April the 24th, 2015, Mons, “groupe de contact FNRS Calcul Intesif”

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Mathematics beyond paper and pencil. A personal view.

Acknowledgments

naXys colleagues, among which:

- Anne-Sophie Libert, Sotiris Sotiriadis

(exoplanets)

- Alexandre Mayer#, Delphine Nicolay

Department of Physics

(GA optics and robotics)

- Julien Blanchard, Annick Sartenaer, Caroline Sainvitu*, Charlotte Beauthier*

* Cenaero

(GA many-variables optimization)

Some informations about naXys :

Namur Center for Complex Systems

- Created in 2010, because of a strong will of researchers from the Department of Mathematics to reorganize their activities in a large and unique research axis: **the complex systems**.

- naXys accounts for ~70 members (~2/3 from math), several faculties and departments

Some research axes & keywords

ARCCOS
Complexity in cosmology

biomedx
Biology, medicine and complex systems

dynamix
Dynamical systems and complex systems

sox
Social sciences, economics and complex systems

xn
Complex networks

…

Some keywords:
Optimization, big data, HPC, models, numerical simulations, theory, …

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Introduction

We are interested in problems: modeling, analysis and theory.

Problem = any computational problem that can be solved with pencil and paper (Church-Turing)

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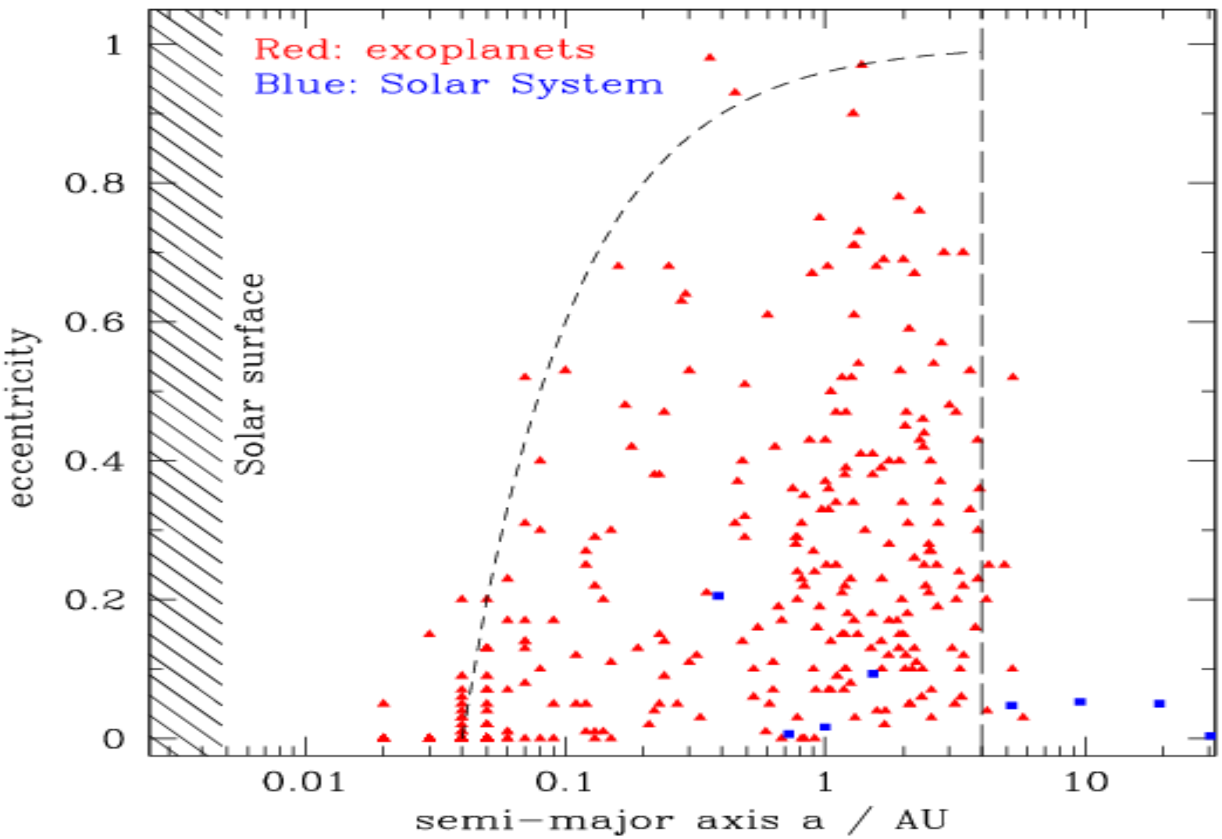
However problems are often based on real operational problems (quick solution, adaptation), with constraints, huge sizes .

