

**IRSN**

INSTITUT  
DE RADIOPROTECTION  
ET DE SÛRETÉ NUCLÉAIRE

*Enhancing nuclear safety*

# Stochastic global optimization practice in nuclear criticality safety assessment

Dr. Y. Richet

Criticality Assessment Study  
and Research Department

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# Overview

## ■ Nuclear criticality-safety assessment and related issues

- Classical approach and basic tools
- Rethinking through « Computer Experiments » framework:
  - ◀ Expert driven ▶ supplemented by « Algorithm assisted» policy

## ■ Components to build an operational workbench

- Front-end GUI
- Grid computing engine & algorithm back-end

## ■ Feedback on two years of daily use

- Adhesion vs. resiliency
- Enhancing robustness with EGO/kriging improvements

## ■ Focus on stochastic optimization

- Related [R] packages
- Integration of stochastic simulator

# Nuclear criticality-safety assessment and related issues

# Nuclear criticality-safety assessment and related issues

## ➤ Classical approach and basic tools

### ■ Nuclear criticality-safety

- Physics = neutron transport, chemistry, materials science
- System = industrial storage, transport cask, ...
- Hypothesis = environment conditions: flooding, earthquake, overloading
- Output of interest = neutrons multiplication factor (aka k-effective),  
criticality means k-effective > 1.0
- Safety demonstration = k-effective *not to exceed 0.95*,  
*in the hypothesis range*

### ■ Assessment: modeling criticality accident risk

Expert knowledge assessment ... supplemented by numerical checking:

- Physics <- criticality simulation code
- System <- input dataset
- Hypothesis <- input dataset variables (dim<10)
- Output of interest <- (scalar) output of the code

# Nuclear criticality-safety assessment and related issues

## ➤ Classical approach and basic tools

### ■ Parametric study for maximization of k-effective

- < 10 scalar, independent & compact parameters
- Non linear & cross effects
- (often) Several local max

### ■ (Mc) Monte Carlo simulation of k-effective

- One calculation point costs 10 s. to 1 h.
- Endpoint simulation maybe:
  - $\text{sd}(k\text{-effective}) < \text{input setting (say } 0.00100)$
  - $\text{quantile}(k\text{-effective}, 0.999) < \text{input setting (say } 0.95000 \text{ or current max.)}$

### ■ Remote/grid calculation issue at IRSN

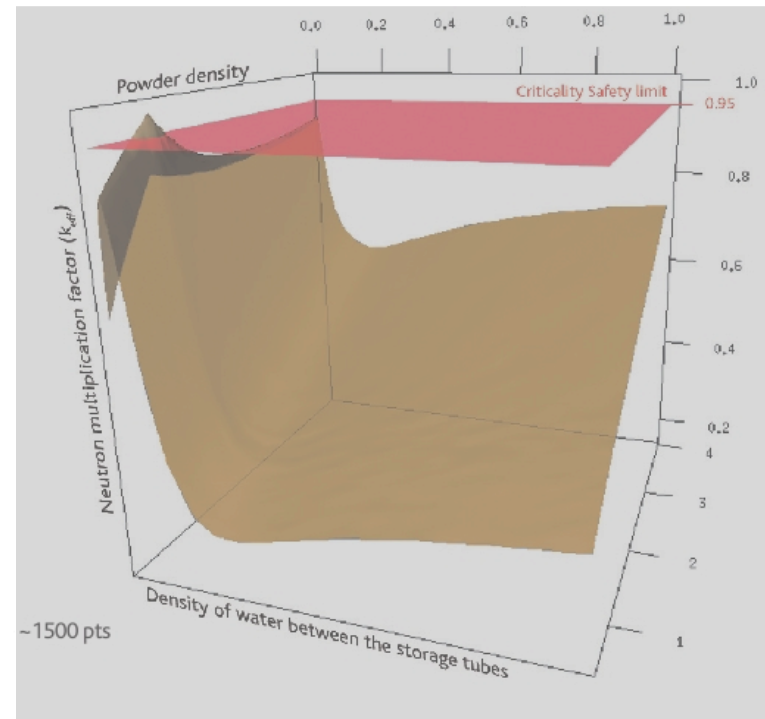
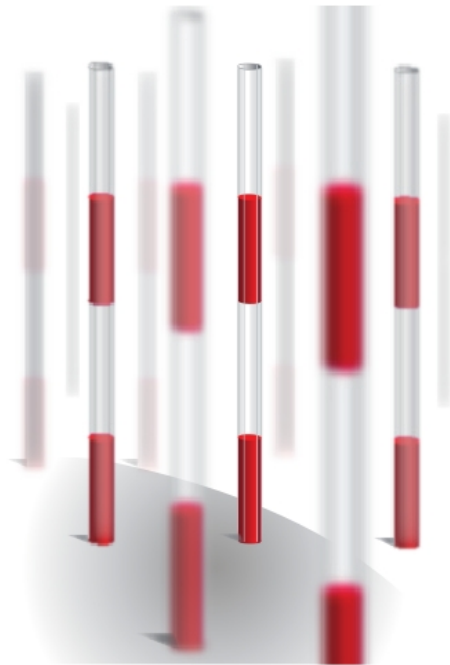
- ~ 80 heterogeneous CPU available
- Not (yet) parallelized code (Markov chain)

# Nuclear criticality-safety assessment and related issues

## ➤ Classical approach and basic tools

■ Case study = interim storage of dry PuO<sub>2</sub> powder, variables being:

- Powder loading as powder density in [0.5,4.0]
- Storage flooding as water density between cans in [0.0,1.0]



# Nuclear criticality-safety assessment and related issues

## ➤ Rethinking through « Computer Experiments » framework

### ■ Expert-driven approach

- OaT maximization
  - 2 or 3 parameters
  - (supposed) penalizing value for other parameters
  - 1 or 2 cycles by hand ...
- Factorial DoE
  - 5 to 10 points / dimension
  - 2 or 3 parameters
  - automated task with dedicated software (including PROMETHEE)

