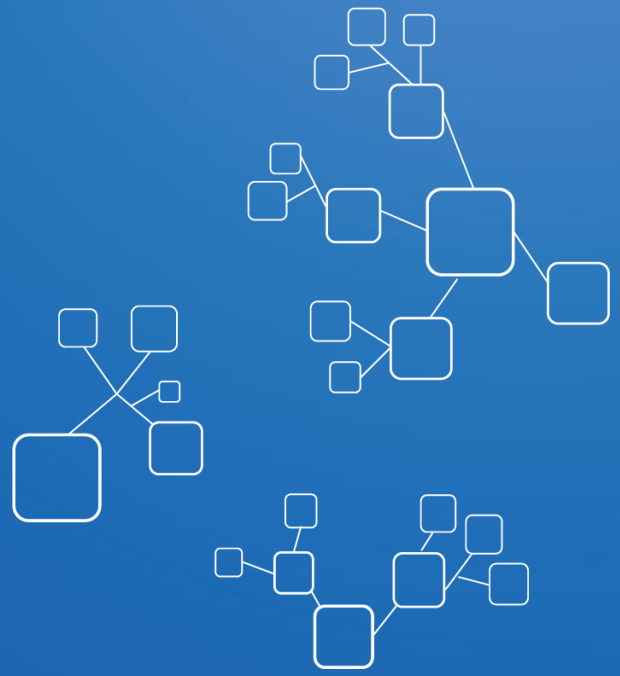
Applications of parallel optimization runs of global stochastic optimization methods

26.08.2013.

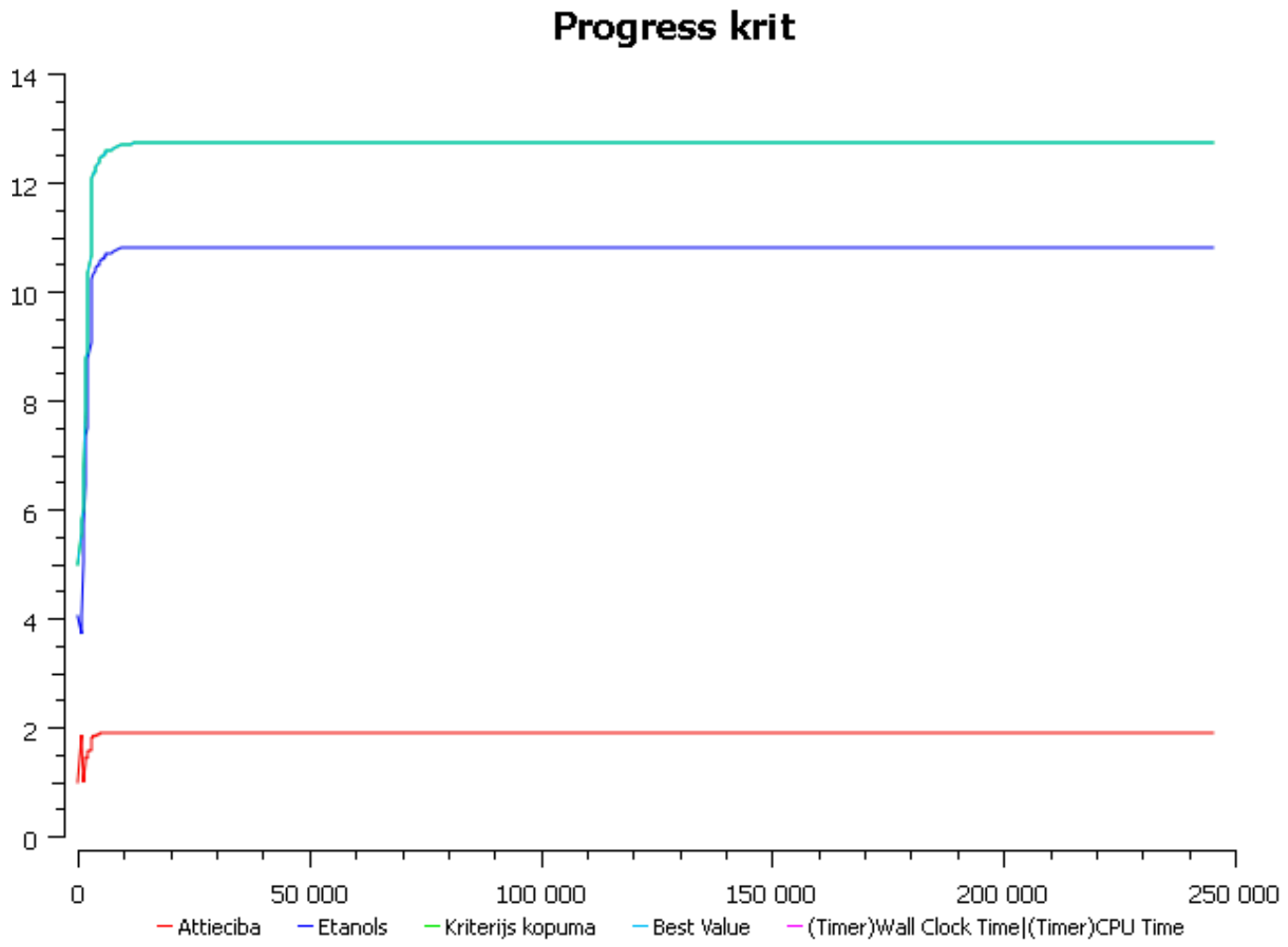


Egils Stalidzans

Biosystems group, Latvia University of Agriculture

within the project „Features of numerical methods optimizing dynamic models of biochemical networks”

When should we stop?



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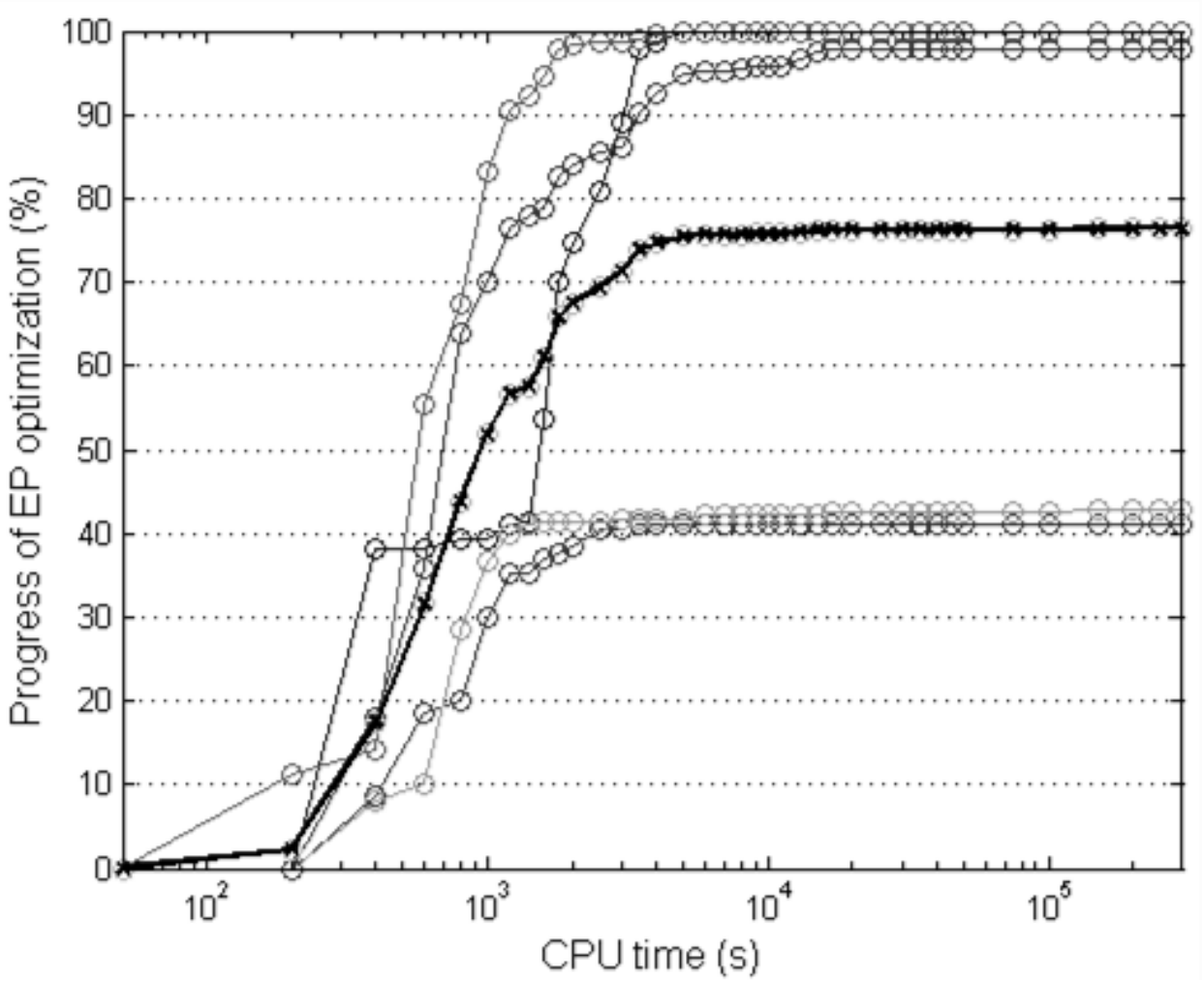
Stagnation example reaches 100%



