Boosting AND/OR-Based Computational Protein Design: Dynamic Heuristics and Generalizable UFO (Supplemental Materials)

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CONTENTS

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1 ADDITIONAL MATERIALS

The following resources can be found in entry **R274** on the Dechter Lab Publications page:

1.1 EXTENDED BACKGROUND (WITH GLOSSARY)

A document that includes a glossary of terms and more in-depth background (found in entry **R274** on the Dechter Lab Publications page).

1.2 EXPLORING UFO'S

A document highlighting some important properties of underflow thresholding and preliminary experiments of UFO on other important graphical model tasks (found in entry **R274** on the Dechter Lab Publications page).

1.3 HIGHLIGHT VIDEO

A highlight video summarizing this work (found in entry **R274** on the Dechter Lab Publications page).

1.4 BENCHMARKS

Released benchmarks that were experimented on (found in entry **R274** on the Dechter Lab Publications page).

2 EXTENDED EMPIRICAL EVALUATION

In this section we present additional empirical evaluations and results extending those presented in the main paper.

2.0.1 Algorithms

We experimented with 5 algorithms: AOBB-K*; AOBB-K*-b (boosted) with an improved wMBE-K*-b heuristic and search enhancements; AOBB-K*-b-DH, AOBB-K*-b with dynamic heuristics; AOBB-K*-b-UFO, AOBB-K*-b empowered with a CPD-specific UFO scheme; and BBK*, state-of-the-art best-first search algorithm in comprehensive CPD software OSPREY 3.0 [Ojewole et al., 2018, Hallen et al., 2018].

Each AOBB-K* derived algorithm was implemented in C++. AOBB-K*-b-DH dynamic heuristic re-computations were regulated with $maxDepth = 2$ and $dhThreshold = 10^{20} \cdot K^*_{wt}$, where K^*_{wt} is the wild-type K* value. The UFO scheme used by AOBB-K*-b-UFO performed binary search in log-space and decreased the resulting threshold with $\delta = 0.2$. Because the AOBB-K*-b algorithms use the wMBE-K*-b heuristic which does not guarantee bounds, they do not guarantee discovery of the optimal K* (ie. they are not complete). Similarly, schemes empowered with UFO lose optimality guarantees.

BBK* is implemented in Java, was set to use rigid rotamers, and given a bound-tightness of 1×10^{-200}[1]. Despite the extremely small bound tightness parameter, BBK* still performs noticeably as an approximate algorithm.

Experiments were run on a 2.66 GHz processor, and given 4 GB of memory and a time limit of 1hr for each problem. As BBK* can take advantage of parallelism, it was given access to 4 CPU cores.

2.0.2 Benchmarks.

We performed empirical evaluation on benchmarks derived from re-design problems for real proteins provided by the Bruce Donald Lab at Duke University. To gradually increase difficulty, small problems with two mutable residues (with five to ten total residues) were incrementally enlarged by making more of the residues mutable. Experiments were performed on the "Expanded" problem set from Pezeshki et al. [2022] consisting of 12 problems with 3 mutable residues, a new set of 32 problems expanded to have 4 mutable residues, and a set of 18 problems expanded to have 5 mutable residues. The names of the newly created benchmarks are shown with three parts: d[g]-[M]-[p] (eg. d27-4-1), where [g] represents the problem design number as obtained from the Donald Lab, [M] indicates the number of mutable residues after enlarging, and [p] is a single digit representing the specific permutation of the M residues that were made mutable. The resulting conformation spaces for these problems ranged from on the order of 10^6 for 3 mutable residues to 10^{11} for 5 mutable residues.

2.0.3 Benchmark Nomenclature

Whereas in the main paper, benchmark names were shortened for brevity, here we include the full design designations for the benchmark names. Below, we describe the nomenclature and relation to the names as appears in the main paper.

General Benchmark-Name Format. Benchmarks are named according to the following format:

<protein PDB>_<base design number>_<extended design specifications_<graphical model formulation>

for example:

1gwc_prepped_00021_4_4-0-1-2-3_1_0_F2_N0_E0_e0_t0e+00_KstarMAP

The <protein PDB> portion (ex: 1gwc_prepped) indicates the protein PDB file used (which is included with the provided benchmark files). A protein PDB (Protein Data Bank) file is a widely used format for storing the three-dimensional structure of proteins as described in Research Collaboratory for Structural Bioinformatics (RCSB) [2023]. It contains detailed information about the arrangement and coordinates of atoms within the protein molecule. This includes the positions of individual atoms, their chemical identities, and how they are connected to form the protein's structure. Additionally, PDB files may include supplementary data like experimental methods used to determine the structure and quality assessments.

[1]BBK*'s bound tightness parameter does not correlate directly with an ω-approximation. See Ojewole et al. [2018].

The <base design number> (ex: 00021) is a number that indicates the original re-design problem as obtained from the Donald Lab (more details to follow).

The <extended design specifications> (ex: 4_4-0-1-2-3_1_0) is an extension that describes how the base design was modified and indicates the number and identity of the mutable residues. This will be described in detail in the following sections.

The <graphical model formulation> (ex: F2_N0_E0_e0_t0e+00_KstarMAP) describes how these design problems were formulated as a graphical model. For all of the problems experimented on, this portion was the same and indicates the graphical model formulation described in the main paper.

CPD design parameters for the 3 mutable residue problems. For the three mutable residue problems (taken from Pezeshki et al. [2022]) the <extended design specifications> were taken as-is to be able to compare directly to results from that work.

CPD design parameters for the 4 or 5 mutable residue problems. The benchmarks experimented on are re-design problems for real proteins obtained by the Bruce Donald Lab. Each problem obtained consists of a PDB file for the protein and re-design specifications in the form of a TOML file [tom, n.d.] that identifies two interacting subunits to be considered (in the file designated as *strand0* and *strand1*), the residues from each to consider, and which residues will be mutable. The obtained problems were named as: <protein PDB>_<base design number> (ex: 1gwc_prepped_00021). Since these original problems were expanded to make more of the residues mutable, the names were appended with <extended design specifications> to more specifically highlight the number and identity of mutable residues (ex. appended with: 4_4-0-1-2-3_1_0). These extended design specifications can be broken into four parts:

<number of residues in strand0>_<number and identity of mutable residues in strand0>_<number of residues in strand1>_<number and identity of mutable residues in strand1>

for example:

4_4-0-1-2-3_1_0

For this example problem, we consider 4 residues within the first subunit (strand0) and 1 residues within the second subunit (strand1). We see that all four residues of the first subunit are made mutable - specifically residues 0, 1, 2, 3 (referring to the index of the residues as would appear in a list with them ordered by their protein residue number according to the PDB file). There are zero mutable residues in the second subunit (ie. the only residue in the second subunit is non-mutable and its amino acid assignment is set).

Instance Names in the Tables Below. For simplicity, instances are referred to by their <base design number>_<extended design specifications portions of their name (ex: 00021_4_4-0-1-2-3_1_0) in the tables below.

Generation and Choice of 4 and 5 Mutable Residue Benchmarks. The larger re-design specifications were generated by expanding the smaller 2 or 3 mutable-residue problems obtained by the Donald Lab and making more residues mutable. A random subset of these benchmarks were chosen and random non-mutable residues (of the strand that already had mutable residues) were made mutable. The final set used was a subset of these generated problems for which BBK* produced a solution for within two hours. OSPREY was used to generate tables for the energies of interactions between the different possible different amino acid rotamers of the residues, and from the re-design specifications and the energy tables a graphical model (as described in the main paper) formed in modified UAI format [Dechter et al., 2022] that includes a .sum file that identifies the conformation variables corresponding to each protein subunit for both when the protein is in its dissociate and complexed form.

2.1 EXPANDED COMPARISON OF THE AOBB-K*-B-[DH/UFO] SCHEMES

Table Description The following tables are extensions of Table 3 from the main paper, expanded to included all benchmarks experimented on. These tables compare the performance of the AOBB-K*-b-[DH/UFO] schemes with each other and BBK*. The results are separated into four tables: Table 1 shows results on the "Expanded" problem set from Pezeshki et al. [2022] with 3 mutable residues, Table 2 (split across two sub tables) shows results on problems expanded to have 4 mutable residues, and Table 3 shows results on problems expanded to have 5 mutable residues. Please see Section 2.0.3 of this document for the description of the instance nomenclature.

For each problem, the AOBB-K*-b-[UFO/DH] solvers are ranked top-down based on their performance (top being best). A solver's rank is first determined by the quality of K* found (higher is better), and then by how fast their respective final solution was first discovered. The columns in the tables are as follows:

M: Number of mutable residues

Problem: Problem instance designation (as described in Section 2.0.3 above)

Algorithm Specific AOBB-K*-b-[DH/UFO] algorithm

i i-bound used for the wMBE-K*-b heuristic

OR Number of residue variable OR nodes explored

AND Number of residue variable AND nodes explored

Soln Algorithm's K* solution. (This value is recomputed using a non-thresholded problem).

Anytime The time (in seconds) at which the final solution was first discovered.

Time The completion time of the algorithm if under 3600 seconds ("timeout" otherwise).

wt K* The wild-type protein's K* value.

Between AOBB-K*-b-[UFO/DH] and BBK* K* solutions, blue font highlights better values and red font worse values. If AOBB-K*-b-[UFO/DH] had a better K* solution compared to BBK*'s and that solution was also found before BBK* terminated, the AOBB-K*-b-[UFO/DH]'s "Anytime" value is also made blue. Similarly, red font highlights worse values. Italics highlights statistics responsible for a higher ranking in the solver orderings.

Table 1: Comparison AOBB-K*-b-[UFO/DH] schemes with BBK* on problems with 3 mutable residues. For each problem, the AOBB-K*-b-[UFO/DH] solvers are ranked top-down based on their performance (top being best). Shown is the i-bound used, traversed residue OR and AND nodes, best-found K* solution (recomputed without underflow-thresholding), the time at which the best-found solution was first discovered ("Anytime"), and the completion time ("Time"). Between AOBB-K*-b-[UFO/DH] and BBK*, blue font highlights better values and red font worse values. Italics highlight statistics responsible for a higher ranking in the solver orderings. For reference, the wild-type K* solution is also shown.

