Optimization for simulation based problems

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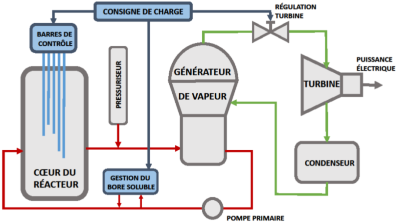
Context

Mobility system

Nuclear energy system



A priori, each domain is very different
But, share :

- Design problems for new perspectives,
- Inaccessible (cost) quantities, scales, etc.

Solving design problems, etc.

Solving optimization problems (mono- or multi-objective)

- Using the cognitive, and social abilities of humans :
  expert knowledges, evaluation of risk, uncertainties, divide into sub-problems, complex reasoning, etc.
- Using the computational, and memorization abilities of machines :
  automatic, data, formal language, speed, multi-scale, etc.

Solving design problems, etc.

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Main AI approaches for automatic solving

- Algebraic approach : algebraic, or formel model
- Digital twin approach : numerical model, and numerical simulation

Comparaison of approaches

Algebraic approach

- Formal model
- Aggregated variables, noice (demand, incertainties), contraints,...
- Artificial or real-like problem instances
- Offline

Tools :
cplex, gurobi, constr. prog., etc.

$$\max \sum_{t\in T}(pf_t) - \sum_{t\in T}\sum_{o\in O}(g_{t,o}u_{t,o} + 5s_{t,o})$$

$$s_{t-1,o} + b_{t,o} = u_{t,o} + s_{t,o} \quad \forall t \in T \setminus t_0,\ \forall o \in O$$

$$i + b_{t_0,o} = u_{t_0,o} + s_{t_0,o} \quad \forall o \in O$$

$$s_{t_e,o} = i \quad \forall o \in O$$

$$\sum_{o\in V} u_{t,o} \leq 200 \quad \forall t \in T$$

$$\sum_{o\in N} u_{t,o} \leq 250 \quad \forall t \in T$$

$$3f_t \leq \sum_{o\in V} h_o u_{t,o} \leq 6f_t \quad \forall t \in T$$

$$\sum_{o\in V} u_{t,o} = f_t \quad \forall t \in T$$

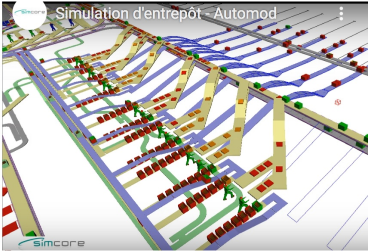
$$b_{t,o}, u_{t,o}, s_{t,o} \geq 0 \quad \forall t \in T,\ \forall o \in O$$

$$f_t \geq 0 \quad \forall t \in T$$

Digital twin approach

- Low level model
- Complex interactions
- Flow of data : sensor, etc.
- Offline, Online

Tools :
simcore, simio, matsim, devs,...



Consequences for automatic solving

$$\max \sum_{t\in T}(pf_t) - \sum_{t\in T}\sum_{o\in O}(g_{t,o}u_{t,o} + 5s_{t,o})$$

$$s_{t-1,o} + b_{t,o} = u_{t,o} + s_{t,o} \quad \forall t \in T \setminus t_0,\ \forall o \in O$$

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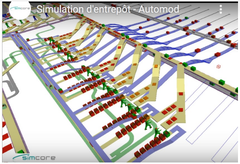


Algebraic approach

Pros :

- Exploitation of the algebraic properties of the model
- Explicit, and synthetic model

Difficulties :

- Design of the model :
  creation of languages, etc.

Digital twin approach

Pros :

- Low level description
- Tests, visualization

Difficulties :

- Black-box : (var., obj.)
- Costly simulation
  (time, energy)

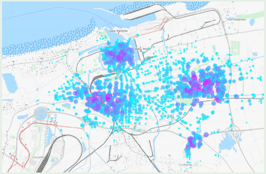
Indeed, not only "solving", but also support of decision making :
before, during, and after the optimization process

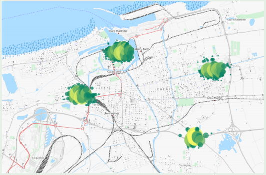
Digital twin for mobility system

F. Leprêtre, V. Marion, C. Fonlupt, S. Verel (LISIC) - thesis 2017 - 2020.
H. Aguirre, R. Armas, K. Tanaka (Shinshu Univ., Nagano, jp)

Partner : Calais City, Marie Capon, (expertise, and funding from PMCO/ULCO)

SIALAC benchmark of mobility





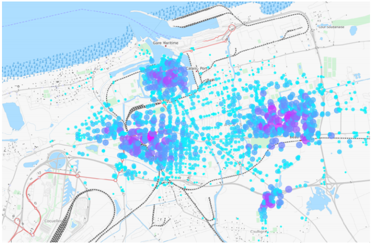
Different and, futur scenario : home, agents, activity

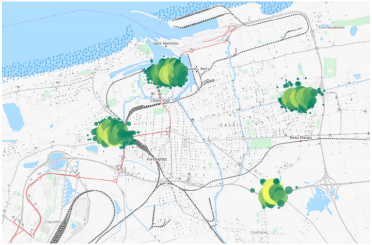
Two problems

- Tuning of traffic light
- Bus stop position

SIALAC benchmark of mobility

Leprêtre, F., et al. Applied Soft Computing, 2019 [6]





