Squaring the engineering optimization circle : distributed global optimization algorithms for computationally expensive problems

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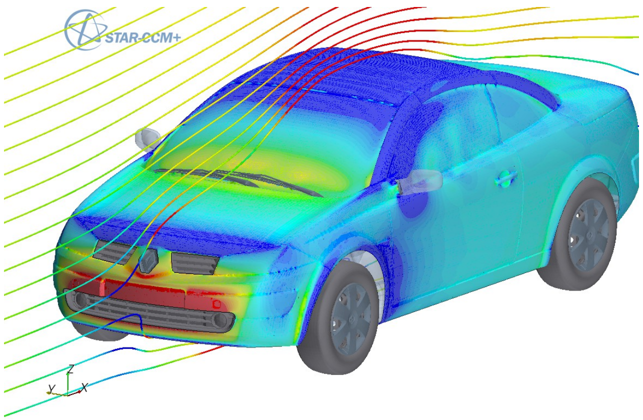
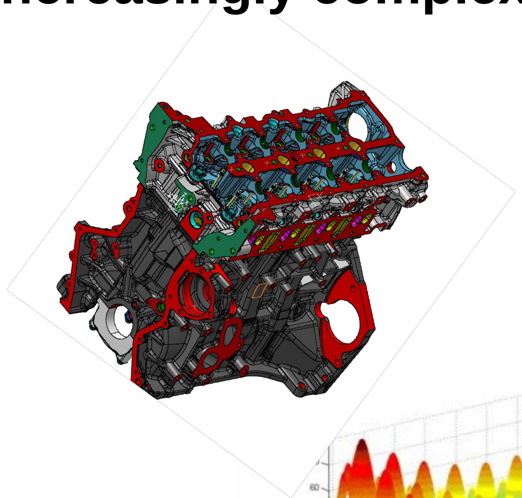
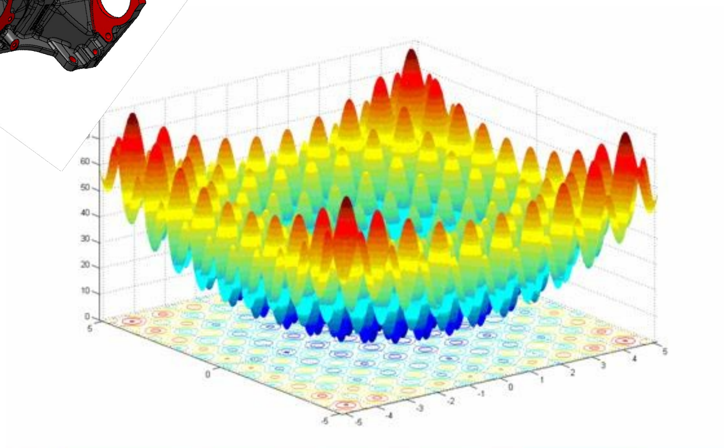
Globally optimal solutions and realistic models : squaring the engineeting optimization circle

There is a demand for optimizing increasingly complex models ...







…. and finding the globally best solution(s)

A realistic simulation takes typically 0,5h
In 10D, global optimization needs (say) 10000 evaluations → ~208 days

Globally optimal solutions and realistic models : squaring the engineeting optimization circle

The computational cost is an endless obstacle to engineering optimization.

Approaches :

- reducing the cost of the simulation : reduced models, metamodels.
- making the optimization problem easier : reducing the number of design variables.
- Having more efficient global optimization algorithms.
- taking advantage of parallel computing infrastructures.

some topics we have been looking at lately

Outline of the talk

metamodel ← kriging

parallelized global optimization algorithms ← parallelized Expected Improvement (EI) algorithms, dynamic partitioning (agents).

1. Introduction to kriging and optimization
2. Synchronous parallel EI
3. Asynchronous parallel EI
4. Embarrassingly parallel EI algorithms
5. An agent-based dynamic partitioning algorithm

centralized

decision

decentralized

Related work

Many in evolutionary computing, e.g., Branke et al., *Distribution of evolutionary algorithms in heterogeneous networks, GECCO 2004* : island models and migration schemes adapted to heterogenous computing ressources. Not adapted to expensive objective functions.

Local pattern search : E.g., Kolda, *Revisiting asynchronous parallel pattern search for nonlinear optimization*, SIAM J. Optimization, 2005.

Deterministic global optimization : E.g., Regis and Shoemaker, *Parallel radial basis function methods for the global optimization of expensive functions*, Eur. J. of OR, 2007. ← Closest contribution to the current work, yet synchronous.

Problem statement, notation

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

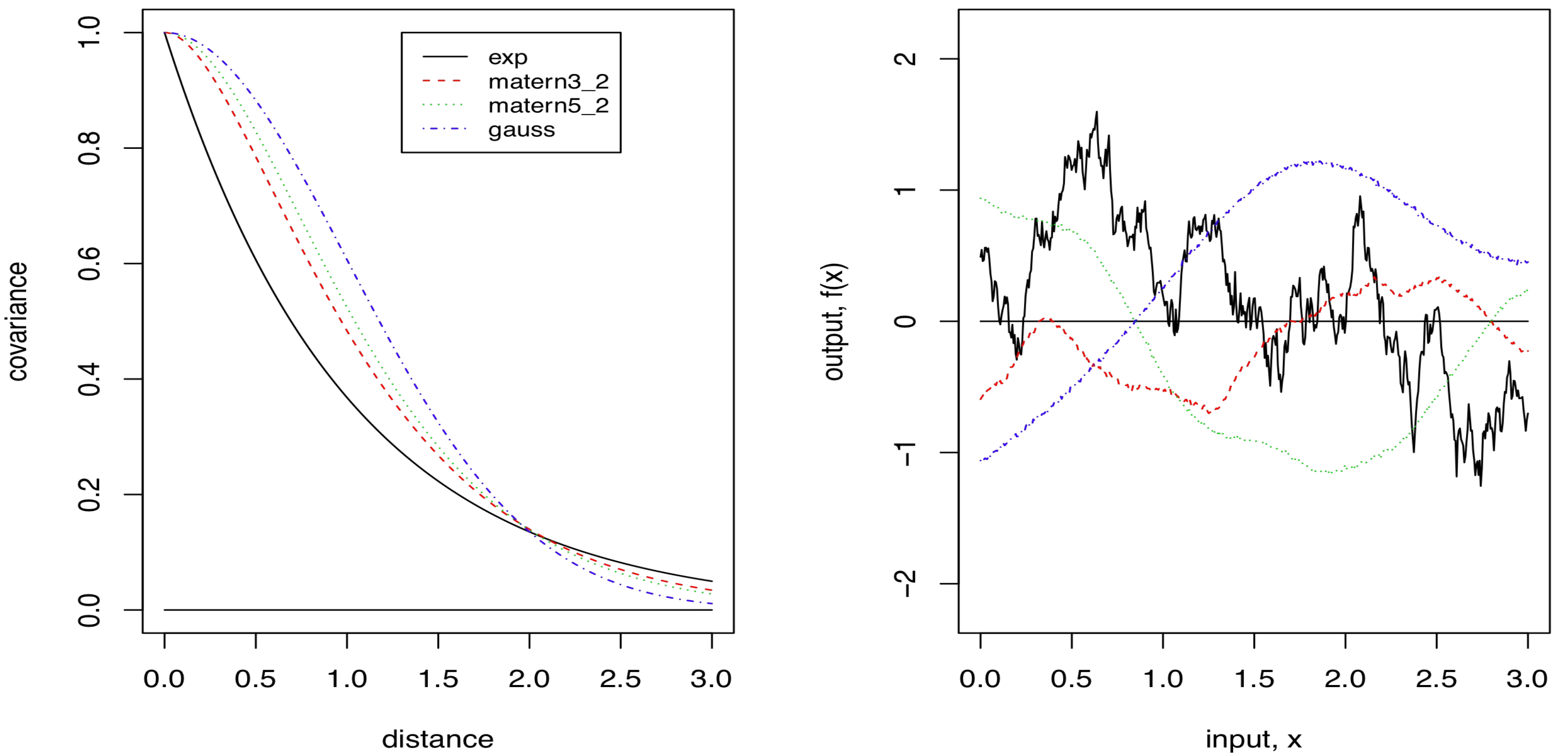
$$g(y(x)) \leq 0$$

x : design variables
y : numerical simulator (analytical, finite elements, coupled sub-models …).
f and g : optimization criteria (objective function and constraints)

Working assumptions : kriging (1)

Assume that *f(x)* can be seen as a trajectory of a stationary Gaussian random process, *F(x)*.

A fairly large class of functions can be represented in this way. They are parameterized by the covariance *Cov(F(x),F(x'))*.



(O. Roustant, HDR, 2011)

Working assumptions : kriging (2)

More precisely, assume that f(x) can be represented by a stationary **conditioned** Gaussian random process (+ linear trend) : kriging,

$$F(x) = a_0 + a_1\mu_1(x) + \ldots + a_L\mu_L(x) + Z(x) \;\Big|\; \begin{pmatrix} F(x^1) = f(x^1) \\ \ldots \\ F(x^m) = f(x^m) \end{pmatrix}$$

$$\Rightarrow \boxed{\left[F(\boldsymbol{x}^{\text{new}}) \mid F(\boldsymbol{x}) = f(\boldsymbol{x})\right] \sim \mathrm{N}\left(m_k(\boldsymbol{x}^{\text{new}}), C_k(\boldsymbol{x}^{\text{new}})\right)}$$

m_k and C_k are analytically known.

For example if the linear trend is known (simple kriging) :

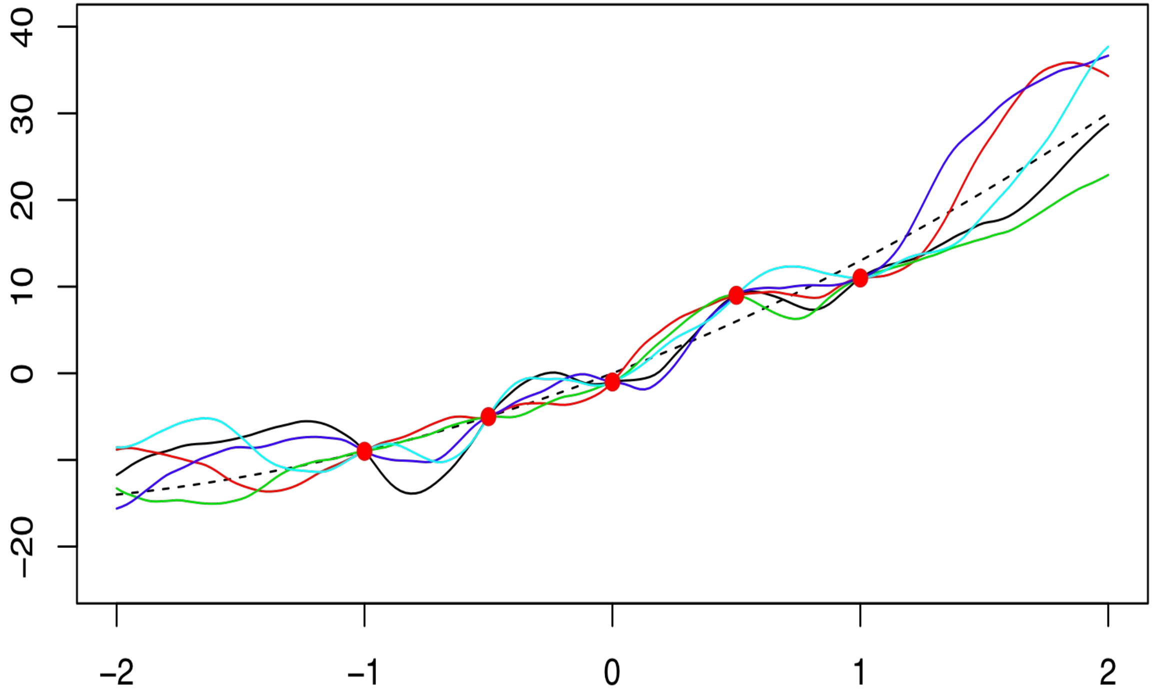
$$m_k(\boldsymbol{x}^{\text{new}}) = \mu(\boldsymbol{x}^{\text{new}}) + c^T(\boldsymbol{x}^{\text{new}})\, C^{-1}\left(f(\boldsymbol{x}) - \mu(\boldsymbol{x})\right)$$
$$C_k(\boldsymbol{x}^{\text{new}}) = C(\boldsymbol{x}^{\text{new}}) - c^T(\boldsymbol{x}^{\text{new}})\, C^{-1} c(\boldsymbol{x}^{\text{new}})$$

Kriging example

Red bullets are calculated points, $\left(x_i, f\left(x_i\right)\right)$

Paths of $\left[F\left(\boldsymbol{x}^{\mathbf{new}}\right) \mid F\left(\boldsymbol{x}\right)=f\left(\boldsymbol{x}\right)\right]$ in colour,

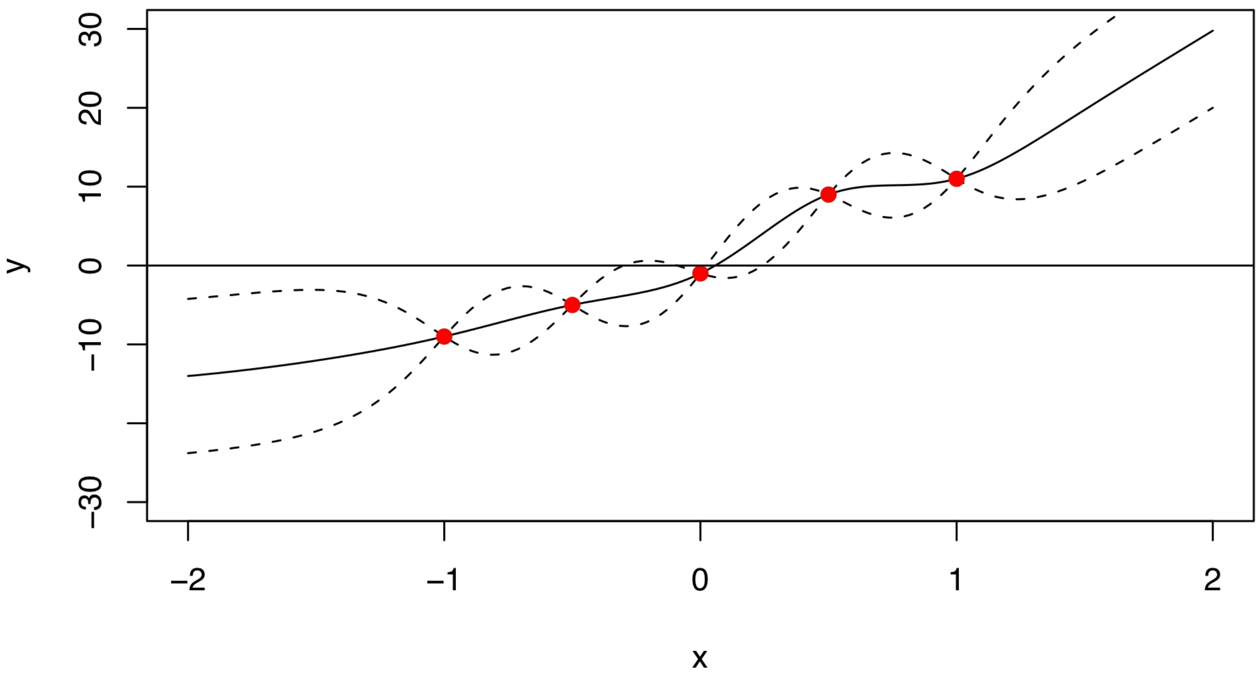
$\mu\left(x\right)$ black dotted line.



Kriging example

$m_k(x)$, kriging average, black line,

$\pm s_k(x)$, $\pm$std dev. prediction interval, dotted lines.

