IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Enhancing nuclear safety

Stochastic global optimization practice in nuclear criticality safety assessment

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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

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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:
  - sd(k-effective) < input setting (say 0.00100)
  - quantile(k-effective,0.999) < input setting (say 0.95000 or current max.)

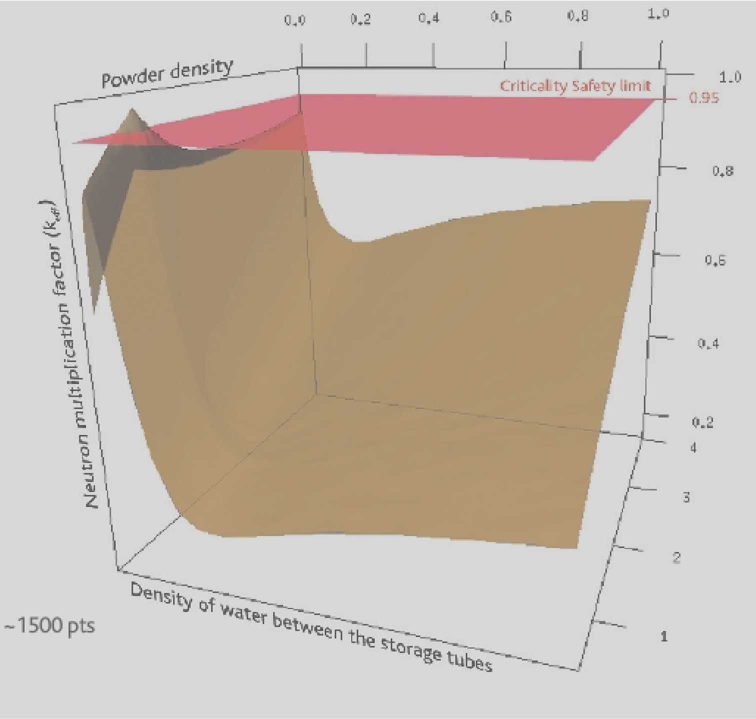
Remote/grid calculation issue at IRSN

- ~ 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 PuO2 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)

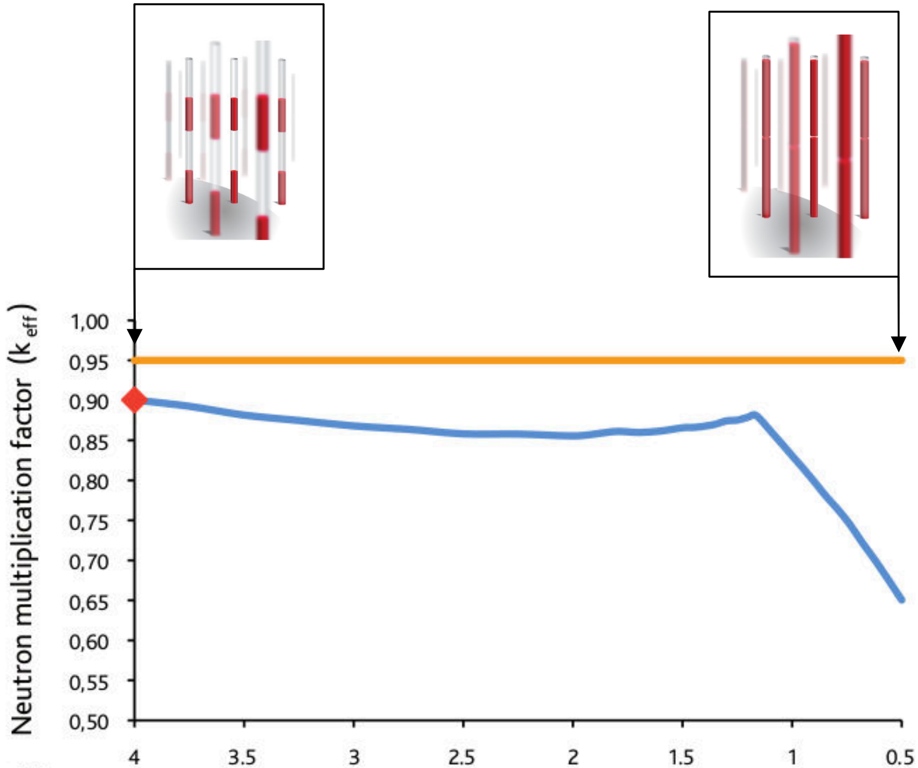
➚ Case study results

Nuclear criticality-safety assessment and related issues

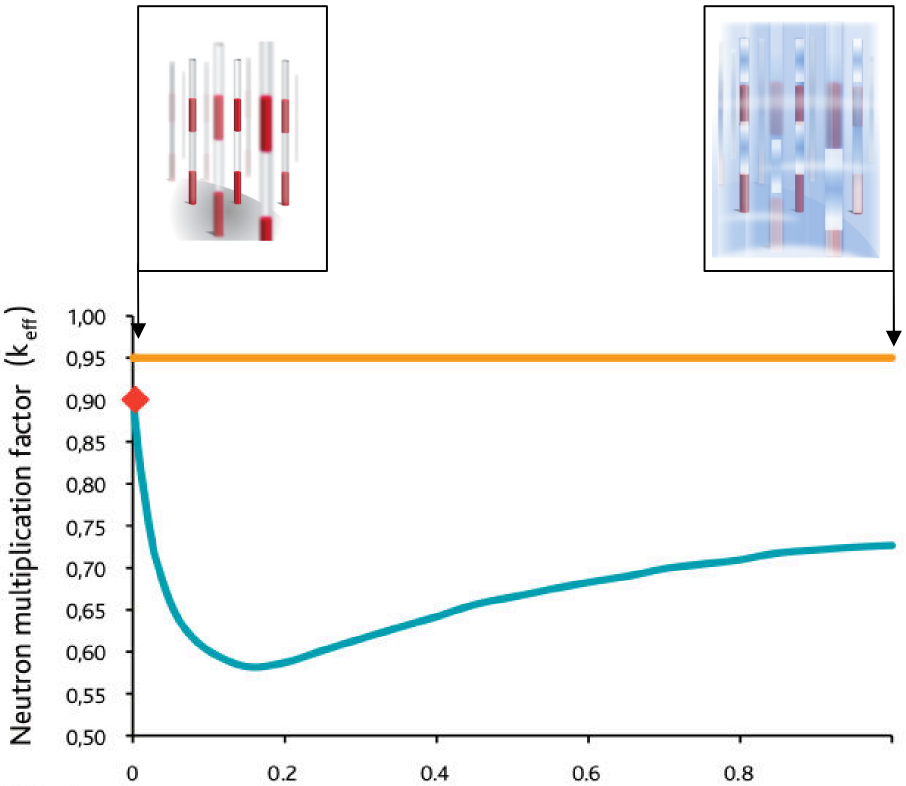
↗ Rethinking through « Computer Experiments » framework

Expert-driven approach – case study results

- OaT maximization



~15 pts



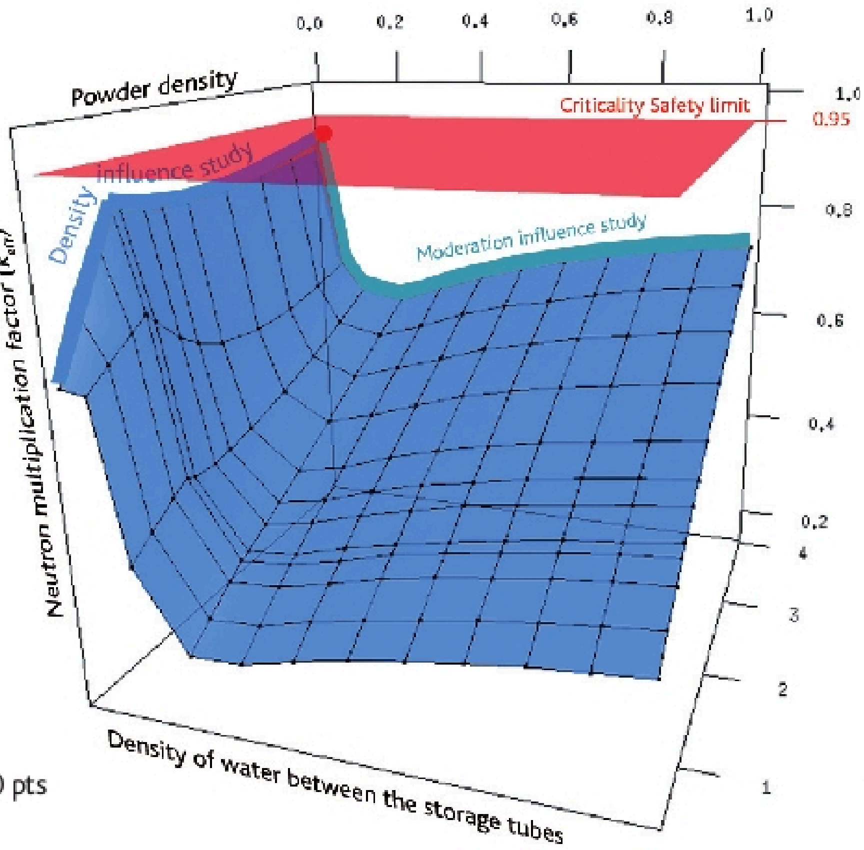
-15 pts

Nuclear criticality-safety assessment and related issues

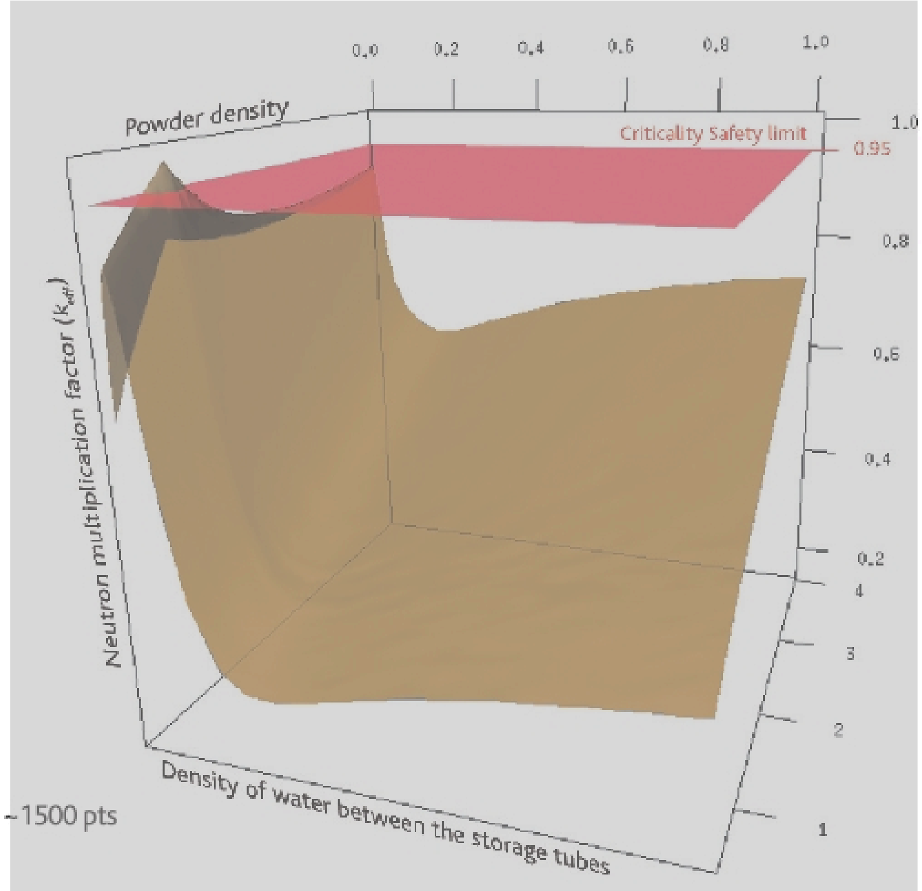
↗ Rethinking through « Computer Experiments » framework

