A Human Computation Framework for Boosting Combinatorial Solvers

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Motivation

There has been **significant progress** in the area of **search**, **constraint satisfaction**, and **automated reasoning**.

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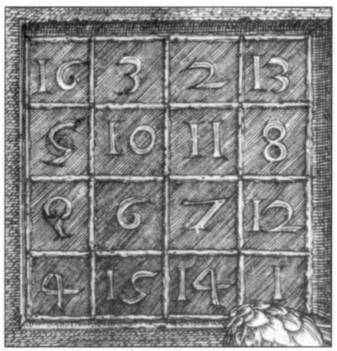
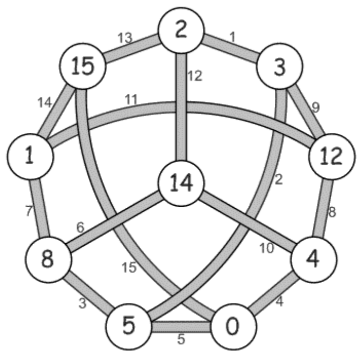
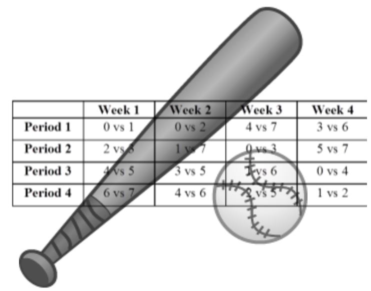


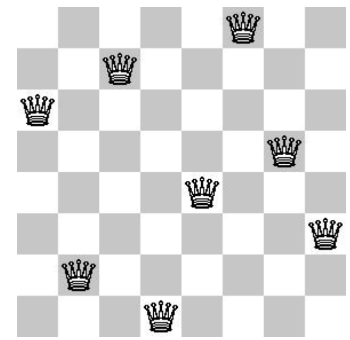
Magic squares



Graceful Graphs



Round-Robin Tournament



N-Queens

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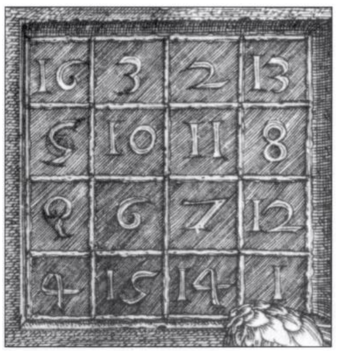

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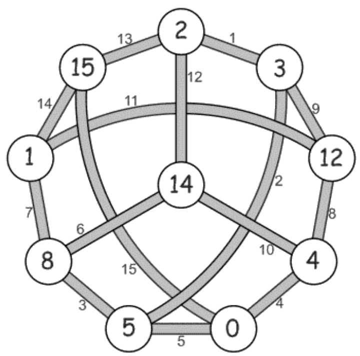

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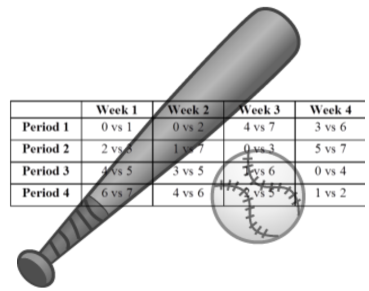
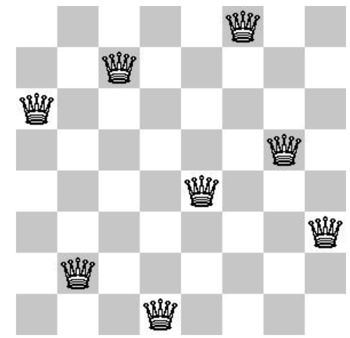


	Week 1	Week 2	Week 3	Week 4
Period 1	0 vs 1	0 vs 2	4 vs 7	3 vs 6
Period 2	2 vs 3	1 vs 7	0 vs 3	5 vs 7
Period 3	4 vs 5	3 vs 5	1 vs 6	0 vs 4
Period 4	6 vs 7	4 vs 6	2 vs 5	1 vs 2

Round-Robin Tournament



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Typically, these combinatorial objects exhibit additional **hidden structure**, beyond the original structure of the problem.

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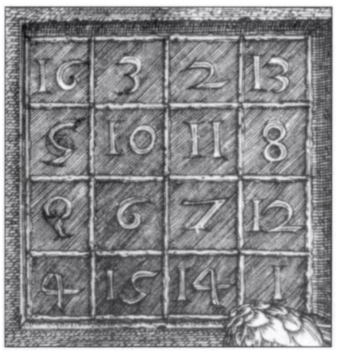

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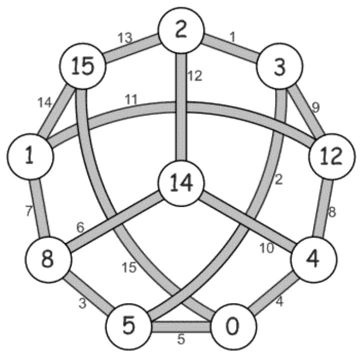

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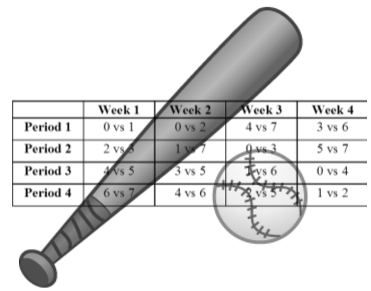

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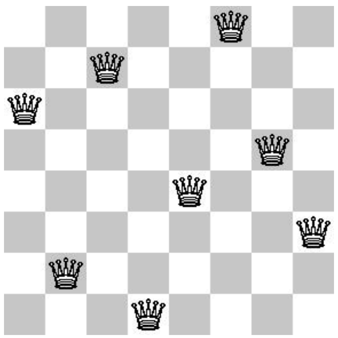

N-Queens

Typically, these combinatorial objects exhibit additional **hidden structure**, beyond the original structure of the problem.