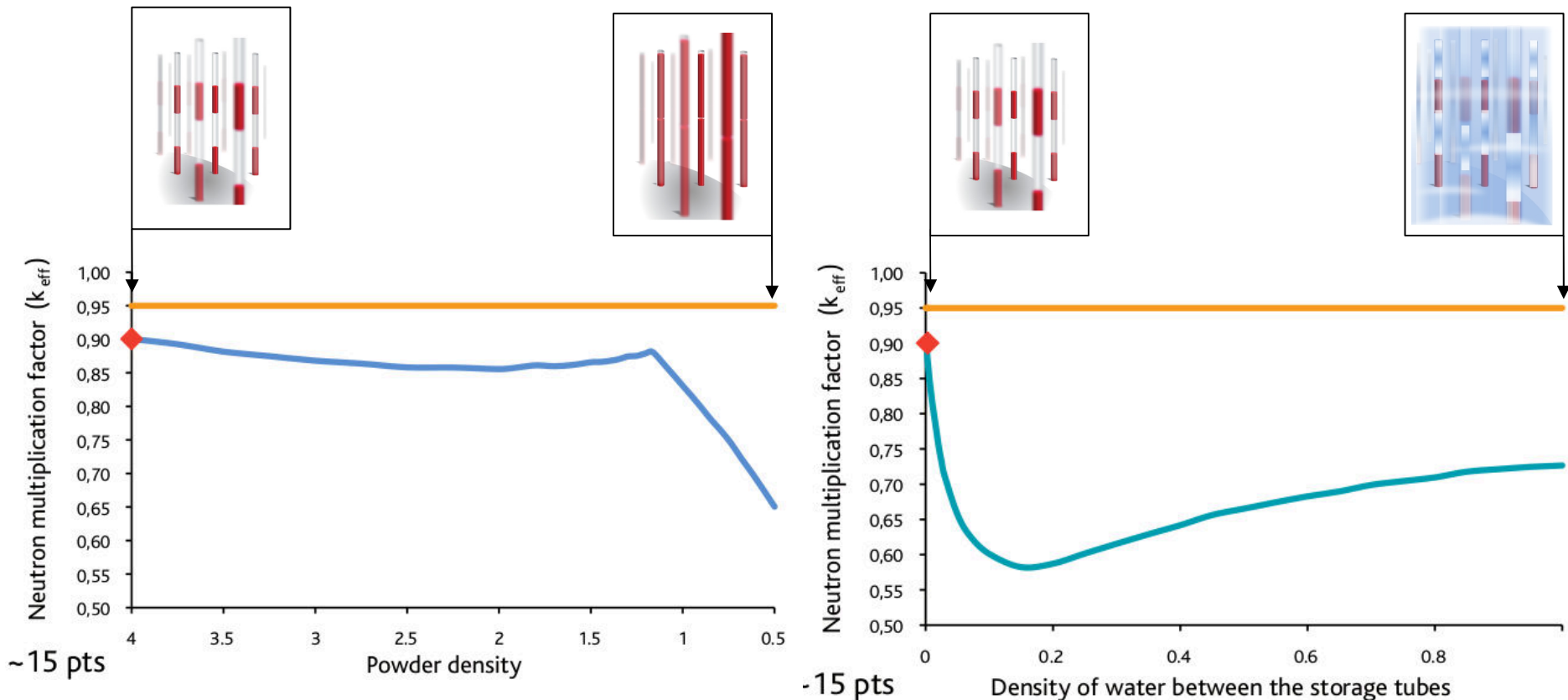
### ➤ Case study results

# Nuclear criticality-safety assessment and related issues

## ➤ Rethinking through « Computer Experiments » framework

### Expert-driven approach - case study results

- OaT maximization



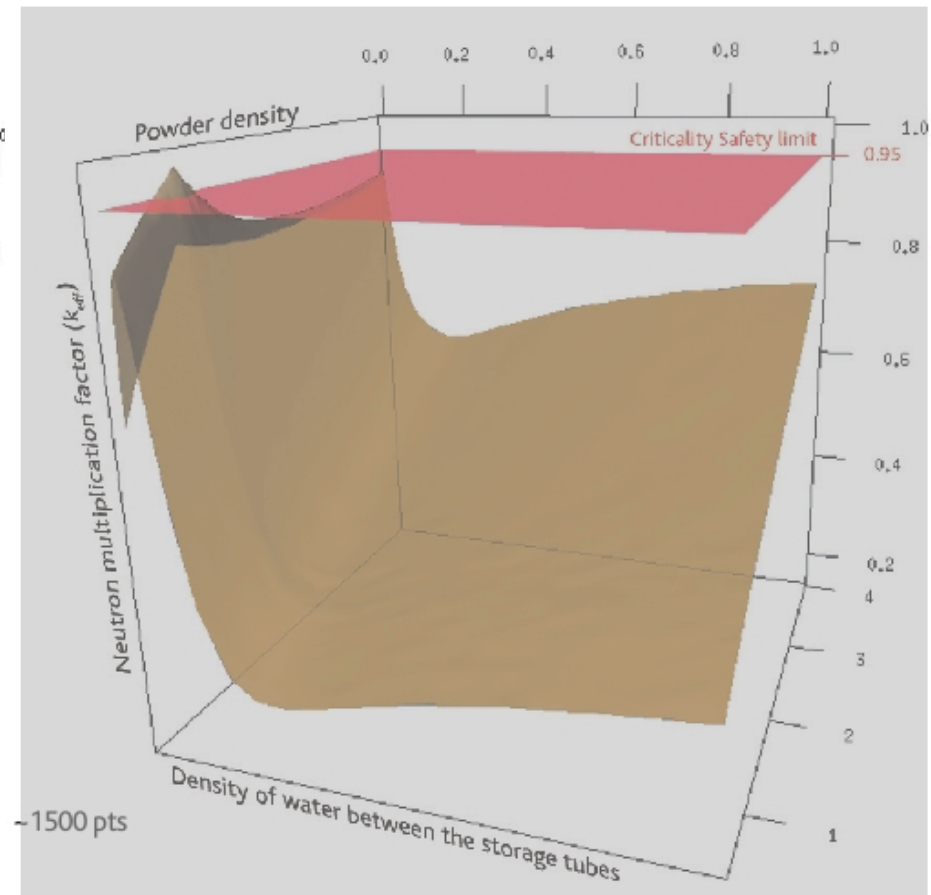
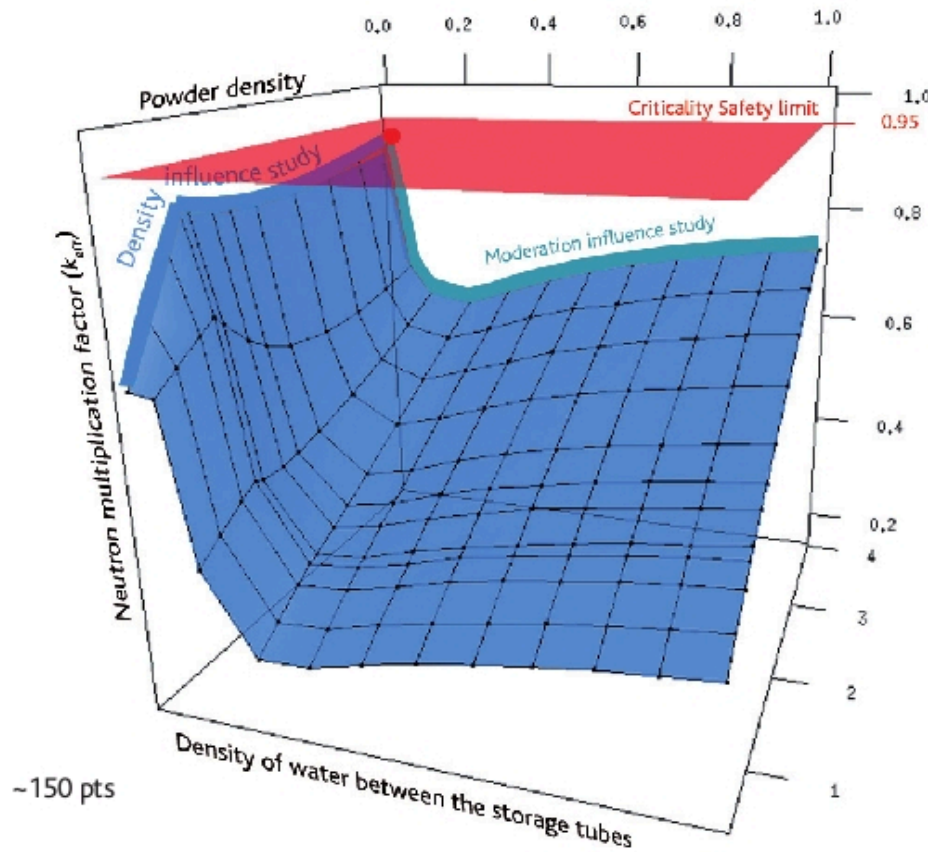


# Nuclear criticality-safety assessment and related issues

## ➤ Rethinking through « Computer Experiments » framework

### Expert-driven approach - case study results

- Factorial DoE



# Nuclear criticality-safety assessment and related issues

## ➤ Rethinking through « Computer Experiments » framework

### ■ EGO-assisted approach

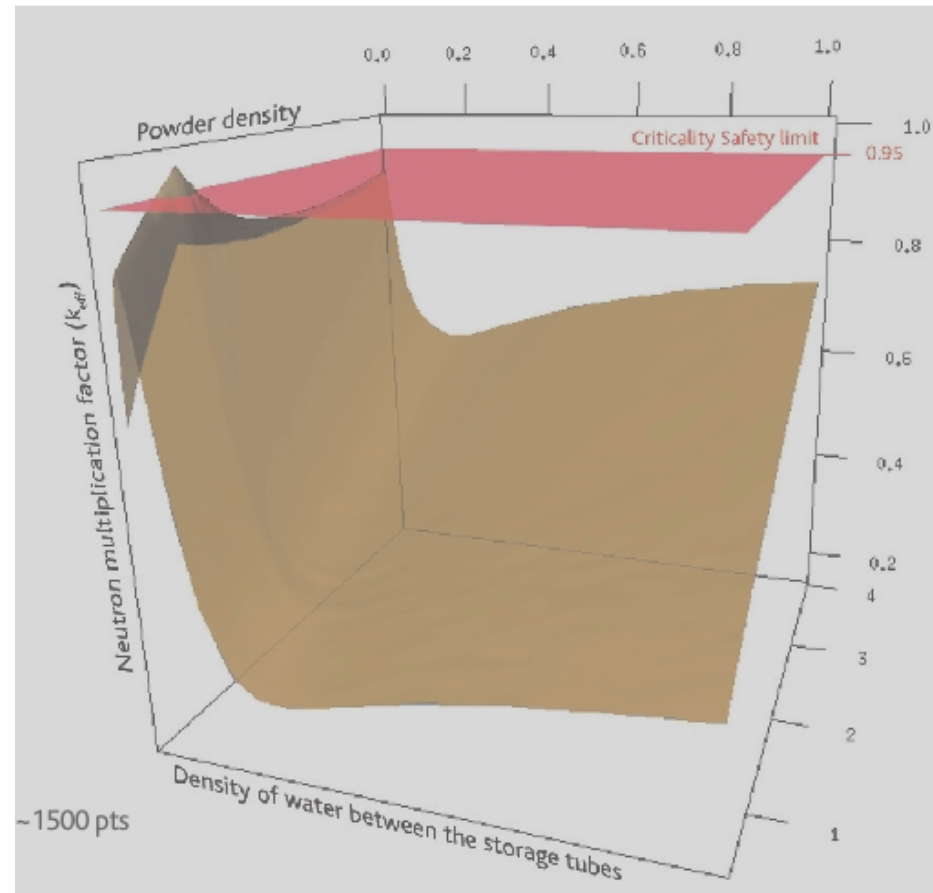
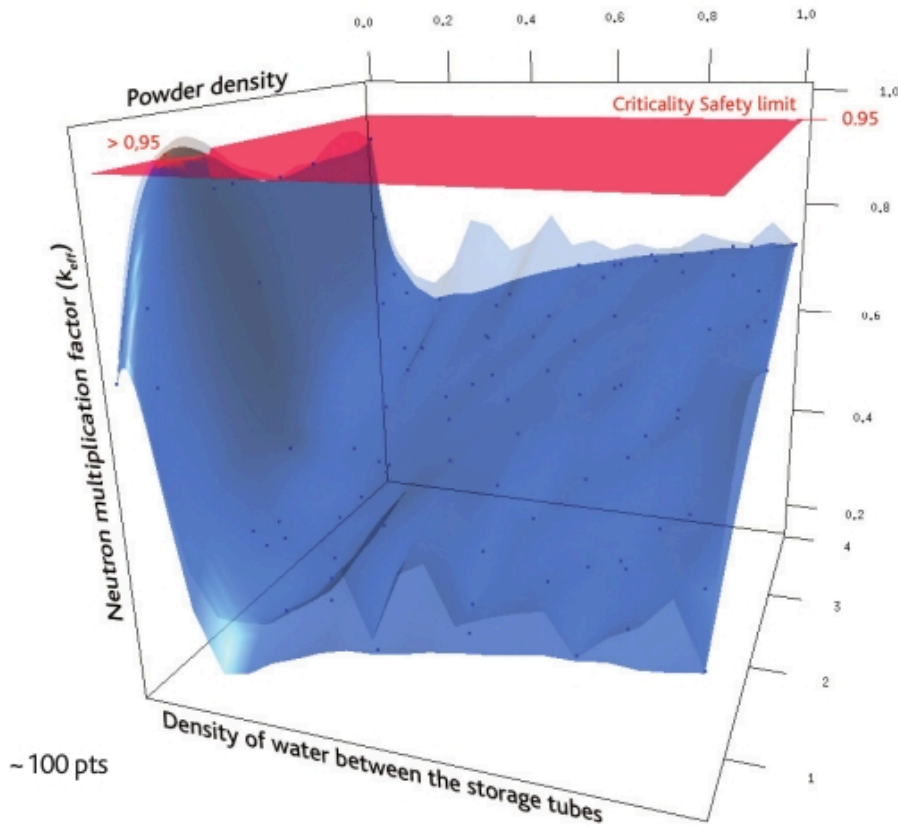
- Initial DoE
  - LHS
  - (cross) Bounds of parameters
- Kriging surrogate of noisy (as MC) experiments
- Maximization of Expected Improvement criterion
- Loop on Kriging/maxEI ...