Expert-driven approach – case study results

- Factorial DoE



~150 pts



~1500 pts

Nuclear criticality-safety assessment and related issues

↗ Rethinking through « Computer Experiments » framework

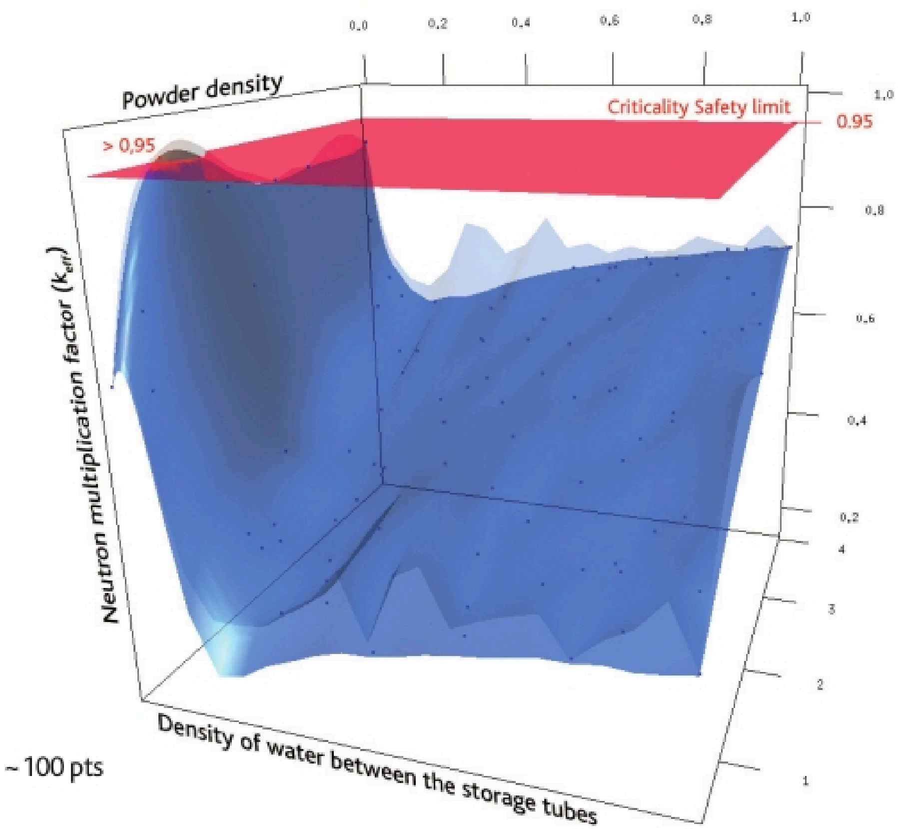
EGO-assisted approach

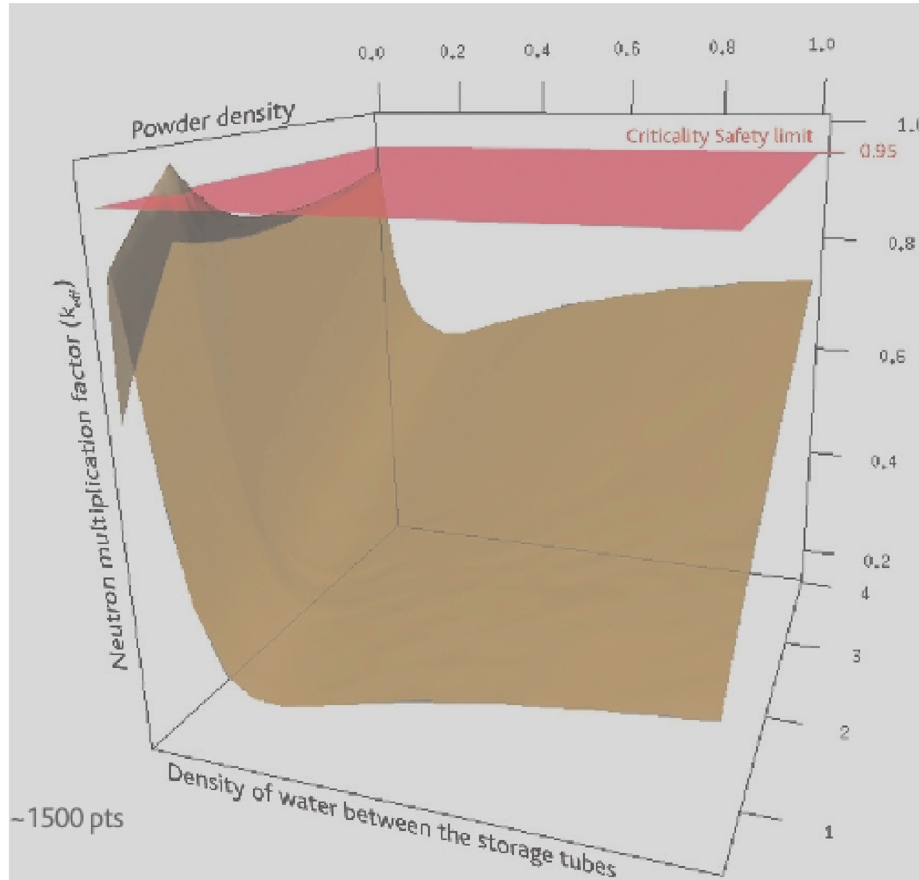
- Initial DoE
  - LHS
  - (cross) Bounds of parameters
- Kriging surrogate of noisy (as MC) experiments
- Maximization of Expected Improvement criterion
- Loop on Kriging/maxEI ...

↗ Case study results

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, …)