Research Question: Can we **crowdsource** the discovery of hidden structure of the problem and **exploit** it to boost combinatorial search?

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Part of a broader **research agenda** focused on harnessing **human insights** to solve **hard combinatorial problems** in scientific discovery:

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1	2	3	4	5	6	7	8	9	10	11
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3	6	9	11	8	5	2	1	4	7	10
4	8	11	7	3	1	5	9	10	6	2
5	10	8	3	2	7	11	6	1	4	9
6	11	5	1	7	10	4	2	8	9	3
7	9	2	5	11	4	3	10	6	1	8
8	7	1	9	6	2	10	5	3	11	4
9	5	4	10	1	8	6	3	11	2	7
10	3	7	6	4	9	1	11	2	8	5
11	1	10	2	9	3	8	4	7	5	6

1 2 4 8 11 22
3 5-7 19 21 23
9 10 12-18 20

Spatially Balanced Latin Squares	**Weak Schur Numbers**
[Smith et al., IJCAI'05] $n \leq 35$	[Eliahou et al., Computers & Math Applications'12] $WS(6) \geq 575$
[L. et al, AAAI'12] Any n s.t. 2n+1 is prime	[L. et al, AAAI'12] $WS(6) \geq 581$

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5	10	8	3	2	7	11	6	1	4	9
6	11	5	1	7	10	4	2	8	9	3
7	9	2	5	11	4	3	10	6	1	8
8	7	1	9	6	2	10	5	3	11	4
9	5	4	10	1	8	6	3	11	2	7
10	3	7	6	4	9	1	11	2	8	5
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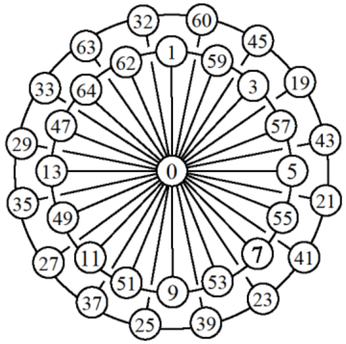

1	20	71	40	51	41	70	30	90	91
92	12	29	62	49	59	32	79	82	9
8	83	23	38	53	48	68	73	13	98
94	17	74	34	47	57	64	24	87	7
6	85	26	65	45	55	36	76	15	96
5	86	75	66	46	56	35	25	16	95
97	84	77	37	54	44	67	27	14	4
93	88	28	63	58	43	33	78	18	3
99	19	22	69	42	52	39	72	89	2
10	11	80	31	60	50	61	21	81	100

Spatially Balanced Latin Squares	Weak Schur Numbers	Graceful Double-Wheel Graphs	Diagonally ordered Magic Squares
[Smith et al., IJCAI'05] $n \leq 35$	[Eliahou et al., Computers & Math Applications'12] $WS(6) \geq 575$	[Heule & Walsh, AAAI'10] $n \leq 24$	[Gomes & Sellmann, CP'04] $n \leq 19$
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6	11	5	1	7	10	4	2	8	9	3
7	9	2	5	11	4	3	10	6	1	8
8	7	1	9	6	2	10	5	3	11	4
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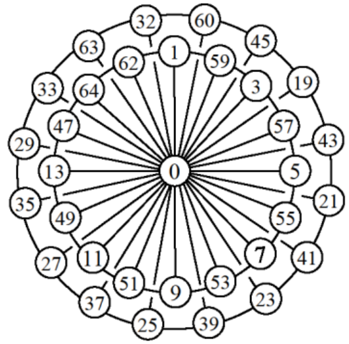

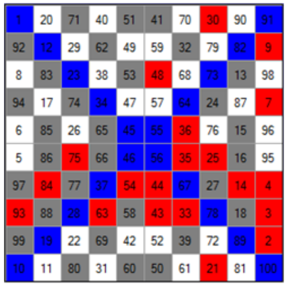

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Spatially Balanced Latin Squares	Weak Schur Numbers	Graceful Double-Wheel Graphs	Diagonally ordered Magic Squares	Erdos Discrepancy Sequences
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[L. et al, AAAI'12] Any n s.t. 2n+1 is prime	[L. et al, AAAI'12] $WS(6) \geq 581$	[L. et al, IJCAI'13] Any $n > 3$	[L. et al, IJCAI'13] Any n s.t. n is doubly even	[L. et al, CP'14] $n \leq 127{,}645$