24h = 86400s

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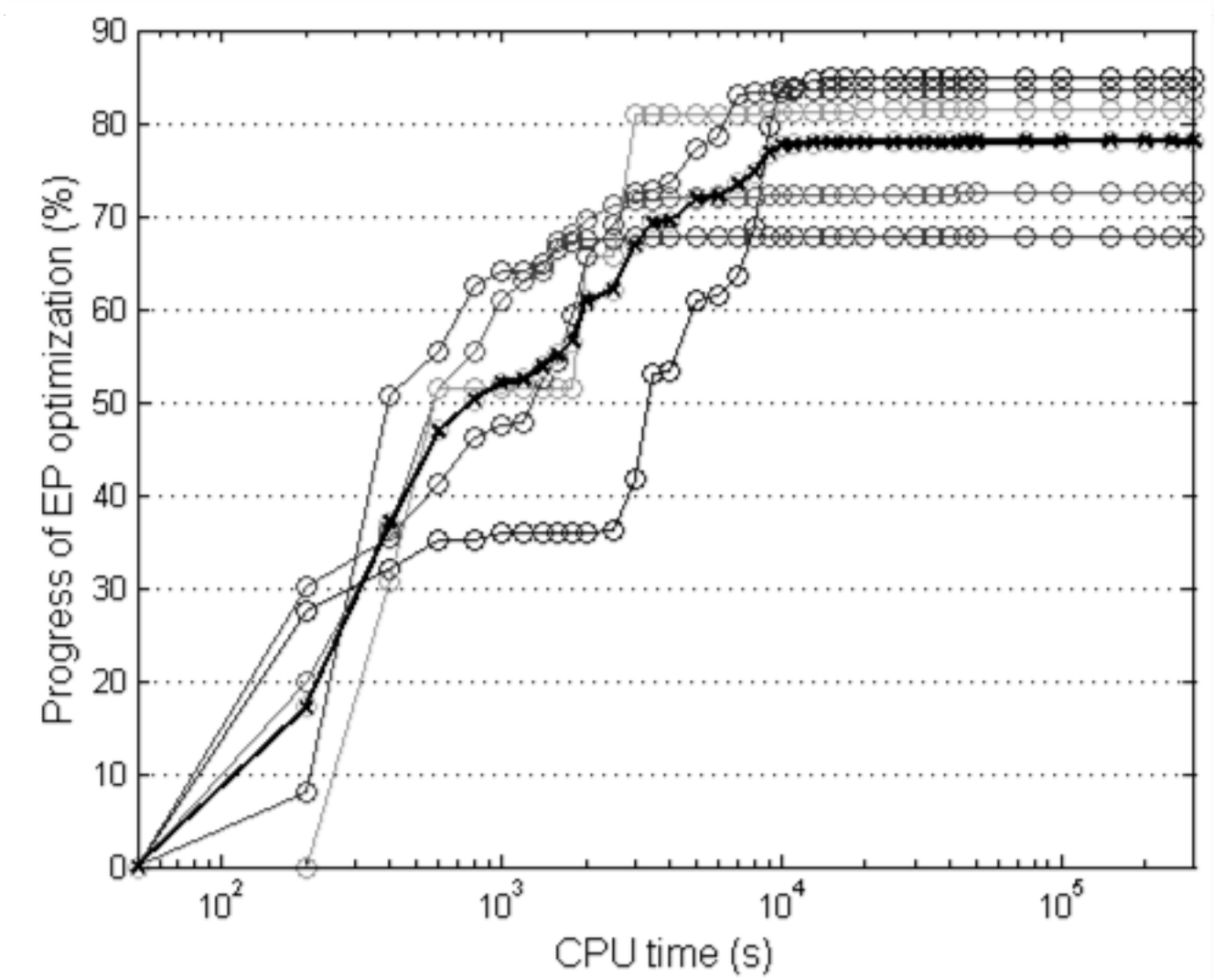
Stagnation sample does not reach 100%



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When should we terminate global stochastic optimization run?

- Reaching of global optimality is not guaranteed -> can not be sure that global optimum is reached
- Stocastic improvement of objective function value -> each run is different and statistics can be applied
- Combinatorial explosion of number of combinations of adjustable parameters (>32000 combinations of up to 15 parameters) -> automatic search and termination is necessary is necessary