### ➤ Case study results

# Nuclear criticality-safety assessment and related issues

## ➤ Rethinking through « Computer Experiments » framework

### ■ EGO-assisted approach - case study results



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# Components to build an operational workbench

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## ➤ Front-end GUI

### ■ End user input

- Based on ASCII input dataset of your code (application field agnostic)
- User free to insert « \$parameter » or formulas anywhere in these file
- Select any DoE policy available for this input parameters / code output
  - Factorial DoE, Efficient Global Optimization
  - ... (SA, determ. optimization, inversion, ...)

### ■ Computing

- (blindly) Launch the grid computing workflow
- (online) Follow intermediate results (if available)

### ■ Analysis

- Get results
- ... and a true applicable conclusion (or a new question :)

# Components to build an operational workbench

The screenshot displays a software interface with several panels and a central text editor. The top menu bar includes 'Configuration' and 'Help'. The 'Data sets' panel on the left shows a table with columns 'Data set', 'State', 'Pts', and 'Variables'. The 'Calculations' panel below it has a table with columns 'Q', 'Data set', 'State', and 'Activity'. The 'Results' panel at the bottom left has a table with columns 'V', 'Data set', 'Size', 'Pts', and 'State'. The central 'Model Define' panel shows 'Model' set to 'Moret\_5A1' and a 'Dataset' list containing 'Puits\_PuO2\_2variables\_grille\_75x75.jd.1'. Below this is a table for 'Output values' and 'Type'. The main text editor area contains a list of model components with their types and volumes.

Data set	State	Pts	Variables
Puits_PuO2_2variable...	new	1	
Puits_PuO2_2variable...	new	1	d.broui.scale d.Pu...

Q	Data set	State	Activity
---	----------	-------	----------

V	Data set	Size	Pts	State
---	----------	------	-----	-------

Model: Moret\_5A1

Dataset: Puits\_PuO2\_2variables\_grille\_75x75.jd.1

Output values	Type
mean_keff	float
sigma_keff	float

```
460  
461 GEOM  
462 MODU 0  
463  
464 * Reflexion par 60 cm de beton  
465 TYPE 10 BOIT 45 45 363  
466 VOLU 10 0 10 1 0. 0. 303  
467 RBOIT 1 1 1 1 0 0  
468 * Interieur de la salle (brouillard de densité variable)  
469 TYPE 11 BOIT 45 45 303  
470 VOLU 11 10 11 2 0. 0. 303  
471  
472 * Puits (acier 5 mm)  
473 TYPE 20 CYLZ 6.8 151.5  
474 VOLU 21 11 20 4 0. 0. 151.5  
475 VOLU 22 11 20 4 0. 0. 454.5  
476 * Interieur Puits (air)  
477 TYPE 30 CYLZ 6.5 150  
478 VOLU 31 21 30 2 0. 0. 153  
479 VOLU 32 22 30 2 0. 0. 456  
480 * Conteneur (acier 2.5 mm)  
481 TYPE 40 CYLZ 5.9 150  
482 VOLU 41 31 40 4 0. 0. 153  
483 VOLU 42 32 40 4 0. 0. 456  
484 * Interieur conteneur (air)  
485 TYPE 50 CYLZ 5.75 150  
486 VOLU 51 41 50 2 0. 0. 153  
487 VOLU 52 42 50 2 0. 0. 456  
488 * Fissile  
489 TYPE 60 CYLZ 5.75 49.8925  
490
```



# Components to build an operational workbench

The screenshot displays a software interface with several panels:

- Data sets:** A table listing data sets with columns for Data set, State, Pts, and Variables. Two entries are visible: "Puits\_PuO2\_2variable..." with State "new" and Pts "1".
- Model Define:** A central panel where the model is set to "Moret\_5A1". It includes a "Dataset" dropdown set to "Puits\_PuO2\_2variables\_grille\_75x75\_jd". Below this are two tables:
 

Input variable	Default value
d.broui.scale	0.0
d.PuO2	4.0

Output values	Type
mean_keff	float
sigma_keff	float
- Calculations:** A panel with a table for tracking calculations, currently empty.
- Results:** A panel with a table for tracking results, currently empty.
- Code Editor:** A large text area containing model definition code. The code includes comments in French and commands like "TYPE", "VOLU", and "RBOIT" with various mathematical expressions and parameters.



# Components to build an operational workbench

Configuration Help

### Data sets

Data set	State	Pts	Variables
Puits_PuO2_2variable...	defining	1	d.broui.scale d.Pu...

### Model Define

#### Input

Name	Engineering	Group	Type	Default value	Values
d.broui.scale	<input checked="" type="checkbox"/>		real	0.0	[0.0 ; 1.0]
d.PuO2	<input checked="" type="checkbox"/>		real	4.0	[0.5 ; 3.5]

### Output

Engineering	Name	Type
<input checked="" type="checkbox"/>	N(mean_keff,s...	GaussianDensity
<input type="checkbox"/>	mean_keff+3*...	Numeric
<input type="checkbox"/>	mean_keff	Numeric
<input type="checkbox"/>	sigma_keff	Numeric

### Calculations

Q	Data set	State	Activity

### Results

V	Data set	Size	Pts	State

### Engineering N(mean\_keff,sigma\_keff) as a function of d.broui.scale d.PuO2

Type	Name
<input type="checkbox"/>	No design of experiments
<input type="checkbox"/>	Sensitivity analysis SRC
<input type="checkbox"/>	<b>Calibration EGI</b>
<input type="checkbox"/>	Calibration Dichotomy
<input type="checkbox"/>	Uncertainties prop... Monte Carlo sampling
<input type="checkbox"/>	Sensitivity analysis FAST
<input type="checkbox"/>	<b>Xautoscale</b>
<input type="checkbox"/>	Uncertainties prop... Monte Carlo sampling with statistic ...
<input type="checkbox"/>	Calibration Bounds dichotomy
<input type="checkbox"/>	Uncertainties prop... Wilks formula
<input type="checkbox"/>	Sensitivity analysis Morris screening
<input type="checkbox"/>	<b>Optimization gradientdescent</b>
<input type="checkbox"/>	Sensitivity analysis PCC
<input checked="" type="checkbox"/>	<b>Optimization Efficient Global Optimization</b>

Computing parameters \ Kriging parameters \ Optimization parameters \ Expert know

