Optimizing
with realistic simulators and kriging

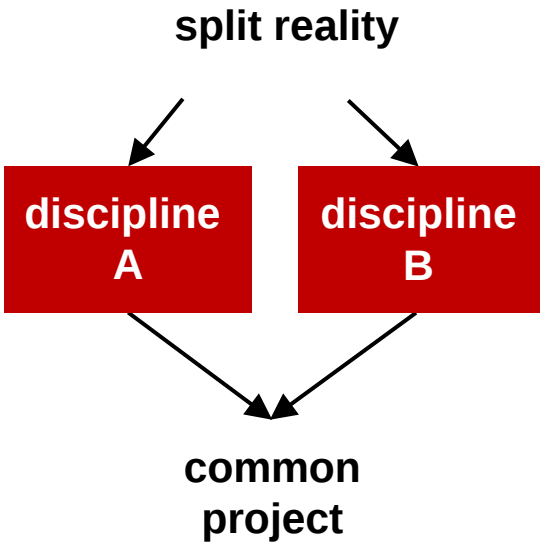
Rodolphe Le Riche
www.emse.fr/~leriche
CNRS and Ecole des Mines de St-Etienne

UTC / Labex MS2T, Feb. 2014

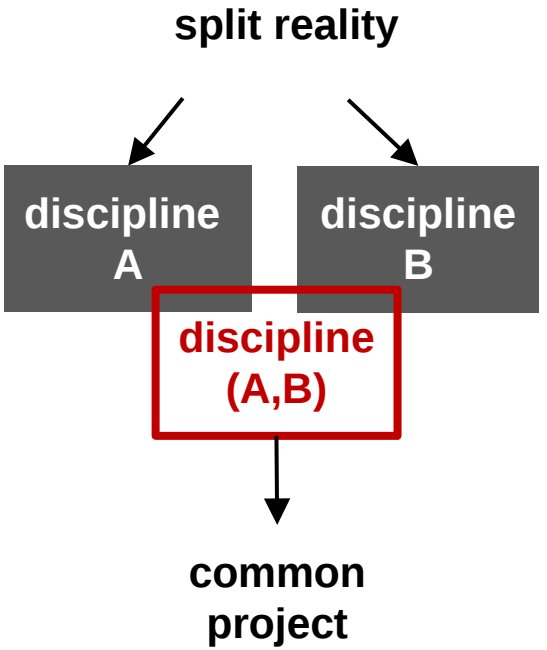
Physical and statistical models for optimization : towards interdisciplinarity

Optimization from numerical simulators is an example where physics and statistics need to collaborate in a pluri and even interdisciplinary effort.

multi



inter



B. Guy et R. Le Riche, *Articulation des rationalités cartésienne et complexe dans les projets associant plusieurs disciplines*, 3ièmes Ateliers sur la Contradiction, St-Etienne, Avril 2013 (in French)

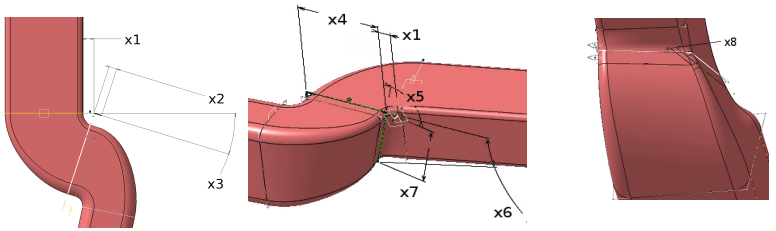
optimization using engineering simulations as a dialog between a physicist / engineer and a statistician

(technical and epistemological content)

Optimizing from engineering simulations

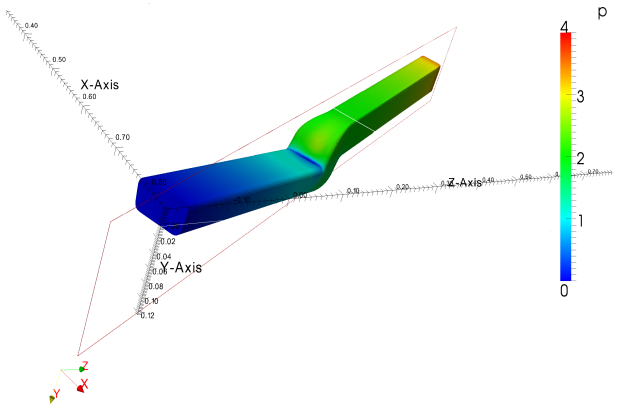
Knowledge about a physical model stored in a simulator with inputs and outputs

x



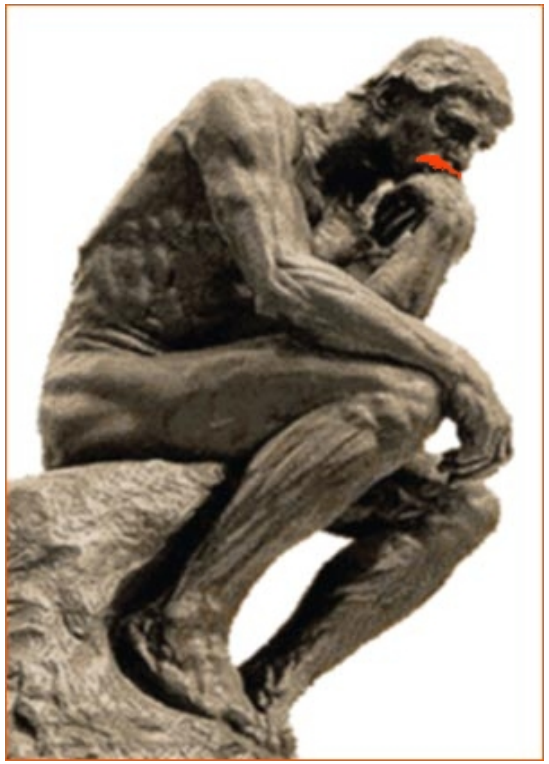
Expl : dimensions of a pipe

Simulation
software
(FE, FVol, BE, ...)
[sec to hours]



Expl : pressure field

The virtual prototyping idea



The physicist / engineer

*The simulation seems fairly realistic. Let's use it to **decide** what is an optimal configuration.*

Mathematical formulation of the optimization

A decision (e.g., a design decision) is **formulated** as an optimization problem :

Mathematical goal : $\min_{x \in S \subset \mathbb{R}^n} f(x)$

f(.), the cost function (pressure drop, masse, constraint violation, distance to goal, cost, risk, ...).

Constraints, $g(x) \leq 0$, are not explicitely discussed in this talk. As a patch, you may assume that

$$\min_{\substack{x \in S \subset \mathbb{R}^n \\ g(x) \leq 0}} f(x) \quad \rightarrow \quad \min_{x \in S \subset \mathbb{R}^n} f(x) + p \times max^2(0, g(x))$$

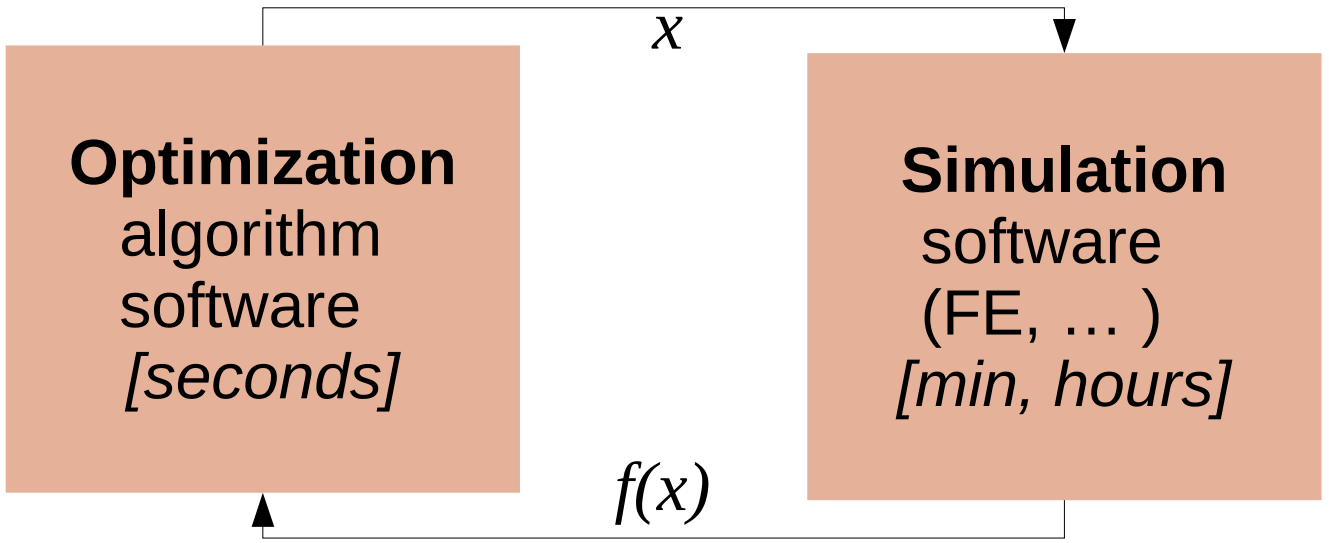
p , a vector of penalty positive scalars.

Constraints satisfaction problem : A. Chaudhuri, R. Le Riche and M. Meunier, *Estimating feasibility using multiple surrogates and ROC curves*, 54th AIAA SDM Conference, Boston, USA, 8-11 April 2013.

Automatic use of the simulator

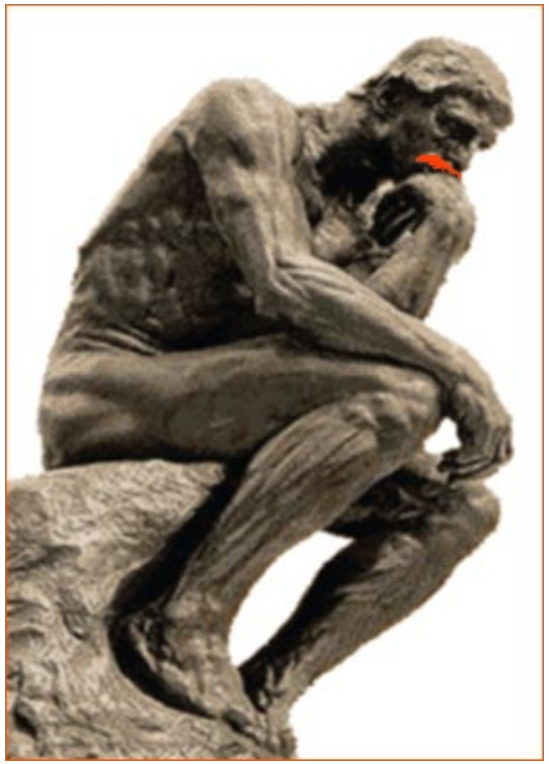
The physicist / engineer : $f(x)$ is not known analytically. Let's try M points and keep the best one, $\arg\min_{i=1,M} f\left(x^i\right)$

An optimization program will automatically call the simulator.



Communication between programs by file, pipe, messages.

By the way, what strategy for the optimization ?



1 call to f takes 1 min.
I have 8 variables, x_i.
I will discretize each variable into 10 possible values and make a grid. That is
$10 \times 10 \times \ldots \times 10 = 10^8$ simulations, i.e.,
… 190 years of calculation !

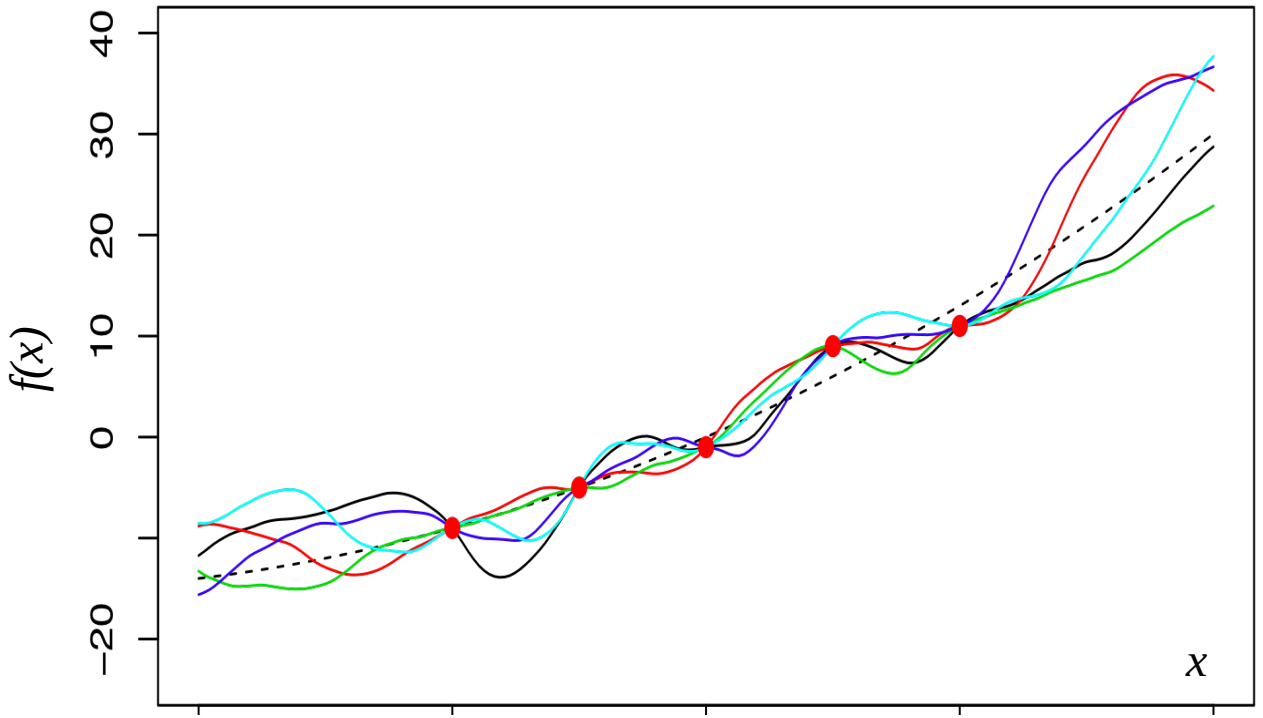
Grids are too expensive, but I will try random points. In 95 % of the cases, I can wait 10h (600 calls to f), I will know the optimum with an accuracy on each variable better than [1] … 50 % of the total range of each variable !

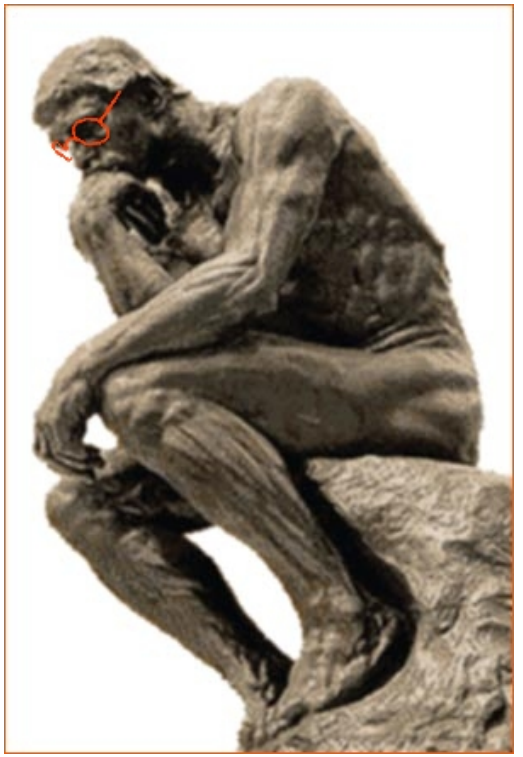
I need a statistician.

The simulation time is the bottleneck. Even 1 min.

[1] Δ , the accuracy, and normalized variables between 0 and 1, then $1-\left(1-\Delta^n\right)^M$ = Confidence

This looks easy ! There are M observations x^i, $f(x^i)$. They are spatially correlated. We can use a Gaussian process indexed by x and conditioned by the observations to guess values of f at unexplored points x





The statistician

!!! only a 1D representation (complexity of dimension is lost in the drawing)
Red bullets = observations, dashed line = true function = *f(x)*, coloured lines = possible functions based on the observations.

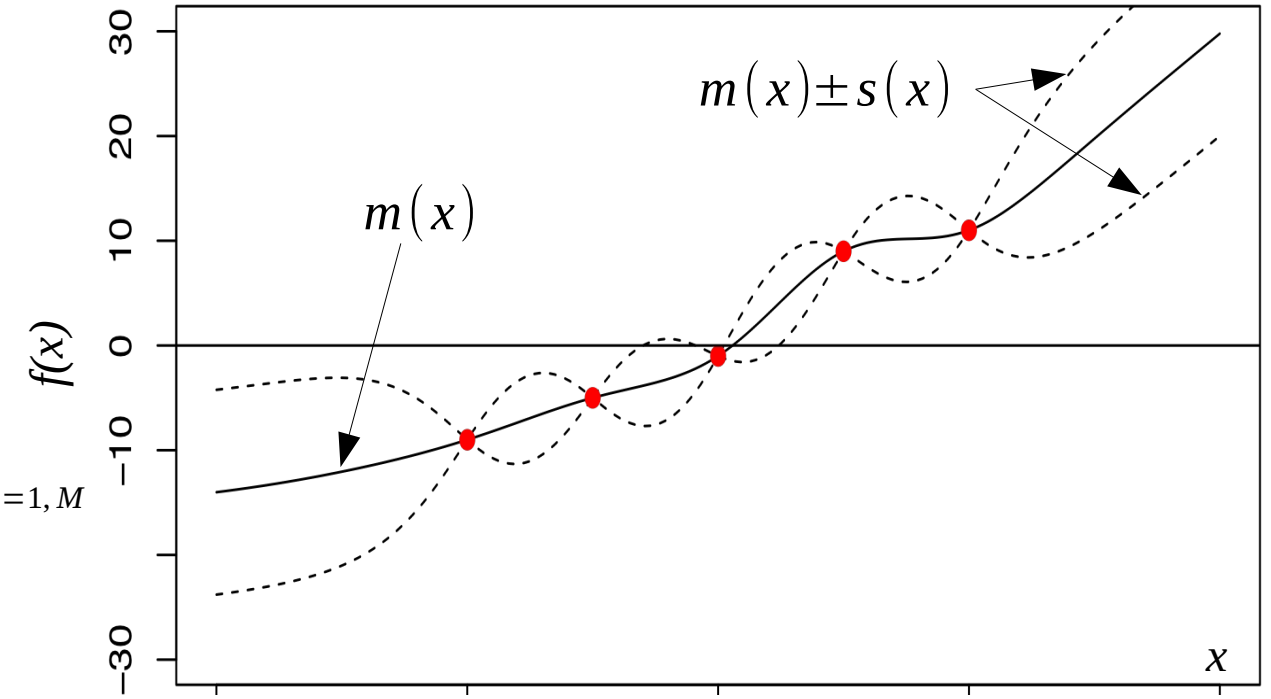
Introduction to kriging (cont.)

