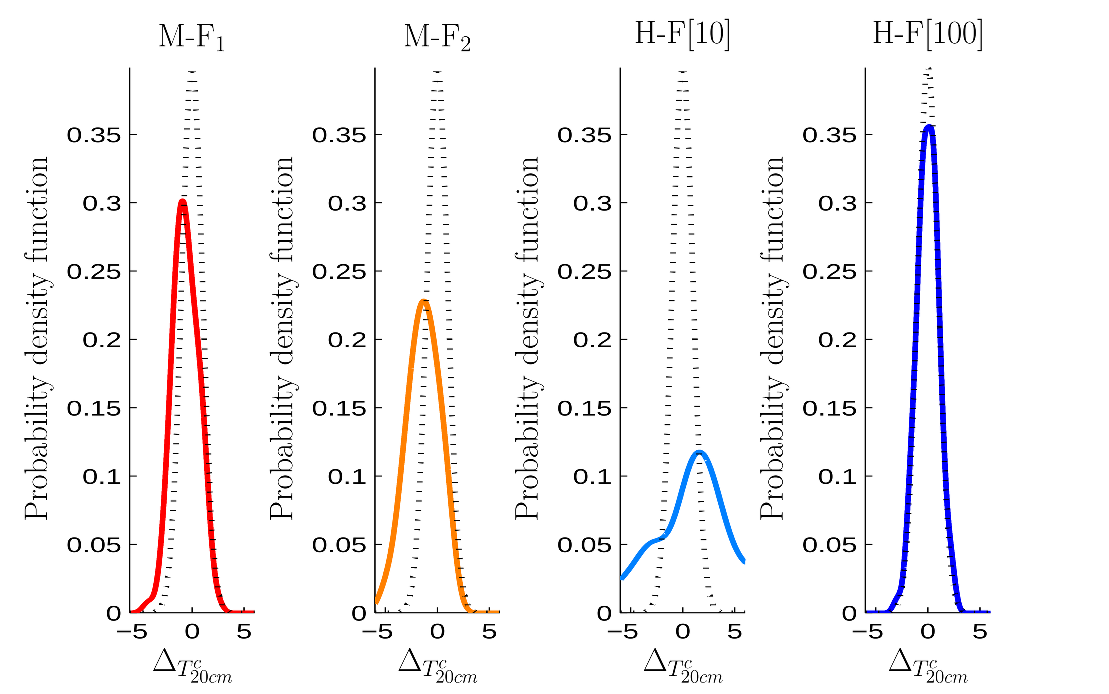
Model validation



Predictions (posterior means) versus observations.

Models are validated by comparing:

- predictions (posterior mean) with observations,
- distributions of normalized residual with the standard normal distribution.



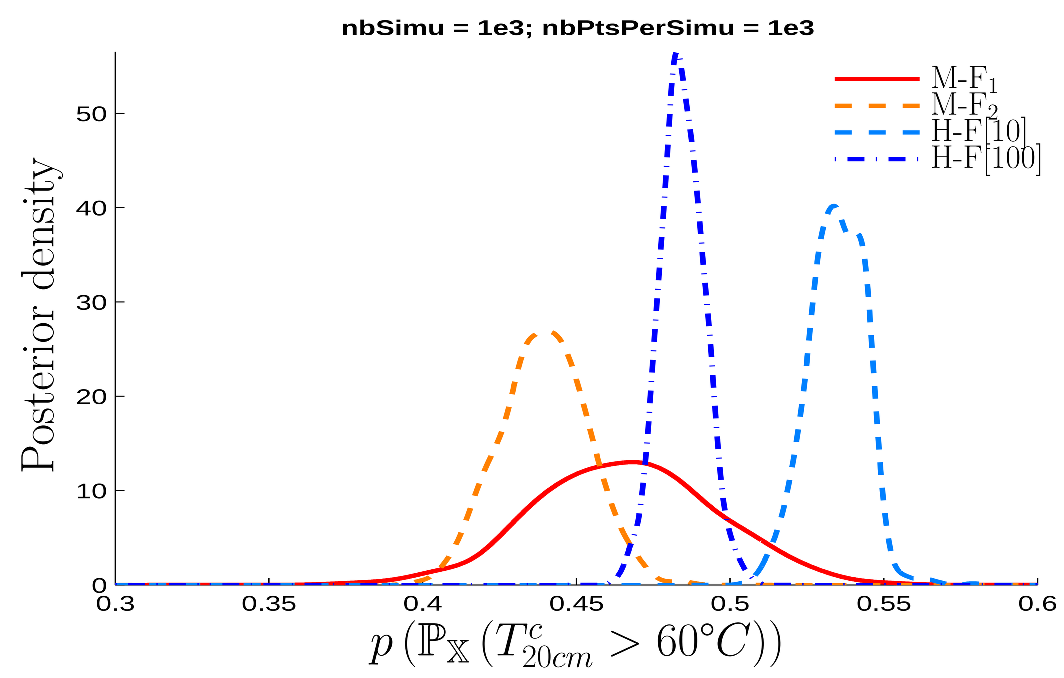
Probability density function of normalized residuals $\Delta_{T^c_{20cm}}$ (colored lines) versus normal distribution (dashed line).

Quality of prediction:

- H-F[10] has bad predictions;
- M-F$_1$ and M-F$_2$ give similar quality of predictions;
- H-F[100] is the best, but its design is 11 times more costly.

Probability to exceed a threshold

Suppose $\mathbb{P}_\mathbb{X}$ a probability distribution on inputs.



Estimation of probability for T^c_{20cm} to exceed $60°C$.

Curves of posterior distributions: 1000 conditional simulations $\times$ 5000 points along $\mathbb{P}_\mathbb{X}$.
By comparison with H-F[100] posterior density:

- H-F[10] and M-F$_2$ have small variance, but their distributions do not agree the posterior distribution of H-F[100];
- M-F$_1$ has a larger variance, but its posterior density maximum is inter the posterior distribution of H-F[100];

$\Rightarrow$ M-F$_1$ provides a better quantification of uncertainty

Conclusion

- Contribution
  - ➭ A Bayesian model for multi-fidelity stochastic simulators has been proposed.
  - ➭ Our model has been shown to provide, in a numerical experiment with FDS, a good quantification of uncertainty on predictions.
- Future work
  - ➭ fully Bayesian inference for hyper-parameters,
  - ➭ sequential design of experiments.

References

Marc C Kennedy and Anthony O'Hagan. Predicting the output from a complex computer code when fast approximations are available. *Biometrika*, 87(1):1–13, 2000.

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.

Rui Tuo, C.F. Jeff Wu, and Dan Yu. Surrogate modeling of computer experiments with different mesh densities. *Technometrics*, 56(3):372–380, 2014.