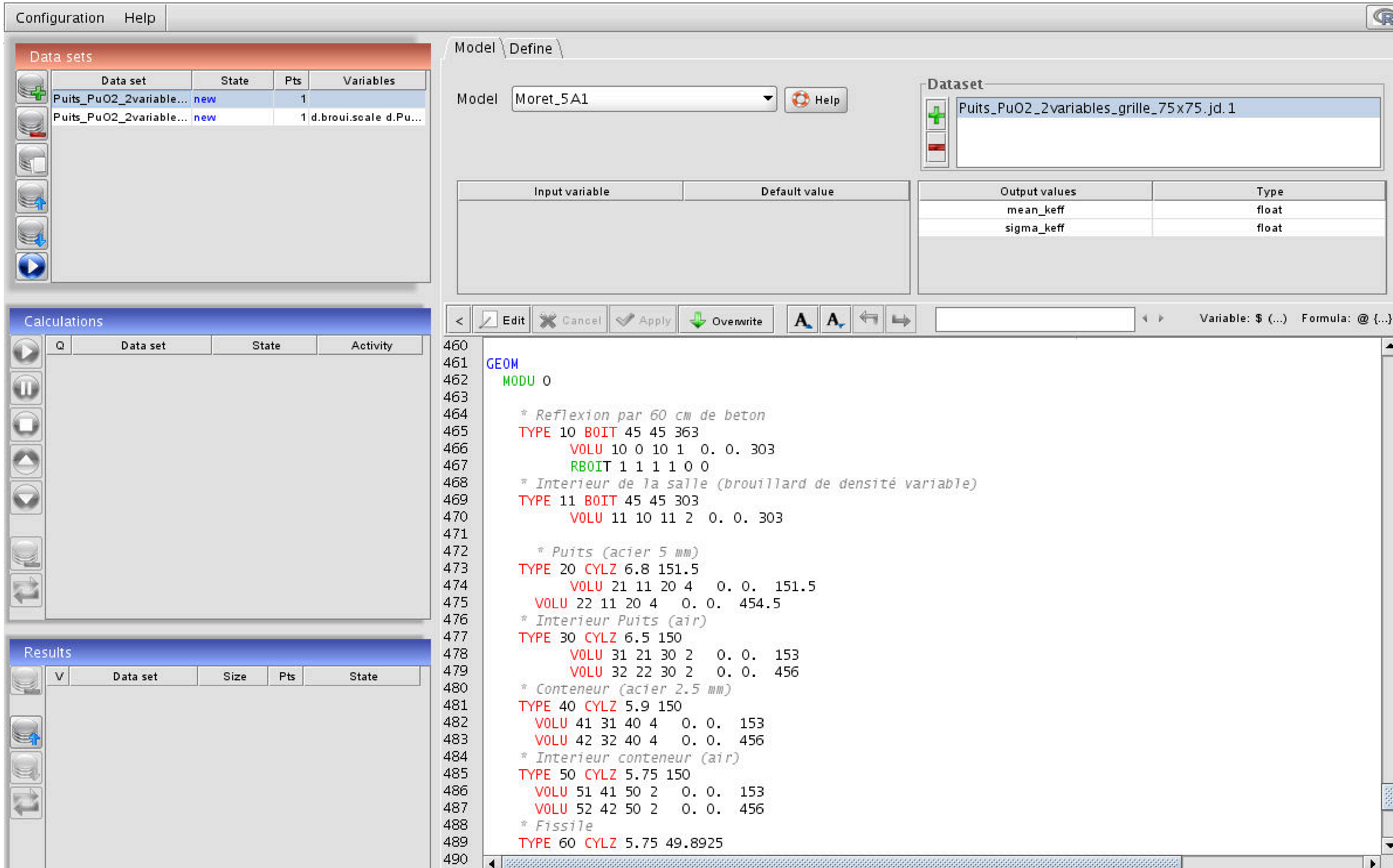
Computing

- (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



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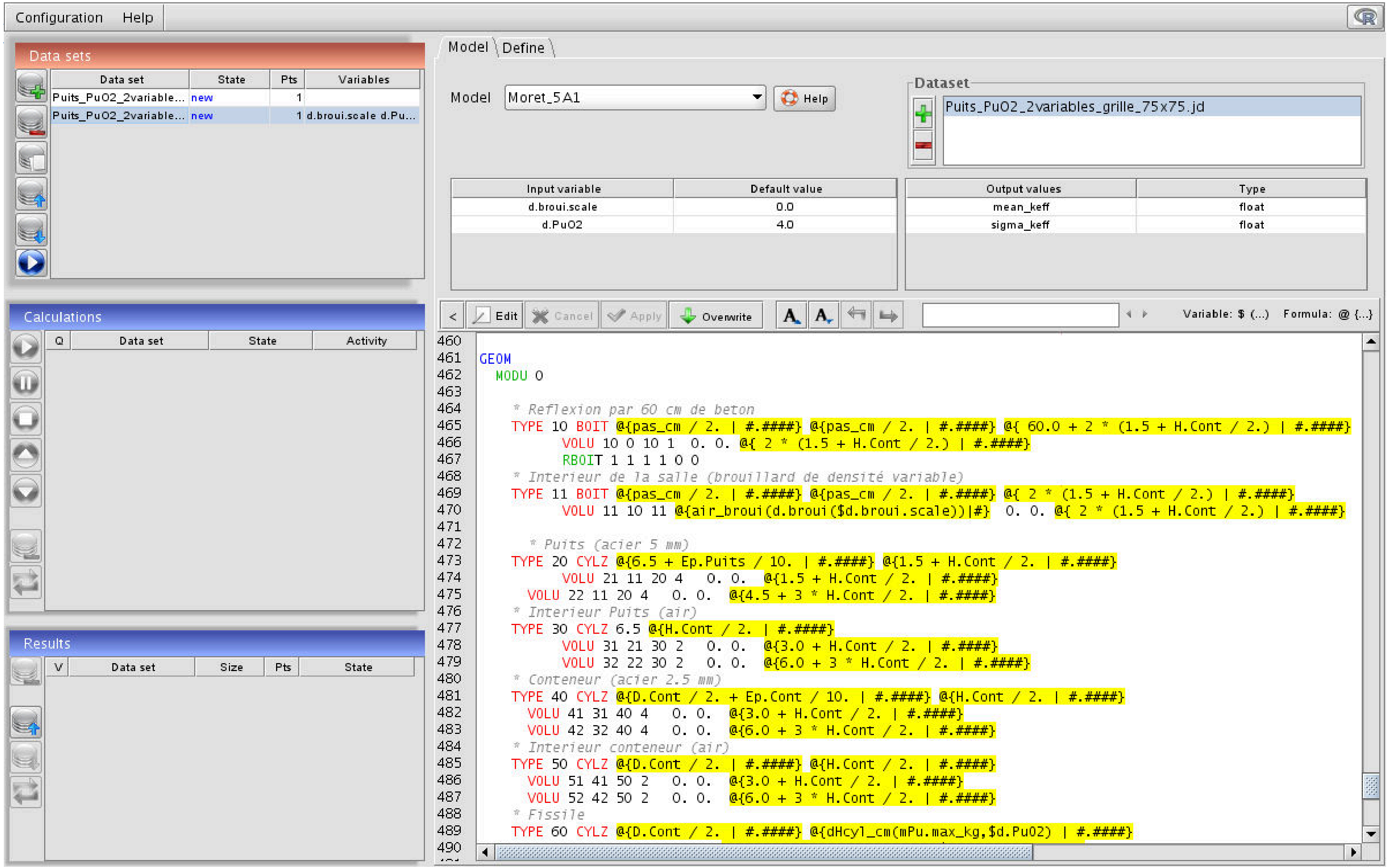

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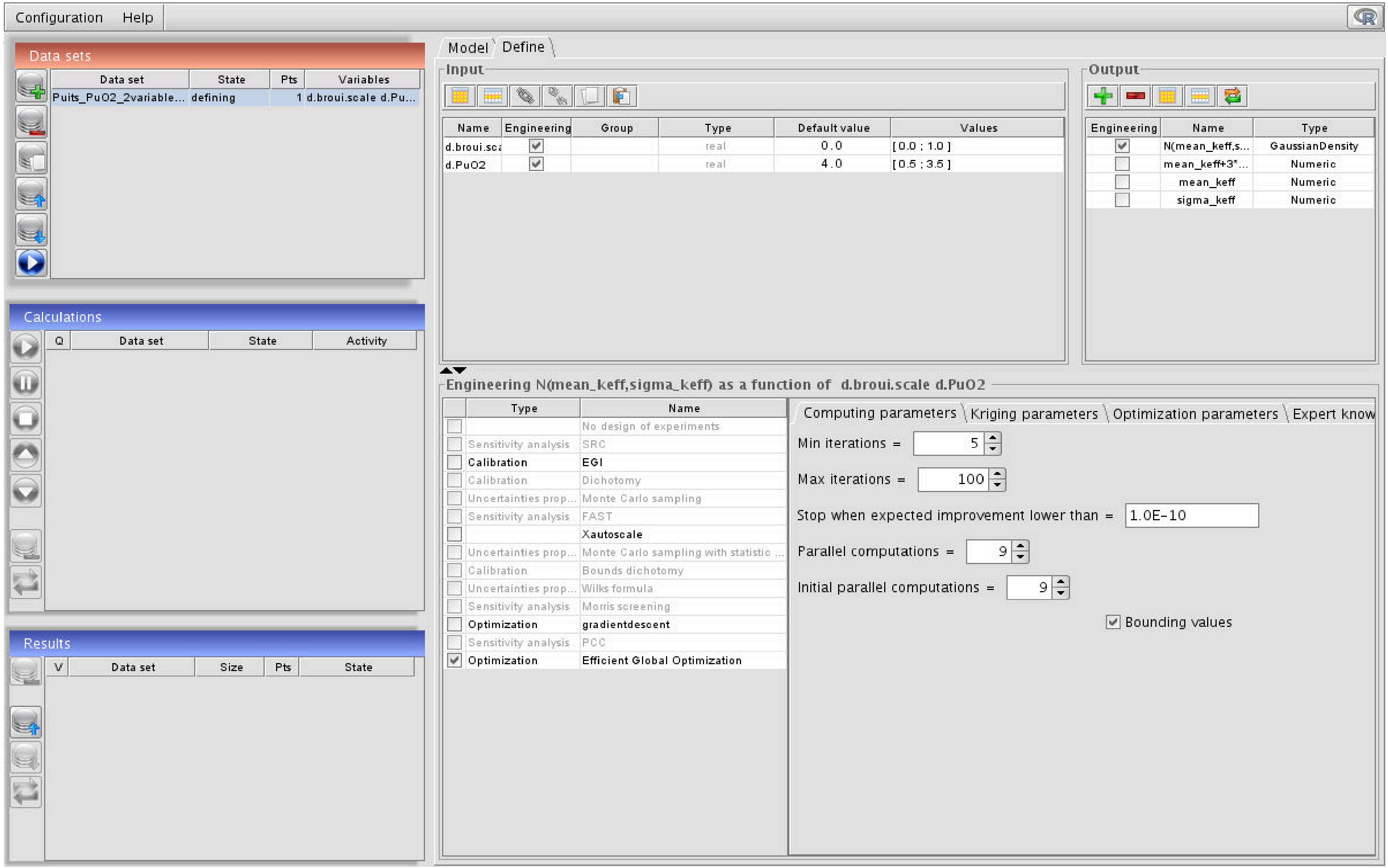

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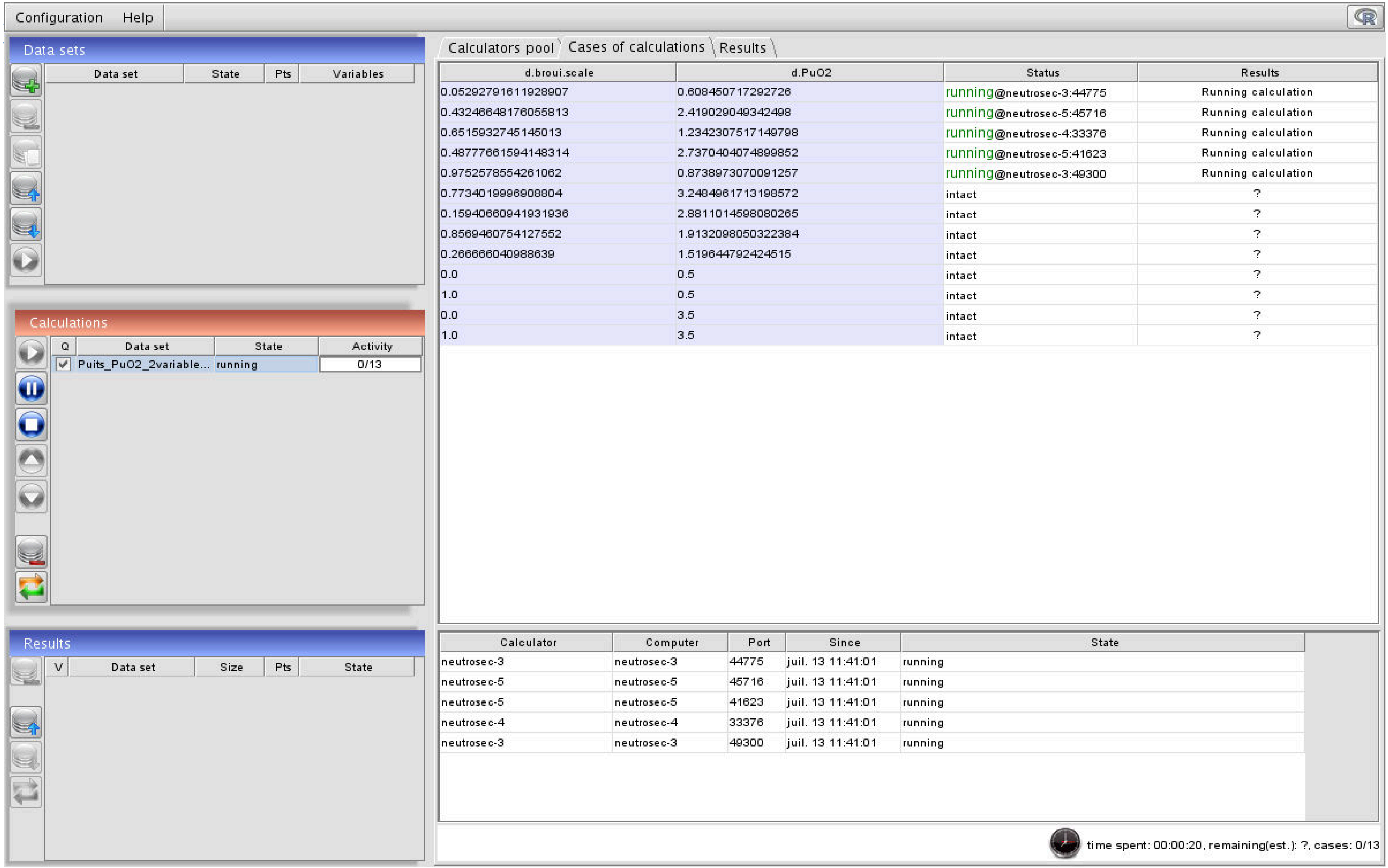

