

Performance of optimisation depending on the size of a model

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LUA

About

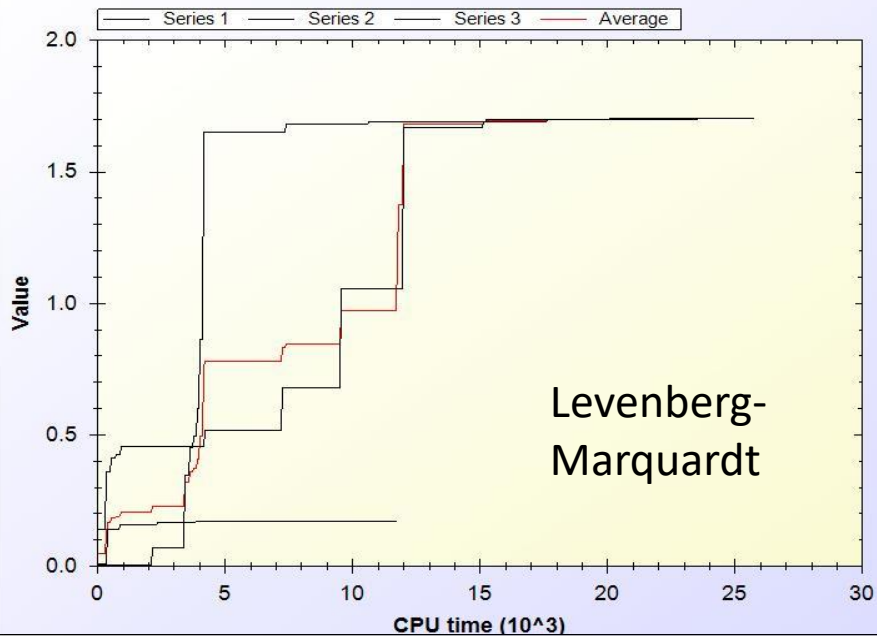
- Hynne model of yeast glycolysis
 - 24 reactions
- Rohwer model of Sucrose accumulation
 - 11 reactions
- 5 parallel runs per optimisation method
- Termination criteria
- Number of Generations 30'000 where applicable

- 4 levels of constraints
 - ✓ Level 1 - no additional constraints
 - ✓ Level 2 - amino acid constraint
 - ✓ Level 3 - metabolite concentration corridor constraint
 - ✓ Level 4 – combined level 2 and level 3 constraints

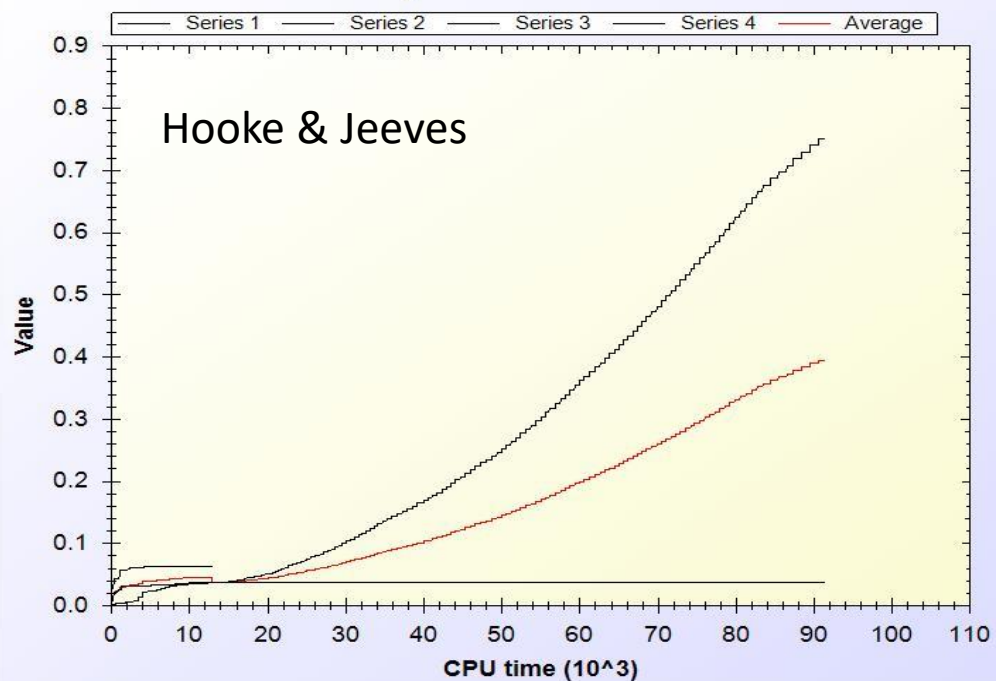
Level 1

- Used all available optimisation methods
- Local methods were unable to reach consensus or feasible results in glycolysis model:
 - Hooke & Jeeves
 - Levenberg-Marquardt
 - Nelder-Mead
 - Praxis
 - Truncated Newton
 - Steepest Descent

