Gemfony scientific

Distributed Parametric Optimization with the Geneva Library Collection

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BoostCon 2011 / Aspen, CO / May 16, 2011

Karlsruhe Institute of Technology (North Campus)

Steinbuch Centre for Computing (SCC)

About Gemfony

- Start-Up
  - A spin-off from KIT
- Founders with many years experience in
  - Modelling complex systems
  - Optimization
  - Cloud- and Grid-Management
  - IT-Security
- Main product: Geneva
  - **G**rid-**en**abled **ev**olutionary **a**lgorithms
  - Accelerated parametric optimization for problems from a wide array of problem domains, both in industry and science
  - Heavily based on Boost

http://www.gridcafe.org

Questions

Who in this room has heard before the term parametric optimization before this talk?

Questions

Who in this room has
used parametric optimization
to improve the results of his/her work ?

Index

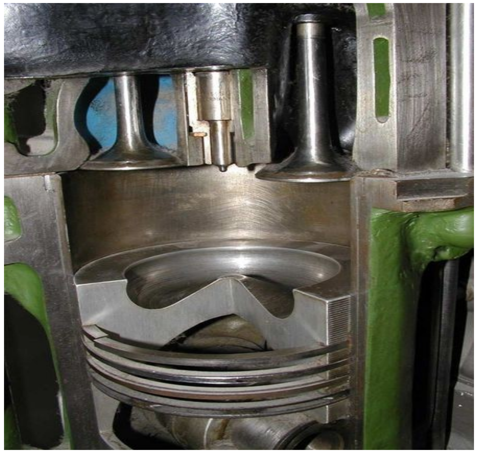
- Defining „parametric optimization“
- Some Use-Cases
- The Geneva Library Collection
  - Design decisions
  - Features
  - Libraries and Architecture
  - Performance
  - Status
- Experiences made with
  - Boost
  - Open Source

Optimization Problems

Optimization problems can be found in just about every field of engineering, natural sciences as well as business and economic scicences (and every other part of life)

Engineering and Simulations

- Optimization of combustion engines
  - Simultaneous adaption of large amounts of parameters
- Simulations
  - E.g. weather, traffic, ...
  - Callibration of „constant“ parameters, so a simulation does better predictions
  - E.g.: let the simulation „predict“ yesterday's weather based on the weather records stored for the past 100 years



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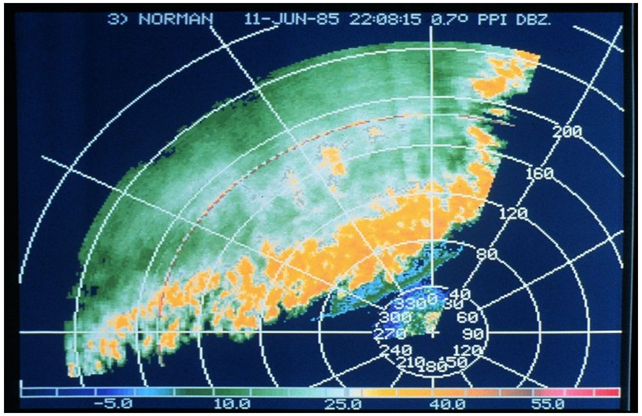
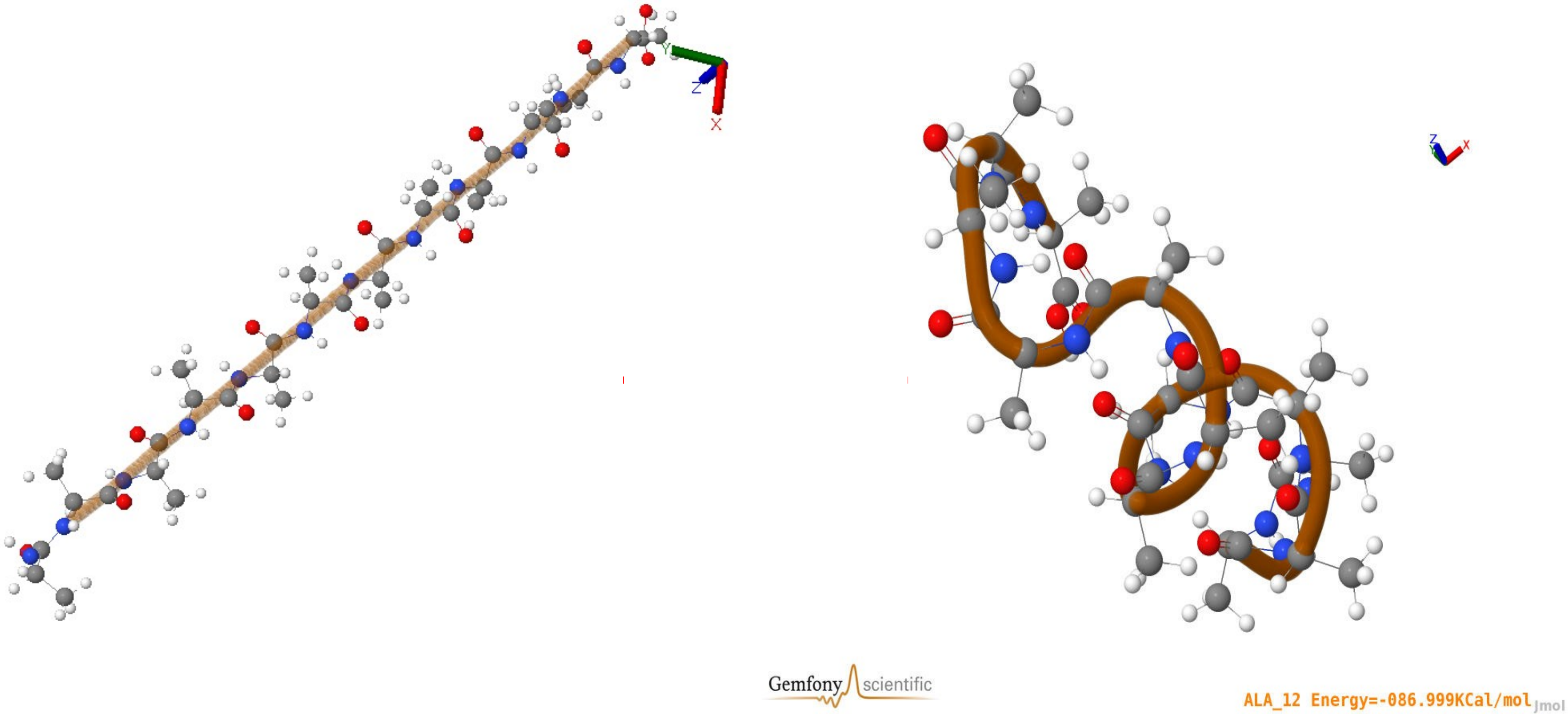
http://de.wikipedia.org/wiki/Sturm (Public domain)

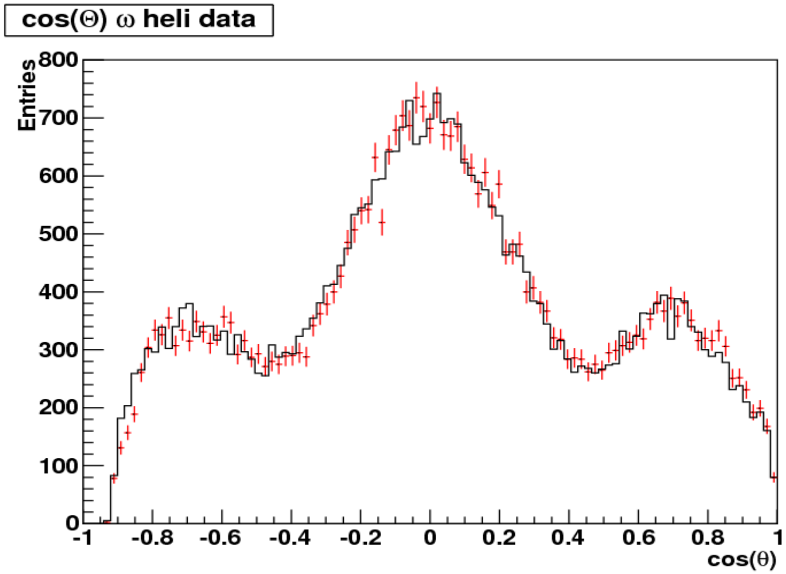


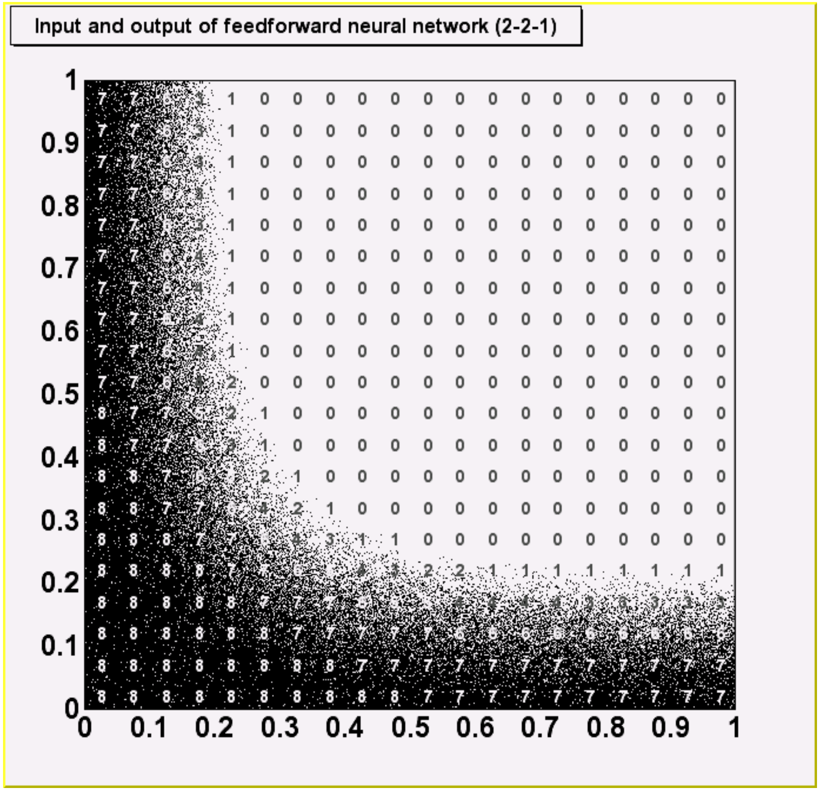
Protein Folding

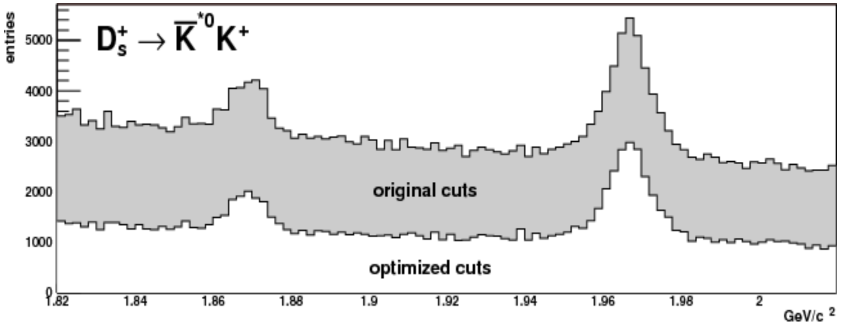


Plots created with the Jmol molecular viewer

Elementary Particle Physics, Neural Networks







Optimization Problems

Many problems can be described in terms of a set of parameters (e.g. floating point, Integer, boolean) and a *computer-implemented* evaluation function that assigns a (usually numeric) quality to them.

$$\left(x_{1,} x_{2,} \ldots, x_n\right) \rightarrow f\left(x_{1,} x_{2,} \ldots, x_n\right)$$

Defining „parametric optimization“

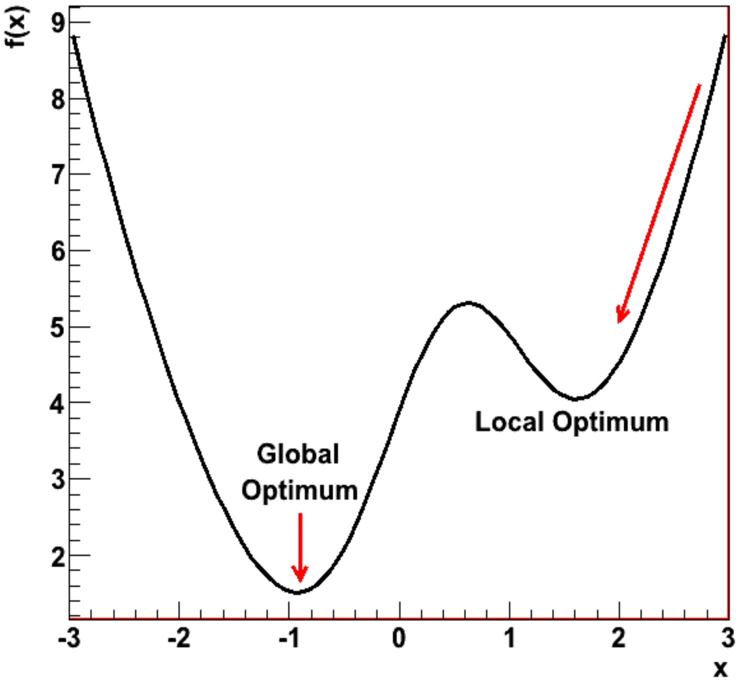
- In the context of this talk:

> Parametric optimization refers to the selection of the best *available* element from a set of alternatives, according to a computer-implemented evaluation criterion *f*

- Closely related to mathematical optimization:
  - Searching for extreme values (maxima or minima) of a function
  - But: We can usually not apply unmodified mathematical algorithms to *f*
- In comparison: The *ideal*“ solution refers to the best possible result

Some similarities

- There can be any number of local optima
- There can be many global optima (although more often there is just one)
- Some „traditional“ algorithms for searching minima/maxima of mathematical functions can be adapted to fit parametric optimization



Why not „brute force“ ?