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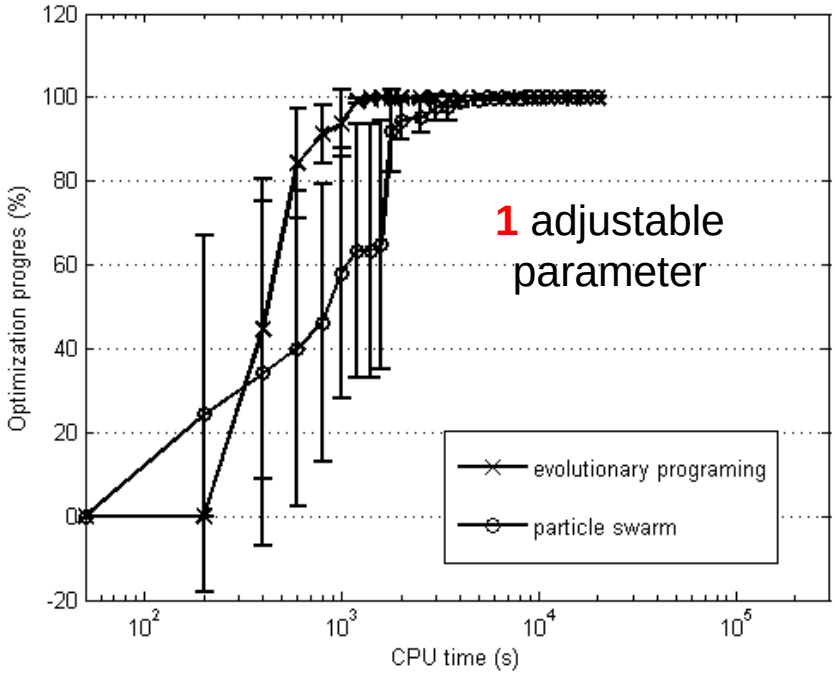
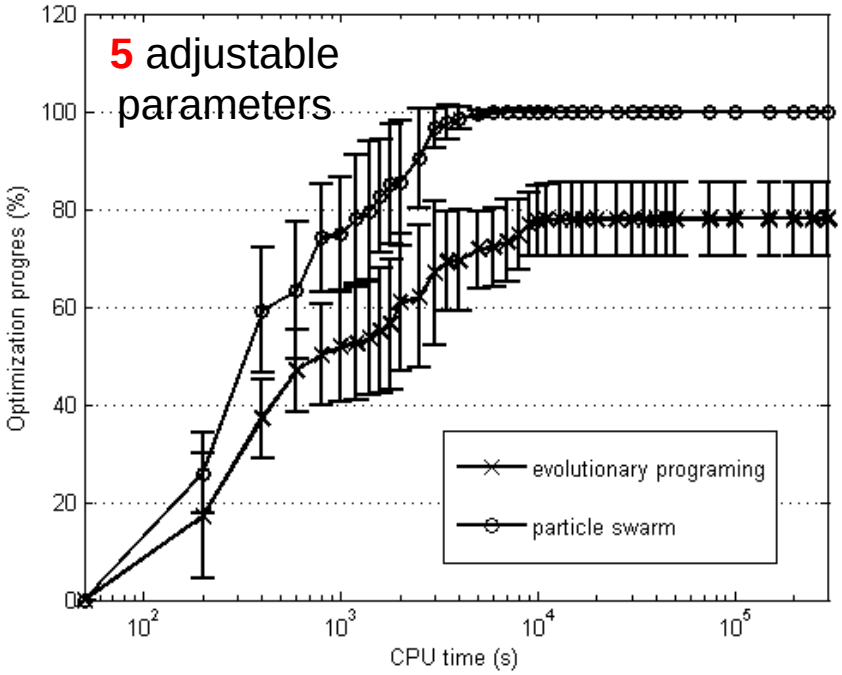
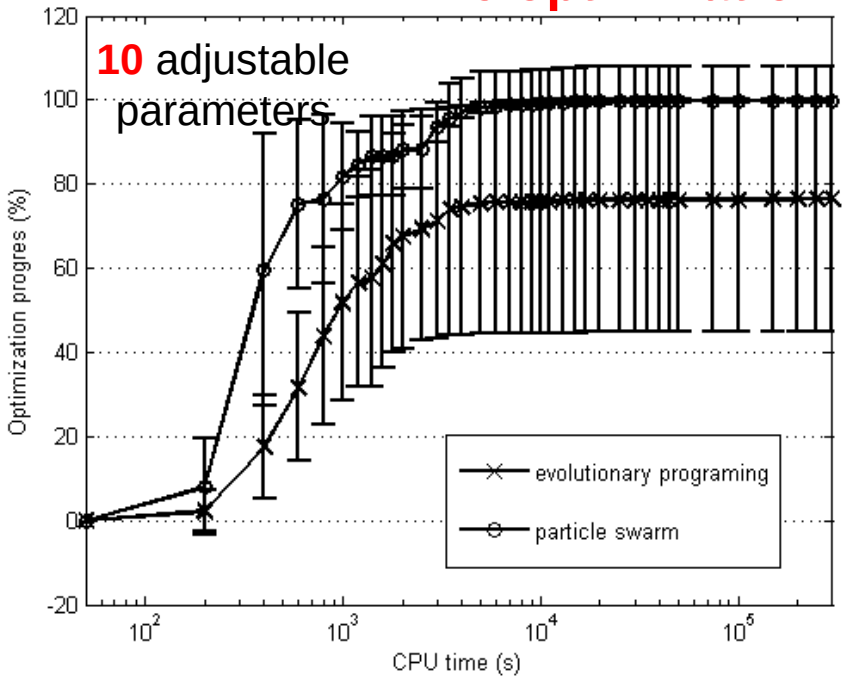
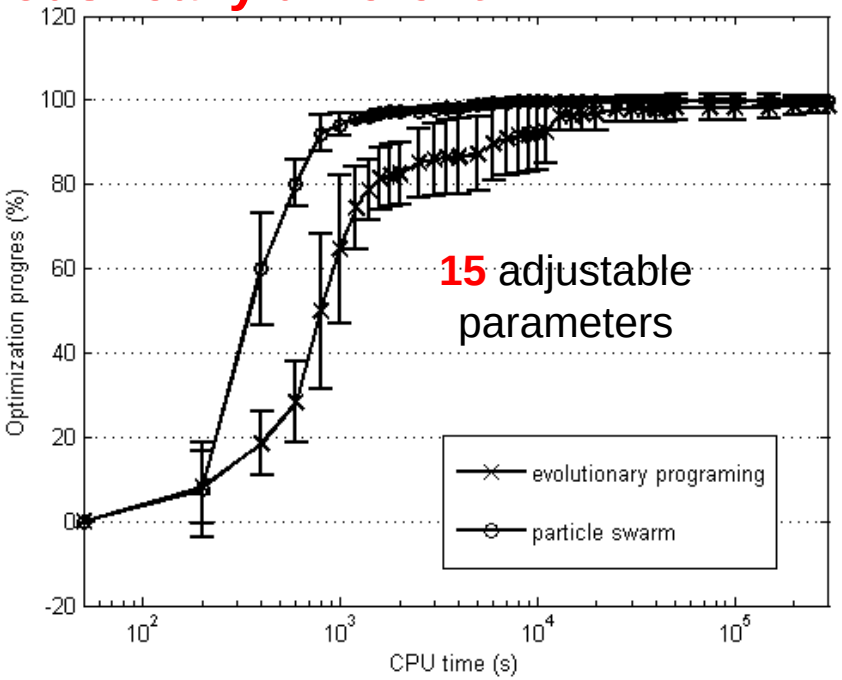




Are optimization methods really different?