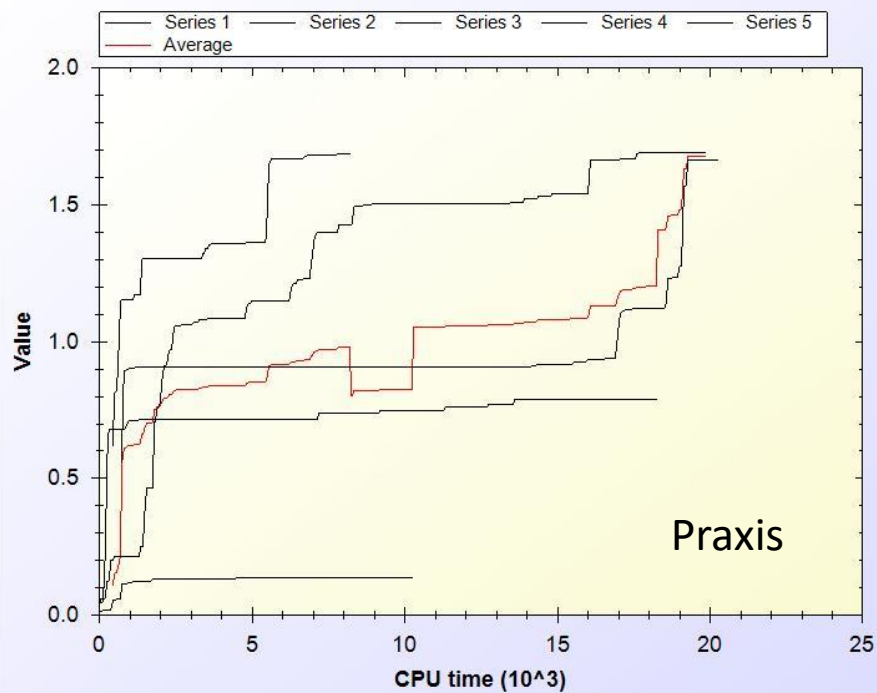
Value dependence on CPU time



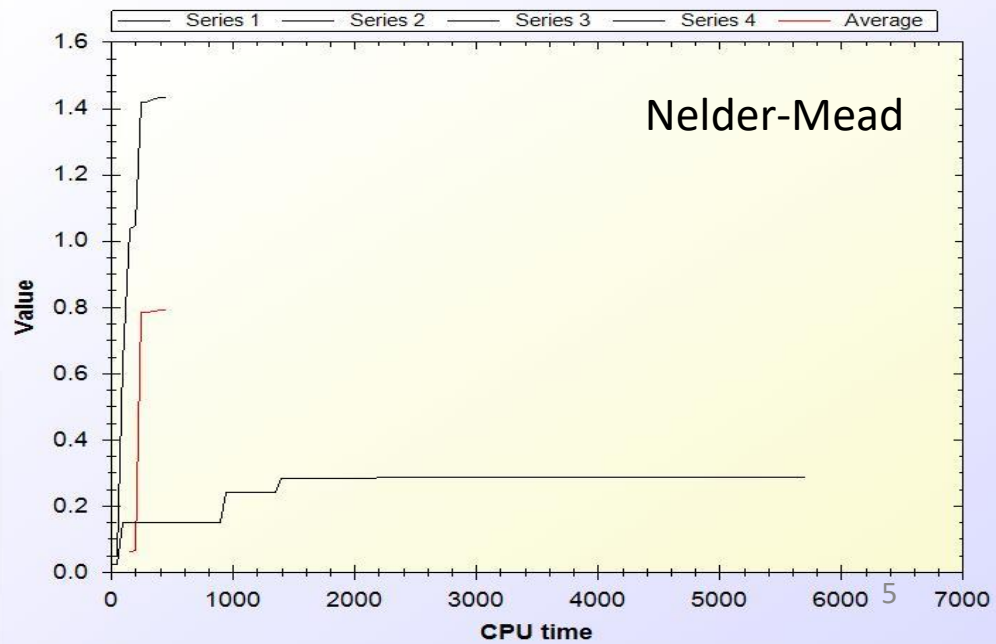
Value dependence on CPU time



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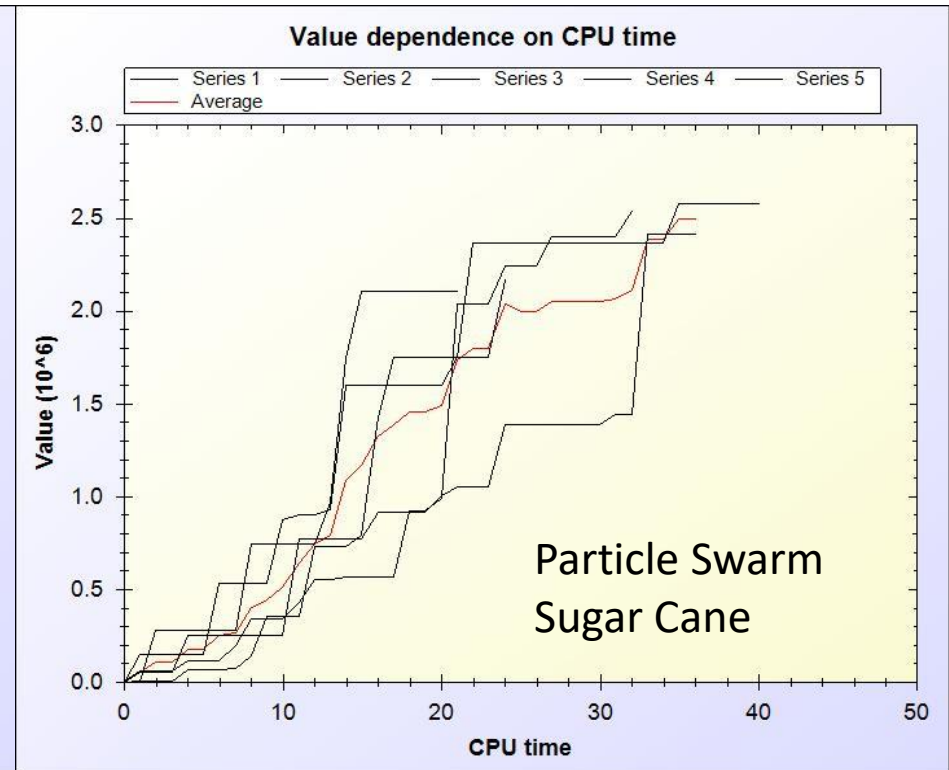
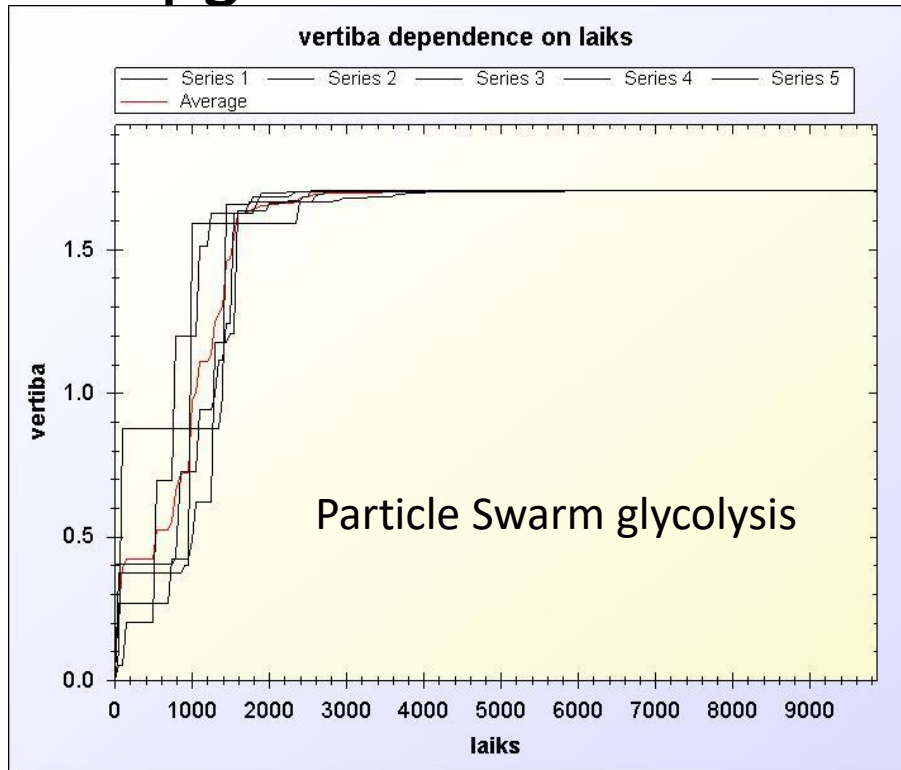