- Imagine an optimization problem with 100 fp-parameters
  - Note: There are many much larger problems
- Let us assume that the evaluation of a single parameter set takes 1 second on a single CPU core
- Now try out just two values per dimension / parameter
  - Means evaluation of 2 to the power of 100 parameter sets
- Equivalent to approx. 40000000000000000000000 years of calculation on a single core
- And noone tells you that the best solution is anywhere near those two parameters you tried
- Some problems have very complex and long-running evaluation functions

We need special algorithms

Special algorithms are needed that avoid visiting every single parameter set (which would be impossible, as we have seen)

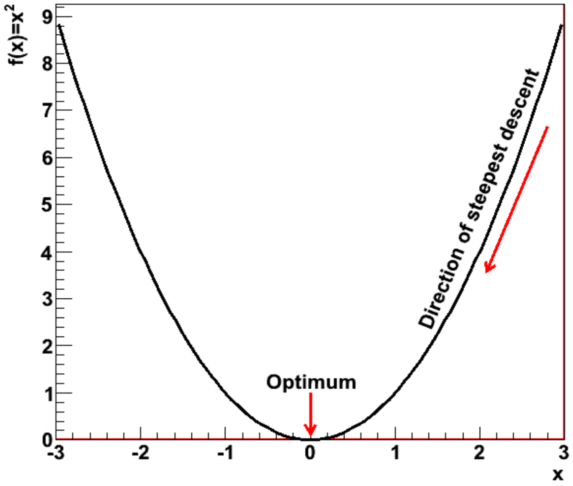
Even better, if they can be easily parallelized

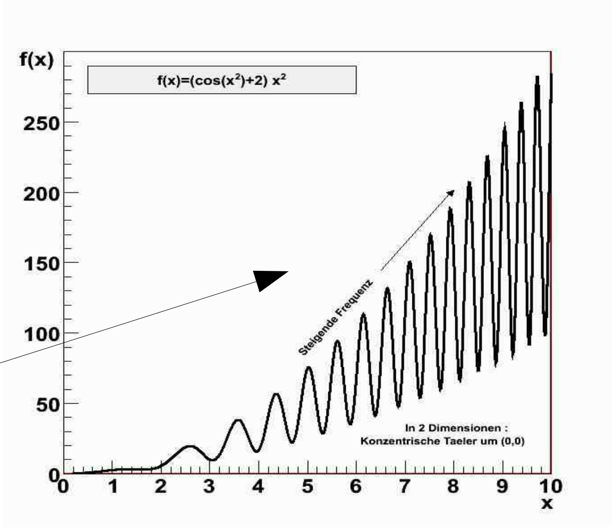
...

A simple solution

- Calculate the direction of steepest descent
  - Simple idea: „walk down-hill“
  - Can be done for computer-implemented evaluation criteria with an approximation

$$\frac{\partial f}{\partial x} \rightarrow \frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

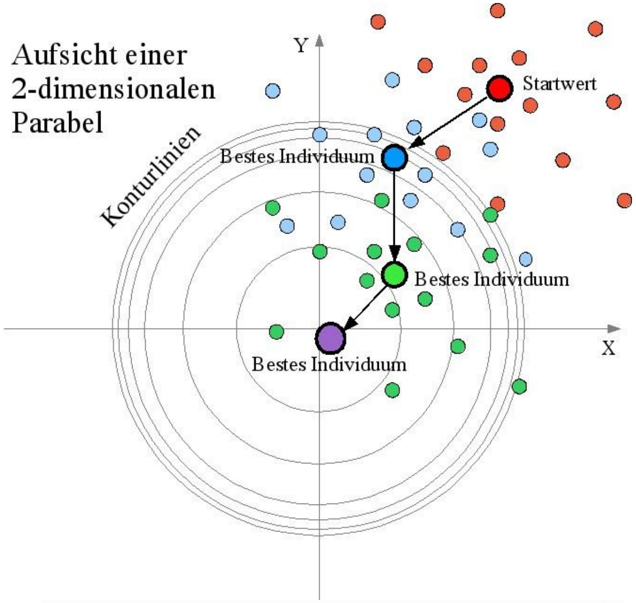


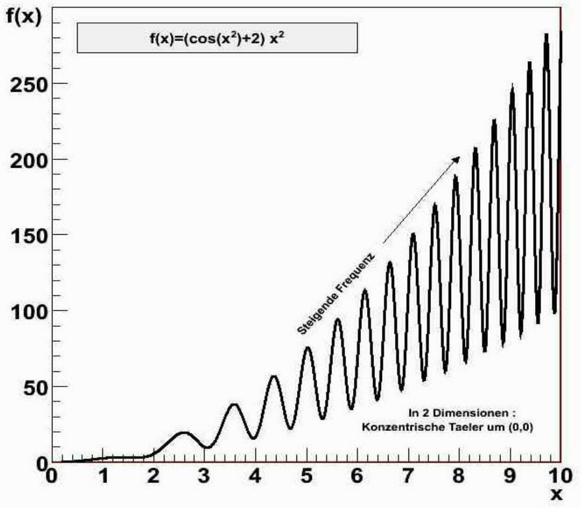


This will fail!

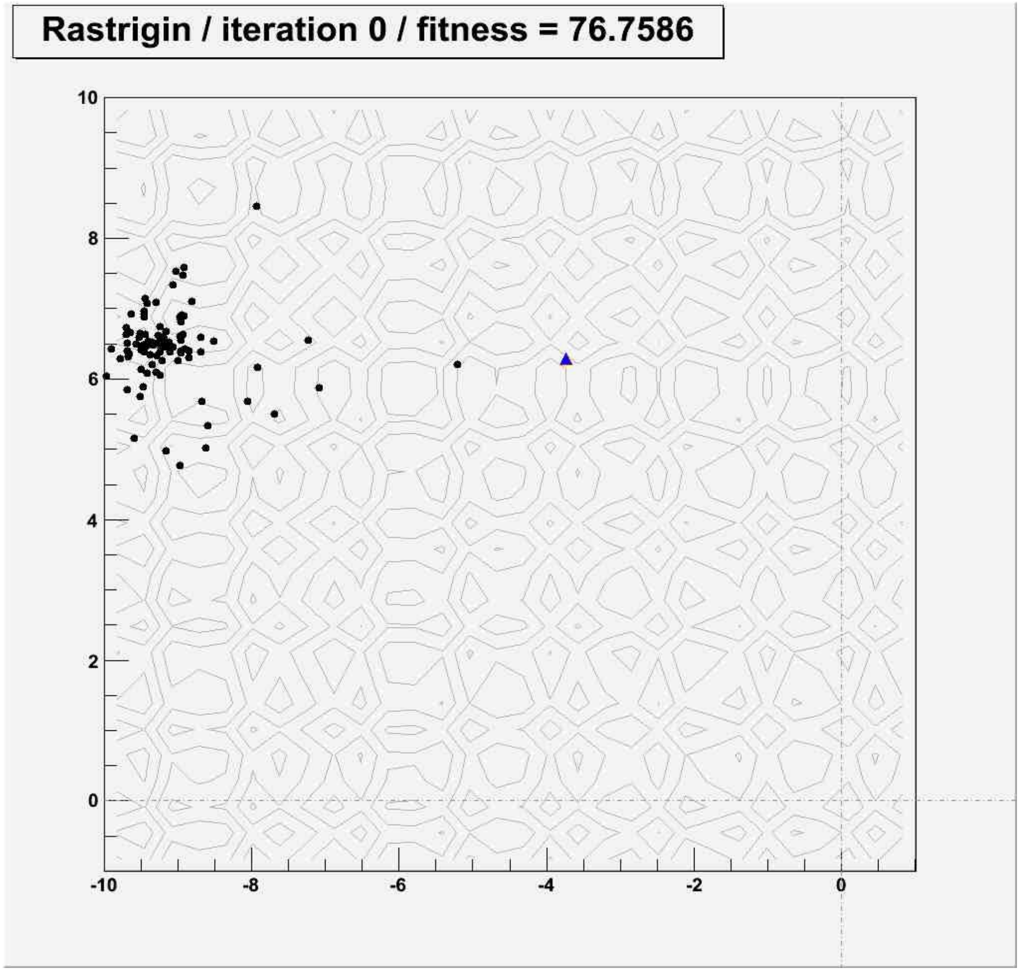
Evolutionary Strategies („ES“)

- Algorithm:
  - Population of parents (best known solutions) and children
  - Cycle of duplication, mutation, selection
  - Mutation usually through addition of gaussian-distributed random numbers
- Advantages:
  - Tolerant wrt. local optima
  - Compute time scales with size of the population
  - Easy to parallelise
- Disadvantages
  - Can be slower than gradient descent for smaller problems
  - Many configuration options (e.g. width of gaussian)





ES: The Rastrigin Function



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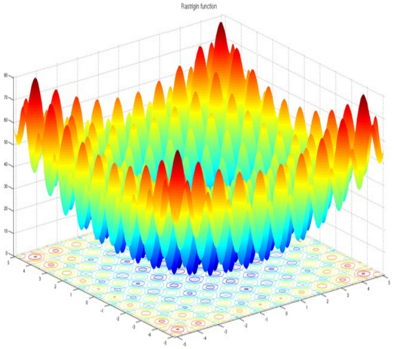
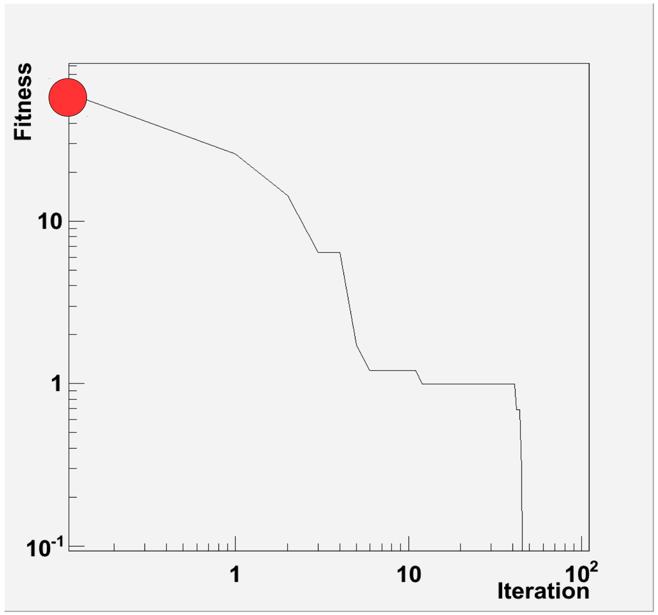
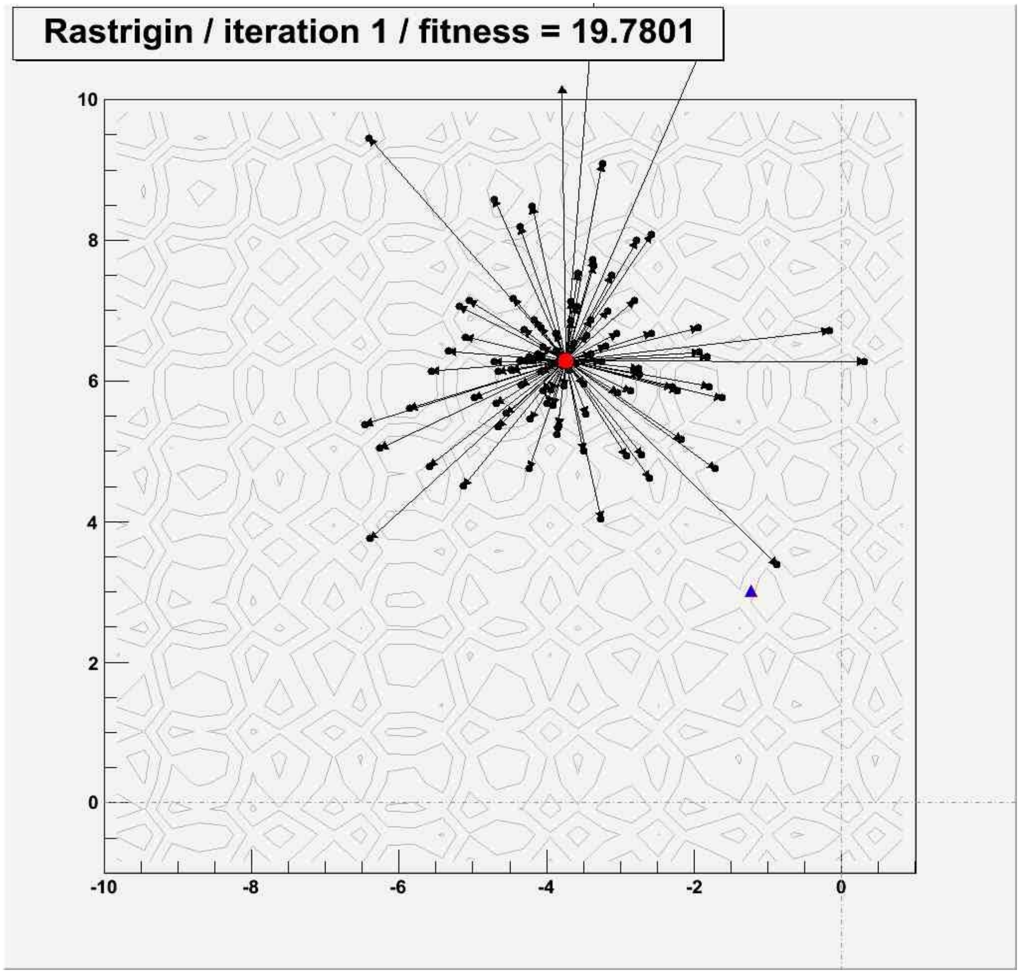
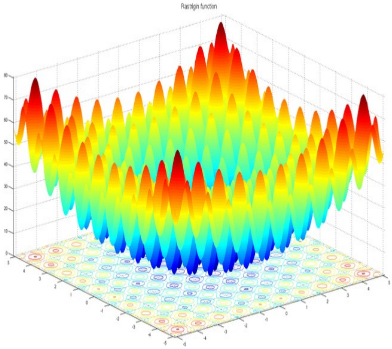


