Solving Atomix with Pattern Databases

Alex Gliesch, Marcus Ritt

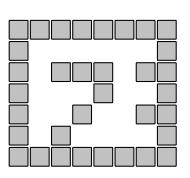
Institute of Informatics
Universidade Federal do Rio Grande do Sul

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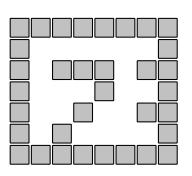
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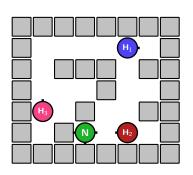
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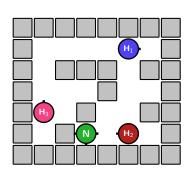
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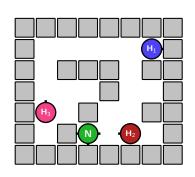
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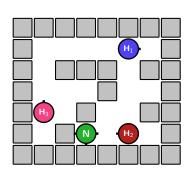
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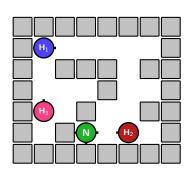
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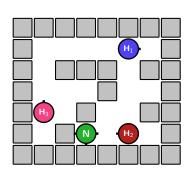
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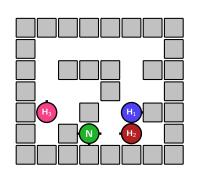
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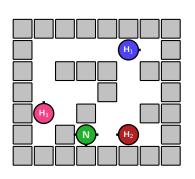
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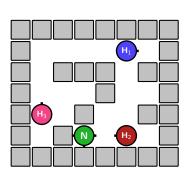
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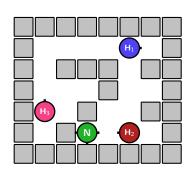
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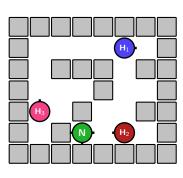


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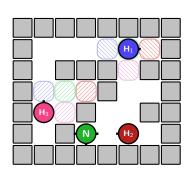


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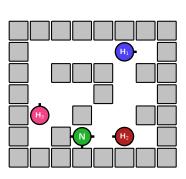
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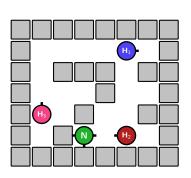
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- ▶ This presentation: focus on PDBs, other contributions with more details in the paper

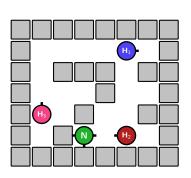
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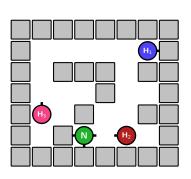
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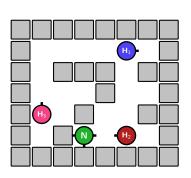
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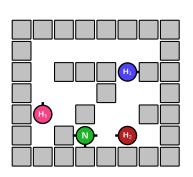
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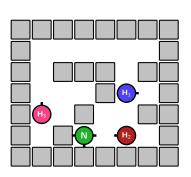
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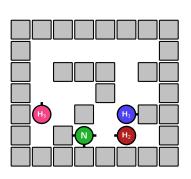
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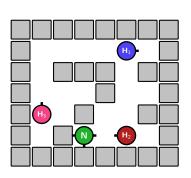
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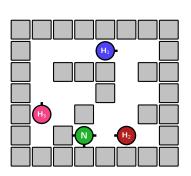
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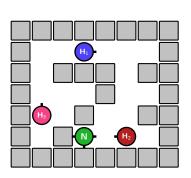
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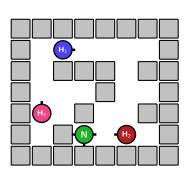
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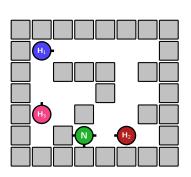
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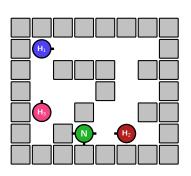
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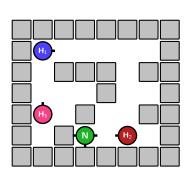
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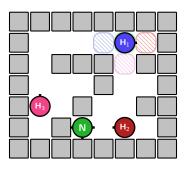


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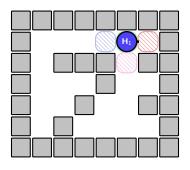