Value dependence on CPU time



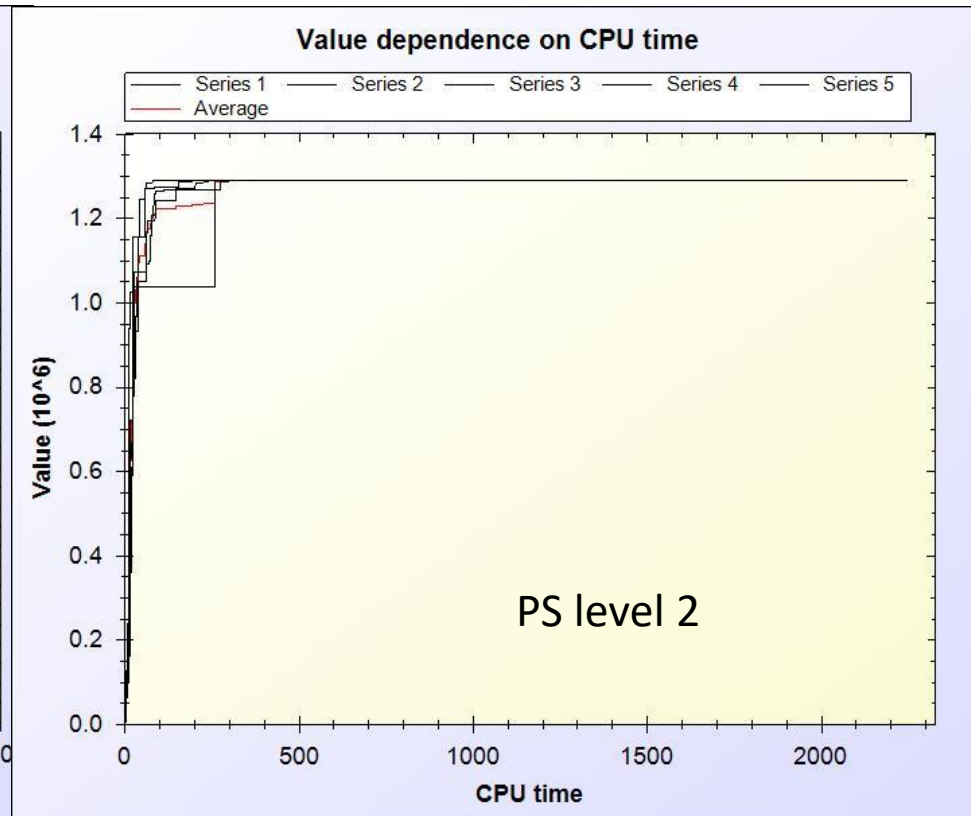
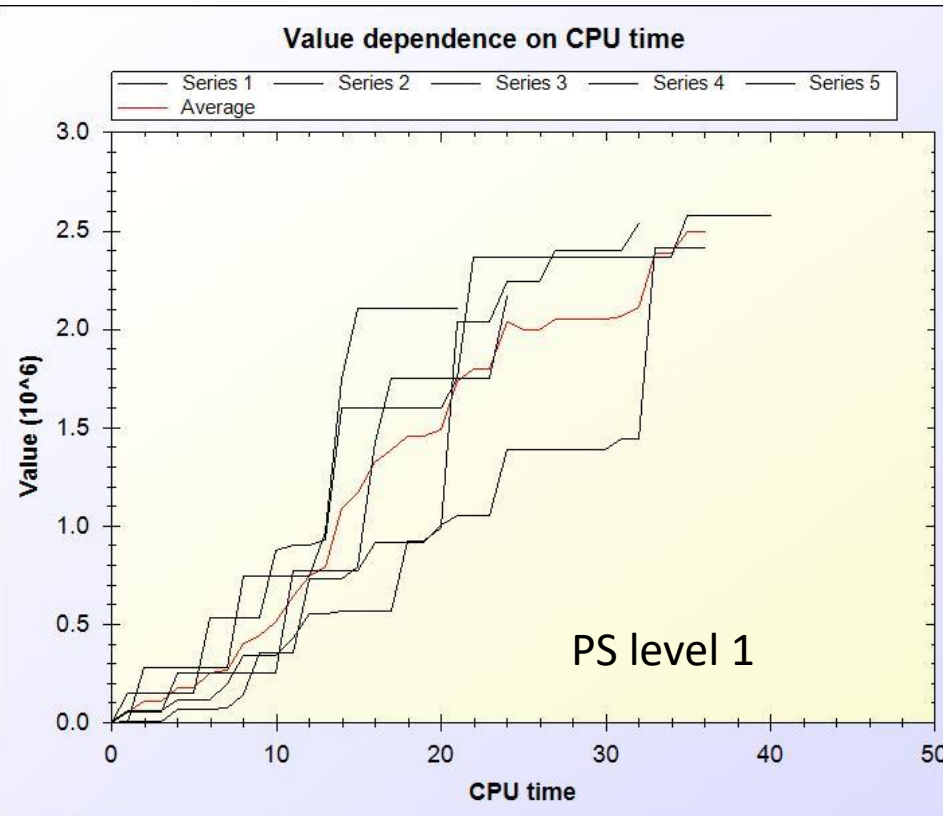
Level 1