AOBB-K*-b-[DH/UFO]										BBK*	
M	Problem	Algorithm	i	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
3	00007_1_0_7_3	AOBB-K*-b-UFO	3	19	364	14.73	*8.22*	333.66	14.08	14.73	369.42
	00007_1_0_7_3	AOBB-K*-b-DH	3	50	503	14.73	*10.38*	2862.36	14.08	14.73	369.42
	00007_1_0_7_3	AOBB-K*-b	4	6	35	14.73	88.55	265.99	14.08	14.73	369.42
	00009_2_0_3_3	AOBB-K*-b-UFO	3	219	3384	4.51	*9.80*	345.61	4.09	4.51	215.82
	00009_2_0_3_3	AOBB-K*-b-DH	3	4	21	4.51	*10.29*	33.11	4.09	4.51	215.82
	00009_2_0_3_3	AOBB-K*-b	4	4	7	4.51	76.84	77.84	4.09	4.51	215.82
	00011_2_0_3_3	AOBB-K*-b-UFO	3	55	185	11.85	*6.38*	23.65	11.75	11.85	26.58
	00011_2_0_3_3	AOBB-K*-b-DH	3	3	15	11.85	*7.70*	24.22	11.75	11.85	26.58
	00011_2_0_3_3	AOBB-K*-b	4	3	5	11.85	99.13	99.14	11.75	11.85	26.58
	00012_3_0_3_3	AOBB-K*-b-DH	3	3	13	*13.93*	*7.45*	21.56	13.93	13.93	11.83
	00012_3_0_3_3	AOBB-K*-b	4	3	4	*13.93*	68.59	68.60	13.93	13.93	11.83
	00012_3_0_3_3	AOBB-K*-b-UFO	3	21	119	13.91	6.06	8.16	13.93	13.93	11.83
	00013_3_0_4_3	AOBB-K*-b-UFO	3	22	416	15.03	*6.11*	89.82	13.25	15.03	39.22
	00013_3_0_4_3	AOBB-K*-b-DH	3	3	5	15.03	*10.15*	10.15	13.25	15.03	39.22
	00013_3_0_4_3	AOBB-K*-b	4	3	5	15.03	99.62	99.63	13.25	15.03	39.22
	00014_3_0_3_3	AOBB-K*-b-UFO	3	25	129	14.36	*6.22*	8.49	13.96	14.36	44.93
	00014_3_0_3_3	AOBB-K*-b-DH	3	3	16	14.36	*8.79*	26.08	13.96	14.36	44.93
	00014_3_0_3_3	AOBB-K*-b	4	3	5	14.36	69.10	69.10	13.96	14.36	44.93
	00017_2_0_4_3	AOBB-K*-b-UFO	3	222	2713	**10.86**	***7.75***	152.26	10.52	10.80	78.00
	00017_2_0_4_3	AOBB-K*-b-DH	3	21	38	**10.86**	***15.80***	41.03	10.52	10.80	78.00
	00017_2_0_4_3	AOBB-K*-b	4	7	10	**10.86**	115.12	115.13	10.52	10.80	78.00
	00019_3_0_3_3	AOBB-K*-b-UFO	3	319	5028	14.99	*6.15*	621.83	14.99	14.99	34.00
	00019_3_0_3_3	AOBB-K*-b-DH	3	8	30	14.99	*11.31*	56.05	14.99	14.99	34.00
	00019_3_0_3_3	AOBB-K*-b	4	3	4	14.99	75.99	76.00	14.99	14.99	34.00
	00020_3_0_3_3	AOBB-K*-b-UFO	3	269	2814	10.96	*13.70*	480.77	10.60	10.96	1388.13
	00020_3_0_3_3	AOBB-K*-b-DH	3	3	44	10.96	*39.67*	339.91	10.60	10.96	1388.13
	00020_3_0_3_3	AOBB-K*-b	4	3	5	10.96	100.02	100.03	10.60	10.96	1388.13
	00021_1_0_4_3	AOBB-K*-b-UFO	3	239	2488	**11.92**	***89.03***	628.59	9.37	11.72	551.27
	00021_1_0_4_3	AOBB-K*-b-DH	3	75	158	**11.92**	***136.44***	1307.45	9.37	11.72	551.27
	00021_1_0_4_3	AOBB-K*-b	4	7	12	**11.92**	**193.83**	196.52	9.37	11.72	551.27
	00025_3_0_4_3	AOBB-K*-b-UFO	3	15	236	**16.18**	***14.02***	64.82	10.74	13.65	880.46
	00025_3_0_4_3	AOBB-K*-b-DH	3	4	23	**16.18**	***51.92***	80.22	10.74	13.65	880.46
	00025_3_0_4_3	AOBB-K*-b	4	4	7	**16.18**	**166.74**	166.75	10.74	13.65	880.46
	00030_4_3_2_0	AOBB-K*-b-UFO	3	180	2178	**11.12**	***8.00***	112.51	10.35	10.97	275.38
	00030_4_3_2_0	AOBB-K*-b-DH	3	70	141	**11.12**	***24.88***	52.57	10.35	10.97	275.38
	00030_4_3_2_0	AOBB-K*-b	4	22	25	**11.12**	**154.05**	154.09	10.35	10.97	275.38

Table 2: Comparison AOBB-K^*-b-[UFO/DH] schemes with BBK^* on problems with 4 mutable residues. For each problem, the AOBB-K^*-b-[UFO/DH] solvers are ranked top-down based on their performance (top being best). Shown is the i-bound used, traversed residue OR and AND nodes, best-found K^* solution (recomputed without underflow-thresholding), the time at which the best-found solution was first discovered ("Anytime"), and the completion time ("Time"). Between AOBB-K^*-b-[UFO/DH] and BBK^*, blue font highlights better values and red font worse values. Italics highlight statistics responsible for a higher ranking in the solver orderings. For reference, the wild-type K^* solution is also shown.

		AOBB-K*-b-[DH/UFO]								BBK*	
M	Problem	Algorithm	i	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
	00007_1_0_7_4-0-1-5-6	AOBB-K*-b-UFO	3	100	1953	***15.92***	1844.58	timeout	14.08	15.60	204.06
	00007_1_0_7_4-0-1-5-6	AOBB-K*-b-DH	3	53	423	*14.25*	348.73	timeout	14.08	15.60	204.06
	00007_1_0_7_4-0-1-5-6	AOBB-K*-b	4	42	172	14.08	163.19	timeout	14.08	15.60	204.06
	00007_1_0_7_4-1-2-3-5	AOBB-K*-b-UFO	3	85	1555	***14.89***	3391.78	timeout	14.08	14.54	278.08
	00007_1_0_7_4-1-2-3-5	AOBB-K*-b-DH	3	28	306	*14.49*	3543.27	timeout	14.08	14.54	278.08
	00007_1_0_7_4-1-2-3-5	AOBB-K*-b	3	12	185	14.49	3293.62	timeout	14.08	14.54	278.08
	00007_1_0_7_4-1-2-5-6	AOBB-K*-b-UFO	3	142	790	*14.95*	577.74	577.75	14.08	15.60	211.31
	00007_1_0_7_4-1-2-5-6	AOBB-K*-b	4	274	1426	*14.49*	302.40	timeout	14.08	15.60	211.31
	00007_1_0_7_4-1-2-5-6	AOBB-K*-b-DH	3	53	391	14.43	3327.38	timeout	14.08	15.60	211.31
	00013_3_0_4_4-0-1-2-3	AOBB-K*-b-UFO	3	345	6058	15.03	*12.69*	1974.43	13.25	15.03	46.46
	00013_3_0_4_4-0-1-2-3	AOBB-K*-b-DH	3	21	23	15.03	*22.05*	79.88	13.25	15.03	46.46
	00013_3_0_4_4-0-1-2-3	AOBB-K*-b	4	21	395	15.03	165.48	timeout	13.25	15.03	46.46
	00017_2_0_4_4-0-1-2-3	AOBB-K*-b-UFO	3	2031	22743	**10.86**	***29.39***	timeout	10.52	10.80	89.94
	00017_2_0_4_4-0-1-2-3	AOBB-K*-b	4	106	1559	**10.86**	*657.54*	timeout	10.52	10.80	89.94
	00017_2_0_4_4-0-1-2-3	AOBB-K*-b-DH	3	132	2208	**10.86**	660.16	timeout	10.52	10.80	89.94
	00018_2_0_6_4-0-1-2-4	AOBB-K*-b-UFO	3	653	5928	***17.02***	2382.08	timeout	15.79	16.58	610.41
	00018_2_0_6_4-0-1-2-4	AOBB-K*-b-DH	3	82	180	***16.60***	1614.68	timeout	15.79	16.58	610.41
	00018_2_0_6_4-0-1-2-4	AOBB-K*-b	3	108	973	16.58	40.78	timeout	15.79	16.58	610.41
	00018_2_0_6_4-0-1-2-5	AOBB-K*-b-UFO	3	245	1110	16.58	*14.38*	140.60	15.79	16.58	581.77
4	00018_2_0_6_4-0-1-2-5	AOBB-K*-b	3	279	1214	16.58	*33.31*	3038.51	15.79	16.58	581.77
	00018_2_0_6_4-0-1-2-5	AOBB-K*-b-DH	3	40	56	16.58	40.13	597.84	15.79	16.58	581.77
	00018_2_0_6_4-1-2-3-5	AOBB-K*-b-UFO	3	6317	12298	*16.20*	154.98	timeout	15.79	16.20	535.01
	00018_2_0_6_4-1-2-3-5	AOBB-K*-b-DH	3	60	451	*16.17*	513.20	timeout	15.79	16.20	535.01
	00018_2_0_6_4-1-2-3-5	AOBB-K*-b	3	46	362	15.79	15.97	timeout	15.79	16.20	535.01
	00021_4_4-0-1-2-3_1_0	AOBB-K*-b-UFO	3	649	10052	***11.92***	***196.30***	timeout	9.37	11.72	687.66
	00021_4_4-0-1-2-3_1_0	AOBB-K*-b-DH	3	122	301	***11.92***	**614.88**	timeout	9.37	11.72	687.66
	00021_4_4-0-1-2-3_1_0	AOBB-K*-b	4	47	751	11.72	264.92	timeout	9.37	11.72	687.66
	00024_4_4-0-1-2-3_3_0	AOBB-K*-b-UFO	3	87	395	**12.96**	***39.06***	43.25	11.79	12.93	128.99
	00024_4_4-0-1-2-3_3_0	AOBB-K*-b	3	94	437	**12.96**	***89.50***	423.39	11.79	12.93	128.99
	00024_4_4-0-1-2-3_3_0	AOBB-K*-b-DH	3	92	251	**12.96**	137.42	415.53	11.79	12.93	128.99
	00027_6_4-0-2-3-5_1_0	AOBB-K*-b-UFO	3	51	126	15.55	*23.85*	43.53	15.48	15.55	476.84
	00027_6_4-0-2-3-5_1_0	AOBB-K*-b	3	57	137	15.55	*79.11*	257.91	15.48	15.55	476.84
	00027_6_4-0-2-3-5_1_0	AOBB-K*-b-DH	3	57	137	15.55	185.02	410.88	15.48	15.55	476.84
	00027_6_4-1-2-3-4_1_0	AOBB-K*-b-UFO	3	89	146	15.64	*16.46*	17.54	15.48	15.64	99.34
	00027_6_4-1-2-3-4_1_0	AOBB-K*-b	3	97	158	15.64	*23.59*	27.62	15.48	15.64	99.34
	00027_6_4-1-2-3-4_1_0	AOBB-K*-b-DH	3	97	158	15.64	193.25	233.56	15.48	15.64	99.34
	00027_6_4-2-3-4-5_1_0	AOBB-K*-b-UFO	3	904	1430	**15.73**	***66.43***	90.34	15.48	15.64	93.40
	00027_6_4-2-3-4-5_1_0	AOBB-K*-b	3	1023	1635	**15.73**	*330.78*	672.67	15.48	15.64	93.40
	00027_6_4-2-3-4-5_1_0	AOBB-K*-b-DH	3	1023	1635	**15.73**	1282.45	2393.03	15.48	15.64	93.40