So (even mathematicians) must use (super)computers to solve problems.

Create new exoplanetary systems to study ours … (I)

The *architecture* of known *exoplanetary systems* is completely different from the one of our Solar System:



- Different orbital spacings and mutual inclinations
- A variety of orbital distances and eccentricities…

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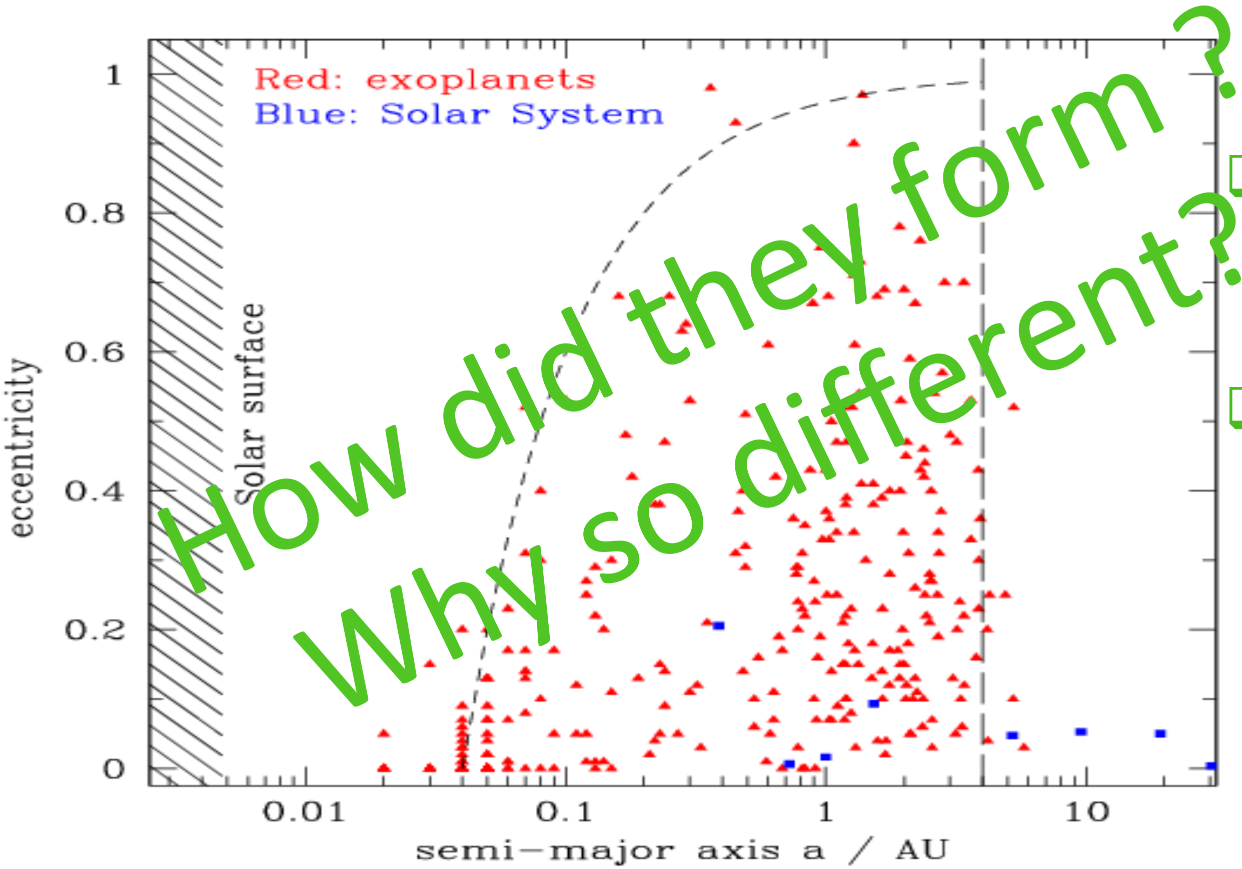