Picture: Wikipedia (public domain)



ES: The Rastrigin Function





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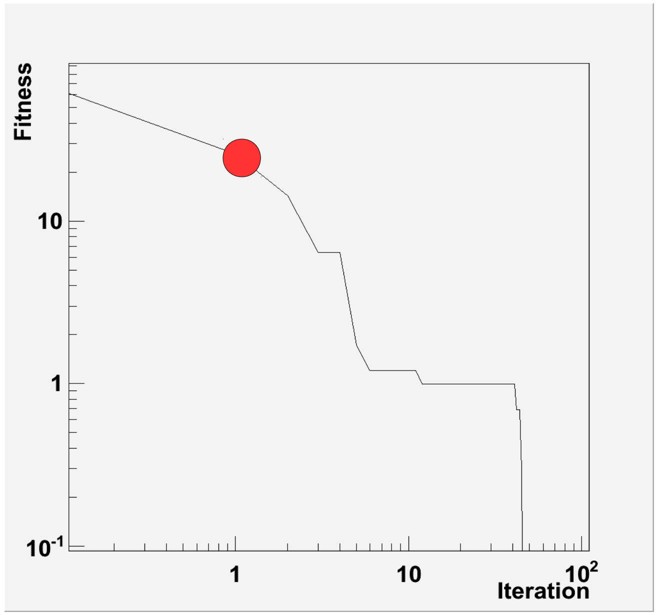

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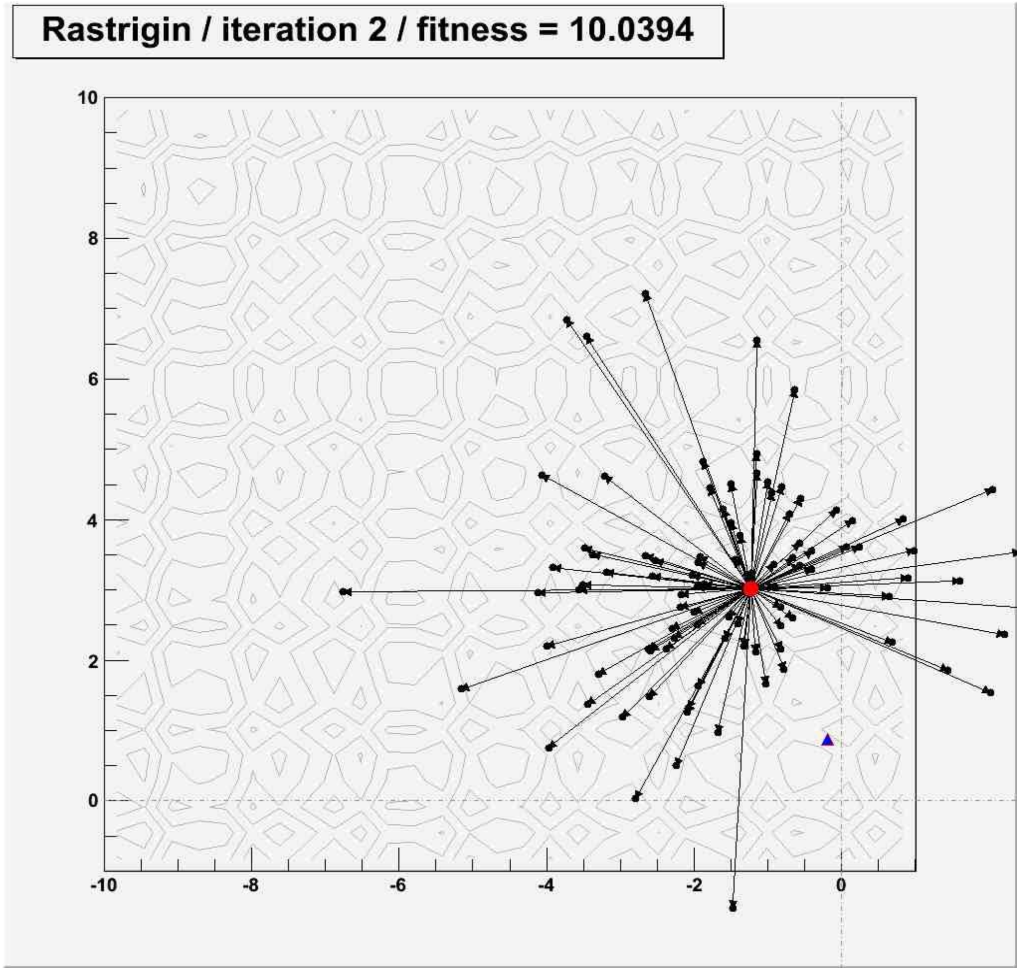

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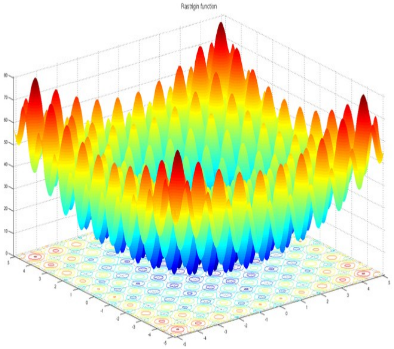

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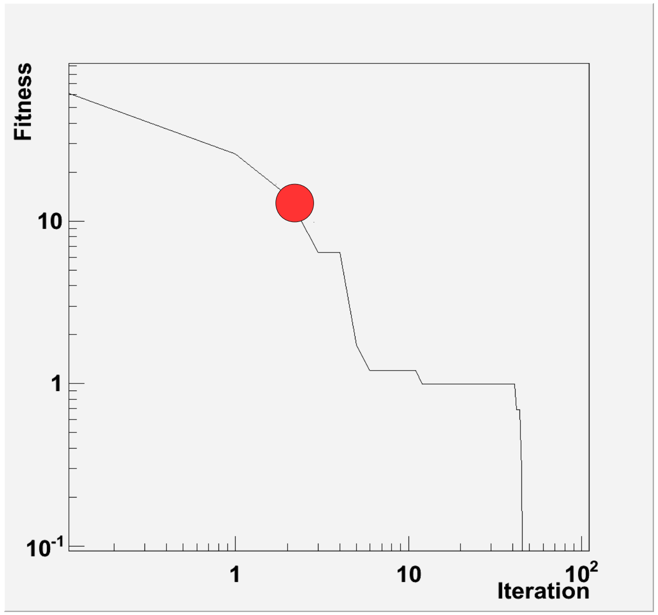

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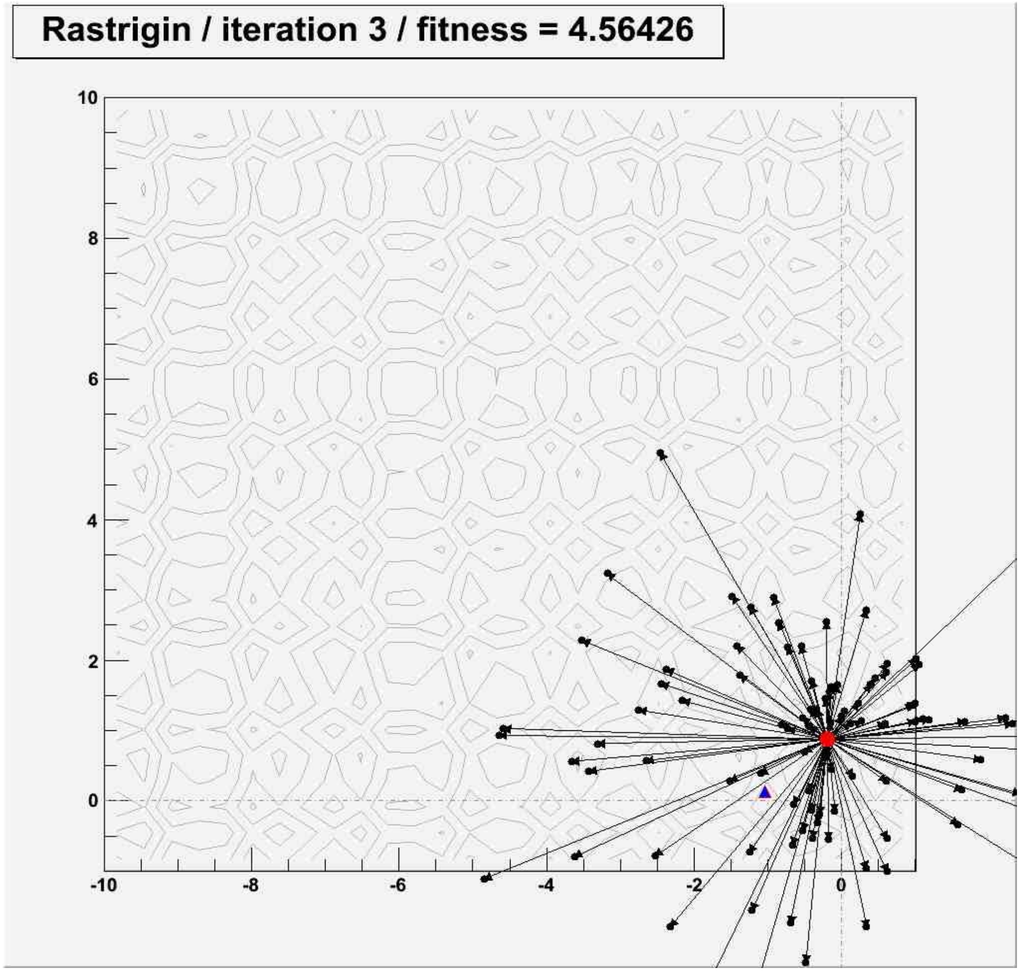

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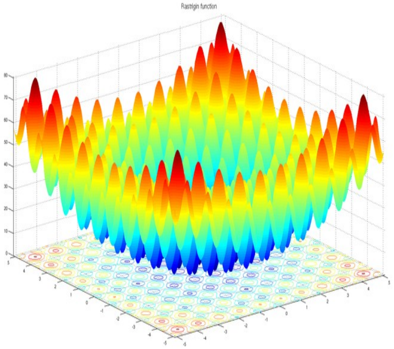

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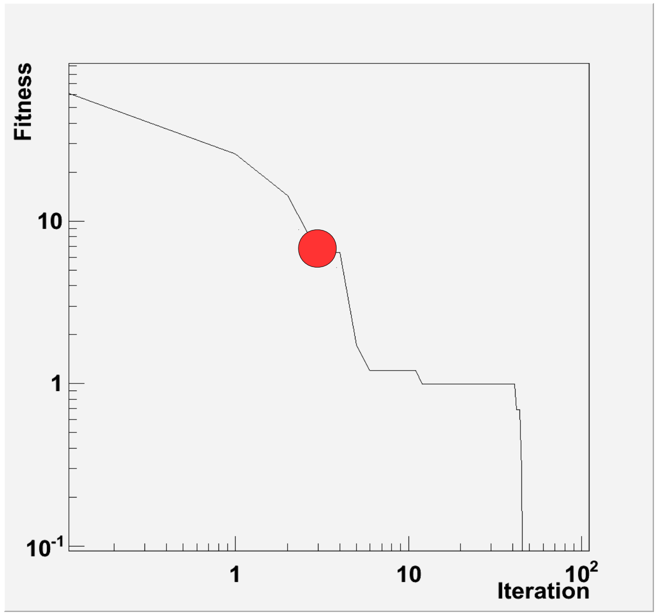
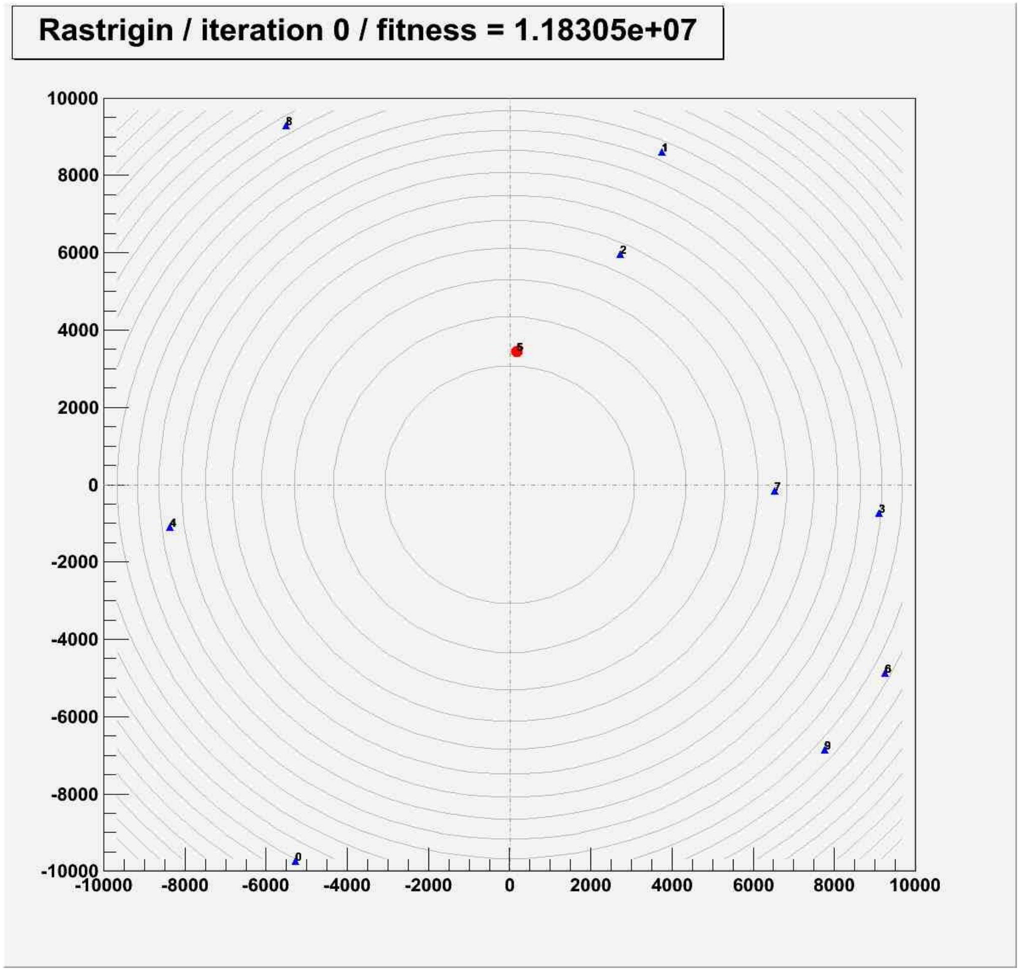