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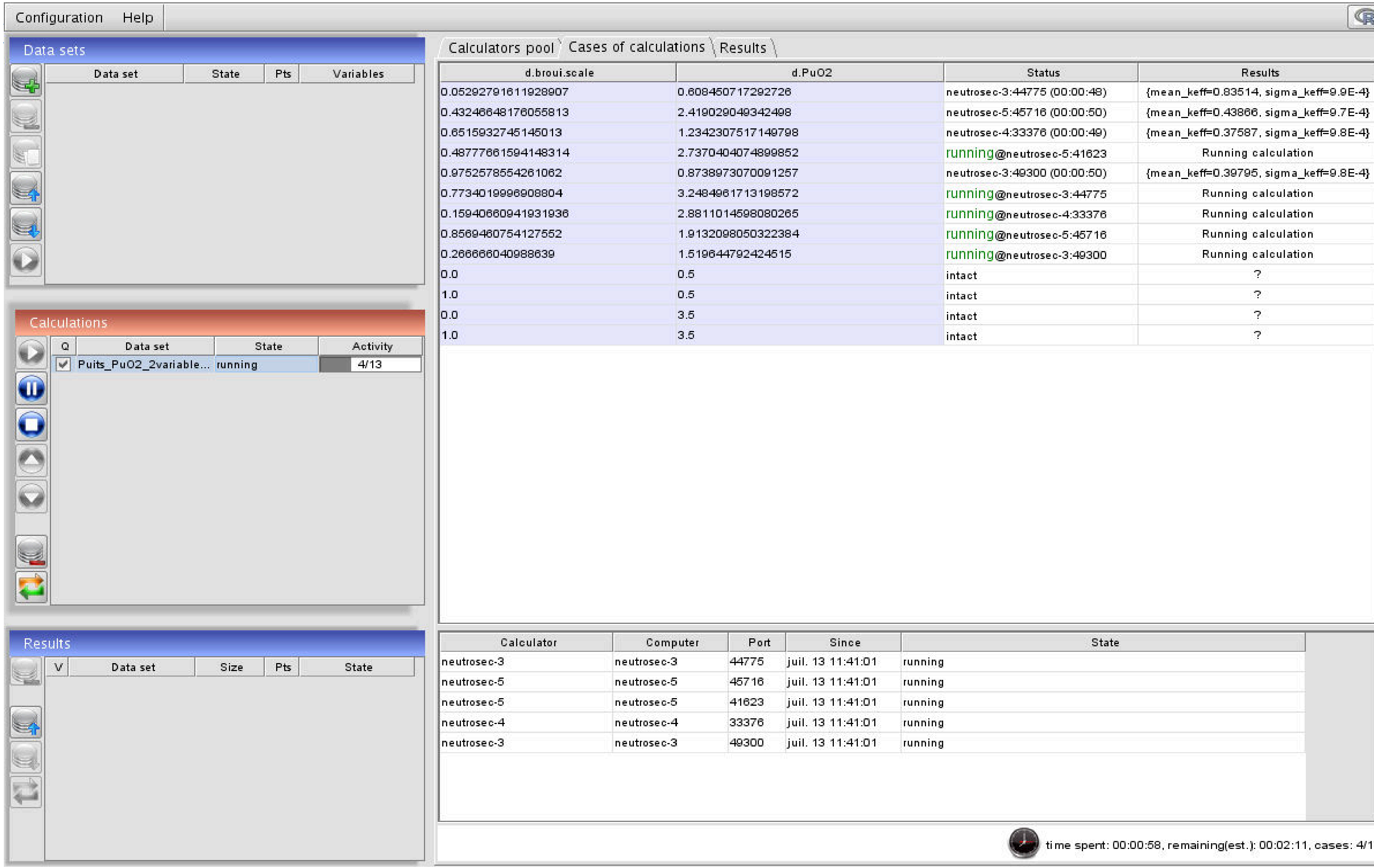

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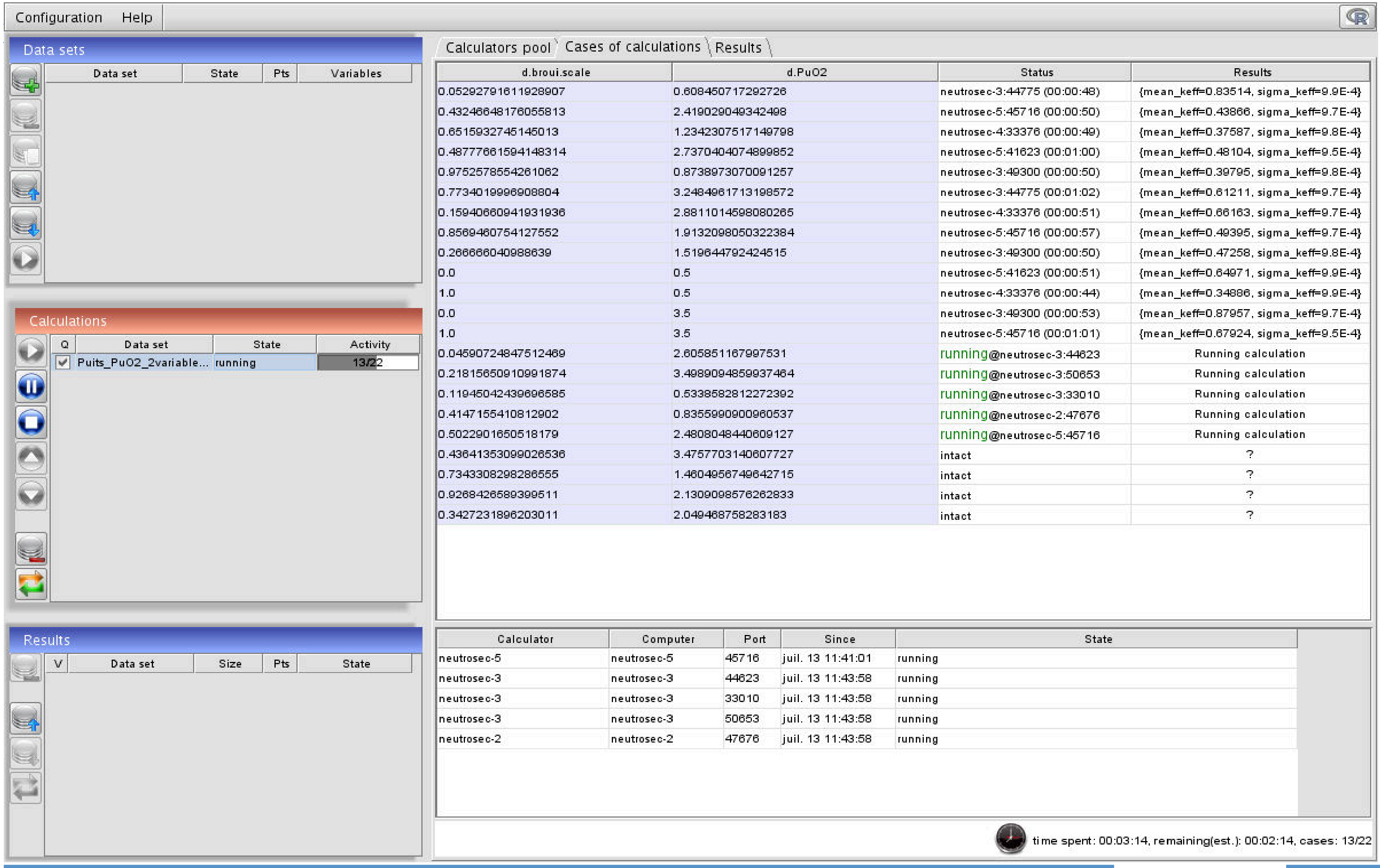
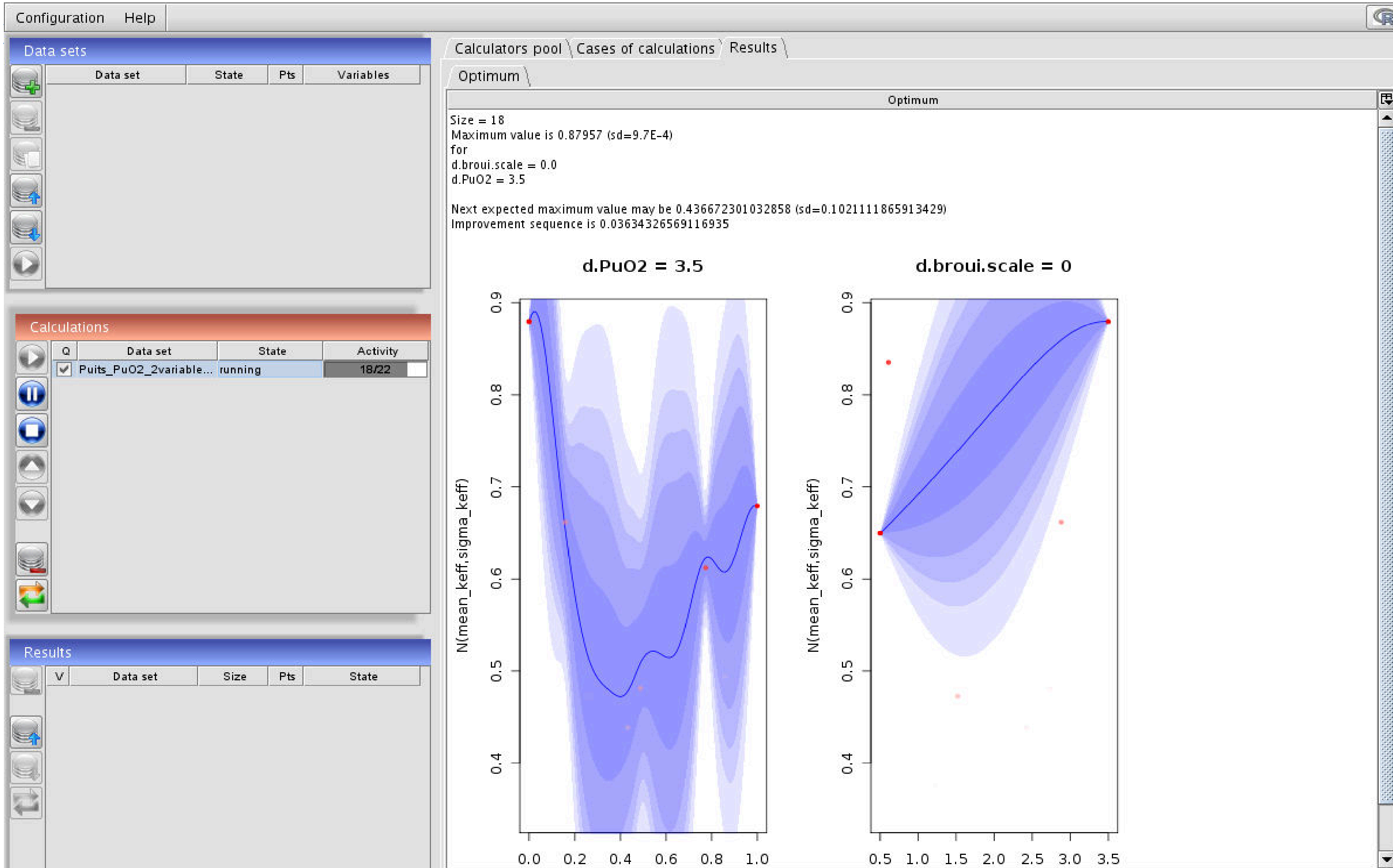


