IRSEN 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





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</p>
- System <- input dataset
- Hypothesis <- input dataset variables (dim<10)
- Output of interest <- (scalar) output of the code



Classical approach and basic tools

- Parametric study for maximization of k-effective
 - < 10 scalar, independent & compact parameters</p>
 - 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)</p>
 - 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)



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]



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Rethinking through « Computer Experiments » framework

Expert-driven approach

- OaT maximization
 - 2 or 3 parameters
 - (supposed) penalizing value for other parameters
 - I 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



Rethinking through « Computer Experiments » framework

Expert-driven approach - case study results

OaT maximization



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Rethinking through « Computer Experiments » framework

Expert-driven approach - case study results



Factorial DoE

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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/maxEl ...
 - 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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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 :)



Configuration Help					R
Data sets	Mod	lel \ Define \			
Data set State Pts Variables				-Dataset	
Puits_Pu02_2variable new 1	Mo	del Moret_5A1	👻 🛟 Help	Puits PuO2 2variables or	tille 75x75 id 1
Puits_PuO2_2variable new 1 d.broui.scale d.Pu		·			me_/3x/3.jd.1
		Input variable	Default value	Output values	Туре
				mean_keff	float
				sigma_keff	float
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	464	* Reflexion par 60	cm de beton		
U	465	TYPE 10 B0IT 45 45	363		
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	400	TYPE 11 BOTT 45 45	303	e Variabie)	
1997 (Sec. 1997)	470	VOLU 11 10 11	1 2 0. 0. 303		
	471				
	472	* Puits (acier 5	mm)		
	473	TYPE 20 CYLZ 6.8 15	51.5		
12 I	4/4	VOLU 21 11 20	0 4 0. 0. 151.5		
	475	* Interiour Puite /	0.0.404.0		
	477	TYPE 30 CYLZ 6.5 15	50		
Results	478	VOLU 31 21 30	0 2 0.0. 153		
V Data set Size Pts State	479	VOLU 32 22 30	020.0.456		
	480	* Conteneur (acier	2.5 mm)		
	481	TYPE 40 CYLZ 5.9 15	0 0 153		
	482		0.0.456		
	484	* Interieur contene	eur (air)		
	485	TYPE 50 CYLZ 5.75 1	150		
	486	VOLU 51 41 50 2	0. 0. 153		88
4-4	487	VOLU 52 42 50 2	0.0.456		1000
	488	" FISSILE TYPE 60 CVL7 5 75 4	10 8075		
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Configuration Help				R		
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	Input variable	Default value	Output values	Туре		
	d.broui.scale	0.0	mean_keff	float		
	d.PuO2	4.0	sigma_keff	float		
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Q Data set State Activity	460			_		
<u> </u>	461 GEOM					
	462 MODU O					
	463 464 * Reflexion par 60 (w de heton				
U	465 TYPE 10 BOIT @{pas_c	m / 2. #.####} @{pas_cm / 2	. #.####} @{ 60.0 + 2 *	(1.5 + H.Cont / 2.) #.####}		
A	466 VOLU 10 0 10 1	1 0. 0. @{ 2 * (1.5 + H.Cont	/ 2.) #.####}			
	467 RB0IT 1 1 1 1	0 0				
	408 * Interfeur de la sa	8 * Interieur de la salle (brouillard de densité variable)				
	470 VOLU 11 10 11	@{air_broui(d.broui(\$d.broui)	scale)) #} 0. 0. @{ 2 *	$(1.5 + H.Cont / 2.) #.####}$		
	471	n <mark>a Maria Canalana (Canalana) (Ca</mark>	abdot to be the			
	472 * Puits (acier 5 #	vm)				
	473 TYPE 20 CYLZ @{6.5 +	- Ep.Puits / 10. #.####} @{1		<mark>}</mark>		
	475 VOLU 21 11 20 475 VOLU 22 11 20 4	4 U.U. $w_{1} + H.Cont / a$	≤• # • #### } 			
	476 * Interieur Puits (a	$\frac{1}{r}$	• • • •••••			
	477 TYPE 30 CYLZ 6.5 @{H	.Cont / 2. #.####}				
Results	478 VOLU 31 21 30	2 0. 0. @{3.0 + H.Cont / 2	2. #.####}			
V Data set Size Pts State	4/9 VOLU 32 22 30	2 0.0. @{6.0 + 3 * H.Con1	z / 2. #.#### }			
Sala	481 TYPE 40 CYL7 MAD Con	(,) mm) 1 / 2 → En Cont / 10 / # ##	##3 @{H Cont / 2 # ####	#1		
	482 VOLU 41 31 40 4	0. 0. @{3.0 + H.Cont / 2. 1	#.####}			
	483 VOLU 42 32 40 4	0. 0. @{6.0 + 3 * H.Cont / 2	. #.####}			
	484 * Interieur conteneu	ır (air)				
	485 TYPE 50 CYLZ @{D.Cor	it / 2. #.####} @{H.Cont / 2	. #.####}	in the second		
	487 V0L0 51 41 50 2	0. 0. $(3.0 + 1.001) / 2.$	#•####} # ####l			
No. of Control of Cont	488 * Fissile	5. 5. eto. + 5 n.conc / 2	· I ····			
	489 TYPE 60 CYLZ @{D.Cor	nt / 2. #.####} @{dHcy1_cm(m	Pu.max_kg,\$d.Pu02) #.###	*** }		
	490					