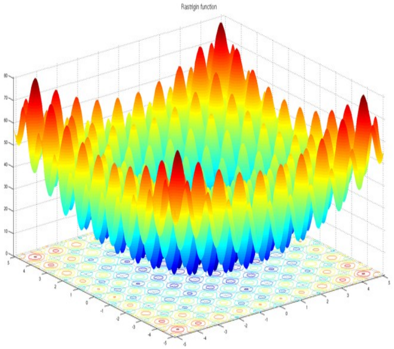
Other Algorithms

- Particle Swarm Algorithms
  - Members of „neighborhoods“ of candidate solutions are drawn in each iteration towards
    - The globally best solution
    - The best solution of the neighborhood
    - A random direction
- Deluge algorithms / Simulated Annealing
- Line search, Simplex, …

(Source: Wikipedia; Author D. Dibenski; public domain)

Swarm: Rastrigin Function





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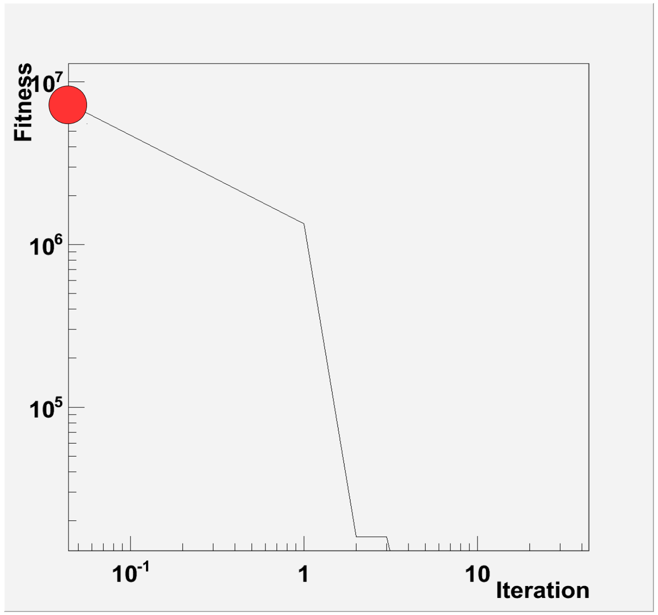

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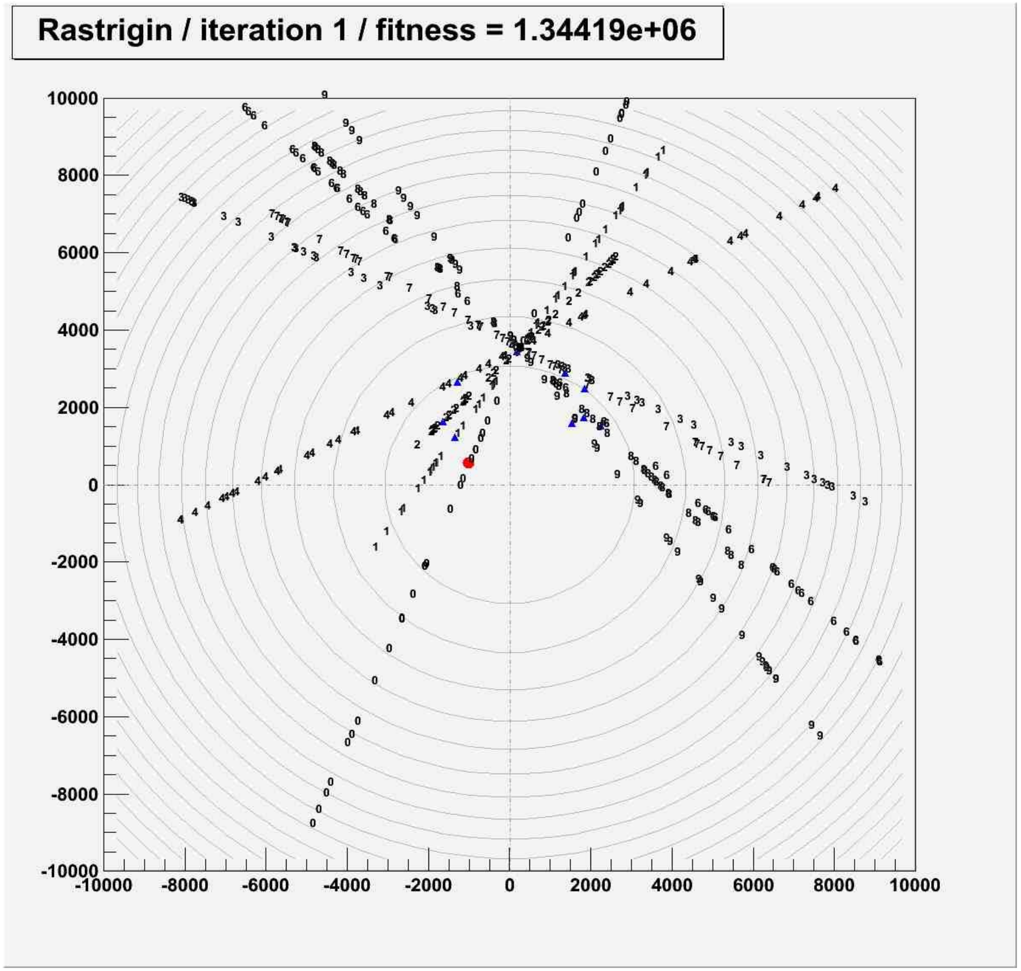
Swarm: Rastrigin Function



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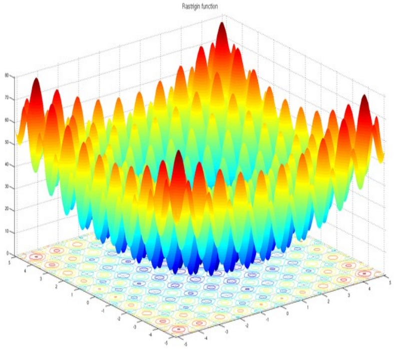

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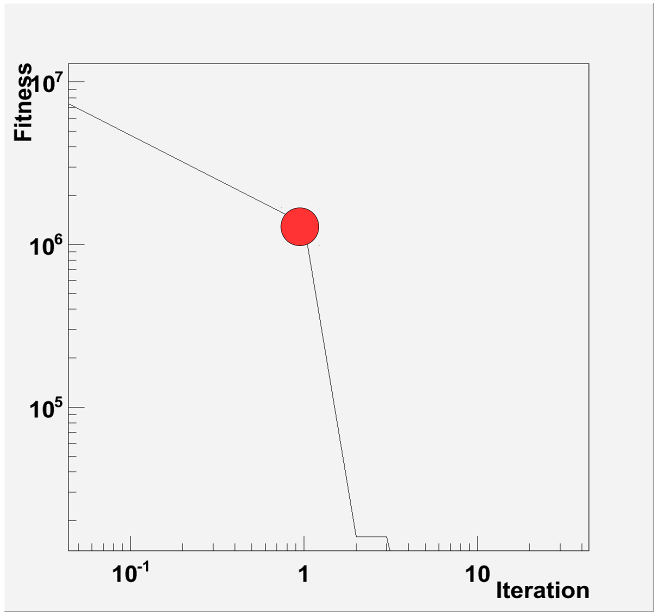
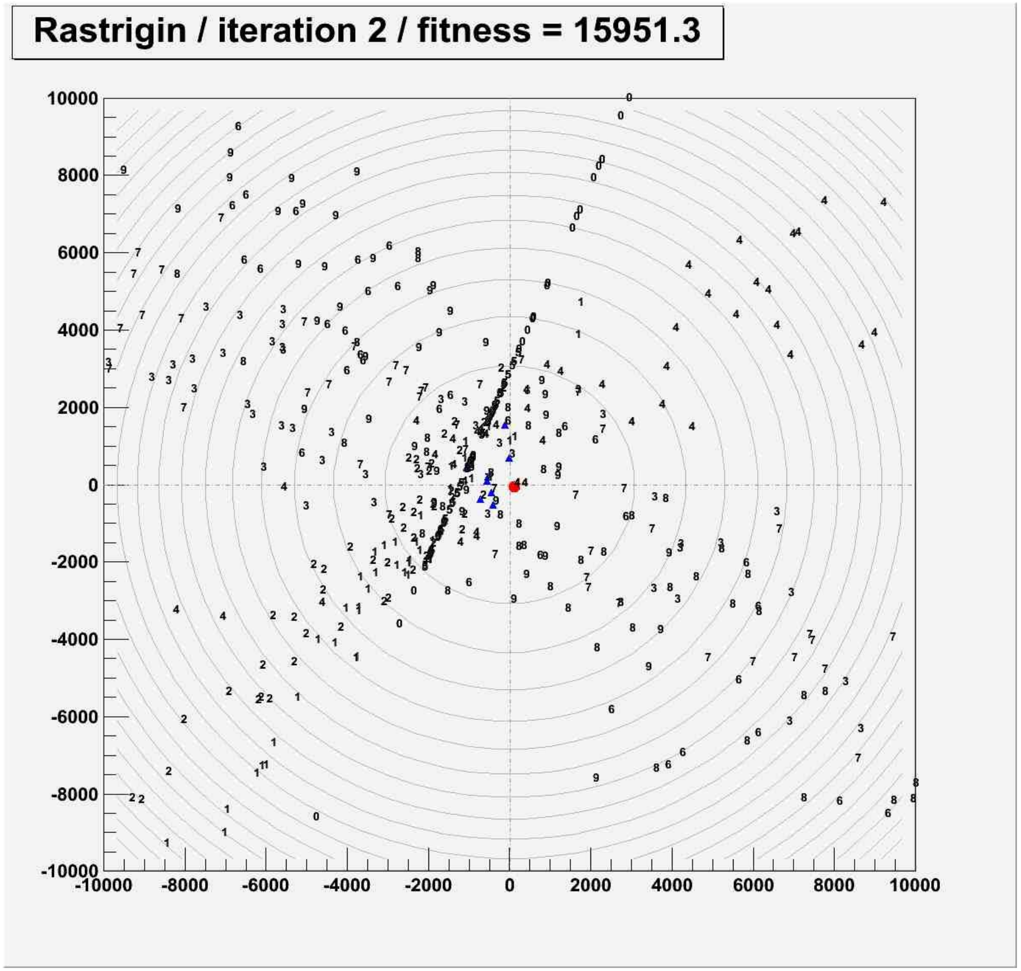


Swarm: Rastrigin Function



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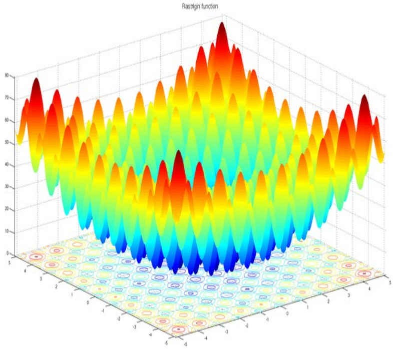