M	Problem	AOBB-K*-b-[DH/UFO] Algorithm	i	OR	AND	Soln	Anytime	Time	wt K*	BBK* Soln	BBK* Time
	00028_1_0_6_4-0-1-2-3	AOBB-K*-b-UFO	3	7	16	15.27	16.34	16.89	15.27	15.27	92.03
	00028_1_0_6_4-0-1-2-3	AOBB-K*-b	3	9	19	15.27	17.33	21.83	15.27	15.27	92.03
	00028_1_0_6_4-0-1-2-3	AOBB-K*-b-DH	3	9	12	15.27	24.90	38.09	15.27	15.27	92.03
	00028_1_0_6_4-0-2-3-5	AOBB-K*-b-UFO	3	80	197	15.27	15.58	47.04	15.27	15.27	95.25
	00028_1_0_6_4-0-2-3-5	AOBB-K*-b	3	93	230	15.27	16.08	337.70	15.27	15.27	95.25
	00028_1_0_6_4-0-2-3-5	AOBB-K*-b-DH	3	93	230	15.27	22.16	514.96	15.27	15.27	95.25
	00028_1_0_6_4-1-2-3-4	AOBB-K*-b-UFO	3	85	133	15.44	16.25	16.34	15.27	15.44	60.18
	00028_1_0_6_4-1-2-3-4	AOBB-K*-b-DH	3	199	282	15.44	222.76	227.07	15.27	15.44	60.18
	00028_1_0_6_4-1-2-3-4	AOBB-K*-b	3	139	164	15.35	14.05	16.82	15.27	15.44	60.18
	00028_1_0_6_4-2-3-4-5	AOBB-K*-b-UFO	3	651	996	15.44	15.95	70.34	15.27	15.44	57.35
	00028_1_0_6_4-2-3-4-5	AOBB-K*-b-DH	3	771	1193	15.44	78.57	1814.41	15.27	15.44	57.35
	00028_1_0_6_4-2-3-4-5	AOBB-K*-b	4	663	977	15.44	175.69	650.49	15.27	15.44	57.35
	00030_4_4-0-1-2-3_2_0	AOBB-K*-b-UFO	3	570	5339	11.12	18.01	905.57	10.35	10.97	253.55
	00030_4_4-0-1-2-3_2_0	AOBB-K*-b	3	277	3413	11.12	227.47	timeout	10.35	10.97	253.55
	00030_4_4-0-1-2-3_2_0	AOBB-K*-b-DH	3	270	2592	11.12	285.82	timeout	10.35	10.97	253.55
	00033_6_4-0-1-2-3_2_0	AOBB-K*-b-UFO	3	73	201	11.38	20.72	60.32	10.48	11.38	2488.59
	00033_6_4-0-1-2-3_2_0	AOBB-K*-b-DH	3	73	277	11.38	96.51	848.47	10.48	11.38	2488.59
	00033_6_4-0-1-2-3_2_0	AOBB-K*-b	3	73	277	11.38	117.15	718.92	10.48	11.38	2488.59
	00033_6_4-0-1-2-4_2_0	AOBB-K*-b-UFO	3	14	43	11.38	17.08	22.82	10.48	11.38	1111.01
	00033_6_4-0-1-2-4_2_0	AOBB-K*-b	3	14	46	11.38	88.64	133.00	10.48	11.38	1111.01
	00033_6_4-0-1-2-4_2_0	AOBB-K*-b-DH	3	14	46	11.38	96.02	163.95	10.48	11.38	1111.01
	00033_6_4-1-2-4-5_2_0	AOBB-K*-b-UFO	3	58	107	10.48	15.42	19.86	10.48	10.48	519.04
	00033_6_4-1-2-4-5_2_0	AOBB-K*-b	3	58	107	10.48	33.52	75.86	10.48	10.48	519.04
	00033_6_4-1-2-4-5_2_0	AOBB-K*-b-DH	3	58	107	10.48	43.87	264.02	10.48	10.48	519.04
	00041_1_0_7_4-0-3-4-5	AOBB-K*-b-UFO	3	62	157	22.73	14.52	76.47	22.73	22.73	883.01
	00041_1_0_7_4-0-3-4-5	AOBB-K*-b	3	59	150	22.73	51.05	timeout	22.73	22.73	883.01
	00041_1_0_7_4-0-3-4-5	AOBB-K*-b-DH	3	98	126	22.73	59.46	443.77	22.73	22.73	883.01
	00042_3_0_7_4-0-1-2-5	AOBB-K*-b-UFO	3	96	383	22.65	13.33	71.43	22.65	22.65	1015.99
4	00042_3_0_7_4-0-1-2-5	AOBB-K*-b	3	27	126	22.65	89.44	timeout	22.65	22.65	1015.99
	00042_3_0_7_4-0-1-2-5	AOBB-K*-b-DH	3	29	80	22.65	98.34	timeout	22.65	22.65	1015.99
	00042_3_0_7_4-1-2-3-4	AOBB-K*-b-DH	3	49	92	22.66	1273.74	timeout	22.65	23.07	2653.46
	00042_3_0_7_4-1-2-3-4	AOBB-K*-b-UFO	3	1178	1893	22.65	16.91	699.97	22.65	23.07	2653.46
	00042_3_0_7_4-1-2-3-4	AOBB-K*-b	3	16	27	22.65	121.30	timeout	22.65	23.07	2653.46
	00043_5_4-0-1-3-4_2_0	AOBB-K*-b-UFO	3	1434	2694	18.19	76.49	484.69	18.04	18.18	119.88
	00043_5_4-0-1-3-4_2_0	AOBB-K*-b-DH	3	1032	2010	18.19	386.49	timeout	18.04	18.18	119.88
	00043_5_4-0-1-3-4_2_0	AOBB-K*-b	3	1042	2032	18.19	896.67	timeout	18.04	18.18	119.88
	00043_5_4-0-2-3-4_2_0	AOBB-K*-b-UFO	3	268	395	18.04	15.15	20.08	18.04	18.04	59.80
	00043_5_4-0-2-3-4_2_0	AOBB-K*-b	3	450	699	18.04	19.07	263.56	18.04	18.04	59.80
	00043_5_4-0-2-3-4_2_0	AOBB-K*-b-DH	3	346	476	18.04	22.48	490.98	18.04	18.04	59.80
	00044_5_4-0-1-3-4_2_0	AOBB-K*-b-UFO	3	2387	4593	18.19	14.97	1340.16	18.19	18.19	67.98
	00044_5_4-0-1-3-4_2_0	AOBB-K*-b	3	1069	2154	18.19	20.75	timeout	18.19	18.19	67.98
	00044_5_4-0-1-3-4_2_0	AOBB-K*-b-DH	3	862	1758	18.19	28.00	timeout	18.19	18.19	67.98
	00044_5_4-1-2-3-4_2_0	AOBB-K*-b-UFO	3	446	3452	18.19	16.46	369.70	18.19	18.19	66.31
	00044_5_4-1-2-3-4_2_0	AOBB-K*-b	3	115	443	18.19	23.50	2611.81	18.19	18.19	66.31
	00044_5_4-1-2-3-4_2_0	AOBB-K*-b-DH	3	265	1574	18.19	33.17	timeout	18.19	18.19	66.31
	00047_2_0_6_4-0-1-2-3	AOBB-K*-b-UFO	3	493	3570	23.08	201.89	timeout	22.70	23.05	1597.58
	00047_2_0_6_4-0-1-2-3	AOBB-K*-b	3	32	219	22.74	161.18	timeout	22.70	23.05	1597.58
	00047_2_0_6_4-0-1-2-3	AOBB-K*-b-DH	3	34	225	22.74	169.41	timeout	22.70	23.05	1597.58
	00047_2_0_6_4-0-1-2-5	AOBB-K*-b-UFO	3	153	793	22.87	72.53	239.88	22.70	22.83	1339.15
	00047_2_0_6_4-0-1-2-5	AOBB-K*-b	3	38	185	22.74	130.95	timeout	22.70	22.83	1339.15
	00047_2_0_6_4-0-1-2-5	AOBB-K*-b-DH	3	35	169	22.74	140.66	timeout	22.70	22.83	1339.15
	00047_2_0_6_4-1-2-3-4	AOBB-K*-b-UFO	3	3558	6719	23.05	94.49	2428.49	22.70	23.05	1440.21
	00047_2_0_6_4-1-2-3-4	AOBB-K*-b	3	64	122	22.80	552.22	timeout	22.70	23.05	1440.21
	00047_2_0_6_4-1-2-3-4	AOBB-K*-b-DH	3	132	254	22.70	50.51	timeout	22.70	23.05	1440.21
	00048_2_0_7_4-1-2-5-6	AOBB-K*-b-UFO	3	328	551	22.81	14.67	146.13	22.81	22.81	404.02
	00048_2_0_7_4-1-2-5-6	AOBB-K*-b-DH	3	111	197	22.81	58.98	timeout	22.81	22.81	404.02
	00048_2_0_7_4-1-2-5-6	AOBB-K*-b	4	56	76	22.81	201.61	554.81	22.81	22.81	404.02

Table 3: Comparison AOBB-K^*-b-[UFO/DH] schemes with BBK^* on problems with 5 mutable residues. For each problem, the AOBB-K^*-b-[UFO/DH] solvers are ranked top-down based on their performance (top being best). Shown is the i-bound used, traversed residue OR and AND nodes, best-found K^* solution (recomputed without underflow-thresholding), the time at which the best-found solution was first discovered ("Anytime"), and the completion time ("Time"). Between AOBB-K^*-b-[UFO/DH] and BBK^*, blue font highlights better values and red font worse values. Italics highlight statistics responsible for a higher ranking in the solver orderings. For reference, the wild-type K^* solution is also shown.