Min iterations =

Max iterations =

Stop when expected improvement lower than =

Parallel computations =

Initial parallel computations =

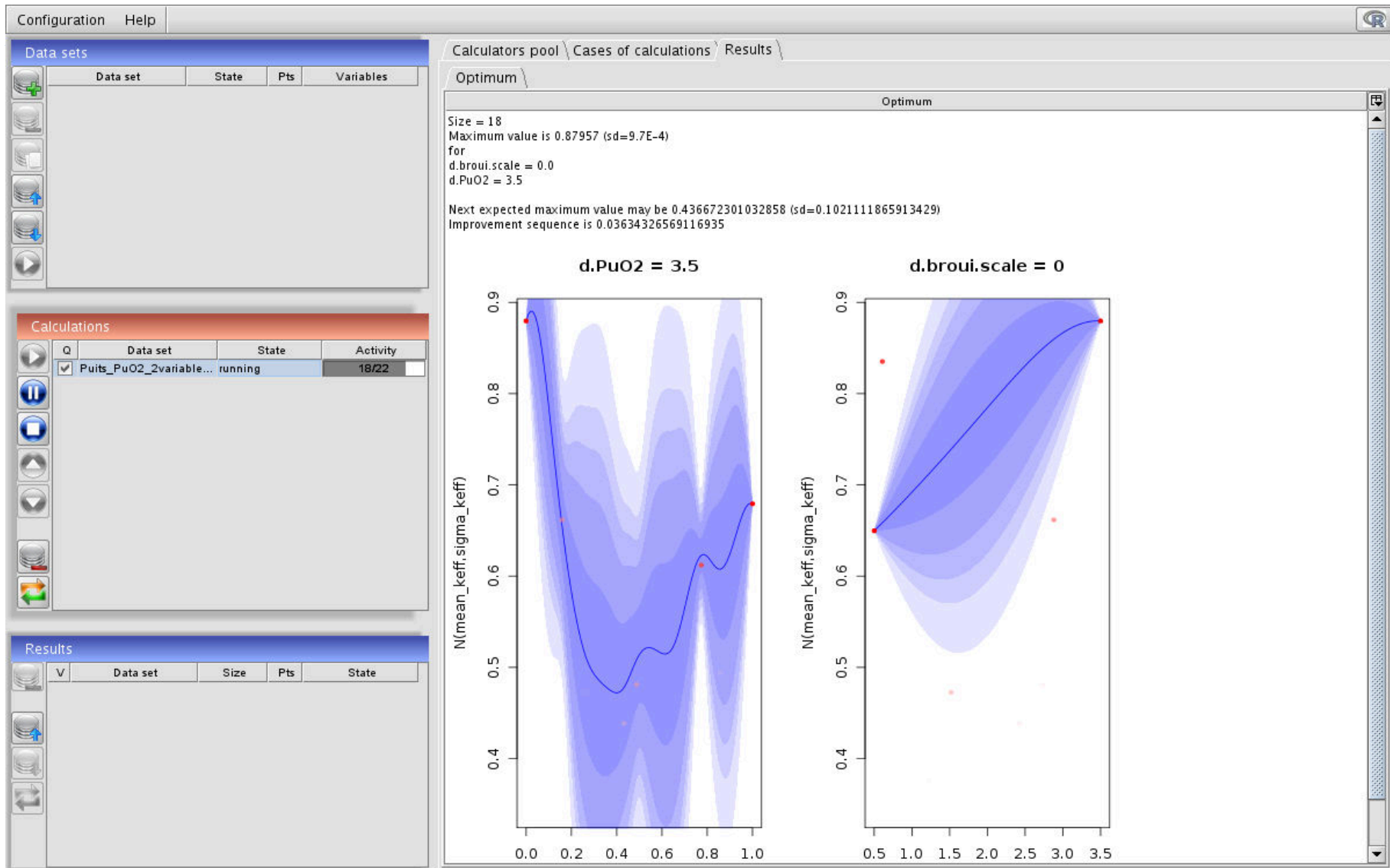
Bounding values







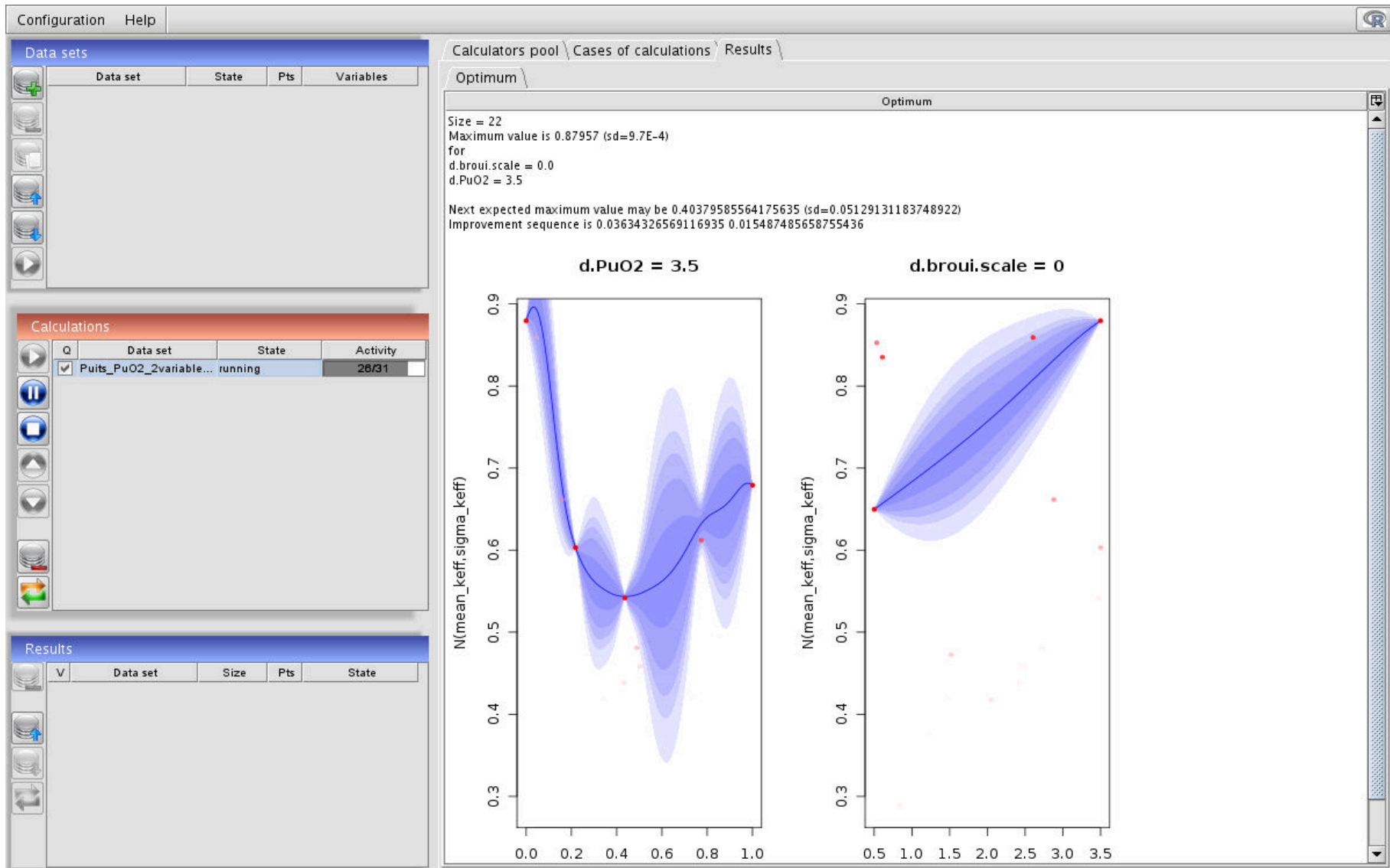
# Components to build an operational workbench