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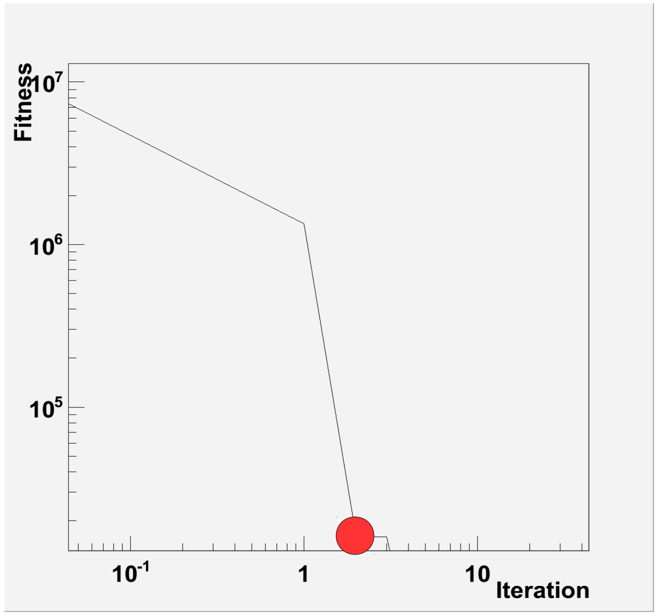
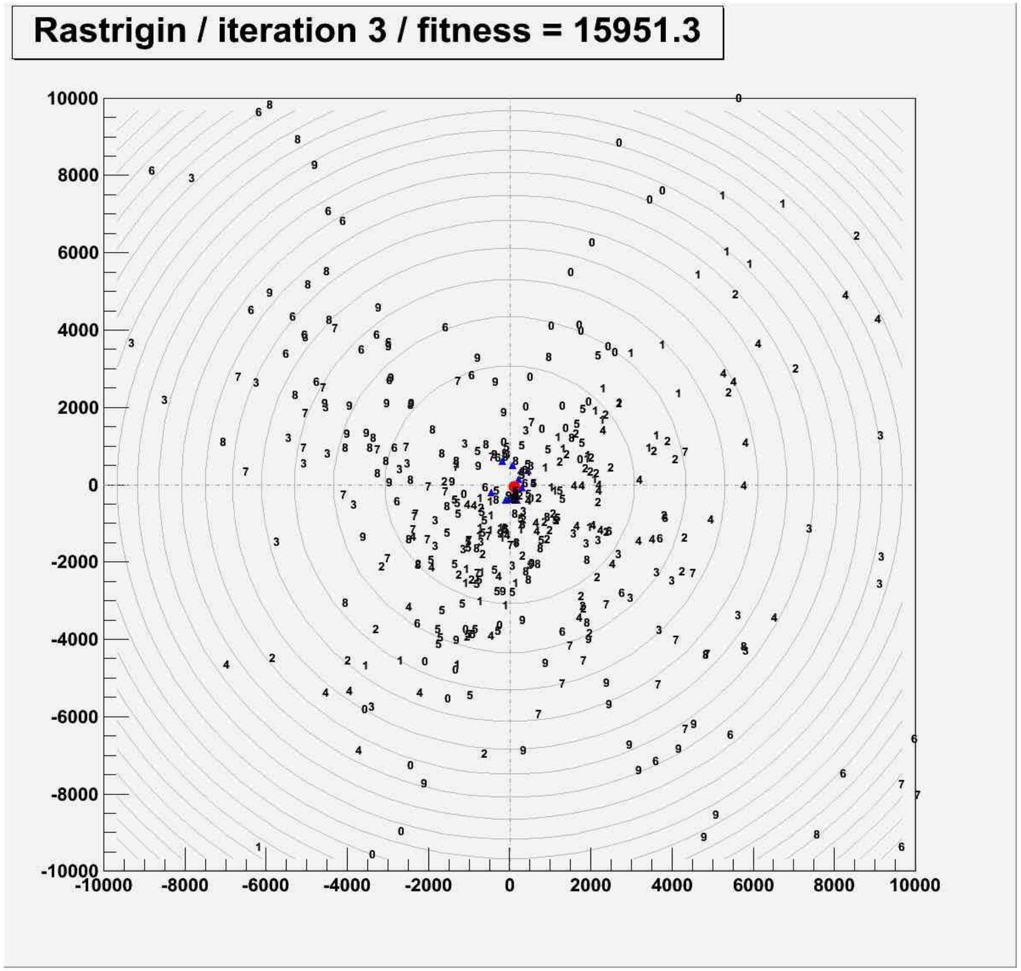


Swarm: Rastrigin Function



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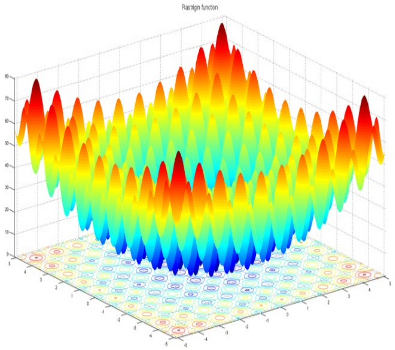
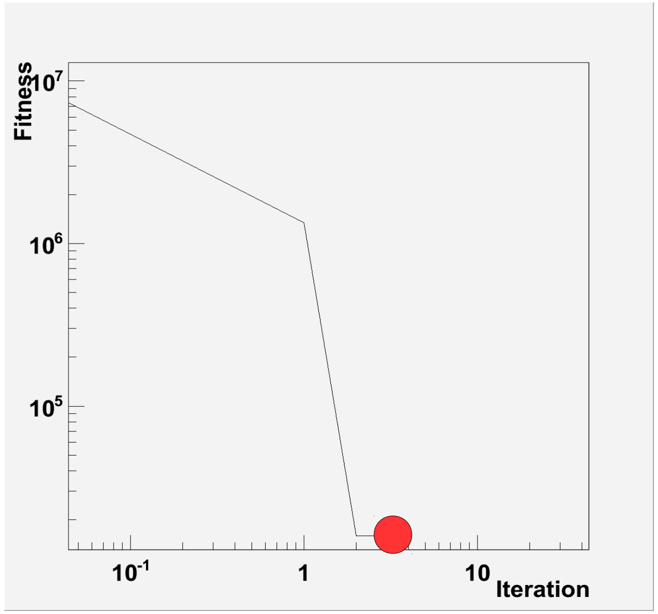


Picture: Wikipedia (public domain)



Geneva

The examples above were calculated
with the Geneva library
of optimization algorithms

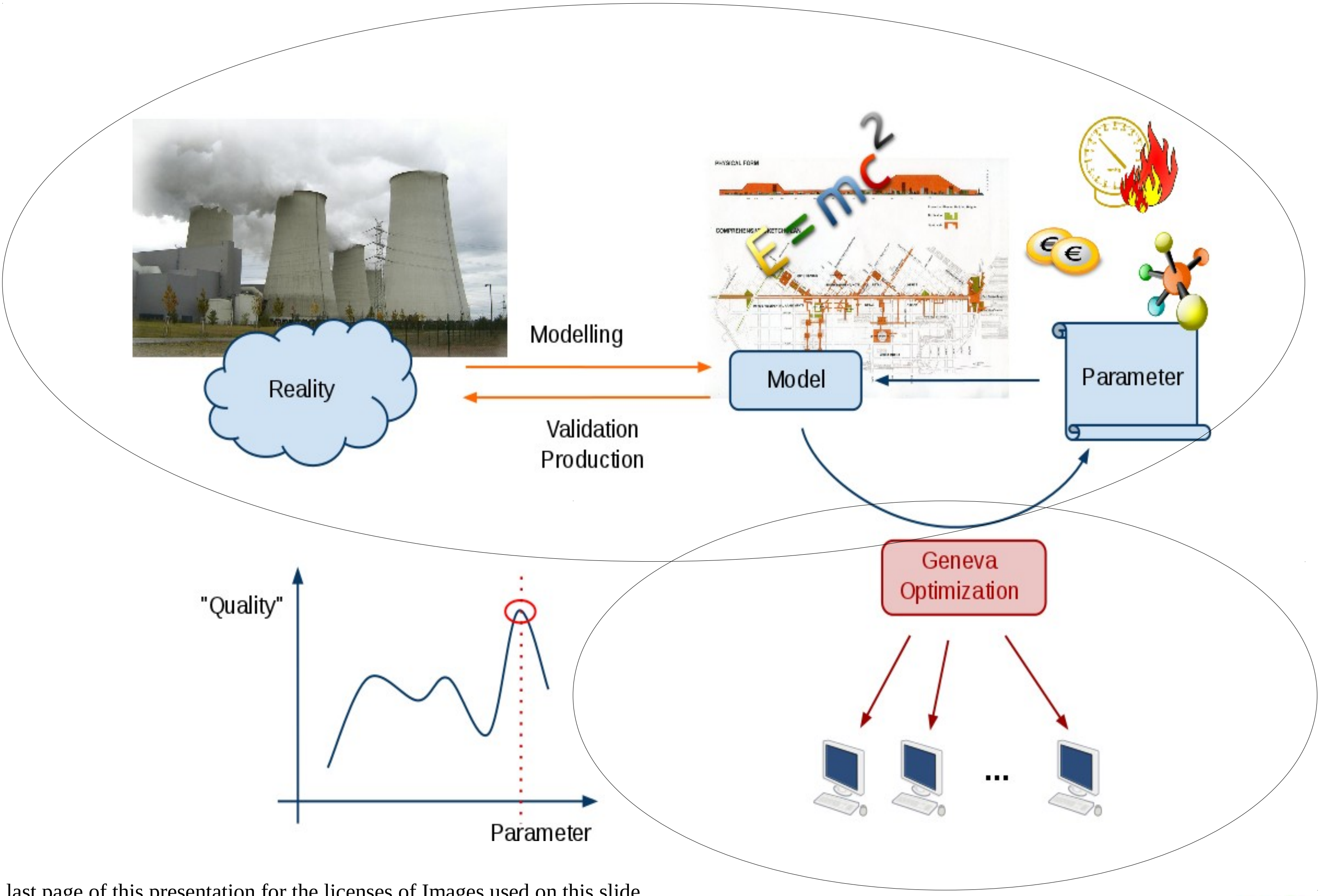
Geneva: Boundary Conditions

- Geneva wants to provide users with an environment that lets them solve optimization problems of any size transparently, as easily on a single core-machine as in the Grid or Cloud.
- Geneva wants to become a „warehouse of optimization algorithms“, all working on the same problem descriptions
- Geneva targets optimization problems, whose figure of merit requires long-lasting computations
- We assume that many very large scale optimization problems so far have not been targetted as
  - Typical single- or multi-core machines do not offer sufficient computing power
  - The complexities of running optimizations in parallel and/or distributed enviroments lead to the assumption that performing such computations is not feasible

Connecting Fields of Knowledge

Problem definition

Optimization



Reality

Modelling

Validation
Production

Model

Parameter

Geneva
Optimization

"Quality"

Parameter

...

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Geneva: Design Criteria

- Focus on long-lasting, computationally expensive evaluation functions
  - Stability *of core library* rated higher than efficiency
  - Suitable for distributed environments
- Serial, multi-threaded and networked execution, transparent to users
  - Implications of networked and multi-threaded execution:
    - No global variables
    - User-defined data structures must be serializable
- Familiar interface
  - STL interface for data, individuals, populations, ...

Geneva: Design Criteria

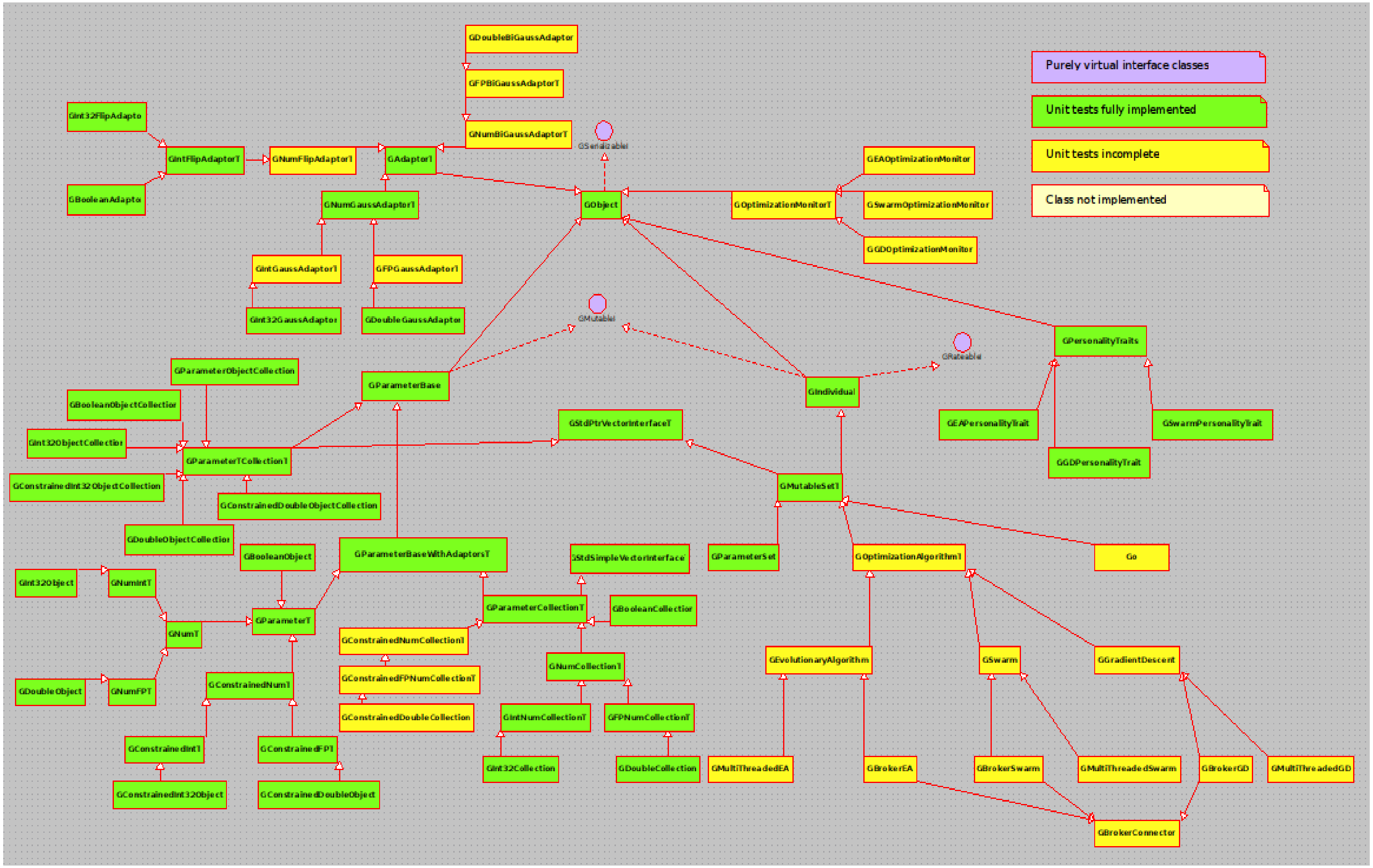
- Fault tolerance of networked execution:
  - Algorithm must be able to repair itself in case of missing or late replies from clients
- Execution of clients in Grid and Cloud:
  - No push mode means: Server needs public IP, clients don't
- Easy, portable build environment:
  - CMake
- Quality assurance:
  - Unit-tests, based on Boost.Test library
  - Can be integrated into user code