- Unlike glycolysis model, sucrose model run values don't reach consensus with GASR and PS



Level 1

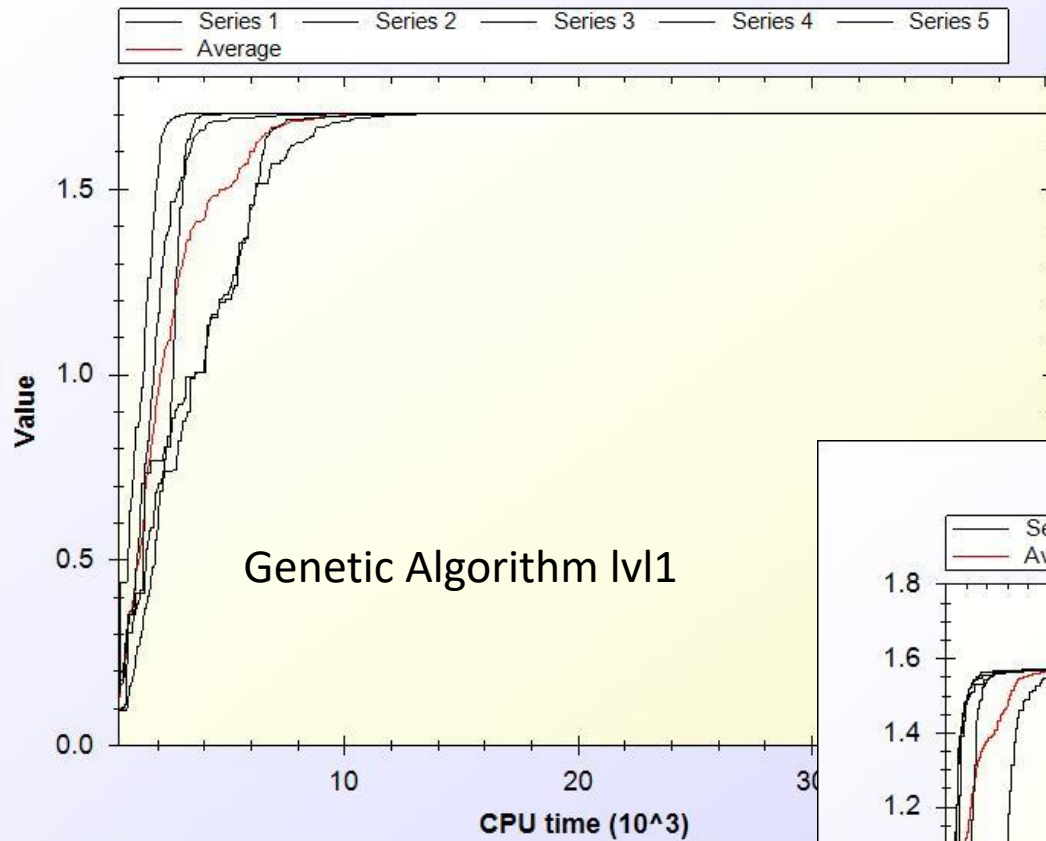
- In sucrose model, PS seems to be working better with level 2, than level 1 constraints