Statistical model of $f(x)$:

$$F(x) \sim N\left(m(x), s^2(x)\right)$$

and F is correlated in space,

$$\boldsymbol{c}(x) = \left[Cov\left(F(x), F(x^i)\right)\right]_{i=1,M}$$
$$\boldsymbol{C} = \left[Cov\left(F(x^i), F(x^j)\right)\right]_{i,j}$$



Kriging average : $m(x) = \mu + \boldsymbol{c}^{\boldsymbol{T}}(x)\boldsymbol{C}^{-1}(\boldsymbol{f} - \mu\,\boldsymbol{1})$

Kriging variance : $s^2(x) = \sigma^2 - \boldsymbol{c}^T(x)\boldsymbol{C}^{-1}\boldsymbol{c}(x)$

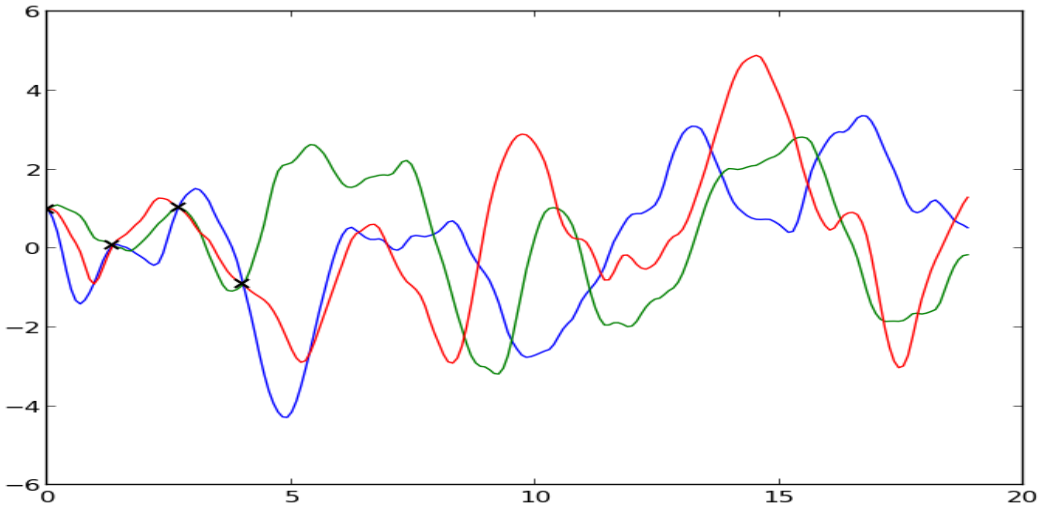
Important : choice of the kernel (stationary)

$$Cov\left(F(x), F(x')\right) = \text{a function of } |x - x'| \text{ and parameters } \theta \text{ (length scale)}$$

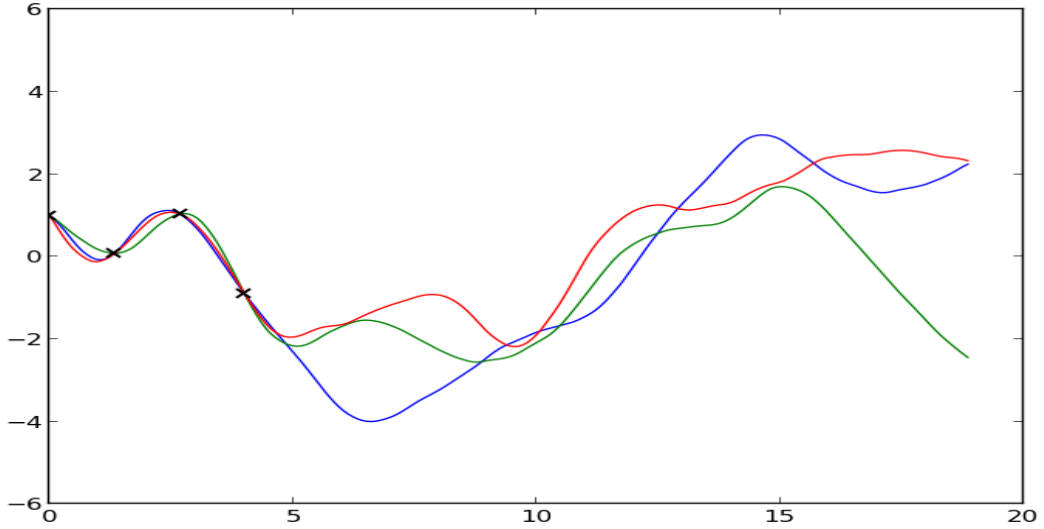
Not all functions are kernel functions.

[see Rasmussen & Williams, *GPML*, 2006 for general explanations, see Mohammadi, Le Riche, Touboul and Bay, *On regularization techniques in statistical learning by GP*, NICST'2013]

From simulator to kernel design



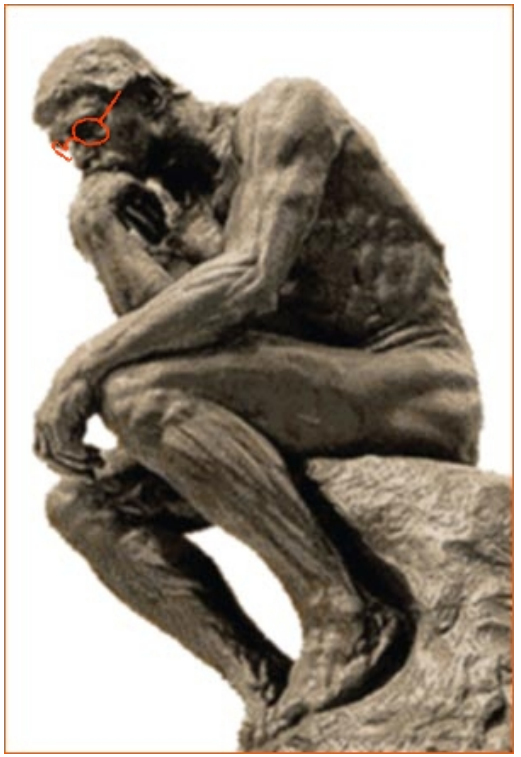
Matern 5/2 kernels, $\sigma^2=4$, **length scale = 1**



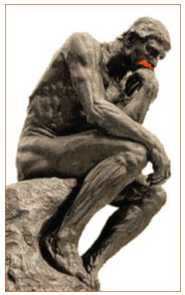
Matern 5/2 kernels, $\sigma^2=4$, **length scale = 3**

My approach is general, yet its prediction properties are sensitive to the kernel choice... and there are so many possible kernels.

I need a physicist / engineer.



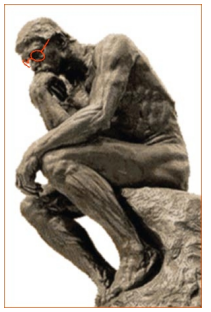
From simulator to kernel design (cont.)

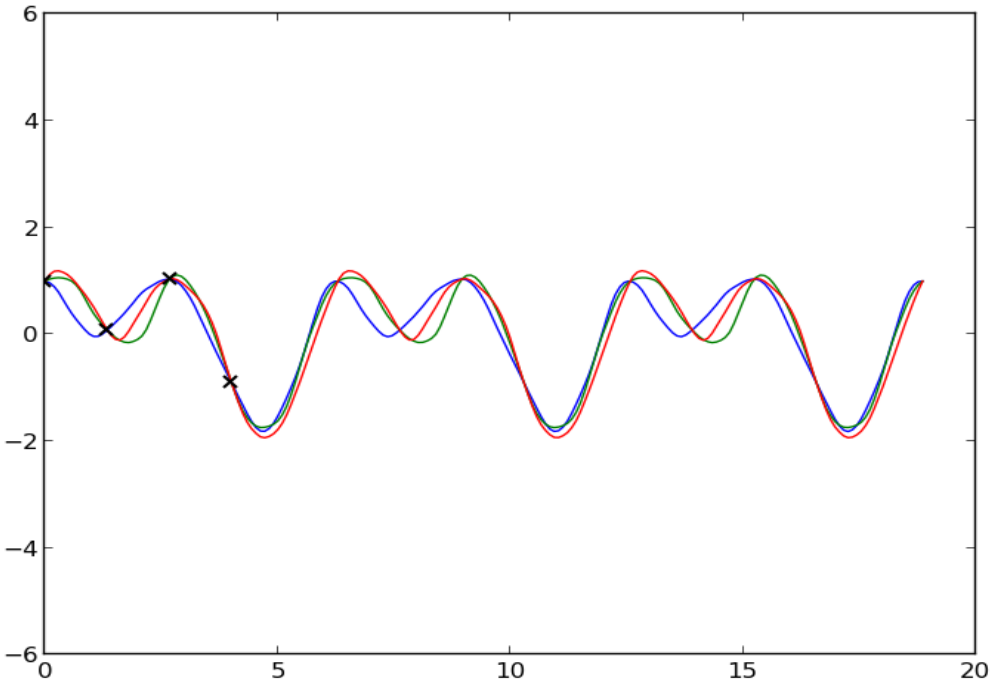


f(x) is periodic (example)

then the kernel could be of the form [2]

$$Cov\left(F\left(x\right),F\left(x'\right)\right)=\sigma^{2}\exp\left(\frac{-1+\cos\left(x-x'\right)}{\theta^{2}}\right)$$





The periodicity knowledge allows to considerably reduce statistical uncertainties.

Other typical expert knowledge : derivatives, symmetries, rotations, PDE's, correlated multi-fidelity simulators, previous designs, ...

Kernel design is an active research domain.

[2] N. Durrande, R. Le Riche and S. Avril, *MRI sequence denoising using Gaussian processes*, Euromech 534 colloquium on Advanced experimental approaches and inverse problems in tissue biomechanics, May 2012.
N. Durrande, J. Hensman, M. Rattray, N. D. Lawrence, *Gaussian process models for periodicity detection*, submitted to JRSSb in 2013.

Epistemic comment

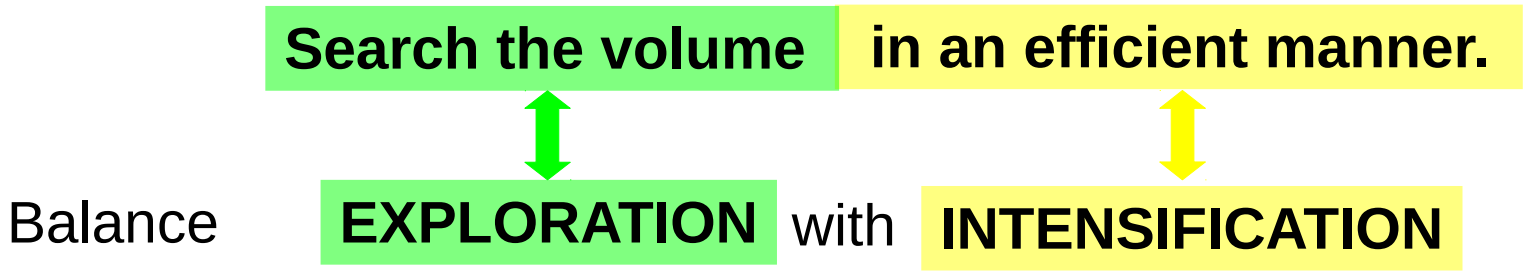
Practical optimization problems use numerical simulators.

In general (no specific mathematical property known such as convexity, monotony, ...), they are difficult.

They should be approached in an interdisciplinary effort (metamodels and simulation) which is the only one that makes the best use of all available knowledge.

Seems obvious, but worth being stated as scientists work in communities...

Kriging and optimization



- **We will deterministically fill the design space in an efficient order.**
- **Other global search principles**
  - **Stochastic searches** : (pseudo)-randomly sample the design space S, use probabilities to intensify search in known high performance regions and sometimes explore unknown regions.
  - (pseudo-)**Randomly restart** local searches.
  - (and mix the above principles)

A state-of-the-art global optimization algorithm using metamodels : EGO

(D.R. Jones et al., JOGO, 1998)

EGO = Efficient Global Optimization = use a « kriging » metamodel to define the Expected Improvement (EI) criterion. Maximize EI to creates new x's to simulate.

EGO deterministically creates a series of design points that ultimately would fill S.

Some opensource implementations :

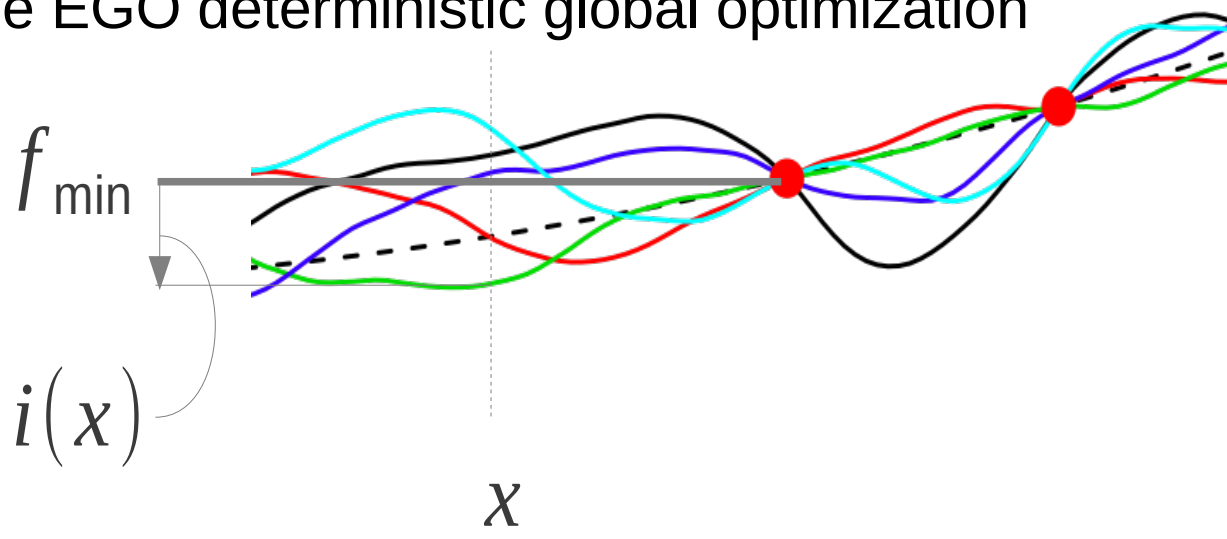
- DiceOptim in R (EMSE & Bern Univ.)
- Krisp in Scilab (Riga Techn. Univ & EMSE)
- STK: a Small (Matlab/GNU Octave) Toolbox for Kriging, (Supelec)

(one point-) Expected improvement

A natural measure of progress : the improvement,

$$I(x) = \left[f_{\min} - F(x) \right]^{+} \mid F(\boldsymbol{x}) = f(\boldsymbol{x}) \quad , \quad \text{where } [.]^{+} \equiv max(0,.)$$

- The expected improvement is known analytically.
- It is a parameter free measure of the exploration-intensification compromise.
- Its maximization defines the EGO deterministic global optimization algorithm.

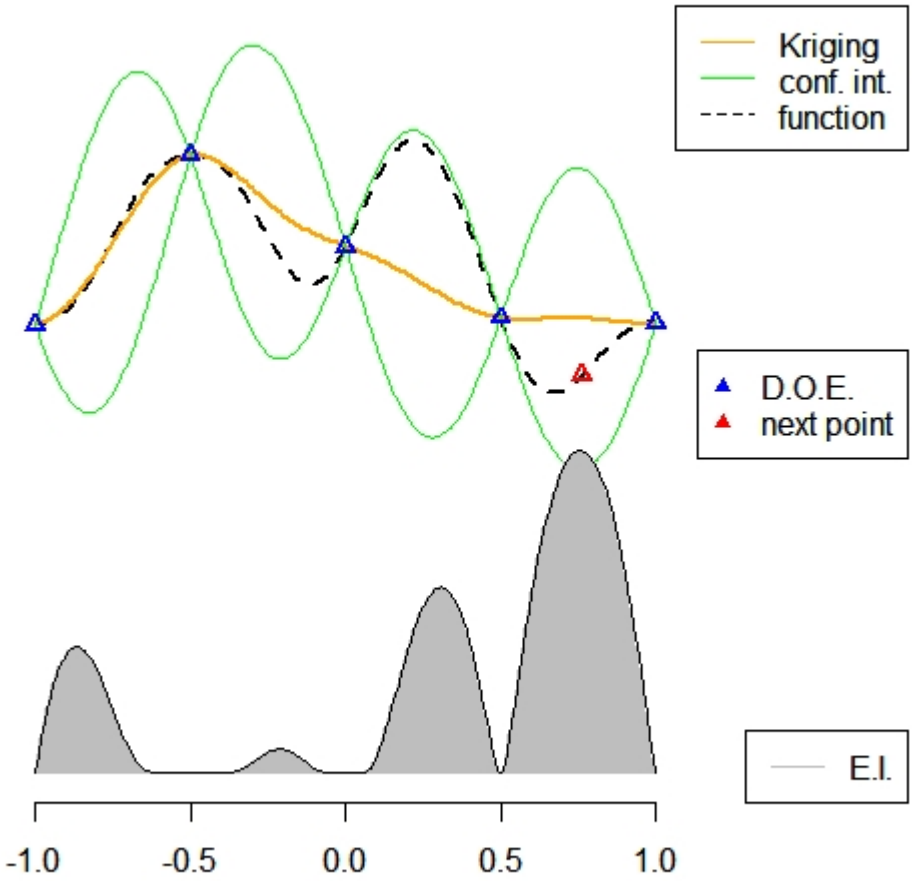


$$EI(x) = s(x) \times \left(u(x)\Phi(u(x)) + \varphi(u(x)) \right) \quad , \quad \text{where } u(x) = \frac{f_{\min} - m_k(x)}{s(x)}$$