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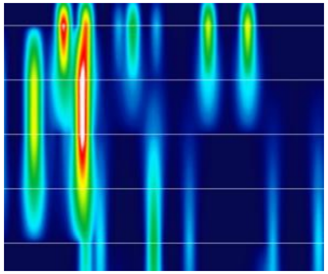


Phase-Map Identification Problem
[Ermon et al., SAT'12] $t_{D2} \approx$ 13 hours
[L. et al, HCOMP'14] $t_{D2} \approx$ 16 minutes

Outline

- Motivation
- Hidden Structure in Hard Combinatorial Problems
- Framework for Boosting Combinatorial Solvers
- Motivating Application
- Empirical Results
- Conclusions and Future Directions

Hidden Structure in Hard Combinatorial Problems

NP-Hard Combinatorial Problems - worst-case intractable (NP-complete) -- exponential time;

Real-world problems have lots of *hidden* tractable sub-structure – often if exploited allows for much shorter solution times.

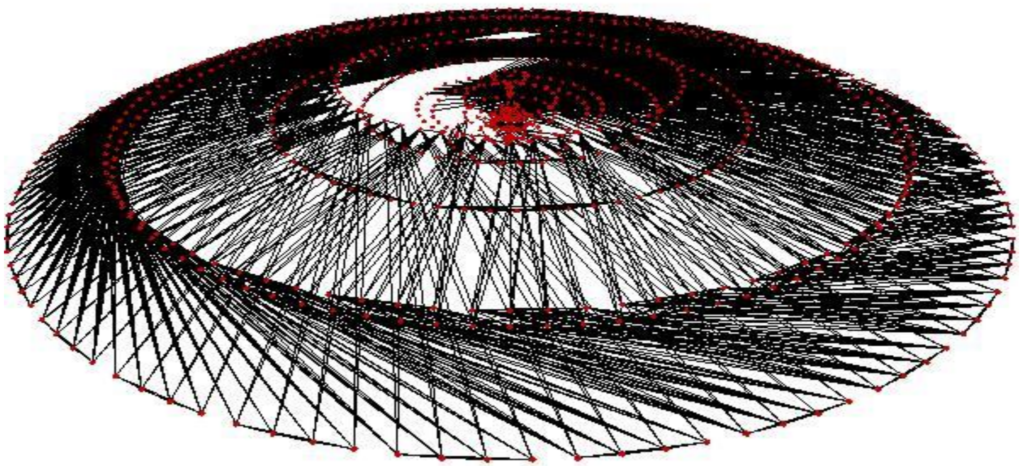
- Key notion: backdoor variables

A backdoor to a given problem is a subset of "critical" variables such that, once assigned values, the remaining instance simplifies to a tractable class.

Backdoor variables represent clever reasoning shortcuts in the search space.

Shown that real world problems can have surprisingly small backdoors.

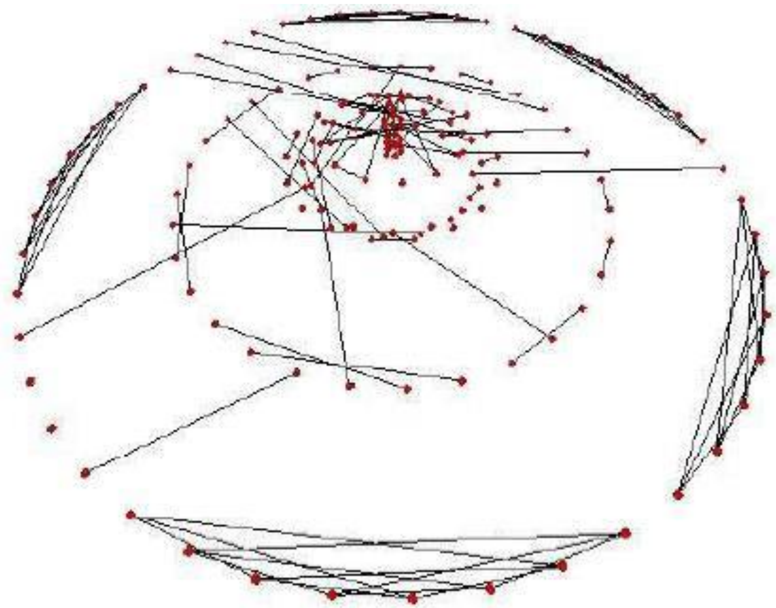
Backdoors - “seeing is believing”



Logistics planning formula.

843 vars, 7,301 constraints, approx. min backdoor 16

Backdoors - "seeing is believing"



After setting just 12 (out of 800+) backdoor vars – problem almost solved.

Finding backdoors in practice

Backdoors explain how a solver can get "clever" and solve very large instances. Rapid restart techniques and variable selection heuristics enable solvers to find small backdoor sets relatively quickly.

However, so far we have not been able to understand the semantics of backdoors.

Can we use Human Computation (with minimal input) to identify backdoors to speed up search of combinatorial solvers?

