Computer-Aided Algorithm Design:

Automated Tuning, Configuration, Selection and Beyond

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for hard problems?

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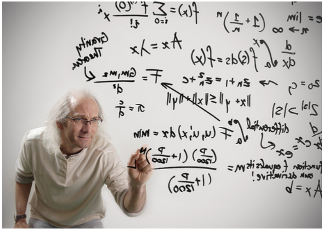

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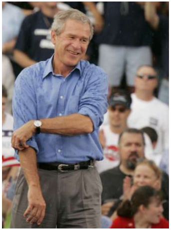

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$\rightsquigarrow$ principled experimentation + generic techniques

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- facilitates principled design of heuristic algorithms
- profoundly changes how we build and use algorithms

High-performance heuristic algorithms are difficult to design

- many design choices (representation / search space; neighbourhoods; search strategy; variable/value selection heuristic; restart rules; pre-processing; data structures; ...)

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- performance can be tricky to assess due to
  - differences in behaviour across problem instances
  - stochasticity

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- resulting algorithms often complex, somewhat ad-hoc, not fully optimised

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- Goal: Minimize expected run-time on 'typical' SAT instances from software verification tool
- Problems:
  - default settings $\rightsquigarrow$ $\approx$ 300 seconds / run
  - good performance on some instances may not generalise

Outline

1. Introduction
2. From traditional to computer-aided algorithm design
3. Design spaces and design patterns
4. Meta-algorithmic search and optimisation procedures
5. Three success stories (SAT, timetabling, MIP)
6. The next step: Programming by Optimisation

From traditional to computer-aided algorithm design

Traditional algorithm design approach:

- iterative, manual process

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- design often starts from generic or broadly applicable problem solving method (*e.g.*, evolutionary algorithm)

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$\rightsquigarrow$ complicated designs, unfulfilled performance potential

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$\rightsquigarrow$ genetic programming, hyper-heuristics, reactive search; learning and intelligent optimisation, SLS engineering; meta-learning; program synthesis

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Meta-algorithmic system:

- explores design space in principled manner
- evaluates candidate design
- finds high-performance designs

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- exploits complementary strengths of different approaches for solving a given problem
- uses principled, fully formalised methods for algorithm design
- can be used to customise algorithms for use in specific applications with minimal human effort

Example: SAT-based software verification

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- manual configuration by algorithm designer
- automated configuration using ParamILS, a generic algorithm configuration procedure

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SPEAR: Empirical results on software verification benchmarks

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- $\approx$ 500-fold speedup through use automated algorithm configuration procedure (ParamILS)
- new state of the art
  (winner of 2007 SMT Competition, QF_BV category)

Design spaces and design patterns

Special cases of computer-aided algorithm design:

- parameter optimisation (for given set of instances)

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- restart strategies

  Luby *et al.* (1993); Gagliolo & Schmidhuber (2007);
  Streeter *et al.* (2007)

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$\rightsquigarrow$ meta-algorithmic design patterns, induce design spaces

Meta-algorithmic search and optimisation procedures

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- use powerful heuristic search and optimisation procedures, combined with significant amounts of computing power
- use machine learning methods (classification, regression), combined with significant amount of training data

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  - advanced stochastic local search procedures
    e.g., ParamILS (Hutter *et al.* 2007)

More examples:

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  - evolutionary algorithms (*e.g.*, Harik & Lobo 1999)

Many open questions:

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- How to best deal with censored, sparse data?

How good are current methods for computer-aided algorithm design?

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Further successes:

- protein structure prediction (Thachuk *et al.* 2007)
- SAT (KhudaBukhsh *et al.* 2009; Xu *et al.* – to appear; Tompkins & HH – to appear)
- TSP (Styles & HH – in preparation)

SATzilla: Portfolio-based algorithm selection for SAT

Xu, Hutter, HH, Leyton-Brown (2008)

Key idea: Instance-based Algorithm Selection (Rice 1976)

- *Given:* set S of algorithms for a problem, problem instance π
- *Select* from S the algorithm expected to solve π *most efficiently*, based on (cheaply computable) *features* of π.