One EGO iteration

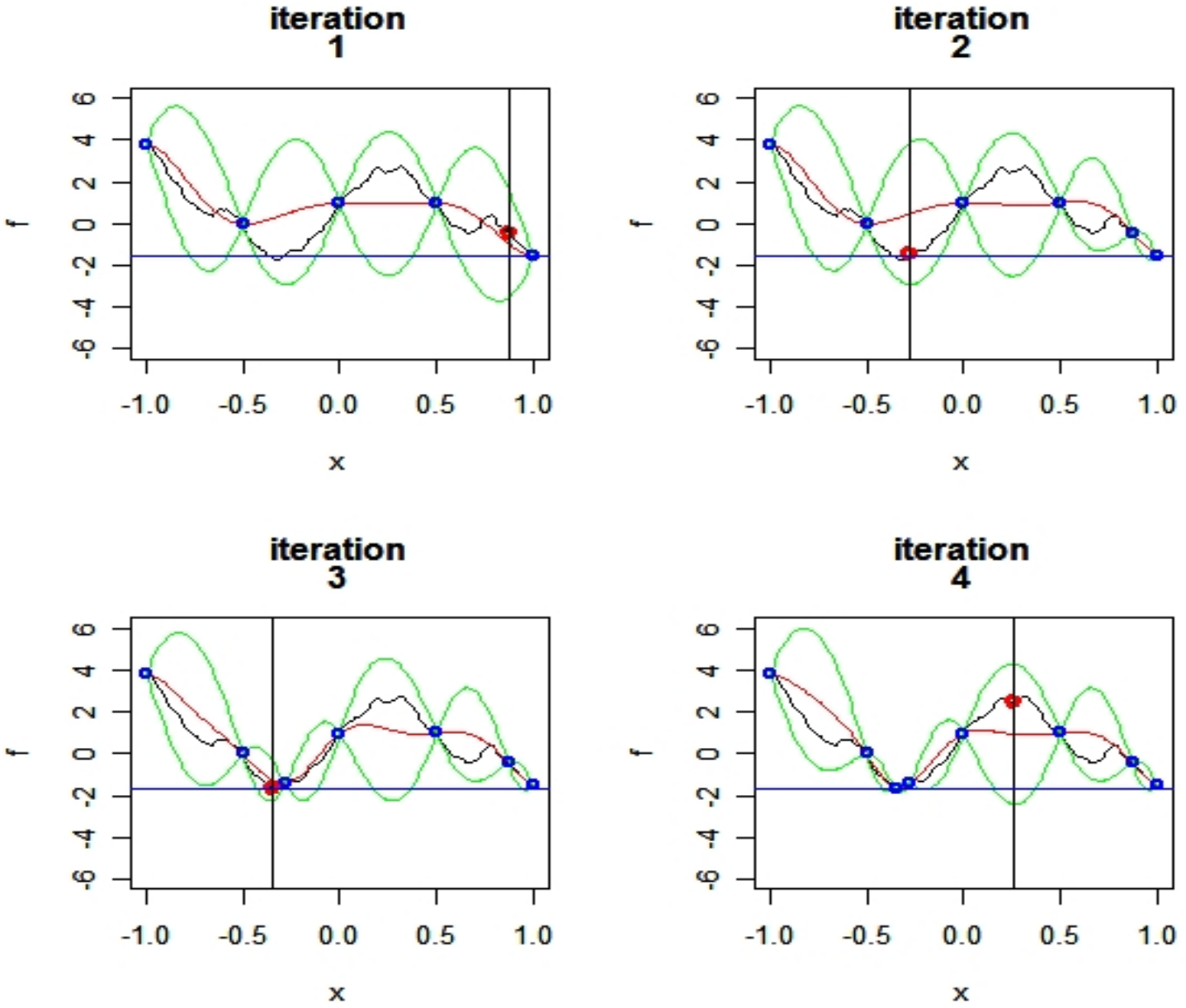
At each iteration, EGO adds to the t known points the one that maximizes EI,

$$x^{t+1} = arg\,max_x\, EI(x)$$



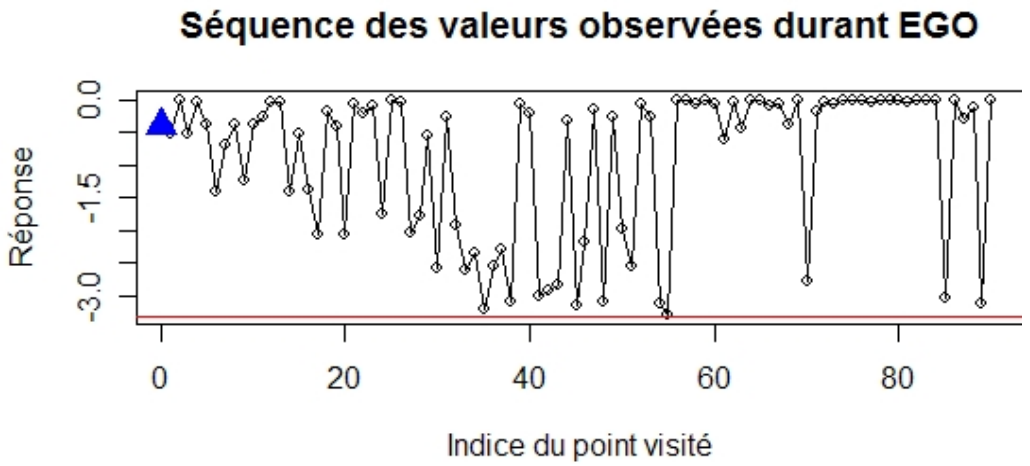
then, the kriging model is updated ...

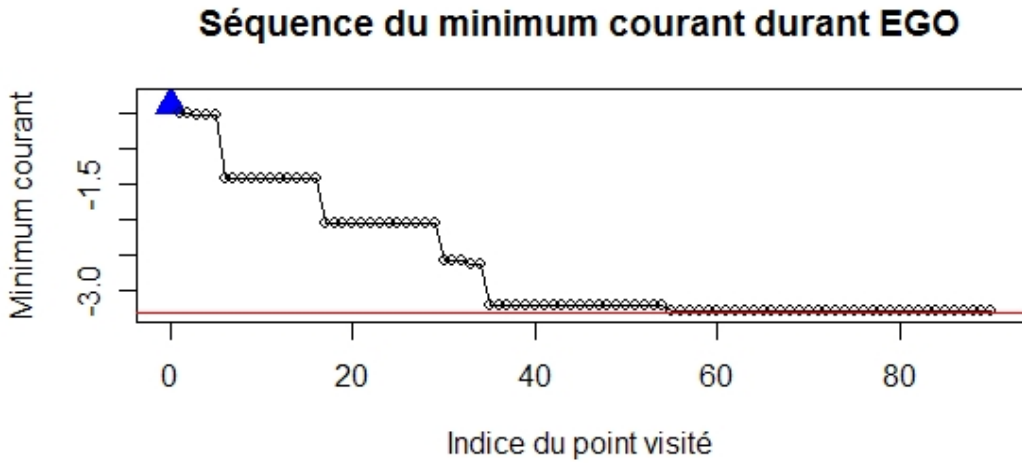
EGO : example

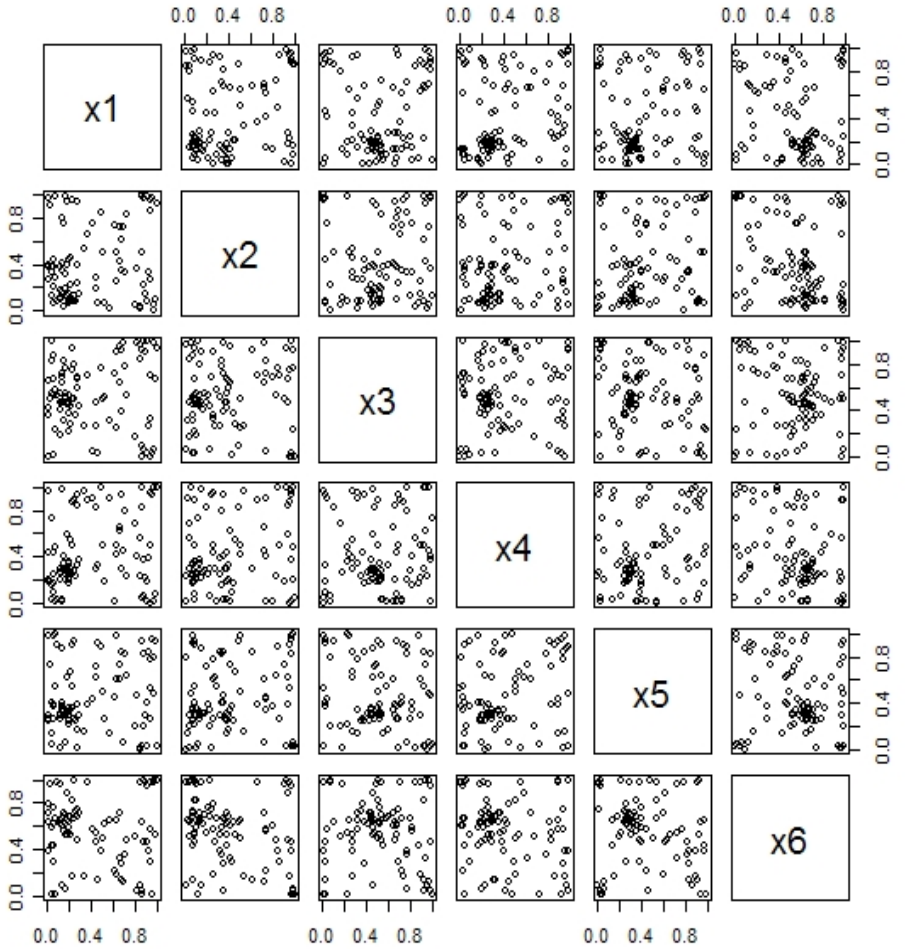

iteration
1
iteration
2
iteration
3
iteration
4
f
x
-6
-4
-2
0
2
4
6
-1.0
-0.5
0.0
0.5
1.0

EGO : exemple en 6D

Fonction de Hartman, $f(x^*)=-3.32$, 10 points dans le plan d'expérience initial.



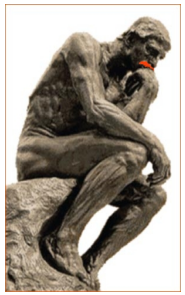




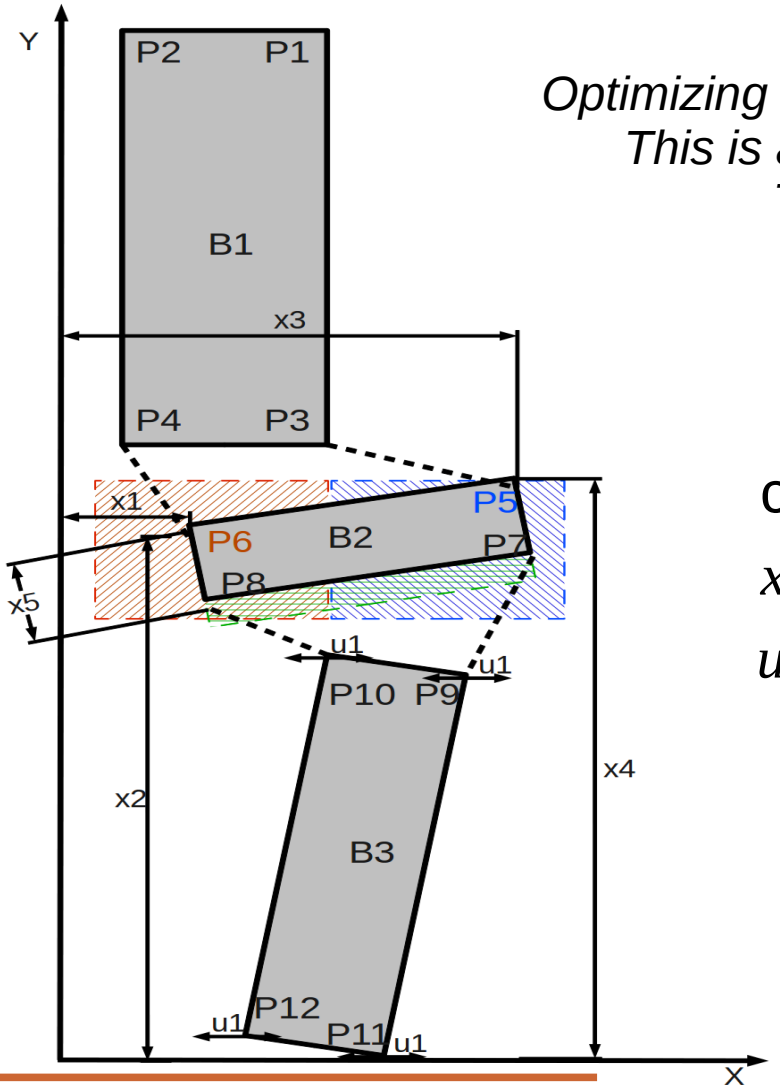
(DiceOptim, D. Ginsbourger, 2009)

Accounting for uncertainties in the optimization

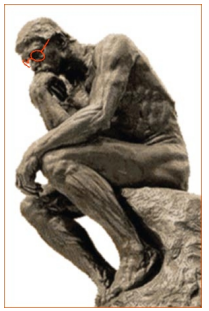
Duct design with uncertain boundary conditions



There is this tricky situation I keep running into.
I am designing a structure, and the boundary conditions are not well controlled …



Optimizing with uncertainties.
This is a difficult problem.
Thanks for asking.

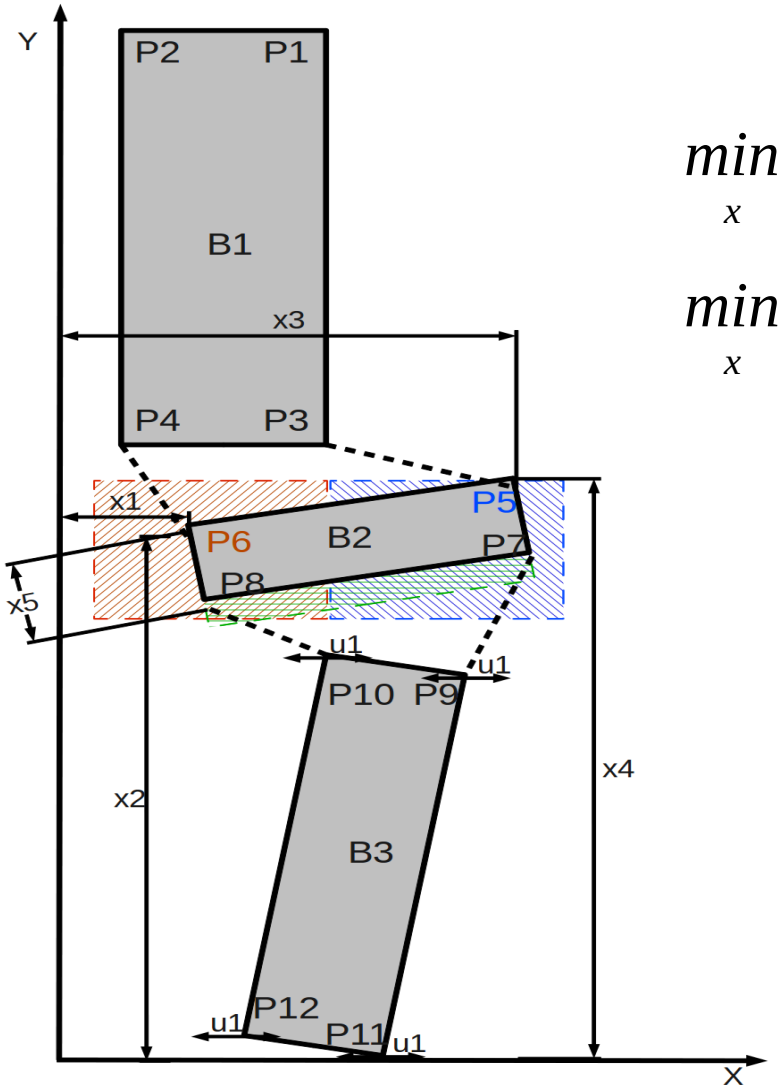


conditioner duct design

x_1 ,..., x_5 : designs variables

u_1 : random noise (Gaussian)
(manufacturing tolerance)

Duct design with uncertain boundary conditions
Problem formulation



$$\min_x E_U\left(\text{normal flow Std Dev @ P9P10}\right)$$

$$\min_x E_U\left(\text{pressure loss P1P2-P11P12}\right)$$

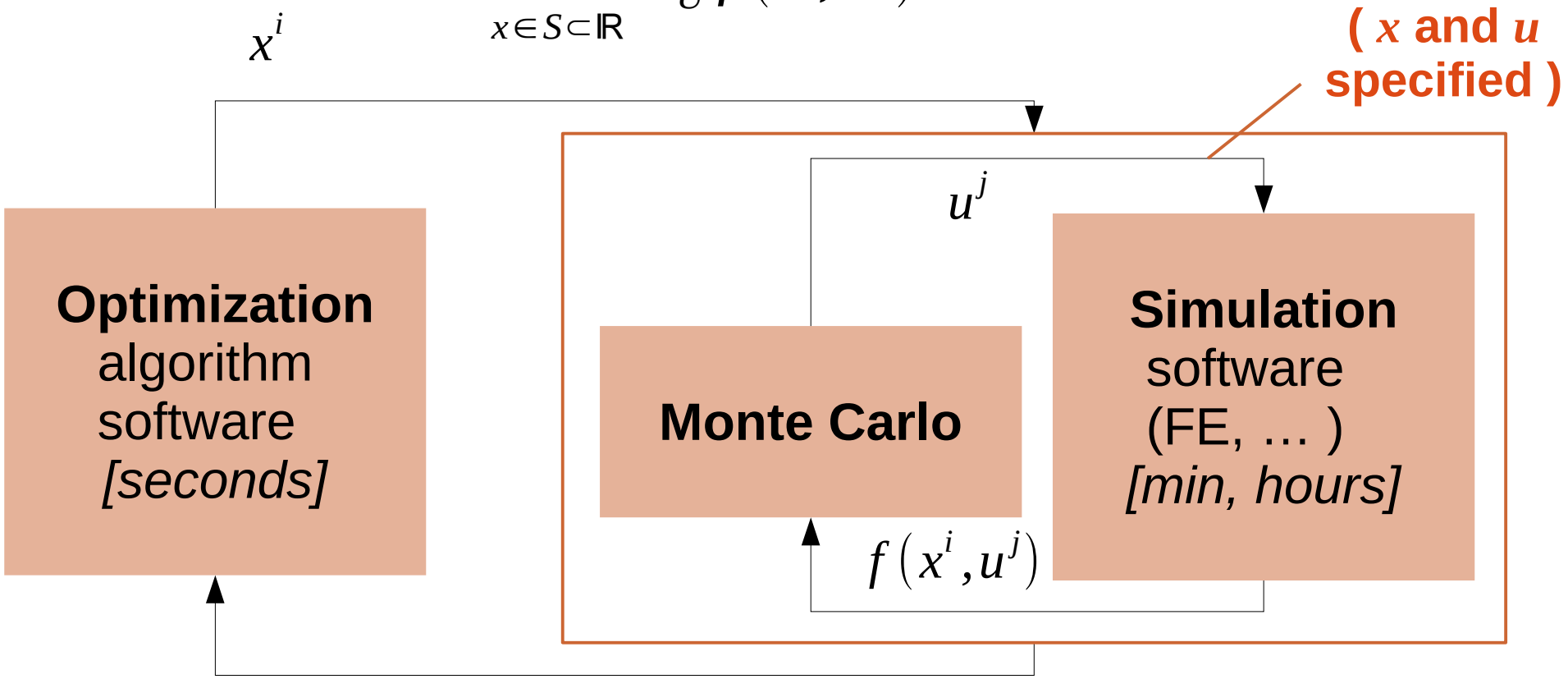
$$\min_x E_U\left(f\left(x,U\right)\right)$$

2 difficult tasks put together : optimization * uncertainty propagation (e.g., Monte Carlo). Inherently 2 imbricated loops.