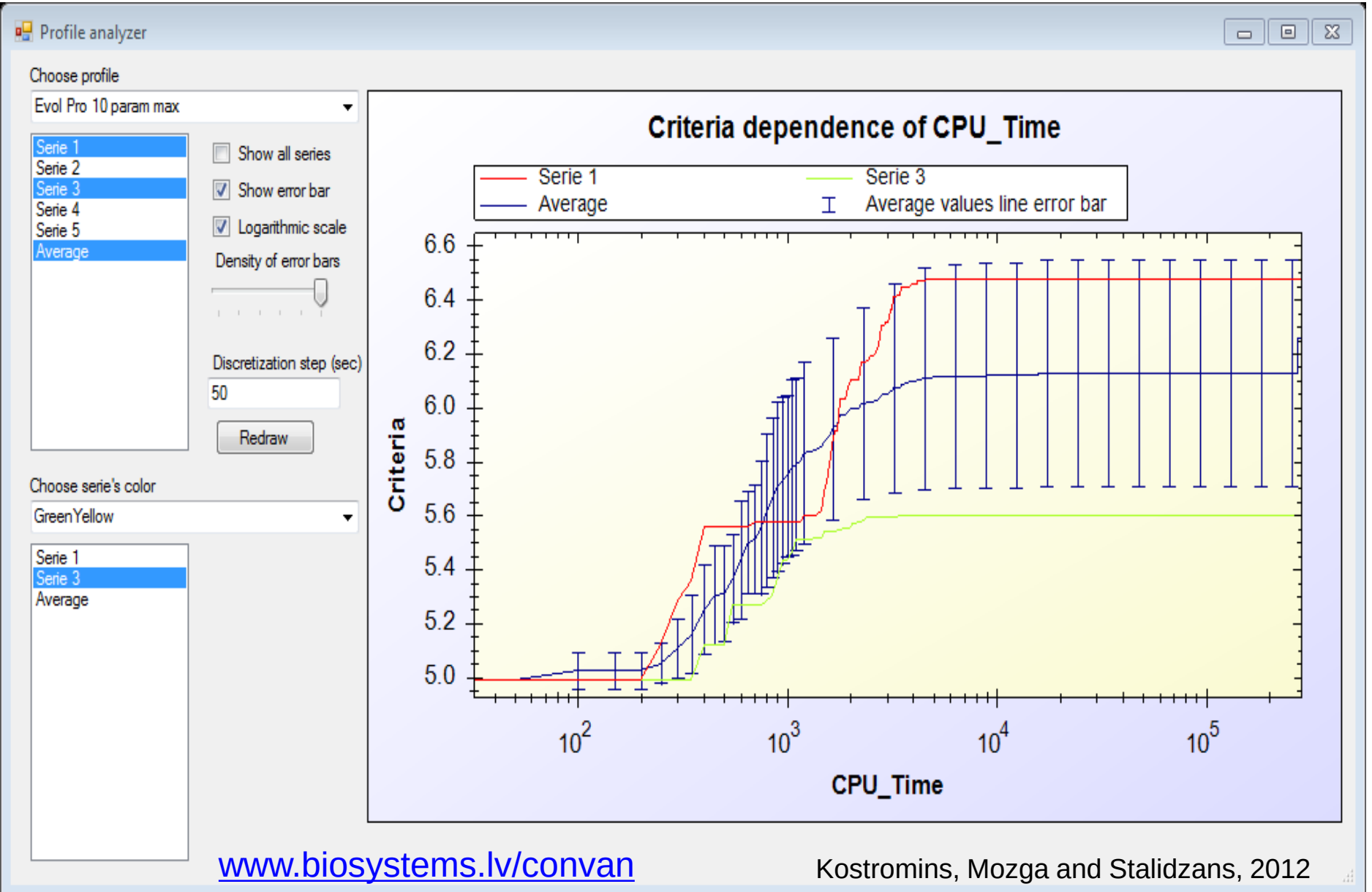




COPASI report file


```
Optimization Task

Problem Description:
Subtask:
Steady-State Task

Problem Description:
    JacobianRequested: 1
    StabilityAnalysisRequested: 1

Method: Enhanced Newton
    Resolution: 1e-009
    Derivation Factor: 0.001
    Use Newton: 1
    Use Integration: 1
    Use Back Integration: 0
    Accept Negative Concentrations: 0
    Iteration Limit: 50
    Maximum duration for forward integration: 1e+006
    Maximum duration for backward integration: 1e+006


Objective Function:
    <CN=Root,Model=Galazzo1990_FermentationPathwayKinetics,Vector=Reactions[Pyruvate kinase],Reference=Flux>

List of Optimization Items:
    0.499 <= (GAPD).Vm5 <= 499; Start Value = 4.00901
    0.317 <= (Phosphofructokinase).Vm4 <= 317; Start Value = 5.44304

Method: Particle Swarm
    Iteration Limit: 300000
    Swarm Size: 50
    Std. Deviation: 1e-006
    Random Number Generator: 1
    Seed: 0

CPU time        [Best Value]    [Function Evaluations]  [Best Parameters]       maximum real part
0.202801        -1.#INF 1       (       4.00901 5.44304 )       1.#QNAN
1.99681 35.3657 9       (       26.647  173.641 )       -0.0545744
10.0621 35.6203 52      (       28.4603 211.739 )       -0.0994227
11.7313 35.636  63      (       238.106 214.546 )       -17.023
14.3521 35.8607 84      (       49.3655 262.869 )       -1.3477
18.0025 36.0415 102     (       187.752 317     )       -15.5993
24.0086 36.0415 161     (       314.255 317     )       -23.0608
24.8354 36.0415 189     (       398.123 317     )       -20.536
25.0538 36.0415 202     (       385.544 317     )       -20.8494
```

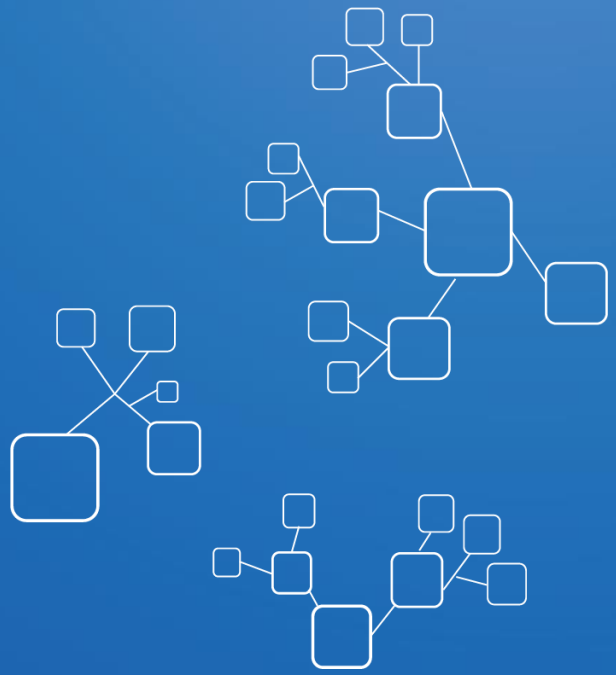
Application of ConvAn for analysis of convergence speed of design task using COPASI report



www.biosystems.lv/convan

Kostromins, Mozga and Stalidzans, 2012

THANK YOU!



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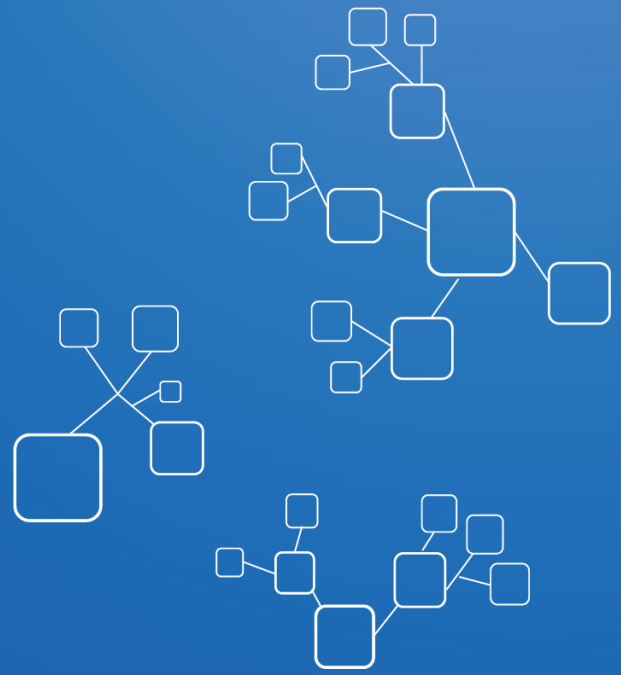
CRITERIA FOR AUTOMATIC TERMINATION OF PARALLEL OPTIMISATION RUNS

26.08.2013.