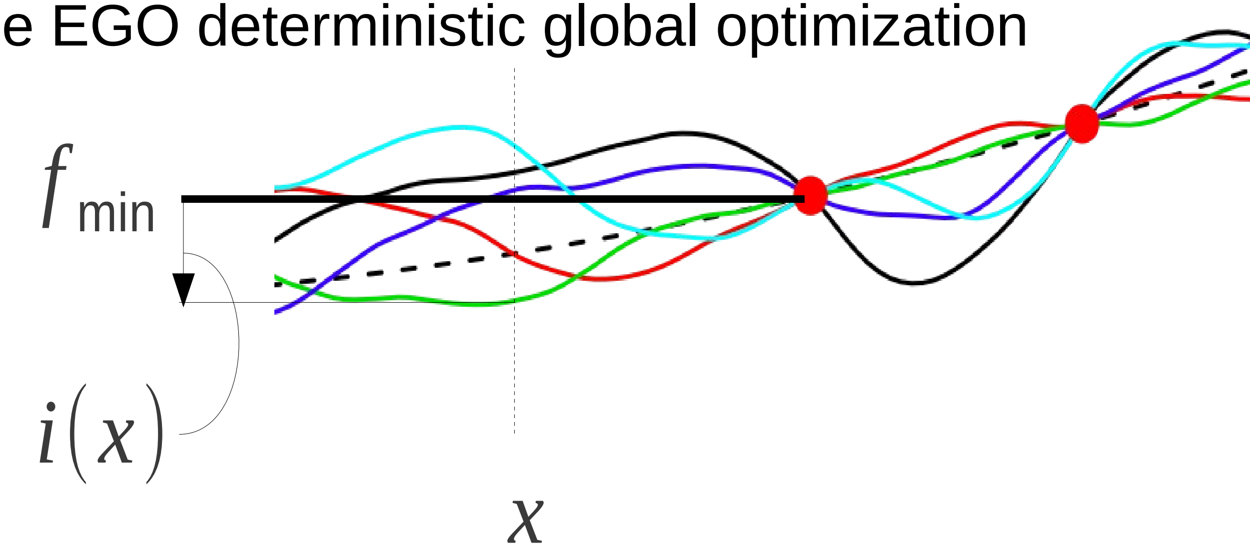


(one point-) Expected improvement

A natural measure of progress : the improvement,

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

- 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 (D. Jones, 1998).
  (sequential)

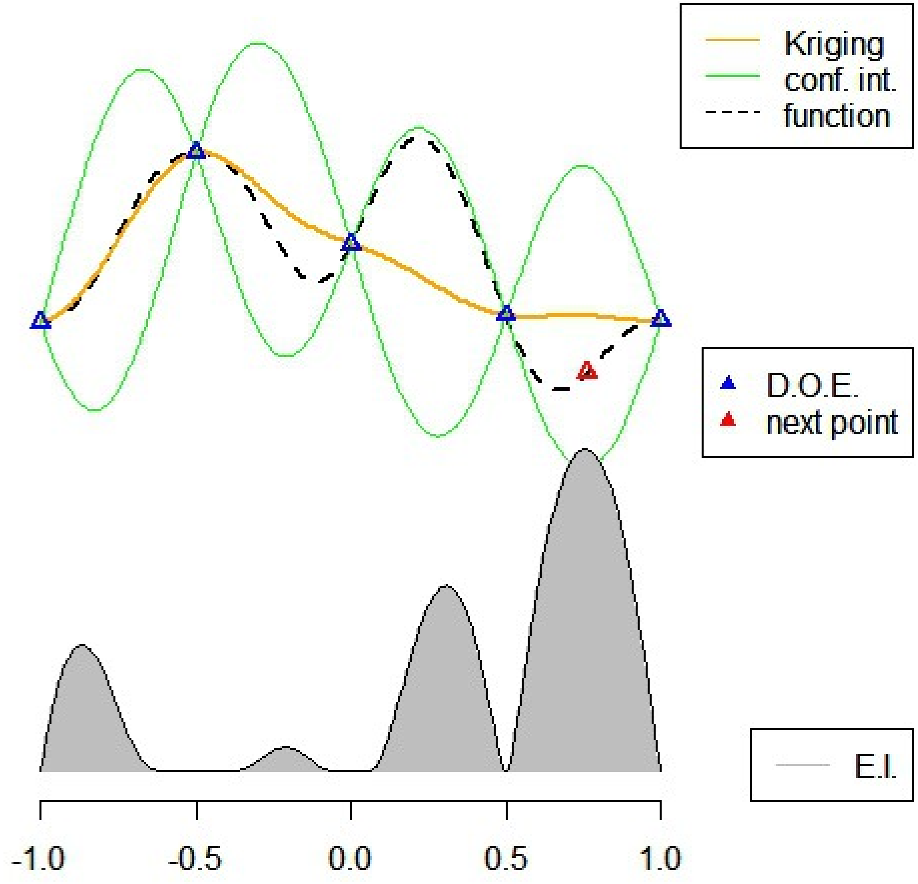


$$EI(x) = s_k(x) \times \left(u(x)\Phi(u(x)) + \varphi(u(x))\right) \quad , \quad \text{where } u(x) = \frac{f_{\min} - m_k(x)}{s_k(x)}$$

One EGO iteration

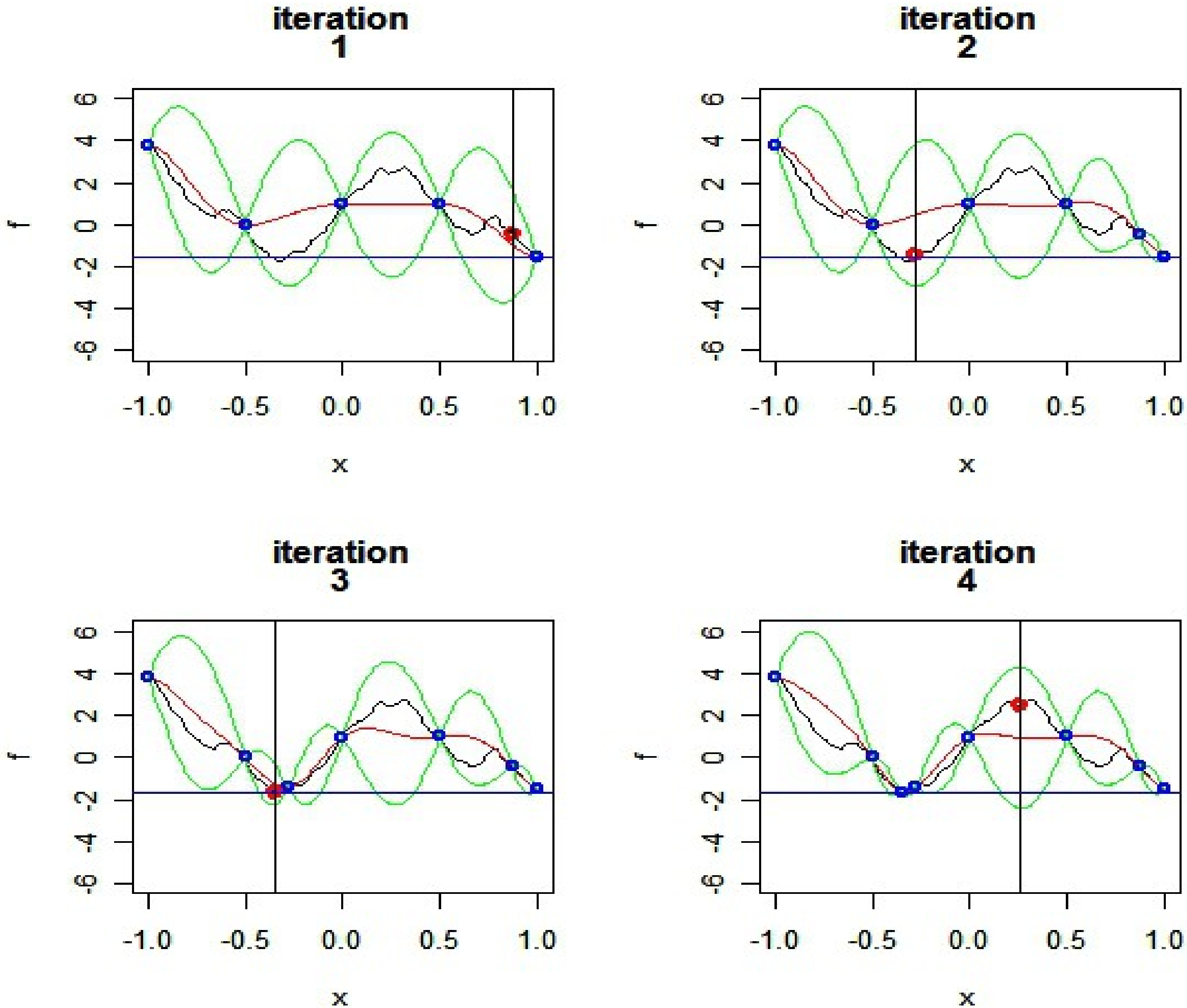
At each iteration, EGO adds to the t known points the one that maximizes EI,

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



then, the kriging model is updated ...

EGO : example


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

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5. An agent-based dynamic partitioning algorithm

From EGO to asynchronous parallel EI algorithm Selected bibliography of the team

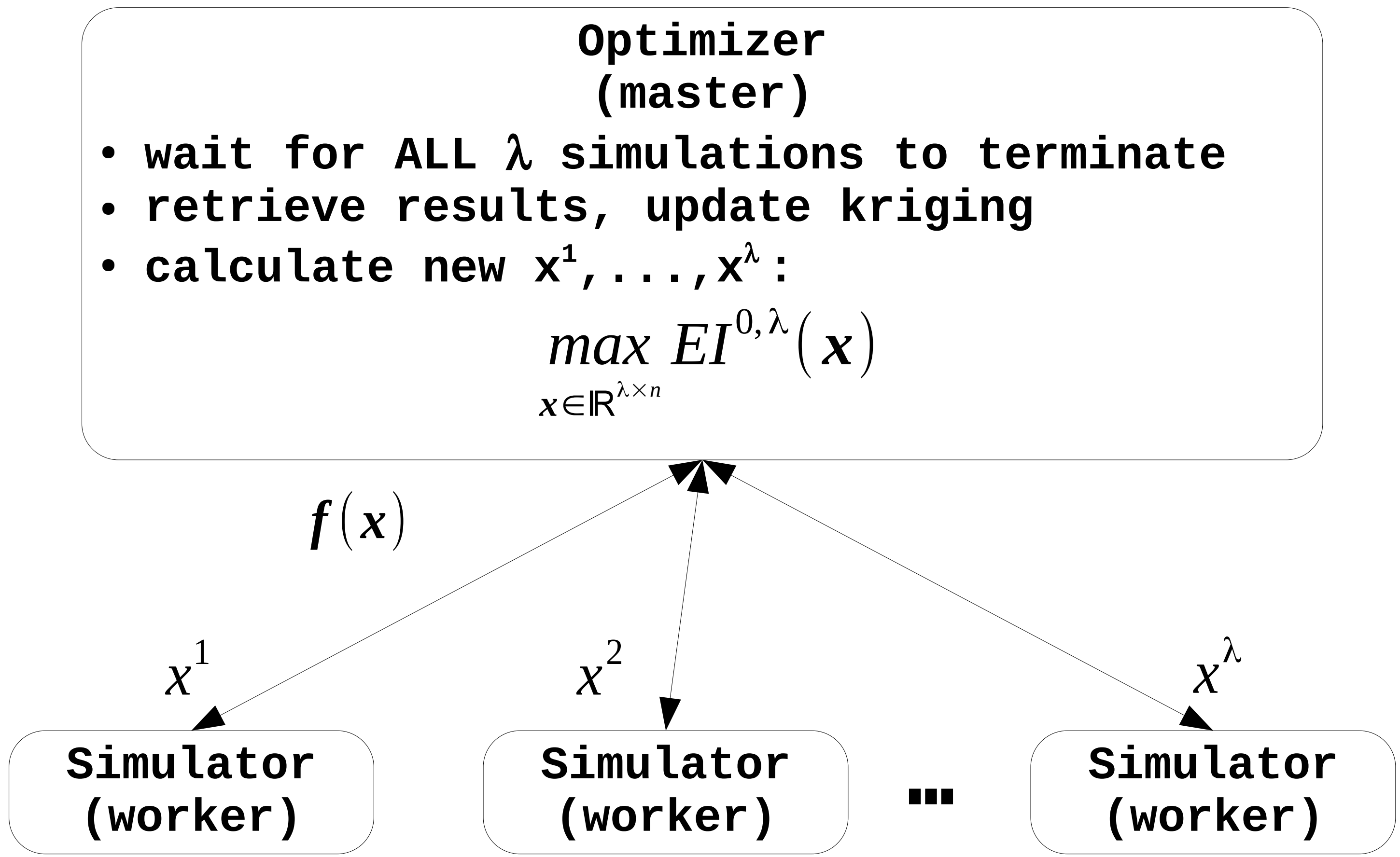
• D. Ginsbourger, R. Le Riche and L. Carraro, Kriging is well-suited to parallelize optimization, CIEOP, 2010.

• D. Ginsbourger, J. Janusevskis and R. Le Riche, Dealing with asynchronicity in parallel Gaussian Process based global optimization, Technical report hal-00507632, 2010.

• Janusevskis, J., Le Riche, R., Ginsbourger, D. and R. Girdziusas, Expected improvements for the asynchronous parallel global optimization of expensive functions : potentials and challenges, to be published in Learning and Intelligent Optimization, selected articles from the LION 6 Conference (Paris, Jan. 16-20, 2012), LNCS 7219, Lecture Notes in Computer Science series, Springer Verlag, Aug. 2012

Synchronous parallel EI : flow chart

A master-worker structure between computing nodes :



Synchronous parallel EI : criterion

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

→ choose $\boldsymbol{x}$ so that they maximize the synchronous λ points EI

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

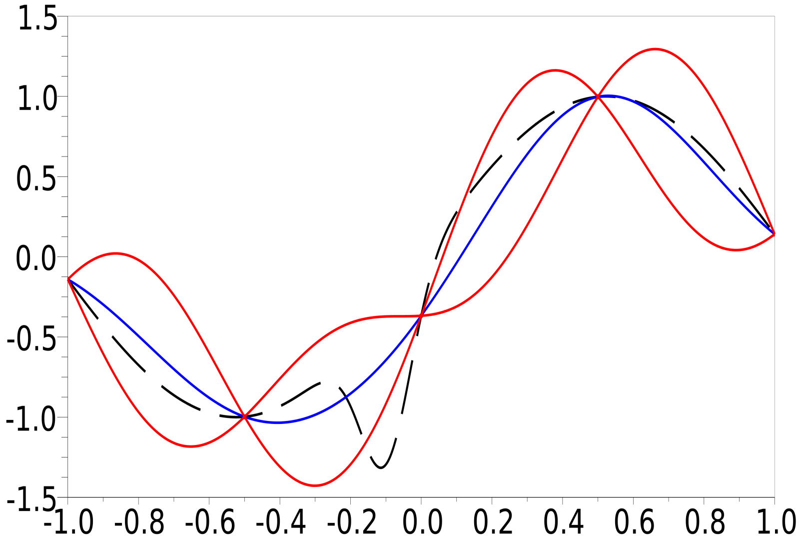
Compare to the sequential 1 point EI, from the EGO algorithm :

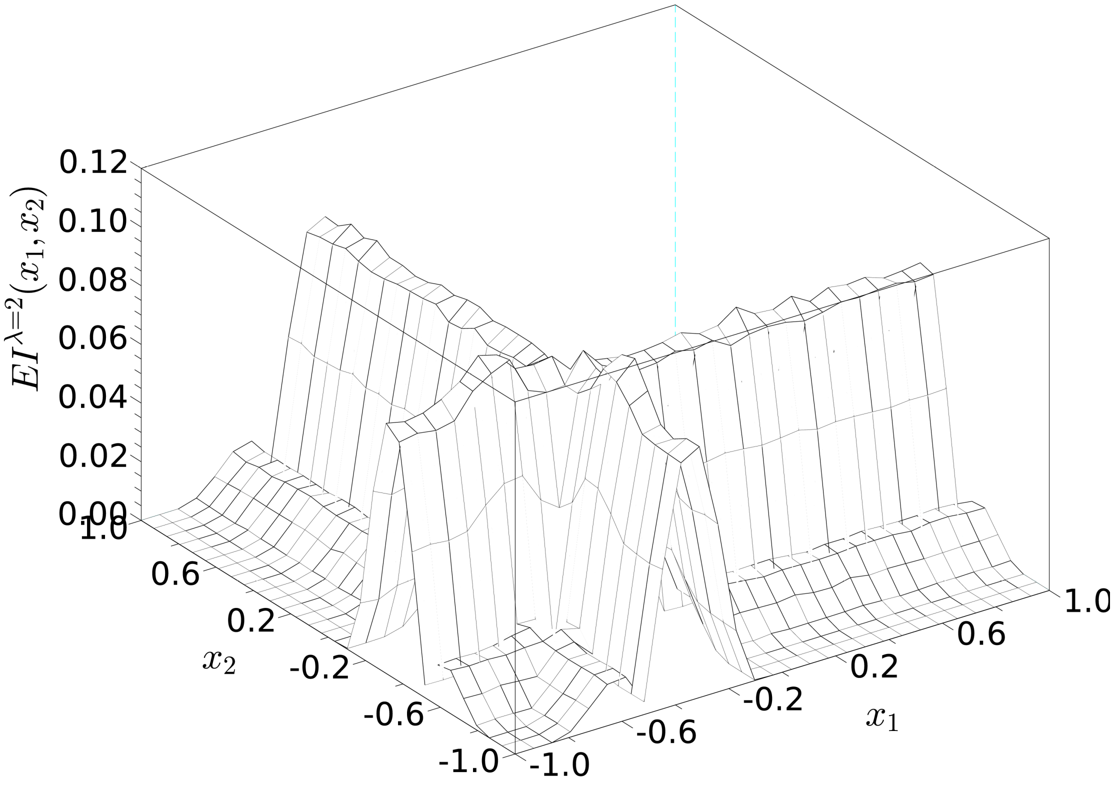
$$EI(x) \equiv EI^{0,1}(x) = E\left[f_{\text{min}} - F(x)\right]^+ \mid F(x^{1\ldots m}) = f(x^{1\ldots m})$$

Numerical estimation of $EI^{0,\lambda}$

$EI^{\mu,\lambda}$ not known analytically (excepted $EI^{0,1}$ and $EI^{0,2}$, recent efficient estimations by C. Chevalier and D. Ginsbourger at Bern Univ.) : Monte Carlo estimation.