Illustrative Example – Edge-Matching Puzzle

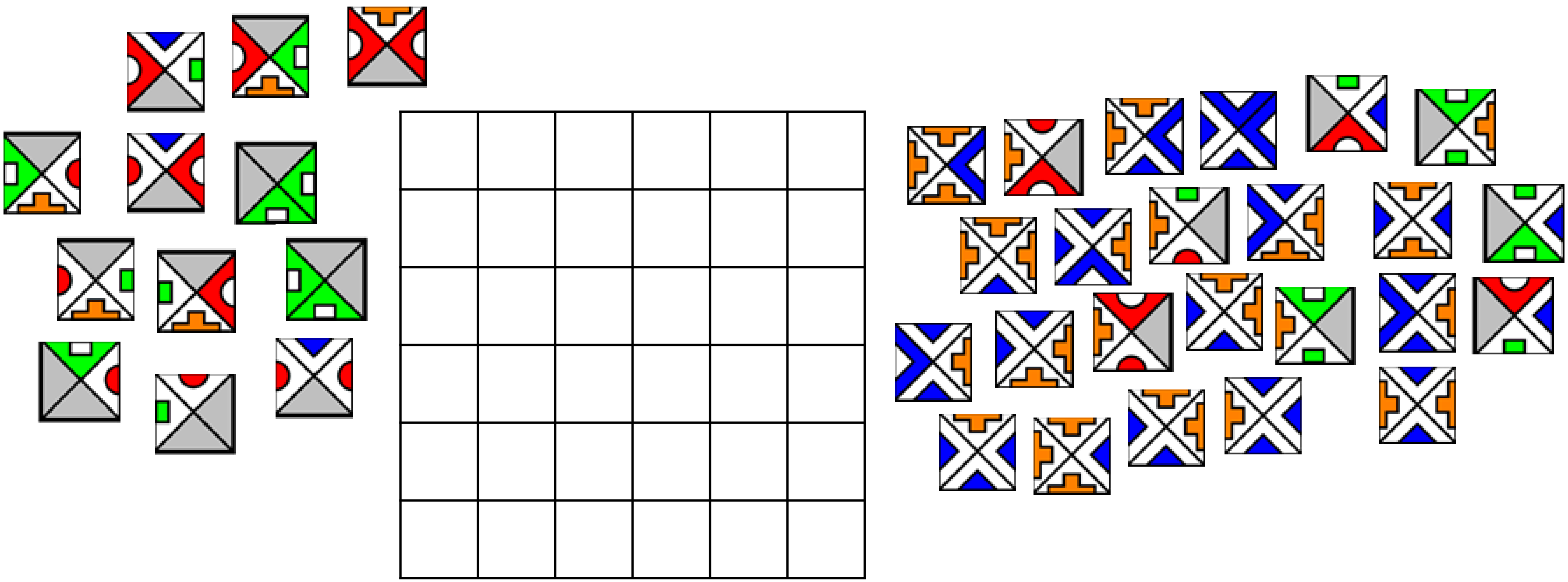


Fig: Example of the Edge-Matching Puzzle

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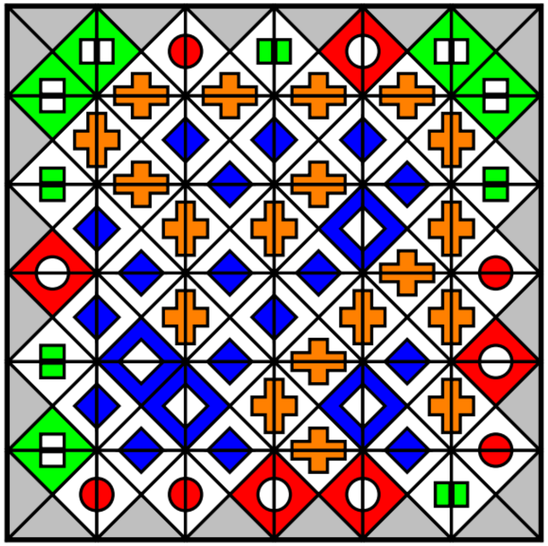

Fig: Solution to the Edge-Matching Puzzle

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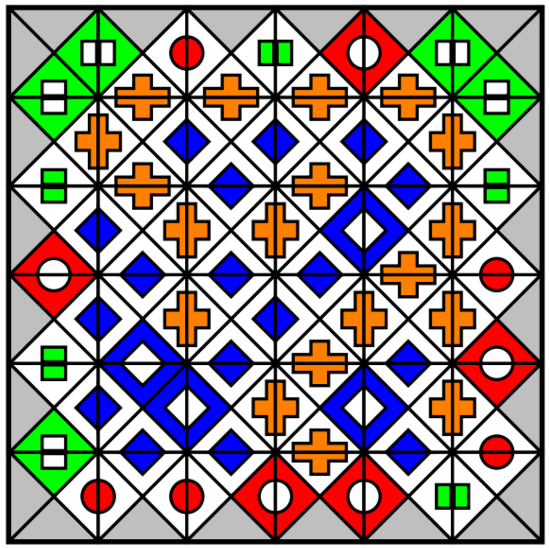


Fig: Solution to the Edge-Matching Puzzle

<u>**SAT formulation:**</u>

- **Variables**: Boolean variables to indicate whether a piece *k* is in cell *(i,j)* with rotation *r*

- **Constraints**:

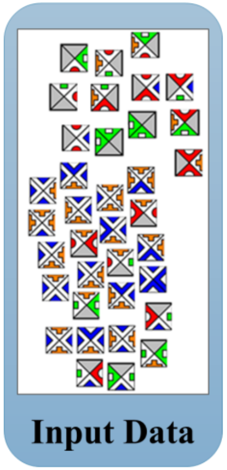
  1) A cell has one puzzle piece

  2) A piece is assigned to one cell

  3) A piece matches its neighbors

  4) Border pieces are not allowed to be assigned to internal cells

Human Computation Framework for Boosting Combinatorial Solvers



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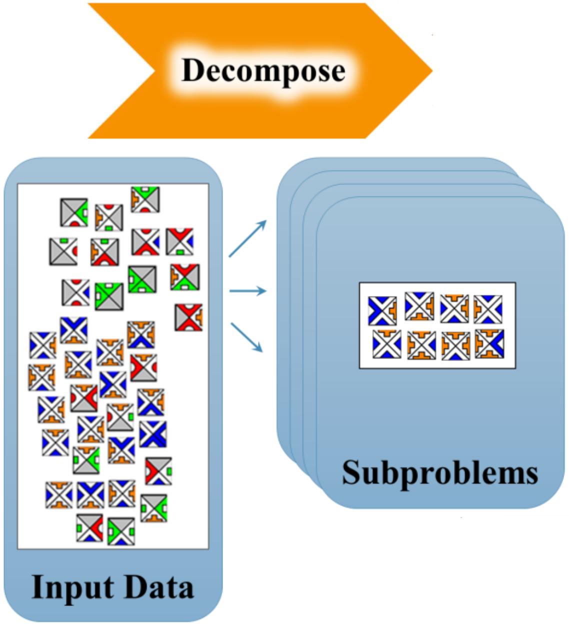

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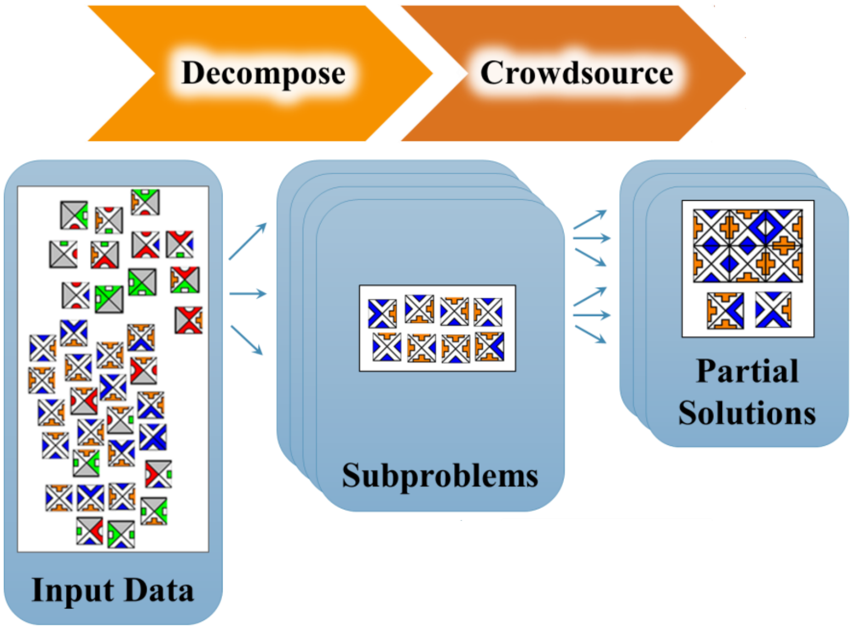

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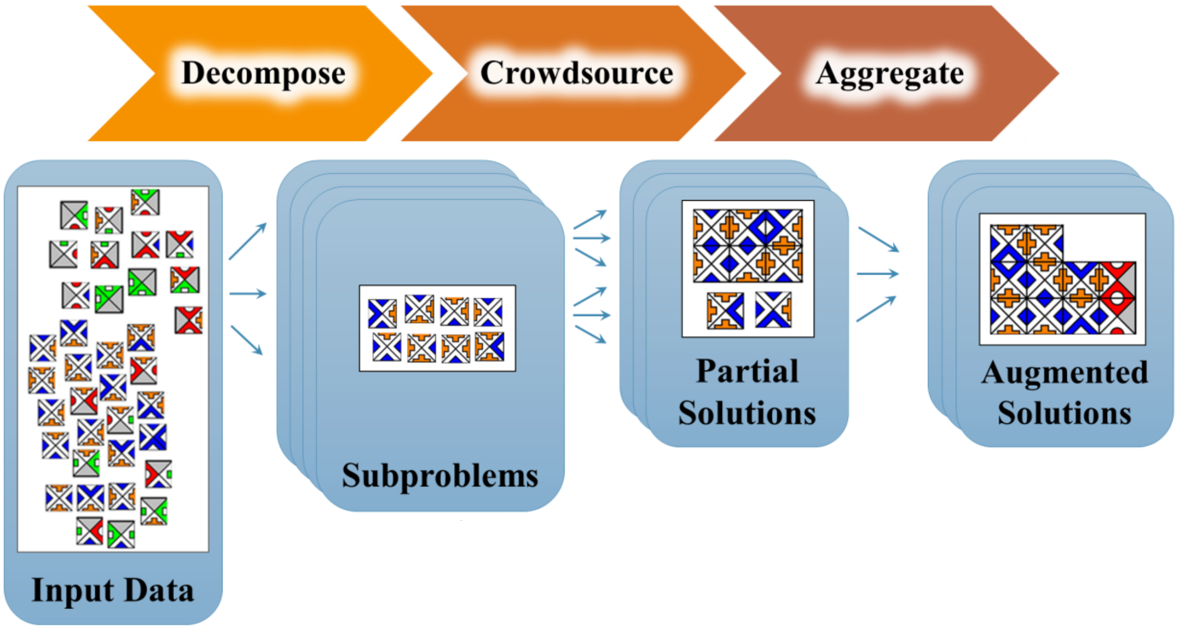