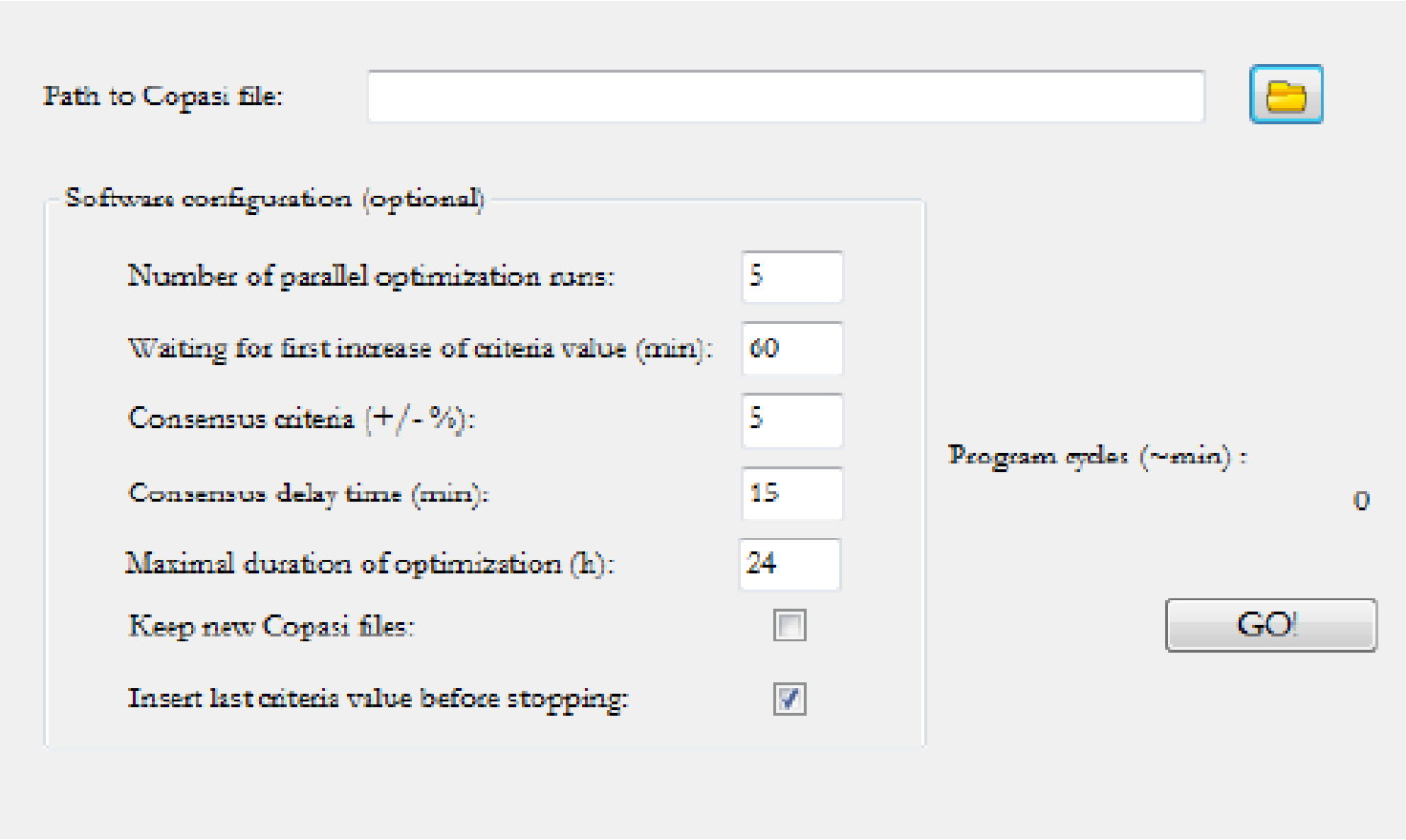
NATALJA BULIPOPA

BIOSYSTEMS GROUP, LATVIA UNIVERSITY OF AGRICULTURE

Baltisch-Deutsches HochschulKontor

within the project „Features of numerical methods optimizing dynamic models of biochemical networks”

CoRunner – parallel optimization run manager for COPASI



www.biosystems.lv/corunner

Sulins and Stalidzans, 2012

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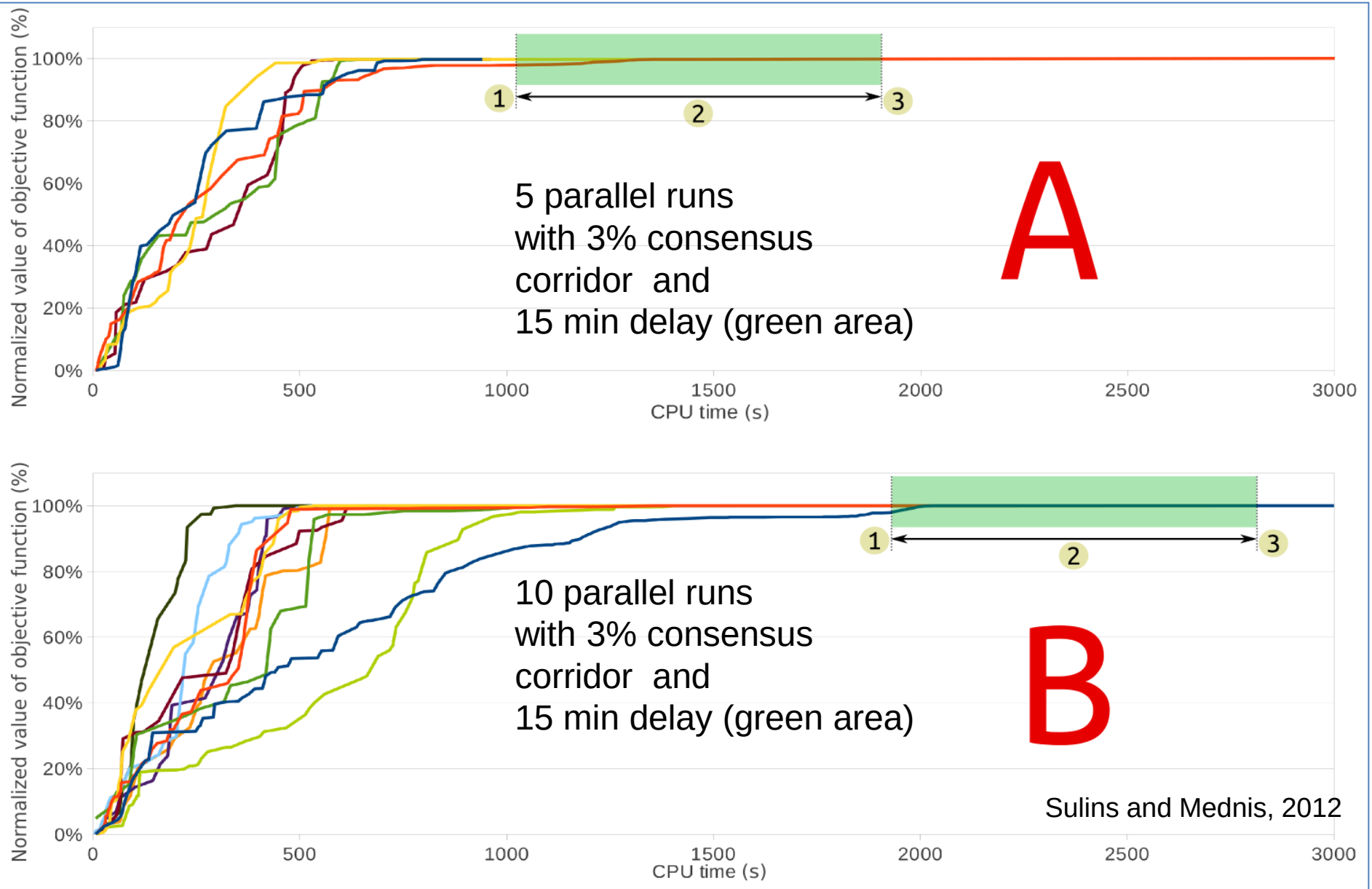
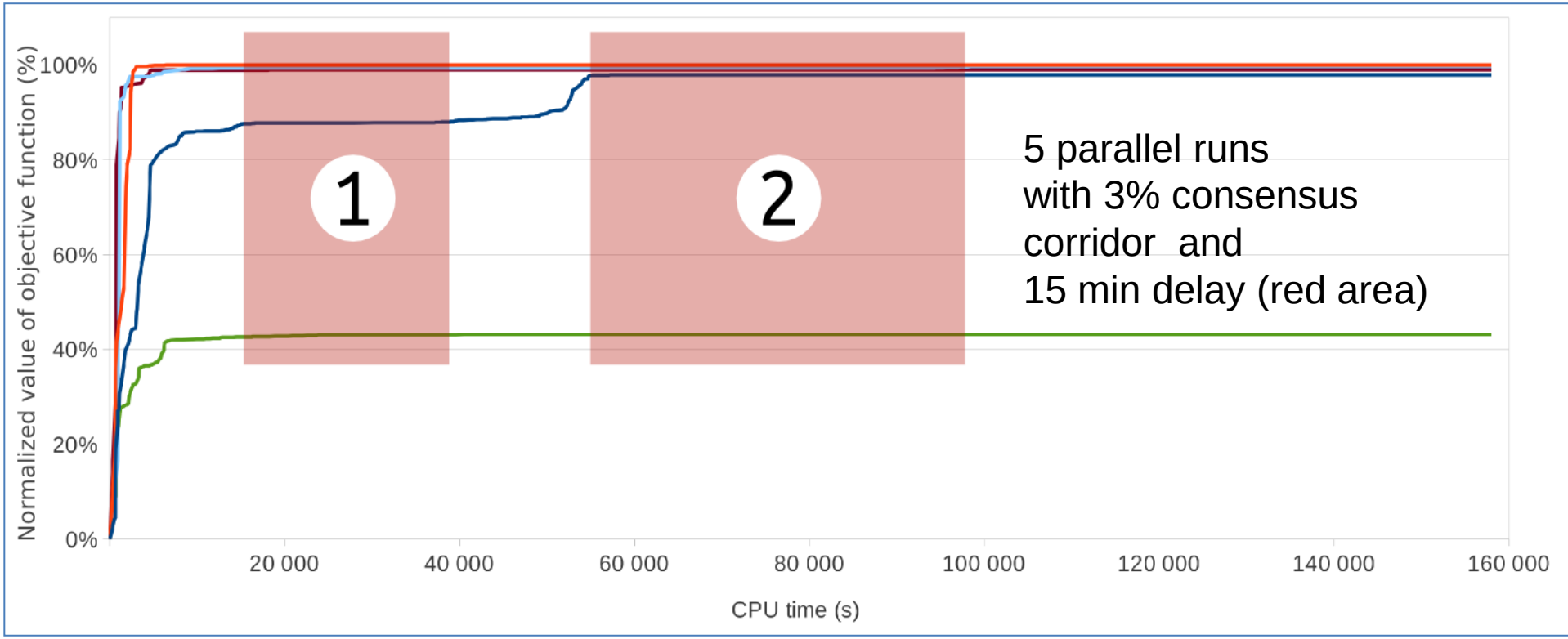
Consensus case (CoRunner)