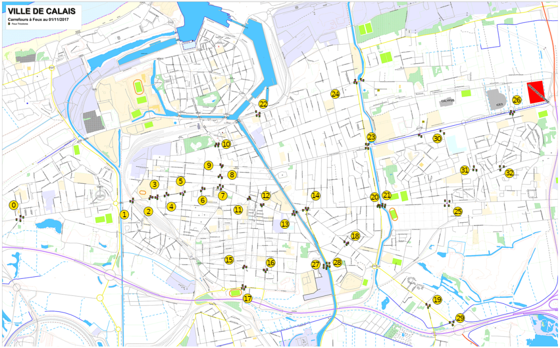
Number of agents	$\{5, 10, 15, 20\} \times 10^3$
Home	$\{1 \text{ cluster}, 4 \text{ clusters}, \text{ uniform}\}$
Activity	$\{1 \text{ cluster}, 4 \text{ clusters}\}$
Signals systems	$\{50\%, 75\%, 100\%\}$

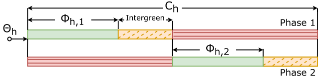
72 scenario using MatSim (Multi-Agent Transport Simulation)

Goal

- Show to the partner what it is possible with such tools
- Design **robust** optimization algorithms for mobility problems

Traffic light problem for Calais, and Quito cities





- Space : 33 (Calais), 70 (Quito) intersections
  search space dim. $\times 4$ integer variables
- Criteria : minimize average travel time (black-box problem)
- Computational time per simulation $\approx$ 1 minute

Gradient free optimization algorithms

Stochastic Hill Climber

$x \leftarrow$ initialize random solution
repeat
$x' \leftarrow$ mutate x
$x \leftarrow x'$ **if** $f(x') < f(x)$
until stopping criterion met

Evolutionary Algorithm

$P = \{x_1, \ldots, x_\mu\} \leftarrow$ rnd. init.
repeat
$P_{genitor} \leftarrow$ selection from P
$P_{children} \leftarrow$ breed $P_{genitor}$
$P \leftarrow$ replace $P \cup P_{children}$
until stopping criterion met

- `mutate` : random variation of candidate solution
- Tradeoff exploration / exploitation : `mutate` / `selection`

How to tune the mutation operator (variables to modify) ?

Structure of real-world problems

Intuitively

Real-world problem instances are often "structured" :

- Local sub-problems are not random,
- Interdependency between sub-problems are not random.

Importance of variables

Consequence : some variables are more impactful than others.

Examples

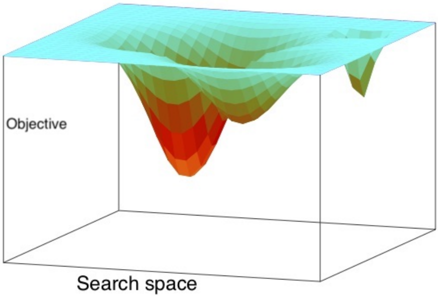
Isolated traffic lights are less impact on travel time
than central traffic lights

How to detect important variable ?
Expert knowledge, or more automatically....

Fitness landscape

Fitness landscape (Wright 1920)

- $\mathcal{S}$: set of candidate solutions, search space
- $f : \mathcal{S} \to \mathbb{R}$: objective function
- $\mathcal{N} : \mathcal{S} \to 2^{\mathcal{S}}$, neighborhood relation between solutions



- Geometry of the fitness landscape :
  Features/metrics are correlated to algorithm performance

$\Rightarrow$ Toward automatic design (tuning/control) of algorithms

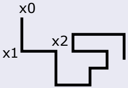
Variable importance metric

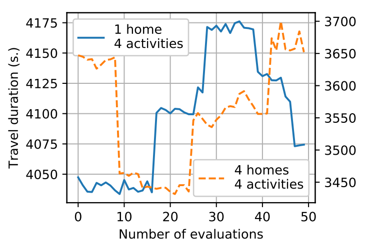
Importance degree of variable i

$$\delta_i = |f(mutate_i(x)) - f(x)|$$

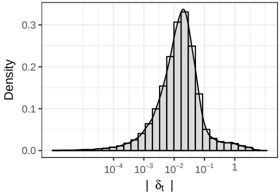
Estimation : Random walk on fitness landscape

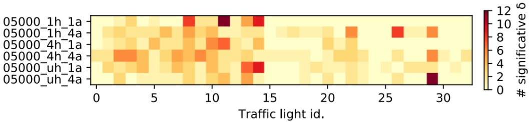
Sequence of neighboring solutions : $(x_0, x_1, x_2, \ldots)$





Explainable model of importance





⇒ Explainable model, communication with the partner

Adaptive algorithm based on importance

Backbone in combinatorial problems :
"good" solutions have some specific variables value

Design of mutation operator

- **Hypothesis** : modify in priority important variables
- **Goal** : automatic learning of expert knowledge

Method

- Divide the set of variables into 3 groups according to importance
- Use adaptive machine learning technique to select the group to mutate.