Cf. J. Janusevskis and R. Le Riche, *Robust optimization of a 2D air conditioning duct using kriging*, technical report hal-00566285, feb. 2011.

Example of naive optimization with uncertainties

$$\min_{x \in S \subset \mathbb{R}} E_U f(x, U)$$



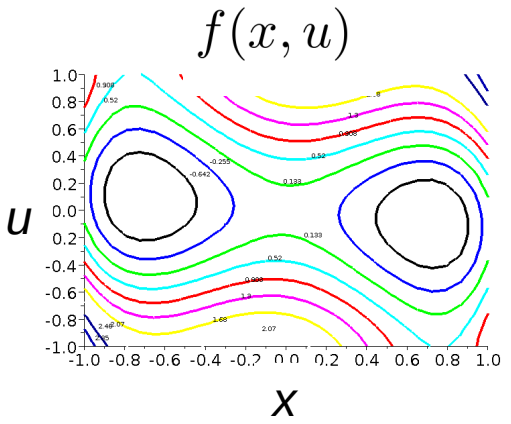
$$E_U f(x^i, U) \approx \frac{1}{N_{MC}} \sum_{j=1}^{N_{MC}} f(x^i, u^j)$$

Drawbacks : the cost of a simulation is multiplied by N_{MC} and the estimation is noisy.

Kriging based optimization with uncertainties
Integrated kriging

Objective : $\min_x \mathbb{E}_U [f(x, U)]$

Principle : work in the joint (x,u) space.



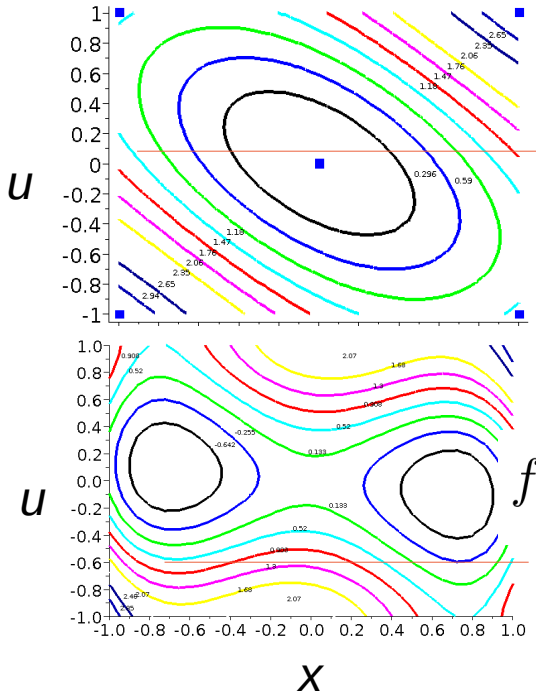
Cf. J. Janusevskis and R. Le Riche, *Simultaneous kriging-based estimation and optimization of mean response*, Journal of Global Optimization, Springer, 2012

Kriging based optimization with uncertainties
Integrated kriging

$\min_x \mathbb{E}_U[f(x,U)]$: **objective**

$Y^t_{(x,u)}(\omega)$: **kriging approximation to deterministic** $f(x,u)$

$Z^t_{(x)}(\omega) = \mathbb{E}_U[Y^t_{(x,U)}(\omega)]$: **integrated process approximation to** $\mathbb{E}_U[f(x,U)]$



integrate

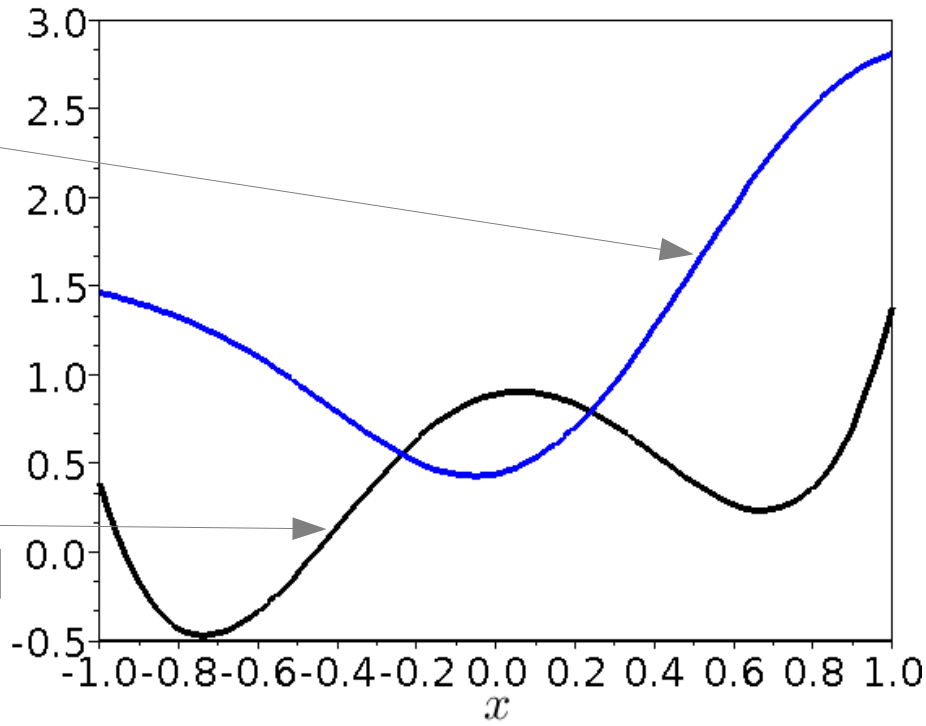
$\mathbb{E}\left(Y^t_{(x,u)}(\omega)\right)$

approximation

$E_\Omega[Z_{(x)}(\omega)]$

$f(x,u)$

objective $E_U[f(x,U)]$



Kriging based optimization with uncertainties
Integrated kriging

Z is a process approximating the objective function $\mathbb{E}_U[f(x,U)]$

Optimize with an Expected Improvement criterion,

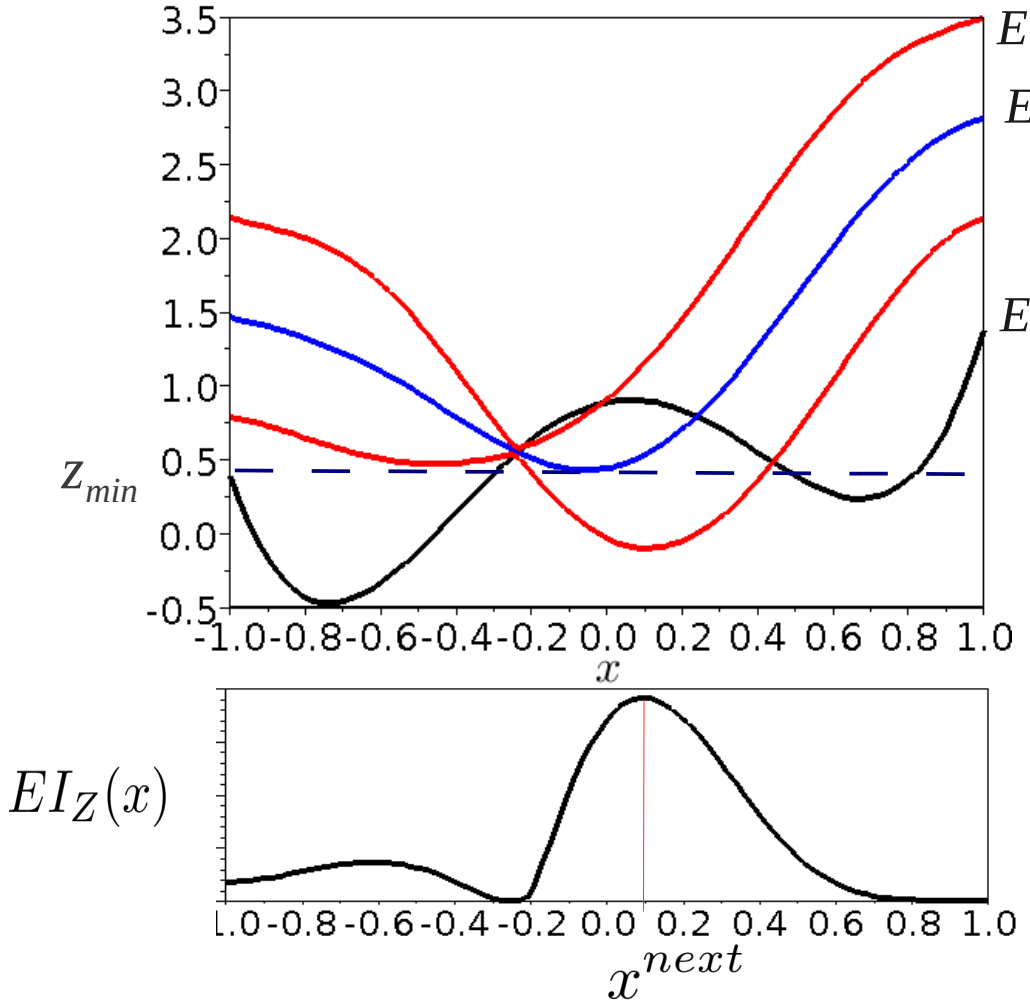
$$x^{next} = \arg\max_x EI_Z(x)$$

Optimize with an Expected Improvement criterion,

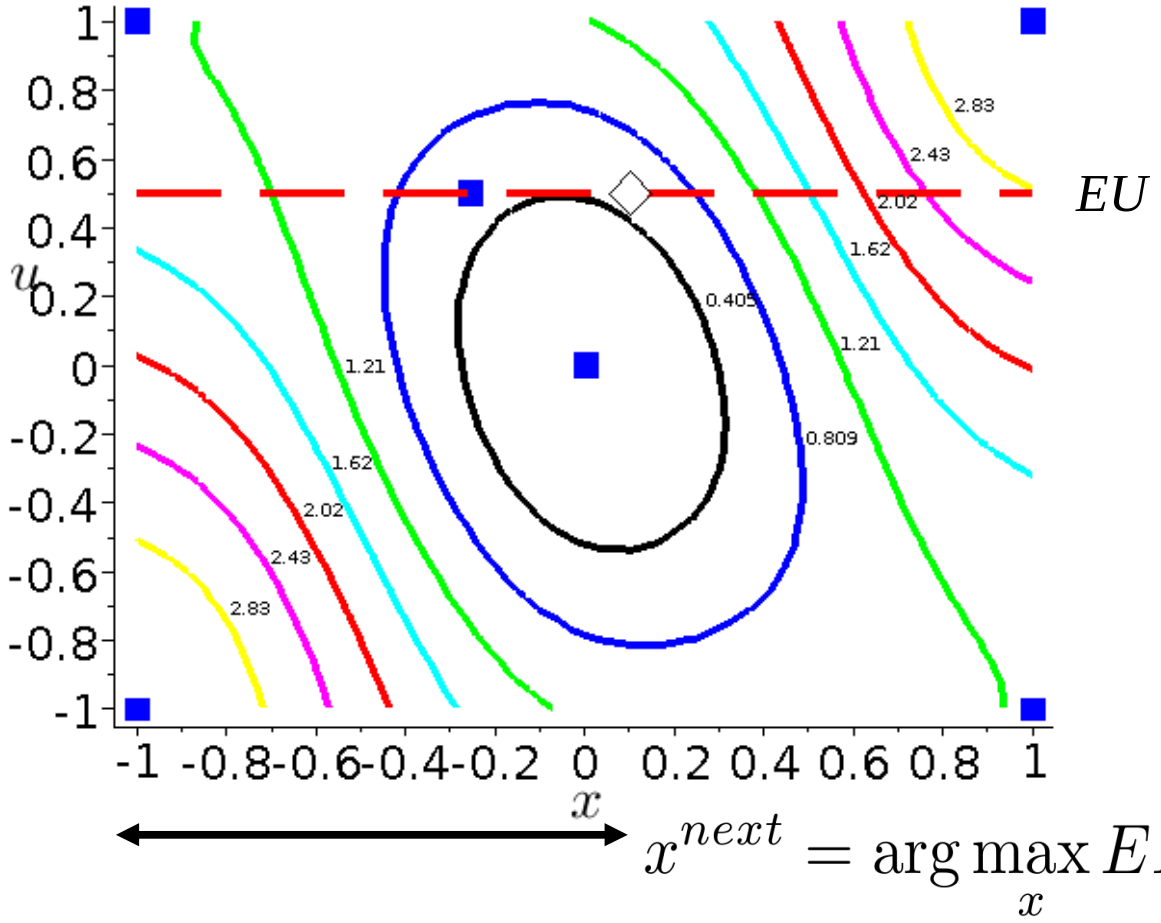
$I_Z(x) = max(z_{min} - Z(x), 0)$, but z_{min} not observed (in integrated space).

$\Rightarrow$ Define $z_{min} = \min_{x^1,\ldots,x^t} E(Z(x))$

Kriging based optimization with uncertainties
Integrated kriging



Kriging based optimization with uncertainties
Integrated kriging



$$x^{next} = \arg\max_x EI_Z^t(x)$$

x ok. What about *u* ? (which we need to call the simulator)

Kriging based optimization with uncertainties
Integrated kriging

x^{next} gives a region of interest from an optimization of the expected f point of view.

One simulation will be run to improve our knowledge of this region of interest → one choice of (x,u).

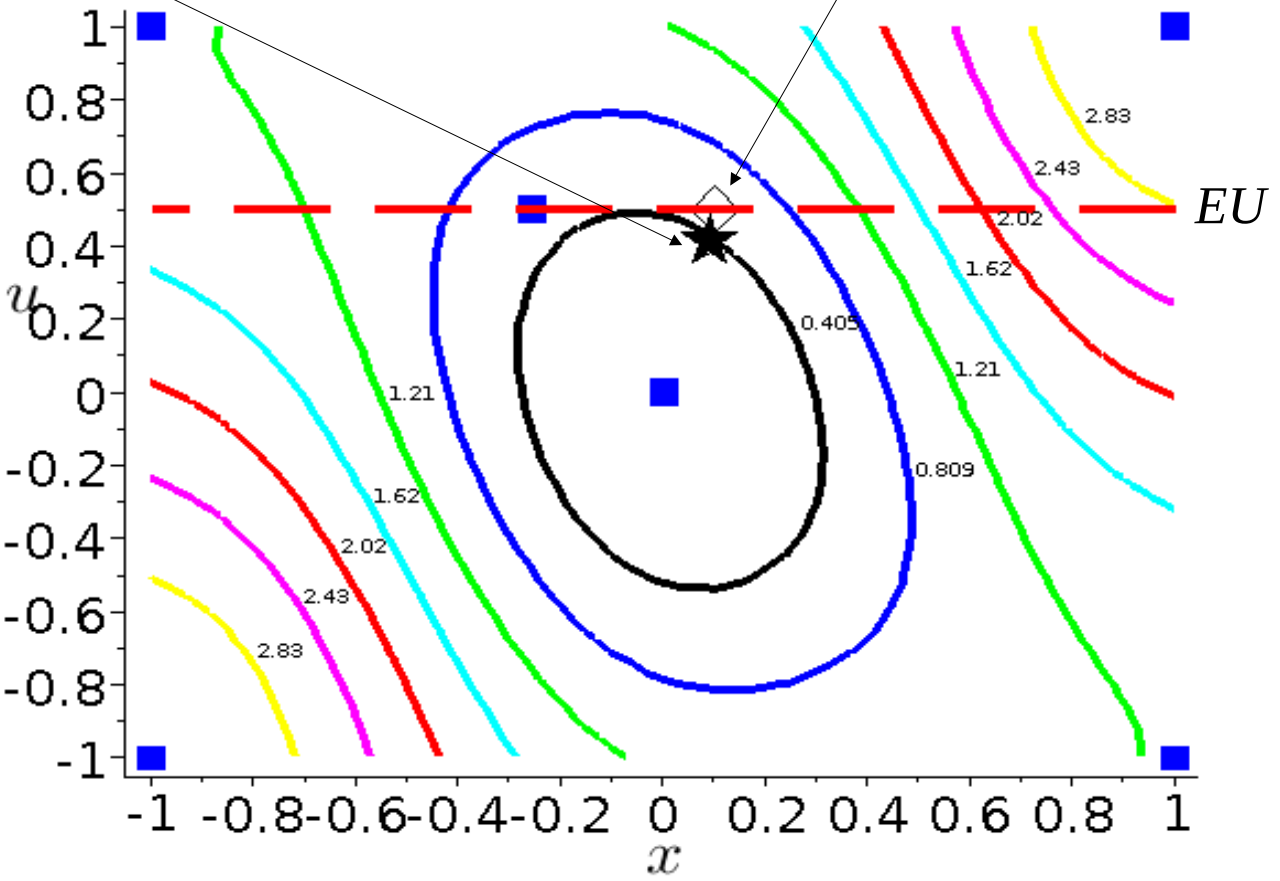
Choose (x^{t+1},u^{t+1}) that provides the most information, i.e., which minimizes the variance of the integrated process at x^{next}
(possible because the variance does not depend on f evaluations, only on the points positions)

$$(x^{t+1}, u^{t+1}) = \arg\min_{x,u} \mathbb{VAR}\ Z^{t+1}_{(x^{next})}(\omega)$$

Kriging based optimization with uncertainties
Integrated kriging

$$x^{next} = \arg\max_{x} EI_Z^t(x)$$

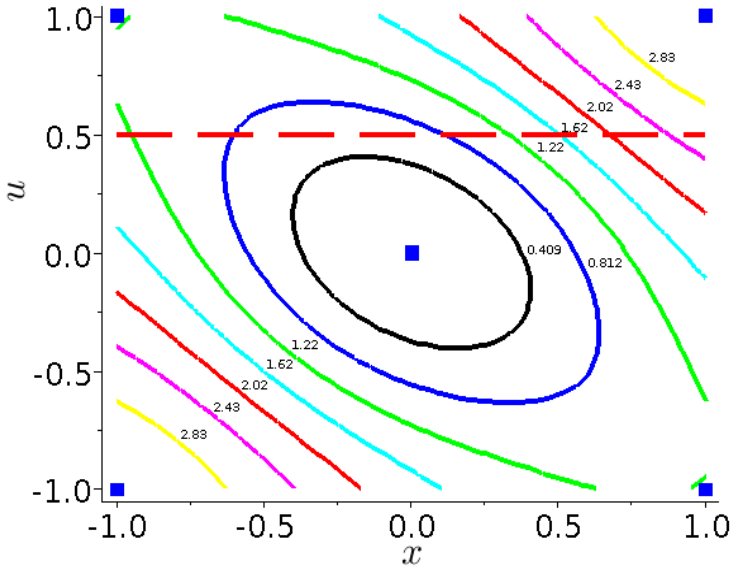
$$(x^{t+1}, u^{t+1}) = \arg\min_{x,u} \mathbb{VAR}\ Z^{t+1}_{(x^{next})}(\omega)$$