Level 2 - amino acid constraint

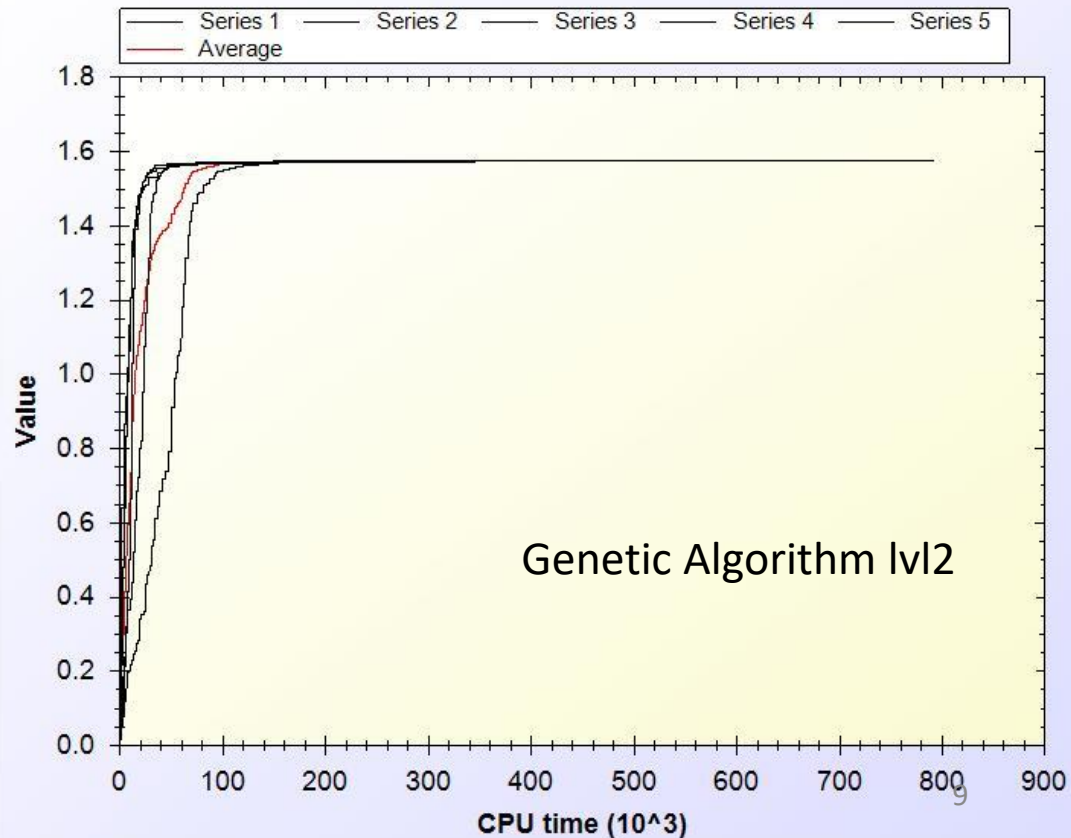
- Use only global methods (lack of results using local methods)
- Only Genetic Algorithm and Particle Swarm reach consensus in glycolysis model
- GA, EP,PS and SRES reach consensus in succrose model
- It takes noticeably more time to reach consensus with constraint than without

Value dependence on CPU time



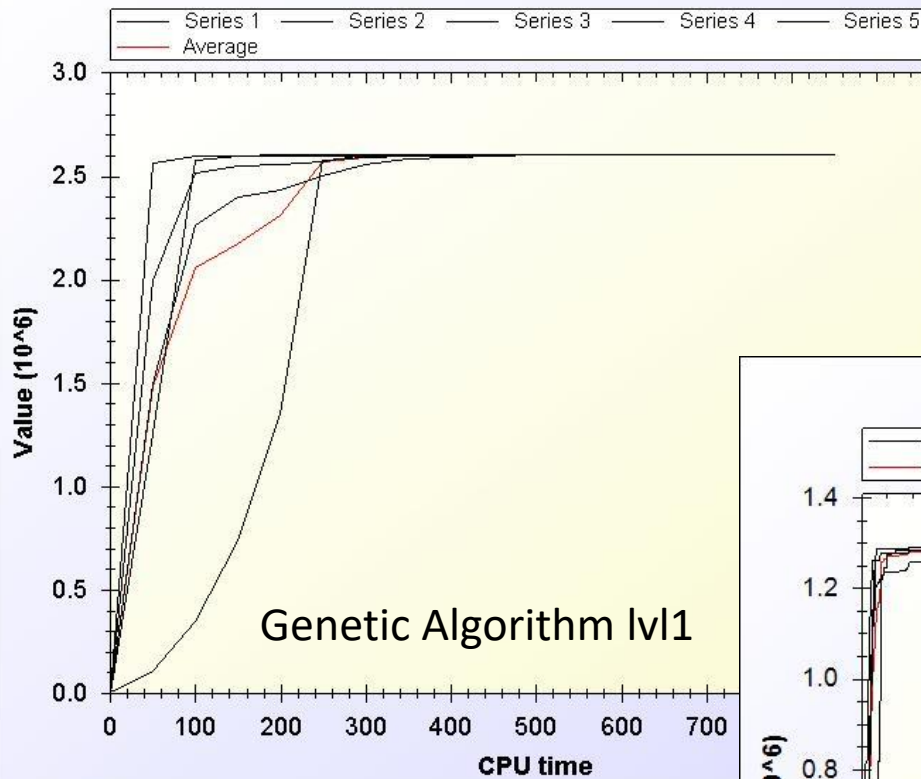
- Optimisation takes approx. 10 times more time to reach consensus with constraint, than without (in case of GA, glycolysis)

Value dependence on CPU time



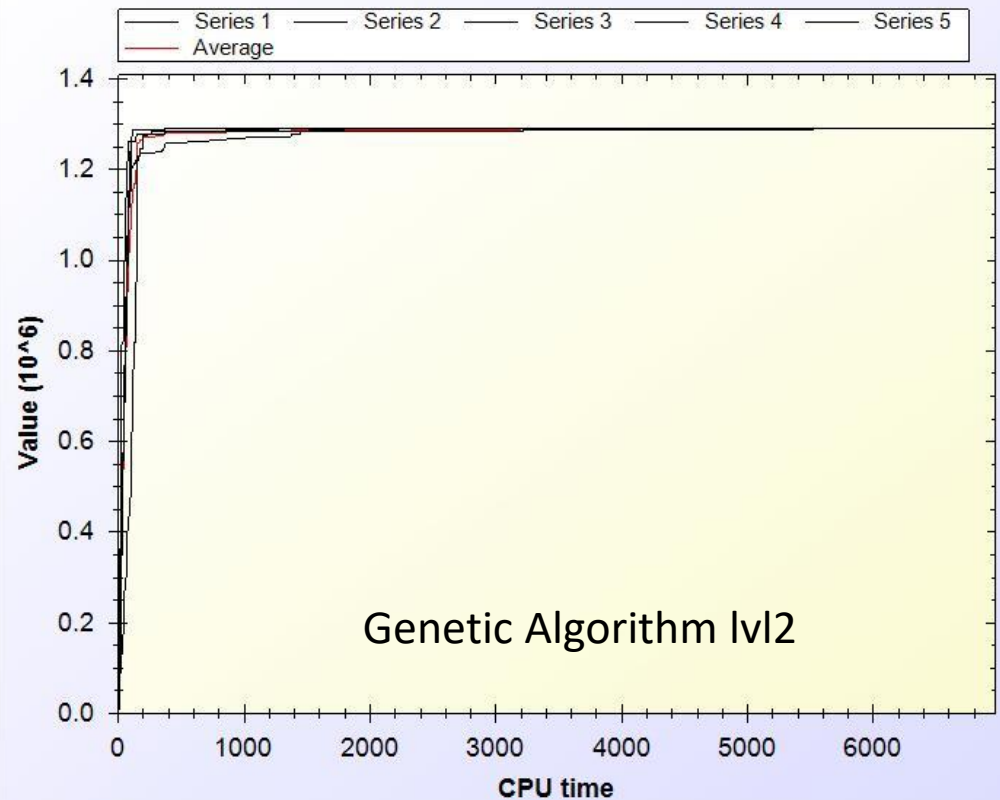
That is not always the case in sucrose model, however, the increase in time consumption can be less than 10 times