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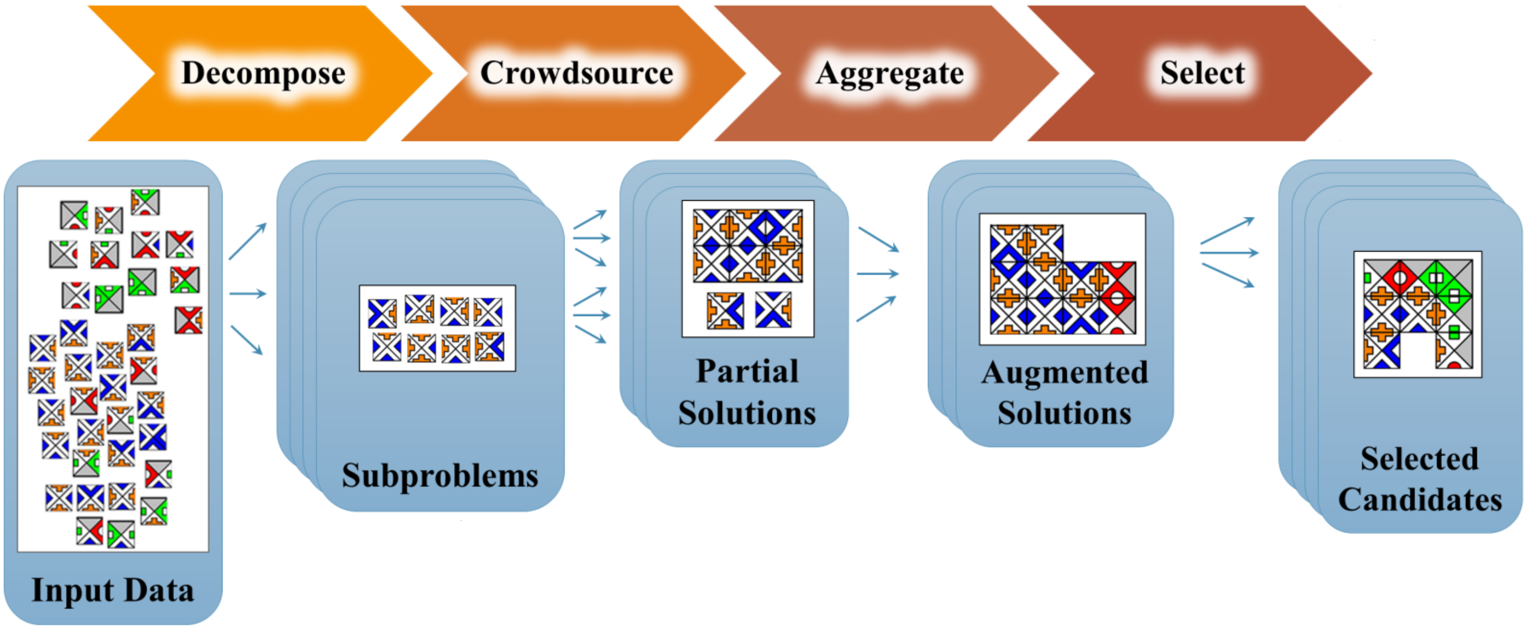