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SATzilla in a nutshell:

- CNF formula $\rightsquigarrow$ 84 polytime-computable instance features
- features $\rightsquigarrow$ performance prediction for set of SAT solvers
- run solver with best predicted performance

Under the hood:

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- Use ridge regression on selected features to predict solver run-times from instance features.
- Use method by Schmee & Hahn (1979) to deal with censored run-time data.

Some bells and whistles:

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$\rightsquigarrow$ prizes in 5 of the 9 main categories of the 2009 SAT Solver Competition (3 gold, 2 silver medals)

Post-Enrolment Course Timetabling

Chiarandini, Fawcett, HH (2008); Fawcett, HH, Chiarandini (in preparation)

Post-Enrolment Course Timetabling:

- students enroll in courses
- courses are assigned to rooms and time slots, subject to *hard constraints*
- preferences are represented by *soft constraints*

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Our solver:

- modular multiphase stochastic local search algorithm
- hard constraint solver: finds feasible course schedules
- soft constraint solver: optimise schedule (maintaining feasibility)

Our first solver:

- developed over ca. 1 month
- starting point: Chiarandini *et al.* (2003)
- *soft constraint solver* unchanged
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- 7 parameters, 50 400 configurations

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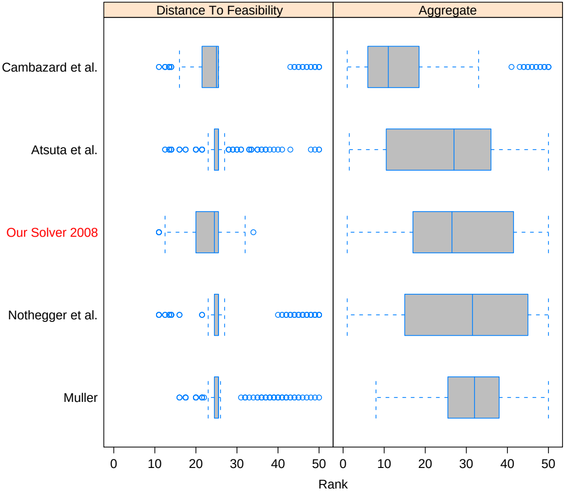
Automated configuration process:

- configurator: FocusedILS 2.3 (Hutter *et al.* 2009)
- performance objective: solution quality after 300 CPU sec

2nd International Timetabling Competition (ITC), Track 2



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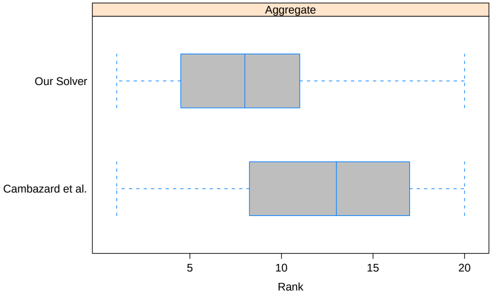
Automated configuration process:

- configurator: FocusedILS 2.4 (new version, multiple stages)
- multiple performance objectives
  (final stage: solution quality after 600 CPU sec)

2-way race against ITC Track 2 winner



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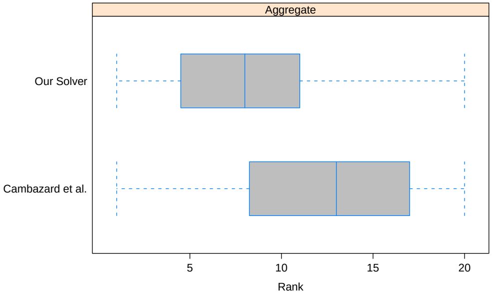

- our solver wins beats ITC winner on 20 out of 24 competition instances
- application to university-wide exam scheduling at UBC
  ($\approx$ 1650 exams, 28 000 students)

Mixed Integer Programming (MIP)

Hutter, HH, Leyton-Brown, Stützle (2009); Hutter, HH, Leyton-Brown (2010)

- MIP is widely used for modelling optimisation problems
- MIP solvers play an important role for solving broad range of real-world problems

CPLEX:

- prominent and widely used commercial MIP solver
- exact solver, based on sophisticated branch & cut algorithm and numerous heuristics
- 159 parameters, 81 directly control search process

"A great deal of algorithmic development effort has been devoted to establishing default ILOG CPLEX parameter settings that achieve good performance on a wide variety of MIP models."