Adaptive bandit descent

Multi-armed bandit problem (reinforcement learning)

UCB strategy to select to relevant arm :

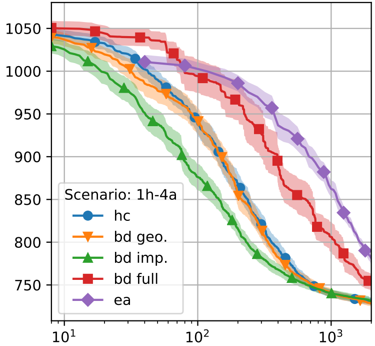
$$\hat{r}_i + C\sqrt{\frac{S}{s_i}}$$

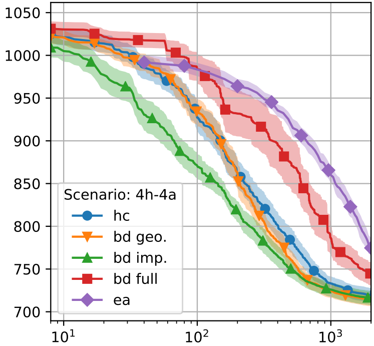
$\hat{r}_i$: reward, s_i : nb. of selection of arm i, and S : total nb. of selection, C : tradeoff parameter

Adaptive algorithm

$G \leftarrow$ split var. into groups
$x \leftarrow$ initialize random solution
repeat
  $g \leftarrow$ select group in G using UCB rule
  $x' \leftarrow$ mutate a variable from g of x
  $x \leftarrow x'$ **if** $f(x') < f(x)$
  Update rewards
until stopping criterion met

Some results





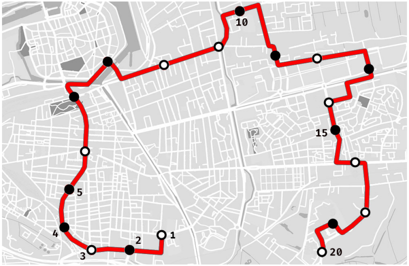
- Speed up the convergence
- Better than "hand made" groups,
  or previous Evolutionary Algorithm
- Robust on different scenario (also for Quito city)

Optimisation with time expensive simulation

- Parallel computation : distribute computation on machines
- Surrogate model : substitution of the original function with an (approximated) function fast to compute

Surrogate model

- A lot of works on numerical optimization :
  $f : \mathbb{R}^d \to \mathbb{R}$
- Few works on discrete/combinatorial optimization :
  $f : \{0,1\}^d \to \mathbb{R}$



Bus stop position problem

- Space : $\{0,1\}^d$ open or close possible stops
- Criterium : min. travel time

Surrogate-assisted opt. of pseudo-boolean problems

Florain Leprêtre, Virginie Marion, Cyril Fonlupt (LISIC),
K. Tanaka, H. Aguirre (Univ. Shinshu), A. Liefooghe, B. Derbel (univ. Lille)

Surrogate-Assisted Optimization

$X \leftarrow$ initial sample
repeat
  $M \leftarrow$ Build model of f from X
  $x^\star \leftarrow$ Optimize *w.r.t.* an acquisition function based on M
  $y^\star \leftarrow f(x^\star)$ using the numerical simulation
  $X \leftarrow X \cup \{(x^\star, y^\star)\}$
until time limit

In numerical optimization :

- Models :
  Gaussian Process, polynomial chaos, NN, RBF net., deep$*$, etc.
- Acquisition function :
  M, Expected improvement, probability impr., UCB, etc.

In discrete optimization :

- Use discrete distance, or numerical variable

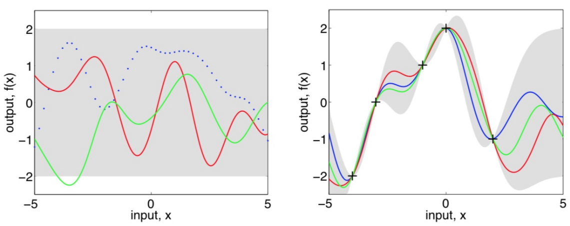
Learn from "small" data : model representation, incertainty

Example : Efficient Global Optimizer

- Model : Gaussian Process $M(x) \approx \mathcal{N}(m(x), K(x,x'))$
- Acquisition function : Expected Improvement

GP : Random variables which have joint Gaussian distribution.

mean : $m(y(x)) = \mu$
covariance : $cov(y(x), y(x')) = exp(-\theta d(x,x')^p)$



(a), prior (b), posterior

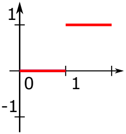
from : Rasmussen, Williams, GP for ML, MIT Press, 2006.

Walsh functions for pseudo-boolean optimization

- Space pseudo-boolean function is a vector space
- Basis : multi-linear functions, $x_{k_1} \dots x_{k_\ell}$ [Baptista, Poloczek, BOCS, ICML 2018]

Multi-linear :

$d = 1$, $\psi_1(x) = x$

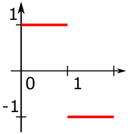


Orthogonal : No

x	ψ_0	ψ_1
0	1	0
1	1	1

Walsh :

$d = 1$, $\varphi_1(x) = (-1)^x$



Orthogonal : Yes

x	φ_0	φ_1
0	1	1
1	1	-1

Extension to dimension d using tensorial product :

$$\psi_{k_1 \dots k_\ell}(x) = x_{k_1} \dots x_{k_\ell} \qquad \varphi_{k_1 \dots k_\ell}(x) = (-1)^{x_{k_1}} \dots (-1)^{x_{k_\ell}}$$

Surrogate model for pseudo-boolean functions

Walsh functions

$$\forall x \in \{0,1\}^d, \quad \varphi_k(x) = (-1)^{\sum_{j=0}^{d-1} k_j x_j}$$