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- A variety of orbital distances and eccentricities…

Create new exoplanetary systems to study ours … (II)

Protoplanetary gas disc

- Gravitational N-body simulations (very high accuracy, *symplectic* integration schemes to avoid errors accumulation over thousands of orbits)
- N-body code → *SyMBA* *(Duncan et al. 1998)*

$$H_{\text{Kep}} = \sum_{i=1}^{n}\left(\frac{|P_i|^2}{2m_i} - \frac{Gm_i m_0}{|Q_i|}\right), \qquad H_{\text{Sun}} = \frac{1}{2m_0}\left|\sum_{i=1}^{n} P_i\right|^2, \qquad H_{\text{int}} = -\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\frac{Gm_i m_j}{|Q_i - Q_j|}.$$

- Study the early stages of the formation of planetary systems

(Extra forces acting on the planets because of the protoplanetary gas disc)

Create new exoplanetary systems to study ours … (III)

Statistical study ($N_{systems} \approx 15000$) to test the possible outcomes for different initial configurations, in order to reproduce the diversity of the observed systems.

- Computational time for 1 system (~$2*10^9$ *time-steps*) ~ 1 day*

*It depends on the cluster and the specific node

- ~350-400 systems/day, hence ~45 day for a "good" investigation of the parameters space

- Software → PGI FORTRAN Compiler

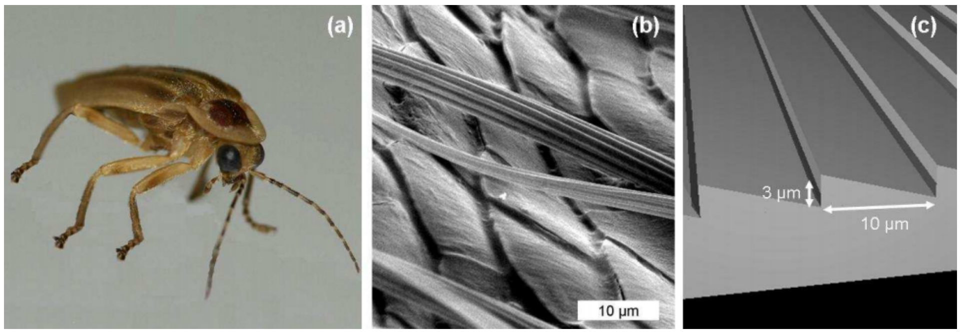
- The code is developed for a ***serial computation*** [*1 CPU core per job*]

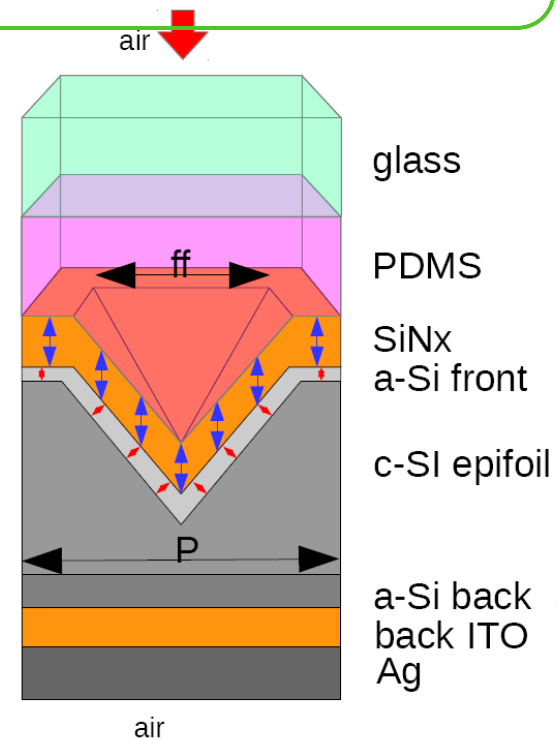
- Small memory usage - [*0.15Mb per job*]