		AOBB-K*-b-[DH/UFO]								BBK*	
M	Problem	Algorithm	i	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b-UFO	3	62	1235	***15.17***	1570.30	timeout	14.08	14.73	401.09
	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b-DH	3	15	234	14.73	*57.91*	timeout	14.08	14.73	401.09
	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b	3	16	268	14.73	62.53	timeout	14.08	14.73	401.09
	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b-UFO	3	100	2031	***14.84***	1284.59	timeout	14.08	14.73	404.03
	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b	3	13	197	14.73	*341.88*	timeout	14.08	14.73	404.03
	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b-DH	3	13	198	14.73	369.87	timeout	14.08	14.73	404.03
	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b-UFO	3	82	1639	*14.84*	891.90	timeout	14.08	15.60	205.56
	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b	3	18	295	14.73	*67.53*	timeout	14.08	15.60	205.56
	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b-DH	3	15	244	14.73	156.68	timeout	14.08	15.60	205.56
	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b-UFO	3	130	2635	14.73	*28.85*	timeout	14.08	15.60	201.04
	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b	3	13	200	14.73	*75.53*	timeout	14.08	15.60	201.04
	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b-DH	3	15	245	14.73	93.41	timeout	14.08	15.60	201.04
	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b-UFO	3	470	5245	***16.60***	2978.16	timeout	15.79	16.58	753.95
	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b	3	15	243	16.58	*61.89*	timeout	15.79	16.58	753.95
	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b-DH	3	15	242	16.58	80.37	timeout	15.79	16.58	753.95
	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b-UFO	3	329	3620	***16.60***	1872.22	timeout	15.79	16.58	628.53
	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b	3	19	302	16.58	*65.70*	timeout	15.79	16.58	628.53
	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b-DH	3	21	354	16.58	82.87	timeout	15.79	16.58	628.53
	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b-UFO	3	709	1378	*16.24*	3365.86	timeout	15.79	16.25	501.48
	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b	3	15	227	15.79	*30.54*	timeout	15.79	16.25	501.48
	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b-DH	3	15	215	15.79	48.73	timeout	15.79	16.25	501.48
	00027_6_5-0-1-2-3-5_1_0	AOBB-K*-b	3	137	423	15.55	*274.30*	timeout	15.48	15.55	1270.65
	00027_6_5-0-1-2-3-5_1_0	AOBB-K*-b-UFO	3	137	423	15.55	*276.91*	timeout	15.48	15.55	1270.65
	00027_6_5-0-1-2-3-5_1_0	AOBB-K*-b-DH	3	132	416	15.55	321.02	timeout	15.48	15.55	1270.65
	00028_1_0_6_5-0-1-2-3-5	AOBB-K*-b	3	362	934	15.27	*44.51*	timeout	15.27	15.27	98.97
	00028_1_0_6_5-0-1-2-3-5	AOBB-K*-b-UFO	3	362	934	15.27	*46.65*	timeout	15.27	15.27	98.97
	00028_1_0_6_5-0-1-2-3-5	AOBB-K*-b-DH	3	357	919	15.27	60.33	timeout	15.27	15.27	98.97
	00028_1_0_6_5-0-2-3-4-5	AOBB-K*-b-UFO	3	1182	3214	15.44	*63.56*	timeout	15.27	15.44	64.50
	00028_1_0_6_5-0-2-3-4-5	AOBB-K*-b	3	877	2417	15.44	*69.11*	timeout	15.27	15.44	64.50
	00028_1_0_6_5-0-2-3-4-5	AOBB-K*-b-DH	3	425	1226	15.44	204.31	timeout	15.27	15.44	64.50
	00028_1_0_6_5-1-2-3-4-5	AOBB-K*-b-UFO	3	1053	3397	15.44	*94.05*	timeout	15.27	15.44	62.30
	00028_1_0_6_5-1-2-3-4-5	AOBB-K*-b	3	1029	3311	15.44	*102.56*	timeout	15.27	15.44	62.30
	00028_1_0_6_5-1-2-3-4-5	AOBB-K*-b-DH	3	1023	3274	15.44	297.86	timeout	15.27	15.44	62.30
	00031_2_0_5_5-0-1-2-3-4	AOBB-K*-b-UFO	3	211	1020	7.88	*22.35*	128.75	7.63	7.88	130.04
	00031_2_0_5_5-0-1-2-3-4	AOBB-K*-b	3	129	876	7.88	*129.43*	timeout	7.63	7.88	130.04
	00031_2_0_5_5-0-1-2-3-4	AOBB-K*-b-DH	3	128	867	7.88	145.63	timeout	7.63	7.88	130.04
	00033_6_5-0-1-2-3-4_2_0	AOBB-K*-b	3	49	117	11.38	*108.93*	218.20	10.48	11.38	1165.00
	00033_6_5-0-1-2-3-4_2_0	AOBB-K*-b-UFO	3	49	117	11.38	*111.01*	220.16	10.48	11.38	1165.00
	00033_6_5-0-1-2-3-4_2_0	AOBB-K*-b-DH	3	49	117	11.38	120.67	419.25	10.48	11.38	1165.00
	00033_6_5-0-1-2-3-5_2_0	AOBB-K*-b	3	612	1349	11.38	*153.84*	555.26	10.48	11.38	1133.88
	00033_6_5-0-1-2-3-5_2_0	AOBB-K*-b-UFO	3	612	1349	11.38	*155.81*	557.34	10.48	11.38	1133.88
	00033_6_5-0-1-2-3-5_2_0	AOBB-K*-b-DH	3	612	1349	11.38	170.78	2017.05	10.48	11.38	1133.88
	00044_5_5-0-1-2-3-4_2_0	AOBB-K*-b	3	1179	2613	18.19	*33.76*	timeout	18.19	18.19	70.22
	00044_5_5-0-1-2-3-4_2_0	AOBB-K*-b-UFO	3	1178	2608	18.19	*35.75*	timeout	18.19	18.19	70.22
	00044_5_5-0-1-2-3-4_2_0	AOBB-K*-b-DH	3	1203	2673	18.19	51.49	timeout	18.19	18.19	70.22
	00047_2_0_6_5-0-1-2-3-4	AOBB-K*-b-UFO	3	339	2371	***23.08***	**2068.22**	timeout	22.70	23.05	6984.35
	00047_2_0_6_5-0-1-2-3-4	AOBB-K*-b	3	11	88	22.74	*222.66*	timeout	22.70	23.05	6984.35
	00047_2_0_6_5-0-1-2-3-4	AOBB-K*-b-DH	3	12	96	22.74	241.88	timeout	22.70	23.05	6984.35
	00047_2_0_6_5-0-1-2-3-5	AOBB-K*-b-UFO	3	370	3160	*22.77*	2645.82	timeout	22.70	23.05	1696.25
	00047_2_0_6_5-0-1-2-3-5	AOBB-K*-b	3	12	149	22.74	*216.61*	timeout	22.70	23.05	1696.25
	00047_2_0_6_5-0-1-2-3-5	AOBB-K*-b-DH	3	18	227	22.74	234.91	timeout	22.70	23.05	1696.25
	00047_2_0_6_5-0-1-2-4-5	AOBB-K*-b-UFO	3	2421	9738	***22.87***	3263.79	timeout	22.70	22.83	1374.29
	00047_2_0_6_5-0-1-2-4-5	AOBB-K*-b	3	20	187	22.74	*216.96*	timeout	22.70	22.83	1374.29
	00047_2_0_6_5-0-1-2-4-5	AOBB-K*-b-DH	3	20	164	22.74	235.27	timeout	22.70	22.83	1374.29

Evaluating Dynamic Heuristics. As highlighted in the main paper, the dynamic heuristic re-computation often influences the search space considerably, sometimes reducing it (ex. 00018_2_0_6_4-0-1-2-5) while in other cases causing an increase in the number of nodes explored (ex. 00044_5_4-1-2-3-4_2_0). The latter case may occur if dynamic heuristic re-computation causes the K* estimate for a node to increase rather than decrease (specifically by decreasing the denominator Z_U estimate which wMBE-K*-b does not guarantee to be a lower bound) preventing nodes from being pruned. The reduction of AOBB-K*-b-DH's performance relative to AOBB-K*-b on progressively larger problems (as can be seen by AOBB-K*-b-DH's relative ranking) can be explained by (1) the fact that, even for the same i-bound, heuristic computations become much more expensive for problems with more mutable residues due to increases in domain size, and (2) the current naive implementation of dynamic heuristic re-computations does not leverage the problem's structure nor re-use portions of the heuristic that are unchanging (recomputing everything from scratch), this later point leaving an open direction for future research. Furthermore, as highlighted in the main paper, the discovery of high levels of determinism in the heuristic messages of the larger problems indicates potential for moving to more compact data structures (such as using a relational representations) that can take advantage of repeating determinism and lead to use of greater i-bounds and potentially improve computation time.

UFO Impact. From the rank-based ordering of the algorithms, the competitiveness of the UFO scheme is apparent. The frequency of blue coloring for UFO shows the algorithms' competitiveness against BBK* on the problems with three, four, and five mutable residues.

AOBB-K*-b Although AOBB-K*-b generally ranked lower than one of other AOBB-K*-b variants, even without augmentation it keeps up with BBK* through problems with 4 mutable residues, and even finds respectable solutions for some 5-mutable-residue problems. This is a significant scalability increase as the original AOBB-K* could not scale up to problems with more than 3 mutable residues.

2.2 DH + UFO COMBINATION EVALUATION

UFO δ Hyper Parameter Choice. To choose the δ to compare for AOBB-K^*-b-UFO and AOBB-K^*-b-DH-UFO, we ran both algorithms with various $\delta \in \{0.001, 0.010, 0.100, 0.250, 0.500, 0.750, 1.000\}$ and, for each, chose the δ that resulted in producing the highest quality K^* solution most frequently (ie. across all problems), and then by the speed at which their final solution was first discovered. For AOBB-K^*-b-UFO this resulted in $\delta = 0.1$, and for AOBB-K^*-b-DH-UFO this resulted in $\delta = 0.01$.