Normal, and orthogonal basis

Any function can be written as :

$$f(x) = \sum_{k=0}^{2^d-1} w_k . \varphi_k(x)$$

with : $w_k = \frac{1}{2^d} \sum_{x\in\{0,1\}^d} f(x).\varphi_k(x)$

Example with order 2, model limited to quadratic interactions :

$$f(x) = w_0 + \sum_{i=1}^{d} w_i.\sigma_i + \sum_{i<j=1} w_{ij}.\sigma_i\sigma_j \text{ with } \sigma_i = (-1)^{x_i}$$

Why Walsh functions ?

$$f(x) = w_0 + \sum_{i=1}^{d} w_i.\sigma_i + \sum_{i<j} w_{ij}.\sigma_i\sigma_j \text{ with } \sigma_i = (-1)^{x_i}$$

- Explicit algebraic model (not black-box) : easy to interpret
  Interaction between variables, intensity of interaction $|w_{i,j}|$
- Efficient algorithms to optimize such problems
- Model of function used in quantum computing
  Also know as Spin-Glasses, or QUBO / UBQP problems

Surrogate model based on Walsh fonctions

Expansion to order ℓ (cf. polynomial chaos, sparse grid, etc.)

$$M(x) = \sum_{k\ :\ \mathrm{ord}(\varphi_k)\leqslant\ell} \widehat{w}_k.\varphi_k(x)$$

- Pros :
  See previous slides
- Cons :
  model dimension (quadratic, cubic, etc.)
  No uncertainty estimation

Estimation of coefficients :
linear regression using sparse techniques : LARS/LASSO, etc.
LASSO : $\hat{w} = \mathrm{argmin}((M(x_i) - y_i)^2 + \alpha||w||_1\ )$

Walsh Surrogate-assisted Optimizer (WSaO)

Surrogate-Assisted Optimization

$X \leftarrow$ initial sample
repeat
  $M \leftarrow$ Build Walsh model of f from X
  $x^\star \leftarrow$ Optimize M using Eff. Hill-Climber
  $y^\star \leftarrow f(x^\star)$ using the numerical simulation
  $X \leftarrow X \cup \{(x^\star, y^\star)\}$
until time limit

Efficient optimization algorithm for Walsh functions

using the additive property :

$$\delta_i(x) = M(x \bigoplus i) - M(x) = -2 \sum_{k \supset i} w_k \varphi_k(x)$$
$$\delta_{ij}(x) = \delta_i(x \bigoplus j) - \delta_i(x) = 4 \sum_{k \supset i \& k \supset j} w_k \varphi_k(x)$$

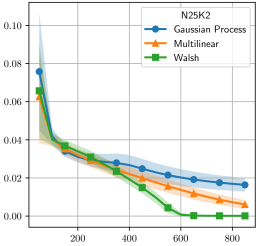
Find best improving move in $O(\ell)$ at each step of the search.
Partition crossover to combine 2 solutions

Chicano, Whitley, Ochoa, and Tinós. "Optimizing one million variable NK landscapes by hybridizing deterministic recombination and local search." In Genetic and Evolutionary Computation Conference, 2017.

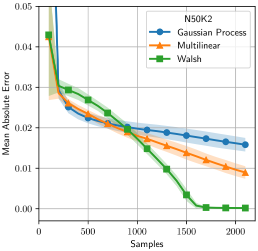
Quality of Walsh regression on academic benchmarks

Mean abs. error on NK-landscapes benchmark

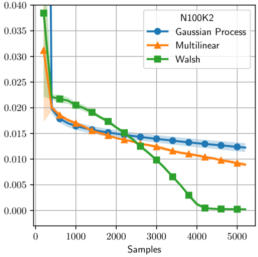
$d = 10$



$d = 25$



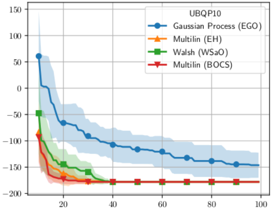
$d = 100$



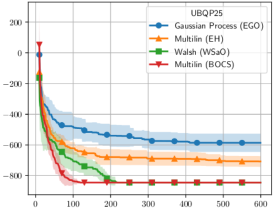
Walsh Surrogate-assisted Optimizer (WSaO)

Performance on UBQP (min.) benchmark

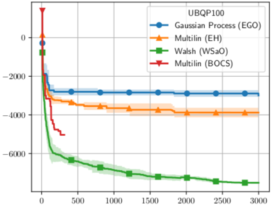
$d = 10$



$d = 25$



$d = 100$

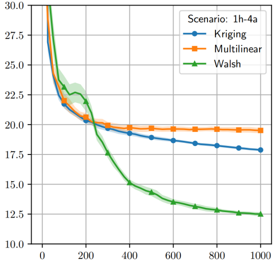


- Krigging : information of distance decreases with dimension
- BOCS : bayesian estimation of multilinear basis, SA opt. alg. (very expensive to compute)