Expl : 1D function (black dotted), $EI^{0,2}(x_{1,}\, x_2)$
10000 MC simulations



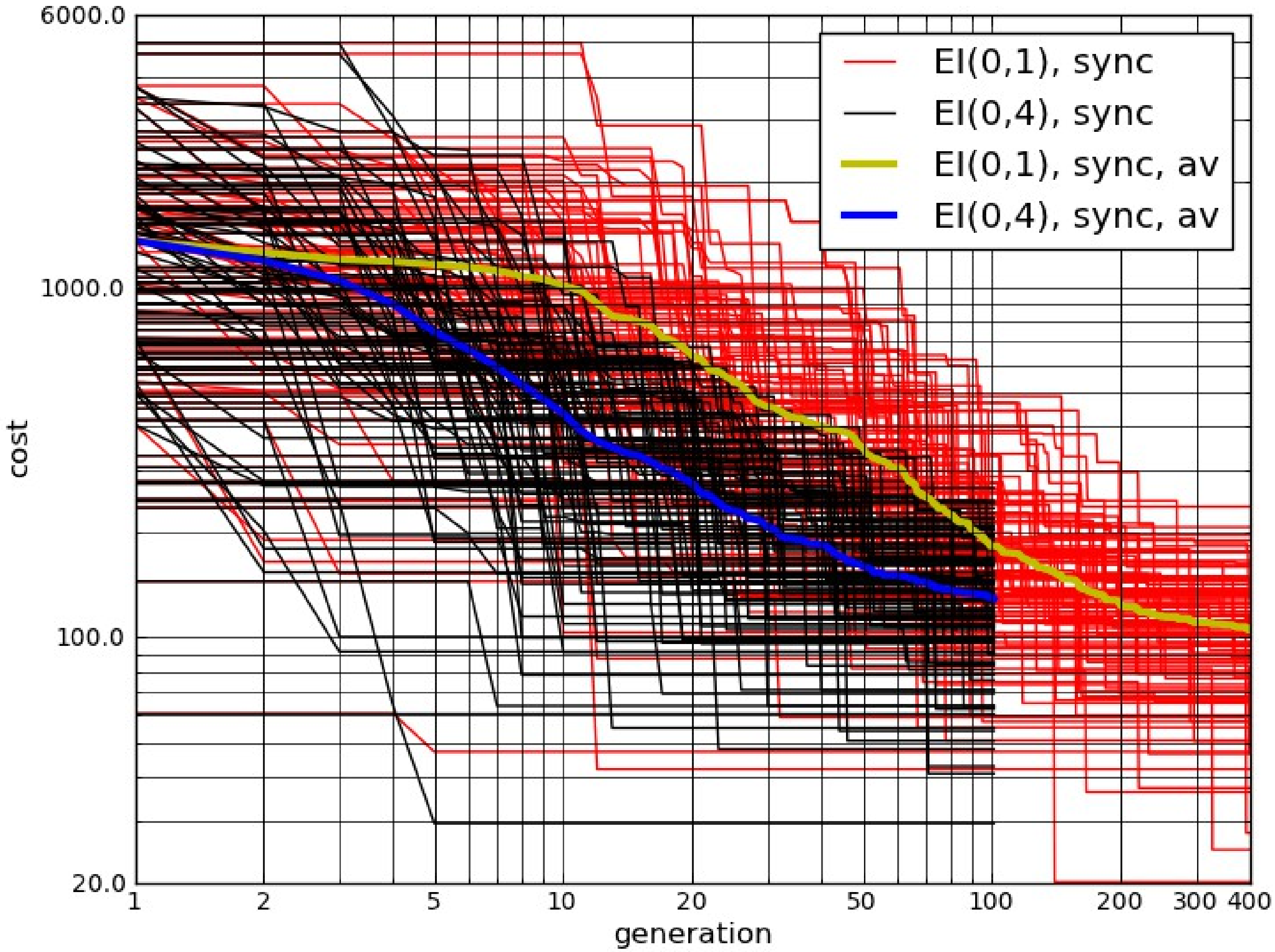


Test functions

Label	Cost function	Domain	Minimal value	Modality
"michalewicz2d"	$\sum_{i=1}^{2} \sin(x_i) \sin^2(i x_i^2/\pi)$	$[0,5]^2$	-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"	$\|\mathbf{A}_{4\times 5} - \mathbf{x}_{1\ldots 4}\mathbf{x}_{5\ldots 9}^T\|_2,\, a_{ij} \sim U(0,1)^1$	$[-1,1]^9$	0.712	bimodal

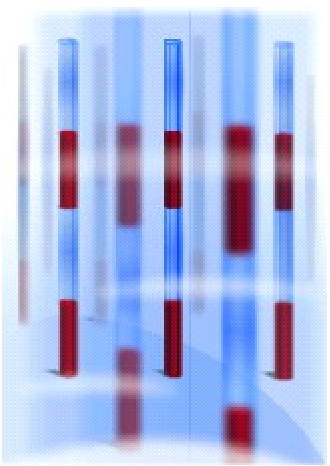
Results with $EI^{0,\mu}$

(6D Rosenbrock function)

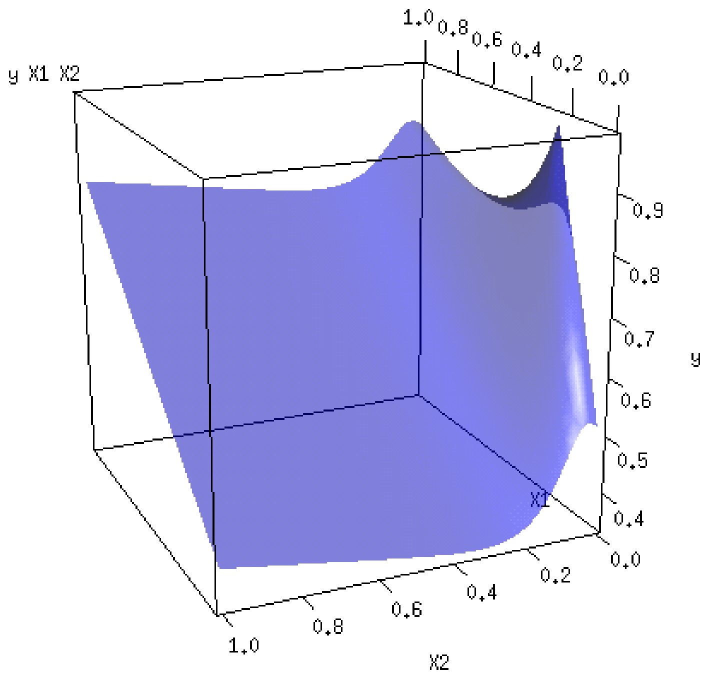


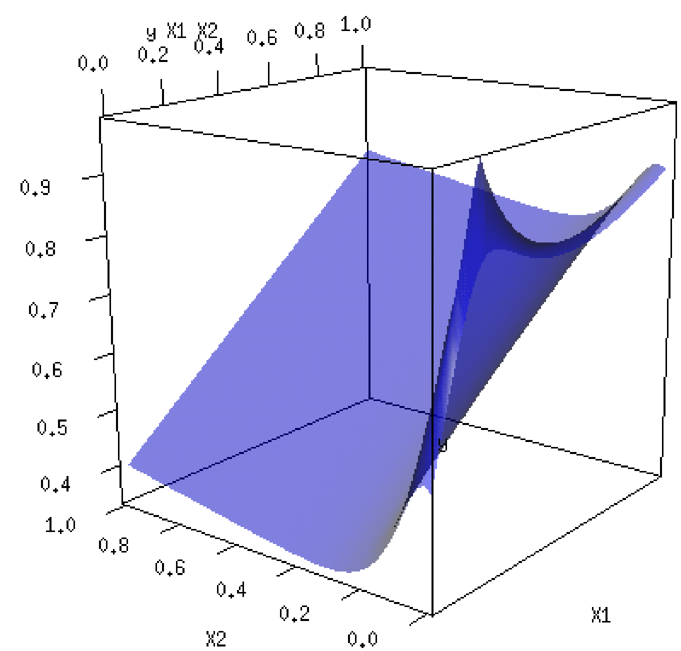
Results with $EI^{0,\lambda}$: nuclear safety test case

(from Yann Richet, IRSN)



- Maximization of 2D criticality model to check safety.
- Plutonium powder in storage can arrays ==> neutronic interaction between neutronic cans.
- x_1 : density of water between cans
- x_2 : density of plutonium powder
- Y : neutronic reactivity of the system (>1.0 means uncontrolled chain reaction, to be avoided)
- « true » maximum is ~0.99 .



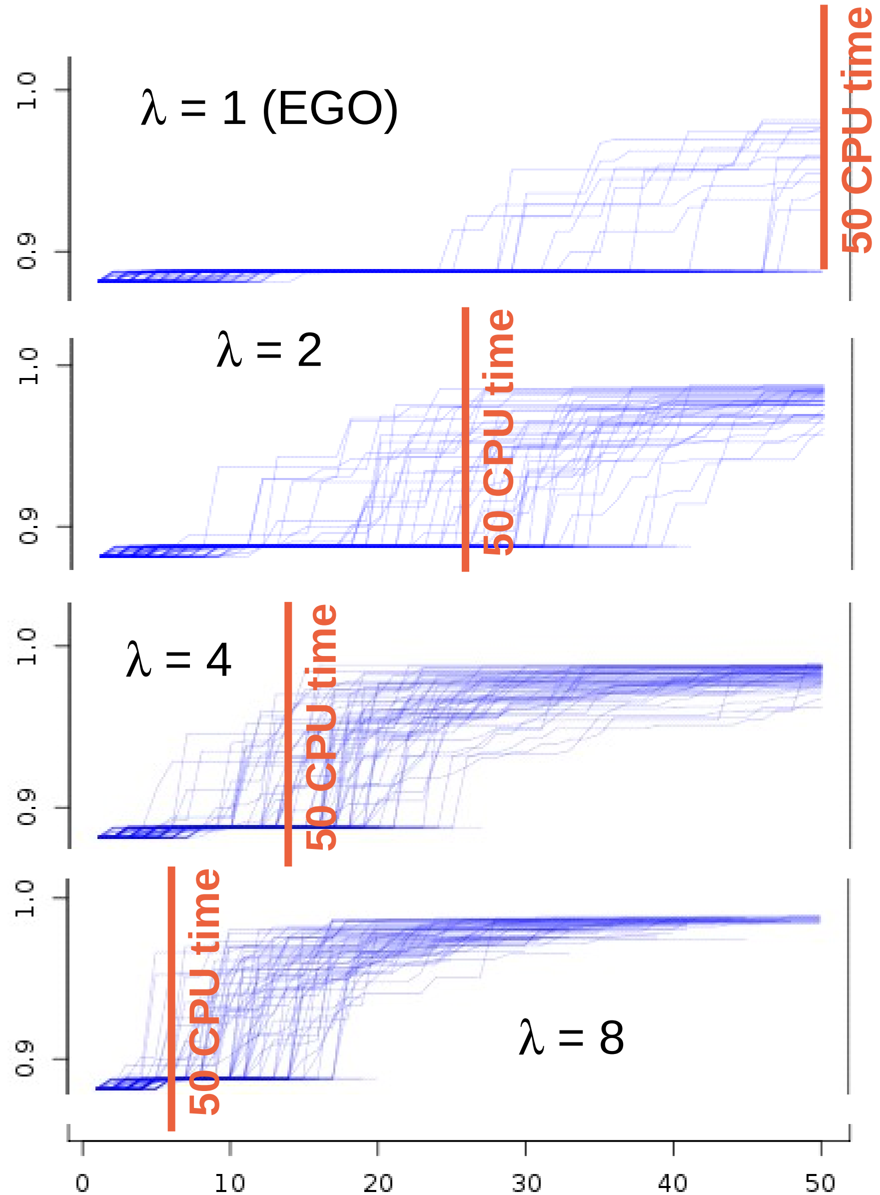


Results with $EI^{0,\lambda}$: nuclear safety test case

(from Yann Richet, IRSN)

100 EGO runs with different starting LHS (9 points + 4 corners)

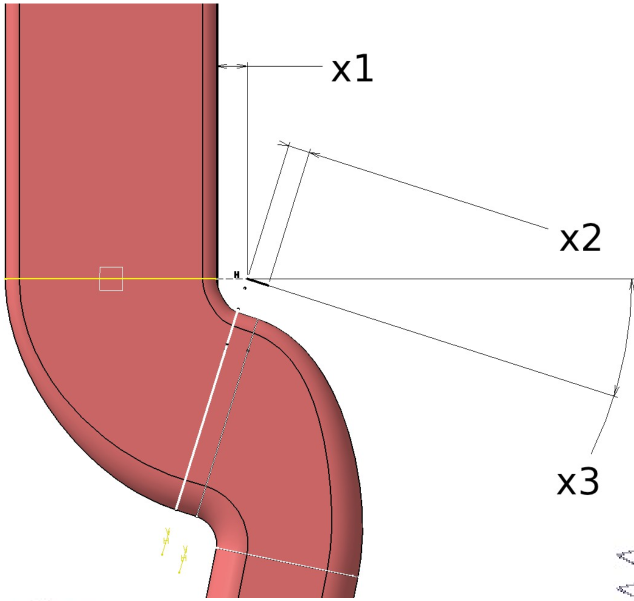
End EGO when
either max(EI(x)) <1.e-20
or > 50 iterations

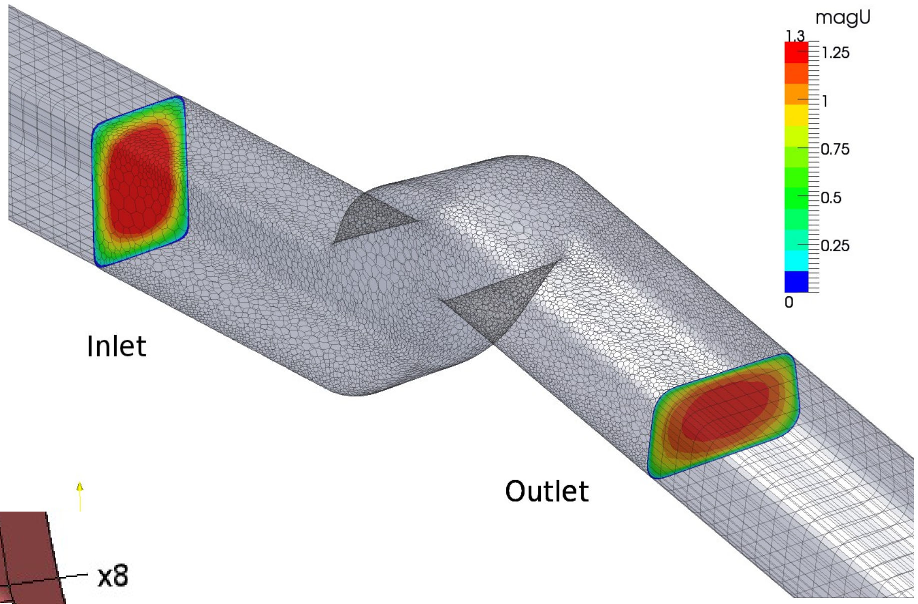


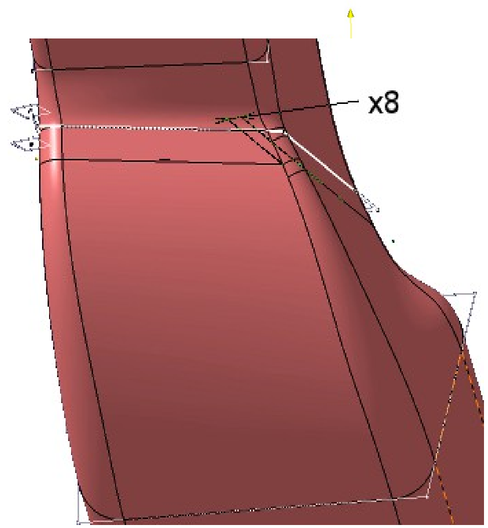
generations ~ wall clock time
if little T spread

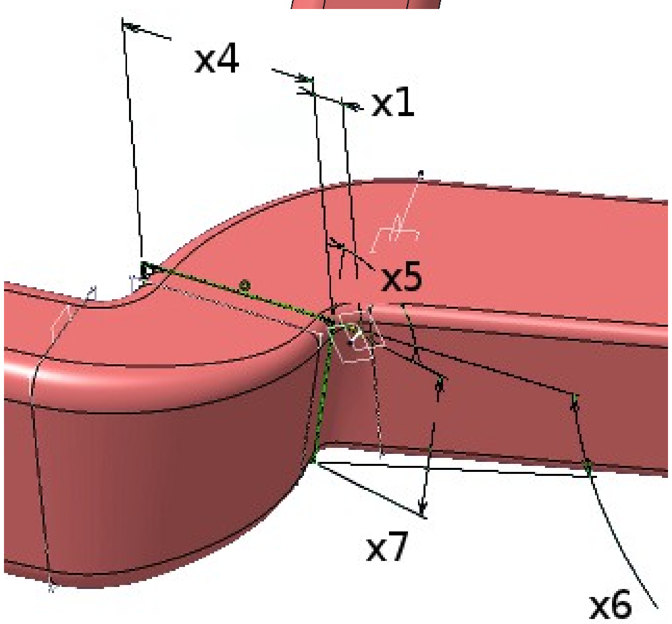
Results with $EI^{0,\lambda}$: air duct design (1)

(from ANR / OMD2 project)









$\boldsymbol{min_{x1,\ldots,x8}}$ pressure loss

viscous, turbulent, incompressible flow (Re=4000, ν=1.6 10^{-4} m^2/s)

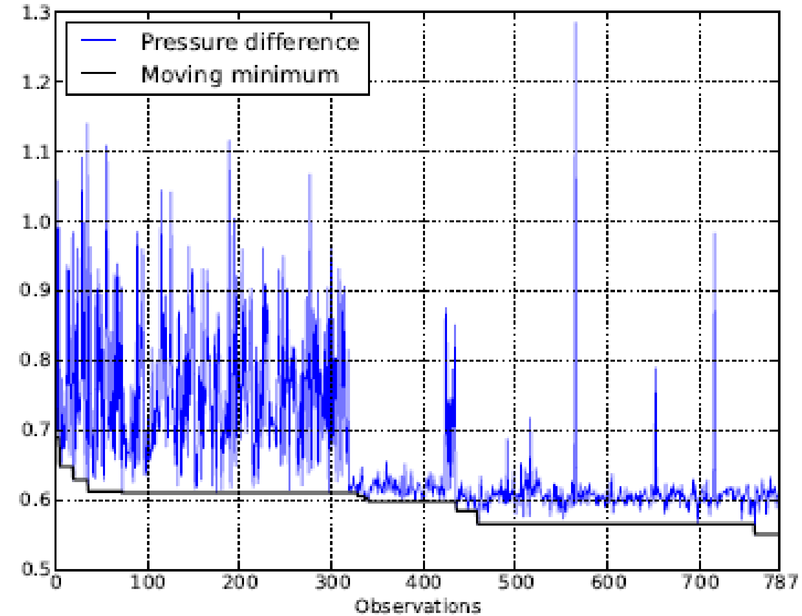
Complete simulation workflow :
Catia (CAO) + StarCCM (mesh) + Openfoam (FE analysis), from 15 to 40 min.
Run on PACA Grid.