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Configuration Help		R						
Data sets	/ Model ^Y Define \							
Data set State Pts Variables	[InputOutput							
Puits_Pu02_2variable defining 1 d.broui.scale d.Pu								
	Name Engineering Group Type Default value	Values Engineering Name Type						
	d.broui.scz V real 0.0	[0.0 ; 1.0] V N(mean_keff,s GaussianDensity						
	d.PuO2 V real 4.0	[0.5 ; 3.5] mean_keff+3* Numeric						
		mean_keff Numeric						
		sigma_keff Numeric						
Calculations								
Q Data set State Activity								
	▲▼ Engineering Monann haff signs haff as a function of discui	ecole d PuOD						
W	Engineering N(mean_Keii,Sigma_Keii) as a function of a.broui	Scale 0.PUO2						
	Type Name Computing pa	arameters \ Kriging parameters \ Optimization parameters \ Expert know						
	No design of experiments							
	Colibration 561	=						
	Calibration Dichotomy Max iterations	= 100						
	Uncertainties prop. Monte Carlo sampling							
	Sensitivity analysis FAST Stop when exp	pected improvement lower than = 1.0E-10						
	Xautoscale							
	Uncertainties prop Monte Carlo sampling with statistic Parallel compl	utations = 9						
	Calibration Bounds dichotomy							
	Uncertainties prop Wilks formula Initial parallel	computations = 9						
	Sensitivity analysis Morris screening							
	Optimization gradientdescent	Bounding values						
Results	Sensitivity analysis PCC							
V Data set Size Pts State	Optimization Efficient Global Optimization							
(ma)								

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Configuration Help						R
Data sets	Calculators pool Case	is of calculations \setminus	$Results \setminus$			
Data set State Pts Variables	d.broui.scale			d.PuO2	Status	Results
	0.05292791611928907	0.6084	507172927:	26	running@neutrosec-3:44775	Running calculation
	0.43246648176055813	2.4190	290493424	98	running@neutrosec-5:45718	Running calculation
	0.6515932745145013	1.2342	307517149	798	running@neutrosec-4:33376	Running calculation
	0.48777661594148314	2.7370	4040748991	852	running@neutrosec-5:41623	Running calculation
	0.9752578554261062	0.8738	973070091:	257	running@neutrosec-3:49300	Running calculation
	0.7734019996908804	3.2484	961713198	572	intact	?
	0.15940660941931936	2.8811	0145980803	265	intact	?
	0.8569460754127552	1.9132	098050322	384	intact	?
	0.266666040988639	1.5196	447924245	15	intact	?
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	neutrosec-3	neutrosec-3	44775	juil. 13 11:41:01	running	
V Data set Size Pts State	neutrosec-5	neutrosec-5	45716	juil. 13 11:41:01	running	
	neutrosec-5	neutrosec-5	41623	juil. 13 11:41:01	running	
	neutrosec-4	neutrosec-4	33376	iuil. 13 11:41:01	running	
	neutrosec-3	neutrosec-3	49300	juil. 13 11:41:01	running	
					time spent:	uu:uu:20, remaining(est.): ?, cases: 0/13