Geneva: Implementation

- C++
  - Heavily uses Boost
  - Efficient (cmp. Java)
  - About 80000 LOC
- So far largely Linux-based
  - But likely portable
  - Tested with various g++, Intel
- Major components
  - Representation of parameter sets
  - Optimization algorithms
  - Parallelization and communication
  - Random number factory

```
int main(int argc, char **argv)
{
      GOptimizer go(argc, argv);

      //-----------------------------------------------
      // Client mode
      if(go.clientRun()) return 0;

      //-----------------------------------------------
      // Server mode

      // Create the first set of individuals.
      for(std::size_t p = 0 ; p<nParents; p++) {
        boost::shared_ptr<GParameterSet>
      functionIndividual_ptr
              =
      GFunctionIndividual<>::getFunctionIndividual();

      // Make the param. collection known to individual
        go.push_back(functionIndividual_ptr);
      }

      // Perform the actual optimization
      boost::shared_ptr<GParameterSet>
      bestFunctionIndividual_ptr
                      = go.optimize();

      // Do something with the best individual
      // [...]

      std::cout << "Done ..." << std::endl;
      return 0;
}
```

Class Hierarchy



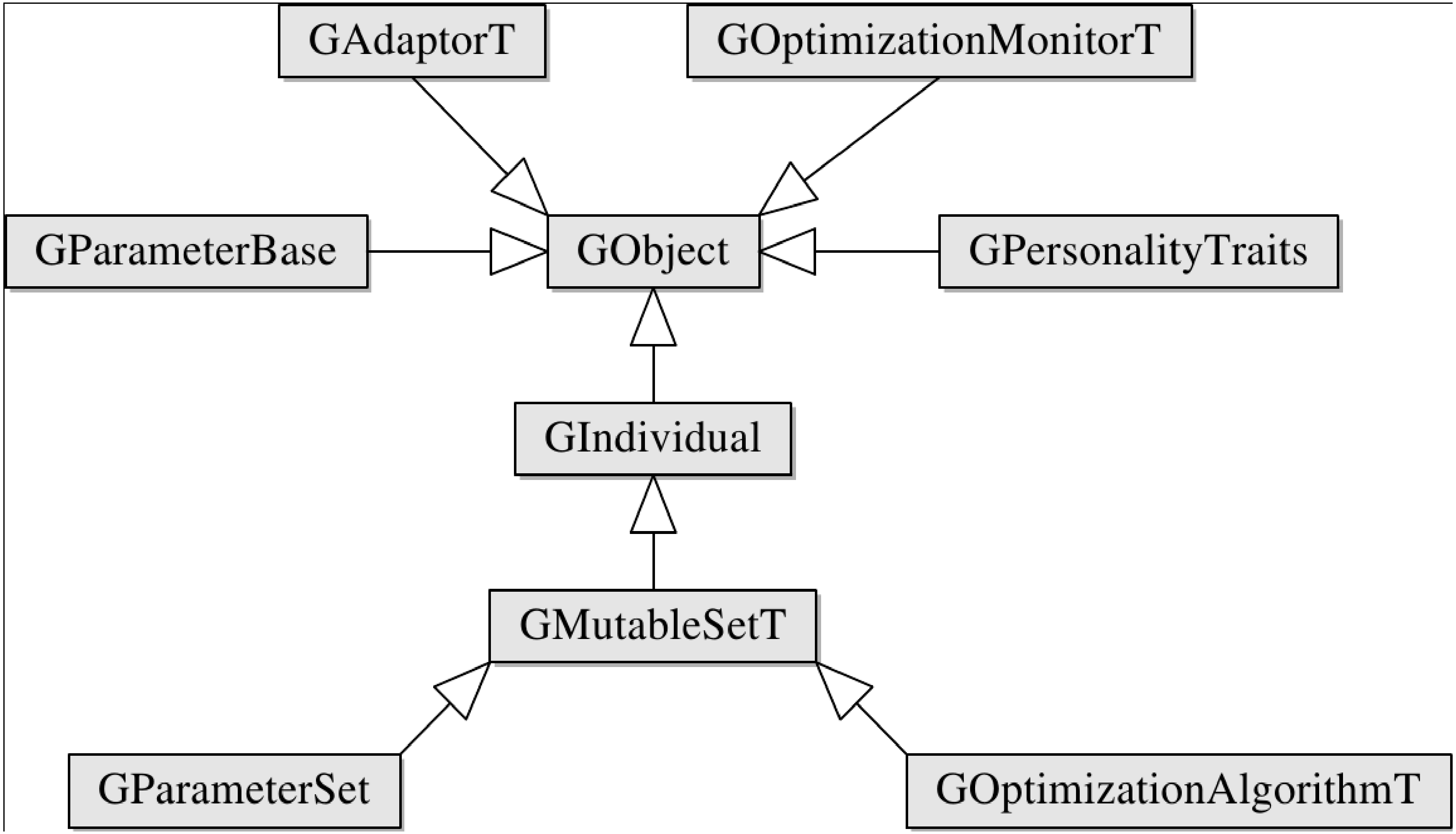
Purely virtual interface classes

Unit tests fully implemented

Unit tests incomplete

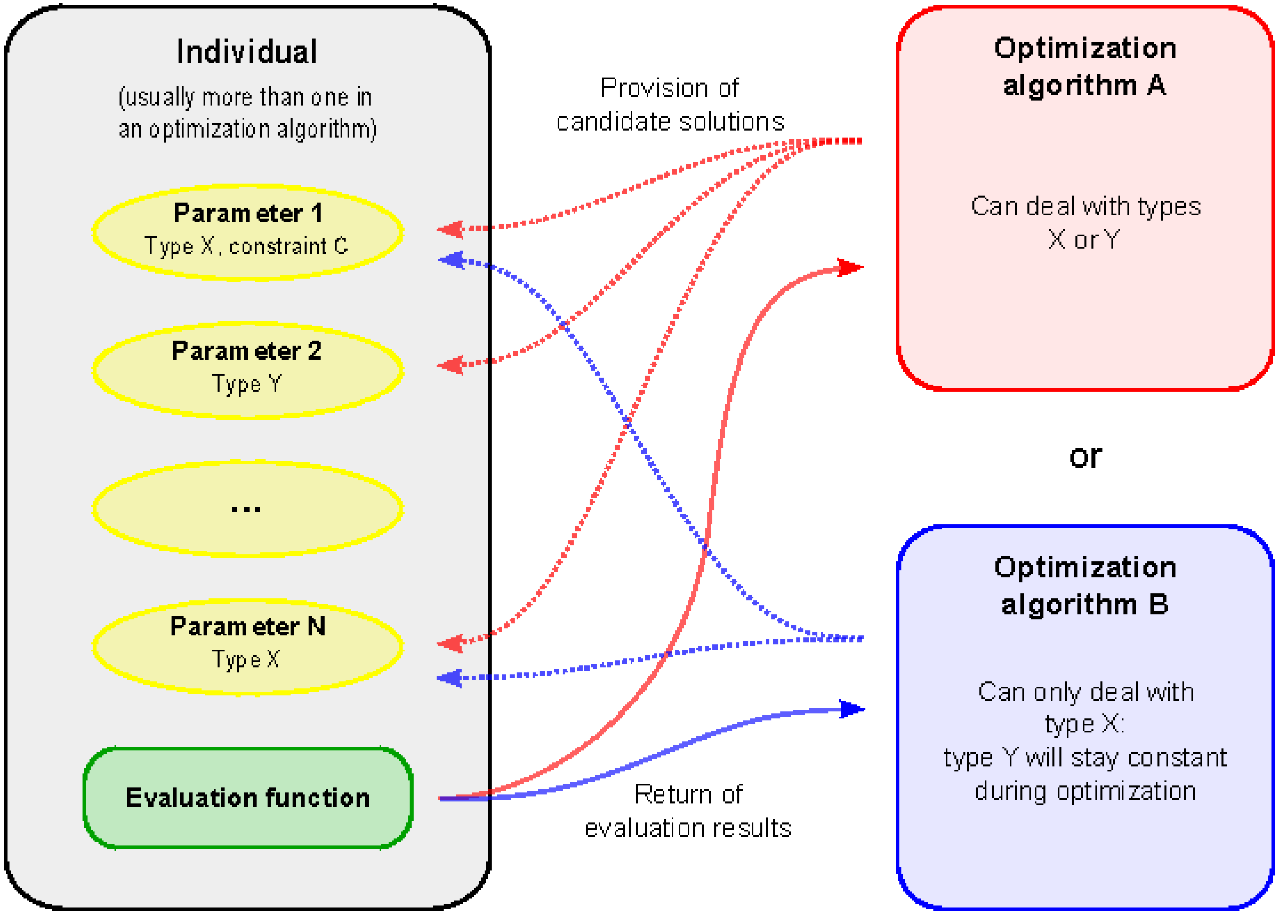
Class not implemented

Core Classes



Parameters vs. Algorithm

Iteration-based optimization



Individual

(usually more than one in an optimization algorithm)

Parameter 1
Type X, constraint C

Parameter 2
Type Y

...