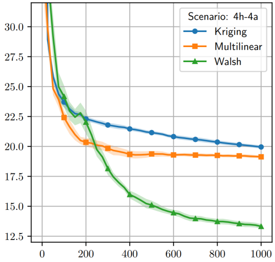
Preliminary results on bus stop problem

Mean abs. error on instances with $d = 20$, 4 activity centers

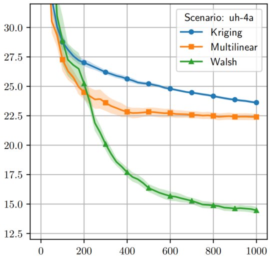
1 home



4 home

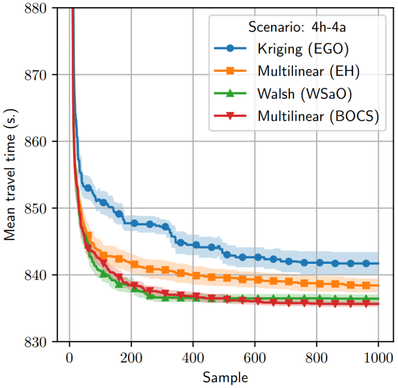


uniform



WSaO on bus stop problem

Preliminary results for small dimension $d = 20$ problem



Comments with surrogate models

- Result with surrogate assisted optimization :
  Near optimal solution, and an explicit model of your problem
  Use non black-box machine learning model are useful !
- Open issues :
  Tradeoff between quality of the model (uncertainty),
  and optimization effort
- Perspectives :
  multi-objective optimization, uncertainty,
  numerical & discret, routing problems, large scale, etc.

Comments with surrogate models

Projects around mobility at LISIC Lab

- ANR project Murdasp

`https://murdasp.univ-littoral.fr/` :
"Pour une mobilité durable et adaptée à un contexte de pandémie",
Moez Kilani, Daniel De Wolf, Cyril Fonlupt (LEM, TVES, LISIC)

- 3 **thesis** starting in oct. 2021 :
  Mobility and communication protocol DEVS simulation/5G
  (F. Condette, E. Ramat/P. Sondi),
  Mobility at local scale DEVS simulation/optim.
  (A. Pestelle, E. Ramat/S. Tari),
  Mobility at region scale using MatSim
  (V. Vendi, C. Fonlupt/S. Verel)

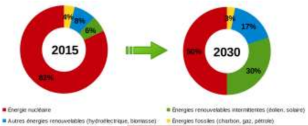
Contexte

Jean-Michel Do, Jean-Charles Le Pallec, CEA Saclay,
Mathieu Muniglia, PhD, 2014 - 2017
Valentin Drouet, PhD, 2017 - 2020

Optimisation multi-objectifs du pilotage des réacteurs nucléaires REP en suivi de charge dans le contexte de la transition énergétique à l'aide d'algorithmes évolutionnaires

Baptiste Gasse, PhD candidate, 2020 - 2023

Optimisation du pilotage des réacteurs nucléaires REP dans un réseau électrique dans le contexte de la transition énergétique



Augmentation de la part d'énergies renouvelables

Intermittence

Déséquilibre potentiel entre la consommation et la production

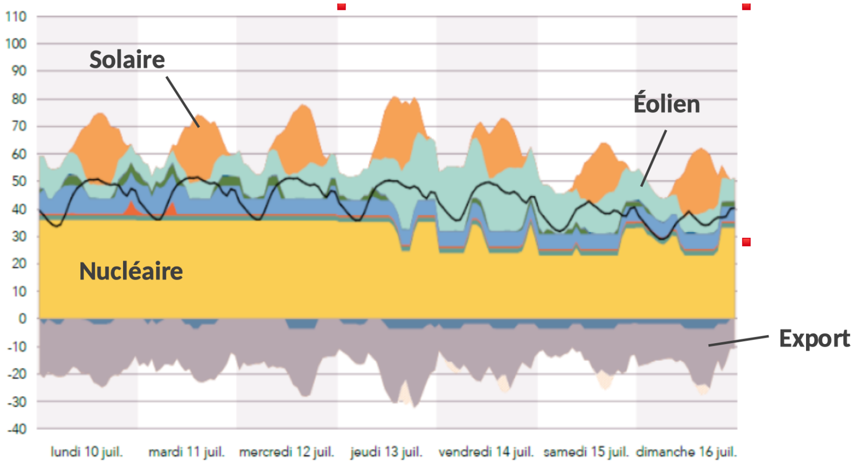
Flexibilité (RTE)

Smart Grids (gestion locale)

Manœuvrabilité des REP

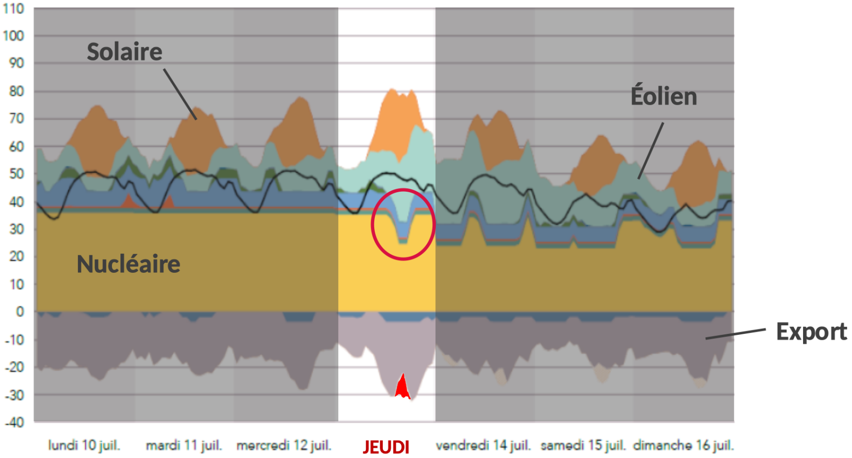
Stockage

Scenario of energetic transition in France



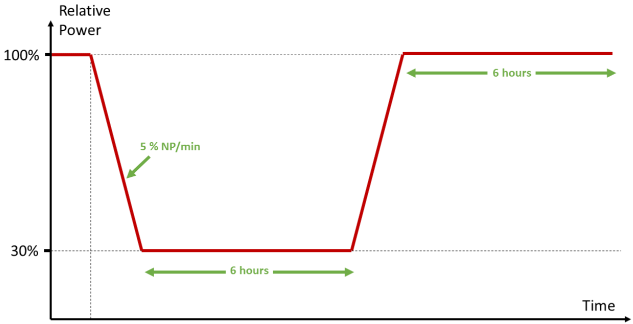
RTE (french electricity transport compagny) prediction for a typical week in 2035 (VOLT scenario)