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- Generalized distance: minimum number of relaxed moves from one position to another
- Heuristic value of a state: sum of generalized distances from every atom, independently, to its final position in a molecule

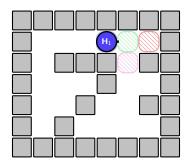




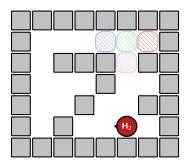
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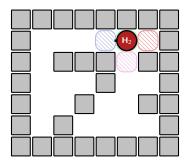


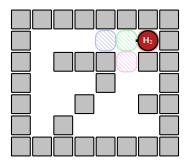
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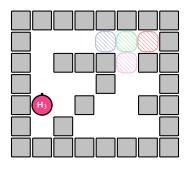


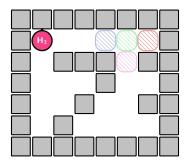
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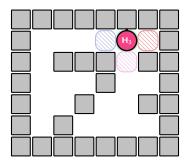


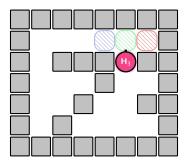


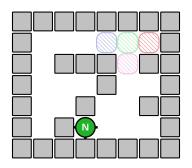






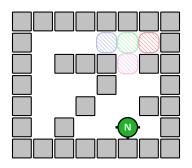






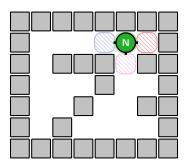
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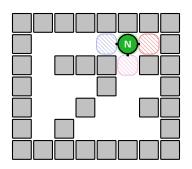
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 Distances are pre-computed before search starts by an all-pairs-shortest-paths algorithm

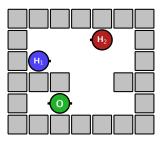
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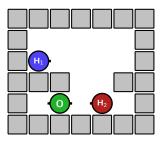
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- In particular, we are interested in additive PDBs: if the abstract states use disjoint sets of pieces, we can add their distances and still be admissible

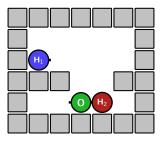
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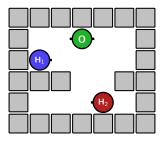
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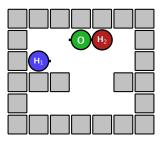
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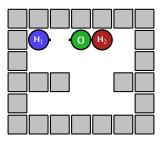
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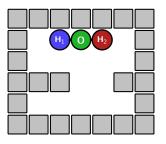
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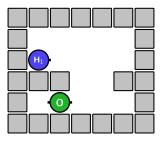
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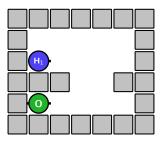
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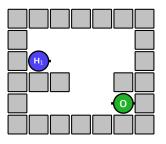
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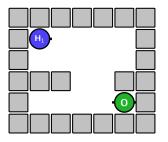
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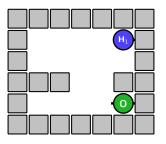
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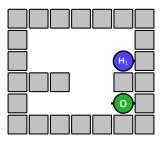
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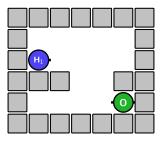
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- A PDB on relaxed Atomix penalizes negative interactions (such as linear conflicts) between atoms within the PDB's set of pieces

Statically-partitioned PDB

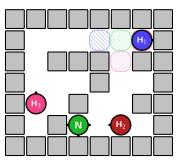
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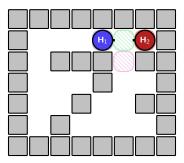
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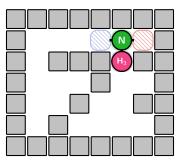
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- ► Chosen patterns of *k* of atoms stay the same during search
 - Some partitions may yield better overall lower bounds than others
 - Would be good to pick a partition that captures more conflicts within the patterns



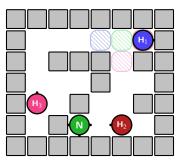
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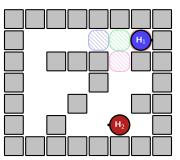
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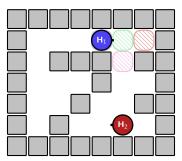
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- ► Same thing for {H₃, N}