Stagnation case (CoRunner)



Sulins and Mednis, 2012

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Automatic termination criteria

- Automatic termination criteria in case of consensus or stagnation of parallel optimization runs have been proposed as criteria for automatic termination.

- It is proposed to modify automatic optimization termination criteria of parallel optimization runs applying upper limit agreement of a number of parallel optimization runs.

Automatic termination criteria

- Automatic application of upper limit agreement would reduce the duration of scanning of the whole space of combination of adjustable parameters.

- This approach is tested on the yeast glycolysis model (Galazzo and Bailey, 1990) with six adjustable parameters using COPASI, CoRunner and ConvAn software for five parallel optimization runs per combination of adjustable parameters.

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Optimization task

- Set according to the *in silico* optimization experiments of ethanol production performed by Rodriguez-Acosta on the same model;
- Concentrations of six enzymes catalyzing reactions *ATPase*, *GAPD*, *Glucose in* (Glu), *Hexokinase* (HK), *Phosphofructokinase* (PFK) and *Pyruvate kinase* (PK) are chosen as adjustable parameters.
- 63 combinations of six adjustable parameters (up to six out of six) are optimized.
- The range of changes of adjustable parameters is set within range from -99% to +900% (from 100-fold decrease to 10-fold increase) from their initial values.
- Maximization of the flow through reaction Pyruvate kinase (PK) (proportional to the ethanol production) is set as the objective function.

Upper level agreement criterion

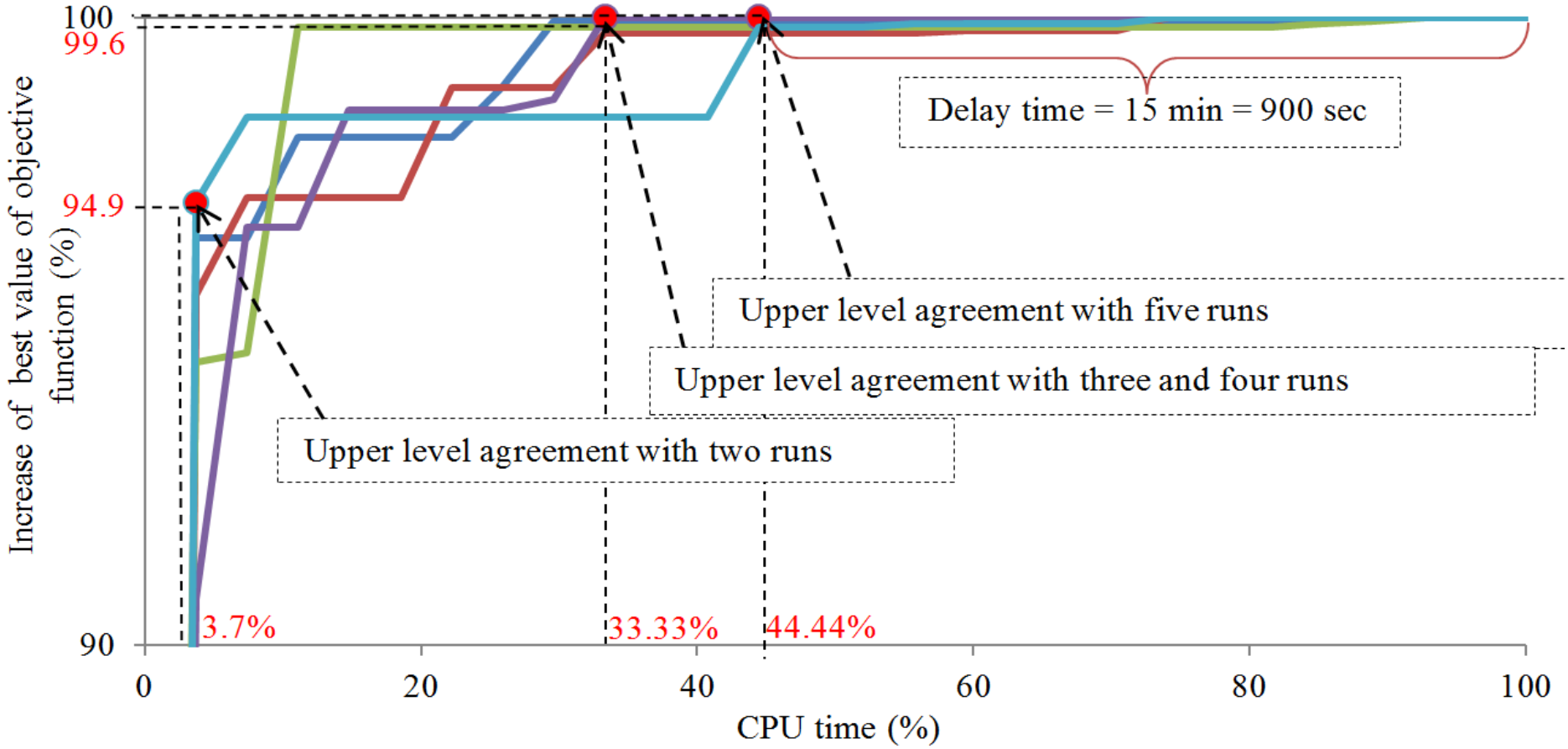

Fig. 1. Determination of upper level agreement for two and more parallel optimization runs and corresponding losses of best value and savings of computational time. 0% and 100% of increase of objective function best value correspond to the value of model before optimization and after delay time of consensus correspondingly. 100% of optimization time correspond to 1620 seconds.