Table Description The following tables compare the performance of various combinations of the AOBB-K^*-b-[DH/UFO] schemes with each other and to BBK^*. The results are separated into six tables: Table 4 shows results on the "Expanded" problem set from Pezeshki et al. [2022] with 3 mutable residues, Table 5 (split across three sub tables) shows results on problems expanded to have 4 mutable residues, and Table 5 (split across two sub tables) shows results on problems expanded to have 5 mutable residues. Please see Section 2.0.3 of this document for the description of the instance nomenclature.

For each problem, the AOBB-K^*-b-[UFO/DH] solvers are ranked top-down based on their performance (top being best). A solver's rank is first determined by the quality of K^* found (higher is better), and then by how fast their respective final solution was first discovered. The columns in the tables are as follows:

M: Number of mutable residues

Problem: Problem instance designation (as described in Section 2.0.3 above)

Algorithm Specific AOBB-K^*-b-[DH/UFO] algorithm

i i-bound used for the wMBE-K^*-b heuristic

δ δ used to decrease the UFO underflow-threshold found

OR Number of residue variable OR nodes explored

AND Number of residue variable AND nodes explored

Soln Algorithm's K^* solution. (This value is recomputed using a non-thresholded problem).

Anytime The time (in seconds) at which the final solution was first discovered.

Time The completion time of the algorithm if under 3600 seconds ("timeout" otherwise).

wt K^* The wild-type protein's K^* value.

Table 4: Comparison of combinations of AOBB-K*-b-[UFO/DH] schemes, and to BBK*, on problems with 3 mutable residues. For each problem, the AOBB-K*-b-[UFO/DH] solvers are ranked top-down based on their performance (top being best). Shown is the i-bound used, δ used to decrease the UFO underflow-threshold found, residue OR and AND nodes traversed, best-found K* solution (recomputed without underflow-thresholding), the time at which the best-found solution was first discovered ("Anytime"), and the completion time ("Time"). Between AOBB-K*-b-[UFO/DH] and BBK*, blue font highlights better values and red font worse values. Italics highlights statistics responsible for a higher ranking in the solver orderings. For reference, the wild-type K* solution is also shown.

	AOBB-K*-b-[DH/UFO]										BBK*	
M	Problem	Algorithm	i	δ	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
3	00007_1_0_7_3	AOBB-K*-b-UFO	3	0.1	19	364	14.73	*7.45*	462.85	14.08	14.73	369.42
3	00007_1_0_7_3	AOBB-K*-b	3	0	19	360	14.73	*8.69*	timeout	14.08	14.73	369.42
3	00007_1_0_7_3	AOBB-K*-b-DH	3	0	50	503	14.73	*10.38*	2862.36	14.08	14.73	369.42
3	00007_1_0_7_3	AOBB-K*-b-DH-UFO	3	0.01	7	76	14.73	10.87	82.15	14.08	14.73	369.42
3	00009_2_0_3_3	AOBB-K*-b-DH-UFO	3	0.01	4	18	4.51	*7.87*	24.94	4.09	4.51	215.82
3	00009_2_0_3_3	AOBB-K*-b-DH	3	0	4	21	4.51	*10.29*	33.11	4.09	4.51	215.82
3	00009_2_0_3_3	AOBB-K*-b-UFO	3	0.1	219	3417	4.51	*10.57*	346.37	4.09	4.51	215.82
3	00009_2_0_3_3	AOBB-K*-b	3	0	238	3138	4.51	74.68	timeout	4.09	4.51	215.82
3	00011_2_0_3_3	AOBB-K*-b	3	0	58	197	11.85	*6.35*	60.55	11.75	11.85	26.58
3	00011_2_0_3_3	AOBB-K*-b-UFO	3	0.1	55	187	11.85	*6.41*	24.99	11.75	11.85	26.58
3	00011_2_0_3_3	AOBB-K*-b-DH	3	0	3	15	11.85	*7.70*	24.22	11.75	11.85	26.58
3	00011_2_0_3_3	AOBB-K*-b-DH-UFO	3	0.01	3	15	11.85	8.00	24.36	11.75	11.85	26.58
3	00012_3_0_3_3	AOBB-K*-b	3	0	21	122	*13.93*	*4.46*	20.73	13.93	13.93	11.83
3	00012_3_0_3_3	AOBB-K*-b-DH	3	0	3	13	*13.93*	*7.45*	21.56	13.93	13.93	11.83
3	00012_3_0_3_3	AOBB-K*-b-DH-UFO	3	0.01	3	14	*13.93*	8.89	23.20	13.93	13.93	11.83
3	00012_3_0_3_3	AOBB-K*-b-UFO	3	0.1	21	119	13.91	6.24	8.57	13.93	13.93	11.83
3	00013_3_0_4_3	AOBB-K*-b-UFO	3	0.1	22	421	15.03	*6.10*	86.24	13.25	15.03	39.22
3	00013_3_0_4_3	AOBB-K*-b	3	0	23	443	15.03	*7.01*	3102.95	13.25	15.03	39.22
3	00013_3_0_4_3	AOBB-K*-b-DH-UFO	3	0.01	3	5	15.03	*9.19*	9.19	13.25	15.03	39.22
3	00013_3_0_4_3	AOBB-K*-b-DH	3	0	3	5	15.03	10.15	10.15	13.25	15.03	39.22
3	00014_3_0_3_3	AOBB-K*-b	3	0	25	132	14.36	*5.82*	21.87	13.96	14.36	44.93
3	00014_3_0_3_3	AOBB-K*-b-UFO	3	0.1	25	130	14.36	*6.20*	8.88	13.96	14.36	44.93
3	00014_3_0_3_3	AOBB-K*-b-DH	3	0	3	16	14.36	*8.79*	26.08	13.96	14.36	44.93
3	00014_3_0_3_3	AOBB-K*-b-DH-UFO	3	0.01	3	16	14.36	9.14	26.37	13.96	14.36	44.93
3	00017_2_0_4_3	AOBB-K*-b-UFO	3	0.1	253	3322	10.86	*7.36*	163.41	10.52	10.80	78.00
3	00017_2_0_4_3	AOBB-K*-b-DH-UFO	3	0.01	8	23	10.86	*8.80*	33.74	10.52	10.80	78.00
3	00017_2_0_4_3	AOBB-K*-b-DH	3	0	21	38	10.86	*15.80*	41.03	10.52	10.80	78.00
3	00017_2_0_4_3	AOBB-K*-b	3	0	182	3145	10.86	154.77	timeout	10.52	10.80	78.00
3	00019_3_0_3_3	AOBB-K*-b-UFO	3	0.1	320	5045	14.99	*6.12*	650.54	14.99	14.99	34.00
3	00019_3_0_3_3	AOBB-K*-b	3	0	174	2551	14.99	*8.30*	timeout	14.99	14.99	34.00
3	00019_3_0_3_3	AOBB-K*-b-DH-UFO	3	0.01	8	30	14.99	*9.22*	45.29	14.99	14.99	34.00
3	00019_3_0_3_3	AOBB-K*-b-DH	3	0	8	30	14.99	11.31	56.05	14.99	14.99	34.00
3	00020_3_0_3_3	AOBB-K*-b-DH-UFO	3	0.01	3	44	10.96	*10.88*	61.36	10.60	10.96	1388.13
3	00020_3_0_3_3	AOBB-K*-b-UFO	3	0.1	261	2657	10.96	*15.40*	483.65	10.60	10.96	1388.13
3	00020_3_0_3_3	AOBB-K*-b-DH	3	0	3	44	10.96	*39.67*	339.91	10.60	10.96	1388.13
3	00020_3_0_3_3	AOBB-K*-b	3	0	127	1510	10.96	305.05	timeout	10.60	10.96	1388.13
3	00021_1_0_4_3	AOBB-K*-b-DH-UFO	3	0.01	78	165	11.92	*59.60*	129.70	9.37	11.72	551.27
3	00021_1_0_4_3	AOBB-K*-b-DH	3	0	75	158	11.92	*136.44*	1307.45	9.37	11.72	551.27
3	00021_1_0_4_3	AOBB-K*-b-UFO	3	0.1	248	2741	11.92	*210.30*	707.73	9.37	11.72	551.27
3	00021_1_0_4_3	AOBB-K*-b	3	0	71	823	11.92	2831.38	timeout	9.37	11.72	551.27
3	00025_3_0_4_3	AOBB-K*-b-DH-UFO	3	0.01	4	12	16.18	*13.43*	22.25	10.74	13.65	880.46
3	00025_3_0_4_3	AOBB-K*-b-DH	3	0	4	23	16.18	*51.92*	80.22	10.74	13.65	880.46
3	00025_3_0_4_3	AOBB-K*-b-UFO	3	0.1	17	268	16.18	*52.08*	76.09	10.74	13.65	880.46
3	00025_3_0_4_3	AOBB-K*-b	3	0	30	492	16.18	2636.07	timeout	10.74	13.65	880.46
3	00030_4_3_2_0	AOBB-K*-b-UFO	3	0.1	207	2718	11.12	*8.39*	140.90	10.35	10.97	275.38
3	00030_4_3_2_0	AOBB-K*-b-DH-UFO	3	0.01	22	39	11.12	*8.99*	33.12	10.35	10.97	275.38
3	00030_4_3_2_0	AOBB-K*-b-DH	3	0	70	141	11.12	*24.88*	52.57	10.35	10.97	275.38
3	00030_4_3_2_0	AOBB-K*-b	3	0	254	3666	11.12	117.20	2014.81	10.35	10.97	275.38

Table 5: Comparison of combinations of AOBB-K*-b-[UFO/DH] schemes, and to BBK*, on problems with 4 mutable residues. For each problem, the AOBB-K*-b-[UFO/DH] solvers are ranked top-down based on their performance (top being best). Shown is the i-bound used, δ used to decrease the UFO underflow-threshold found, residue OR and AND nodes traversed, best-found K* solution (recomputed without underflow-thresholding), the time at which the best-found solution was first discovered ("Anytime"), and the completion time ("Time"). Between AOBB-K*-b-[UFO/DH] and BBK*, blue font highlights better values and red font worse values. Italics highlights statistics responsible for a higher ranking in the solver orderings. For reference, the wild-type K* solution is also shown.