naxys Namur Center for Complex Systems

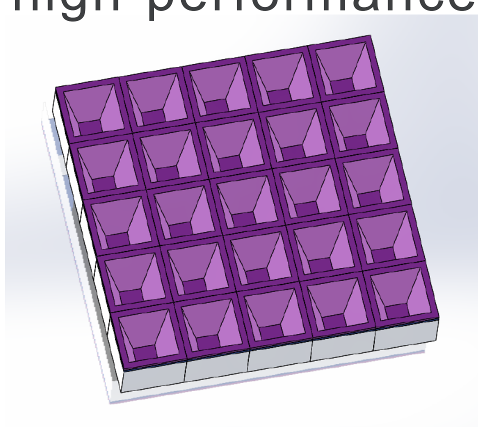
Copy twice Nature to build optimized optical designs (I)

Bio-inspired surface texturation of Light Emitting Diodes (LED) for the optimization of light extraction





Waffle-shaped structures with conformal coatings of cermets and SnO2 for the development of high-performance solar thermal collectors

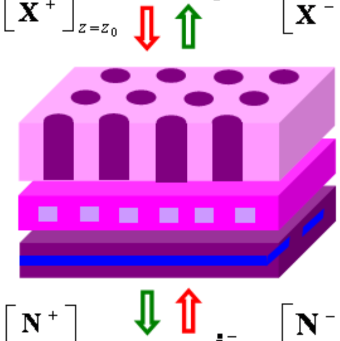


Optimized structures based on thin films of c-Si for the development of high-performance photovoltaics

Copy twice Nature to build optimized optical designs (II)

Rigorous Coupled Waves Analysis for modeling the interaction of electromagnetic radiations with three-dimensional structures

$$\mathbf{i}^+ = \begin{bmatrix} \mathbf{N}^+ \\ \mathbf{X}^+ \end{bmatrix}_{z=z_0} \qquad \mathbf{r}^- = \begin{bmatrix} \mathbf{N}^- \\ \mathbf{X}^- \end{bmatrix}_{z=z_0}$$



$$\begin{bmatrix} \mathbf{t}^+ \\ \mathbf{r}^- \end{bmatrix} = \begin{bmatrix} \mathbf{S}^{++} & \mathbf{S}^{+-} \\ \mathbf{S}^{-+} & \mathbf{S}^{--} \end{bmatrix} \begin{bmatrix} \mathbf{i}^+ \\ \mathbf{i}^- \end{bmatrix}$$

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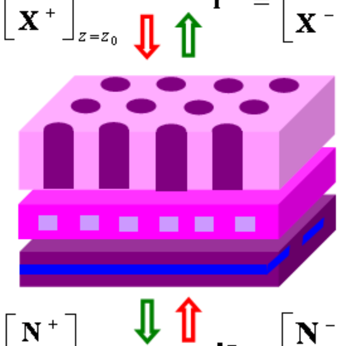

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Parameters optimization by a Genetic Algorithm

$$\text{Find } \{x_i\}_{i=1}^n \text{ such that } f(x_1, x_2, \dots, x_n) \text{ is the global maximum of } f.$$

Genetic algorithms (heuristic method): to work with a population of solutions(=individuals). Each individual represents of a given set of physical parameters. The best individuals are selected. They generate new individuals for the next generation possibly through random mutations. Generation after generation, the population should converge to the **global optimum** of a problem.

Copy twice Nature to build optimized optical designs (III)