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Configuration Help						R
Data sets	Calculators pool Case	s of calculations \setminus	Results \			
Data set State Pts Variables	d.broui.scale			d.PuO2	Status	Results
	0.05292791611928907	0.6084	507172927:	26	neutrosec-3:44775 (00:00:48)	{mean_keff=0.83514, sigma_keff=9.9E-4}
	0.43246648176055813	2.4190	290493424	98	neutrosec-5:45716 (00:00:50)	{mean_keff=0.43866, sigma_keff=9.7E-4}
	0.6515932745145013	1.2342	307517149	798	neutrosec-4:33376 (00:00:49)	{mean_keff=0.37587, sigma_keff=9.8E-4}
	0.48777661594148314	2.7370	404074899	352	running@neutrosec-5:41623	Running calculation
	0.9752578554261062	0.8738	973070091:	257	neutrosec-3:49300 (00:00:50)	{mean_keff=0.39795, sigma_keff=9.8E-4}
	0.7734019996908804	3.2484	961713198	572	running@neutrosec-3:44775	Running calculation
	0.15940660941931936	2.8811	0145980803	265	running@neutrosec-4:33376	Running calculation
	0.8569460754127552	1.9132	098050322	384	running@neutrosec-5:45716	Running calculation
	0.266666040988639	1.5196	447924245	15	running@neutrosec-3:49300	Running calculation
	0.0	0.5			intact	?
	1.0	0.5			intact	?
Calculations	0.0	3.5			intact	?
	1.0	3.5			intact	?
Results	Calculator	Computer	Port	Since	State	
V Data set Size Pts State	neutrosec-3	neutrosec-3	44775	juil. 13 11:41:01	running	
	neutrosec-5	neutrosec-5	45716	juil. 13 11:41:01	running	
	neutrosec-5	neutrosec-5	41623	juil. 13 11:41:01	running	
	neutrosec-4	neutrosec-4	33376	juil. 13 11:41:01	running	
	neutrosec-3	neutrosec-3	49300	juil. 13 11:41:01	running	
	L				🖉 time spent: 00):00:58, remaining(est.): 00:02:11, cases: 4/13

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Configuration Help							R	
Data sets	Calculators pool Case	Calculators pool Cases of calculations Results						
Data set State Pts Variables	d.broui.scale			d.PuO2	Status	Results		
	0.05292791611928907	0.6084	507172927	26	neutrosec-3:44775 (00:00:48)	{mean_keff=0.83514, sigma_keff=9.	.9E-4}	
	0.43246648176055813	2.4190	2.419029049342498		neutrosec-5:45716 (00:00:50)	{mean_keff=0.43866, sigma_keff=9.	.7E-4}	
	0.6515932745145013	1.2342	307517149	798	neutrosec-4:33376 (00:00:49)	{mean_keff=0.37587, sigma_keff=9.	.8E-4}	
	0.48777661594148314	2.7370	404074899	852	neutrosec-5:41623 (00:01:00)	{mean_keff=0.48104, sigma_keff=9.	.5E-4}	
	0.9752578554261062	0.8738	973070091	257	neutrosec-3:49300 (00:00:50)	{mean_keff=0.39795, sigma_keff=9.	.8E-4}	
	0.7734019996908804	3.2484	961713198	572	neutrosec-3:44775 (00:01:02)	{mean_keff=0.61211, sigma_keff=9.	.7E-4}	
	0.15940660941931936	2.8811	014598080	265	neutrosec-4:33376 (00:00:51)	{mean_keff=0.66163, sigma_keff=9.	.7E-4}	
	0.8569460754127552	1.9132	098050322	384	neutrosec-5:45716 (00:00:57)	{mean_keff=0.49395, sigma_keff=9.	.7E-4}	
	0.266666040988639	1.5196	447924245	15	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}	
Calculations	0.0	3.5			neutrosec-3:49300 (00:00:53)	{mean_keff=0.87957, sigma_keff=9.	.7E-4}	
Contract State Automatic	1.0	3.5			neutrosec-5:45716 (00:01:01)	{mean_keff=0.67924, sigma_keff=9.	.5E-4}	
Puits Pu02 2variable running	0.04590724847512469	2.6058	511679975	31	running@neutrosec-3:44623	Running calculation	- D	
	0.21815650910991874	3.4989	094859937	464	running@neutrosec-3:50653	Running calculation		
W	0.11945042439696585	0.5338	582812272	392	running@neutrosec-3:33010	Running calculation	1)	
	0.4147155410812902	0.8355	990900960	537	running@neutrosec-2:47676	Running calculation		
	0.5022901650518179	2.4808	048440609	127	running@neutrosec-5:45716	Running calculation	- D	
	0.43641353099026536	3.4757	703140607	727	intact	?		
	0.7343308298286555	1.4604	956749642	715	intact	7	1]	
	0.9268426589399511	2.1309	098576262	833	intact	?		
	0.3427231896203011	2.0494	687582831	83	intact	3	ji	
Results	Calculator	Computer	Port	Since	State			
V Data set Size Pts 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			
					time spent: 00:0)3:14, remaining(est.): 00:02:14, case:	s: 13/22	