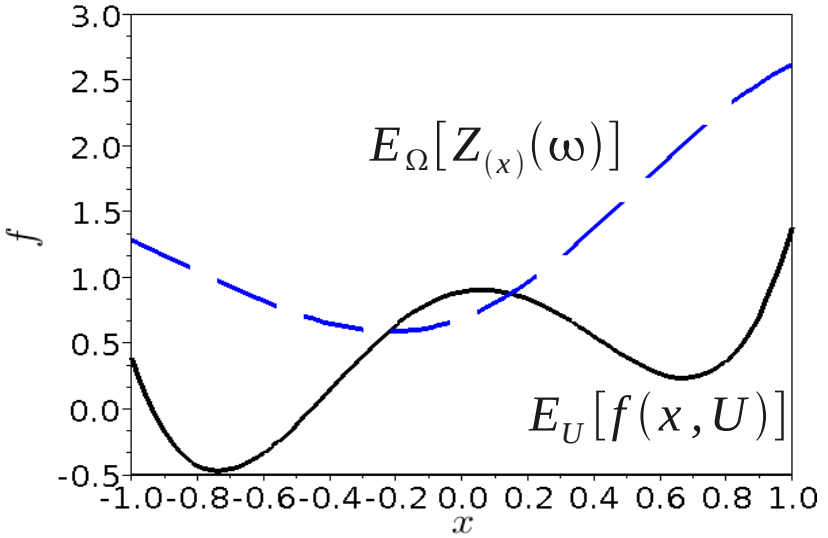


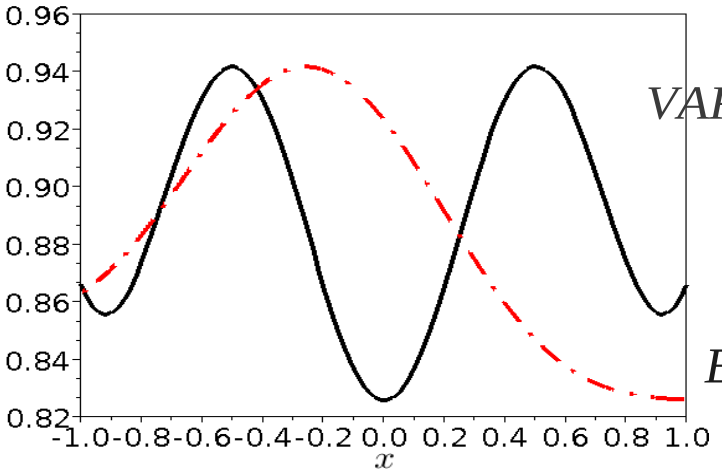
Kriging based optimization with uncertainties, U controlled

2D Expl, simultaneous optimization and sampling

DOE and $E[Y(x,u)]$



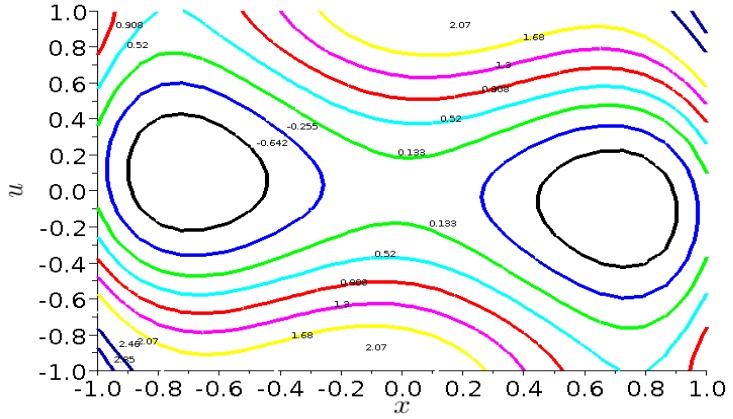




$VAR_\Omega[Z_{(x)}(\omega)]$

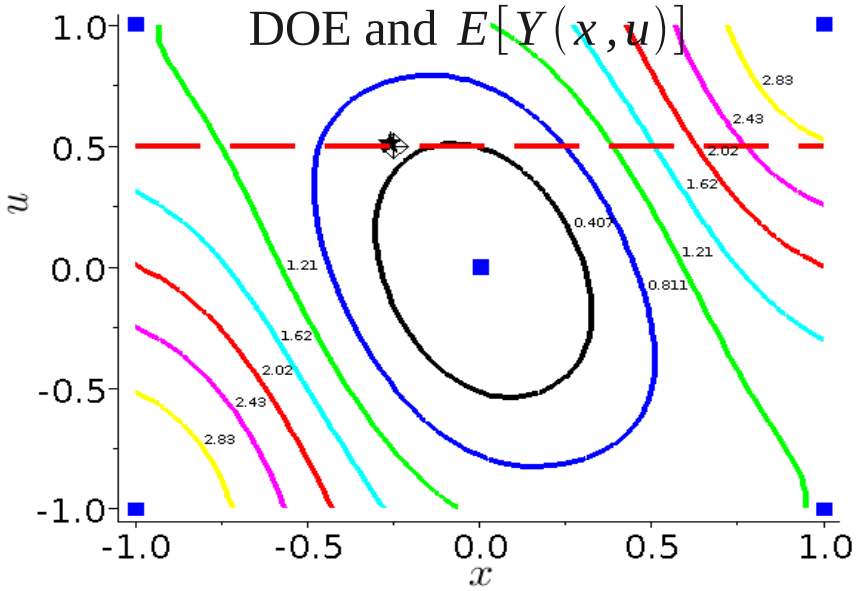
$EI_Z(x)$

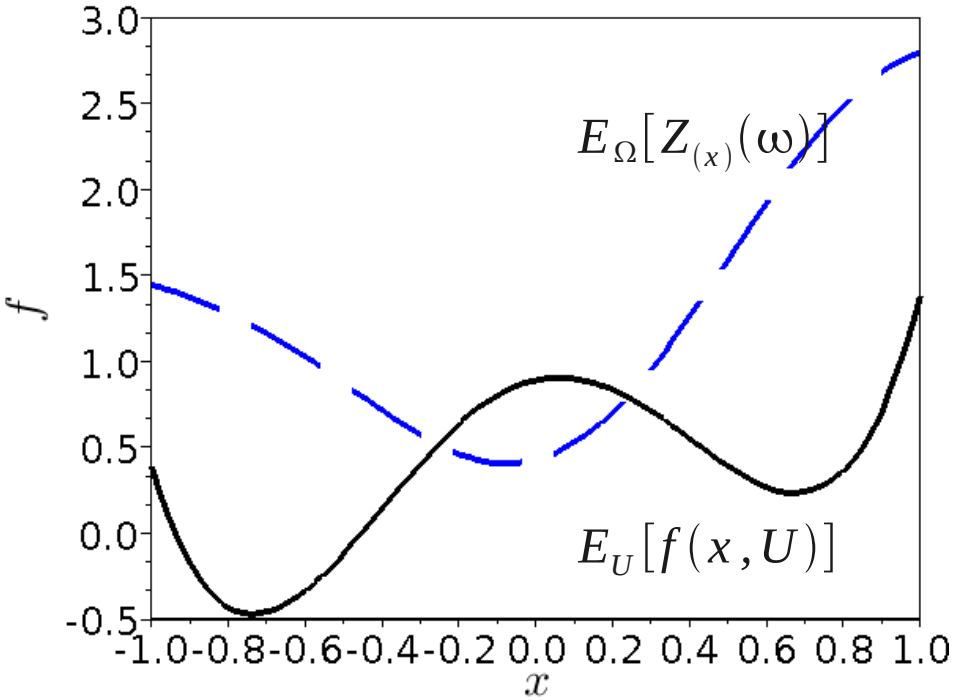
test function

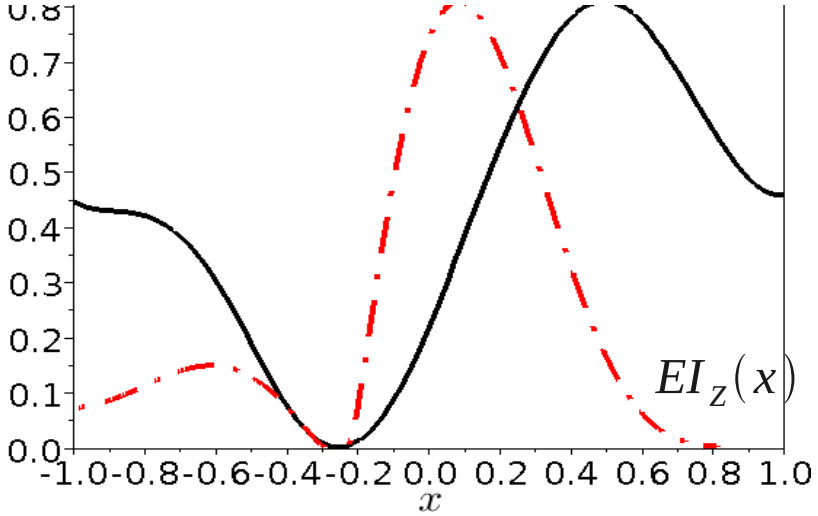


Kriging based optimization with uncertainties, U controlled

1st iteration







$VAR_\Omega[Z_{(x)}(\omega)]$

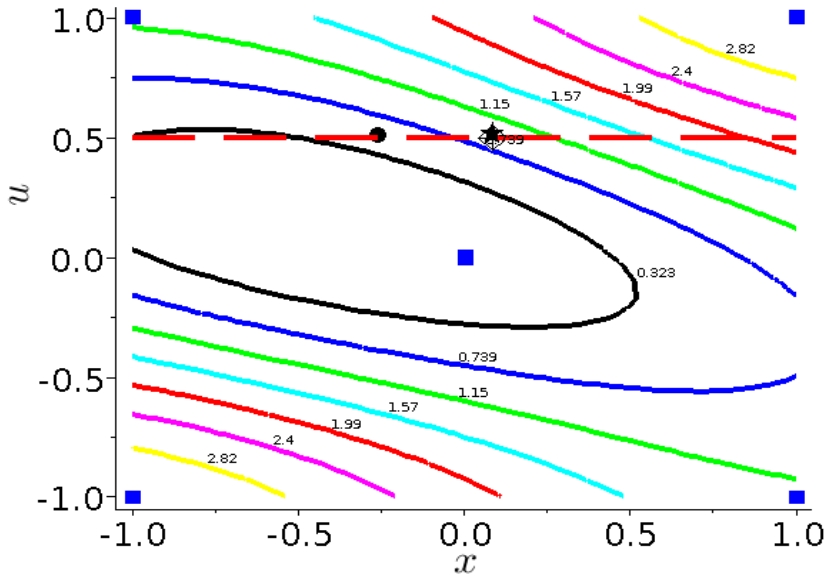
$\diamond$ – (x^{next}, μ)

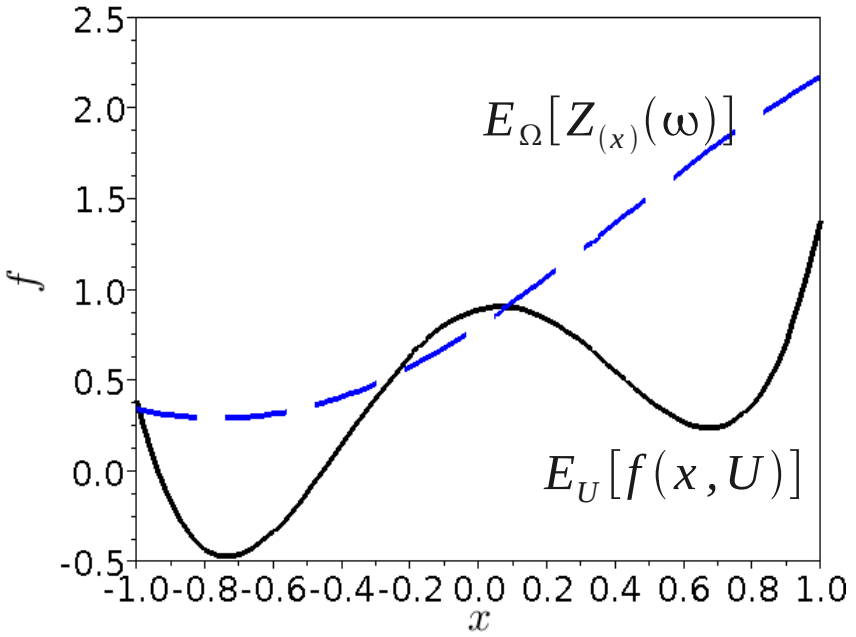
★ – (x^{t+1}, u^{t+1})

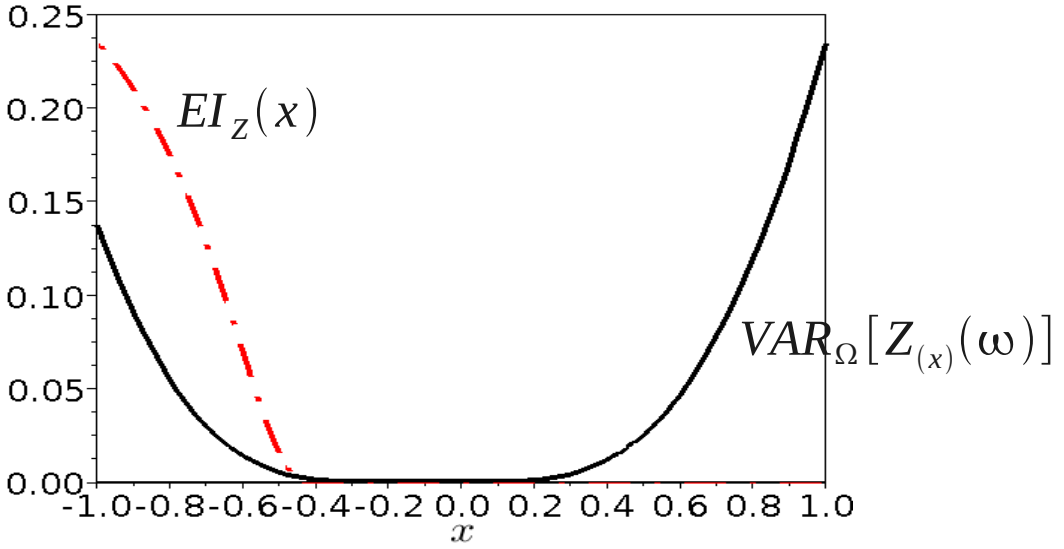
Kriging based optimization with uncertainties, U controlled

2nd iteration

DOE and $E[Y(x,u)]$







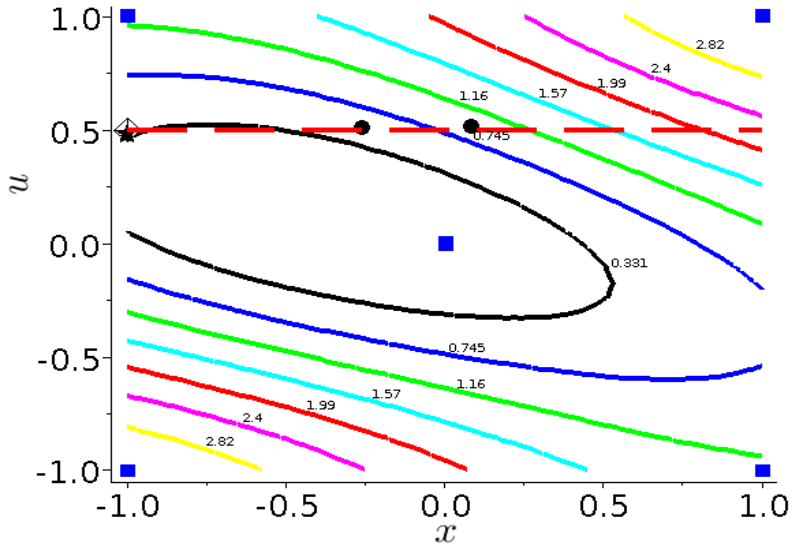
$-\ (x^{next}, \mu)$

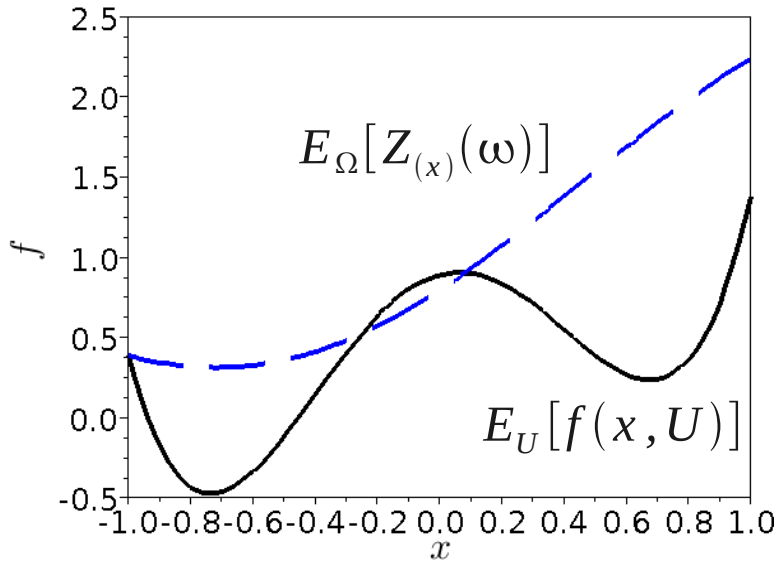
$-\ (x^{t+1}, u^{t+1})$

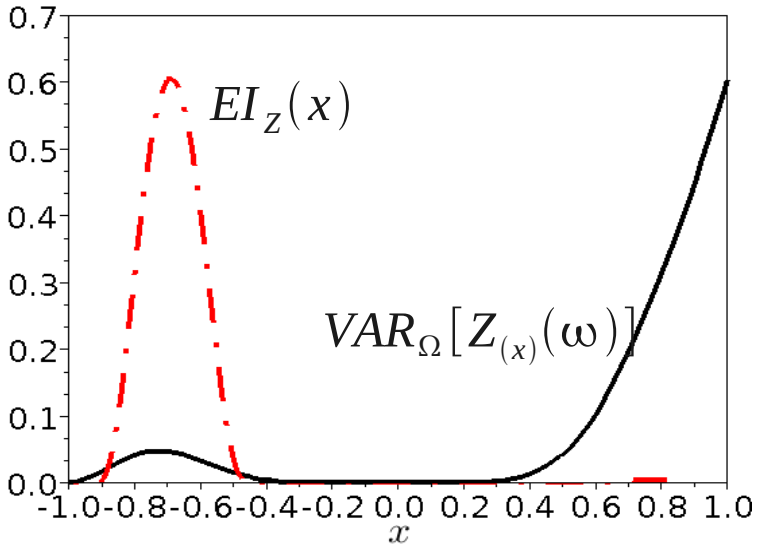
Kriging based optimization with uncertainties, U controlled