d.broui.scale	d.PuO2	Status	Results
0.05292791611928907	0.608450717292726	neutrosec-3:44775 (00:00:48)	{mean_keff=0.83514, sigma_keff=9.9E-4}
0.43246648176055813	2.419029049342498	neutrosec-5:45716 (00:00:50)	{mean_keff=0.43866, sigma_keff=9.7E-4}
0.6515932745145013	1.2342307517149798	neutrosec-4:33376 (00:00:49)	{mean_keff=0.37587, sigma_keff=9.8E-4}
0.48777661594148314	2.7370404074899852	neutrosec-5:41623 (00:01:00)	{mean_keff=0.48104, sigma_keff=9.5E-4}
0.9752578554261062	0.8738973070091257	neutrosec-3:49300 (00:00:50)	{mean_keff=0.39795, sigma_keff=9.8E-4}
0.7734019996908804	3.2484961713198572	neutrosec-3:44775 (00:01:02)	{mean_keff=0.61211, sigma_keff=9.7E-4}
0.15940660941931936	2.8811014598080265	neutrosec-4:33376 (00:00:51)	{mean_keff=0.66163, sigma_keff=9.7E-4}
0.8569460754127552	1.9132098050322384	neutrosec-5:45716 (00:00:57)	{mean_keff=0.49395, sigma_keff=9.7E-4}
0.266666040988639	1.519644792424515	neutrosec-3:49300 (00:00:50)	{mean_keff=0.47258, sigma_keff=9.8E-4}
0.0	0.5	neutrosec-5:41623 (00:00:51)	{mean_keff=0.64971, sigma_keff=9.9E-4}
1.0	0.5	neutrosec-4:33376 (00:00:44)	{mean_keff=0.34886, sigma_keff=9.9E-4}
0.0	3.5	neutrosec-3:49300 (00:00:53)	{mean_keff=0.87957, sigma_keff=9.7E-4}
1.0	3.5	neutrosec-5:45716 (00:01:01)	{mean_keff=0.67924, sigma_keff=9.5E-4}
0.04590724847512469	2.605851167997531	running@neutrosec-3:44623	Running calculation
0.21815650910991874	3.4989094859937464	running@neutrosec-3:50653	Running calculation
0.11945042439696585	0.5338582812272392	running@neutrosec-3:33010	Running calculation
0.4147155410812902	0.8355990900960537	running@neutrosec-2:47676	Running calculation
0.5022901650518179	2.4808048440609127	running@neutrosec-5:45716	Running calculation
0.43641353099026536	3.4757703140607727	intact	?
0.7343308298286555	1.4604956749642715	intact	?
0.9268426589399511	2.1309098576262833	intact	?
0.3427231896203011	2.049468758283183	intact	?

Calculator	Computer	Port	Since	State
neutrosec-5	neutrosec-5	45716	juil. 13 11:41:01	running
neutrosec-3	neutrosec-3	44623	juil. 13 11:43:58	running
neutrosec-3	neutrosec-3	33010	juil. 13 11:43:58	running
neutrosec-3	neutrosec-3	50653	juil. 13 11:43:58	running
neutrosec-2	neutrosec-2	47676	juil. 13 11:43:58	running

Components to build an operational workbench



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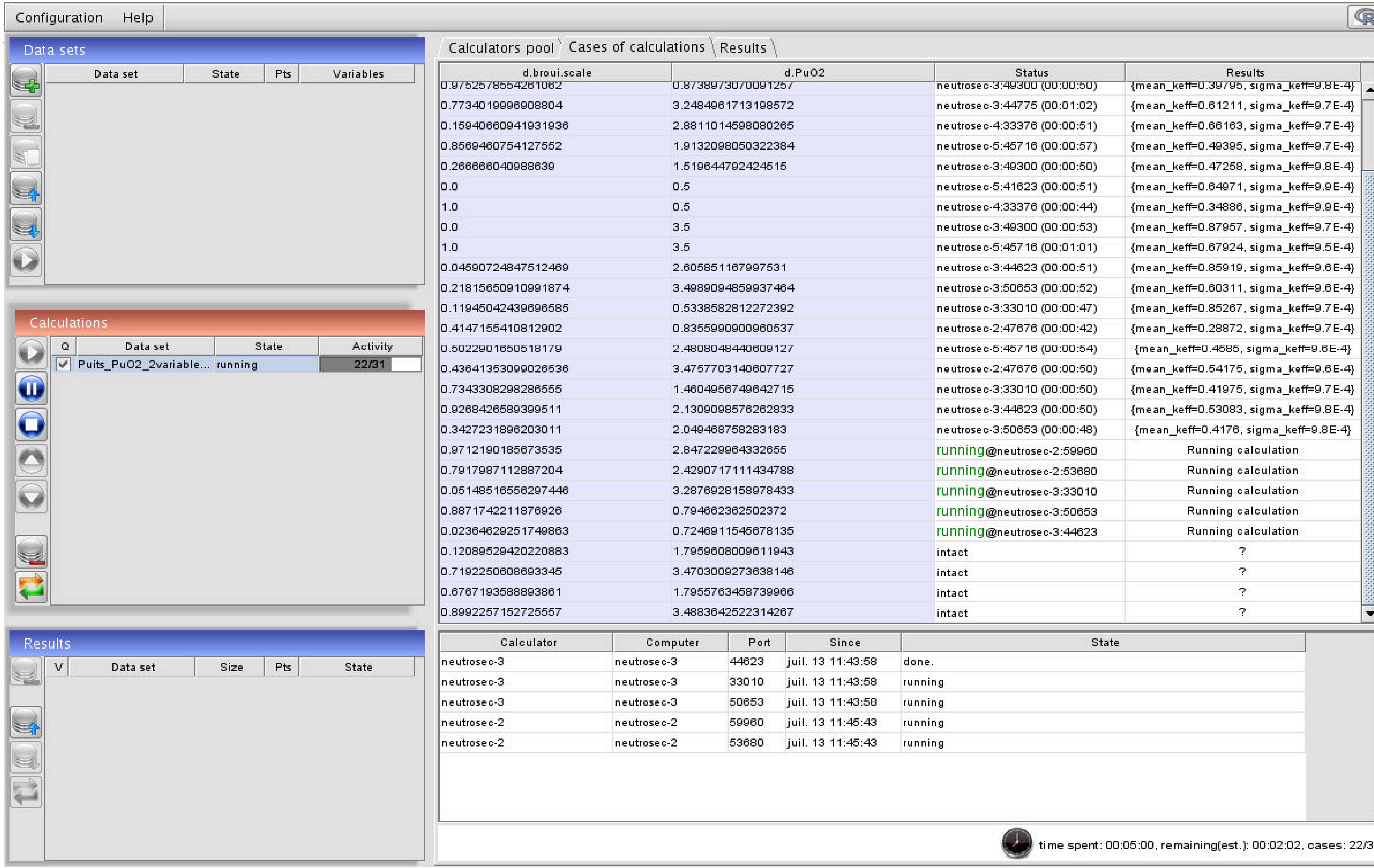

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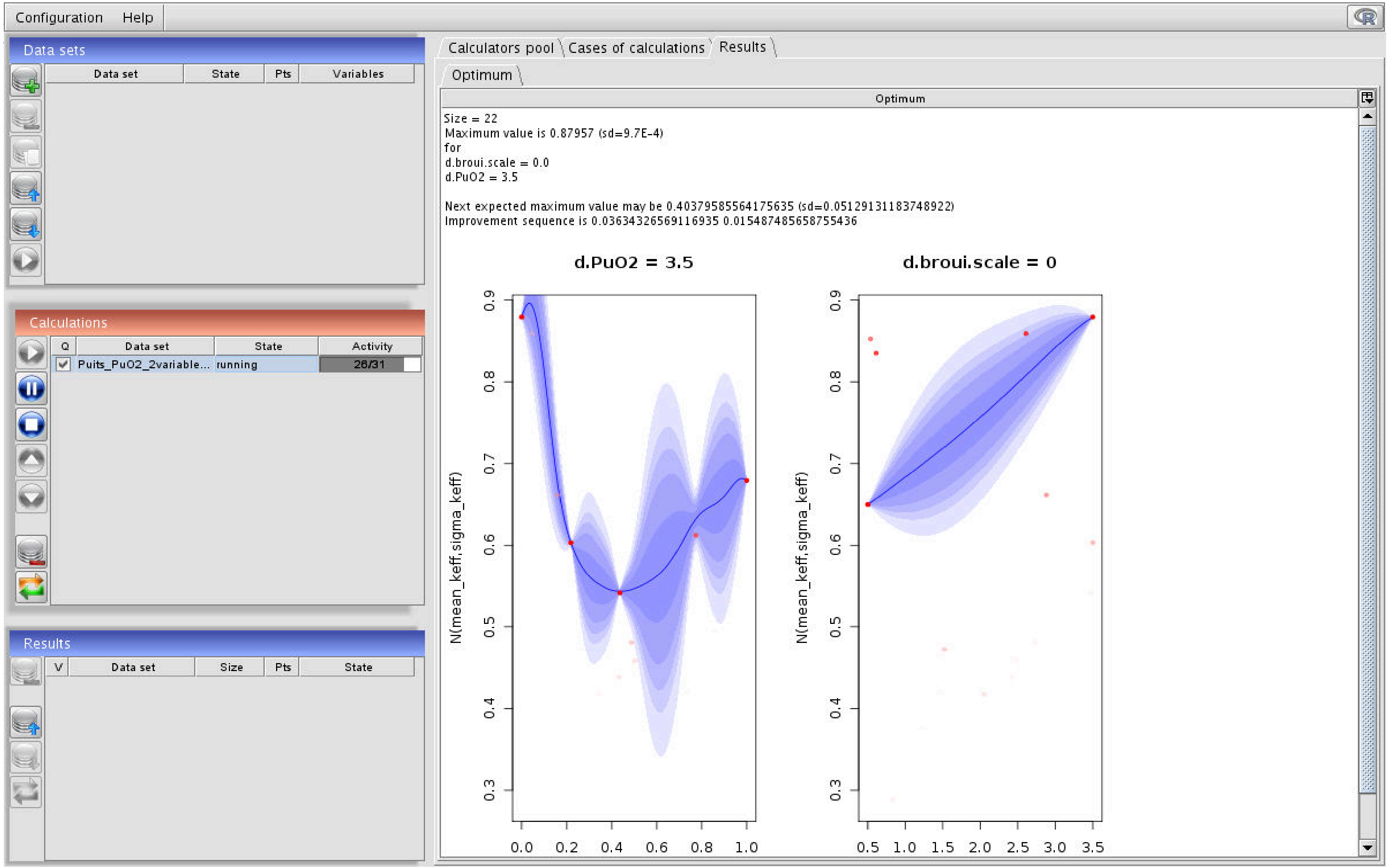