Results with $EI^{0,\lambda}$: air duct design (2)

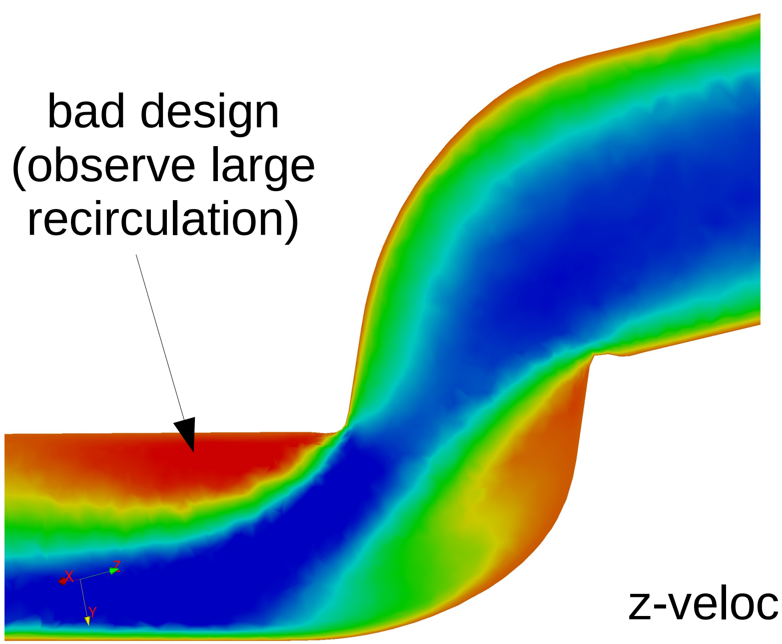
λ=4
320 LHS points in initial DOE

Simulation crashes : from 15 % at the beginning to 60 % at the end.

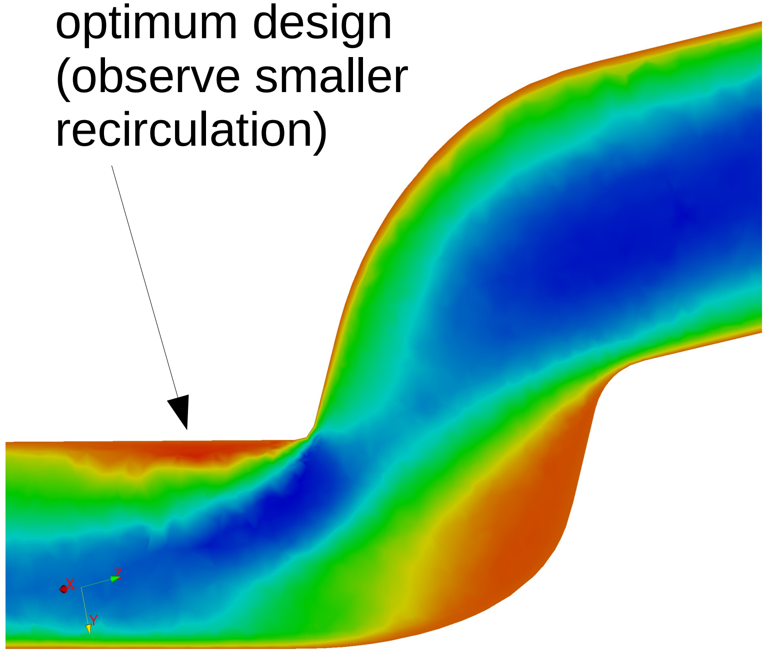
← multi-points EI are more robust to simulation crashes than single point EI.



bad design (observe large recirculation)



optimum design (observe smaller recirculation)



z-velocity maps

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

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 , $T \sim U[t_{min}, t_{max}]$

$t_O =$ time for 1 optimization

T_{WC} : wall clock time for 1 generation

$$T_{WC} = t_O + \max_{i=1,\lambda}(t^i) \quad , \quad E(T_{WC}) = t_O + \frac{\lambda}{\lambda+1}(t_{max} - t_{min}) + t_{min} \sim O(t_O + t_{max})$$

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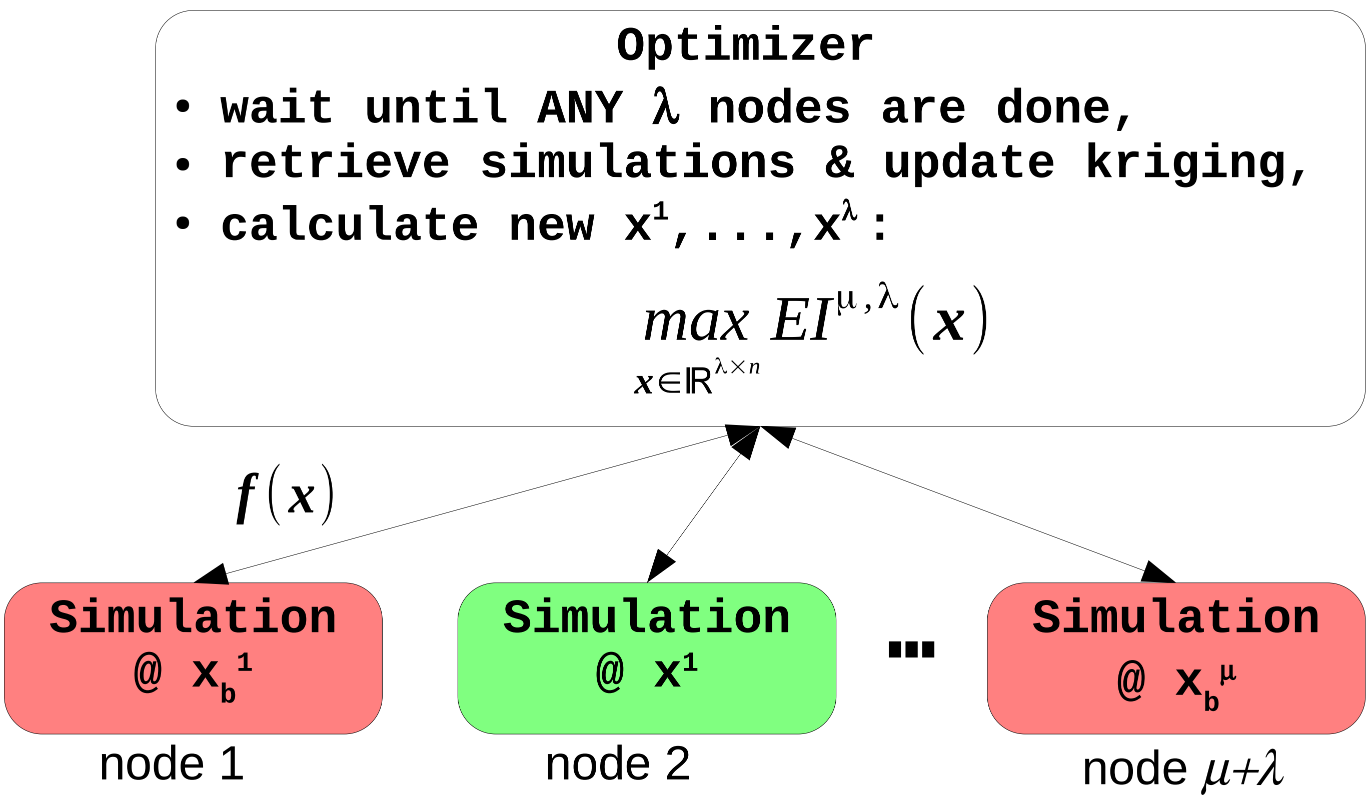
Asynchronous parallel EI : flow chart

- 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).

- $EI^{\mu,\lambda}$ takes full account of past and on-going simulations.



Asynchronous parallel EI : criterion

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

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

Recall the 1 point sequential EI and the synchronous EI :

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

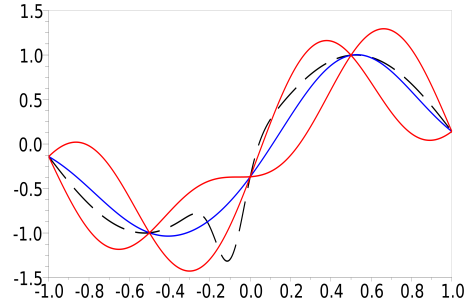
$$EI^{0,\lambda}(\boldsymbol{x}) = E\left[f_{\text{min}} - min\left(F(\boldsymbol{x})\right)\right]^+ \ | \ F(x^{1\ldots m}) = f(x^{1\ldots m})$$

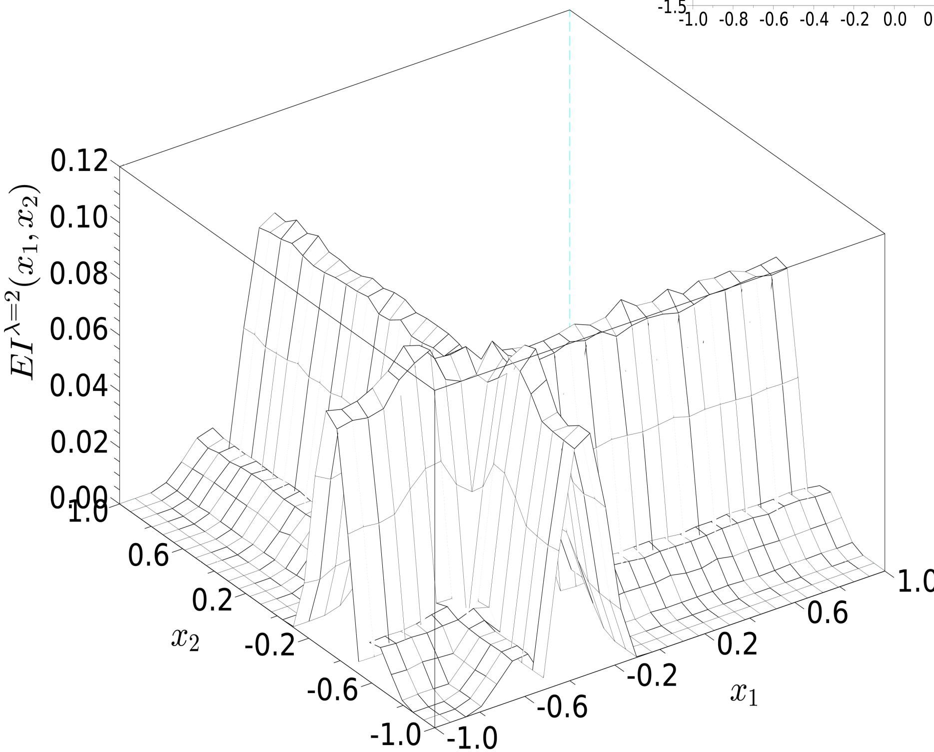
Property : $EI^{\mu,\lambda}(\boldsymbol{x}) \rightarrow 0^+$ as $\boldsymbol{x} \rightarrow \boldsymbol{x_b}$
(the search is pushed away from already sampled points which are being evaluated)

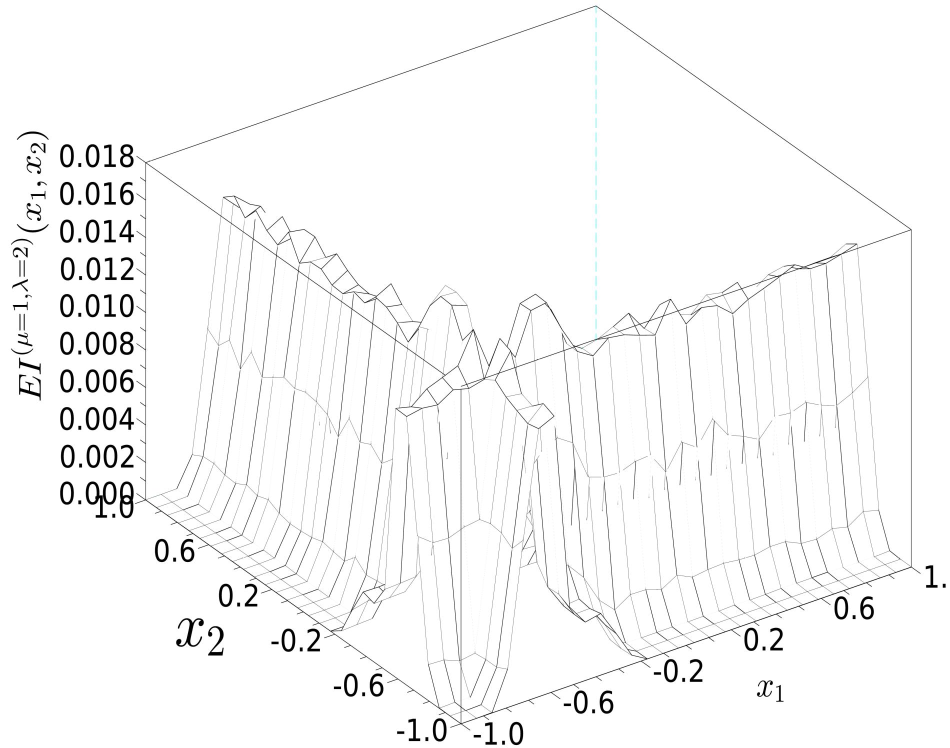
Numerical estimation of $EI^{\mu,\lambda}$

Expl : 1D function (black dotted), $EI^{1,2}(x_1, x_2)$, $x_b = -0.34$

10000 Monte Carlo simulations

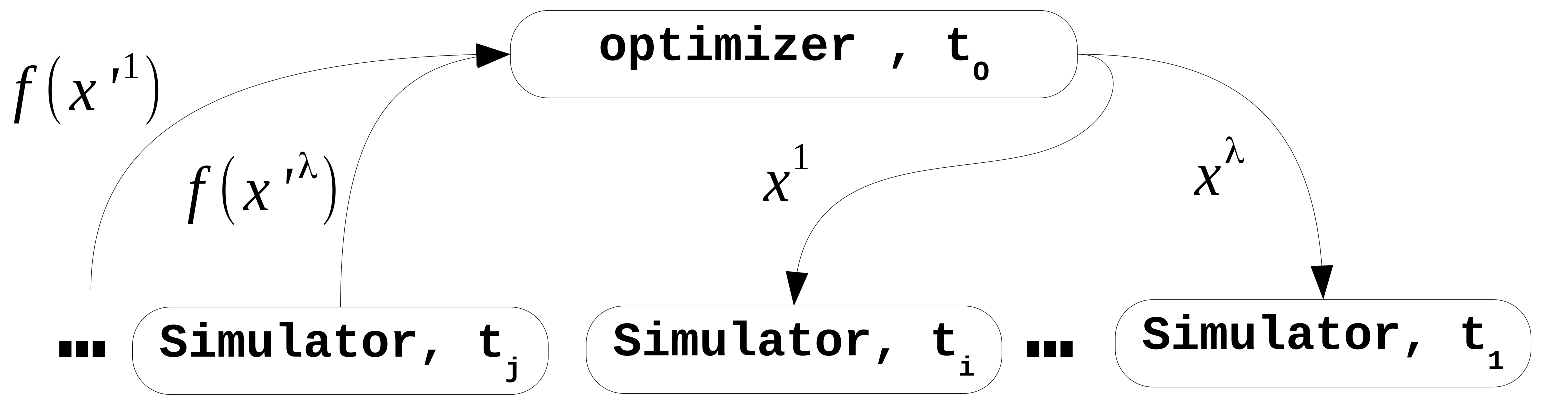






Time model of $EI^{\mu,\lambda}$ (1)

If time simulations $\gg$ time optimizer, use $EI^{\mu,1}$,
if time simulations $\ll$ time optimizer, use $EI^{0,\lambda}$,
otherwise, use $EI^{\mu,\lambda}$ for task allocation.