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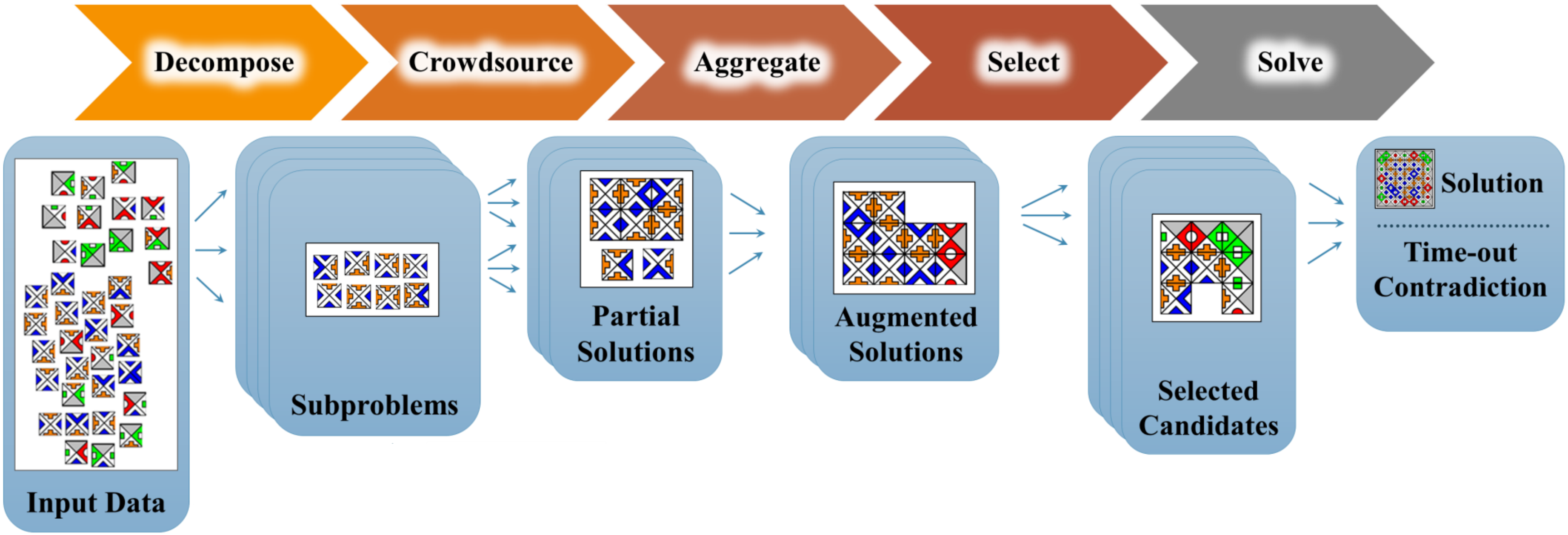

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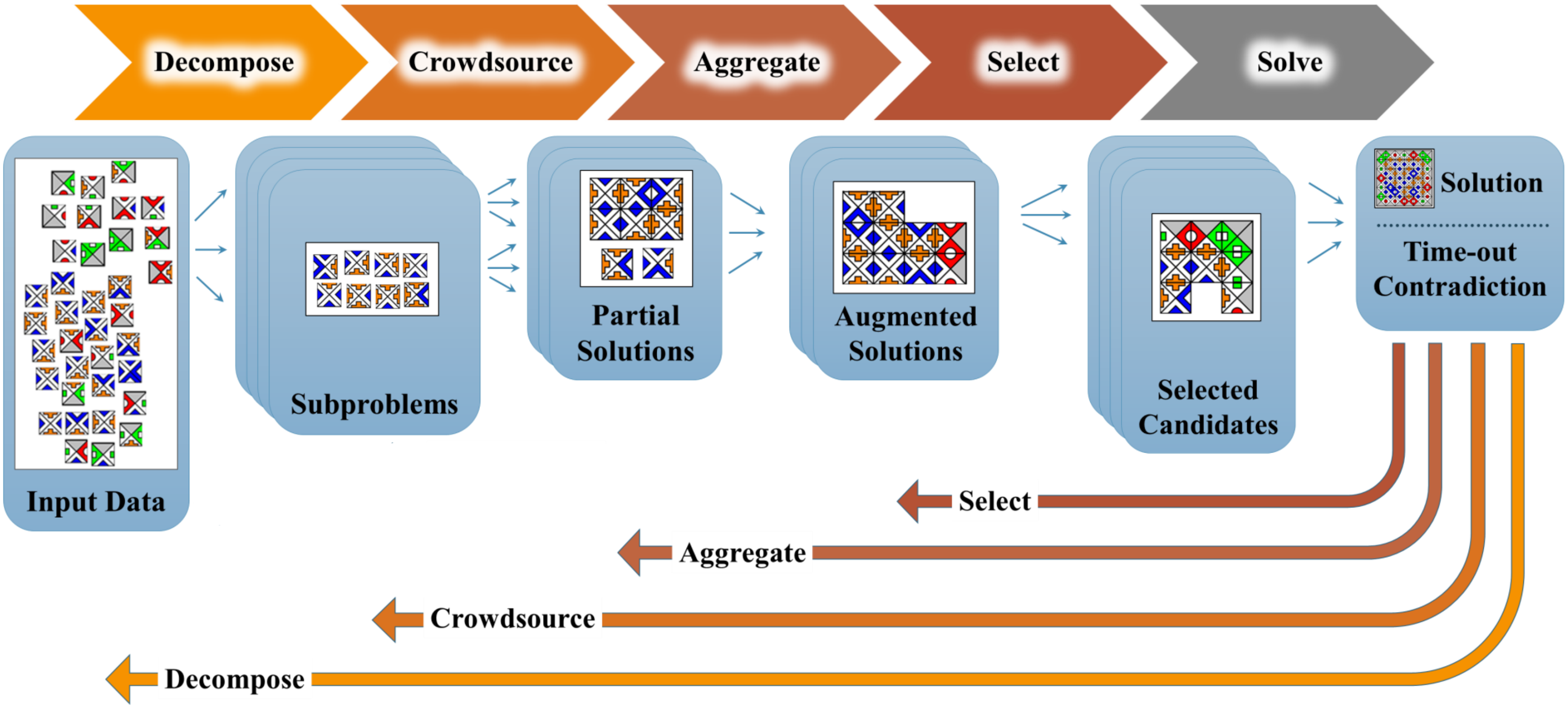