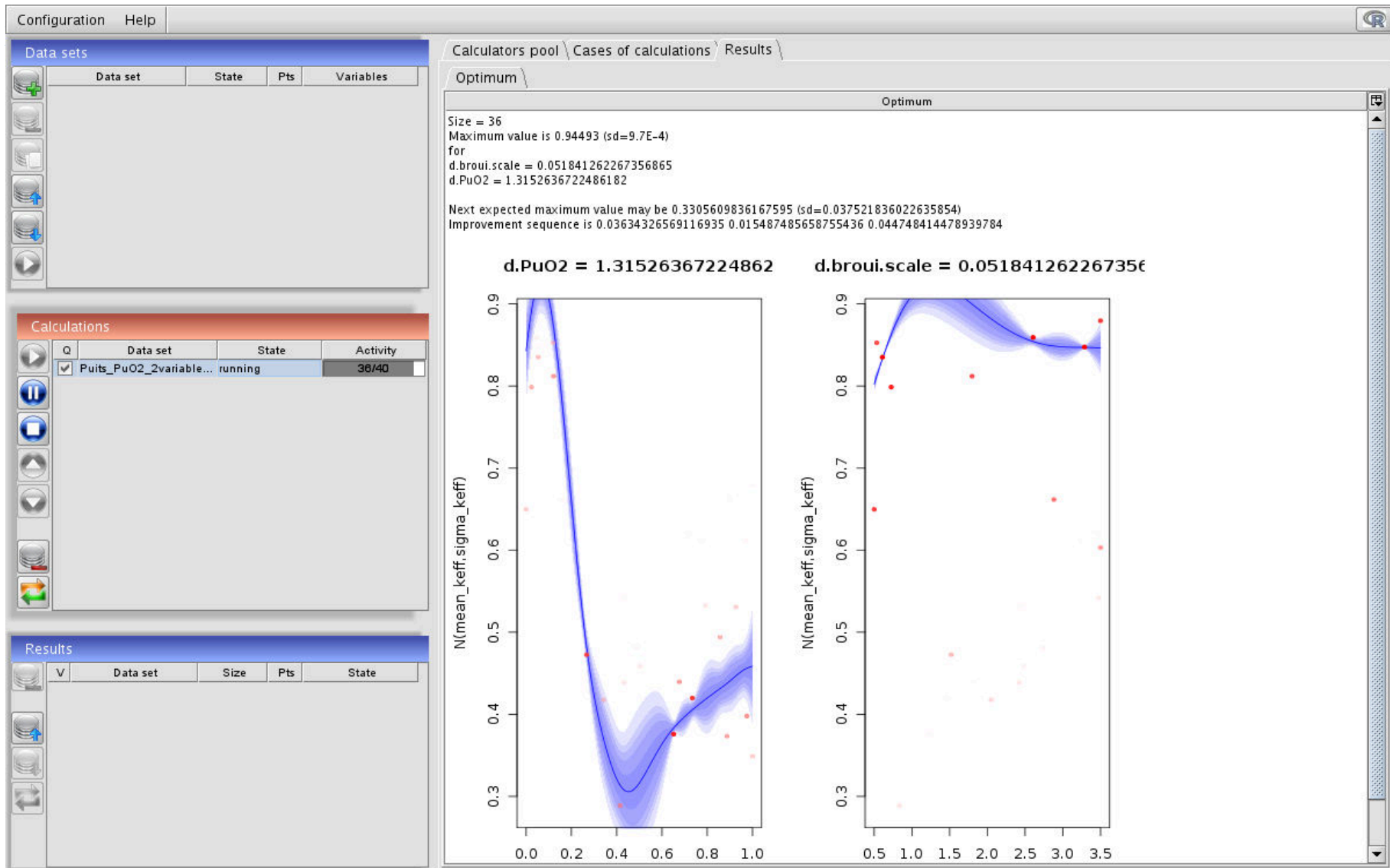




# Components to build an operational workbench

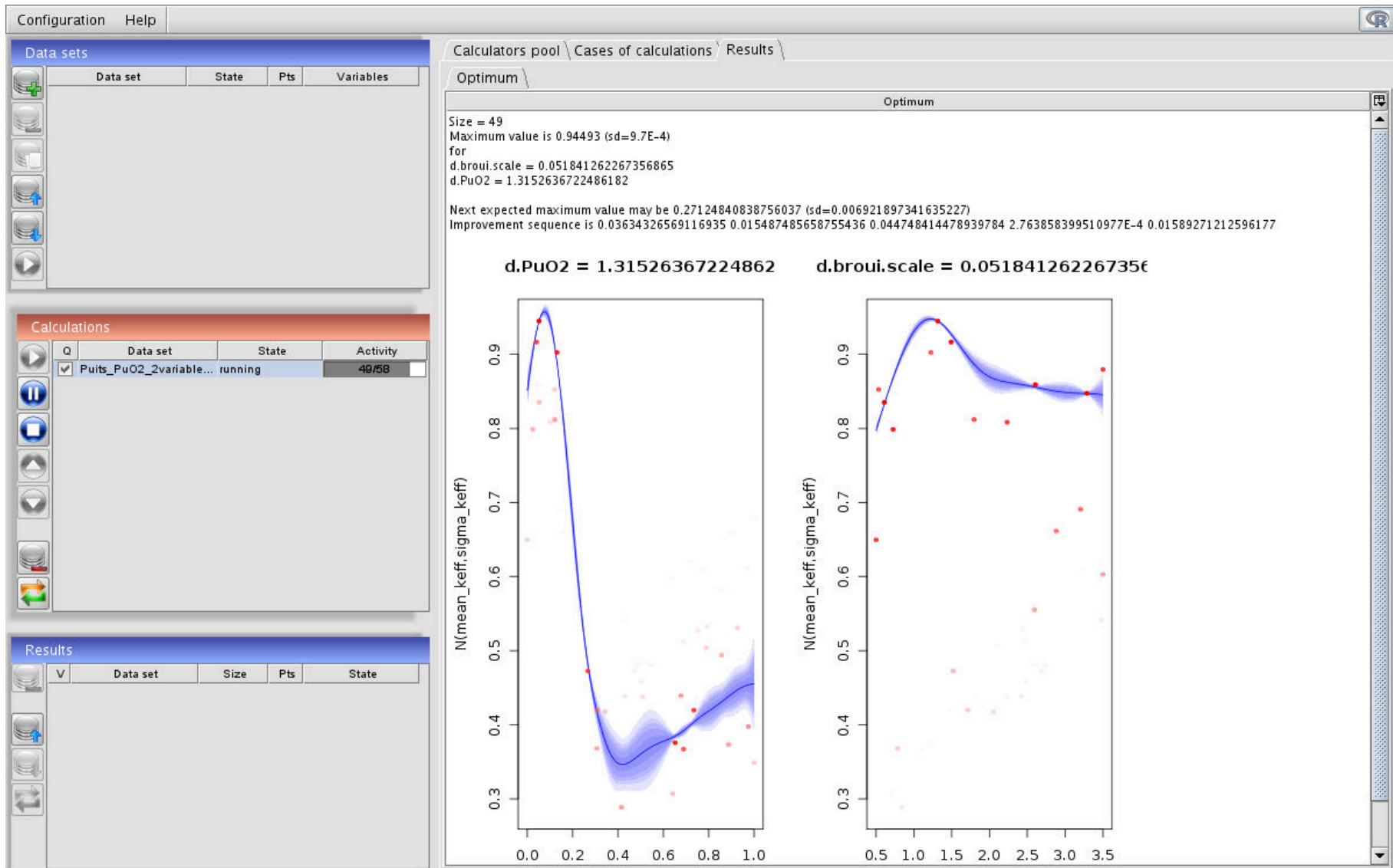


# Components to build an operational workbench

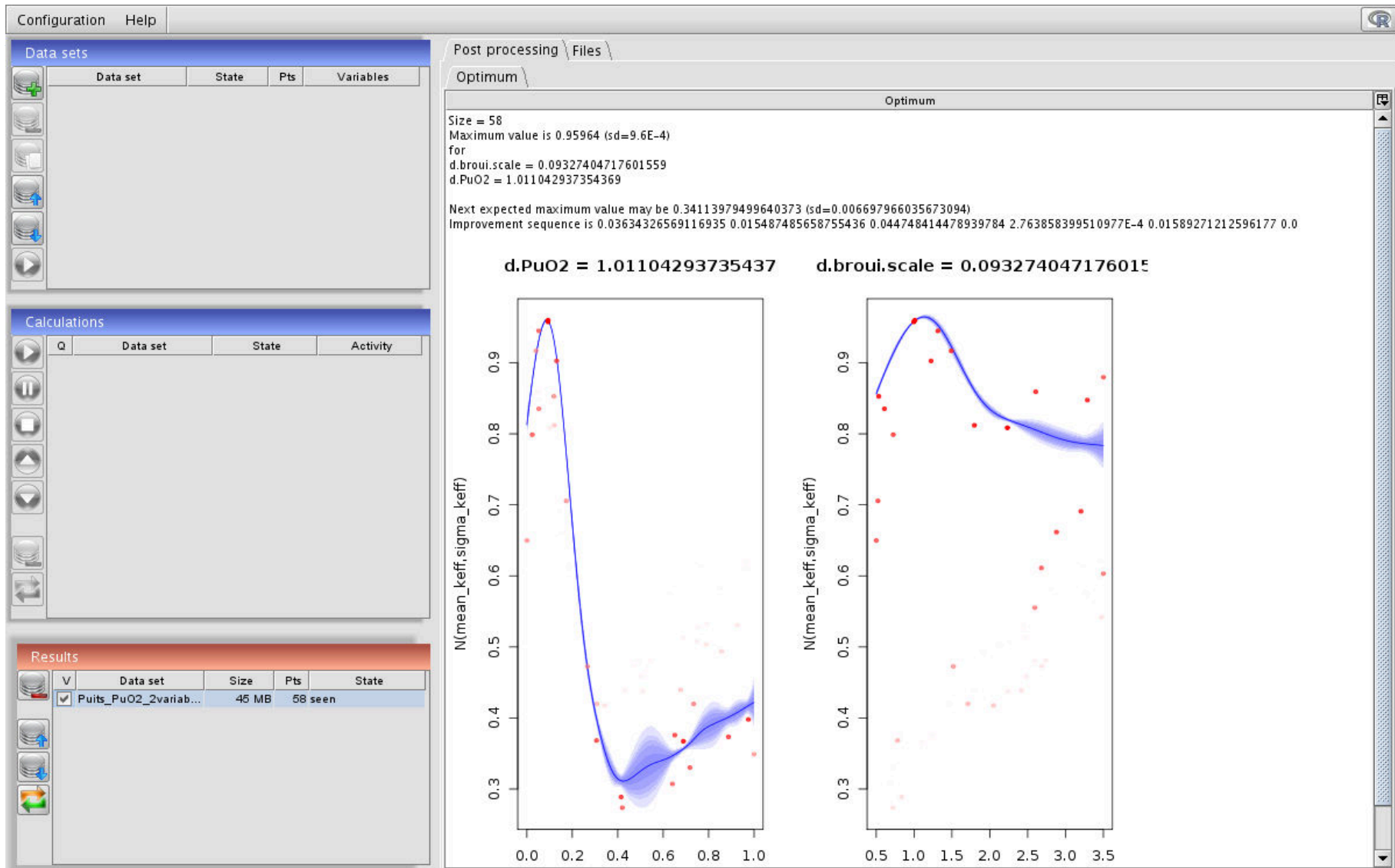




# Components to build an operational workbench



# Components to build an operational workbench



# Components to build an operational workbench

Configuration Help

Data sets

Data set	State	Pts	Variables
----------	-------	-----	-----------

Calculations

Q	Data set	State	Activity
---	----------	-------	----------

Results

V	Data set	Size	Pts	State
✓	Puits_PuO2_2variab...	45 MB	58 seen	

Post processing Files

Find:

Find:

- d.broui.scale=0.05292791611928907
  - d.PuO2=0.608450717292726
    - input
    - info.txt
    - output
- EGO1\_1389836095.Rdata
- d.broui.scale=0.9268426589399511
- km0\_1389836095.Rdata
- d.broui.scale=0.13092024480849992
- d.broui.scale=0.6288579581305385
- d.broui.scale=0.6887877064291388
- d.broui.scale=0.7917987112887204
- d.broui.scale=0.02364629251749863
- d.broui.scale=0.7173223637510091
- d.broui.scale=0.09327404717601559
- d.broui.scale=0.09272100515632431
- d.broui.scale=0.42006798810325563
- EGO0\_1389836095.Rdata
- d.broui.scale=0.7734019996908804
- d.broui.scale=0.6429818482138216
- d.broui.scale=0.5022901650518179
- d.broui.scale=0.3080500189680606
- d.broui.scale=0.4147155410812902
- d.broui.scale=0.17350012273527682
- EGO3\_1389836095.Rdata
- d.broui.scale=0.5092528564855456
- d.broui.scale=0.48777661594148314
- d.broui.scale=0.6877512203063816
- d.broui.scale=0.7343308298286555
- km4\_1389836095.Rdata
- d.broui.scale=0.7478248702827841
- d.broui.scale=0.2277417614286053
- d.broui.scale=0.266666040988639
- d.broui.scale=0.9752578554261062
- d.broui.scale=0.7888243941124529
- d.broui.scale=0.6515932745145013
- d.broui.scale=0.14221573271788657

```
1 #Tue Jul 13 11:41:50 CEST 2010
2 state=4
3 start=1279014061873
4 code=moret5
5 input.d.broui.scale=0.05292791611928907
6 duration=48759
7 end=1279014110632
8 calc=neutrosec-3\;44775
9 input.d.PuO2=0.608450717292726
10 output.sigma_keff=9.9E-4
11 output.mean_keff=0.63514
12
```

# Components to build an operational workbench

## ➤ Grid computing engine & algorithm back-end

### ■ Distributed computing engine

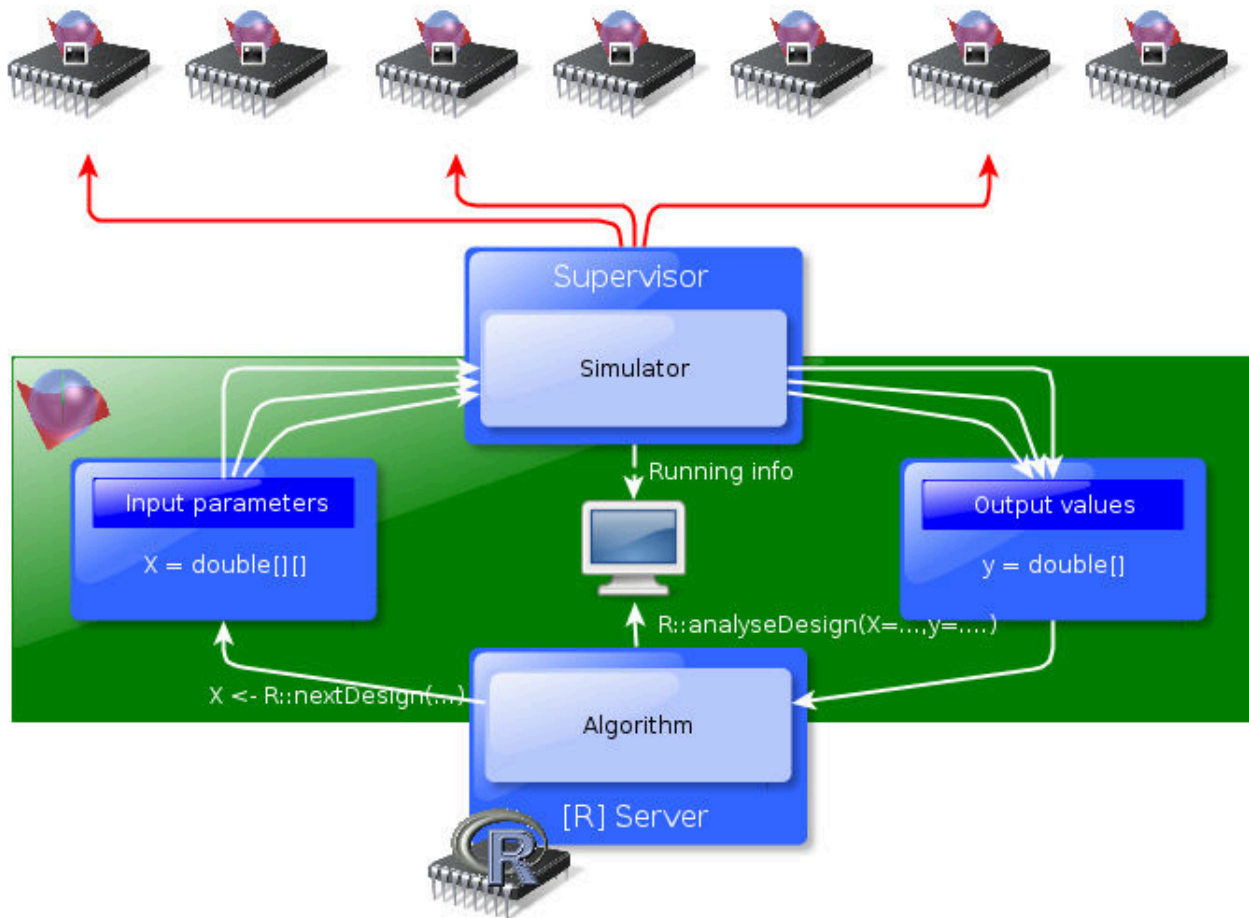
- Asynchronous, remote & parallel distribution
- Back-end daemon compatible with larger set of CPU boxes :  
server, workstation, grid, cluster, ... and even Windows office desktop
- Dynamic merge of heterogeneous computing power
- Failover

### ■ Algorithm back-end

- [R] (remote or local)
- Light wrapping script

# Components to build an operational workbench

## ➤ Grid computing engine & algorithm back-end



# Components to build an operational workbench

## ➤ Grid computing engine & algorithm back-end

```
#' constructor and initializer of R session
init <- function() {
  library(lhs)
  ...
}

#' first design building. All variables are set in [0,1]. d is the dimension, or number of variables
#' @param d number of variables
#' @return next design of experiments
buildInitialDesign <- function(d) {
  set.seed(1)
  lhs <- maximinLHS(n=initBatchSize,k=d)
  ...
}

#' iterated design building.
#' @param X data frame of current doe variables (in [0,1])
#' @param Y data frame of current results
#' @return next doe step
prepareNextDesign <- function(X,Y) {
  ...
  return(as.matrix(Xnext))
}

#' final analysis. All variables are set in [0,1]. Return HTML string
#' @param X data frame of doe variables (in [0,1])
#' @param Y data frame of results
#' @return HTML string of analysis
analyseDesign <- function(X,Y) {
  ...
  html=paste(sep="<br/>",paste("<HTML>... ",m),..., "</HTML>")
  ...
  return(paste(html,plot))
}
```

# Components to build an operational workbench

## ➤ Grid computing engine & algorithm back-end

```
buildInitialDesign <- function(d) {...}
```

```
#' iterated design building.
```

```
#' @param X data frame of current doe variables (in [0,1])
```

```
#' @param Y data frame of current results
```

```
#' @return next DoE step
```

```
prepareNextDesign <- function(X,Y) {
```

```
  if (iEGO > iterations) return();
```

```
  iEGO <- iEGO + 1
```

```
  ...
```

```
  noise.var <- as.array(Y[,2])
```

```
  if (search_min) {y=Y[,1]} else {y=-Y[,1]}
```

```
  ...
```

```
  kmi <- km(design=X, response=y, trend, optim.method='gen',... )
```

```
  EGOi <- max_qEI.CL(model=kmi, npoints=batchSize, L=liar(as.array(Y[,1])), ...)
```

```
  return(as.matrix(EGOi$par))
```

```
}
```

```
#' final analysis. All variables are set in [0,1]. Return HTML string
```

```
#' @param X data frame of doe variables (in [0,1])
```

```
#' @param Y data frame of results
```

```
#' @return HTML string of analysis
```

```
analyseDesign <- function(X,Y) {
```

```
  analyse.files <- paste("sectionview_",iEGO-1, ".png", sep="")
```

```
  png(file=analyse.files,bg="transparent",height=resolution,width = resolution)
```

```
  ...
```

```
  html <- paste(sep="<br/>",paste("<HTML>minimum is ",m),...)
```