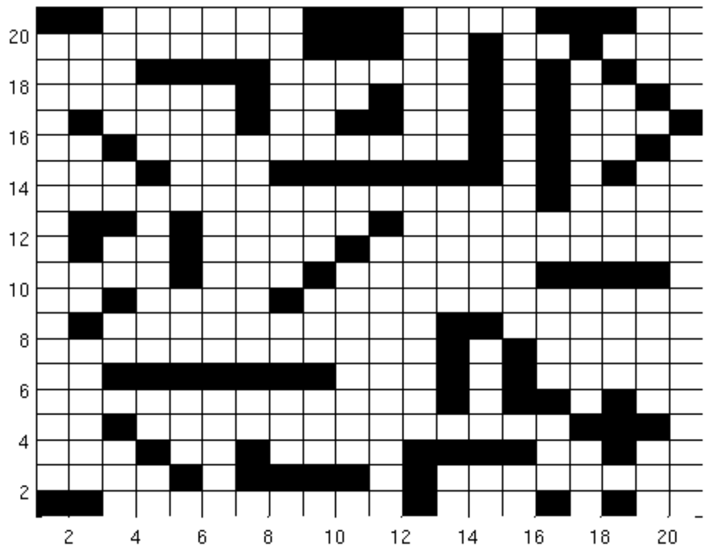
	LED	solar thermal collector	photovoltaic module
Average CPU time for one optical simulation	20 h	30 h	10 h
Memory required	2 GB	10 GB	4 GB
Number of possible parameter combinations	50.418.836.005.356	48.763.605.000	16.120.700.046
Actual number of evaluations by the GA	2235	2377	5195
Population size	100	100	200
Infrastructure	HPC (Hercules)	HPC (Hercules)	Tier-1

- All individuals/solutions are evaluated in **parallel** to speed up GA.
- High performance on the **CECI** and **Tier-1** supercalculator was achieved by multi-agent implementation of the GA (**massively parallel computing**).
- 60 generations are typically required by the GA.
- **Fortran 90** (GA code) & **bash** (scripts for submitting recursively large arrays of jobs - one job for each evaluation of the fitness).
- A **multi-objective genetic algorithm** was implemented to deal with problems that require the consideration of different quality criteria.
- The actual **time** and **memory** requirements are essentially determined by the application.
- From CECI to Tier-1 only need to adapt submission scripts (SLURM vs PBS)

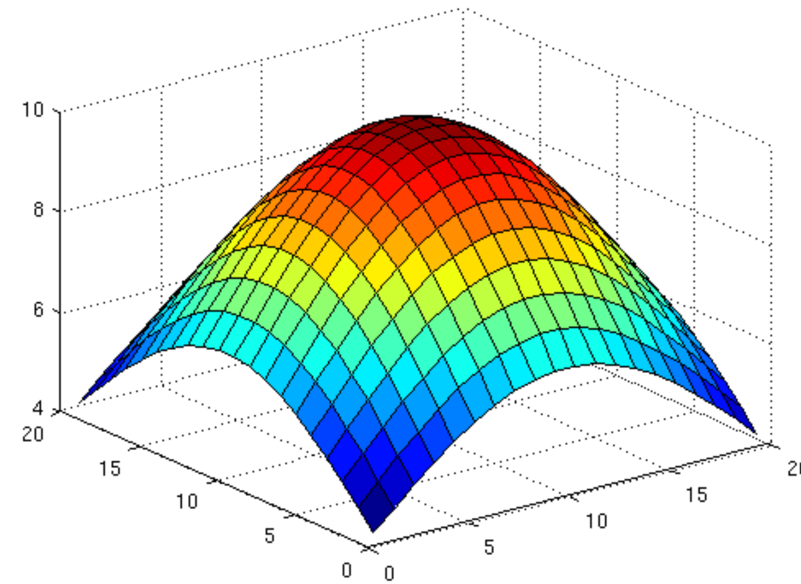
Let's robots to learn tasks by themselves (I)

Robots move on an virtual 2D-arena (discretized grid, periodic boundary conditions, 8 neighbors) aimed at:

- Reaching the maximum height level (T1)
- Avoiding forbidden zones (T2)