[CPLEX 12.1 user manual, p. 478]

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CPLEX on various MIPS benchmarks

Benchmark	Default performance [CPU sec]	Optimised performance [CPU sec]	Speedup factor
BCOL/CONIC.SCH	5.37	2.35 (2.4 ± 0.29)	2.2
BCOL/CLS	712	23.4 (327 ± 860)	30.4
BCOL/MIK	64.8	1.19 (301 ± 948)	54.4
CATS/REGIONS200	72	10.5 (11.4 ± 0.9)	6.8
RNA-QP	969	525 (827 ± 306)	1.8

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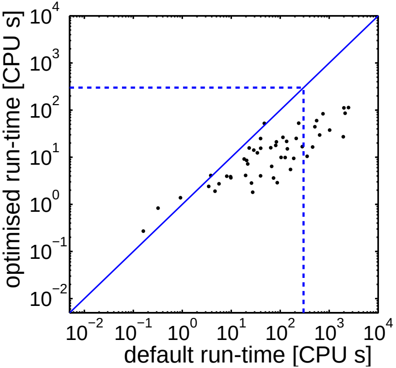
CPLEX on BCOL/CLS



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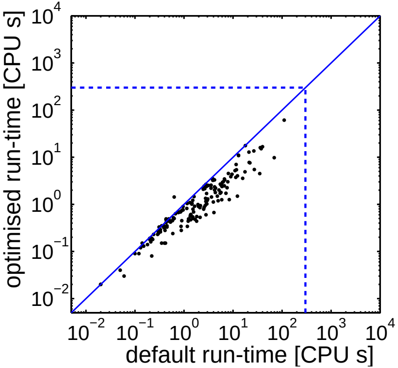
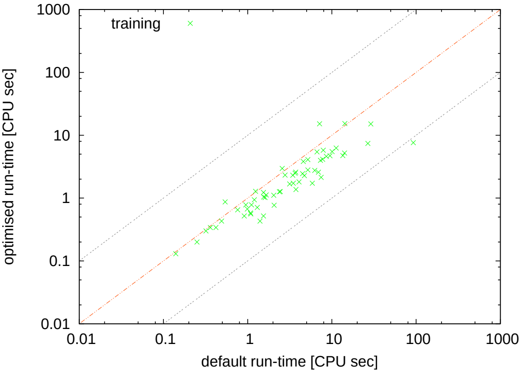


Latest results: Gurobi on BCOL/MIK



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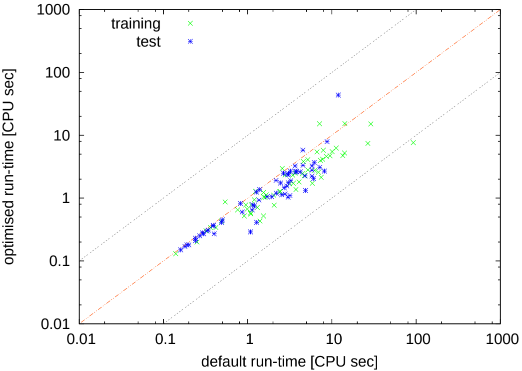

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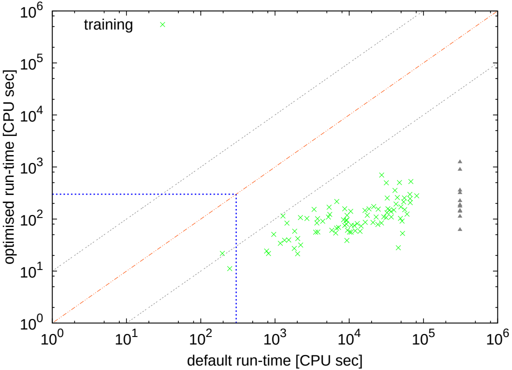