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# Feedback on two years of daily use

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## ➤ Adhesion vs. Resiliency

### ■ Resiliency of « old school » practices

- Coverage: Only 50-80% of assessment practice is covered by the « computer experiments » framework...
  - => **Let users do whatever they want (including previous old practice)**
- Quality Insurance: workflow is already mapped on existing tools...
  - => The workbench have to be **flexible enough** to permit same level of QI
- Users: to master new concepts, the learning curve is sometimes too steep
  - => **Take time to explain...**

### ■ Adhesion to this “new” assessment framework

- <at first> focus on early adopters (easier 20% of target)
- <then> capitalize on « real world » feedback, to adapt the solution
- <try to> convince wider and wider... adapt again and again...
- <finally> involve people in R&D policy
- Efficiency measure based on « real world » test cases
- Smooth (software) transition between *old* and *new* practices

# Feedback on two years of daily use

## ➤ Enhancing robustness with EGO/kriging improvements

### ■ Noisy kriging

- Noise to model random Gaussian output of MC code
- Heteroscedasticity to support arbitrary « fidelity » of experiments

### ■ Automatic input « scaling »

- Support for input parameters transformations  
log/exp/logistic emulated as local 2<sup>nd</sup> degree splines
- To be published in DiceKriging 1.2 (soon)

### ■ Parallel EGO

- Constant Liar heuristic
- Tunnable deepening of EGO

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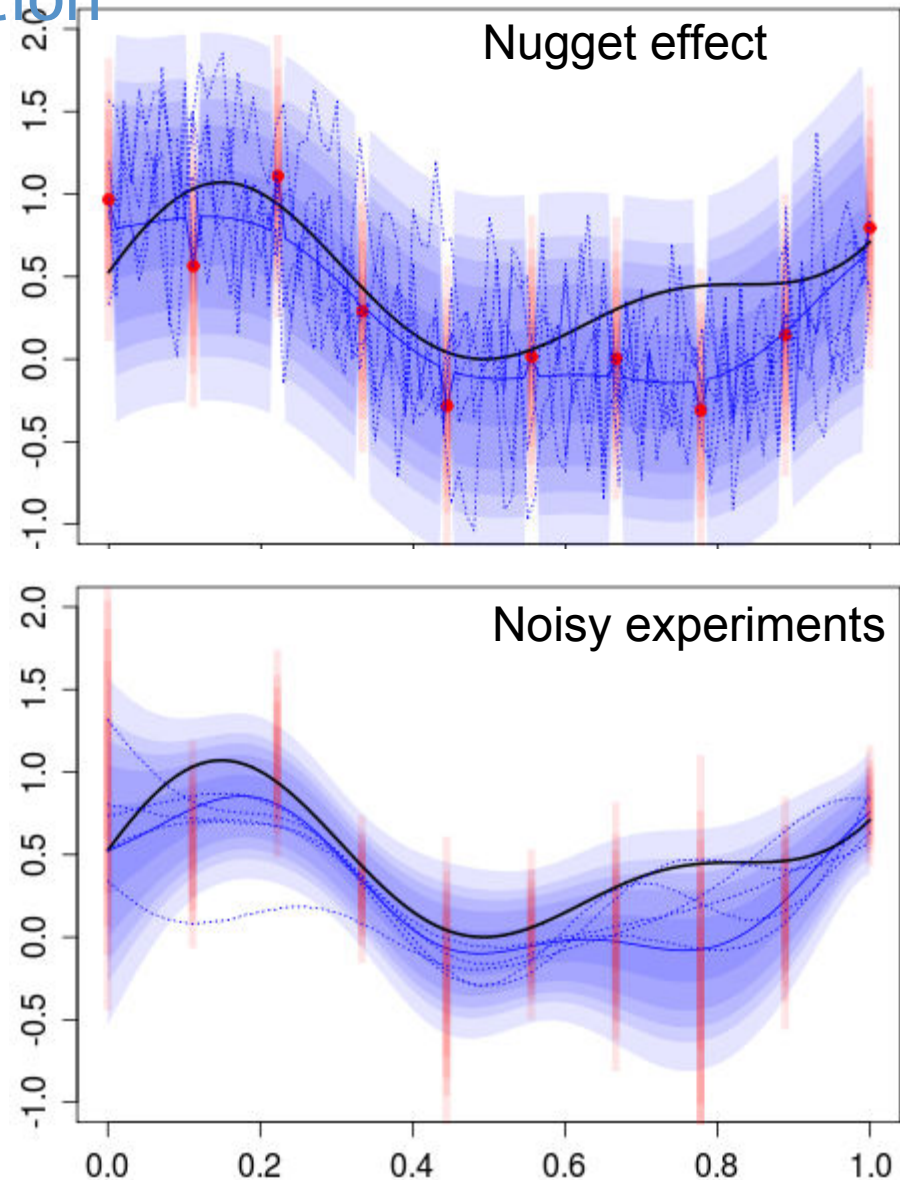
## ➤ Related [R] packages

### ■ DiceKriging

- Ordinary / Universal kriging
- Nugget / Noise

- Kernel:

- Exponential
- Gauss
- Power-exponential
- Matern 3/2
- Matern 5/2



# Focus on stochastic optimization

## ➤ Related [R] packages

### ■ DiceKriging

- Ordinary / Universal kriging
- Nugget / Noise
- Kernel:  $C(x, y) = s^2 k(x, y)$

- Exponential

$$k(h=|x-y|) = e^{-\frac{h}{\theta}}$$

- Gauss

$$k(h=|x-y|) = e^{-\left(\frac{h}{\theta}\right)^2}$$

- Power-exponential  $\left(\frac{h}{\theta}\right)^p$

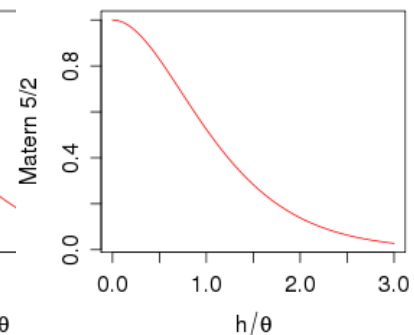
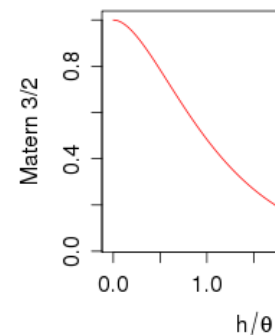
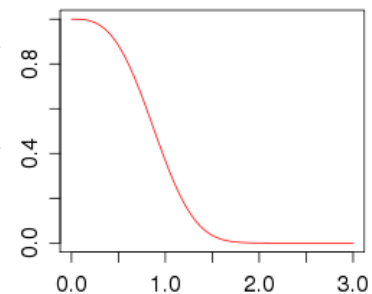
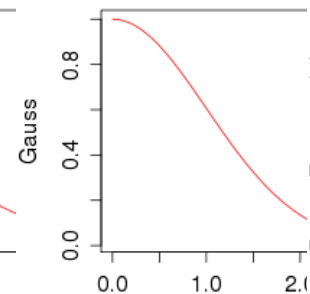
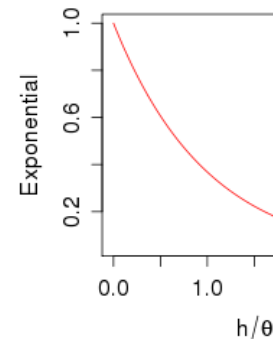
$$k(h=|x-y|) = e^{-\left(\frac{h}{\theta}\right)^p}$$

- Matern 3/2

$$k(h=|x-y|) = \left(1 + \sqrt{3} \frac{h}{\theta}\right) e^{-\sqrt{3} \frac{h}{\theta}}$$

- Matern 5/2

$$k(h=|x-y|) = \left(1 + \sqrt{5} \frac{h}{\theta} + \frac{5}{3} \left(\frac{h}{\theta}\right)^2\right) e^{-\sqrt{5} \frac{h}{\theta}}$$



# Focus on stochastic optimization

## ➤ Related [R] packages

### ■ DiceKriging

- Ordinary / Universal kriging
- Nugget / Noise
- Kernel:  $C(x, y) = s^2 k(x, y)$