$M=\lambda+\mu$ nodes
T : time for 1 simulation, random variable , $T\sim U[t_{min}, t_{max}]$
t_O = time for 1 optimization

T_{WC} : wall clock time for 1 generation. Model :
$T_{WC} = t_O + t_{\lambda:M}$, then $t_{\lambda+1\ldots M:M} \leftarrow max[0 , t_{\lambda+1\ldots M:M} - T_{WC}]$

Time model of $EI^{\mu,\lambda}$ (2)

$M = \lambda + \mu$ nodes

T : time for 1 simulation, random variable, $T \sim U[t_{min}, t_{max}]$, $t_{min} = 10$

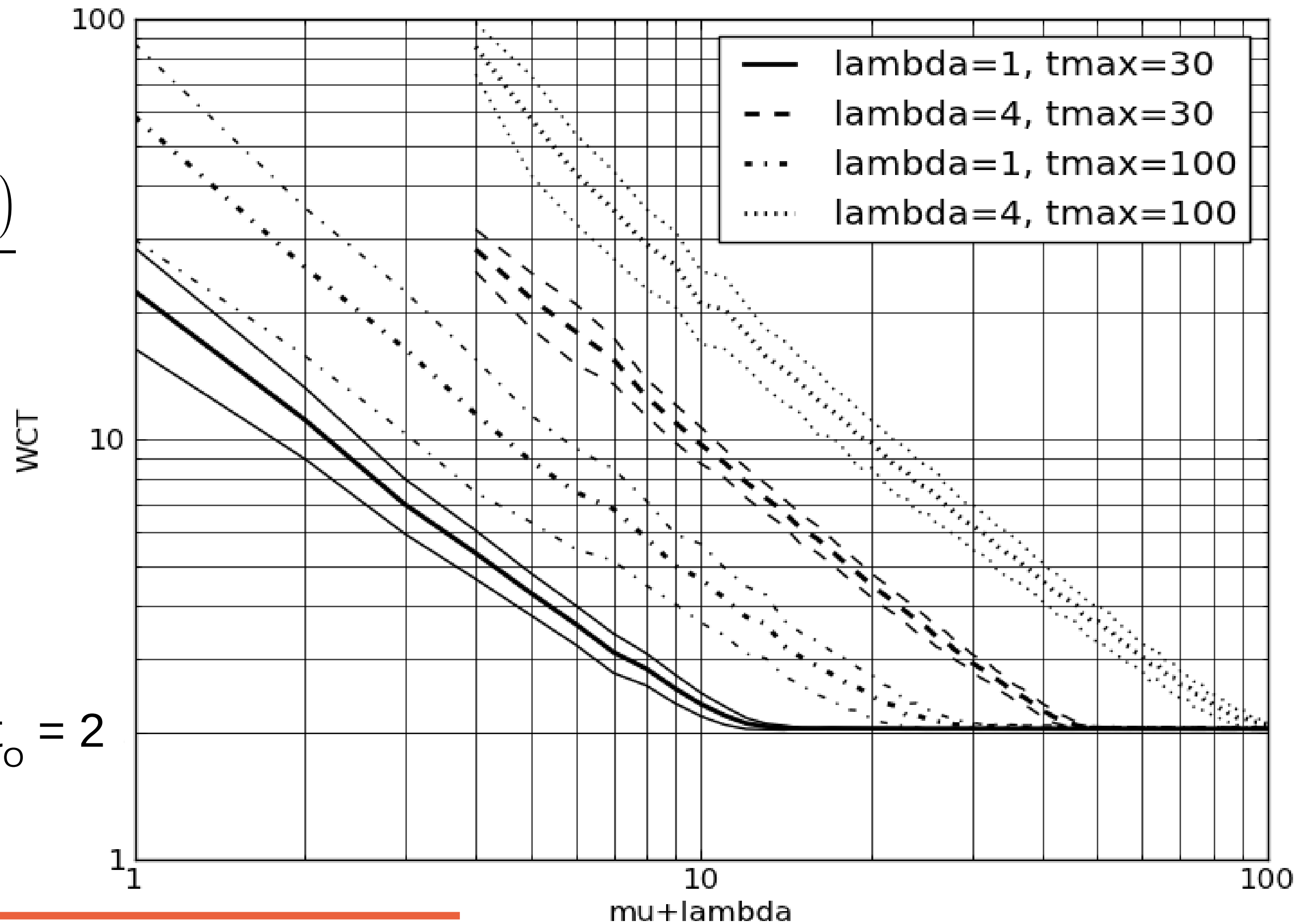
t_O = time for 1 optimization

T_{WC} : wall clock time for 1 generation. Model :

$T_{WC} = t_O + t_{\lambda:M}$, then $t_{\lambda+1\ldots M:M} \leftarrow max[0 \, , \, t_{\lambda+1\ldots M:M} - T_{WC}]$

$$E(T_{WC}) \approx t_O + \frac{E(T_{\lambda:M})}{M}$$

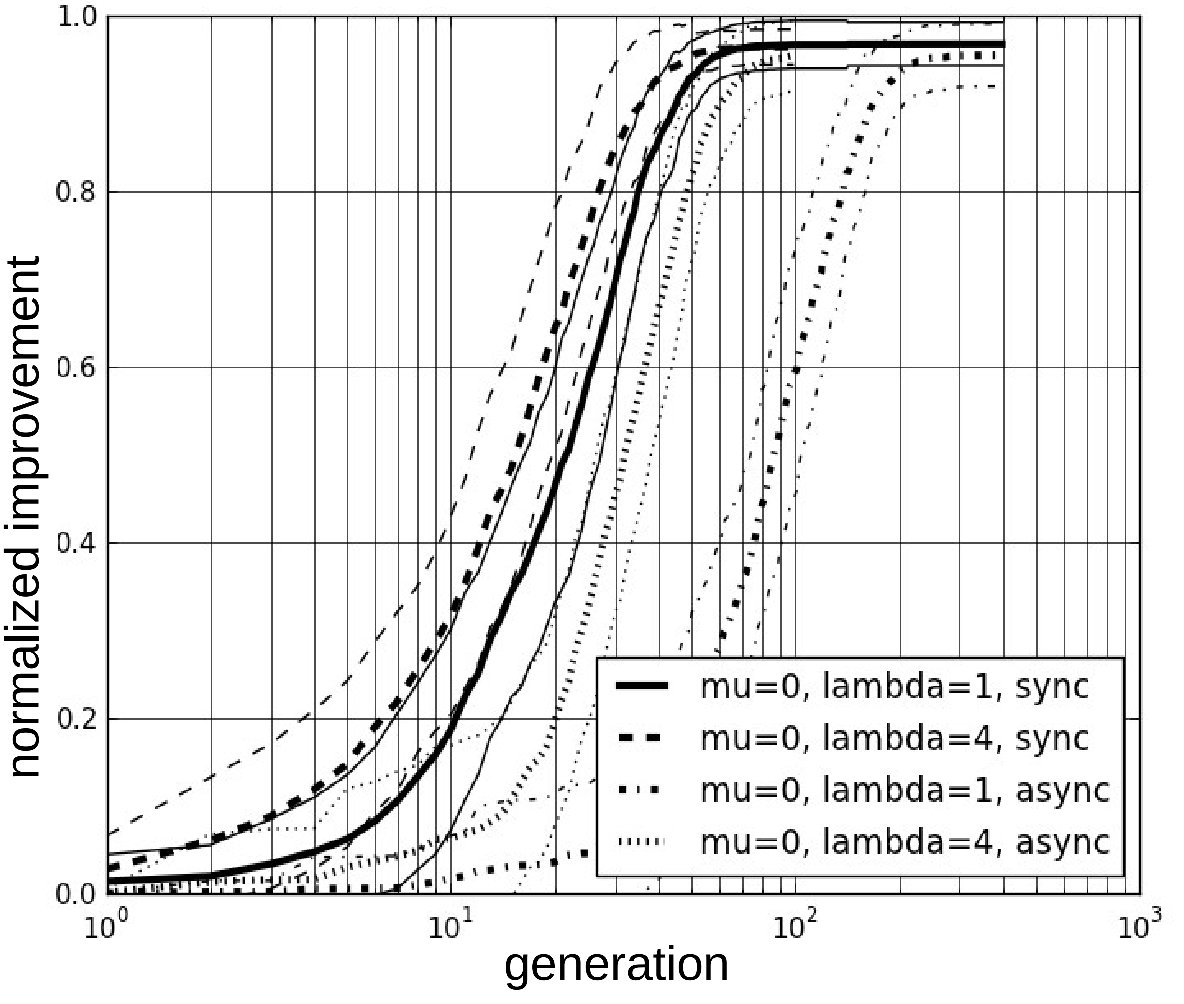
Scaling :
$E(T_{WC}) \underset{M\to\infty}{\to} t_O$



$t_O = 2$

Synchronous vs. asynchronous EI's (1)

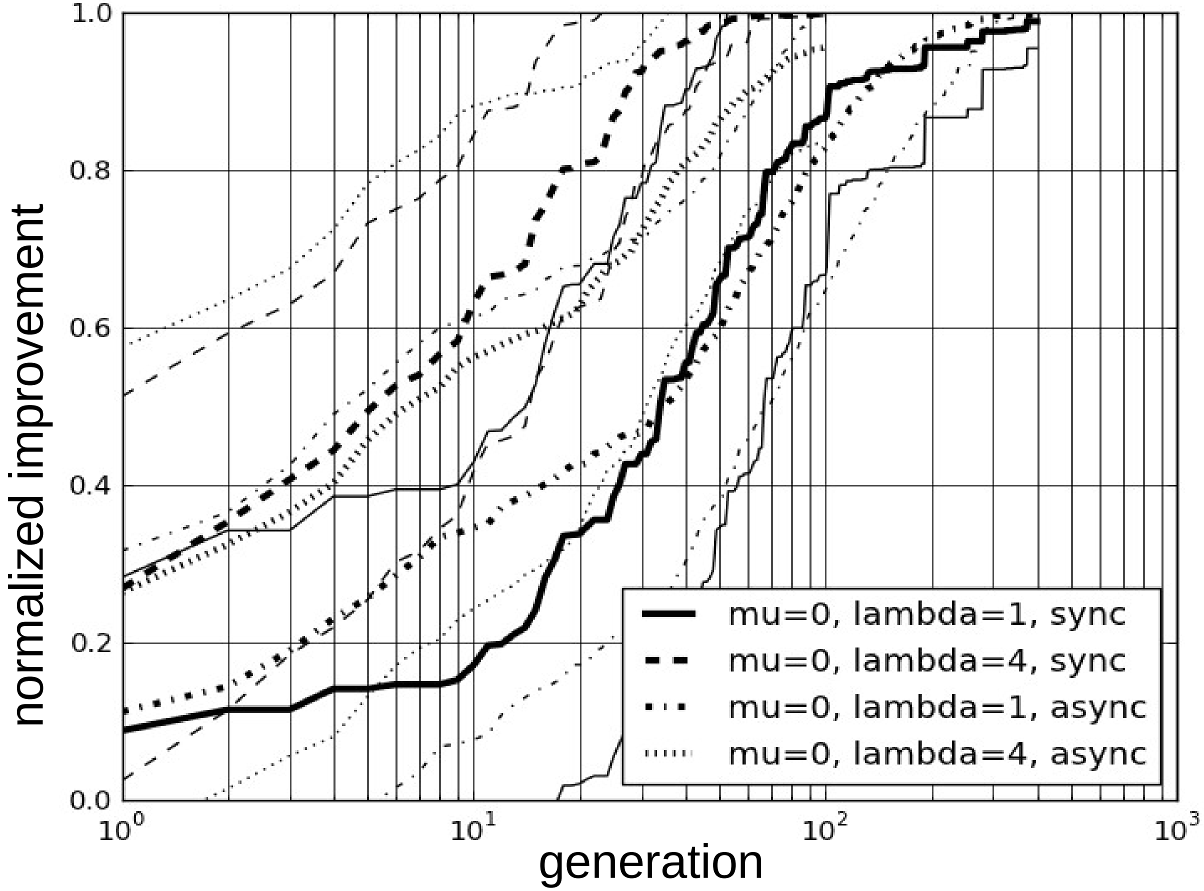
Ex : Rank1, 9D
(idem on Michalewicz
2D and Rosenbrock 6D)



Generation wise, asynchrony slows down the search because all demanded points are not evaluated.
But the wall clock time is much lower (× 0.093 and 0.13 for λ=1 and 4, M=32)

Synchronous vs. asynchronous EI's (2)

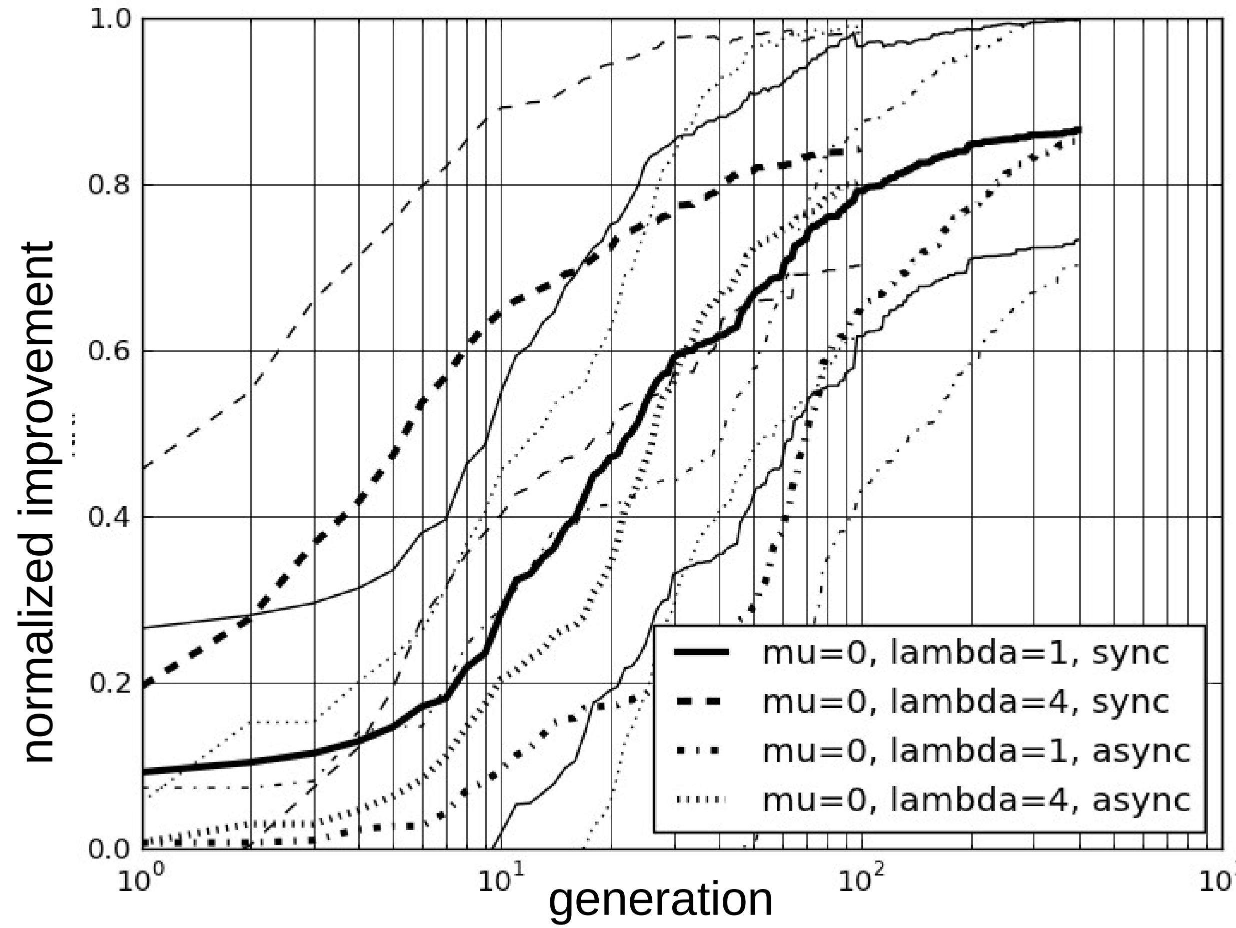
Ex : Michalewicz 2D



Generation wise, asynchrony slows down the search because all demanded points are not evaluated.
But the wall clock time is much lower (× 0.093 and 0.13 for λ=1 and 4, M=32)

Synchronous vs. asynchronous EI's (3)