3rd iteration

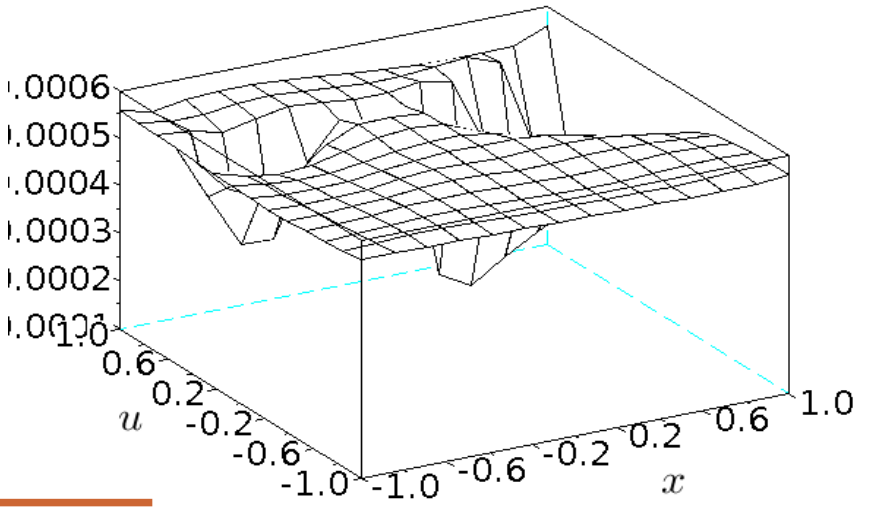
DOE and $E[Y(x,u)]$







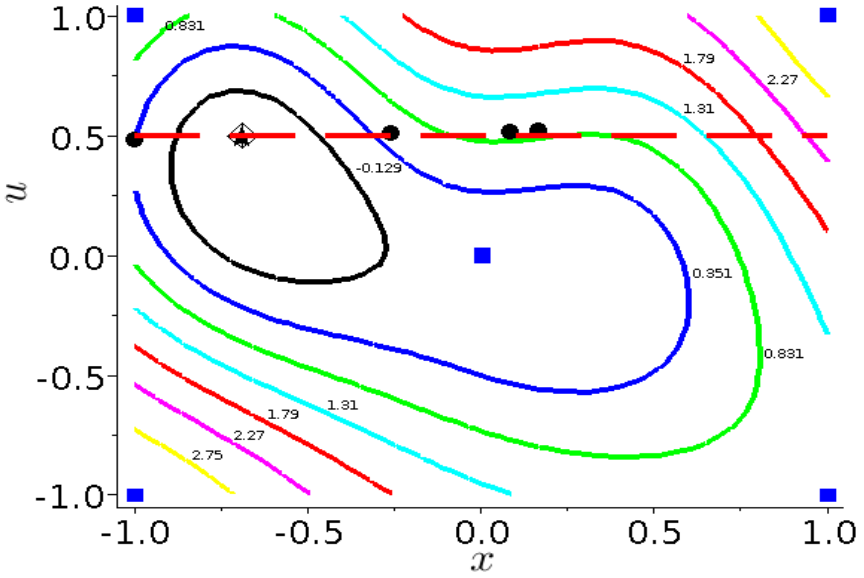
$VAR[Z(xnext)](x,u)$

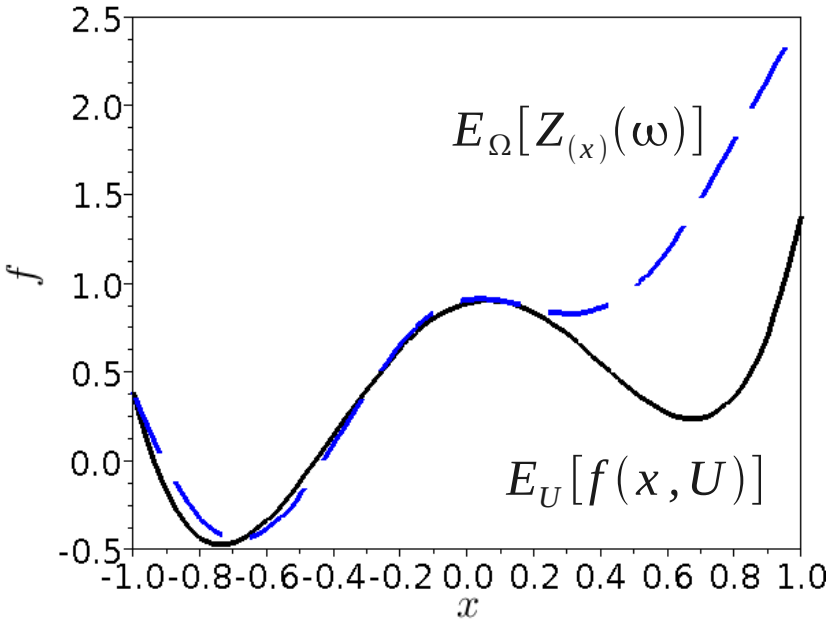


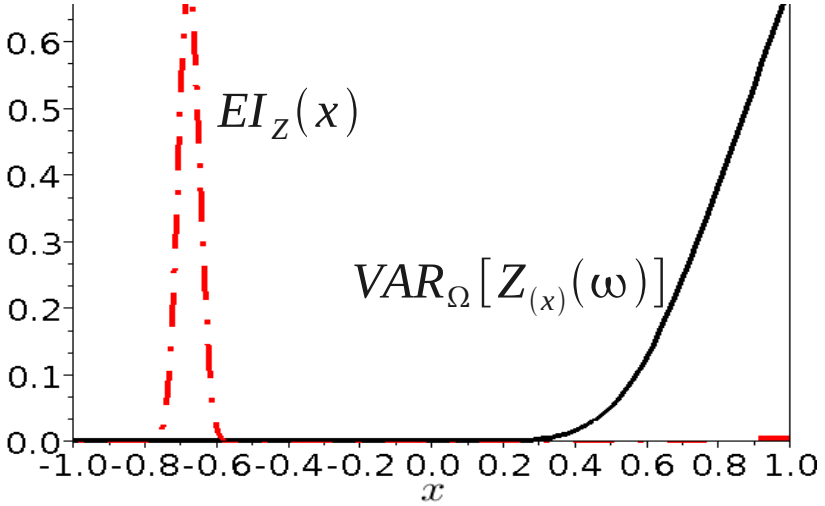
Kriging based optimization with uncertainties, U controlled

5th iteration

DOE and $E[Y(x,u)]$







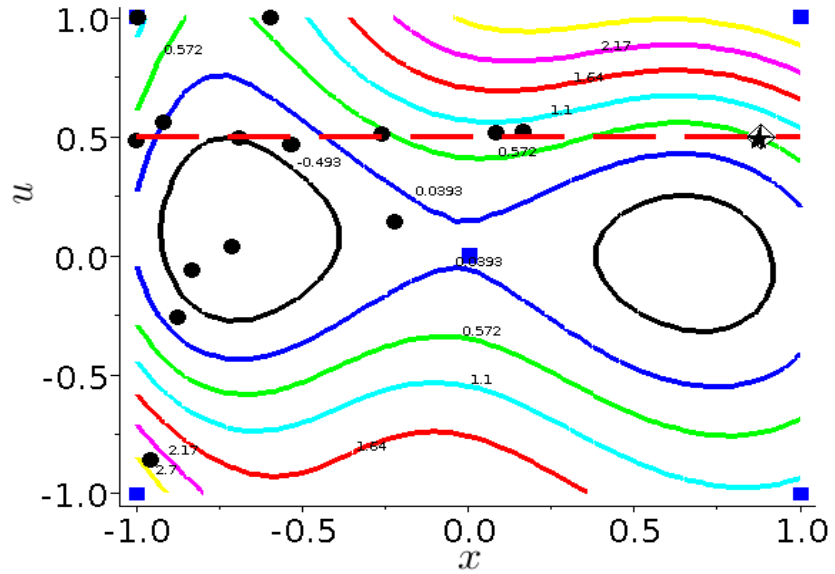
$-\ (x^{next}, \mu)$

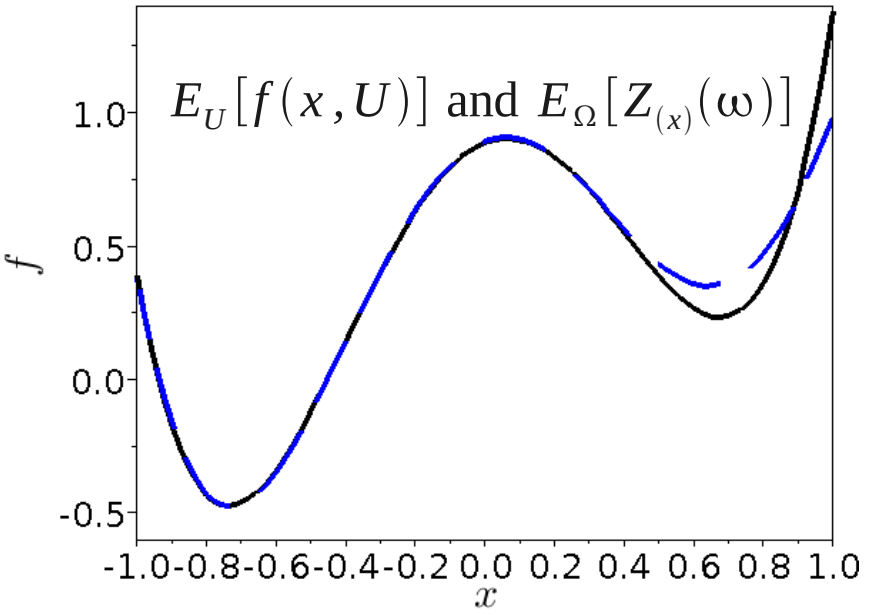
$-\ (x^{t+1}, u^{t+1})$

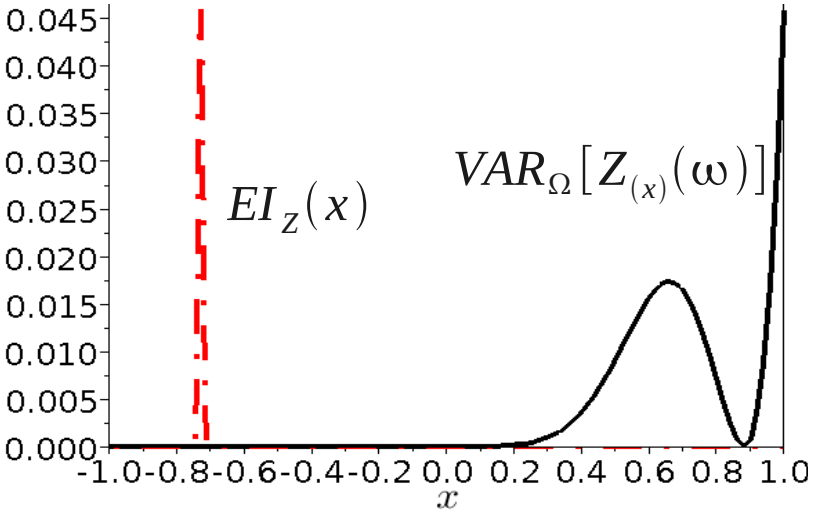
Kriging based optimization with uncertainties, U controlled

17th iteration

DOE and $E[Y(x,u)]$



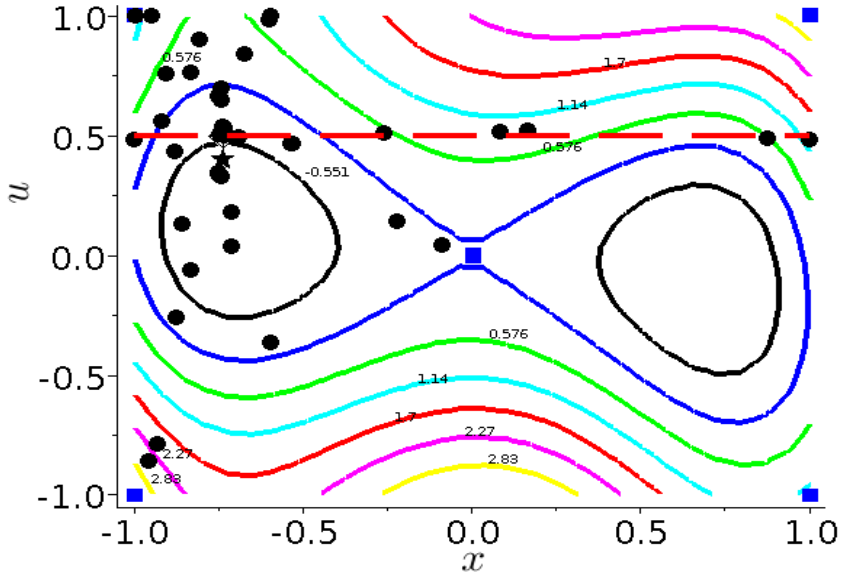




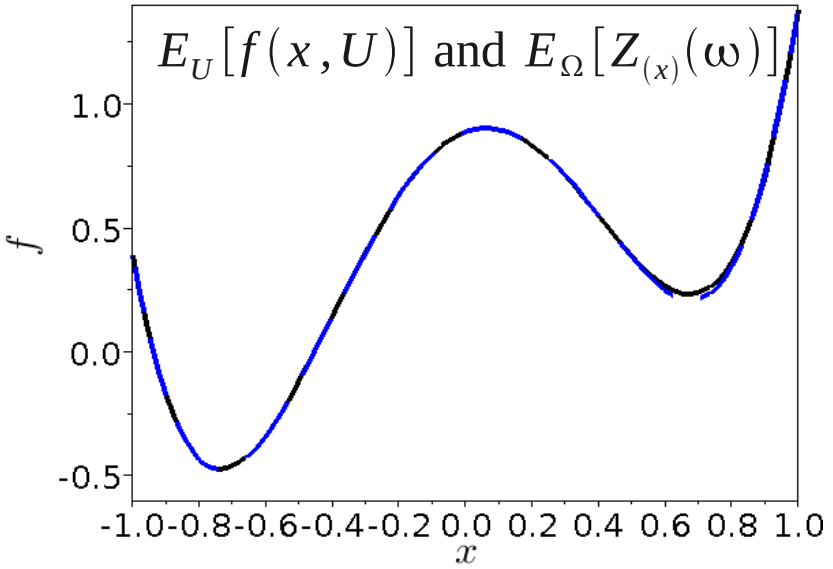
Kriging based optimization with uncertainties, U controlled

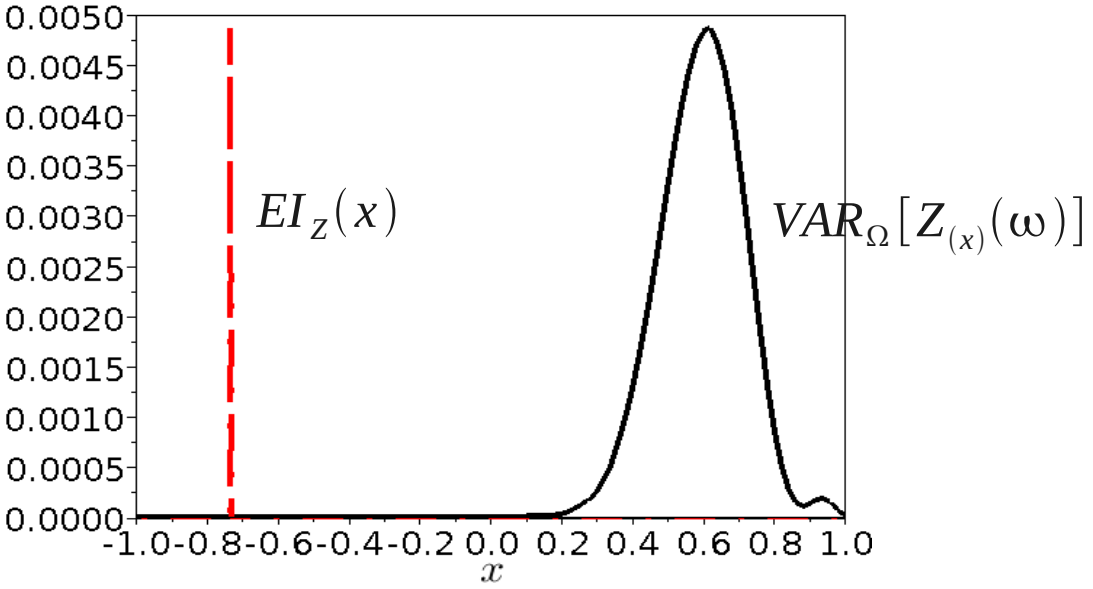
50th iteration

DOE and $E[Y(x,u)]$



$E_U[f(x,U)]$ and $E_\Omega[Z_{(x)}(\omega)]$



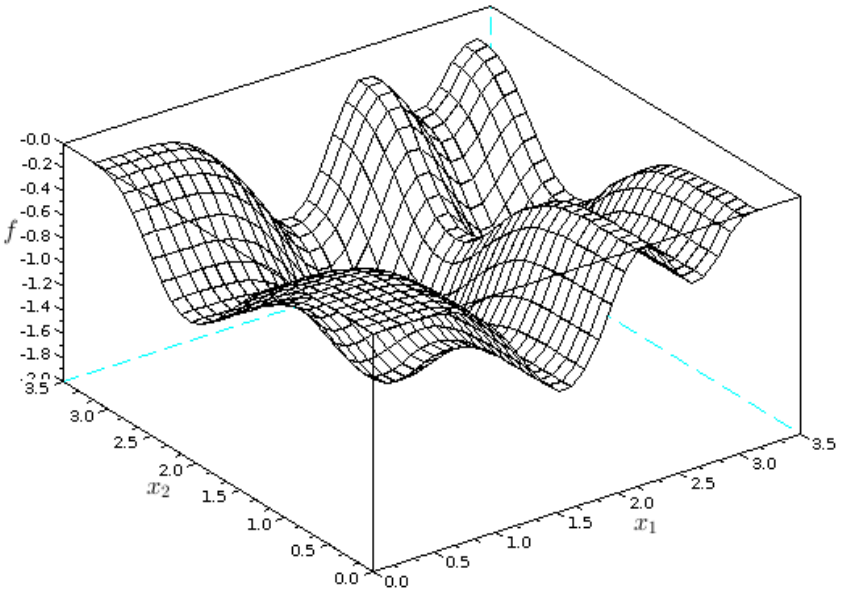


Test functions

Test cases based on Michalewicz function

$$f(x) = -\sum_{i=1}^{n} \sin(x_i)\left[\sin\left(ix_i^2/\pi\right)\right]^2$$

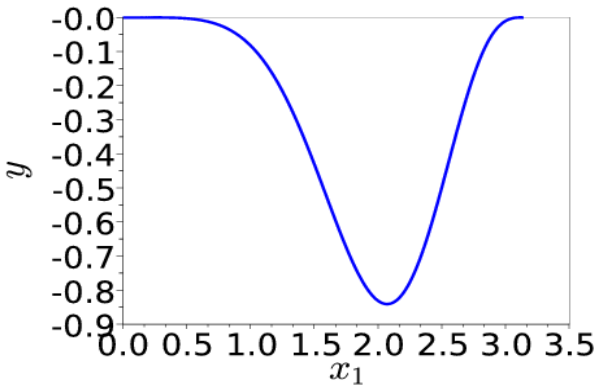
$$f(x,u) = f(x) + f(u)$$

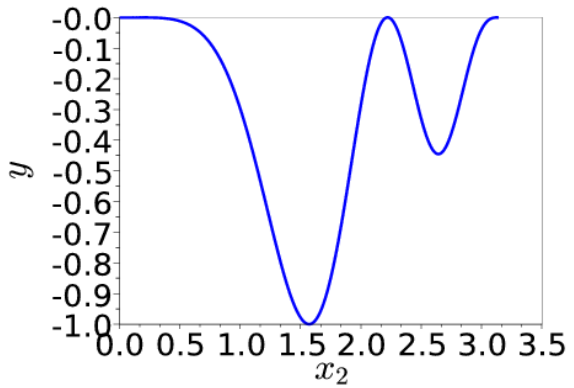


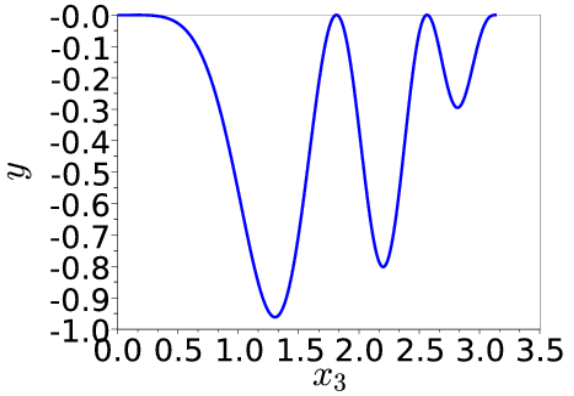
2D: $n_x=1 \;\; n_u=1 \;\; \mu=1.5 \;\; \sigma=0.2$