Bulipopa and Sulins, 2013

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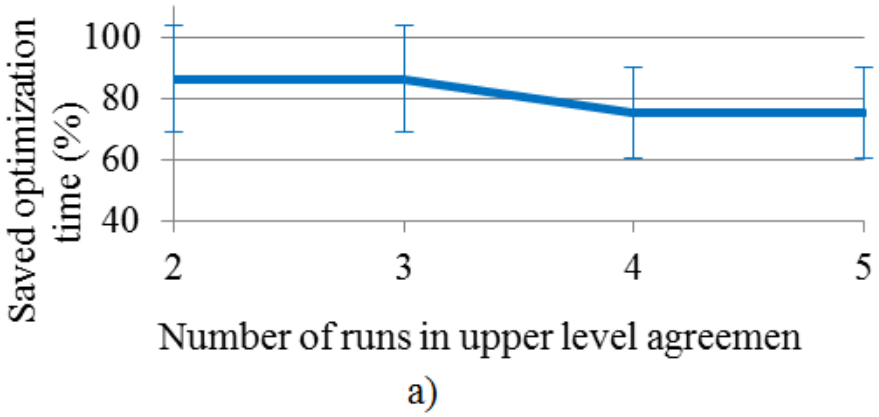
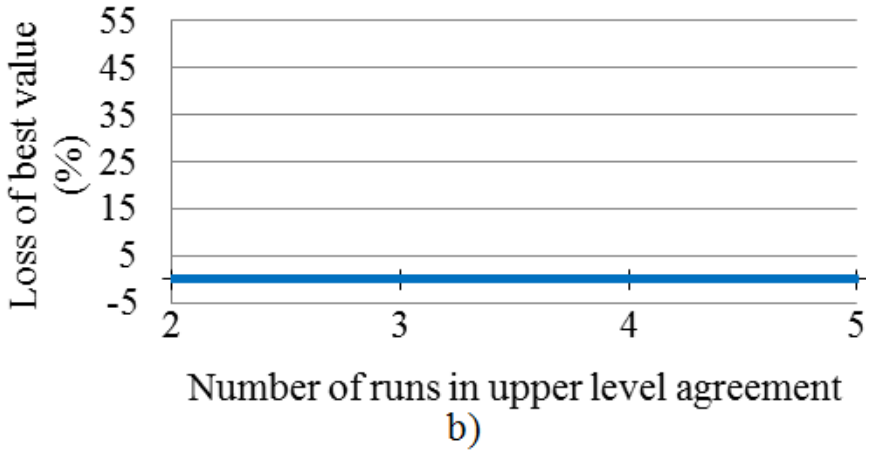
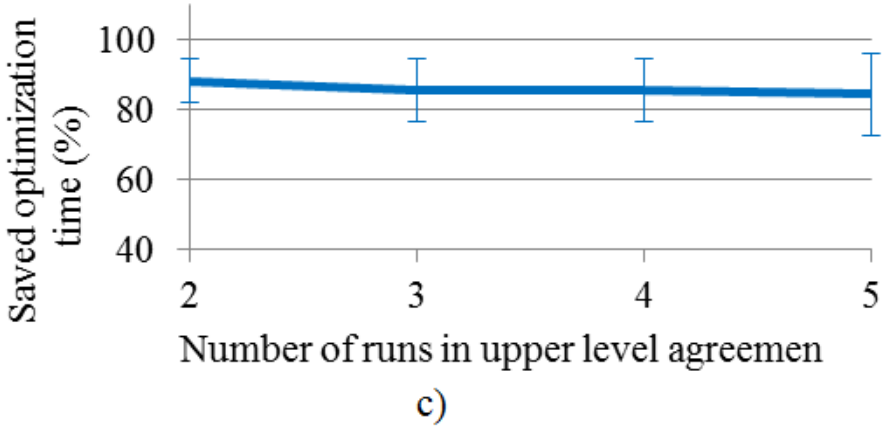
Gains and losses







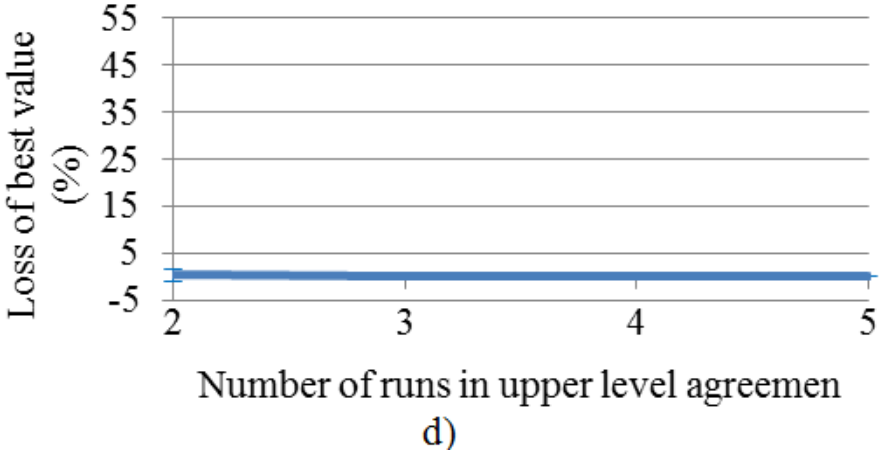


Fig. 2. Reduction of objective function value and on the increase of optimization time for one (a and b) and two (c and d). Error bars demonstrate the standard deviation at n=6 for one, n=15 for two, n=20 for three, n=15 for four and n=6 for five parameters.

Bulipopa and Sulins, 2013

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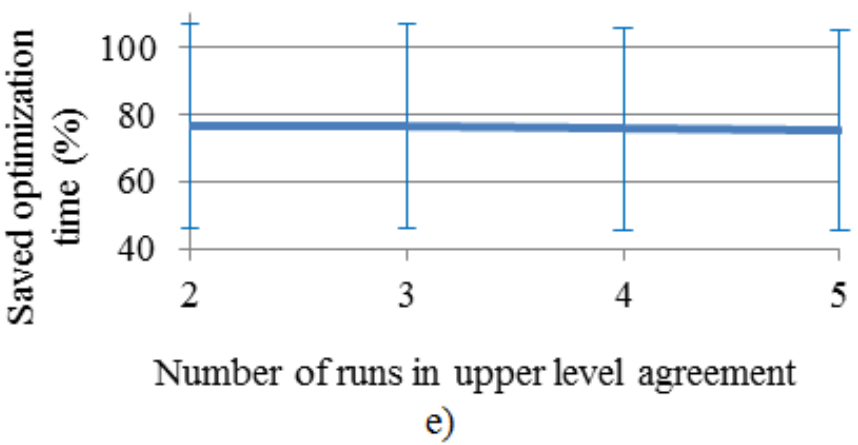
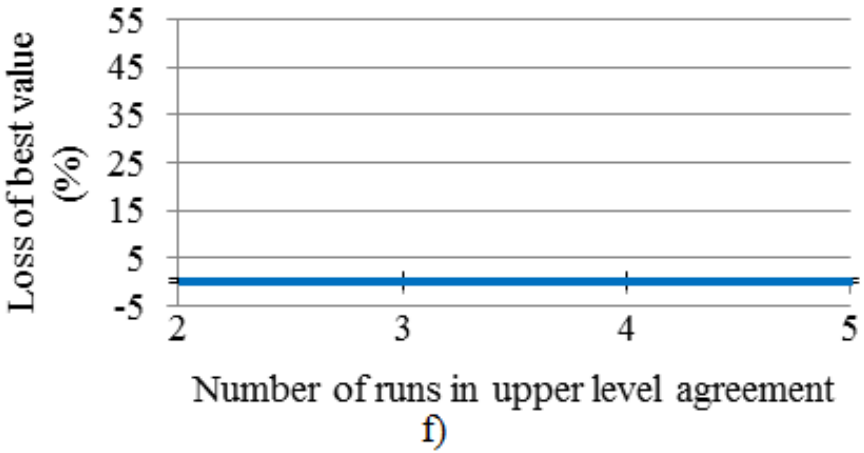
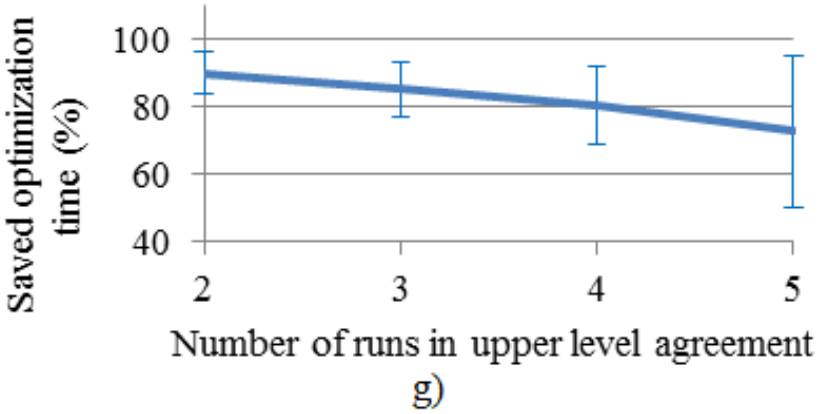
Gains and losses