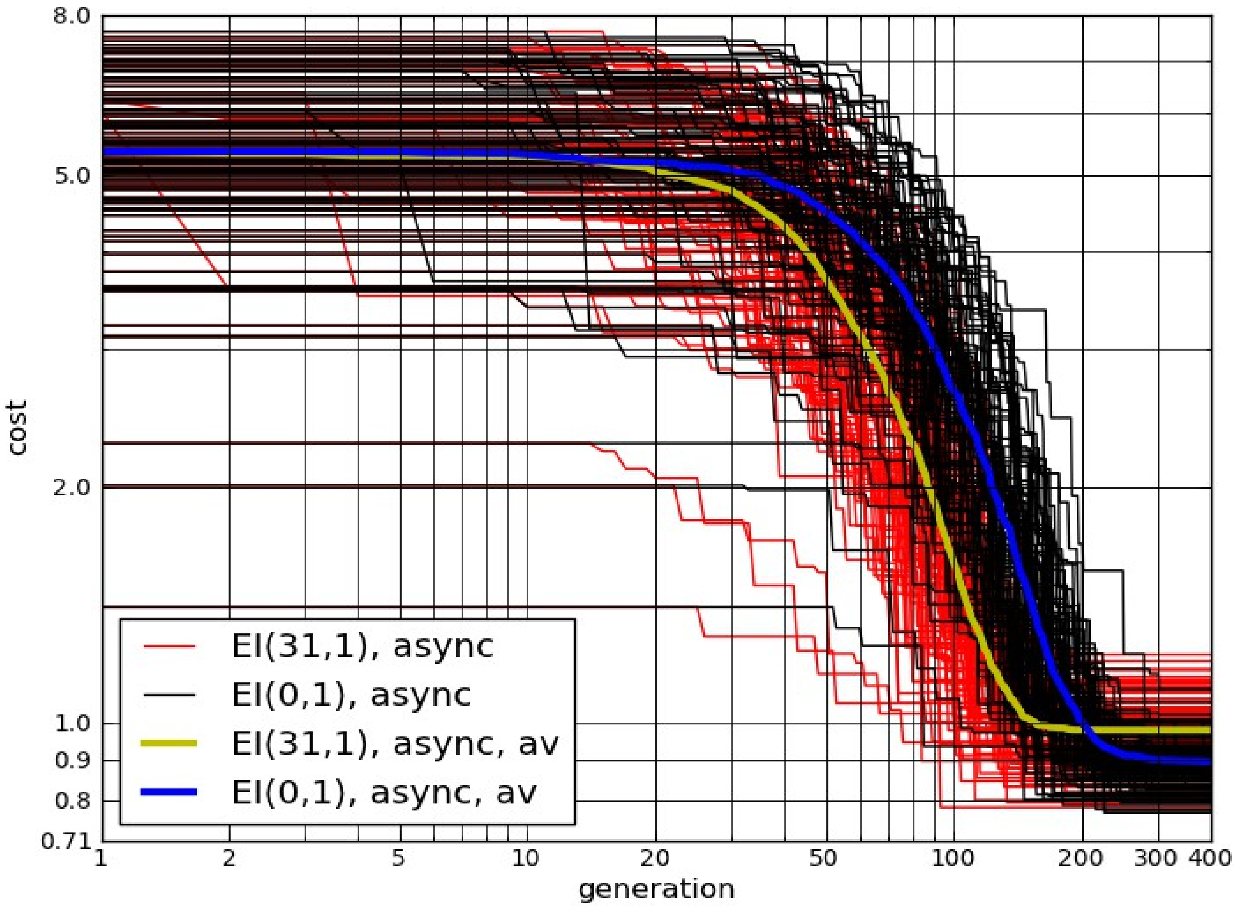
Ex : Rosenbrock 6D



Generation wise, asynchrony slows down the search because all demanded points are not evaluated.
But the wall clock time is much lower (× 0.093 and 0.13 for λ=1 and 4, M=32)

Effect of the μ busy points in $EI^{\mu,\lambda}$

100 runs, $EI^{0,1}$ asynchronous vs. $EI^{31,1}$ asynchronous, rank1 function in 9D



$EI^{31,1}$ is slightly faster than $EI^{0,1}$ because it avoids sending duplicates to the nodes for evaluation.

Partial conclusions

• We have presented an asynchronous parallel expected improvement algorithm for global optimization.

• Thanks to kriging and parallelization, it is adapted to computationally costly objective functions (and not adapted to high dimensions).

• It has a master-slave structure, with one optimizer only.

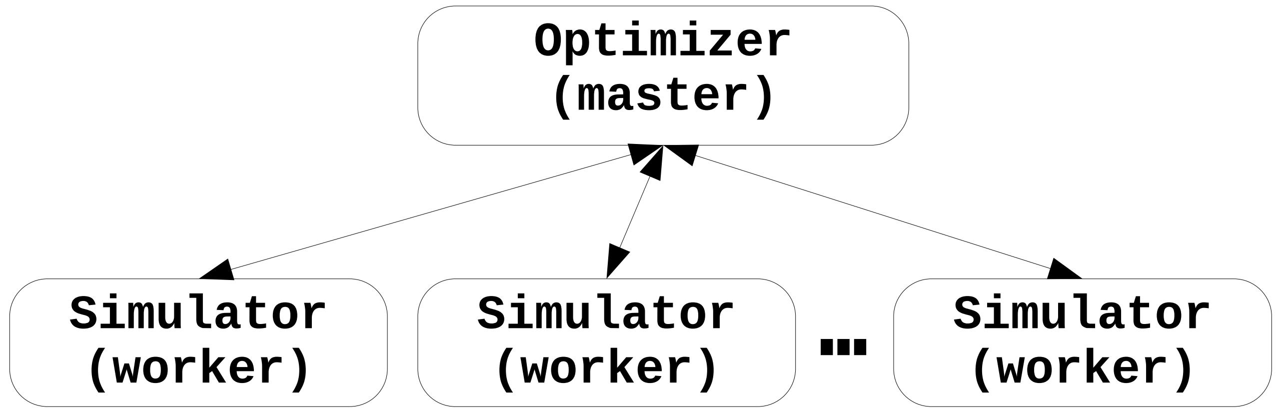
• Scaling : when the number of nodes increases the optimization time becomes the blocking factor.

• Solutions :
  • design fast mono-optimizers
  • **design algorithms with many optimizers.** ← **discussed next**

Algorithms with multiple optimizers

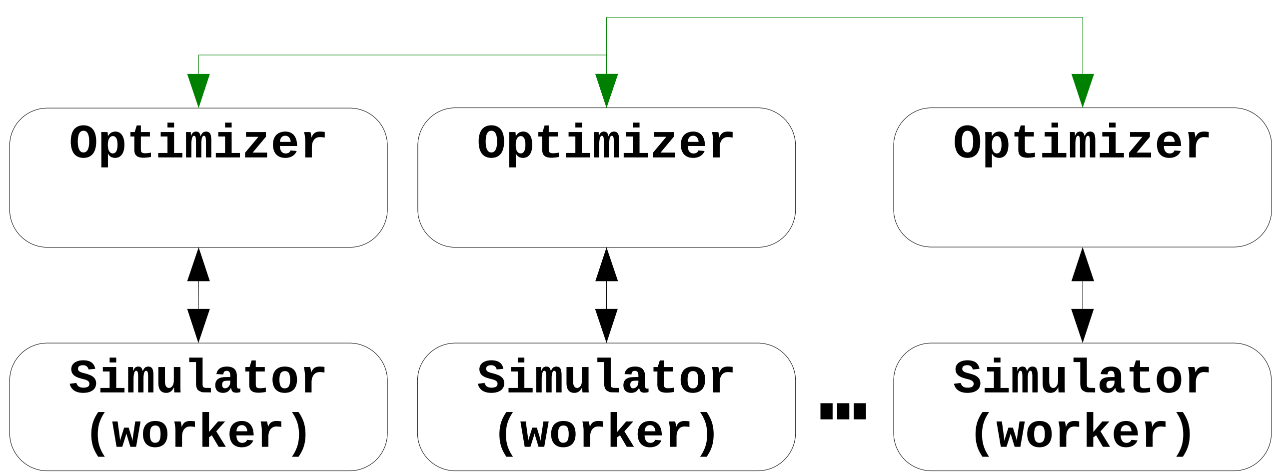
one optimizer

+ : decision with all information and ressources
- : t_o does not scale with M



Many optimizers
with coordination

+ : both optimizer and simulators scale with M
- : decision with partial information / limited ressources

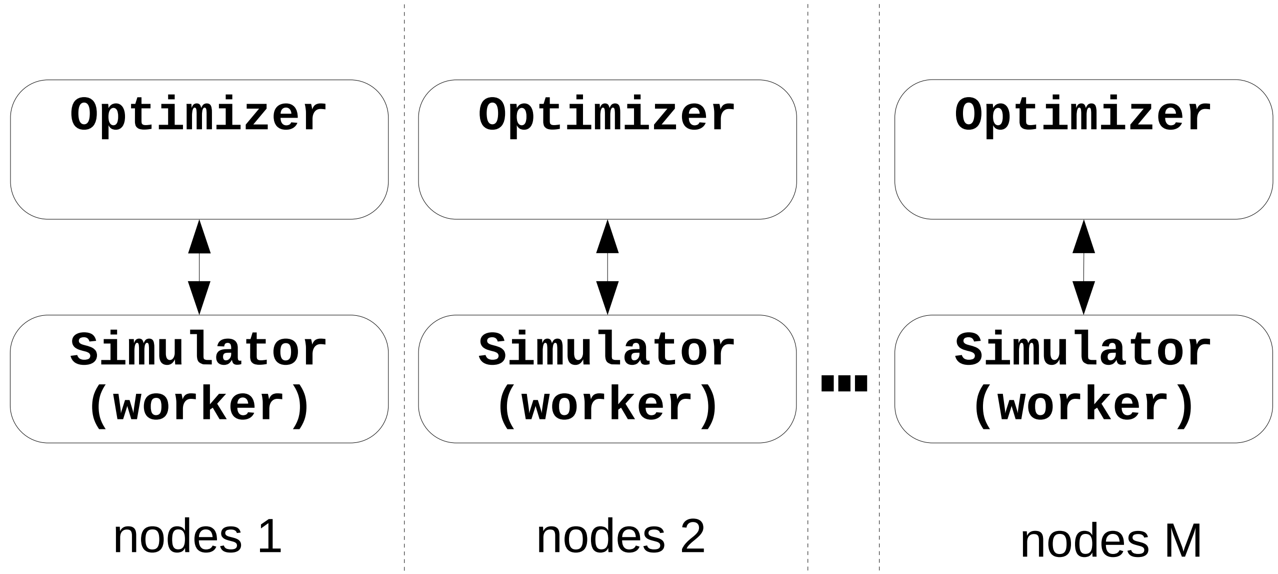


Outline of the talk

1. Introduction to kriging and optimization
2. Synchronous parallel EI
3. Asynchronous parallel EI
4. Embarrassingly parallel EI algorithms
5. An agent-based dynamic partitioning algorithm

Embarrassingly parallel EI algorithms

embarrassingly
=
no coordination

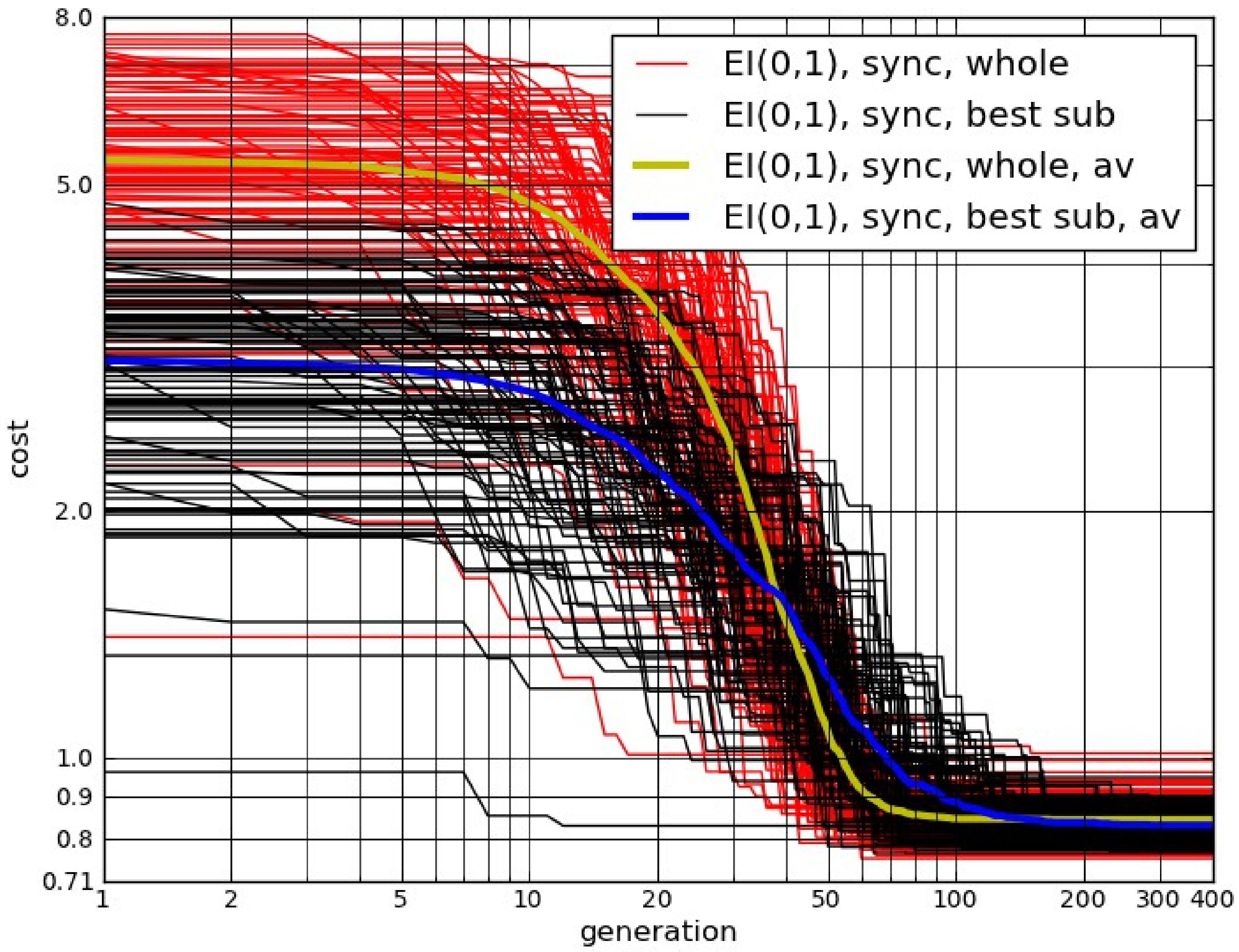


How to do it ?

• Change the initial DOE ← too costly (*size(DOE)* × *M* simulations to start).
• Divide the design space S into M fixed subdomains ← M-1 optimizations are useless, no observed gain.
• **Use M different covariance functions** ← interesting research direction.

Examples follow.

Fixed search space partition : example



9D Rank1 test function, 100 runs.

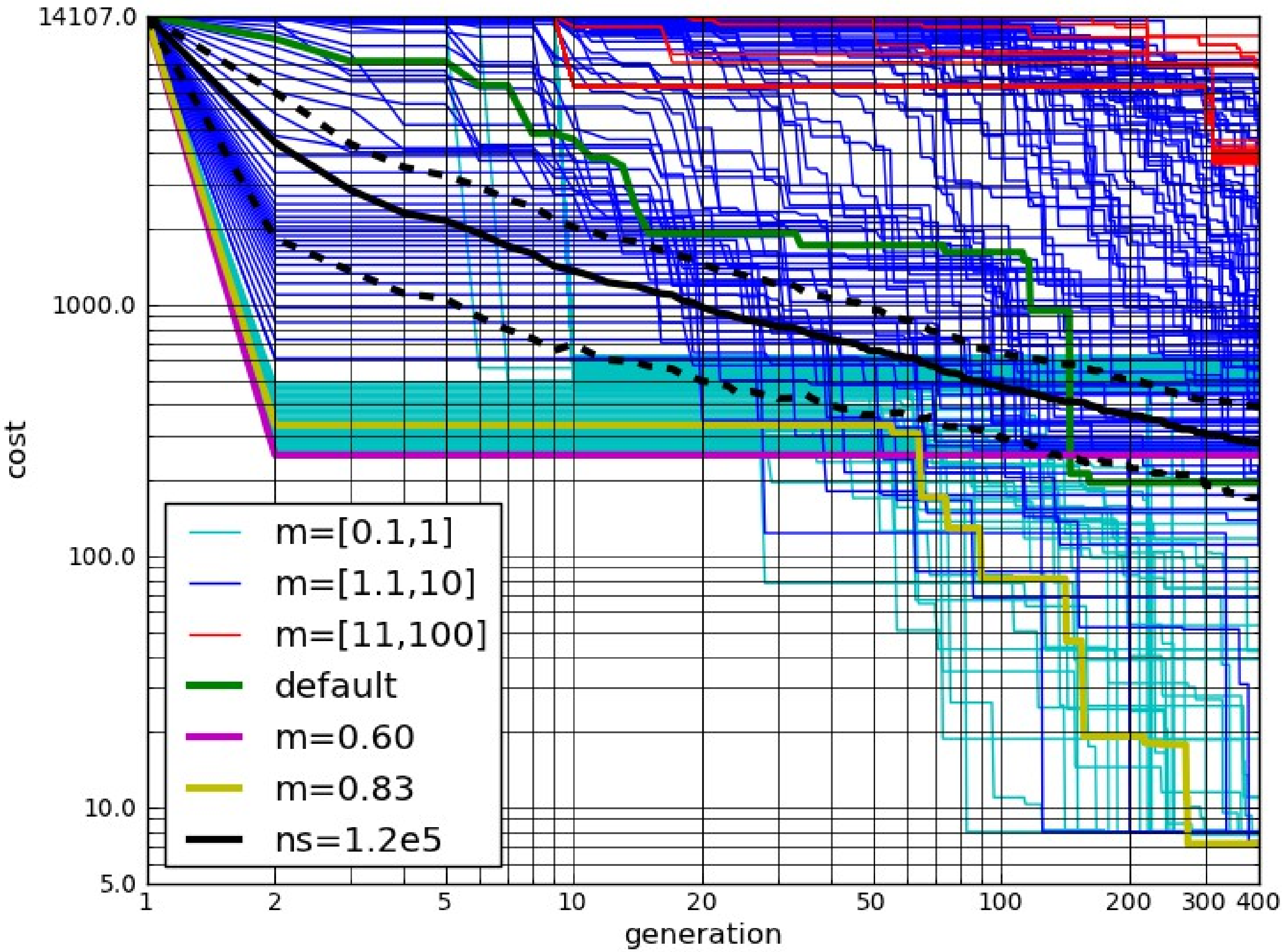
→ No gain observed after 40 iterations.