4D: $n_x=2 \;\; n_u=2 \;\; \mu=[1.5,\ 2.1] \;\; \sigma=[0.2,\ 0.2]$

6D: $n_x=3 \;\; n_u=3 \;\; \mu=[1.5,\ 2.1,\ 2] \;\; \sigma=[0.2,\ 0.2,\ 0.3]$

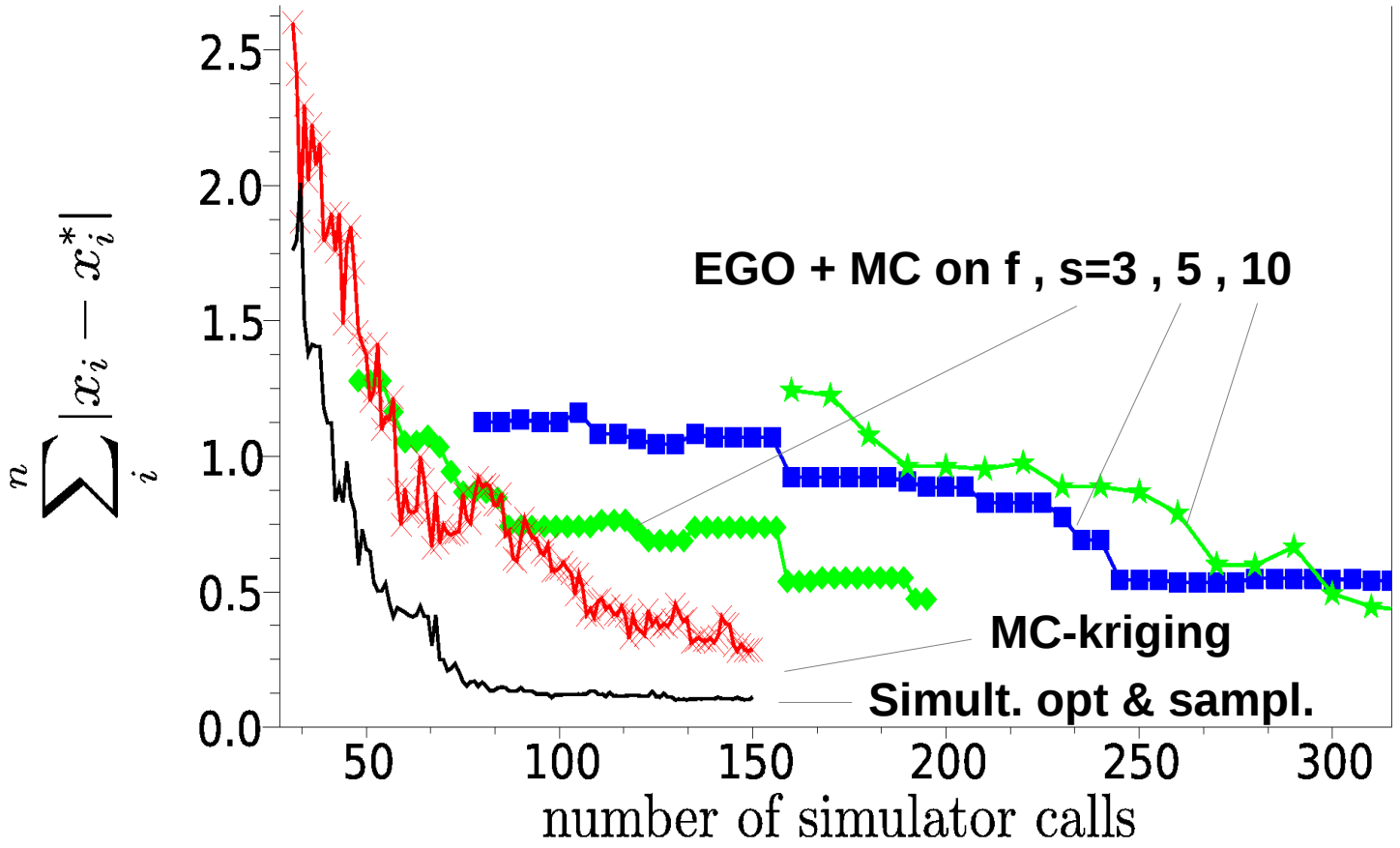






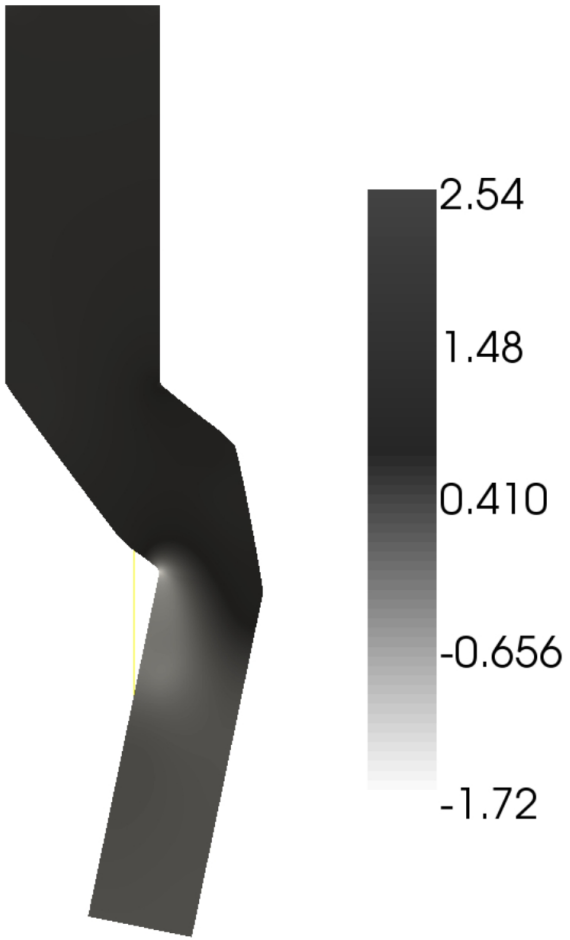
Test results

6D Michalewicz test case, $n_{x=3}$ =3 , n_U =3 .
Initial DOE: RLHS , m=(n_x+n_U)*5 = (3+3)*5 = 30;
10 runs for every method.



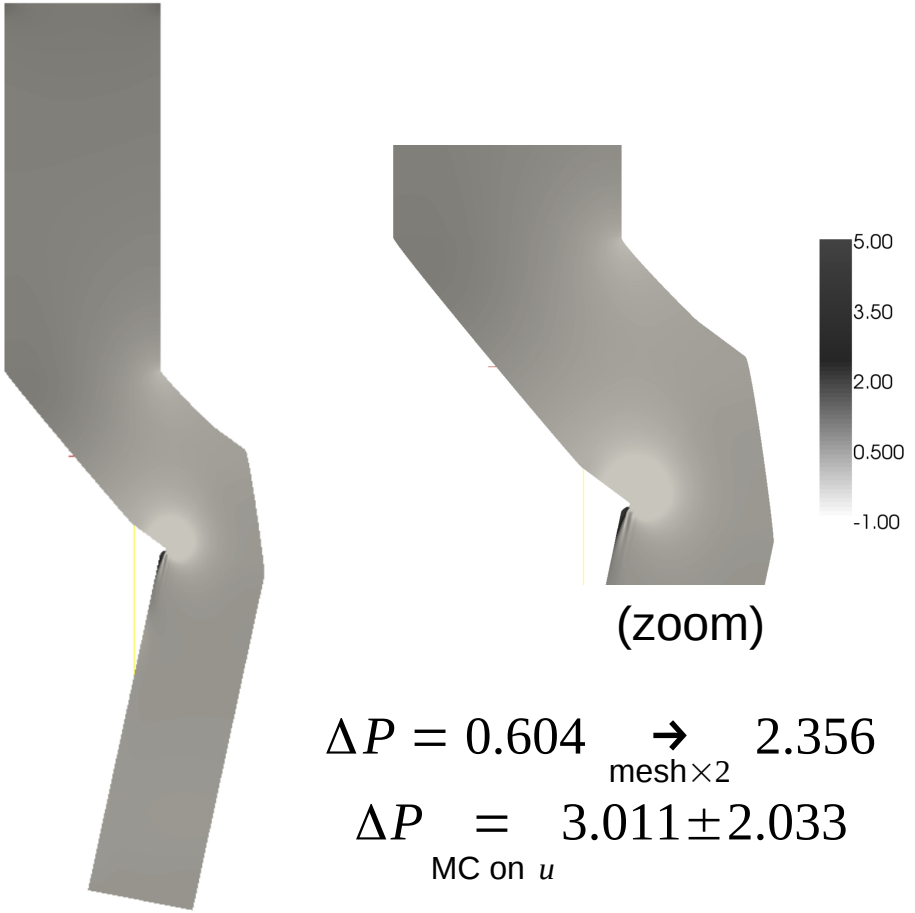
Duct design with uncertain boundary conditions
Pressure loss results

robust design



$$\Delta P \underset{\text{MC on } u}{=} 1.198 \pm 0.069$$

deterministic design for u=0



(zoom)

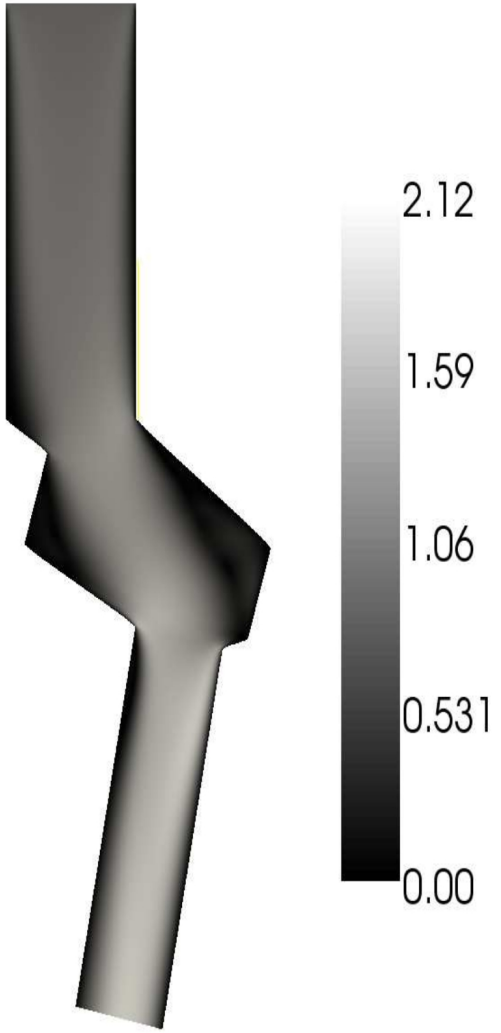
$$\Delta P = 0.604 \underset{\text{mesh}\times 2}{\rightarrow} 2.356$$

$$\Delta P \underset{\text{MC on } u}{=} 3.011 \pm 2.033$$

The result is not stable w.r.t. mesh changes.
The optimization exploits meshing flaws.

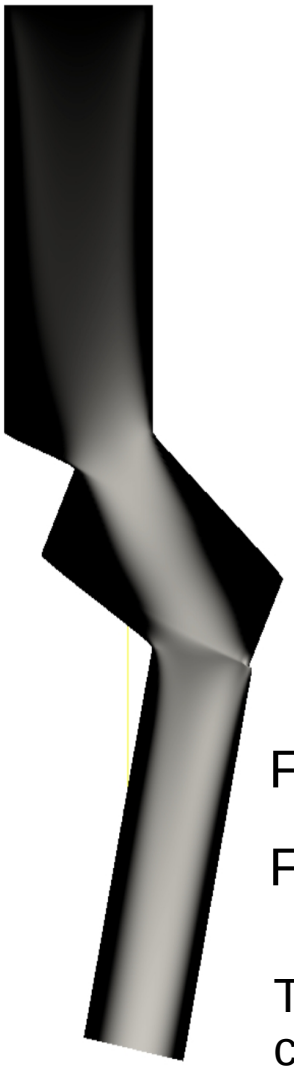
Duct design with uncertain boundary conditions
Flow uniformity results

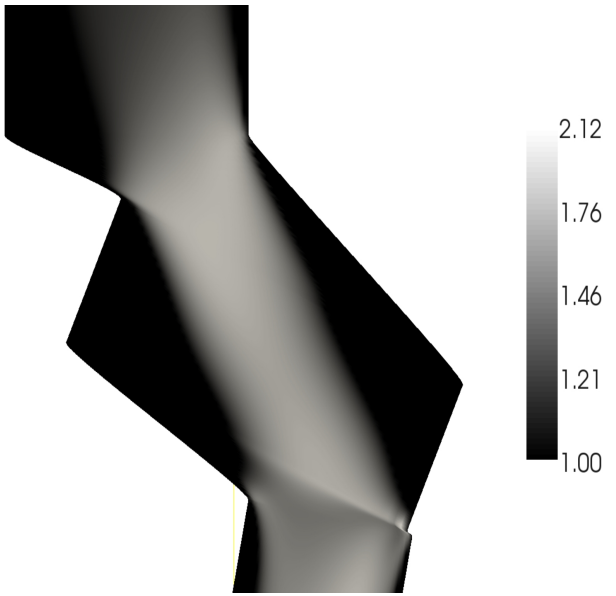
robust design



Flow Std Dev $\underset{\text{MC on } u}{=} 0.155 \pm 0.003$

deterministic design for u=0





(zoom)

Flow Std Dev $\underset{u=0}{=} 0.142 \xrightarrow[\text{mesh}\times 2]{} 0.532$

Flow Std Dev $\underset{\text{MC on } u}{=} 0.243 \pm 0.112$

The result is not stable w.r.t. mesh changes. The optimization exploits meshing flaws.

partial conclusion

Accounting for uncertainties in design

mechanics → statistics

- is a practical issue (there are always model uncertainties or inherent randomnesses)
- raises difficult challenges that foster research

statistics → mechanics

- the collaboration between physical and statistical models will continue to bring new ideas : optimizers are stringent tests for simulators, noise on u as a way to reduce mesh sensitivity, …

U controlled : J. Janusevskis and R. Le Riche, *Simultaneous kriging-based estimation and optimization of mean response*, Journal of Global Optimization, Springer, 2012

U not controlled : Le Riche, Picheny, Ginsbourger, Meyer, Kim, *Gears design with shape uncertainties using Monte Carlo simulations and kriging*, SDM, AIAA-2009-2257.

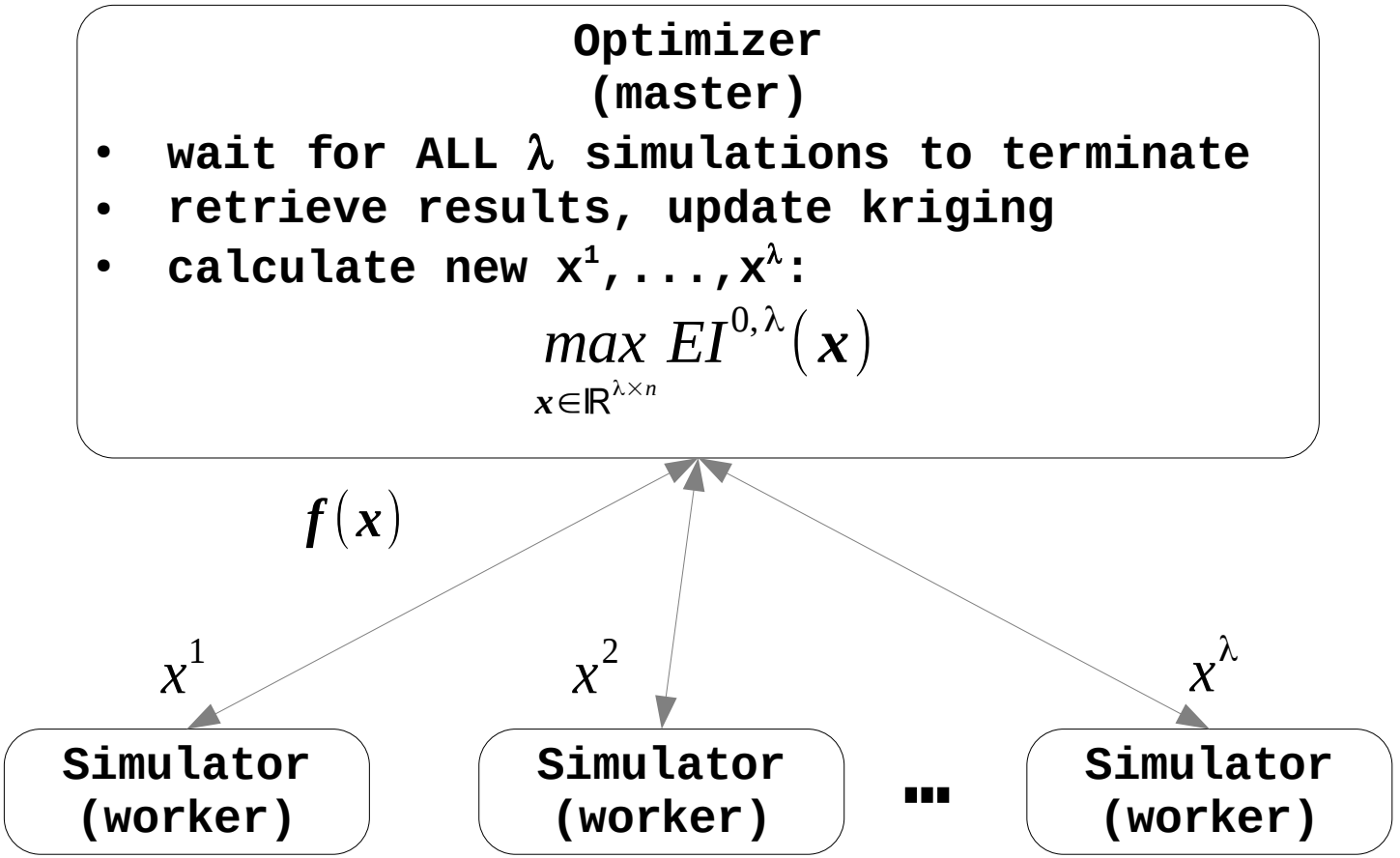
Noisy optimization : D. Salazar, R. Le Riche, G. Pujol and X. Bay, *An empirical study of the use of confidence levels in RBDO with Monte Carlo simulations*, in Multidisciplinary Design Optimization in Computational Mechanics, Wiley/ISTE Pub., 2010.