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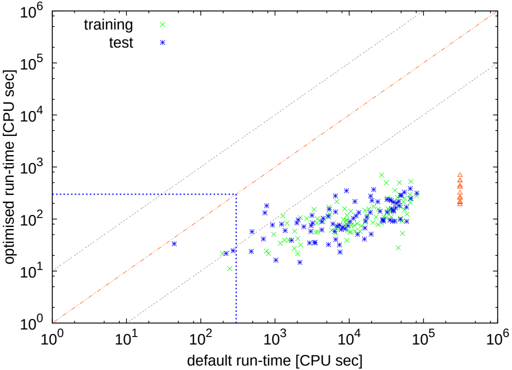

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How to use computer-aided algorithm design?

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application context

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application context

$+$

design space

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optimisation procedure

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success

The next step: Programming by Optimisation

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Need effective support for ...

- specification of rich design spaces

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HAL: High-performance Algorithm Lab

Nell, Fawcett, HH, Leyton-Brown (under review)

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HAL 1.0

HAL 1.0	home	1q/3r	?

New Tasks

Evaluate algorithm performance
Analyse performance of an algorithm on an instance set.

Compare algorithm performance
Compare the performance of two algorithms on an instance set.

Configure algorithm
Optimize parameter settings to maximize algorithm performance on an instance set.

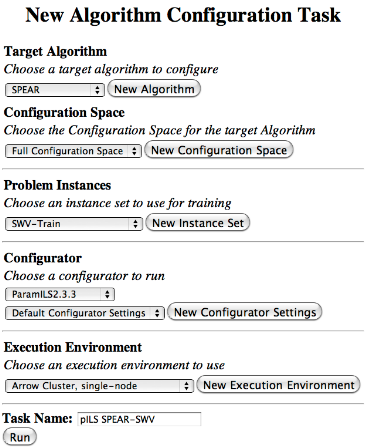
Active Tasks

Status	ID	Name	Start Time	CPU Time	
queued	5	Compare GGA/PILS SPEAR	N/A	0 s	
99%	3	ParamILS SPEAR SWV	2010-04-02 17:25:05.0	258122.70 s	KILL
97%	4	GGA SPEAR SWV	2010-04-02 17:31:31.0	253904.81 s	KILL
8%	6	Compare GGA/PILS SATenstein	2010-04-05 08:47:26.0	1322.16 s	KILL

Completed Tasks

Status	ID	Name	Start Time	CPU Time
done	1	ParamILS SATenstein QCP	2010-04-02 15:07:35.0	188920.02 s
done	2	GGA SATenstein QCP	2010-04-02 15:08:41.0	181342.54 s

HAL 1.0


New Algorithm Configuration Task
Target Algorithm
Choose a target algorithm to configure
SPEAR
New Algorithm
Configuration Space
Choose the Configuration Space for the target Algorithm
Full Configuration Space
New Configuration Space
Problem Instances
Choose an instance set to use for training
SWV-Train
New Instance Set
Configurator
Choose a configurator to run
ParamILS2.3.3
Default Configurator Settings
New Configurator Settings
Execution Environment
Choose an execution environment to use
Arrow Cluster, single-node
New Execution Environment
Task Name:
pILS SPEAR-SWV
Run

HAL 1.0

HAL 1.0 home 1q/3r ?