Different covariance functions : example

9D Rosenbrock test function

EI(0,1) = EGO
300 values of fixed covariance scale parameter (Gaussian kernel)

ns : random search for 300*400 trials.



→ Good covariance functions (e.g., m=0.83 here) yield very efficient optimizations.
Simple parallel implementation is a rough way to estimate them.

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Multiple optimizers with coordination : An agent-based dynamic partitioning algorithm

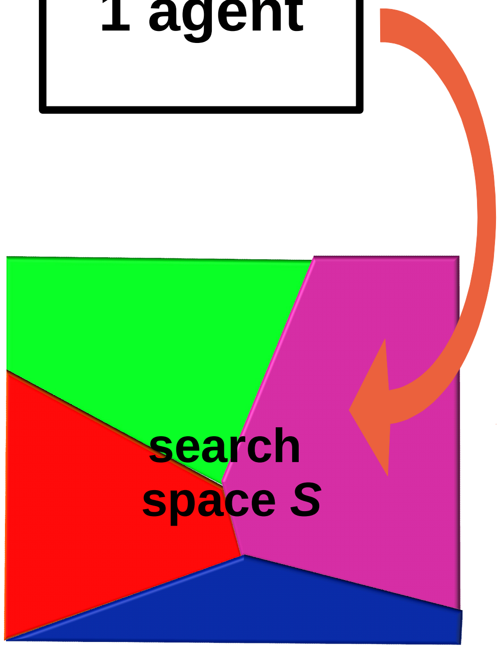
Villanueva, Le Riche, Picard and Haftka, *Dynamic partitioning for balancing exploration and exploitation in constrained optimization*, 14th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Sept. 17-19, 2012, Indianapolis, USA.

Multiple optimizers with coordination : An agent-based dynamic partitioning algorithm

1 subregion
+ 1 surrogate
+ 1 local constrained optimizer
+ 1 simulator

=

1 agent



Agents work in parallel to collectively solve the optimization problem :

$$\min_{x \in S \subset \mathbb{R}^n} f(x)$$
$$g(x) \leq 0$$

Agent coordination through :

- update of the partition
- agent creation
- agent deletion

(let's say 1 agent is affected to a set of computing nodes)

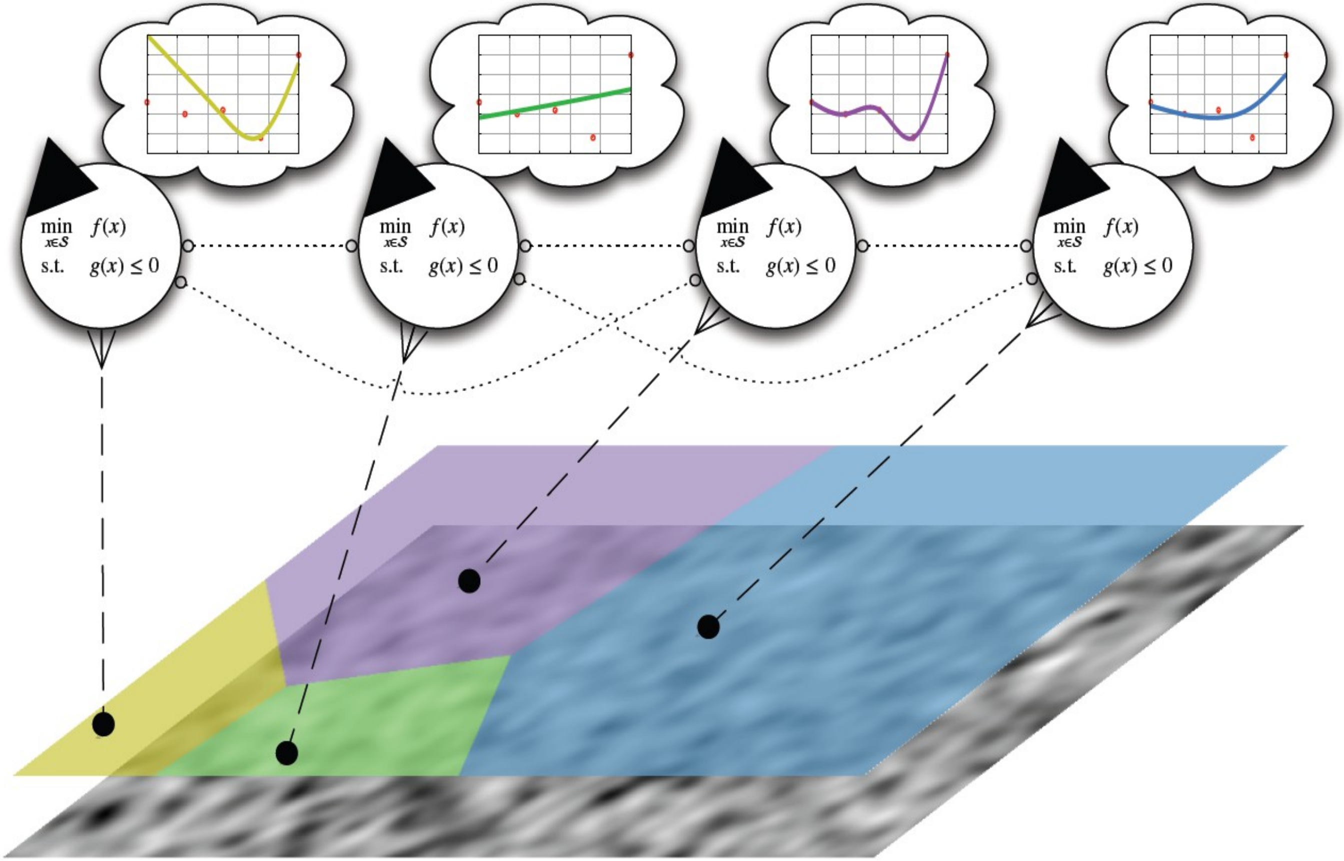
Agent-based dynamic partitioning algorithm
Goals

Solve a global optimization problem AND locate local optima
A method that can be used for expensive problems (thanks to the surrogates)

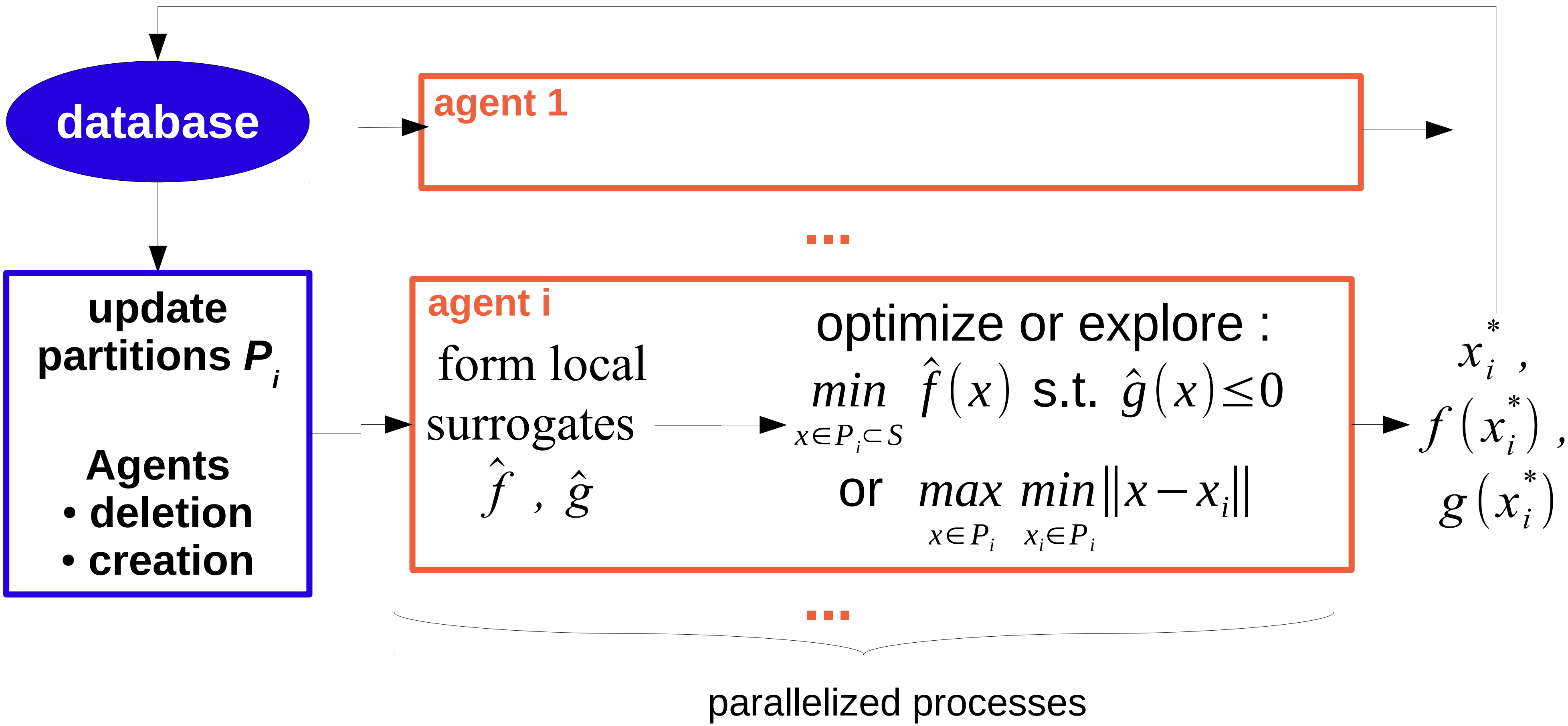
The search space partitioning allows :

1) to share the effort of finding local optima

2) to have surrogates defined locally (better for non stationary problems).



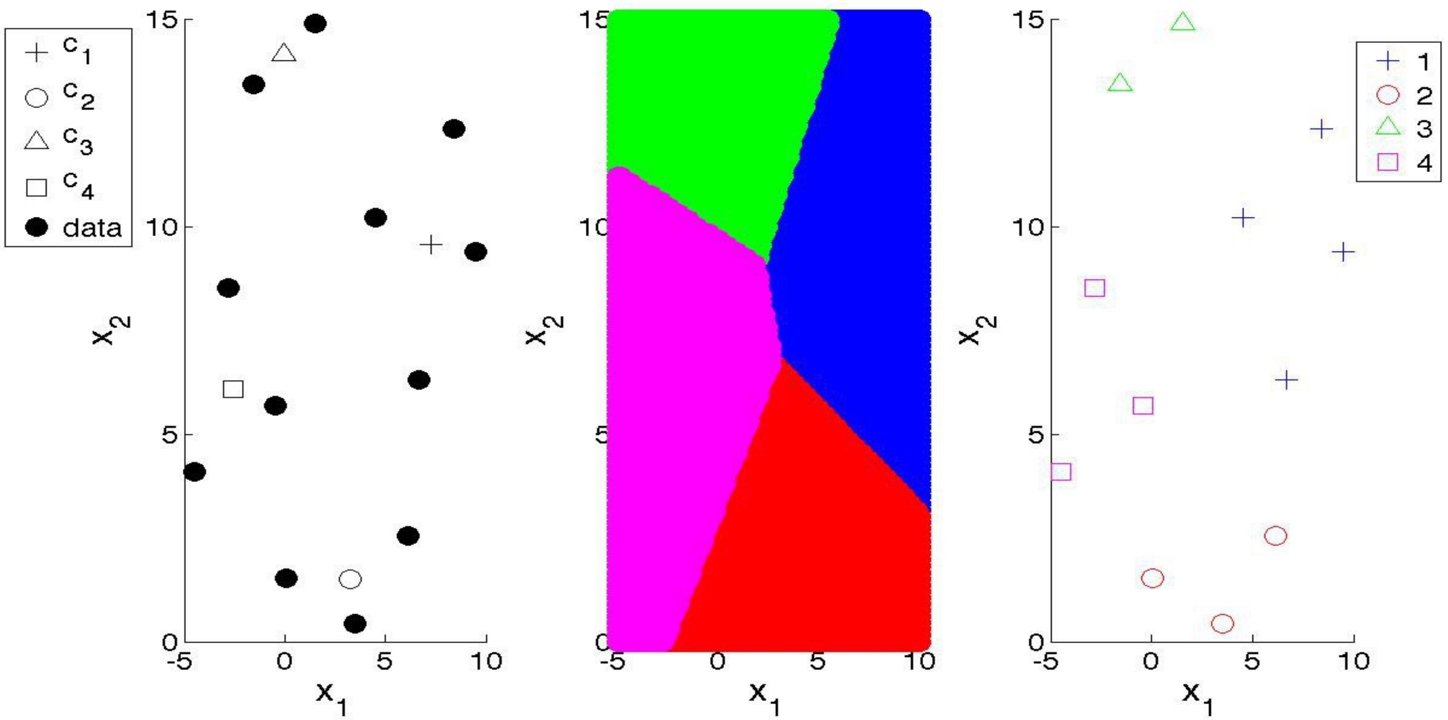
Agent-based dynamic partitioning algorithm
Global flow chart



optimize : SQP.
surrogates : polynomial response surface (orders 1, 2 and 3), kriging (linear or quad. trend), chosen based on cross-validation error.

Subregion definition

Subregions P_i are essentially defined by the centers c_i of the subregions : P_i is the set of points closer to c_i than to other centers. P_i are Voronoi cells.



Dynamic partitioning

The partitioning is updated by moving the centers to the best point in their subregion :

current = current center
new = point added to P_i at the last iteration and not on boundary of P_i

```
if current is infeasible then
   if new is less infeasible then move to new
elseif current is feasible then
   if new is feasible & has better f then move
to new
end
```

Property : agents will stabilize at local optima.

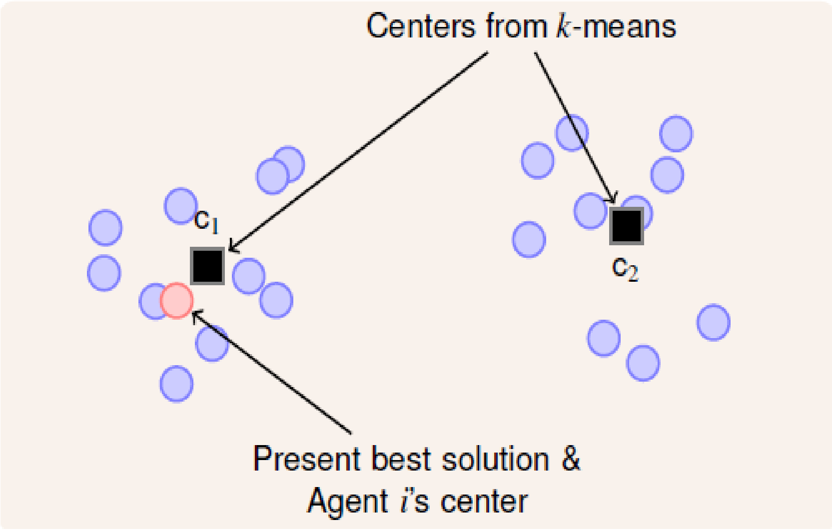
Agent deletion and creation

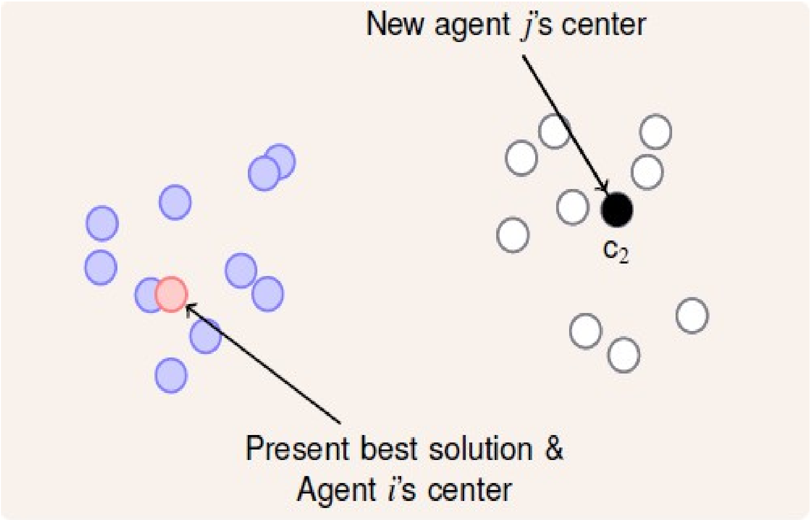
Deletion

If two agent centers are getting too close to each other, delete the worst.

Creation

Principle : the existence of 2 clusters in a subregion is a sign of at least 2 basins of attraction → split the subregion by creating a new agent.
Implementation : K-means + check on inter vs. intra class inertia + move centers at data points.