Value dependence on CPU time



Genetic Algorithm lvl1

Value dependence on CPU time

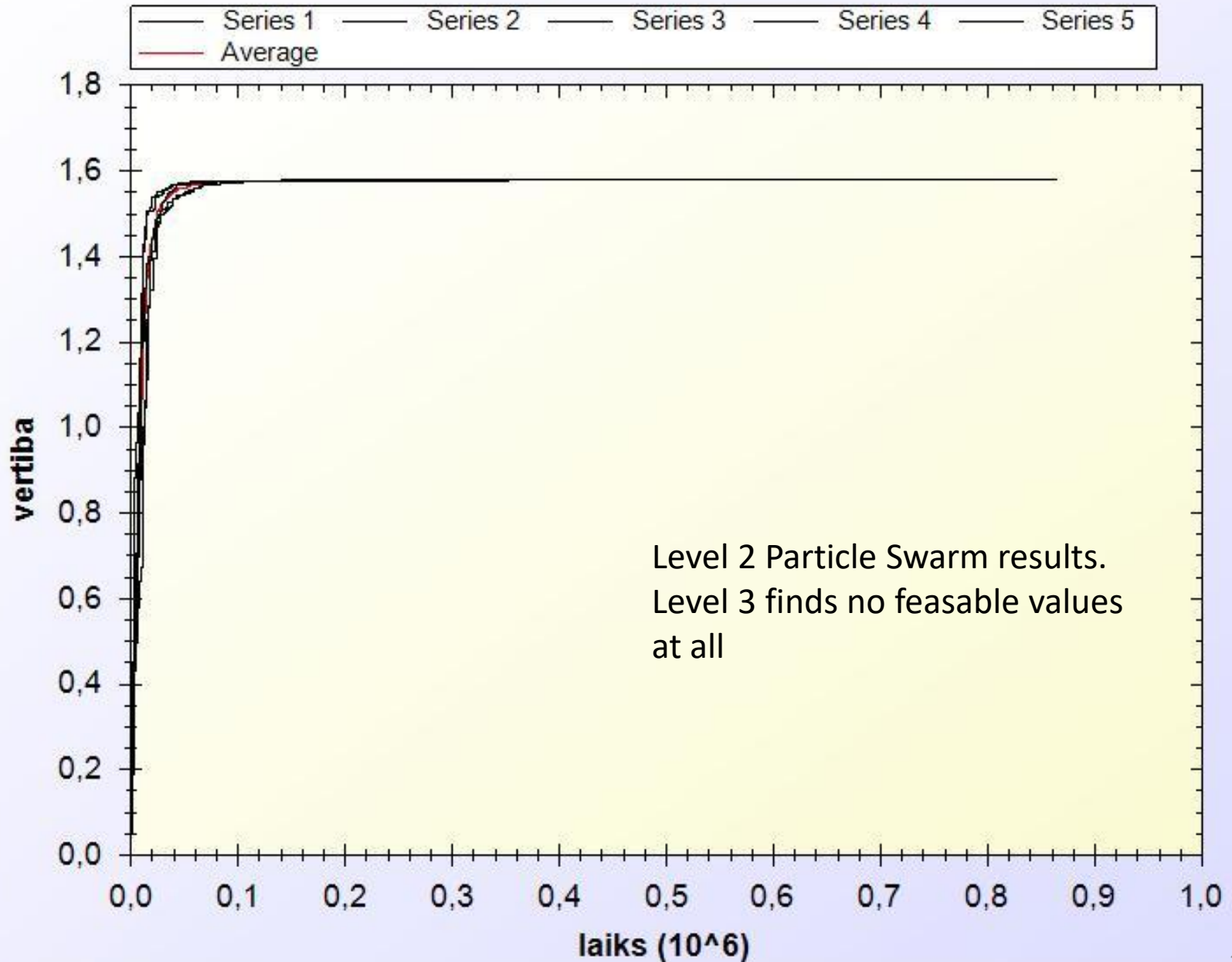


Genetic Algorithm lvl2

Level 3 - metabolite concentration corridor constraint

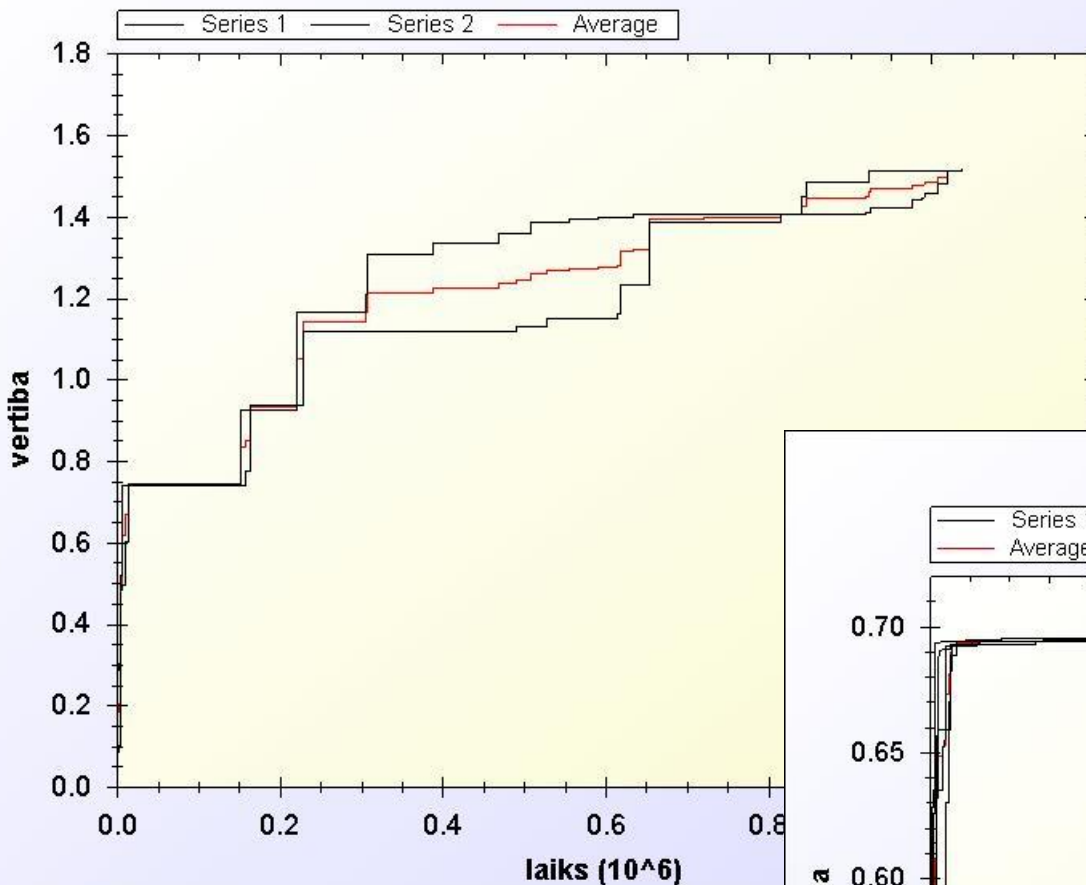
- No result given by Particle Swarm, Random Search and Evolutionary Programming