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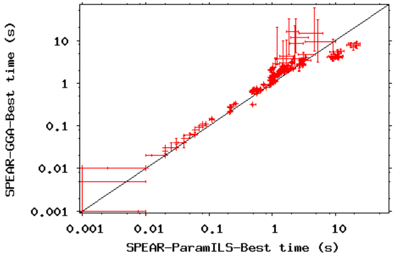
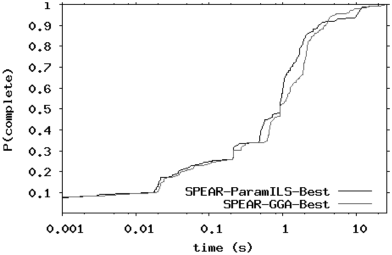
HAL 1.0

Wilcoxon signed-rank test: p=2.63E-15
Wilcoxon winner: SPEAR-ParamILS-Best
Spearman correlation test: p=2.22E-208

	q10	q25	q50	q75	q90	mean	sd
SPEAR-ParamILS-Best	0.017	0.104	0.922	1.670	3.171	1.712	3.216
SPEAR-GGA-Best	0.019	0.135	0.926	2.073	3.888	1.747	3.052





Programming by Optimisation (PbO)

HH (work in progress)

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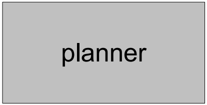
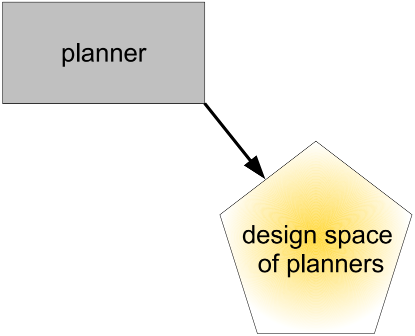
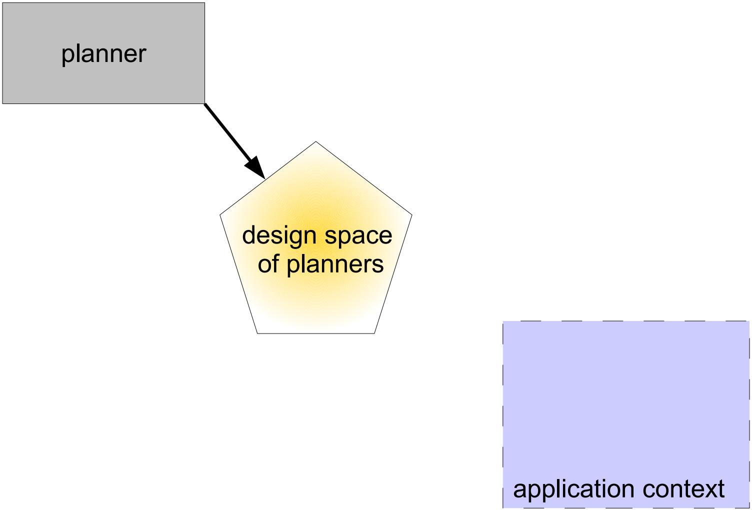
  $\rightsquigarrow$ HAL + compute power