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Con	figuration Help							R
Da	ta sets	Calculators pool Case	s of calculations $ar{}$	Results \				
	Data set State Pts Variables	d.broui.scale			d.PuO2	Status	Results	
		0.9752578554261062	0.87389	73070091:	257	neutrosec-3:49300 (00:00:50)	{mean_keff=0.39795, sigma_keff=9.8E	-4}
Second.		0.7734019996908804	3.24849	061713198	572	neutrosec-3:44775 (00:01:02)	{mean_keff=0.61211, sigma_keff=9.7E	-4}
		0.15940660941931936	2.88110	145980803	265	neutrosec-4:33376 (00:00:51)	{mean_keff=0.66163, sigma_keff=9.7E	:-4}
1		0.8569460754127552	1.91320	980503223	384	neutrosec-5:45716 (00:00:57)	{mean_keff=0.49395, sigma_keff=9.7E	:-4}
1		0.266666040988639	1.51964	147924245	15	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}
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		0.04590724847512469	2.60585	5116799753	31	neutrosec-3:44623 (00:00:51)	{mean_keff=0.85919, sigma_keff=9.6E	-4}
-		0.21815650910991874	3.49890	948599374	464	neutrosec-3:50653 (00:00:52)	{mean_keff=0.60311, sigma_keff=9.6E	-4}
-		0.11945042439696585	0.53385	5828122723	392	neutrosec-3:33010 (00:00:47)	{mean_keff=0.85267, sigma_keff=9.7E	-4}
C	alculations	0.4147155410812902	0.83559	909009608	537	neutrosec-2:47676 (00:00:42)	{mean_keff=0.28872, sigma_keff=9.7E	-4}
S	Q Data set State Activity	0.5022901650518179	2.48080	48440609	127	neutrosec-5:45716 (00:00:54)	{mean_keff=0.4585, sigma_keff=9.6E-	-4}
-	Puits_Pu02_2variable running 22/31	0.43641353099026536	3.47577	031406077	727	neutrosec-2:47676 (00:00:50)	{mean_keff=0.54175, sigma_keff=9.6E	-4}
		0.7343308298286555	1.46049	567496427	715	neutrosec-3:33010 (00:00:50)	{mean_keff=0.41975, sigma_keff=9.7E	-4}
		0.9268426589399511	2.13090	985762628	833	neutrosec-3:44623 (00:00:50)	{mean_keff=0.53083, sigma_keff=9.8E	-4}
		0.3427231896203011	2.04946	875828318	83	neutrosec-3:50653 (00:00:48)	{mean_keff=0.4176, sigma_keff=9.8E-	-4}
		0.9712190185673535	2.84722	2996433265	55	running@neutrosec-2:59960	Running calculation	
		0.7917987112887204	2.42907	7171114343	788	running@neutrosec-2:53680	Running calculation	
C		0.05148516556297446	3.28769	281589784	433	running@neutrosec-3:33010	Running calculation	
		0.8871742211876926	0.79466	3236250237	72	running@neutrosec-3:50653	Running calculation	
		0.02364629251749863	0.72469	911545678	135	running@neutrosec-3:44623	Running calculation	
6		0.12089529420220883	1.79596	3080096119	943	intact	?	
		0.7192250608693345	3.47030	09273638	146	intact	?	
		0.6767193588893861	1,79557	63458739	966	intact	?	
	3	0.8992257152725557	3,48836	3425223142	267	intact	?	
De		Calculates	Computer	Det	Cinco			
Re	suits	Deutrosec-3	neutrosec-3	44623	inil 13 11:43:58	done		
	V Data set Size Pts State	neutrosec-3	neutrosec-3	33010	juil 13 11:43:59	upping		
		neutrosec-3	neutrosec-3	50852	juil 12 11:42:50	running		
		neutrosec-3	neutrosec-3	50060	juit 13 11:45:43	numing		
		neutrosec-2	neutrosec-2	53800	juii. 13 11:45:43			
		neutrosec-2	neutrosec-2	53060	Jun. 13 11.40.43	lunning		
12								
-								
						time spent: 0	0:05:00, remaining(est.): 00:02:02. cases	5: 22/31
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Stochastic global optimization practice in nuclear criticality safety assessment