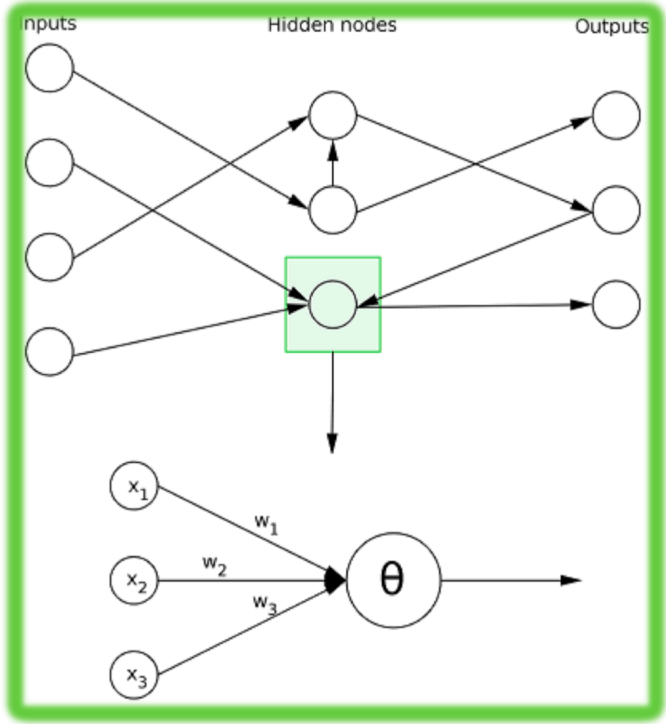
Task 2

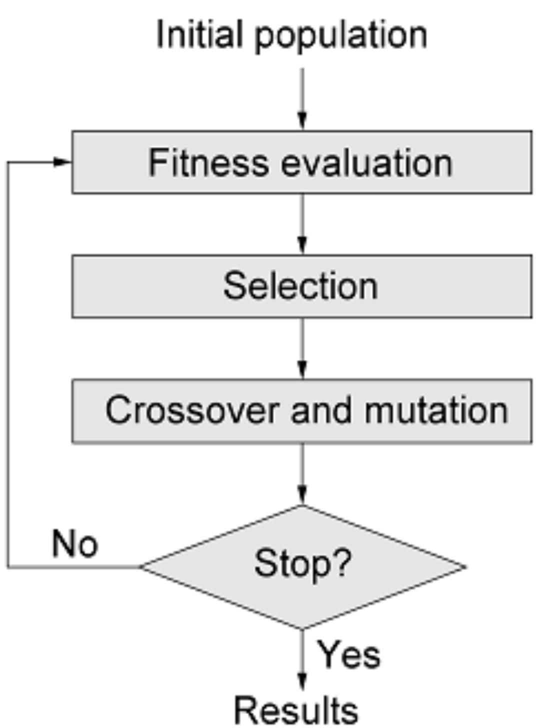


Task 1

Let’s robots to learn tasks by themselves (II)

Robots are controlled by artificial neural networks:
- 17 inputs
- 4 outputs
- 22 hidden nodes
- (possibly) ~1800 weighted synapses





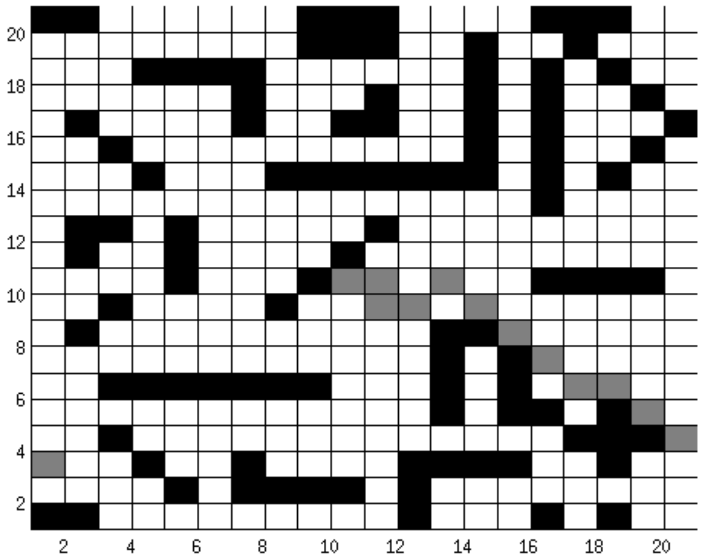
- Weights and thresholds
- Network topology