- Simulated Annealing returns surprisingly good results

vertiba dependence on laiks



Level 2 Particle Swarm results.
Level 3 finds no feasible values
at all

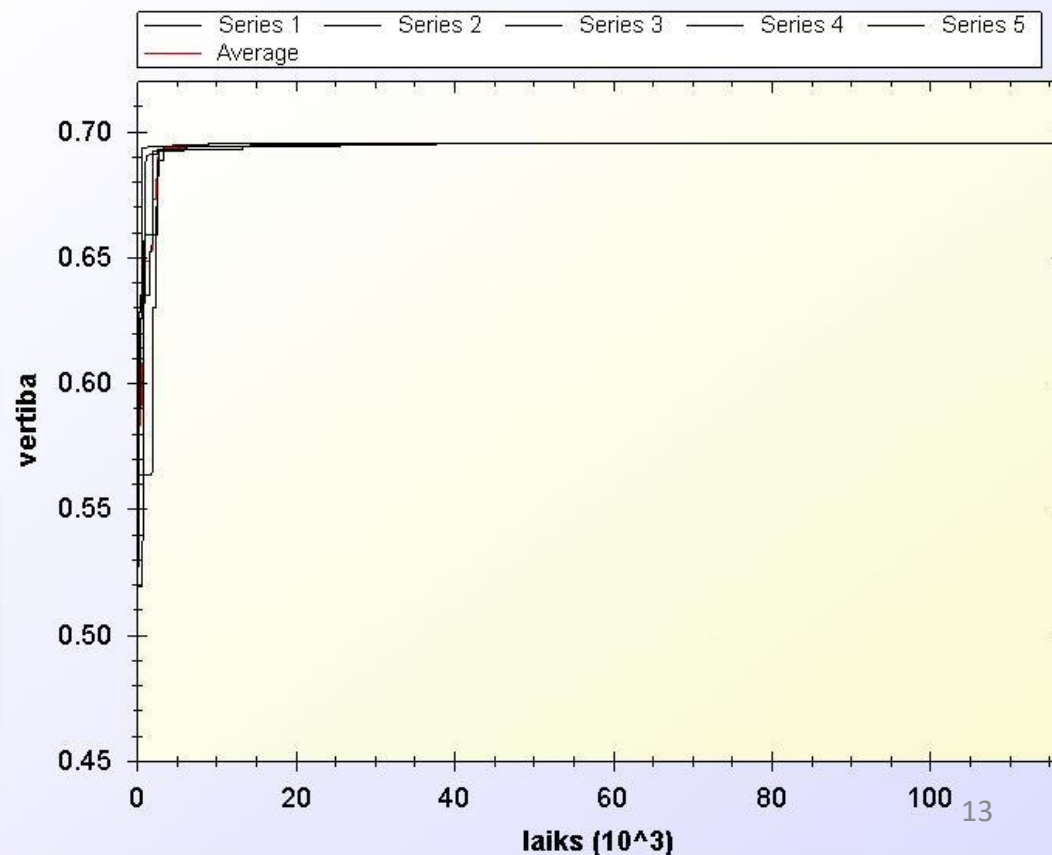
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- Simulated Annealing works several times better and faster with metabolite constraints, than with amino acid one