Scenario of energetic transition in France



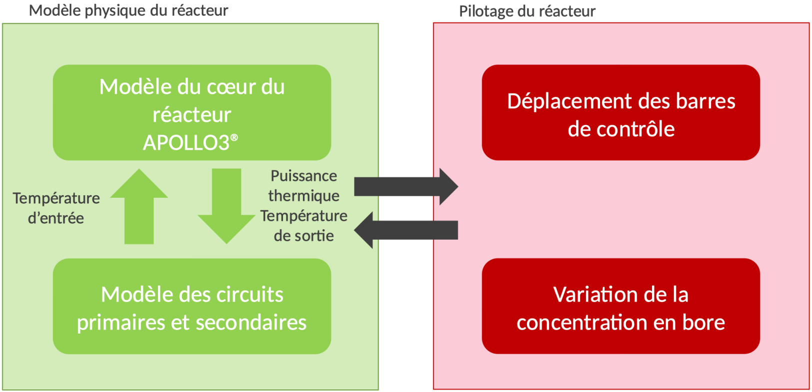
RTE (french electricity transport compagny) prediction for a typical week in 2035 (VOLT scenario)

Target production transient



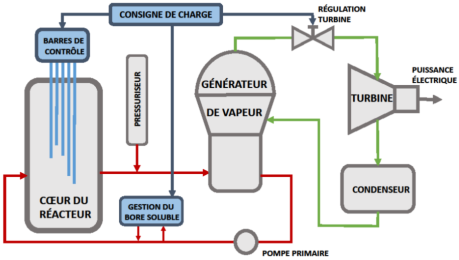
24h of production : most penalizing possible transient

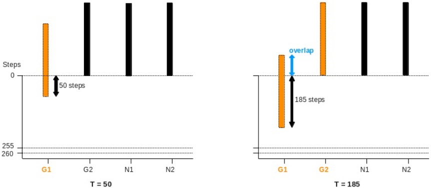
Multi-physic simulator



Around 10min for the simulation of one transient

Optimization problem





Possible criteria

More than 7 criteria can be used :

related to cost, safety, and stability

Available control parameters

- Power Shimming Rods :
  - Recouvrements (x3)
  - Speed control (x4)
- Temperature Regulation Rods :
  - maneuvering band (x1)

Search space size $\approx 10^{12}$

Fitness landscape analysis

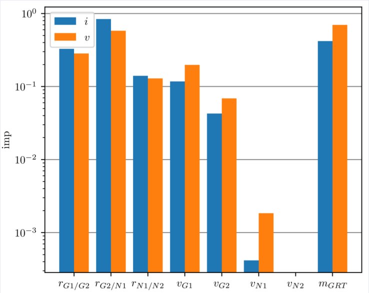
Using random walk sampling

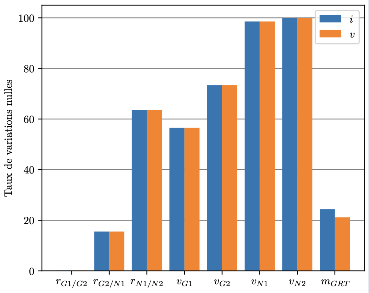
Objective correlation

	v	N_R	C_{IPG}	ΔT	f_T	i	F_v
v	1.0	-0.75	-0.91	-0.14	0.12	-0.06	-0.01
N_R	-0.75	1.0	0.7	0.68	0.17	0.14	0.4
C_{IPG}	-0.91	0.7	1.0	0.12	-0.17	-0.02	-0.1
ΔT	-0.14	0.68	0.12	1.0	0.7	0.51	0.79
f_T	0.12	0.17	-0.17	0.7	1.0	0.83	0.72
i	-0.06	0.14	-0.02	0.51	0.83	1.0	0.58
F_v	-0.01	0.4	-0.1	0.79	0.72	0.58	1.0

2 groups are highly correlated

Variable importance

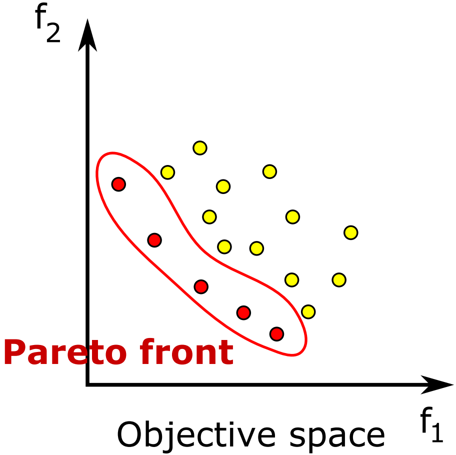




Reduce the dimension to 6, and better understanding of the system

Allow to tune the mutation parameters

Multiobjective optimization

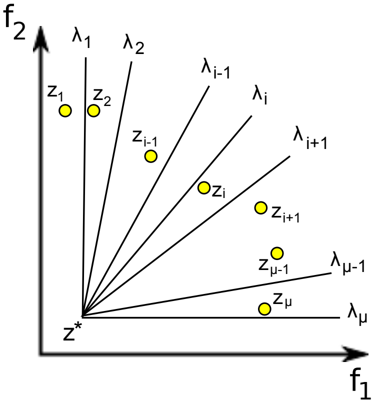


Goal

No a priori on the order/importance of the objectives,
Decision a posteriori based on the optimal Pareto solutions.