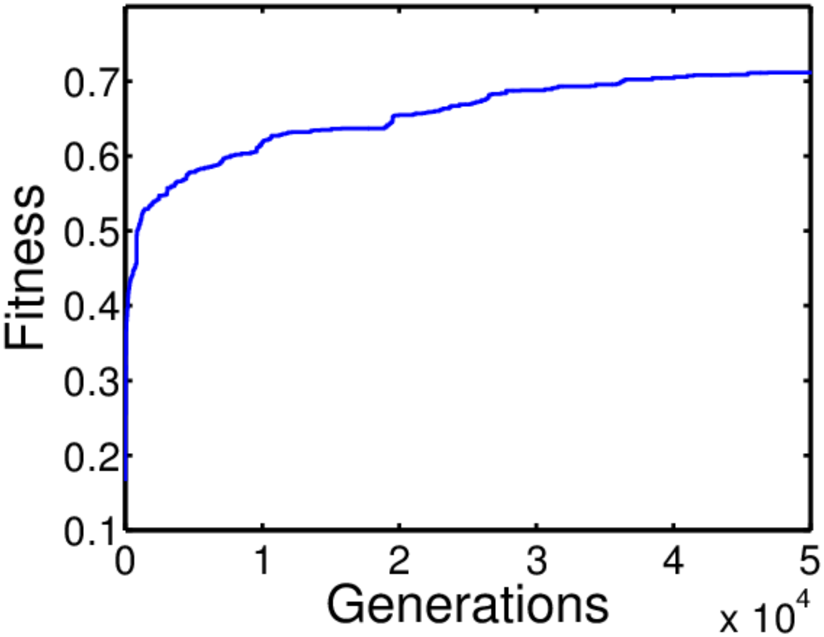
optimized using GA

1 run is
- 50 000 generations / 100 neural nets per generation / 10 replicas for each learning task
- serial job / Matlab / single processor / ~100MB / 3 CPU days

Let's robots to learn tasks by themselves (III)

One robot's path





Fitness evolution

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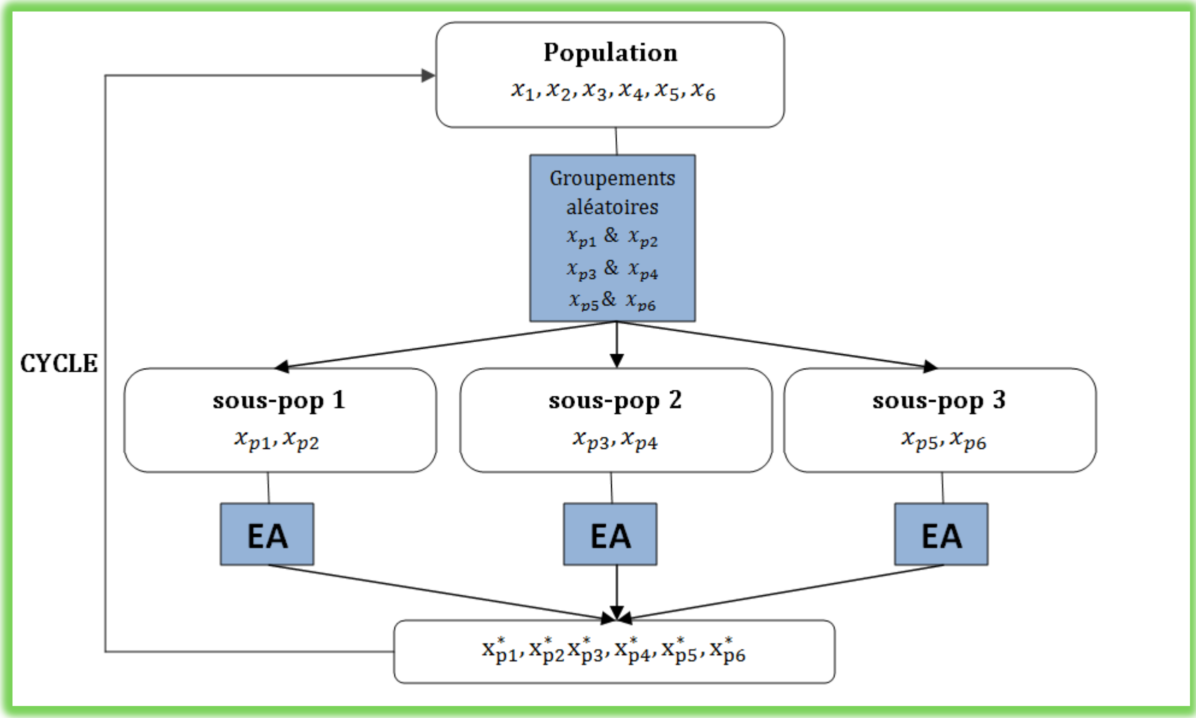
Tackle the curse of dimensionality using GA (I)