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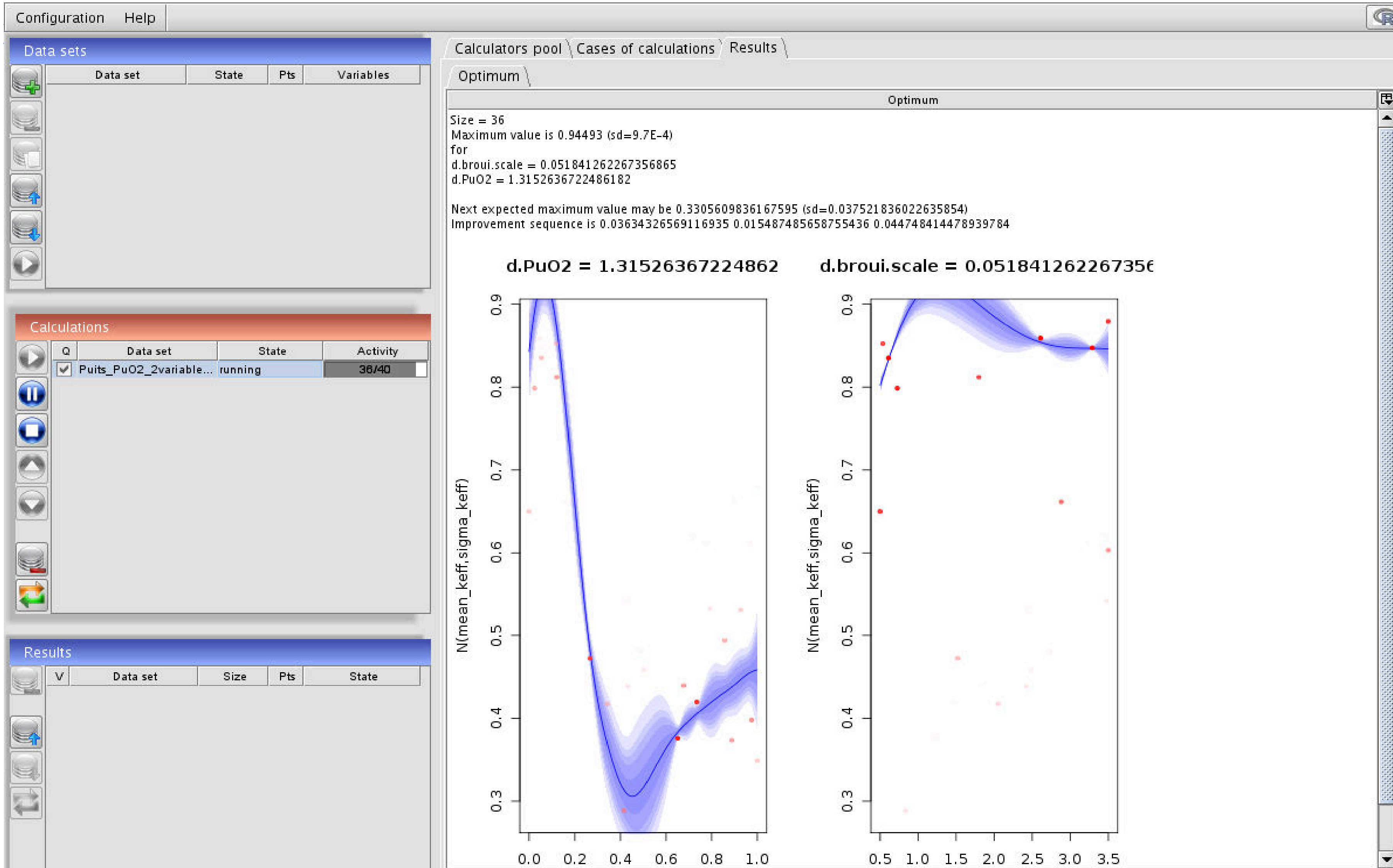

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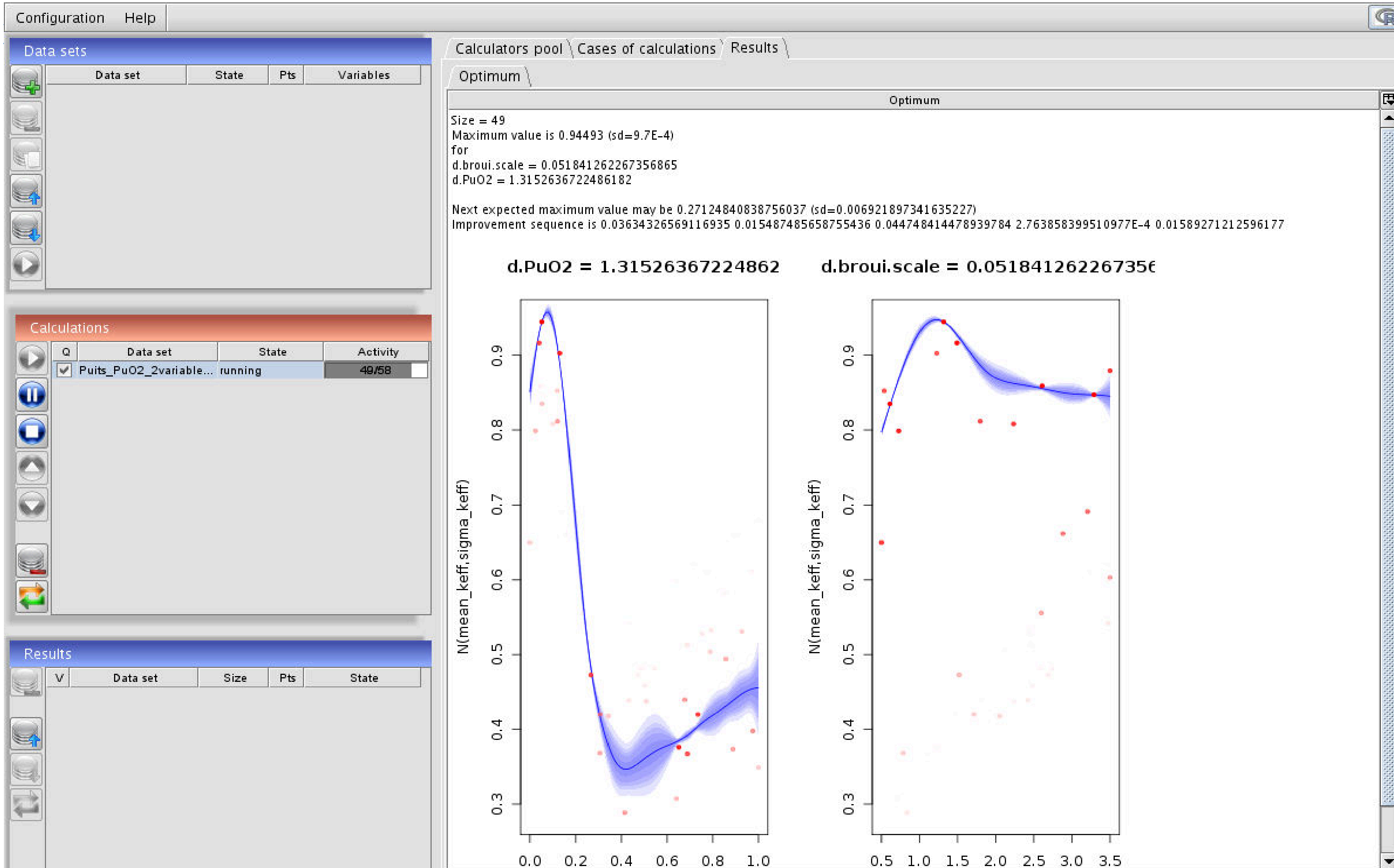

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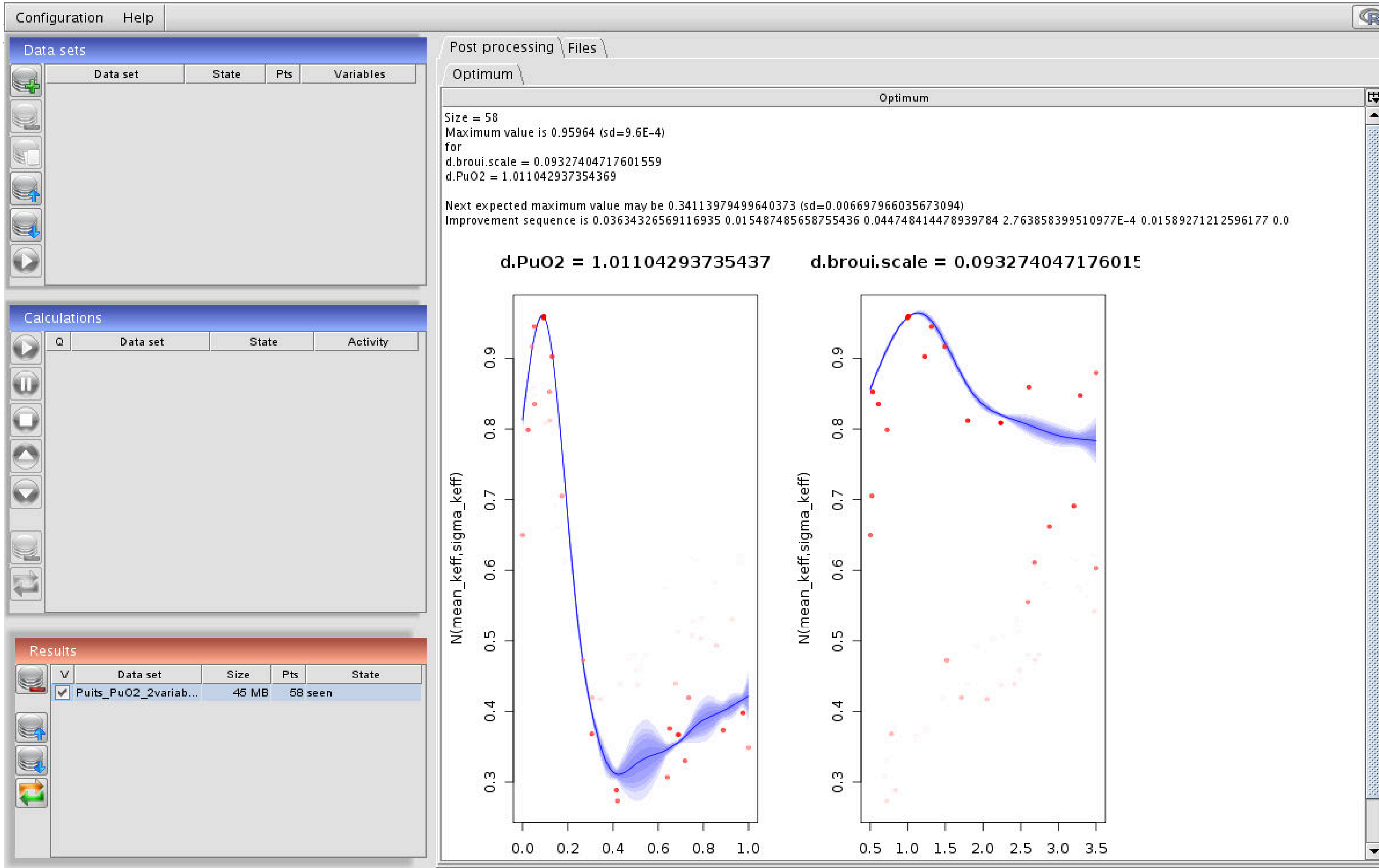