- Exponential

$$k(h=|x-y|) = e^{-\frac{h}{\theta}}$$

- Gauss

$$k(h=|x-y|) = e^{-\left(\frac{h}{\theta}\right)^2}$$

- Power-exponential

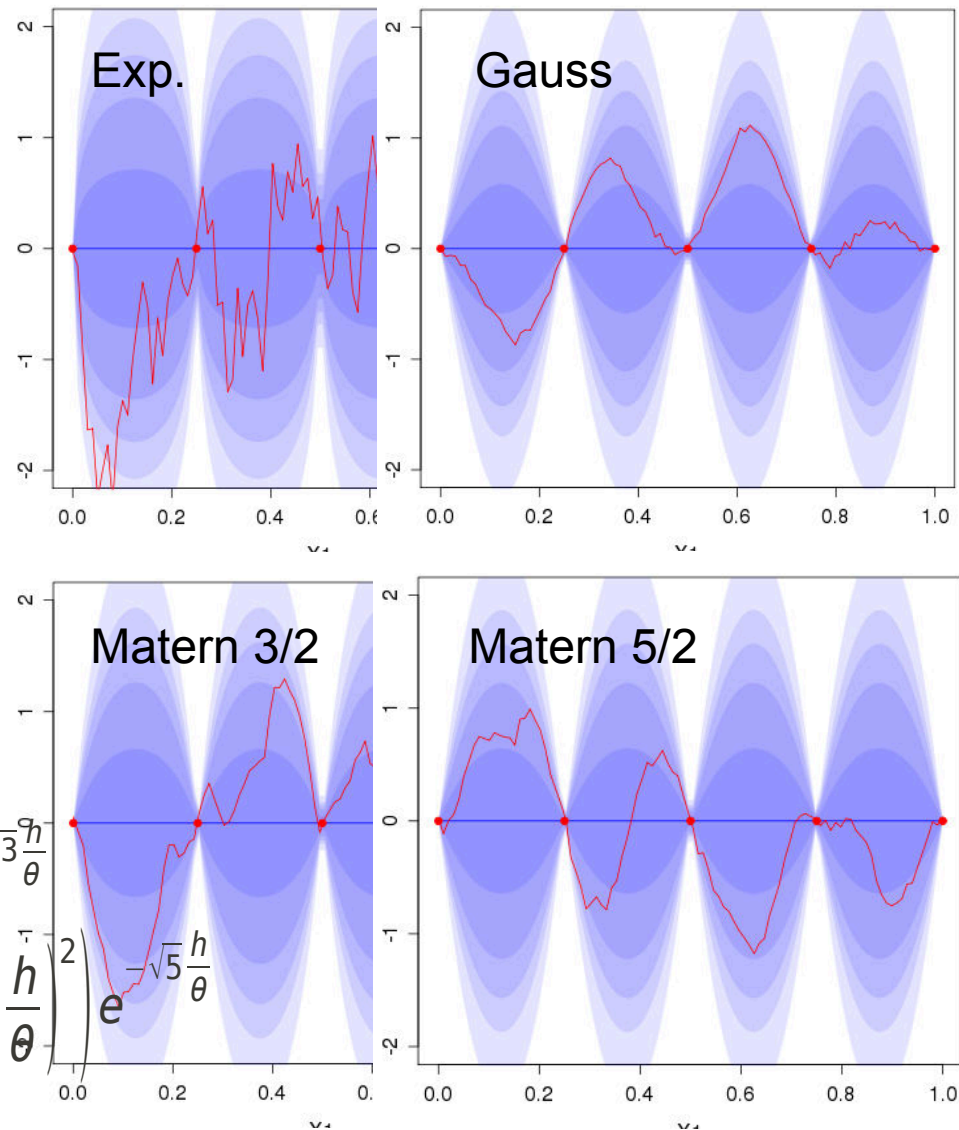
$$k(h=|x-y|) = e^{-\left(\frac{h}{\theta}\right)^p}$$

- Matern 3/2

$$k(h=|x-y|) = \left(1 + \sqrt{3} \frac{h}{\theta}\right) e^{-\sqrt{3} \frac{h}{\theta}}$$

- Matern 5/2

$$k(h=|x-y|) = \left(1 + \sqrt{5} \frac{h}{\theta} + \frac{5}{3} \left(\frac{h}{\theta}\right)^2\right) e^{-\sqrt{5} \frac{h}{\theta}}$$





# Focus on stochastic optimization

## ➤ Related [R] packages

### ■ DiceOptim

- Expected Improvement (local) criterion
  - Low cost criterion (compared to global ones)
  - Maybe extended to noisy kriging
- Parallel maximization of EI based on « Constant Liar » heuristic
  - min/max/mean/kriging mean/...
  - Used as a tuning parameter for global/local optimization
- Integrated / Decoupled call of cost function
  - Suitable for « computer experiments » framework

# Focus on stochastic optimization

## ➤ Related [R] packages

### ■ DiceView

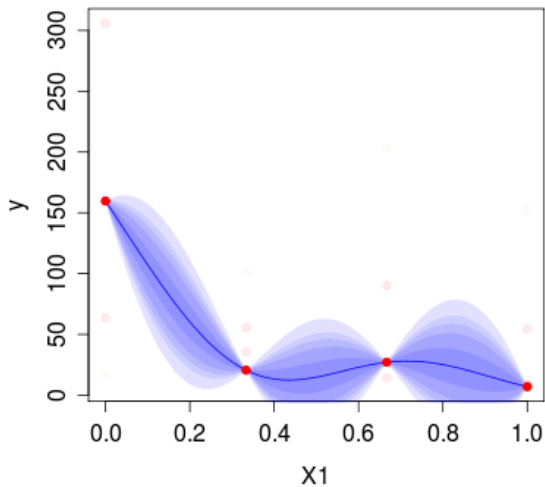
```
d <- 2; n <- 16
design.fact <- expand.grid(seq(0, 1, length = 4), seq(0, 1, length = 4))
design.fact <- data.frame(design.fact); names(design.fact) <- c("x1", "x2")
y <- branin(design.fact)

m <- km(design = design.fact, response = y)

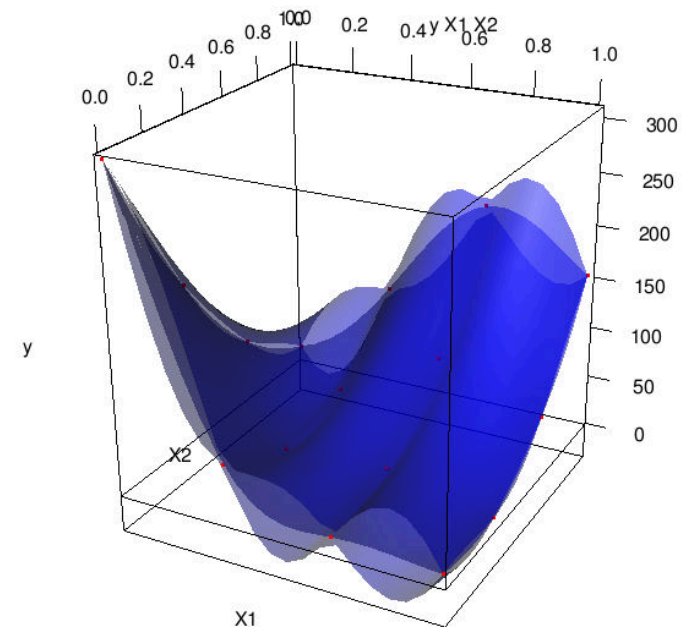
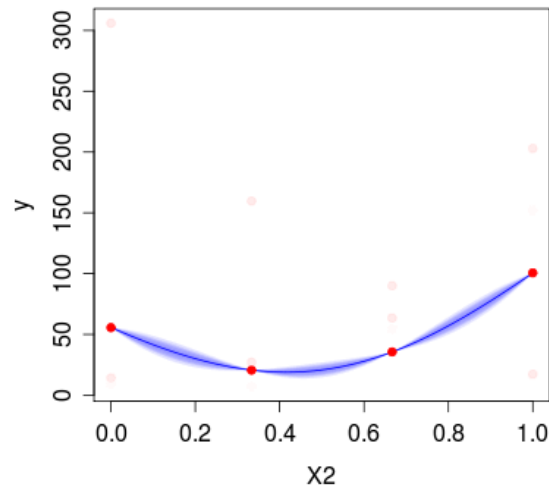
sectionview(m, center = c(.3, .3))

sectionview3d(m)
```

X2 = 0.3



X1 = 0.3



# Focus on stochastic optimization

## ➤ Integration of stochastic simulator

### ■ Controlled convergence heuristic for MC criticality code

- MC code => sd estimator of Gaussian output (k-effective) is available  
(each MC sample increase, for instance)
  - Code endpoint may be
    - Sample size :(
    - Estimator sd target
    - Estimator quantile (0.999) target
  - Early endpoint reached when k-effective 99.9%-quantile  $\ll$  1.0
- OR
- Early endpoint reached when k-effective 99.9%-quantile  $\ll$  current max.

### ■ Resource-constraint optimization using simulator fidelity

- On-line control of experiments fidelity using « Start & Stop »
- Quantile based Expected Improvement
- *To be published in Technometrics 2011*

■ **Promethee** workbench <http://www.irsn.fr/promethee>

■ **Dice\*** kriging packages (<http://dice.emse.fr/>)

### **DiceKriging**

<http://cran.r-project.org/web/packages/DiceKriging/index.html>

### **DiceOptim**

<http://cran.r-project.org/web/packages/DiceOptim/index.html>

### **DiceView**

<http://cran.r-project.org/web/packages/DiceView/index.html>