Find $\{x_i\}_{i=1}^{n}$ such that $f(x_1, x_2, \ldots, x_n)$ is the global maximum of f.

where n is huge

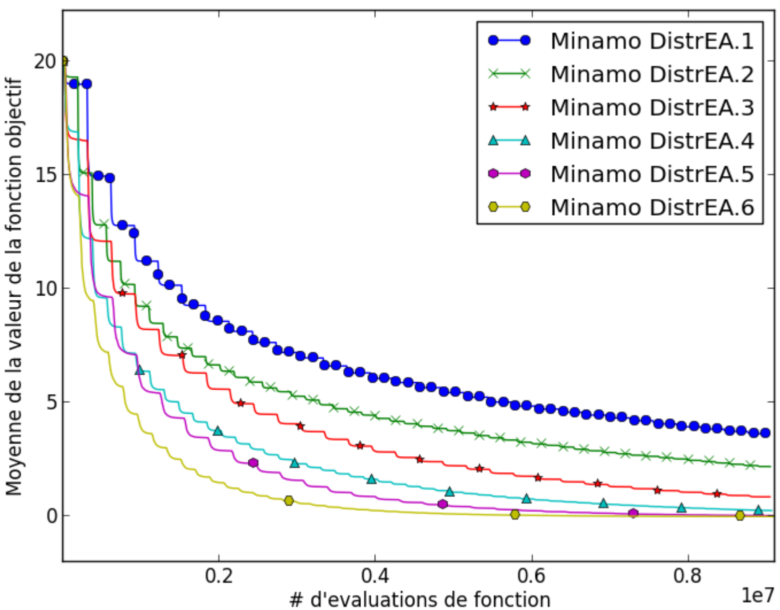
- Idea: divide the problem into sub problems

Cooperative/Distributed evolutionary algorithms (EA)

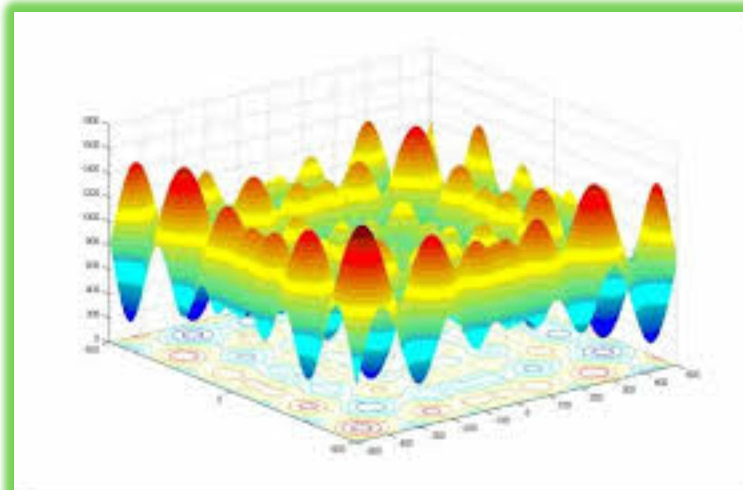


Tackle the curse of dimensionality using GA (II)

- Time: between 1h30 and 6h for 1 optimization (depending on the function and on the EA parameters)
- Memory: 300 Mb for 1 optimization
- 100 replicas for each optimization to estimate the performances
- Massively parallel computing using TIER-I (100 parallel jobs)



Benchmark Schwefel function (n=500)



Take home messages

- We need HPC resources to model and to analyze problems (luckily not to make proofs)
- Need for massively parallel computing
- Need for numerous but short jobs

Thank you

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