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Configuration Help		R						
Data sets	Post processing \Files \							
Data set State Pts Variables	Optimum							
	Optimum							
	Size = 58 Maximum value is 0.95964 (sd=9.6E-4)							
	for d.broui.scale = 0.09327404717601559	88888						
	d.PuO2 = 1.011042937354369							
	Next expected maximum value may be 0.34113979499640373 (sd=0.006697966035673094)							
	d.PuO2 = 1.01104293735437 d.broui.scale = 0.093274047176015							
		10000						
Calculations		0000						
U		200000						
	E E							
	<u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u><u></u></u>	200000						
	eff eff							
Results	Ž 0 Z 0 Z 0 Z 0 Z 0 Z 0 Z 0 Z 0 Z 0 Z 0							
V Data set Size Pts State								
Puits_Pu02_2variab 45 MB 58 seen		00000						
	0.0 0.2 0.4 0.6 0.8 1.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5	-						



Configuration Help	
Data sets Post processing	Files
Data set State Pts Variables	Find:
Image: Constraint of the state of the	S292791611928907 #Tue Jul 13 11:41:50 CEST 2010 state=4 state=1279014061873 code=moret5 input. d. broui.scale=0.05292791611928907 duration=48759 end=127901401632 calc=neutrosec-3::44775 input. d. Pu02=0.608450717292726 output.sigma_keff=9.9E-4 output.mean_keff=0.83514
Calculations a d.broui.scale=0.8 a Data set State Activity d.broui.scale=0.7 a d.broui.scale=0.0 d.broui.scale=0.0 a d.broui.scale=0.0 d.broui.scale=0.0 a d.broui.scale=0.0 d.broui.scale=0.0 b d.broui.scale=0.0 d.broui.scale=0.0 b d.broui.scale=0.0 d.broui.scale=0.0 b d.broui.scale=0.1 d.broui.scale=0.1 b d.broui.scale=0.2 d.broui.scale=0.7 b d.broui.scale=0.5 d.broui.scale=0.5 b d.broui.scale=0.5 d.broui.scale=0.3	282877064291385 887877064291388 917987112887204 2364629251749863 3237404717601559 9272100515632431 2006798810325563 95.Rdata 734019996908804 429818482138216 022901650518179 080500189680606
Image: State Image: State	147155410812002 7360012273527682 96.Rdata 092528564855456 8777681594148314 877512203063818 343308298286555 .Rdata
d.broui.scale=0.7 d.broui.scale=0.2 d.broui.scale=0.2 d.broui.scale=0.2 d.broui.scale=0.9 d.broui.scale=0.7 d.broui.scale=0.7 d.broui.scale=0.6 d.broui.scale=0.1	478248702827841 277417614286053 866666040988639 752578564261062 888243941124529 515932745145013 4221573271788657



7 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





Grid computing engine & algorithm back-end

```
#' constructor and initializer of R session
init <- function() {</pre>
    library(lhs)
     . . .
3
#' 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) {</pre>
    set.seed(1)
    lhs <- maximinLHS(n=initBatchSize,k=d)</pre>
     . . .
#' iterated design building.
#' @param X data frame of current doe variables (in [0,1])
#' Oparam Y data frame of current results
#' @return next doe step
prepareNextDesign <- function(X,Y) {</pre>
    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))
```

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Grid computing engine & algorithm back-end

buildInitialDesign <- function(d) {...}</pre>

```
#' iterated design building.
#' Oparam 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) {</pre>
    if (iEGO > iterations) return();
    iEGO <<- iEGO + 1
    . . .
    noise.var <<- as.array(Y[,2])</pre>
    if (search min) {y=Y[,1]} else {y=-Y[,1]}
    ...
    kmi <- km(design=X, response=y, trend, optim.method='gen',...)</pre>
    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])
#'
   Oparam 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/>br/>",paste("<HTML>minimum is ",m),...
```



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



Feedback on two years of daily use



Feedback on two years of daily use

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 <u>adapt</u> 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

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Automatic input « scaling »

- Support for input parameters transformations log/exp/logistic emulated as local 2nd 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



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

Related [R] packages

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



0.0

1.0

h/0



1.0

h/0

2.0

3.0

0.0

Related [R] packages

- DiceKriging
 - Ordinary / Universal kriging
 - Nugget / Noise
 - Kernel: $C(x, y) = s^2 k(x, y)$
 - Exponential $k(h=|x-y|)=e^{-\frac{h}{\theta}}$
 - $k(h=|x-y|)=e^{-\left(\frac{h}{\theta}\right)^2}$ • Gauss

• Matern 3/2

 Power-exponential h p k(h=|x-y|)=e



0.2

0.4

0.

V.

0.0

0.0



0.6

0.8

1.0

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0.2

0.4

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



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)</pre>
```

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

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

sectionview3d(m)





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.</p>

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