- All 5 runs behave similarly, thus making result more reliable

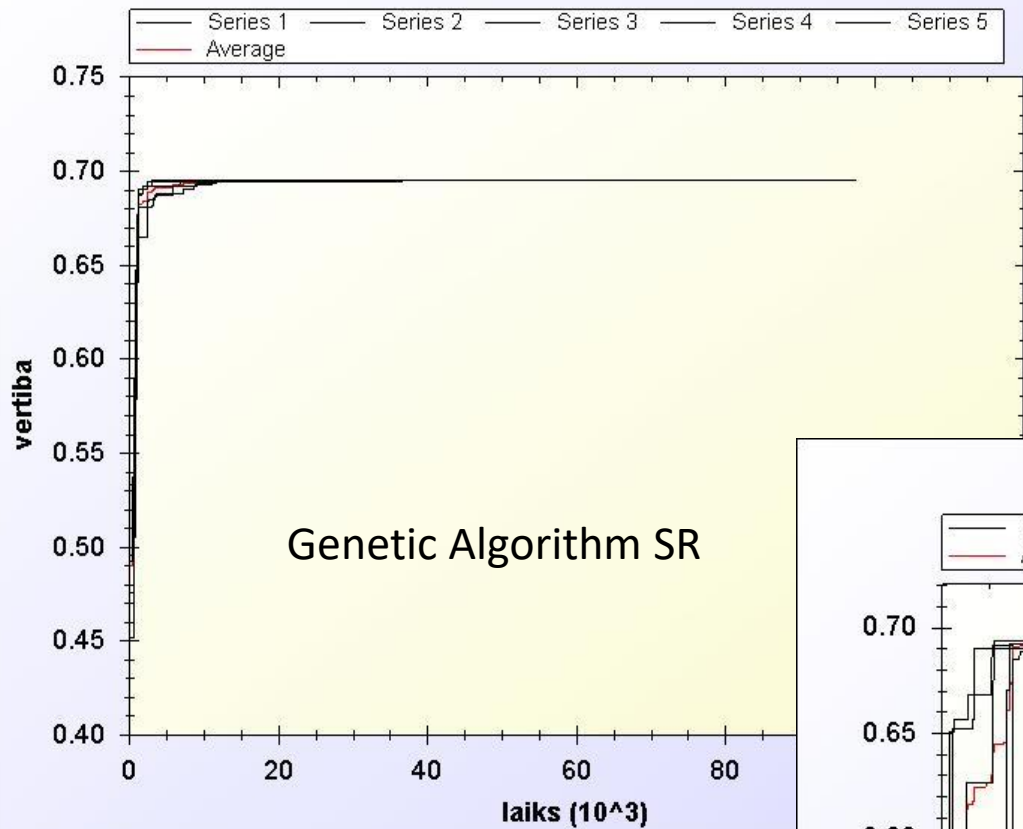
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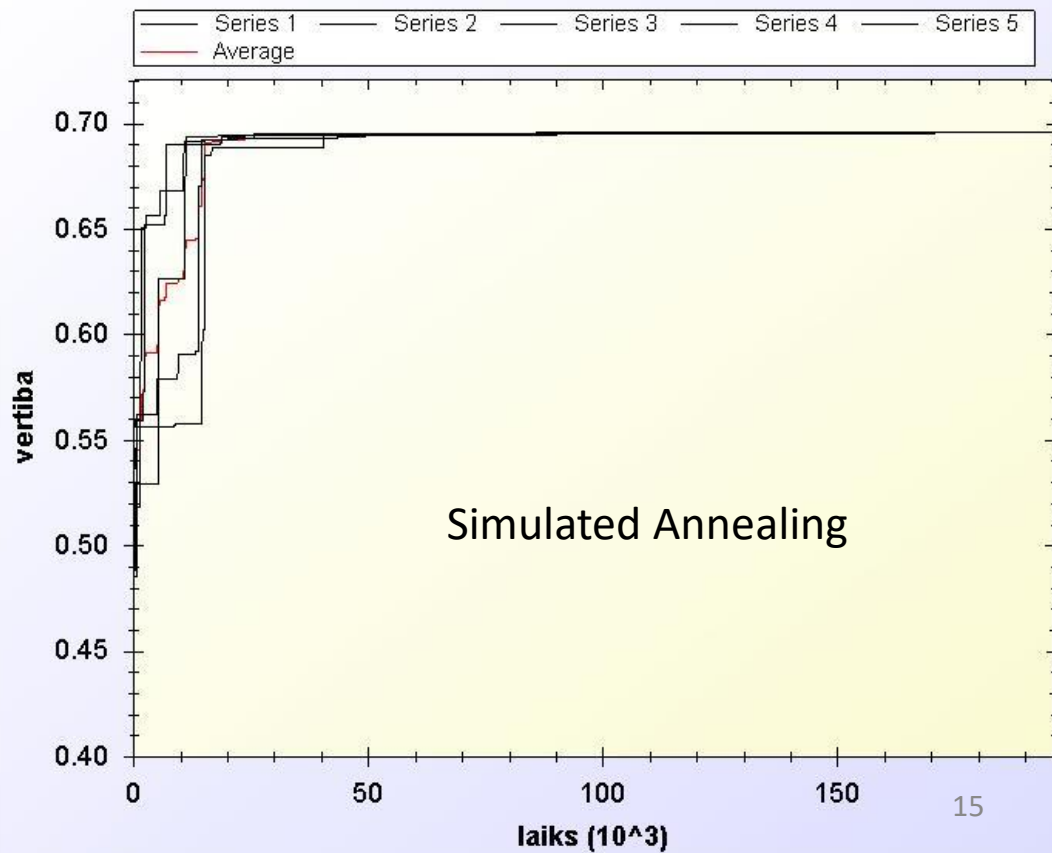
Level 4

- EP, PS and RS still don't give any results
- Fastest results given by Genetic Algorithm SR
- Genetic Algorithm reaches supposed maximum, but 3 out of 5 runs haven't given any results

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- GASR gives results in every level except nr.2 (amino acid constraint)
- Simulated Annealing works very good with metabolite concentration corridor constraints
- Random search doesn't give feasible results in any level

Thank you for attention