Parameter N
Type X

Evaluation function

Provision of candidate solutions

Return of evaluation results

Optimization algorithm A

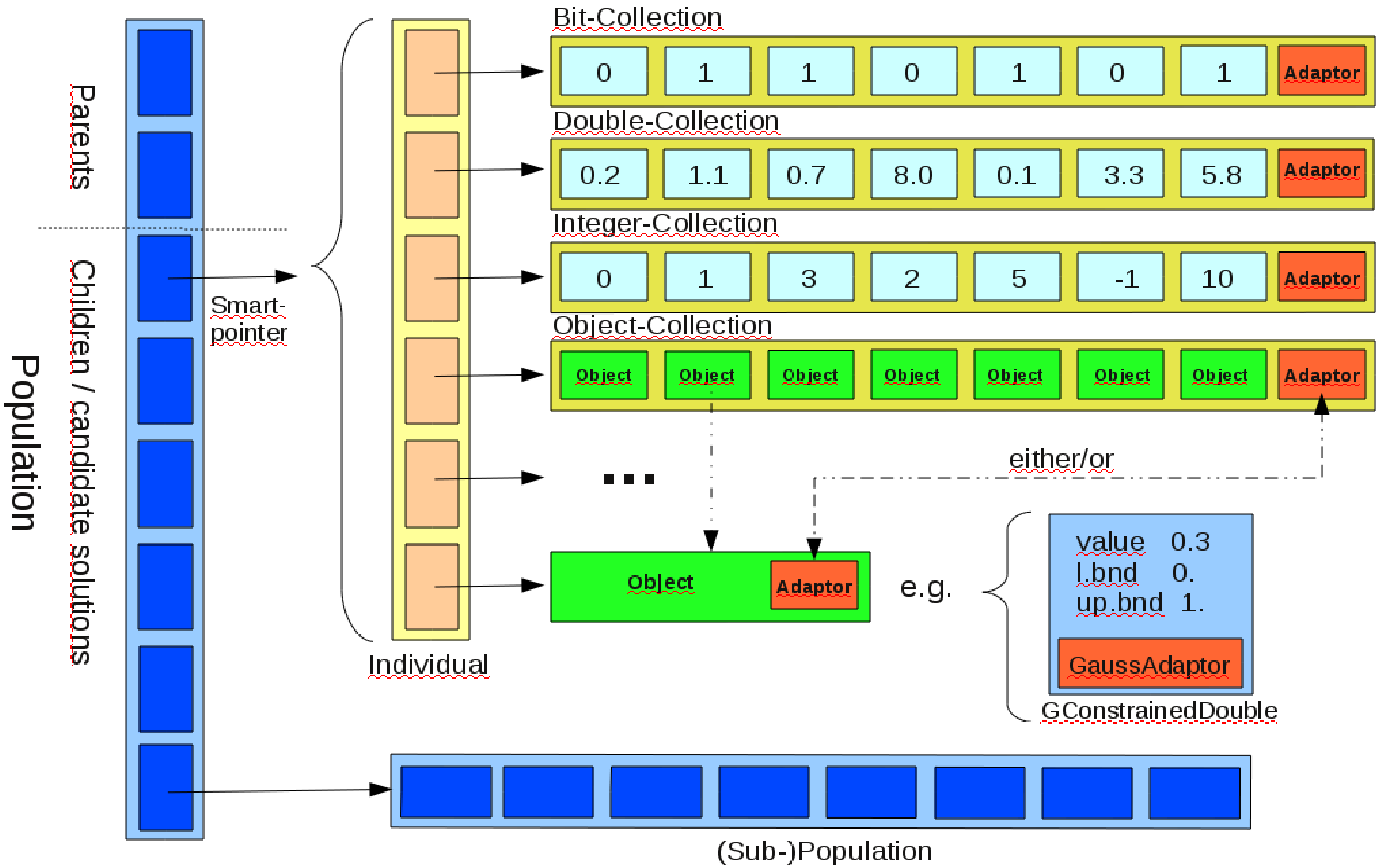
Can deal with types X or Y

or

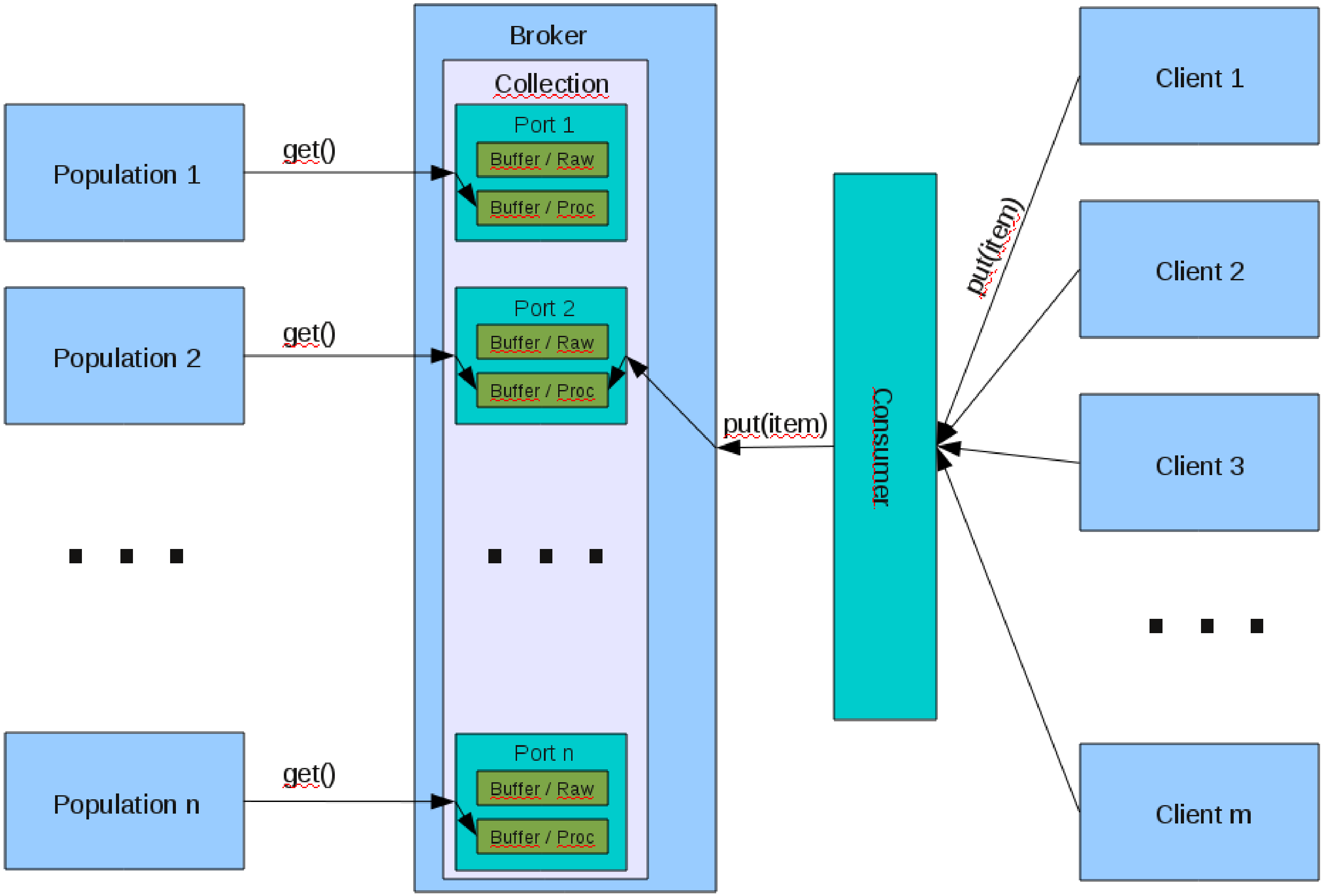
Optimization algorithm B

Can only deal with type X:
type Y will stay constant during optimization

ES: Data Representation / Mixed Parameter Sets



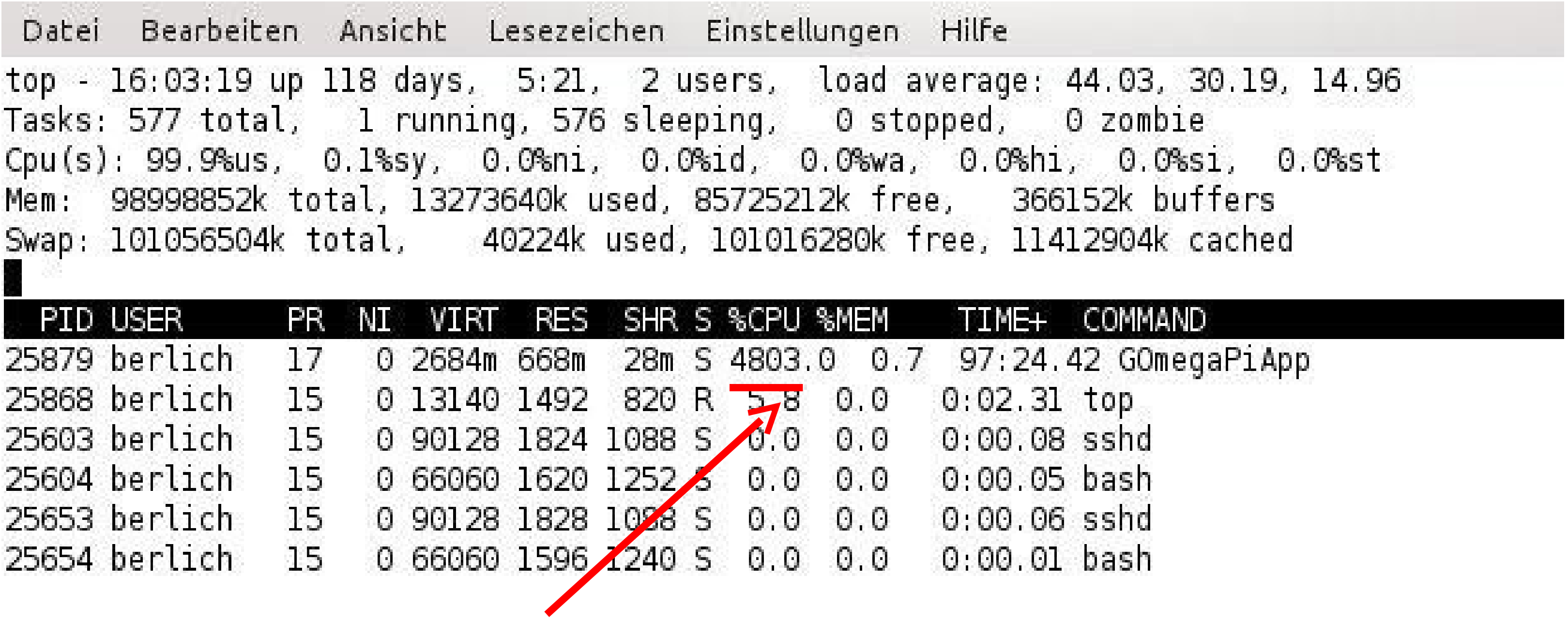
TheBroker


Broker
Collection
Port 1
Buffer / Raw
Buffer / Proc
Port 2
Buffer / Raw
Buffer / Proc
Port n
Buffer / Raw
Buffer / Proc
Population 1
Population 2
Population n
get()
get()
get()
put(item)
put(item)
Consumer
Client 1
Client 2
Client 3
Client m

Capabilities

- Geneva today implements
  - Evolutionary Algorithms
  - Particle Swarm Optimization
  - Gradient Descent
  - Simulated Annealing
- Execution in
  - Serial mode
  - Multithreaded mode
  - Networked mode
- Mixed problem descriptions
  - May contain different parameter types
- Meta-Evolution

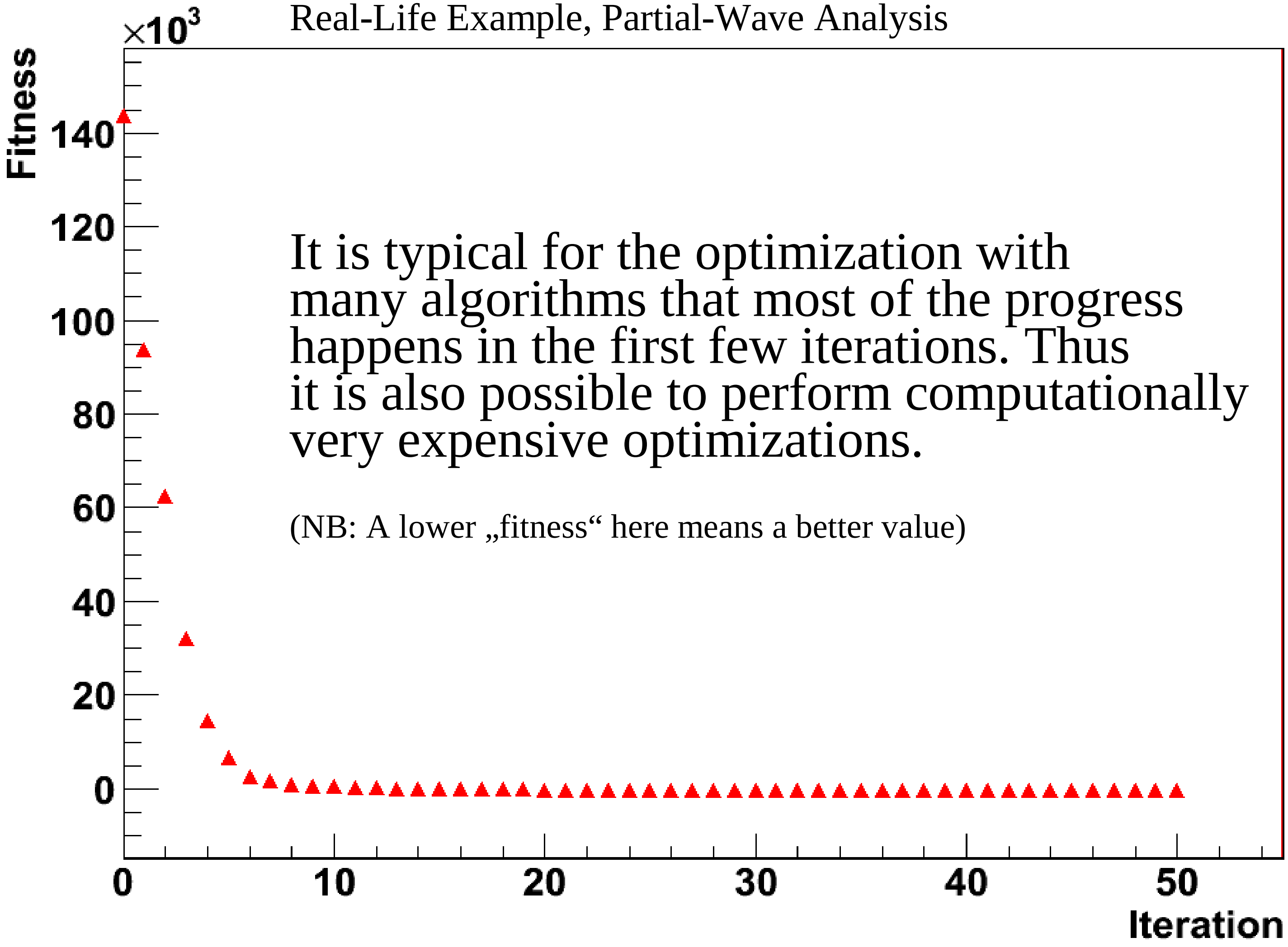
Performance / Multithreading



```
top - 16:03:19 up 118 days,  5:21,  2 users,  load average: 44.03, 30.19, 14.96
Tasks: 577 total,   1 running, 576 sleeping,   0 stopped,   0 zombie
Cpu(s): 99.9%us,  0.1%sy,  0.0%ni,  0.0%id,  0.0%wa,  0.0%hi,  0.0%si,  0.0%st
Mem:  98998852k total, 13273640k used, 85725212k free,   366152k buffers
Swap: 101056504k total,    40224k used, 101016280k free, 11412904k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
25879 berlich   17   0 2684m 668m  28m S 4803.0  0.7  97:24.42 GOmegaPiApp
25868 berlich   15   0 13140 1492  820 R  5.8  0.0   0:02.31 top
25603 berlich   15   0 90128 1824 1088 S  0.0  0.0   0:00.08 sshd
25604 berlich   15   0 66060 1620 1252 S  0.0  0.0   0:00.05 bash
25653 berlich   15   0 90128 1828 1088 S  0.0  0.0   0:00.06 sshd
25654 berlich   15   0 66060 1596 1240 S  0.0  0.0   0:00.01 bash
```

- 48 Core AMD Sytem (Magni Cours)
- Here: Evolutionary Algorithms
- Example from High-Energy Physics (Partial Wave Analysis / RUB, Uni Mainz, GSI Darmstadt)

Optimization Progress

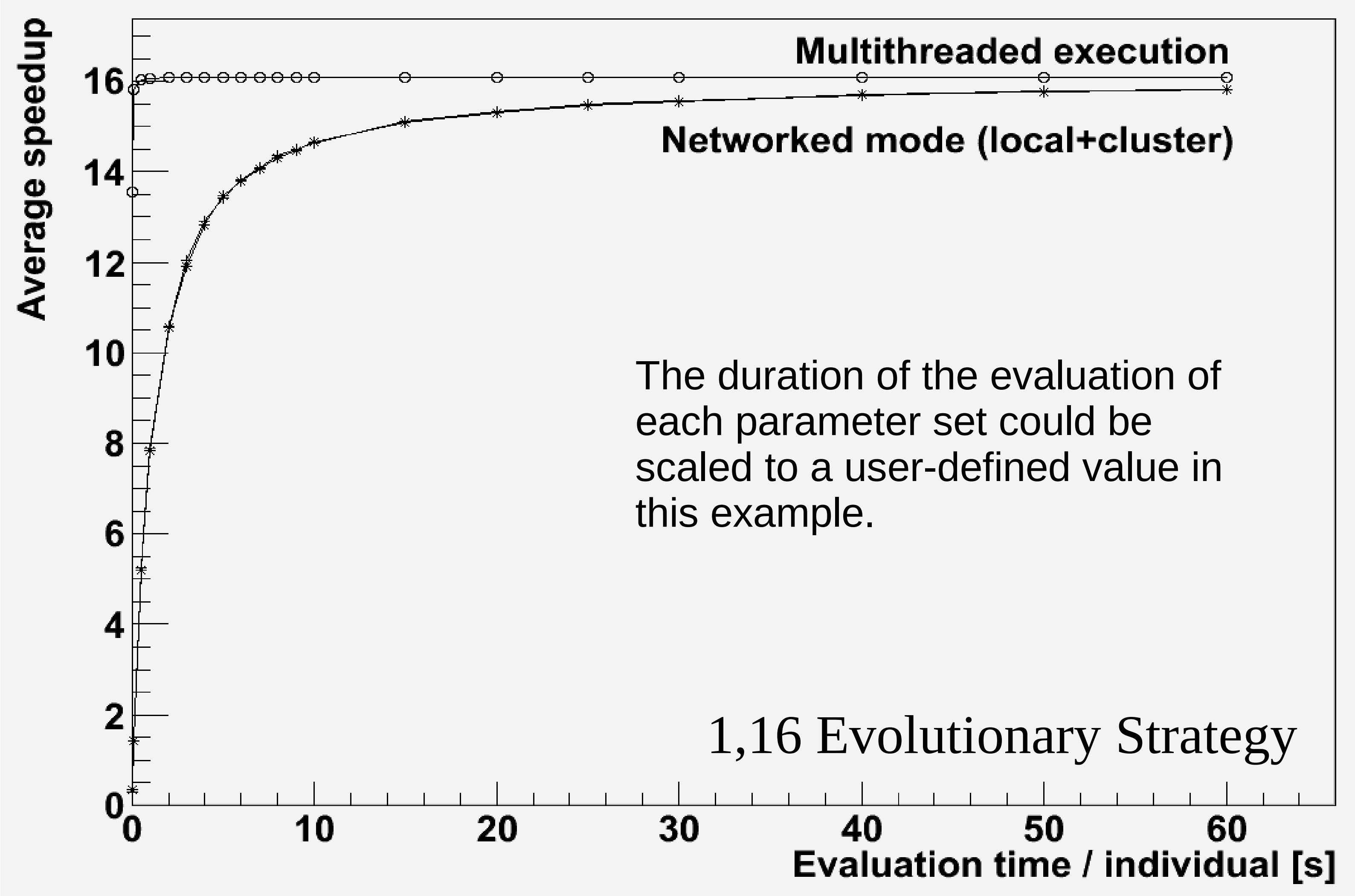


Real-Life Example, Partial-Wave Analysis

It is typical for the optimization with many algorithms that most of the progress happens in the first few iterations. Thus it is also possible to perform computationally very expensive optimizations.