MOEA/D : Multi-Obj. Evo. Algo. based on Decomposition

A lot of MO algo. :
Pareto based (NSGAII,...), indicator based (IBEA,...), and



Population at iteration t

- One solution x_i for each sub pb. i of direction λ_i
- Scalar function g :
  Weighted Tchebycheff
- Representation of solutions in objective space : $z_i = g(x_i|\lambda_i, z_i^\star)$
- Same reference point for all sub-pb. $z^\star = z_1^\star = \ldots = z_\mu^\star$
- Neighborhood size $\sharp B(i) = T = 3$

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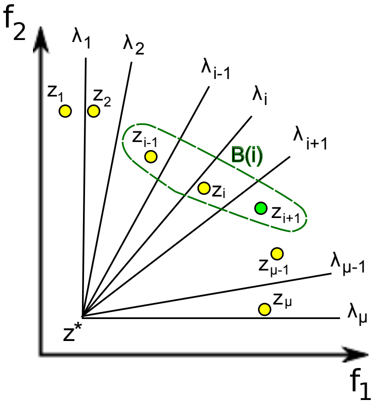

From the neigh. $B(i)$ of sub-pb. i, x_{i+1} is selected

- One solution x_i for each sub pb. i of direction λ_i
- Scalar function g :
  Weighted Tchebycheff
- Representation of solutions in objective space : $z_i = g(x_i | \lambda_i, z_i^\star)$
- Same reference point for all sub-pb. $z^\star = z_1^\star = \ldots = z_\mu^\star$
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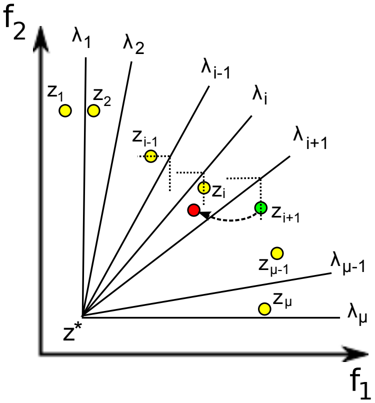

The mutated solution y is created

- One solution x_i for each sub pb. i of direction λ_i
- Scalar function g :
  Weighted Tchebycheff
- Representation of solutions in objective space : $z_i = g(x_i|\lambda_i, z_i^\star)$
- Same reference point for all sub-pb. $z^\star = z_1^\star = \ldots = z_\mu^\star$
- Neighborhood size $\sharp B(i) = T = 3$

MOEA/D : Multi-Obj. Evo. Algo. based on Decomposition

A lot of MO algo. :
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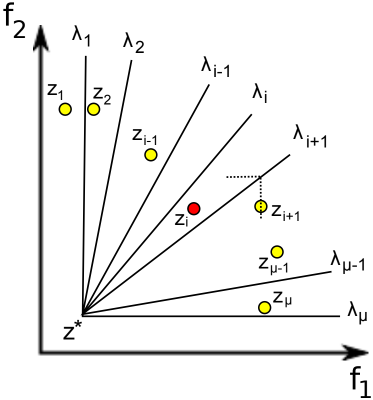
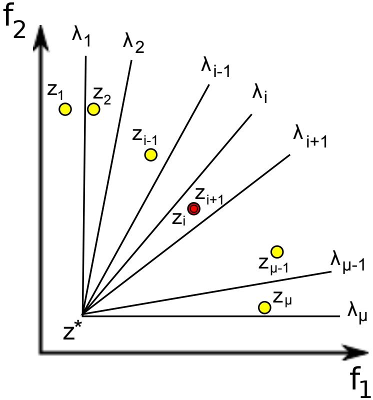


According to scalar fonction,
y is worst than x_{i-1},
y is better than x_i and replaces it.

- One solution x_i for each sub pb. i of direction λ_i
- Scalar function g :
  Weighted Tchebycheff
- Representation of solutions in objective space : $z_i = g(x_i | \lambda_i, z_i^\star)$
- Same reference point for all sub-pb. $z^\star = z_1^\star = \ldots = z_\mu^\star$
- Neighborhood size $\sharp B(i) = T = 3$

MOEA/D : Multi-Obj. Evo. Algo. based on Decomposition

A lot of MO algo. :
Pareto based (NSGAII,...), indicator based (IBEA,...), and



According to scalar fonction,
y is also better than x_{i+1}
and replaces it for the next iteration.

- One solution x_i for each sub pb. i of direction λ_i
- Scalar function g :
  Weighted Tchebycheff
- Representation of solutions in objective space : $z_i = g(x_i | \lambda_i, z_i^\star)$
- Same reference point for all sub-pb. $z^\star = z_1^\star = \ldots = z_\mu^\star$
- Neighborhood size $\sharp B(i) = T = 3$

Massively parallel algorithm

Optimization of problems based on expensive simulation

- Relevant tuning of parameters of the algorithm
- Surrogate model
- Parallel computing

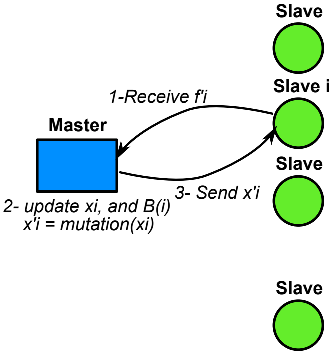
Here,
Simulation for one burnup : 10 min
Simulation of 4 burnups (life cycle) : 40min

Massive parallel system

Algorithms for the TGCC (GENCI Projet),
2 500 000 hours of available computation
1008 cores for 24h of computation.