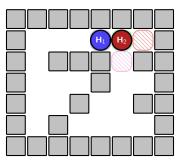
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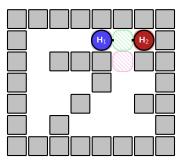
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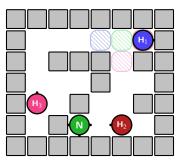
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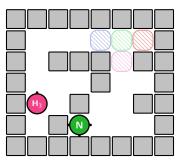
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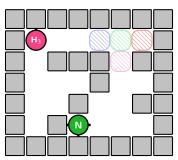
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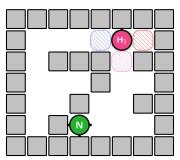
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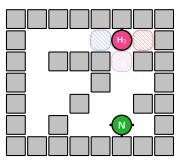
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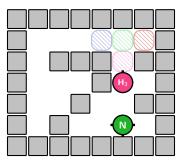
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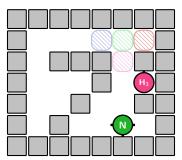
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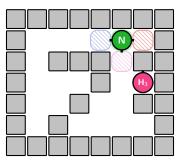
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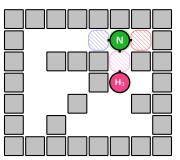
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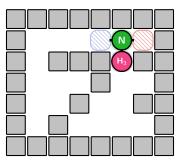
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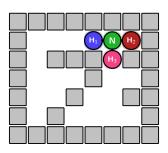
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- ▶ To compute heuristic of state, add heuristic of corresponding abstract states $\{H_1, H_2\}$ and $\{H_3, N\}$



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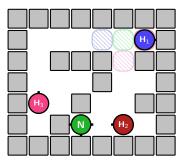
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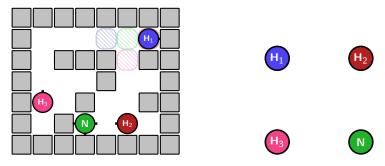
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- ► Final heuristic: 3 for {H₁, H₂} and 8 for {H₃, N} , total 11. Recall that without PDBs it was 8

Dynamically-partitioned PDB

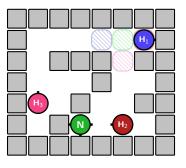
- ▶ Build PDB for all possible $\binom{n}{k}$ partitions of the *n* atoms
- ► At every heuristic call, choose the partition with maximum heuristic value
- For k = 2, the best heuristic is obtained by a maximum weight perfect matching

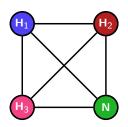


▶ Build a full graph where:

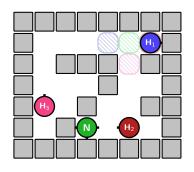


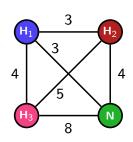
- ► Build a full graph where:
- ► Each atom is a node



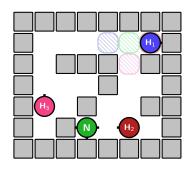


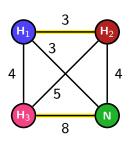
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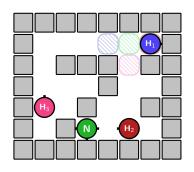


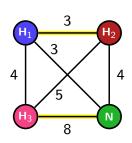
- Build a full graph where:
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- Weight of each edge is the solution of the abstract state using only the two atoms that edge connects
- ▶ Compute maximum cost perfect matching, in $O(n^3)$
- ▶ If $k \ge 3$, matching is NP-hard: better use heuristic methods

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- ► Tests limited to 1h execution time and 10GB memory
- ▶ 10 replications of each run

PDB Results

	Static $k = 3$	Dynamic $k = 2$	No PDB
# Solved	82.8	71	77
Avg. rel. deviation $(\%)$	0.58	1.72	1.47
Avg. initial heuristic (%)	24.04	23.39	26.23
Time (s)	2,952	17,405	3,420
Nodes expanded ($\times 10^8$)	3.39	2.39	8.72

Comparison with Hüffner et al. (2001)

	This work (w/ static PDB)	Hüffner et al.
# Solved	82.8	75
Avg. rel. deviation (%)	0.56	1.67
Time (s)	9,211	12,962
Nodes expanded ($\times 10^8$)	6.79	47.18

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- ▶ Dynamic PDB yields even better lower bounds, even with smaller k, but is very slow to compute $(O(n^3))$
- Static PDB solves 7.8 more instances and expands, on average, 6.94 times fewer nodes compared to previous state of the art

Questions?