planner


planner
design space
of planners


planner
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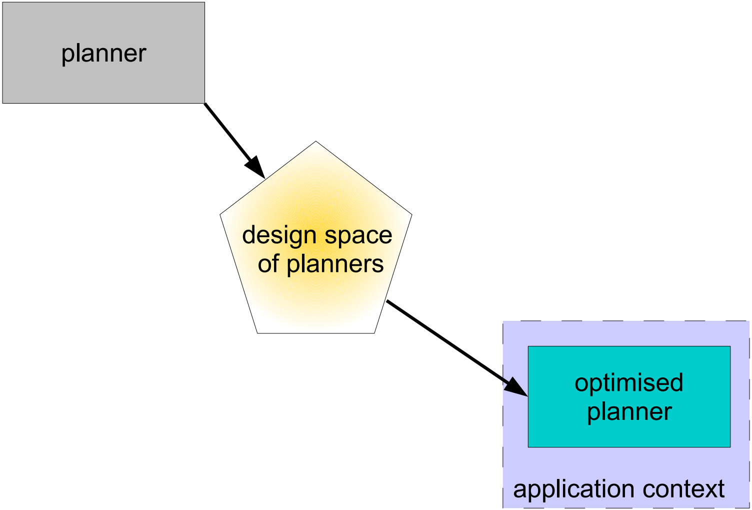
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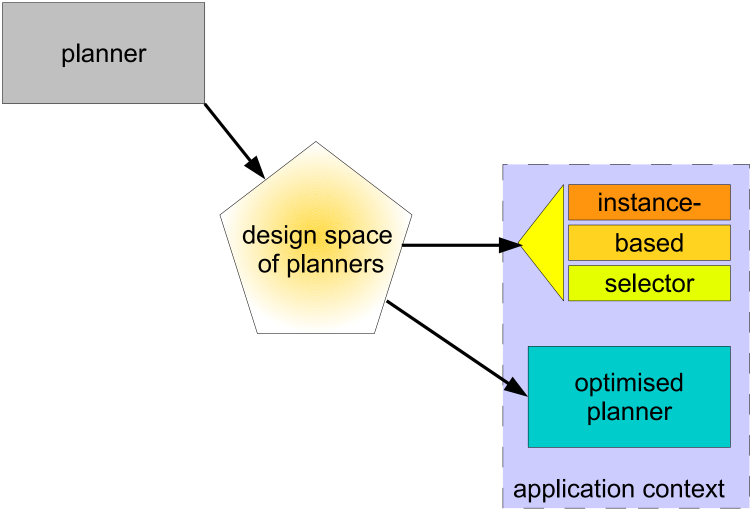
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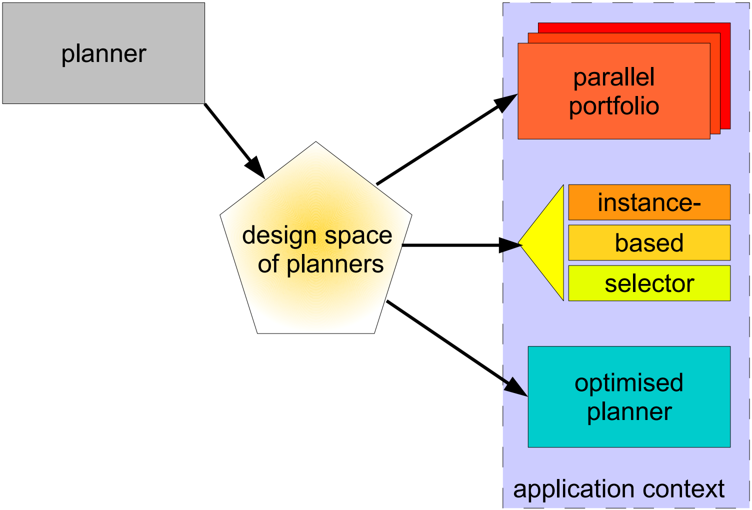
planner
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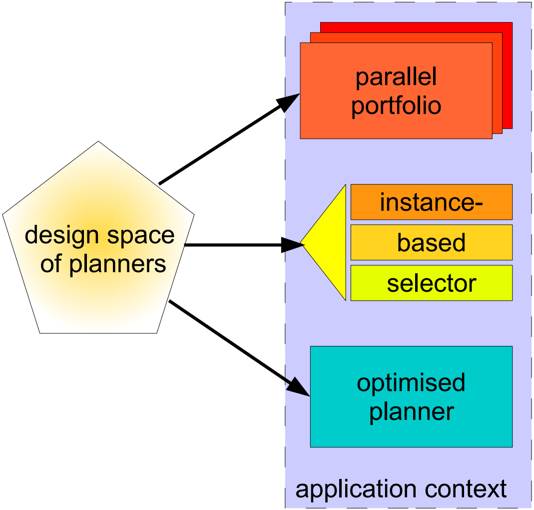
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Computationally too expensive?

Recent example: Hydra SAT solver (Xu *et al.* – to appear)

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- profoundly changes how we build and use algorithms

Acknowledgements

Collaborators:

- Domagoj Babic
- Alex Devkar
- Chris Fawcett
- Frank Hutter
- Chris Nell
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- Alena Shmygelska
- Chris Thachuk
- James Styles
- Lin Xu

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- Marco Chiarandini
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- Kevin Murphy
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- Thomas Stützle
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- WestGrid