Extensions of kriging-based optimization to parallel computing

- since the cost of calculating the objective function is a stumbling block
- Kriging key feature for distribution : joint information brought by a set of points can be measured

Synchronous parallel EI : flow chart

A master-worker structure between computing nodes :



Synchronous parallel EI : criterion

λ nodes are available for new simulations at $x^1,\ldots,x^\lambda \ (\equiv \boldsymbol{x})$

$\rightarrow$ choose $x^1, \ldots, x^\lambda$ so that they maximize the synchronous λ points EI

$$EI^{0,\lambda}(\boldsymbol{x}) = E\left[f_{\min} - min\left(F(x^1),\ldots,F(x^\lambda)\right) \right]^+ \mid F(x^{1\ldots M}) = f(x^{1\ldots M})$$

Compare to the sequential 1 point EI, from the EGO algorithm :

$$EI(x) \equiv EI^{0,1}(x) = E\left[f_{\min} - F(x) \right]^+ \mid F(x^{1\ldots m}) = f(x^{1\ldots m})$$

[cf. D. Ginsbourger, R. Le Riche and L. Carraro, Kriging is well-suited to parallelize optimization, CIEOP, 2010]

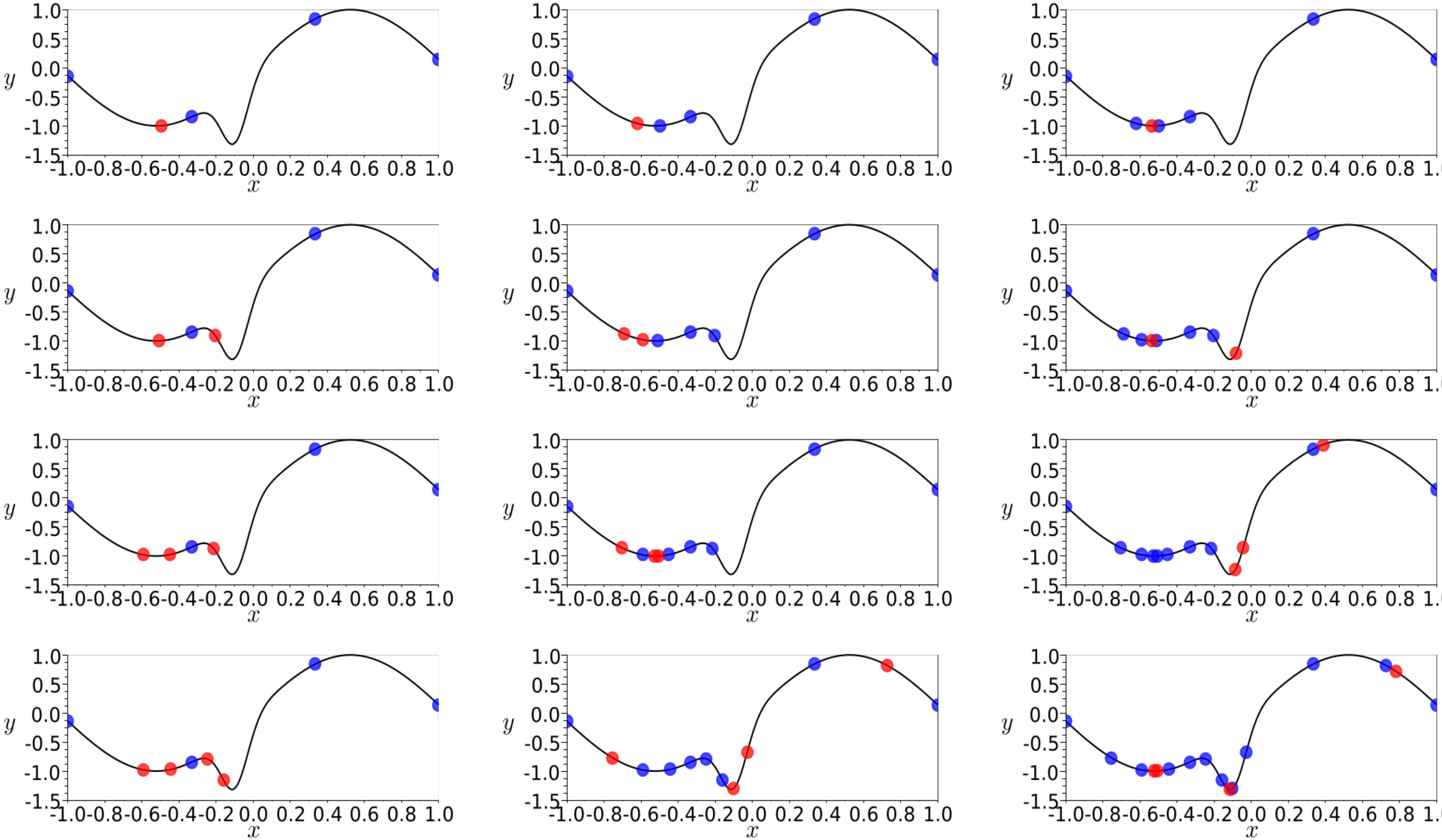
$\mathrm{EI}^{0,\lambda}$ is different from repeated $\mathrm{EI}^{0,1}$

$\lambda = 1$

$\lambda = 2$

$\lambda = 3$

$\lambda = 4$



Limitations of $EI^{0,\lambda}$

The number of nodes that can be used is limited by the problem to be solved

$$\max_{\boldsymbol{x} \in \mathbb{R}^{\lambda \times n}} EI^{0,\lambda}(\boldsymbol{x})$$

which is in dimension $\lambda \times n$.

The computing nodes have different speeds and the simulations different durations.

Time model :

λ nodes

T : time for 1 simulation, random variable, $T \sim U\left[t_{min}, t_{max}\right]$

$t_O =$ time for 1 optimization

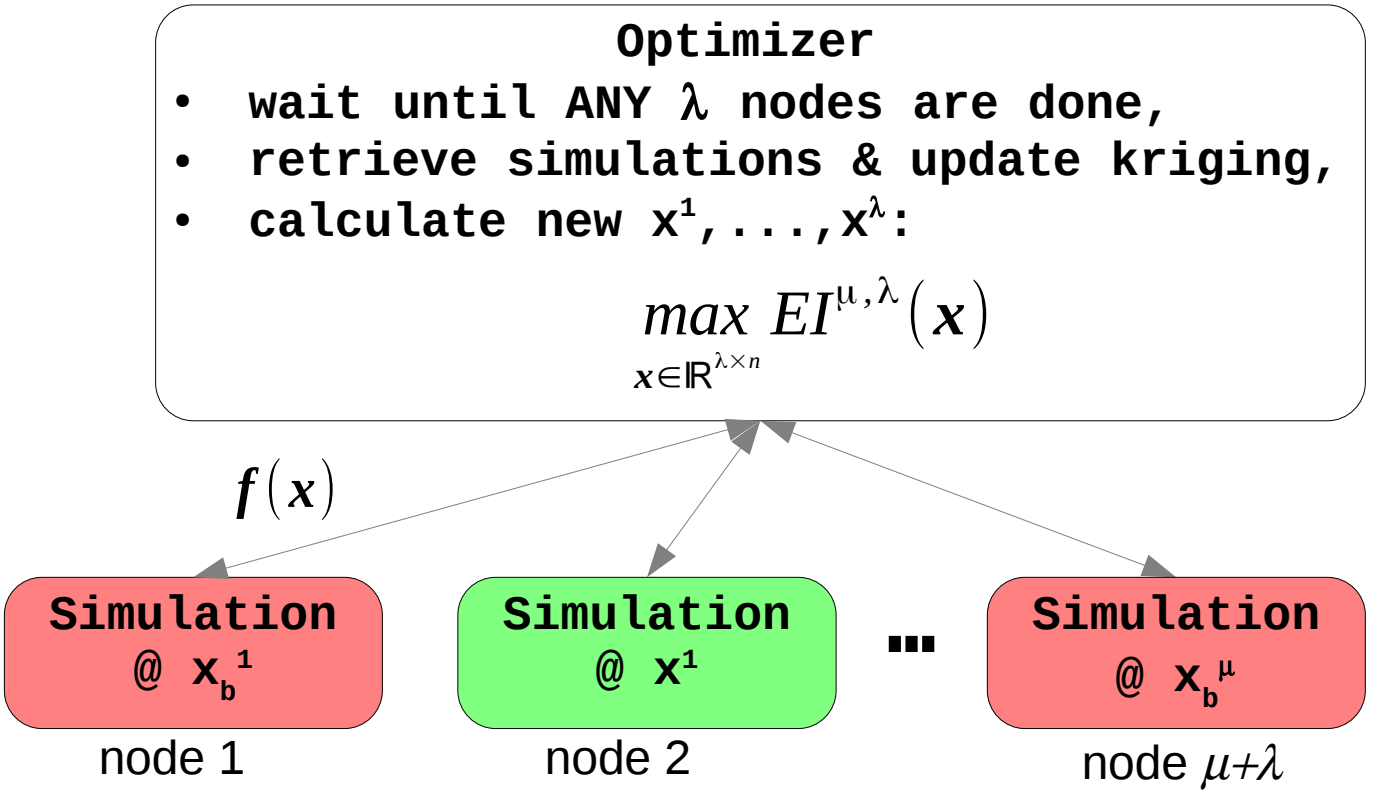
T_{WC} : wall clock time for 1 generation

$E(T_{WC}) = t_O + E(T_{\lambda:\lambda}) \underset{\lambda \gg 1}{\rightarrow} O(t_O + t_{max})$

Asynchronous parallel EI : flow chart

- It allows to use $m > \lambda+\mu$ nodes (actually ok for any optimizer that is not sensitive to the order of return of the points).

- *But* $EI^{\mu,\lambda}$ takes full account of past and on-going simulations and « optimally » (w.r.t. EI criterion) handles $\lambda+\mu$ nodes.



Asynchronous parallel EI : criterion

λ nodes are available for new simulations at $x^1,\dots,x^\lambda \ (\equiv \boldsymbol{x})$
μ nodes are busy running simulations at $x_b^1,\dots,x_b^\mu \ (\equiv \boldsymbol{x_b})$

$$EI^{\mu,\lambda}(\boldsymbol{x}) = E\left[min\left(f_{\min}, F(\boldsymbol{x_b})\right) - min\left(F(\boldsymbol{x})\right)\right]^+ \ | \ F\left(x^{1\dots M}\right) = f\left(x^{1\dots M}\right)$$

Recall the 1 point sequential EI and the synchronous EI :

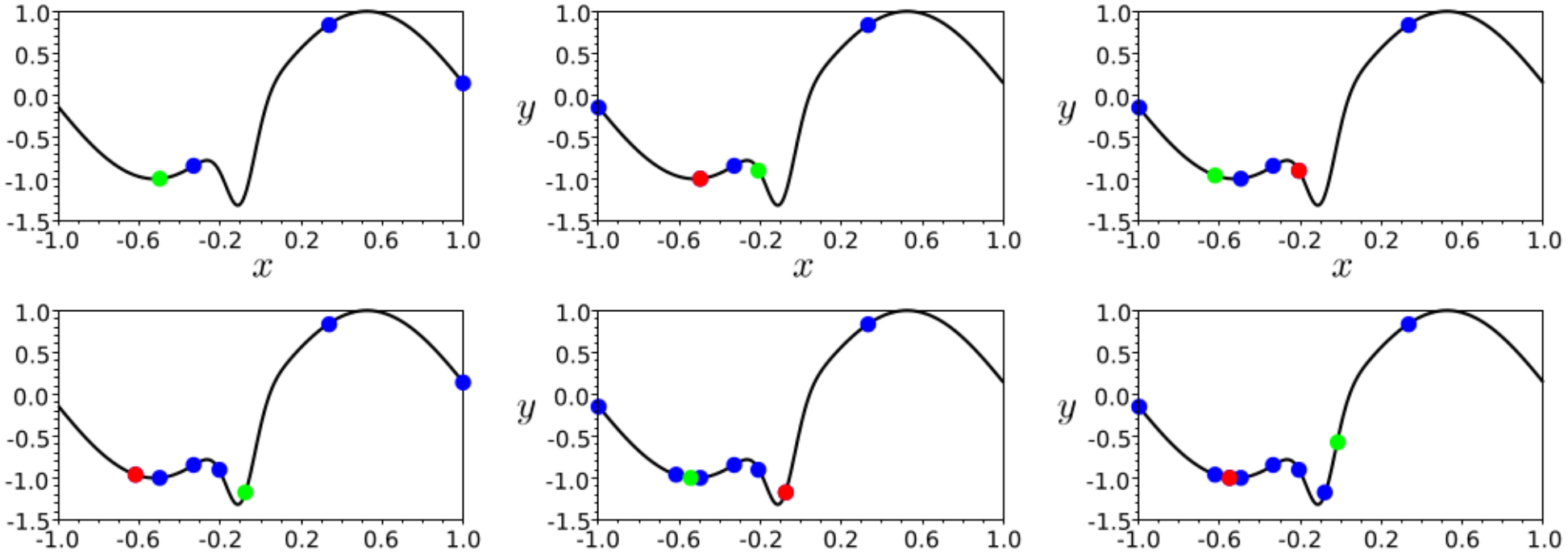
$$EI(x) \equiv EI^{0,1}(x) = E\left[f_{\min} - F(x)\right]^+ \ | \ F\left(x^{1\dots m}\right) = f\left(x^{1\dots m}\right)$$

$$EI^{0,\lambda}(\boldsymbol{x}) = E\left[f_{\min} - min\left(F(\boldsymbol{x})\right)\right]^+ \ | \ F\left(x^{1\dots m}\right) = f\left(x^{1\dots m}\right)$$

Property : $EI^{\mu,\lambda}(\boldsymbol{x}) \to 0^+$ as $\boldsymbol{x} \to \boldsymbol{x_b}$
(the search is pushed away from already sampled points which are being evaluated)

Asynchronous parallel EI : illustration

$$x^{t+1} = \underset{x \in S \subset \mathbb{R}^n}{arg\ max}\ EI^{\mu,\lambda}(\boldsymbol{x}) \quad \text{where} \quad \mu = 1 \quad \text{and} \quad \lambda = 1$$



Advantages of $EI^{\mu,\lambda}$ over $EI^{0,\lambda}$

The number of nodes used ($m > \mu+\lambda$) is not limited by

$$\max_{\boldsymbol{x}\in\mathbb{R}^{\lambda\times n}} EI^{\mu,\lambda}(\boldsymbol{x})$$

which is in dimension $\lambda \times n$ ($\lambda = 1$ as best default strategy)

Time model in $O(m^{-1})$:

$m > \mu+\lambda$ nodes

T : time for 1 simulation, random variable, $T \sim U\left[t_{min}, t_{max}\right]$

$t_O =$ time for 1 optimization

T_{WC} : wall clock time for 1 generation

$$E\left(T_{WC}\right) \approx t_O + \frac{E\left(t_{\lambda:m}\right)}{m}$$

Asynchronous parallel EI : results

100 independant runs on 3 functions, m = 32 computing nodes

Label	Cost function	Domain	Minimal value	Modality
"michalewicz2d"	$\sum_{i=1}^{2} \sin(x_i) \sin^2(ix_i^2/\pi)$	$[0,5]^2$	-1.841	multimodal
"rosenbrock6d"	$\sum_{i=1}^{5} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2$	$[0,5]^6$	0	unimodal
"rank1approx9d"	$\|\mathbf{A}_{4\times5} - \mathbf{x}_{1\ldots4}\mathbf{x}_{5\ldots9}^T\|_2, a_{ij} \sim U(0,1)^1$	$[-1,1]^9$	0.712	bimodal

S_G ; S_T = generation speed up ; time speed up w.r.t. $EI^{0,1}$ sync (EGO)

	micha2D S_G ; S_T	rosen6D S_G ; S_T	rank1 S_G ; S_T
$EI^{0,1}$ sync	1 ; 1	1 ; 1	1 ; 1
$EI^{0,4}$ sync	3.8 ; 3.0	2.9 ; 2.3	1.3 ; 1.0
$EI^{31,1}$ async	0.8 ; 8.3	0.4 ; 4.4	0.4 ; 4.1
$EI^{28,4}$ async	2.58 ; 20.4	1.2 ; 9.2	0.8 ; 6.4

- **$EI^{\mu,\lambda}$ is better generation wise than $EI^{\mu,1}$**
- **asynchronous algos are slower generation wise than synchronous algos**
- **asynchronous algos are faster in wall-clock time than synchronous algos**

Asynchronous parallel EI algorithm
Selected bibliography

$EI^{\mu,\lambda}$

analytical bounds

- J. Janusevskis, R. Le Riche and D. Ginsbourger, *Parallel expected improvements for global optimization: summary, bounds and speed-up*, HAL technical report no. hal-00613971, Aug. 2011.

Bayes approach, analytical bounds

- Janusevskis, J., Le Riche, R., Ginsbourger, D. and R. Girdziusas, *Expected improvements for the asynchronous parallel global optimization of expensive functions : potentials and challenges*, selected articles from the LION 6 Conference, LNCS 7219, Aug. 2012

MC evaluation

- J. Janusevskis, R. Girdziusas and R. Le Riche, *On integration of multi-point improvements*, NIPS workshop on Bayesian Optimization and Decision Making, Lake Tahoe, USA, dec. 2012.

time model, empirical tests

- R. Le Riche, R. Girdziusas and J. Janusevskis, *A study of asynchronous budgeted optimization* , NIPS workshop on Bayesian Optimization and Decision Making, Lake Tahoe, USA, dec. 2012.

Conclusions

Thanks to its spatial convariance, kriging is a rich approach for optimizing with real simulators :

- mathematical framework for metamodel uncertainties
- reconciles design of experiments and optimization

Perspectives :

- high dimensions, large number of analyses
- optimization efficiency (e.g., BBOB contests)
- adding expert knowledge to the kernel choice
- multi-fidelity models and kriging based optimization