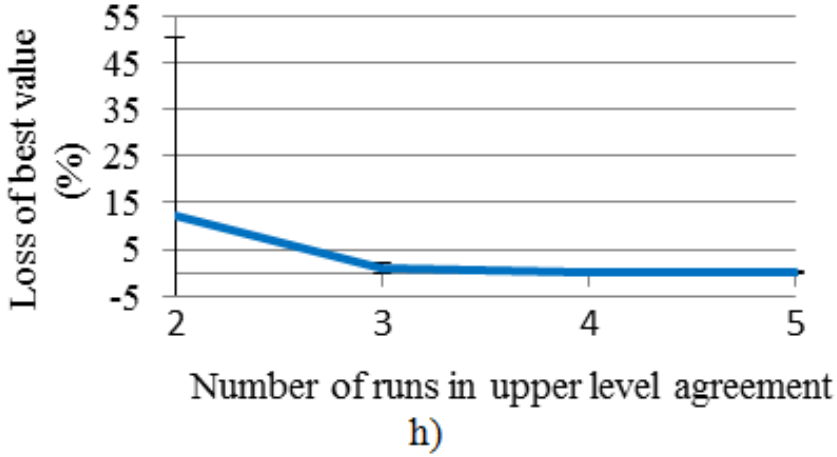


Fig. 3. Reduction of objective function value and on the increase of optimization time for three (e and f) and four (g and h) parameters correspondingly. Error bars demonstrate the standard deviation at n=6 for one, n=15 for two, n=20 for three, n=15 for four and n=6 for five parameters.

Bulipopa and Sulins, 2013

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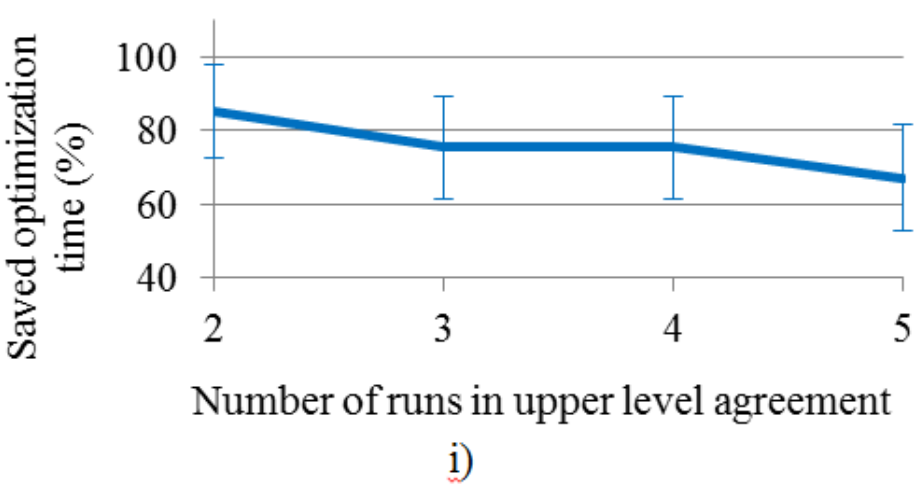
Gains and losses



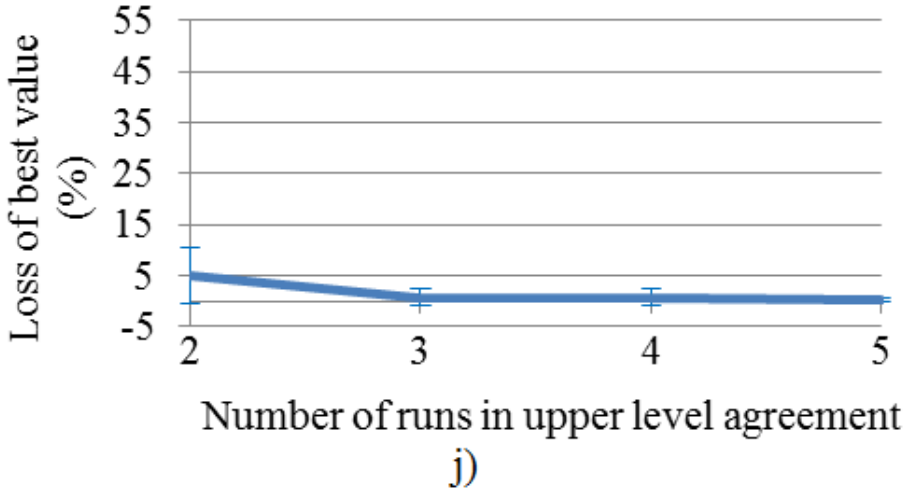


Fig. 4. Reduction of objective function value and on the increase of optimization time for five (i and j) parameters correspondingly. Error bars demonstrate the standard deviation at n=6 for one, n=15 for two, n=20 for three, n=15 for four and n=6 for five parameters.

Bulipopa and Sulins, 2013

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Conclusions

- Significant time can be saved in case of approximate estimation of the best value of objective function for a particular combination of adjustable parameters using upper limit agreement criterion.
- Consensus of all parallel runs generally is a special case of upper level agreement criterion when all the parallel runs come to upper level agreement.
- Computational experiments demonstrate that upper level agreement of at least three parallel optimization runs reduces the necessary optimization time by 60-90% and reduces the best value of objective function just by up to 1% compared to consensus within 1% of five parallel runs with delay time of 15 minutes. More extensive experiments would be needed to generalize this statement.
- The optimization termination algorithm can be executed automatically.

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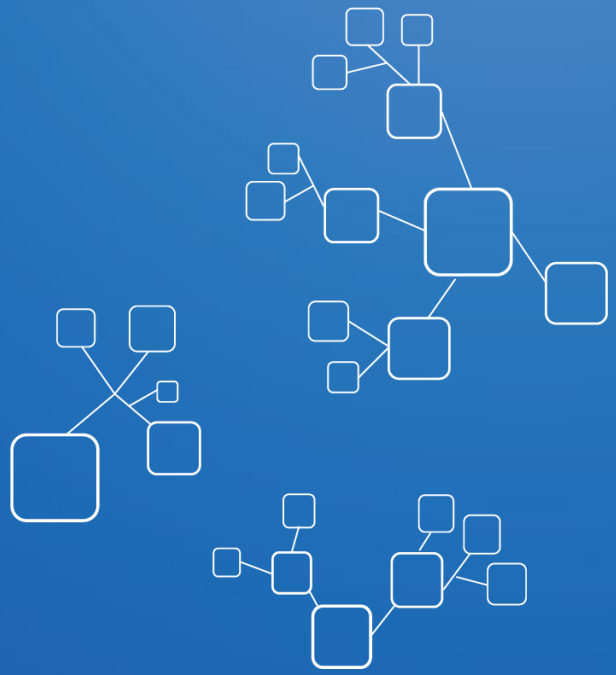
THANK YOU!



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