AOBB-K*-b-[DH/UFO]											BBK*	
M	Problem	Algorithm	i	δ	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
4	00007_1_0_7_4-0-1-5-6	AOBB-K*-b-UFO	3	0.1	123	2422	*15.66*	1891.16	timeout	14.08	15.60	204.06
4	00007_1_0_7_4-0-1-5-6	AOBB-K*-b-DH-UFO	3	0.01	52	386	*15.34*	968.59	1081.68	14.08	15.60	204.06
4	00007_1_0_7_4-0-1-5-6	AOBB-K*-b-DH	3	0	53	423	*14.25*	348.73	timeout	14.08	15.60	204.06
4	00007_1_0_7_4-0-1-5-6	AOBB-K*-b	3	0	69	618	14.08	13.88	timeout	14.08	15.60	204.06
4	00007_1_0_7_4-1-2-3-5	AOBB-K*-b-DH-UFO	3	0.01	268	2053	*14.59*	649.16	timeout	14.08	14.54	278.08
4	00007_1_0_7_4-1-2-3-5	AOBB-K*-b-UFO	3	0.1	78	1428	*14.53*	2403.87	timeout	14.08	14.54	278.08
4	00007_1_0_7_4-1-2-3-5	AOBB-K*-b-DH	3	0	28	306	*14.49*	3543.27	timeout	14.08	14.54	278.08
4	00007_1_0_7_4-1-2-3-5	AOBB-K*-b	3	0	12	185	14.49	3293.62	timeout	14.08	14.54	278.08
4	00007_1_0_7_4-1-2-5-6	AOBB-K*-b-UFO	3	0.1	143	795	*14.93*	739.77	739.78	14.08	15.60	211.31
4	00007_1_0_7_4-1-2-5-6	AOBB-K*-b-DH-UFO	3	0.01	129	697	*14.67*	967.54	1056.77	14.08	15.60	211.31
4	00007_1_0_7_4-1-2-5-6	AOBB-K*-b	3	0	53	391	14.43	*3324.07*	timeout	14.08	15.60	211.31
4	00007_1_0_7_4-1-2-5-6	AOBB-K*-b-DH	3	0	53	391	14.43	3327.38	timeout	14.08	15.60	211.31
4	00013_3_0_4_4-0-1-2-3	AOBB-K*-b-UFO	3	0.1	346	6147	15.03	*12.45*	2085.58	13.25	15.03	46.46
4	00013_3_0_4_4-0-1-2-3	AOBB-K*-b	3	0	23	437	15.03	*14.82*	timeout	13.25	15.03	46.46
4	00013_3_0_4_4-0-1-2-3	AOBB-K*-b-DH-UFO	3	0.01	21	23	15.03	*19.32*	73.71	13.25	15.03	46.46
4	00013_3_0_4_4-0-1-2-3	AOBB-K*-b-DH	3	0	21	23	15.03	22.05	79.88	13.25	15.03	46.46
4	00017_2_0_4_4-0-1-2-3	AOBB-K*-b-UFO	3	0.1	2044	24496	10.86	*23.31*	timeout	10.52	10.80	89.94
4	00017_2_0_4_4-0-1-2-3	AOBB-K*-b-DH-UFO	3	0.01	1732	16826	10.86	*45.14*	timeout	10.52	10.80	89.94
4	00017_2_0_4_4-0-1-2-3	AOBB-K*-b	3	0	38	636	10.86	*186.07*	timeout	10.52	10.80	89.94
4	00017_2_0_4_4-0-1-2-3	AOBB-K*-b-DH	3	0	132	2208	10.86	660.16	timeout	10.52	10.80	89.94
4	00018_2_0_6_4-0-1-2-4	AOBB-K*-b-DH-UFO	3	0.01	736	1613	*17.02*	*1447.78*	3385.86	15.79	16.58	610.41
4	00018_2_0_6_4-0-1-2-4	AOBB-K*-b-UFO	3	0.1	581	5284	*17.02*	2997.10	timeout	15.79	16.58	610.41
4	00018_2_0_6_4-0-1-2-4	AOBB-K*-b-DH	3	0	82	180	*16.60*	1614.68	timeout	15.79	16.58	610.41
4	00018_2_0_6_4-0-1-2-4	AOBB-K*-b	3	0	108	973	16.58	40.78	timeout	15.79	16.58	610.41
4	00018_2_0_6_4-0-1-2-5	AOBB-K*-b-UFO	3	0.1	245	1110	16.58	*14.17*	160.99	15.79	16.58	581.77
4	00018_2_0_6_4-0-1-2-5	AOBB-K*-b-DH-UFO	3	0.01	40	56	16.58	*17.90*	90.14	15.79	16.58	581.77
4	00018_2_0_6_4-0-1-2-5	AOBB-K*-b	3	0	279	1214	16.58	*33.31*	3038.51	15.79	16.58	581.77
4	00018_2_0_6_4-0-1-2-5	AOBB-K*-b-DH	3	0	40	56	16.58	40.13	597.84	15.79	16.58	581.77
4	00018_2_0_6_4-1-2-3-5	AOBB-K*-b-DH-UFO	3	0.01	3851	7487	*16.20*	*150.65*	timeout	15.79	16.20	535.01
4	00018_2_0_6_4-1-2-3-5	AOBB-K*-b-UFO	3	0.1	5736	11167	*16.20*	183.44	timeout	15.79	16.20	535.01
4	00018_2_0_6_4-1-2-3-5	AOBB-K*-b-DH	3	0	60	451	*16.17*	513.20	timeout	15.79	16.20	535.01
4	00018_2_0_6_4-1-2-3-5	AOBB-K*-b	3	0	46	362	15.79	15.97	timeout	15.79	16.20	535.01

		AOBB-K*-b-[DH/UFO]									BBK*	
M	Problem	Algorithm	i	δ	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
4	00021_4_4-0-1-2-3_1_0	AOBB-K*-b-DH-UFO	3	0.01	355	1095	***11.92***	***72.76***	2151.32	9.37	11.72	687.66
4	00021_4_4-0-1-2-3_1_0	AOBB-K*-b-UFO	3	0.1	484	8275	***11.92***	***234.60***	timeout	9.37	11.72	687.66
4	00021_4_4-0-1-2-3_1_0	AOBB-K*-b-DH	3	0	122	301	***11.92***	**614.88**	timeout	9.37	11.72	687.66
4	00021_4_4-0-1-2-3_1_0	AOBB-K*-b	3	0	19	352	11.72	259.49	timeout	9.37	11.72	687.66
4	00024_4_4-0-1-2-3_3_0	AOBB-K*-b-UFO	3	0.1	87	395	**12.96**	***37.12***	44.19	11.79	12.93	128.99
4	00024_4_4-0-1-2-3_3_0	AOBB-K*-b	3	0	94	437	**12.96**	***89.50***	423.39	11.79	12.93	128.99
4	00024_4_4-0-1-2-3_3_0	AOBB-K*-b-DH-UFO	3	0.01	85	242	**12.96**	*135.42*	150.76	11.79	12.93	128.99
4	00024_4_4-0-1-2-3_3_0	AOBB-K*-b-DH	3	0	92	251	**12.96**	137.42	415.53	11.79	12.93	128.99
4	00027_6_4-0-2-3-5_1_0	AOBB-K*-b-UFO	3	0.1	51	126	15.55	*25.26*	49.11	15.48	15.55	476.84
4	00027_6_4-0-2-3-5_1_0	AOBB-K*-b	3	0	57	137	15.55	*79.11*	257.91	15.48	15.55	476.84
4	00027_6_4-0-2-3-5_1_0	AOBB-K*-b-DH-UFO	3	0.01	51	126	15.55	*122.98*	188.72	15.48	15.55	476.84
4	00027_6_4-0-2-3-5_1_0	AOBB-K*-b-DH	3	0	57	137	15.55	185.02	410.88	15.48	15.55	476.84
4	00027_6_4-1-2-3-4_1_0	AOBB-K*-b-UFO	3	0.1	89	146	15.64	*16.17*	17.22	15.48	15.64	99.34
4	00027_6_4-1-2-3-4_1_0	AOBB-K*-b	3	0	97	158	15.64	*23.59*	27.62	15.48	15.64	99.34
4	00027_6_4-1-2-3-4_1_0	AOBB-K*-b-DH-UFO	3	0.01	89	146	15.64	*162.82*	198.27	15.48	15.64	99.34
4	00027_6_4-1-2-3-4_1_0	AOBB-K*-b-DH	3	0	97	158	15.64	193.25	233.56	15.48	15.64	99.34
4	00027_6_4-2-3-4-5_1_0	AOBB-K*-b-UFO	3	0.1	906	1433	**15.73**	***65.67***	88.96	15.48	15.64	93.40
4	00027_6_4-2-3-4-5_1_0	AOBB-K*-b	3	0	1023	1635	**15.73**	*330.78*	672.67	15.48	15.64	93.40
4	00027_6_4-2-3-4-5_1_0	AOBB-K*-b-DH	3	0	1023	1635	**15.73**	*1282.45*	2393.03	15.48	15.64	93.40
4	00027_6_4-2-3-4-5_1_0	AOBB-K*-b-DH-UFO	3	0.01	909	1437	**15.73**	1305.61	1633.88	15.48	15.64	93.40
4	00028_1_0_6_4-0-1-2-3	AOBB-K*-b-UFO	3	0.1	7	16	15.27	*16.25*	16.98	15.27	15.27	92.03
4	00028_1_0_6_4-0-1-2-3	AOBB-K*-b	3	0	9	19	15.27	*17.33*	21.83	15.27	15.27	92.03
4	00028_1_0_6_4-0-1-2-3	AOBB-K*-b-DH-UFO	3	0.01	7	9	15.27	*23.20*	30.22	15.27	15.27	92.03
4	00028_1_0_6_4-0-1-2-3	AOBB-K*-b-DH	3	0	9	12	15.27	24.90	38.09	15.27	15.27	92.03
4	00028_1_0_6_4-0-2-3-5	AOBB-K*-b-UFO	3	0.1	83	200	15.27	*15.50*	54.27	15.27	15.27	95.25
4	00028_1_0_6_4-0-2-3-5	AOBB-K*-b	3	0	93	230	15.27	*16.08*	337.70	15.27	15.27	95.25
4	00028_1_0_6_4-0-2-3-5	AOBB-K*-b-DH	3	0	93	230	15.27	*22.16*	514.96	15.27	15.27	95.25
4	00028_1_0_6_4-0-2-3-5	AOBB-K*-b-DH-UFO	3	0.01	85	203	15.27	22.76	273.31	15.27	15.27	95.25
4	00028_1_0_6_4-1-2-3-4	AOBB-K*-b-UFO	3	0.1	85	133	*15.44*	*16.43*	16.54	15.27	15.44	60.18
4	00028_1_0_6_4-1-2-3-4	AOBB-K*-b-DH-UFO	3	0.01	88	137	*15.44*	*195.69*	199.40	15.27	15.44	60.18
4	00028_1_0_6_4-1-2-3-4	AOBB-K*-b-DH	3	0	199	282	*15.44*	*222.76*	227.07	15.27	15.44	60.18
4	00028_1_0_6_4-1-2-3-4	AOBB-K*-b	3	0	139	164	15.35	14.05	16.82	15.27	15.44	60.18
4	00028_1_0_6_4-2-3-4-5	AOBB-K*-b-UFO	3	0.1	702	1057	15.44	*15.88*	75.98	15.27	15.44	57.35
4	00028_1_0_6_4-2-3-4-5	AOBB-K*-b	3	0	771	1193	15.44	*26.52*	570.92	15.27	15.44	57.35
4	00028_1_0_6_4-2-3-4-5	AOBB-K*-b-DH	3	0	771	1193	15.44	*78.57*	1814.41	15.27	15.44	57.35
4	00028_1_0_6_4-2-3-4-5	AOBB-K*-b-DH-UFO	3	0.01	705	1061	15.44	84.63	1493.68	15.27	15.44	57.35
4	00030_4_4-0-1-2-3_2_0	AOBB-K*-b-UFO	3	0.1	715	7454	**11.12**	***18.81***	1254.35	10.35	10.97	253.55
4	00030_4_4-0-1-2-3_2_0	AOBB-K*-b-DH-UFO	3	0.01	756	6817	**11.12**	***28.43***	1515.99	10.35	10.97	253.55
4	00030_4_4-0-1-2-3_2_0	AOBB-K*-b	3	0	277	3413	**11.12**	***227.47***	timeout	10.35	10.97	253.55
4	00030_4_4-0-1-2-3_2_0	AOBB-K*-b-DH	3	0	270	2592	**11.12**	285.82	timeout	10.35	10.97	253.55
4	00033_6_4-0-1-2-3_2_0	AOBB-K*-b-UFO	3	0.1	73	201	11.38	*20.72*	62.29	10.48	11.38	2488.59
4	00033_6_4-0-1-2-3_2_0	AOBB-K*-b-DH-UFO	3	0.01	73	205	11.38	*28.50*	193.16	10.48	11.38	2488.59
4	00033_6_4-0-1-2-3_2_0	AOBB-K*-b-DH	3	0	73	277	11.38	*96.51*	848.47	10.48	11.38	2488.59
4	00033_6_4-0-1-2-3_2_0	AOBB-K*-b	3	0	73	277	11.38	117.15	718.92	10.48	11.38	2488.59
4	00033_6_4-0-1-2-4_2_0	AOBB-K*-b-UFO	3	0.1	14	46	11.38	*16.99*	23.29	10.48	11.38	1111.01
4	00033_6_4-0-1-2-4_2_0	AOBB-K*-b-DH-UFO	3	0.01	14	46	11.38	*27.49*	49.17	10.48	11.38	1111.01
4	00033_6_4-0-1-2-4_2_0	AOBB-K*-b	3	0	14	46	11.38	*88.64*	133.00	10.48	11.38	1111.01
4	00033_6_4-0-1-2-4_2_0	AOBB-K*-b-DH	3	0	14	46	11.38	96.02	163.95	10.48	11.38	1111.01
4	00033_6_4-1-2-4-5_2_0	AOBB-K*-b-UFO	3	0.1	58	107	10.48	*15.26*	19.95	10.48	10.48	519.04
4	00033_6_4-1-2-4-5_2_0	AOBB-K*-b-DH-UFO	3	0.01	58	107	10.48	*24.25*	180.20	10.48	10.48	519.04
4	00033_6_4-1-2-4-5_2_0	AOBB-K*-b	3	0	58	107	10.48	*33.52*	75.86	10.48	10.48	519.04
4	00033_6_4-1-2-4-5_2_0	AOBB-K*-b-DH	3	0	58	107	10.48	43.87	264.02	10.48	10.48	519.04