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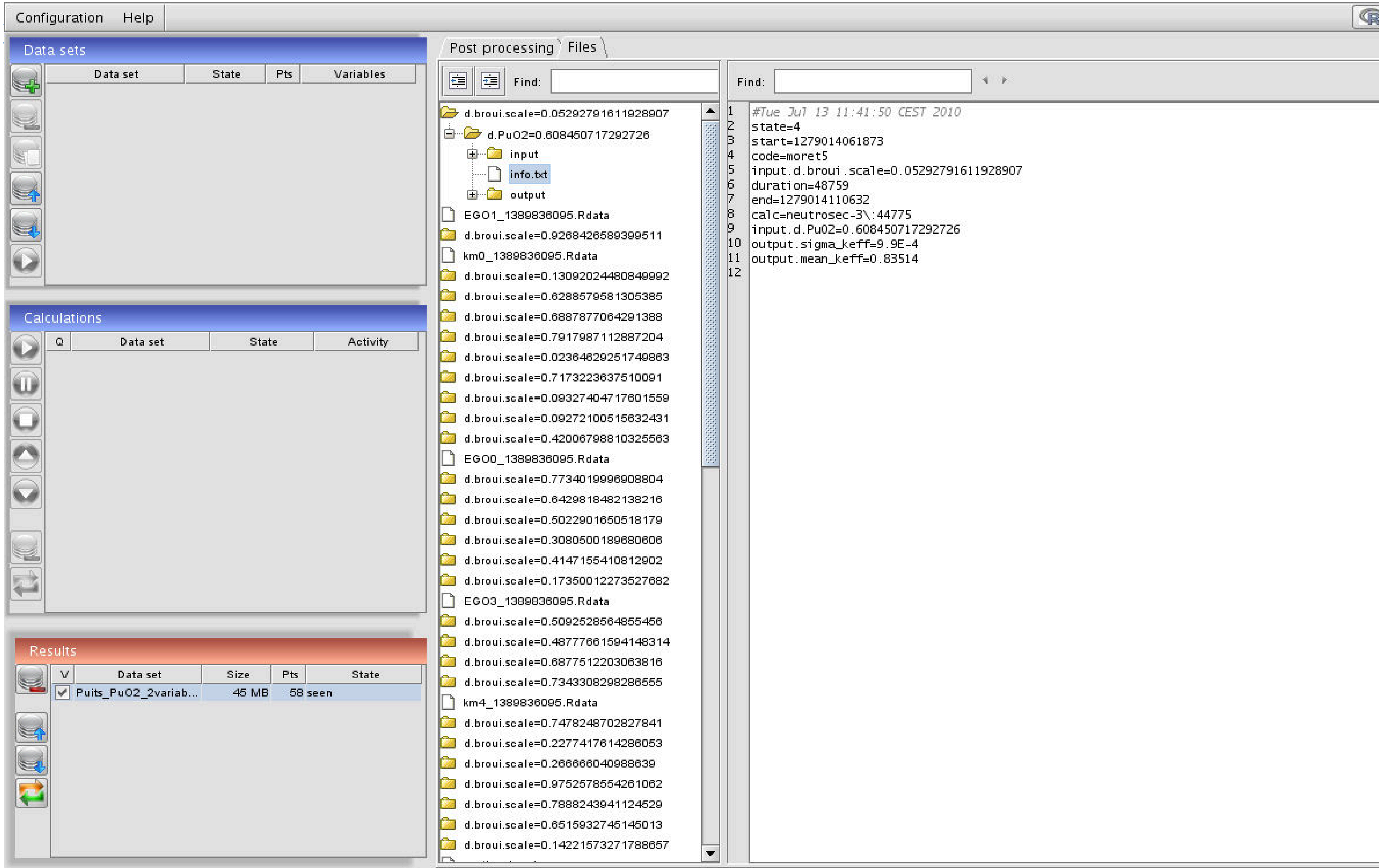


Components to build an operational workbench

Grid computing engine & algorithm back-end

Distributed computing engine

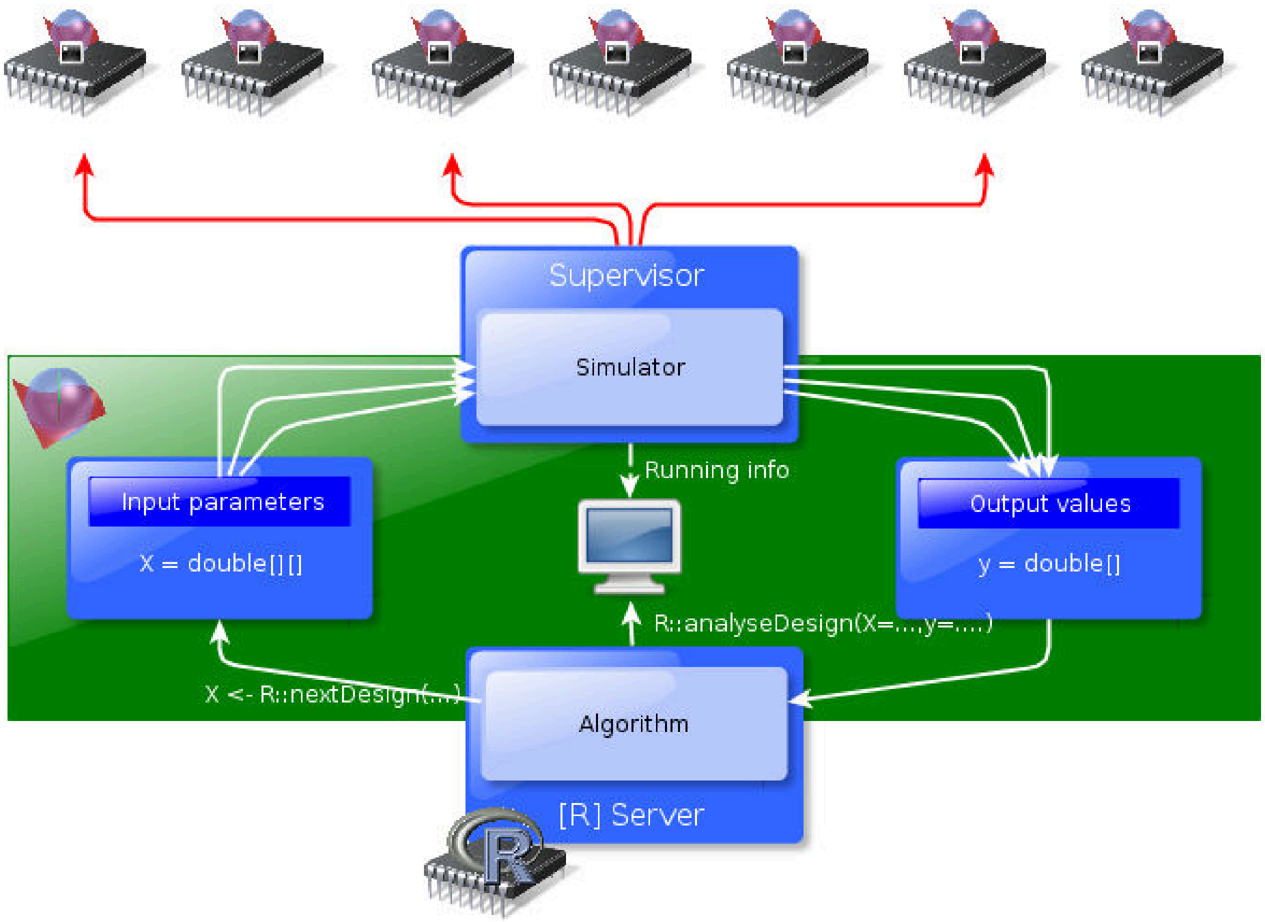
- Asynchronous, remote & parallel distribution
- Back-end daemon compatible with larger set of CPU boxes :
  server, workstation, grid, cluster, ... and even Windows office desktop
- Dynamic merge of heterogeneous computing power
- Failover