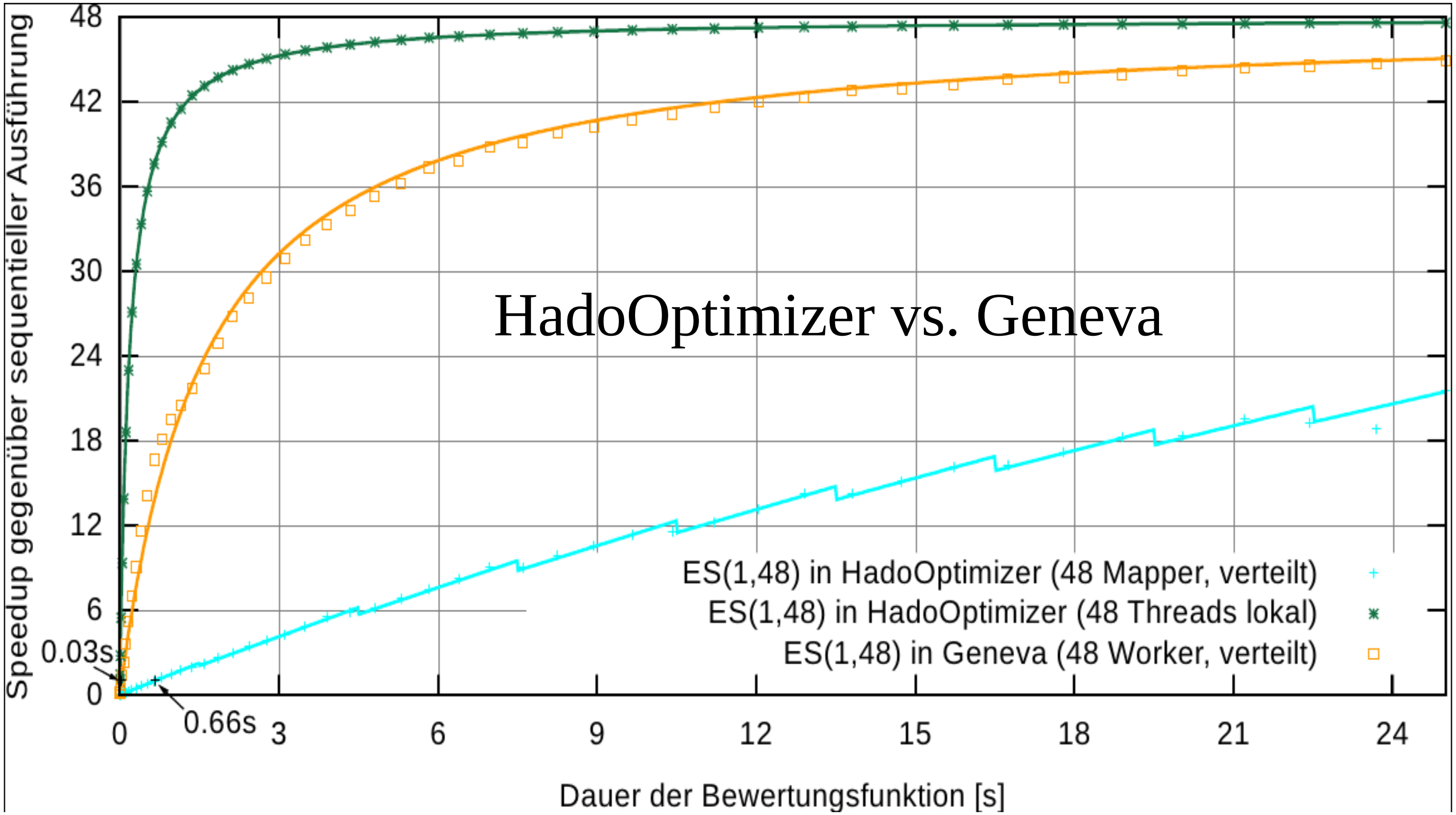
(NB: A lower „fitness“ here means a better value)

Performance:
Speedup in a Cluster



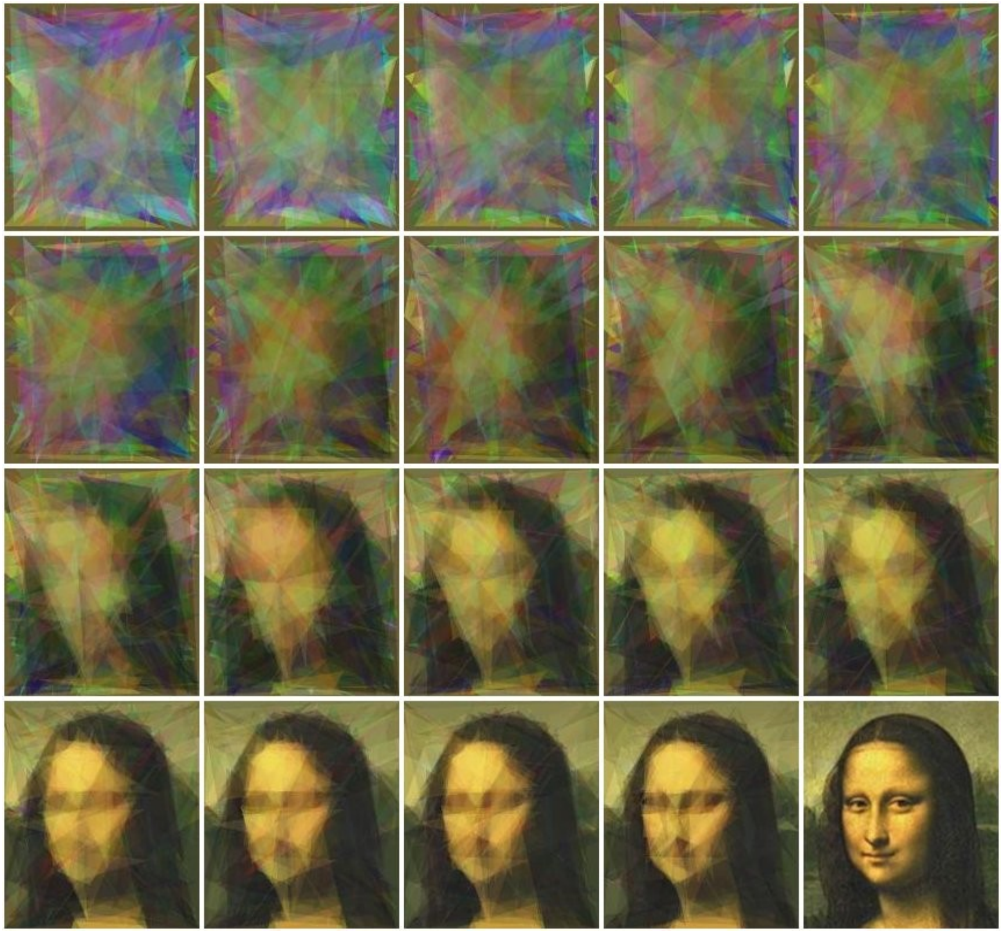
The duration of the evaluation of each parameter set could be scaled to a user-defined value in this example.

Performance: Comparison with Hadoop ES implementation (Java)



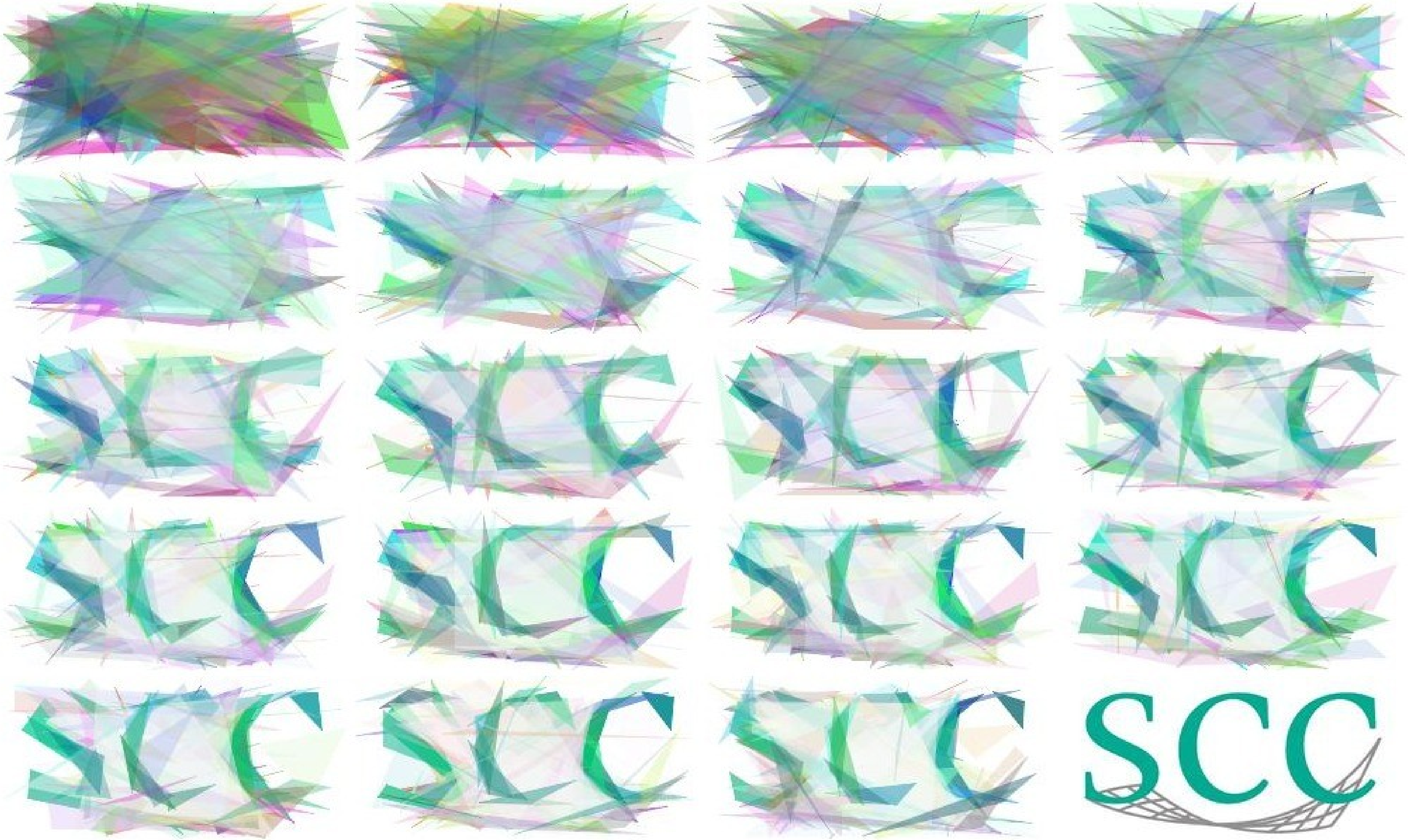
Thanks to Christian Kumpe for the permission to use this plot

Modelling the Mona Lisa



- Goal of the optimization
  - 300 semi-transparent triangles should be superimposed in such a way that they resemble a given target picture
  - 10 parameters / triangle: alpha-channel, coordinates and colors
  - Means that suitable values for 3000 parameters must be found, with no known start value

Modelling the SCC Logo



Geneva and Boost

- Only real external dependency
- Geneva uses (in no particular order)
  - ASIO
  - Serialization
  - Threads
  - Smart pointers
  - Casts
  - Bind, Function, ...
- Has tremendeously sped up development
  - First approach in case of some required feature:
    Check the Boost libraries, whether it already exists
- Development of Geneva would not have been possible without Boost

Geneva is Open Source

- No vendor lock-in
- Availability of source code independent of success of Gemfony
- Full control over what happens
- Customer-driven development
  - Can benefit from third-party suggestions
  - Can initiate own ideas
- Users can sometimes be suspicious ...

Summary

- Shorter Development Cycles
  - Parallelization
  - Good results often within first few cycles
- Robust Optimization Algorithms
  - Local optima
  - Missing responses
- ES probably the most mature algorithm!
- Good scalability for computationally expensive problems
  - Ease of use of distributed resources
  - Better coverage of available resources
- Wide spectrum of deployment scenarios – virtually generic
  - Independence of optimization algorithm and optimization problem
- None of this would have been possible without Boost

Questions ?

Questions!

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Thank you!

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