2D example with disconnected feasible regions

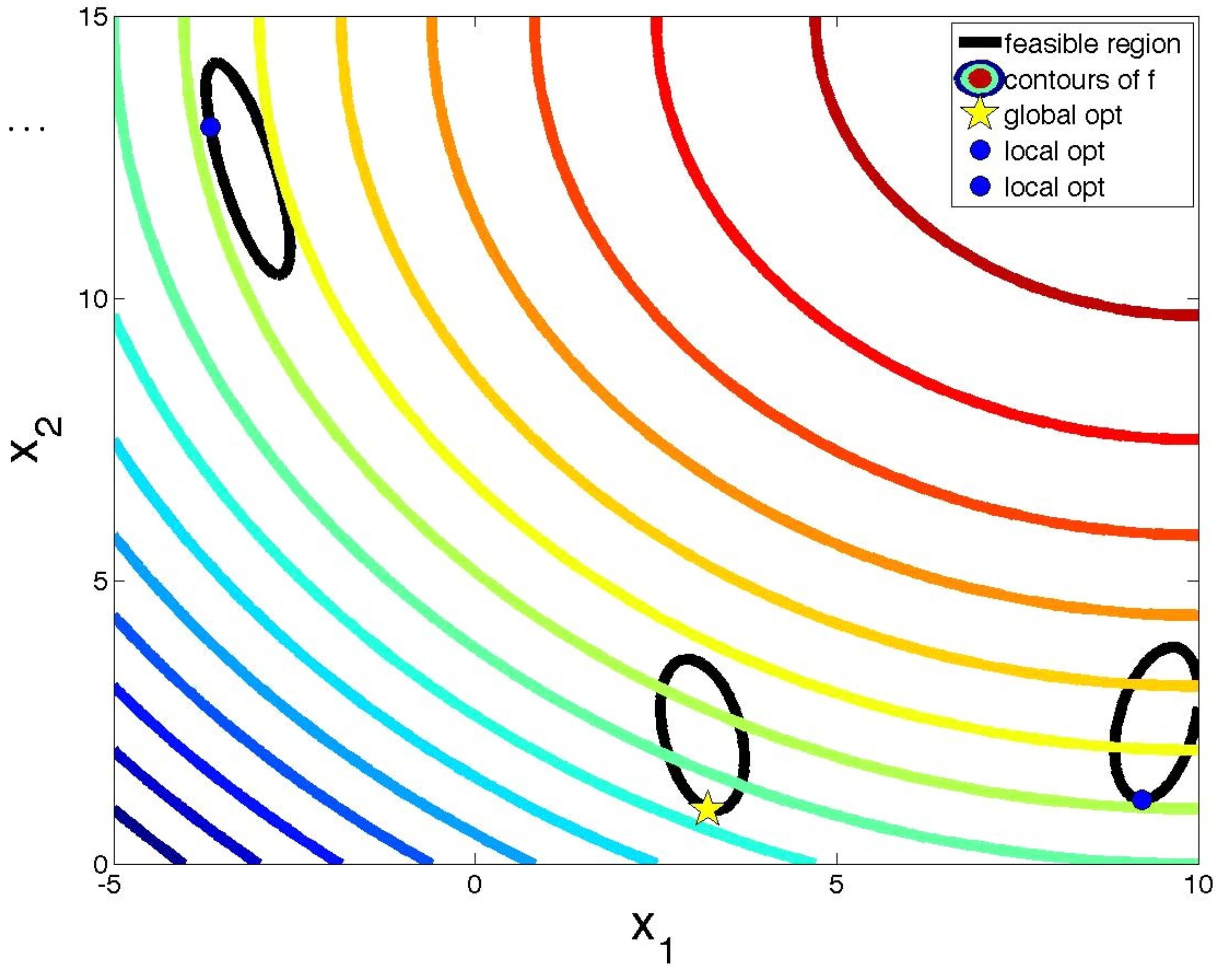
$$\underset{x}{\text{minimize}} \quad f(x) = -(x_1 - 10)^2 - (x_2 - 15)^2$$

$$\text{subject to} \quad g(x) = \left(x_2 - \frac{5.1}{4\pi^2}x_1^2 + \frac{5}{\pi}x_1 - 6\right) + \cdots$$

$$10\left(1 - \frac{1}{8\pi}\right) cos(x_1) + 10 - 2 \leq 0$$

$$-5 \leq x_1 \leq 10$$

$$0 \leq x_2 \leq 15$$

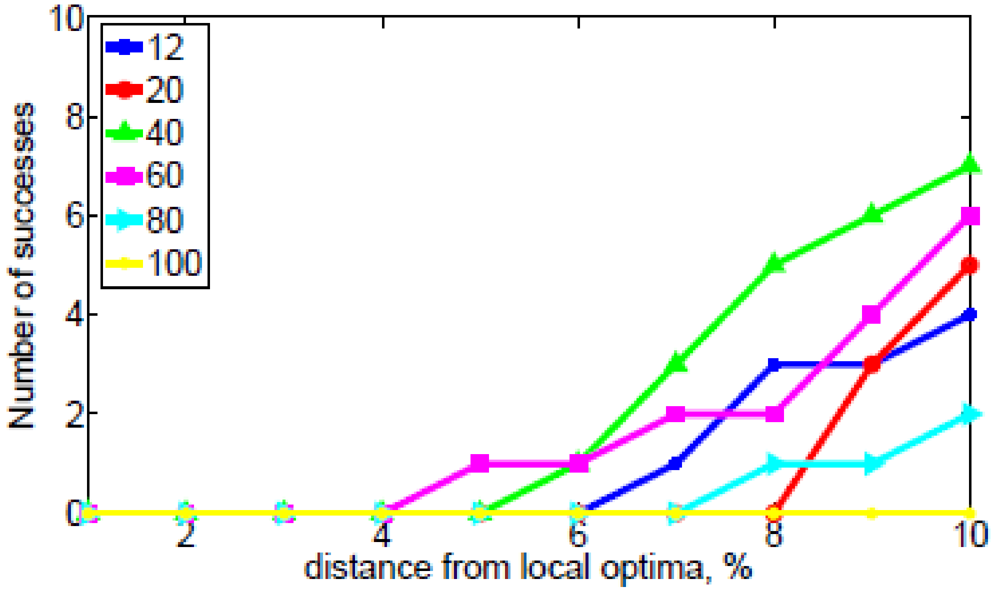


Both *f* and *g* are considered expensive → approximated with surrogates.

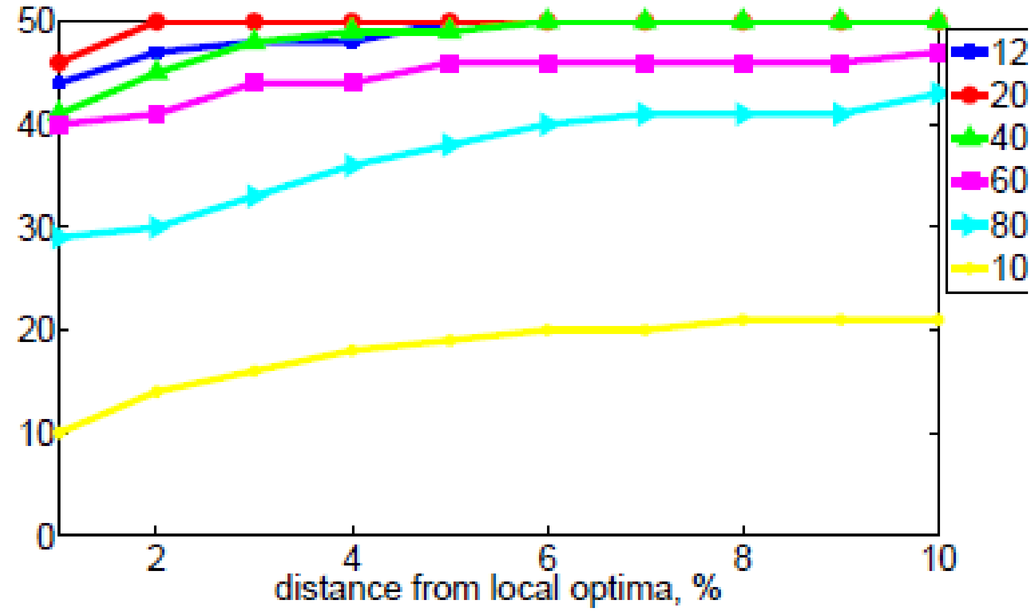
from Sasena, Papalembros, Goovaerts, Global optimization of problems with disconnected feasible regions via surrogate modeling, 9th AIAA/ISSMO symposium on Multidisciplinary Analysis and Optimization, AIAA-2002-5573.

Success at finding all local optima

1 agent



System of agents

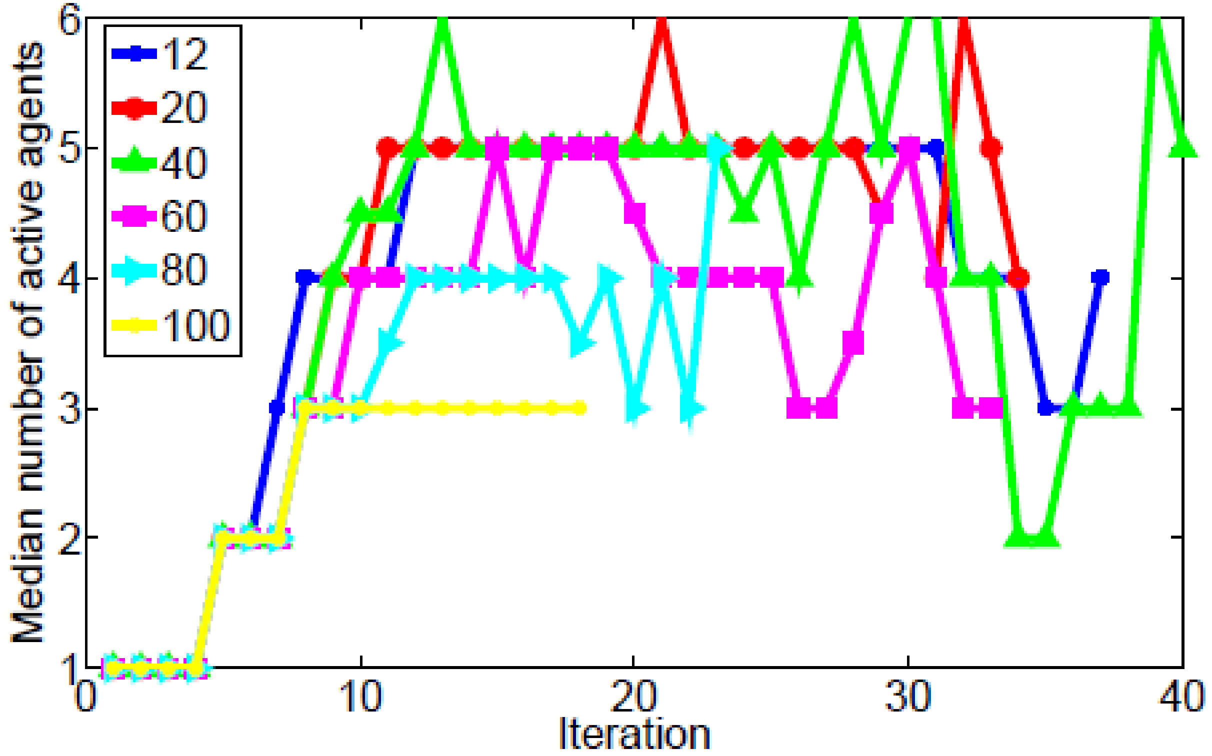


Different curves (colors) = size of initial DOE.
Fair comparisons : size of initial DOE + sum$_{\text{iterations}}$ nb. agents = 132 (constant).
Each curve is the median of 50 repetitions.

- **The partitioning is more efficient at finding all optima than repeated local searches + exploration.**

- **The algorithm benefits from small initial DOEs.**

Agent dynamics : number of agents

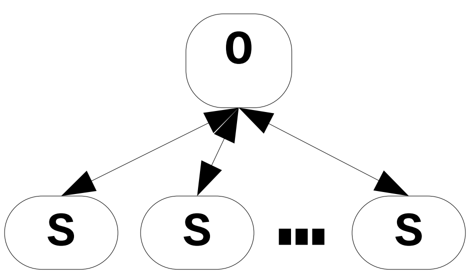


The median number of agents is between 3 and 5.

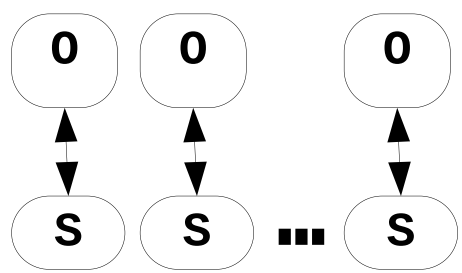
Note : there are 3 local optima.

Concluding remarks

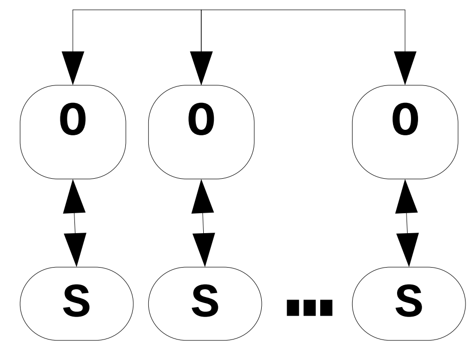
We have shown examples of parallelized global optimization algorithms that are adapted to expensive functions because they use surrogates. They follow the three patterns :



master-slave
$EI^{\mu,\lambda}$



embarrassingly //
different surrogates
(cov. functions) for EI



// + coordination
dynamic partitioning
of the search space

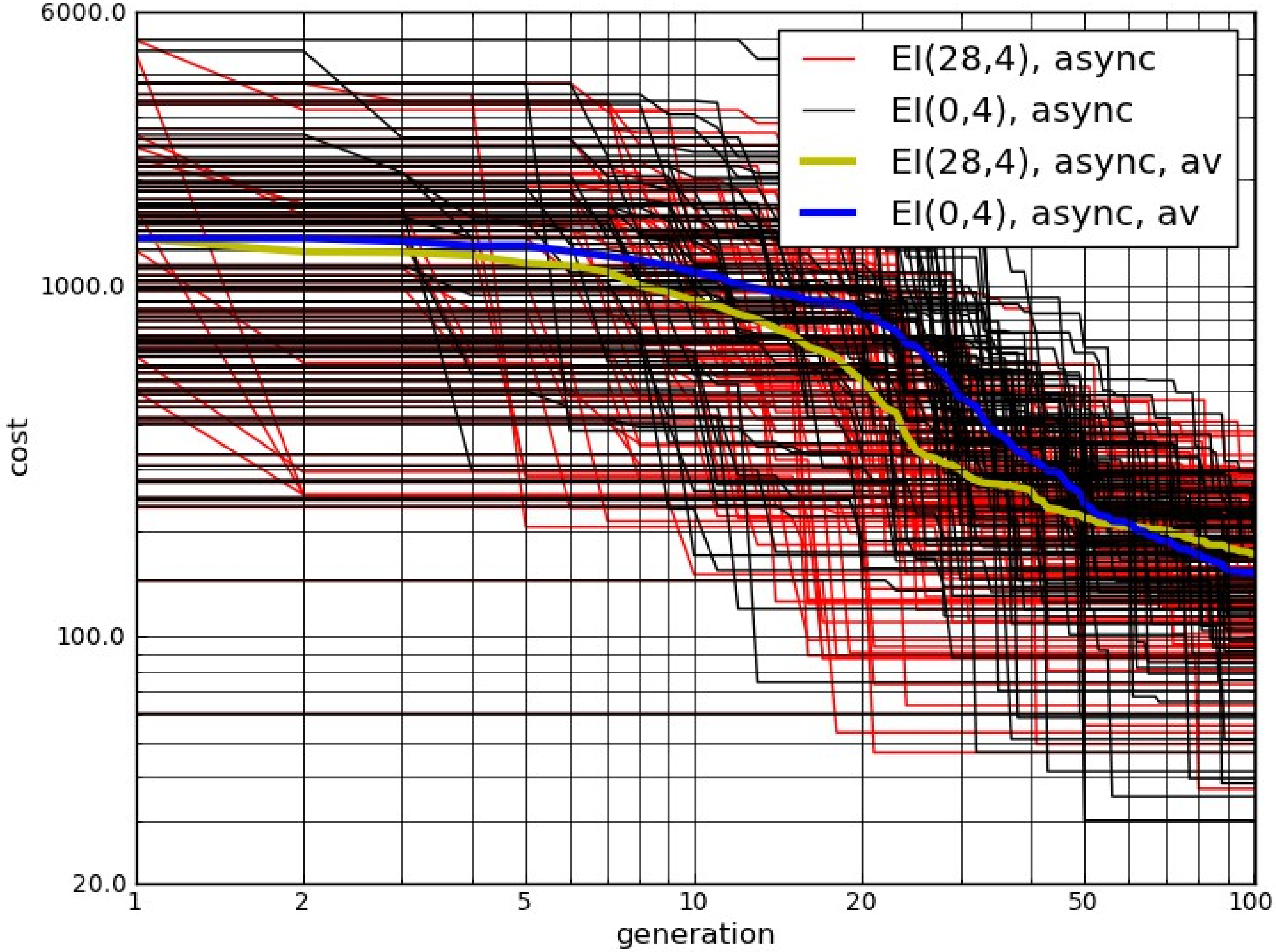
Perspective : better understand what strategy is the best considering

- a function landscape,
- a computational cost / budget,
- a computing infrastructure.

Additional slides

Effect of the μ busy points in $EI^{\mu,\lambda}$

100 runs, $EI^{0,4}$ asynchronous vs. $EI^{28,4}$ asynchronous, Rosenbrock function in 6D



W.r.t. $EI^{0,4}$, $EI^{28,4}$ better avoids sending duplicates to the nodes for evaluation.