		AOBB-K*-b-[DH/UFO]									BBK*	
M	Problem	Algorithm	i	δ	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
4	00041_1_0_7_4-0-3-4-5	AOBB-K*-b-UFO	3	0.1	63	165	22.73	*14.62*	97.66	22.73	22.73	883.01
4	00041_1_0_7_4-0-3-4-5	AOBB-K*-b-DH-UFO	3	0.01	37	54	22.73	*23.35*	108.41	22.73	22.73	883.01
4	00041_1_0_7_4-0-3-4-5	AOBB-K*-b	3	0	59	150	22.73	*51.05*	timeout	22.73	22.73	883.01
4	00041_1_0_7_4-0-3-4-5	AOBB-K*-b-DH	3	0	98	126	22.73	59.46	443.77	22.73	22.73	883.01
4	00042_3_0_7_4-0-1-2-5	AOBB-K*-b-UFO	3	0.1	100	392	22.65	*13.09*	76.54	22.65	22.65	1015.99
4	00042_3_0_7_4-0-1-2-5	AOBB-K*-b-DH-UFO	3	0.01	30	31	22.65	*21.11*	120.87	22.65	22.65	1015.99
4	00042_3_0_7_4-0-1-2-5	AOBB-K*-b	3	0	27	126	22.65	*89.44*	timeout	22.65	22.65	1015.99
4	00042_3_0_7_4-0-1-2-5	AOBB-K*-b-DH	3	0	29	80	22.65	98.34	timeout	22.65	22.65	1015.99
4	00042_3_0_7_4-1-2-3-4	AOBB-K*-b-DH-UFO	3	0.01	1820	3512	*22.96*	183.56	timeout	22.65	23.07	2653.46
4	00042_3_0_7_4-1-2-3-4	AOBB-K*-b-DH	3	0	49	92	*22.66*	1273.74	timeout	22.65	23.07	2653.46
4	00042_3_0_7_4-1-2-3-4	AOBB-K*-b-UFO	3	0.1	901	1339	22.65	*16.59*	345.13	22.65	23.07	2653.46
4	00042_3_0_7_4-1-2-3-4	AOBB-K*-b	3	0	16	27	22.65	121.30	timeout	22.65	23.07	2653.46
4	00043_5_4-0-1-3-4_2_0	AOBB-K*-b-DH-UFO	3	0.01	1507	2836	**18.19**	***63.96***	1184.58	18.04	18.18	119.88
4	00043_5_4-0-1-3-4_2_0	AOBB-K*-b-UFO	3	0.1	1473	2768	**18.19**	***79.08***	521.49	18.04	18.18	119.88
4	00043_5_4-0-1-3-4_2_0	AOBB-K*-b-DH	3	0	1032	2010	**18.19**	*386.49*	timeout	18.04	18.18	119.88
4	00043_5_4-0-1-3-4_2_0	AOBB-K*-b	3	0	1042	2032	**18.19**	896.67	timeout	18.04	18.18	119.88
4	00043_5_4-0-2-3-4_2_0	AOBB-K*-b-UFO	3	0.1	288	420	18.04	*14.83*	20.02	18.04	18.04	59.80
4	00043_5_4-0-2-3-4_2_0	AOBB-K*-b-DH-UFO	3	0.01	256	311	18.04	*18.08*	401.72	18.04	18.04	59.80
4	00043_5_4-0-2-3-4_2_0	AOBB-K*-b	3	0	450	699	18.04	*19.07*	263.56	18.04	18.04	59.80
4	00043_5_4-0-2-3-4_2_0	AOBB-K*-b-DH	3	0	346	476	18.04	22.48	490.98	18.04	18.04	59.80
4	00044_5_4-0-1-3-4_2_0	AOBB-K*-b-UFO	3	0.1	2406	4631	18.19	*14.47*	1428.82	18.19	18.19	67.98
4	00044_5_4-0-1-3-4_2_0	AOBB-K*-b	3	0	1069	2154	18.19	*20.75*	timeout	18.19	18.19	67.98
4	00044_5_4-0-1-3-4_2_0	AOBB-K*-b-DH-UFO	3	0.01	2458	4732	18.19	*21.46*	2749.93	18.19	18.19	67.98
4	00044_5_4-0-1-3-4_2_0	AOBB-K*-b-DH	3	0	862	1758	18.19	28.00	timeout	18.19	18.19	67.98
4	00044_5_4-1-2-3-4_2_0	AOBB-K*-b-UFO	3	0.1	465	3545	18.19	*16.05*	398.80	18.19	18.19	66.31
4	00044_5_4-1-2-3-4_2_0	AOBB-K*-b	3	0	115	443	18.19	*23.50*	2611.81	18.19	18.19	66.31
4	00044_5_4-1-2-3-4_2_0	AOBB-K*-b-DH-UFO	3	0.01	417	1937	18.19	*24.66*	461.01	18.19	18.19	66.31
4	00044_5_4-1-2-3-4_2_0	AOBB-K*-b-DH	3	0	265	1574	18.19	33.17	timeout	18.19	18.19	66.31
4	00047_2_0_6_4-0-1-2-3	AOBB-K*-b-UFO	3	0.1	360	2477	***23.08***	**171.92**	timeout	22.70	23.05	1597.58
4	00047_2_0_6_4-0-1-2-3	AOBB-K*-b-DH-UFO	3	0.01	265	1735	*23.01*	1875.78	timeout	22.70	23.05	1597.58
4	00047_2_0_6_4-0-1-2-3	AOBB-K*-b	3	0	32	219	22.74	*161.18*	timeout	22.70	23.05	1597.58
4	00047_2_0_6_4-0-1-2-3	AOBB-K*-b-DH	3	0	34	225	22.74	169.41	timeout	22.70	23.05	1597.58
4	00047_2_0_6_4-0-1-2-5	AOBB-K*-b-UFO	3	0.1	153	793	***22.87***	***92.87***	296.57	22.70	22.83	1339.15
4	00047_2_0_6_4-0-1-2-5	AOBB-K*-b-DH-UFO	3	0.01	153	811	***22.87***	**244.76**	892.85	22.70	22.83	1339.15
4	00047_2_0_6_4-0-1-2-5	AOBB-K*-b	3	0	38	185	22.74	*130.95*	timeout	22.70	22.83	1339.15
4	00047_2_0_6_4-0-1-2-5	AOBB-K*-b-DH	3	0	35	169	22.74	140.66	timeout	22.70	22.83	1339.15
4	00047_2_0_6_4-1-2-3-4	AOBB-K*-b-UFO	3	0.1	3595	6793	*23.05*	*117.06*	3129.46	22.70	23.05	1440.21
4	00047_2_0_6_4-1-2-3-4	AOBB-K*-b-DH-UFO	3	0.01	1745	3337	*23.05*	382.01	timeout	22.70	23.05	1440.21
4	00047_2_0_6_4-1-2-3-4	AOBB-K*-b	3	0	64	122	*22.80*	552.22	timeout	22.70	23.05	1440.21
4	00047_2_0_6_4-1-2-3-4	AOBB-K*-b-DH	3	0	132	254	22.70	50.51	timeout	22.70	23.05	1440.21
4	00048_2_0_7_4-1-2-5-6	AOBB-K*-b-UFO	3	0.1	353	601	22.81	*14.55*	184.58	22.81	22.81	404.02
4	00048_2_0_7_4-1-2-5-6	AOBB-K*-b-DH-UFO	3	0.01	331	527	22.81	*23.08*	639.41	22.81	22.81	404.02
4	00048_2_0_7_4-1-2-5-6	AOBB-K*-b	3	0	75	100	22.81	*49.97*	399.52	22.81	22.81	404.02
4	00048_2_0_7_4-1-2-5-6	AOBB-K*-b-DH	3	0	111	197	22.81	58.98	timeout	22.81	22.81	404.02