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

```r
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

- Adhesion vs. resiliency
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Focus on stochastic optimization

- Related [R] packages
- Integration of stochastic simulator

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^{nd} degree splines
- To be published in DiceKriging 1.2 (soon)

Parallel EGO

- Constant Liar heuristic
- Tunnable deepening of EGO

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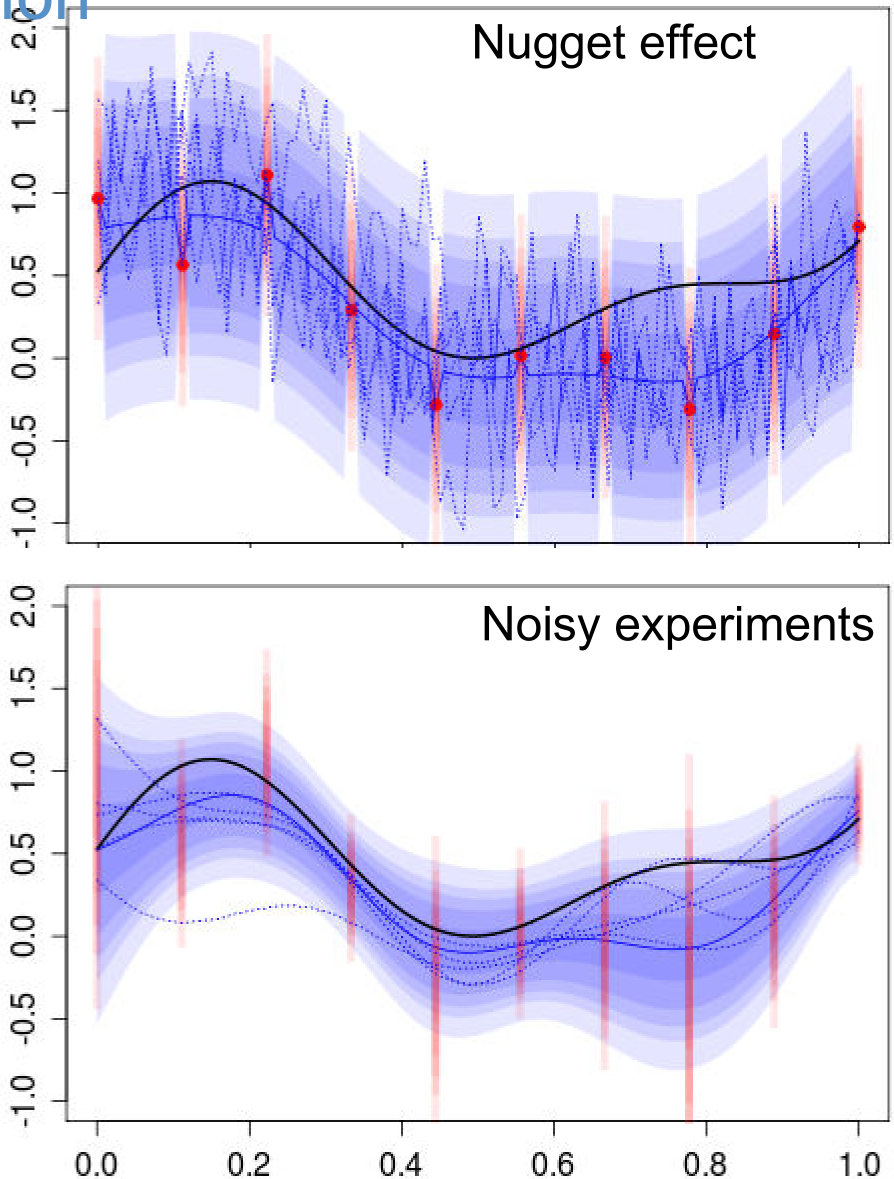
DiceKriging

- Ordinary / Universal kriging
- Nugget / Noise



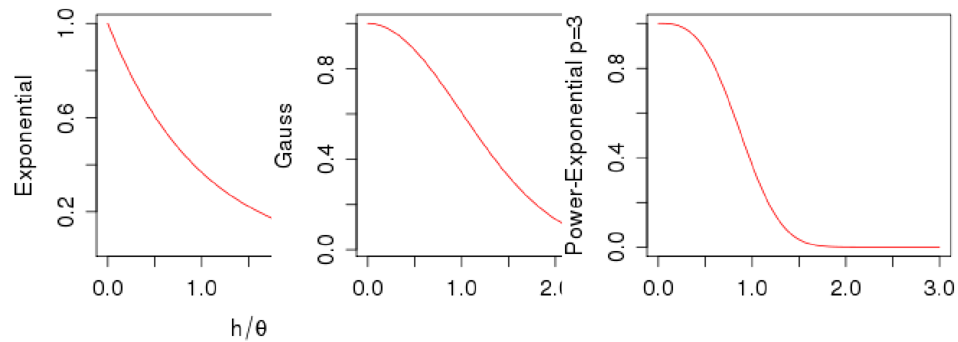
- Kernel:
  - Exponential
  - Gauss
  - Power-exponential
  - Matern 3/2
  - Matern 5/2

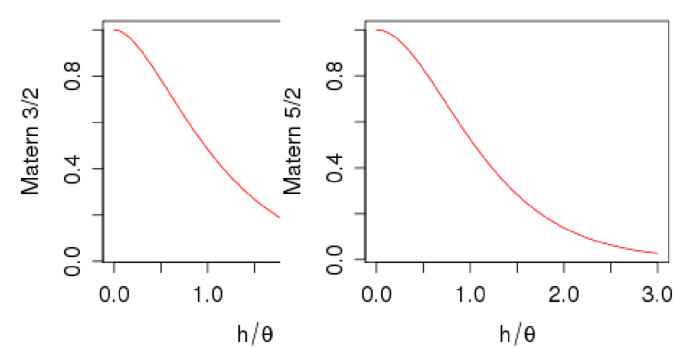
Focus on stochastic optimization

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





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➚ Related [R] packages

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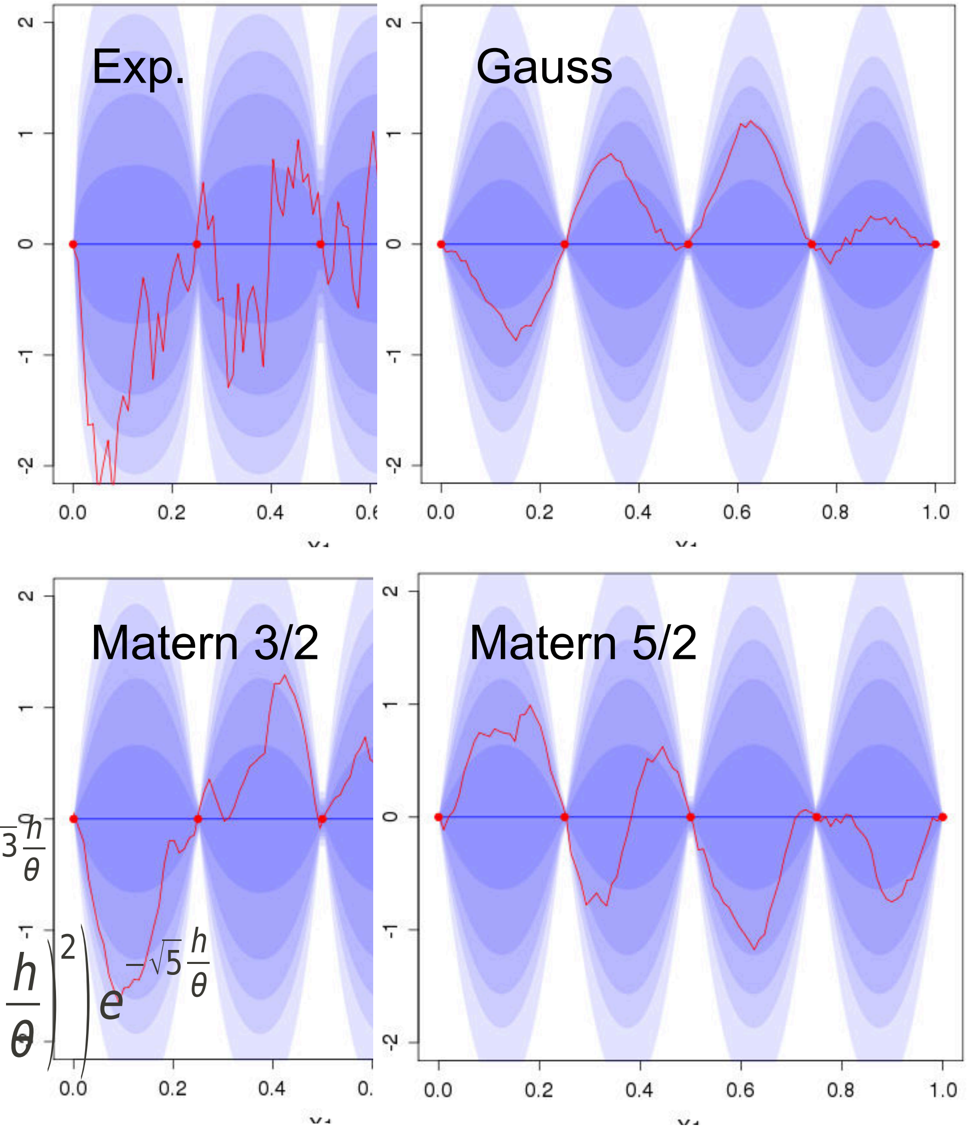


Focus on stochastic optimization

Related [R] packages

DiceOptim

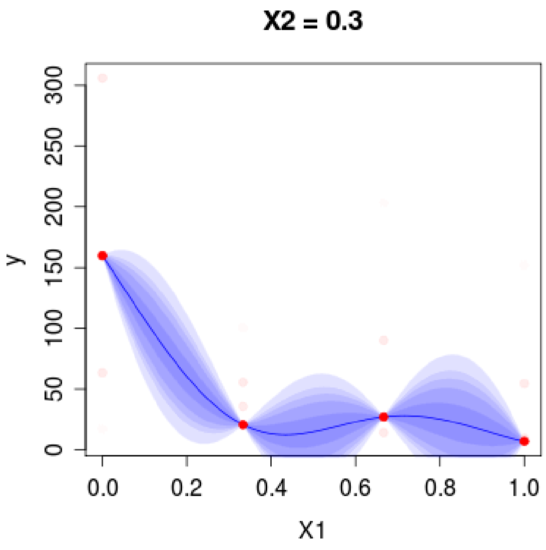
- Expected Improvement (local) criterion
  - Low cost criterion (compared to global ones)
  - Maybe extended to noisy kriging
- Parallel maximization of EI based on « Constant Liar » heuristic
  - min/max/mean/kriging mean/...
  - Used as a tunning parameter for global/local optimization
- Integrated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

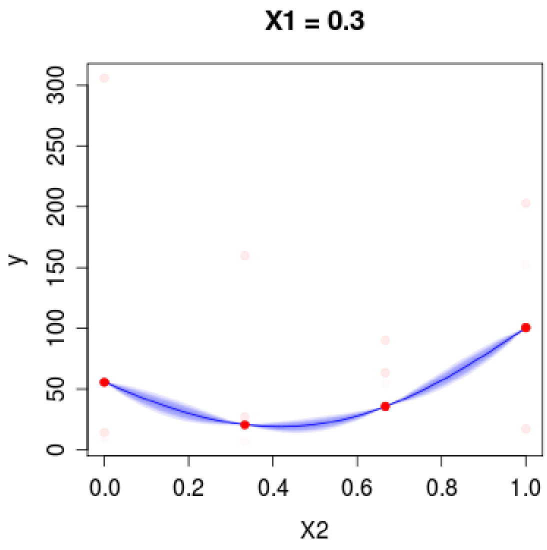
Focus on stochastic optimization

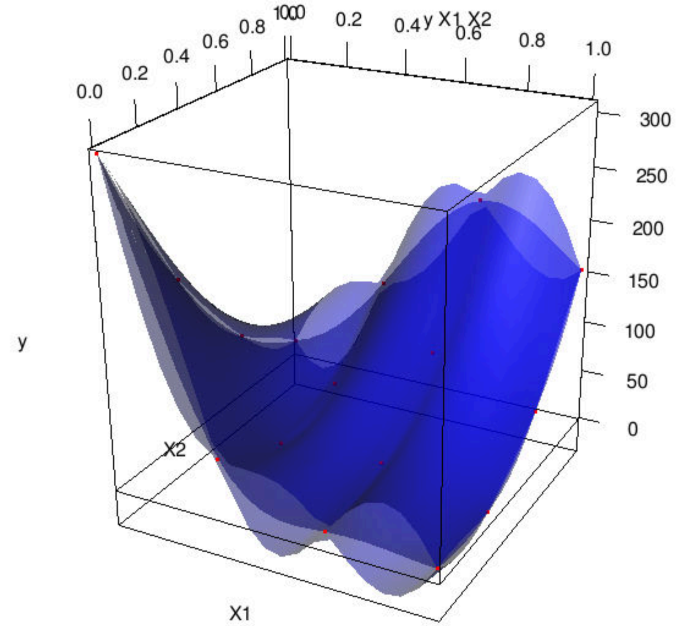
↗ Related [R] packages

- 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)
```







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 << 1.0

OR

- Early endpoint reached when k-effective 99.9%-quantile << 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