Asynchronous MOEA/D

Master-slaves architecture



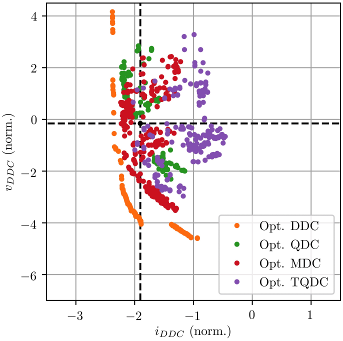
Algorithm on Master

$\{x_1, \ldots, x_\lambda\} \leftarrow$ **Initialization**()
for $i = 1..\lambda$ **do**
  Send (Non-blocking) x_i to slave S_i
end for
repeat
  if there is a pending mess. from S_i **then**
    Receive fitness f_i' of x_i' from S_i
    Update x_i, and $x_j \in B(i)$ with (x_i', f_i')
    $x_i' \leftarrow \texttt{mutation}(x_i)$
    Send (Non-blocking) x_i' to slave S_i
  end if
until time limit

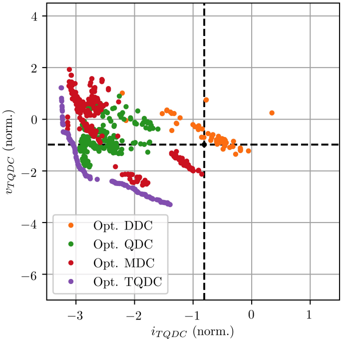
Drouet, V., S. Verel, and J-M. Do. "Surrogate-assisted asynchronous multiobjective algorithm for nuclear power plant operations.", In gecco 2020.

Results at different burnups

At the beginning of exploitation



At the end of exploitation



Optimization on the whole cycle is necessary

Asynchronous MOEA/D with surrogate model

Algorithm on Master

$\{x_1, \ldots, x_\lambda\} \leftarrow$ **Initialization**()
for $i = 1..\lambda$ **do**
  Send (Non-blocking) x_i to slave S_i
end for
repeat
  if there is a pending mess. from S_i **then**
    Receive fitness f_i' of x_i' from S_i
    Add (x_i', f_i') to sample S
    Update x_i, and $x_j \in B(i)$ with (x_i', f_i')
    Train model M with Sample S
    if $|S| < N_{start}$ **then**
      $x_i' \leftarrow \texttt{mutation}(x_i)$
    else
      Select x_i' using model M
    end if
    Send (Non-blocking) x_i' to slave S_i
  end if
until time limit

Criteria

Weighted Volume,
Maximum of instability

Surrogate model

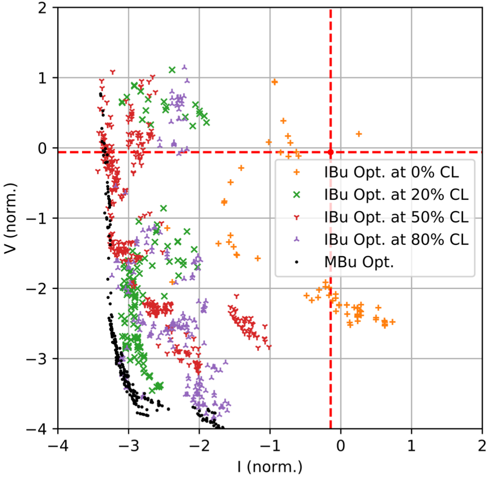
Random forest

Tuning of using offline data

Acceleration of convergence
Double the prob. of improv.

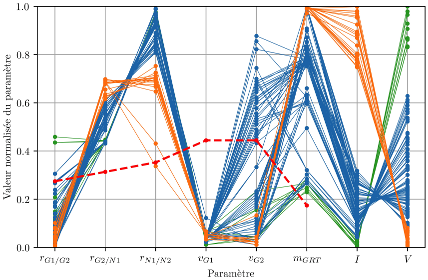
Init. | Random mutation | Surrogate assisted

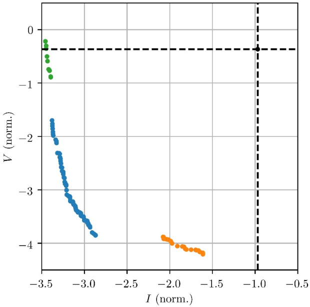
Results on whole exploitation cycle



Reduce Volume of effluent, and Instability (axial offset) from current setting

Analysis of decision variables





A posterio interpretation of the candidate solutions on Pareto front

Conclusion

Optimization, machine learning techniques to solve design problems with digital twins

- Main tools :
  Analysis fitness landscape to understand pb., and tune algo.
  Use surrogate models, to accelerate the search, and bring an algebraic model
  Parallel, and distributed computation
- A good algorithm is a tradeoff between :
  Final decision making
  Search space dimension, and its properties
  Computation time, and power.
- Digital twins, and AI offers a lot of perspectives
  How to combine different methods ?
  How to better understand systems ? ...

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