Table 6: Comparison of combinations of AOBB-K*-b-[UFO/DH] schemes, and to BBK*, on problems with 5 mutable residues. For each problem, the AOBB-K*-b-[UFO/DH] solvers are ranked top-down based on their performance (top being best). Shown is the i-bound used, δ used to decrease the UFO underflow-threshold found, residue OR and AND nodes traversed, best-found K* solution (recomputed without underflow-thresholding), the time at which the best-found solution was first discovered ("Anytime"), and the completion time ("Time"). Between AOBB-K*-b-[UFO/DH] and BBK*, blue font highlights better values and red font worse values. Italics highlights statistics responsible for a higher ranking in the solver orderings. For reference, the wild-type K* solution is also shown.

AOBB-K*-b-[DH/UFO]											BBK*	
M	Problem	Algorithm	i	δ	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b-UFO	3	0.1	65	1268	***15.17***	3582.63	timeout	14.08	14.73	401.09
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b-DH-UFO	3	0.01	61	1210	***14.73***	2071.67	timeout	14.08	14.73	401.09
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b-DH	3	0	15	234	14.73	*57.91*	timeout	14.08	14.73	401.09
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b	3	0	16	268	14.73	62.53	timeout	14.08	14.73	401.09
5	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b-UFO	3	0.1	67	1321	***14.84***	*1792.80*	timeout	14.08	14.73	404.03
5	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b-DH-UFO	3	0.01	57	1127	***14.84***	2295.92	timeout	14.08	14.73	404.03
5	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b	3	0	13	197	14.73	*341.88*	timeout	14.08	14.73	404.03
5	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b-DH	3	0	13	198	14.73	369.87	timeout	14.08	14.73	404.03
5	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b-UFO	3	0.1	61	1210	*14.84*	*1104.51*	timeout	14.08	15.60	205.56
5	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b-DH-UFO	3	0.01	56	1088	*14.84*	2002.66	timeout	14.08	15.60	205.56
5	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b	3	0	18	295	14.73	*67.53*	timeout	14.08	15.60	205.56
5	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b-DH	3	0	15	244	14.73	156.68	timeout	14.08	15.60	205.56
5	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b-UFO	3	0.1	121	2465	14.73	*34.09*	timeout	14.08	15.60	201.04
5	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b-DH-UFO	3	0.01	100	2027	14.73	*45.06*	timeout	14.08	15.60	201.04
5	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b	3	0	13	200	14.73	*75.53*	timeout	14.08	15.60	201.04
5	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b-DH	3	0	15	245	14.73	93.41	timeout	14.08	15.60	201.04
5	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b-DH-UFO	3	0.01	226	2499	***16.98***	3154.16	timeout	15.79	16.58	753.95
5	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b-UFO	3	0.1	429	4782	***16.60***	3243.13	timeout	15.79	16.58	753.95
5	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b	3	0	15	243	16.58	*61.89*	timeout	15.79	16.58	753.95
5	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b-DH	3	0	15	242	16.58	80.37	timeout	15.79	16.58	753.95
5	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b-DH-UFO	3	0.01	199	2149	***16.61***	**602.13**	timeout	15.79	16.58	628.53
5	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b-UFO	3	0.1	302	3340	***16.60***	2080.88	timeout	15.79	16.58	628.53
5	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b	3	0	19	302	16.58	*65.70*	timeout	15.79	16.58	628.53
5	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b-DH	3	0	21	354	16.58	82.87	timeout	15.79	16.58	628.53
5	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b-DH-UFO	3	0.01	536	1041	***16.62***	1884.35	timeout	15.79	16.25	501.48
5	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b-UFO	3	0.1	686	1333	*16.24*	3370.66	timeout	15.79	16.25	501.48
5	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b	3	0	15	227	15.79	*30.54*	timeout	15.79	16.25	501.48
5	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b-DH	3	0	15	215	15.79	48.73	timeout	15.79	16.25	501.48

		AOBB-K*-b-[DH/UFO]										BBK*	
M	Problem	Algorithm	i	δ	OR	AND	Soln	Anytime	Time	wt K*	Soln	Time
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b-UFO	3	0.1	65	1268	***15.17***	3582.63	timeout	14.08	14.73	401.09
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b-DH-UFO	3	0.01	61	1210	***14.73***	2071.67	timeout	14.08	14.73	401.09
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b-DH	3	0	15	234	14.73	*57.91*	timeout	14.08	14.73	401.09
5	00007_1_0_7_5-0-1-2-3-5	AOBB-K*-b	3	0	16	268	14.73	62.53	timeout	14.08	14.73	401.09
5	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b-UFO	3	0.1	67	1321	***14.84***	*1792.80*	timeout	14.08	14.73	404.03
5	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b-DH-UFO	3	0.01	57	1127	***14.84***	2295.92	timeout	14.08	14.73	404.03
5	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b	3	0	13	197	14.73	*341.88*	timeout	14.08	14.73	404.03
5	00007_1_0_7_5-0-1-3-4-5	AOBB-K*-b-DH	3	0	13	198	14.73	369.87	timeout	14.08	14.73	404.03
5	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b-UFO	3	0.1	61	1210	*14.84*	*1104.51*	timeout	14.08	15.60	205.56
5	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b-DH-UFO	3	0.01	56	1088	*14.84*	2002.66	timeout	14.08	15.60	205.56
5	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b	3	0	18	295	14.73	*67.53*	timeout	14.08	15.60	205.56
5	00007_1_0_7_5-0-1-3-5-6	AOBB-K*-b-DH	3	0	15	244	14.73	156.68	timeout	14.08	15.60	205.56
5	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b-UFO	3	0.1	121	2465	14.73	*34.09*	timeout	14.08	15.60	201.04
5	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b-DH-UFO	3	0.01	100	2027	14.73	*45.06*	timeout	14.08	15.60	201.04
5	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b	3	0	13	200	14.73	*75.53*	timeout	14.08	15.60	201.04
5	00007_1_0_7_5-0-1-4-5-6	AOBB-K*-b-DH	3	0	15	245	14.73	93.41	timeout	14.08	15.60	201.04
5	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b-DH-UFO	3	0.01	226	2499	***16.98***	3154.16	timeout	15.79	16.58	753.95
5	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b-UFO	3	0.1	429	4782	***16.60***	3243.13	timeout	15.79	16.58	753.95
5	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b	3	0	15	243	16.58	*61.89*	timeout	15.79	16.58	753.95
5	00018_2_0_6_5-0-1-2-3-4	AOBB-K*-b-DH	3	0	15	242	16.58	80.37	timeout	15.79	16.58	753.95
5	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b-DH-UFO	3	0.01	199	2149	***16.61***	**602.13**	timeout	15.79	16.58	628.53
5	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b-UFO	3	0.1	302	3340	***16.60***	2080.88	timeout	15.79	16.58	628.53
5	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b	3	0	19	302	16.58	*65.70*	timeout	15.79	16.58	628.53
5	00018_2_0_6_5-0-1-2-3-5	AOBB-K*-b-DH	3	0	21	354	16.58	82.87	timeout	15.79	16.58	628.53
5	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b-DH-UFO	3	0.01	536	1041	***16.62***	1884.35	timeout	15.79	16.25	501.48
5	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b-UFO	3	0.1	686	1333	*16.24*	3370.66	timeout	15.79	16.25	501.48
5	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b	3	0	15	227	15.79	*30.54*	timeout	15.79	16.25	501.48
5	00018_2_0_6_5-1-2-3-4-5	AOBB-K*-b-DH	3	0	15	215	15.79	48.73	timeout	15.79	16.25	501.48

AOBB-K*-b-DH-UFO Analysis. For eight of the twelve 3-mutable-residue problems that AOBB-K*-b-DH-UFO first finds its solution in less than ten seconds, all four algorithms performed relatively similarly in terms of solution quality and the reported "Anytime" time. However, out of the four problems (00007_*, 00020_*, 00021_*, 00025_*) AOBB-K*-b-DH-UFO took longer than 10 seconds to first find its solution (ie. "Anytime" > 10.0), it was fastest for three of the problems (00020_*, 00021_*, 00025_*) with an "Anytime" at most 75% of that of the next fastest solver.

Within the 4-mutable-residue problems, results begin to vary slightly. For three out of the thirty-two problems (00007_1_0_7_4-0-1-5-6, 00007_1_0_7_4-1-2-5-6, 00047_2_0_6_4-0-1-2-3), AOBB-K*-b-DH-UFO finds a sub optimal as compared to AOBB-K*-b-UFO, but still finding a better solution than both AOBB-K*-b and AOBB-K*-b-DH. For two problems (00007_1_0_7_4-1-2-3-5 and 00042_3_0_7_4-1-2-3-4), it finds a better solution than all three of the other algorithms. For all other problems, the solution matches the best found solution among the other three algorithms.

Within the 18 5-mutable-residue problems, for 2 out of the 32 problems (00007_1_0_7_5-0-1-2-3-5 and 00047_2_0_6_5-0-1-2-3-4), AOBB-K*-b-DH-UFO finds a sub optimal as compared to AOBB-K*-b-UFO, but still finding a solution as good or better than AOBB-K*-b and AOBB-K*-b-DH. For 4 problems (00018_2_0_6_5-0-1-2-3-4, 00018_2_0_6_5-0-1-2-3-5, 00018_2_0_6_5-1-2-3-4-5, and 00047_2_0_6_5-0-1-2-3-5), it finds a better solution than all three of the other algorithms. For all other problems, the solution matches the best found solution among the other three algorithms.

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