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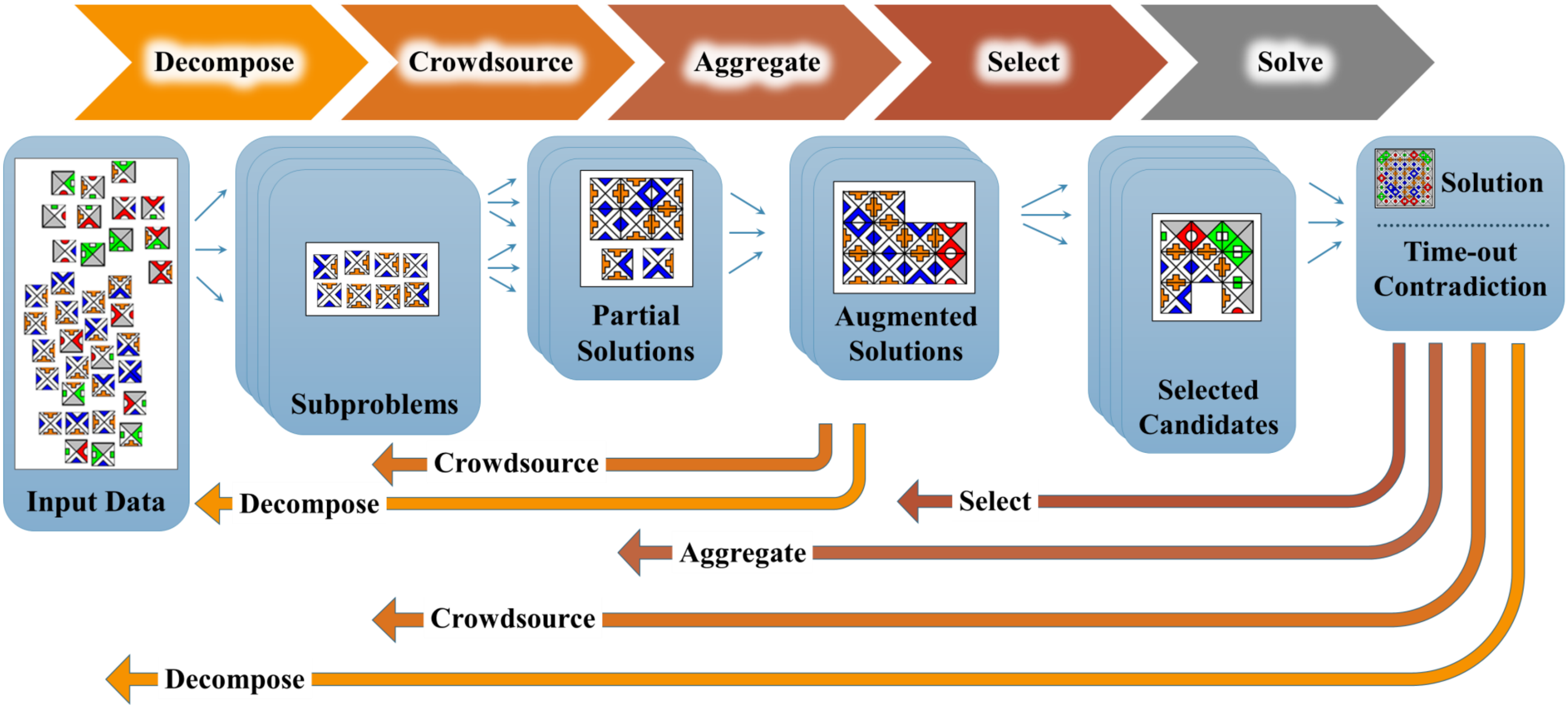
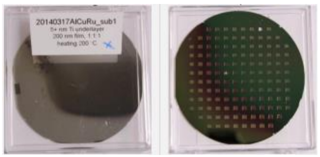


Motivating Application:
High-Throughput Materials Discovery

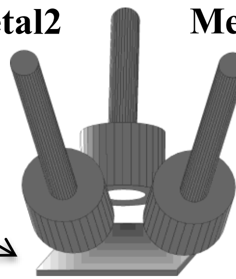


Silicon Wafer

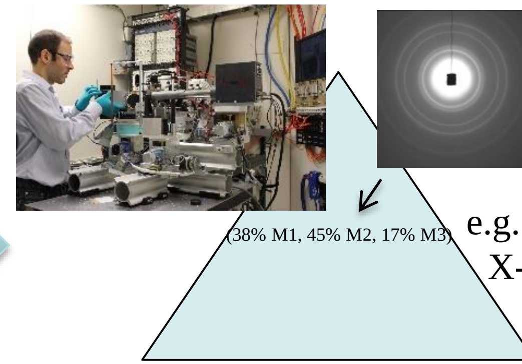
Metal1

Metal2

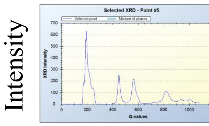
Metal3



**High-Throughput
Materials Synthesis**



Beam Intensity



Diffraction angle

e.g. Electromagnetic
X-Ray Diffraction

**High-Throughput
Characterization of Materials**

BIG Challenge:
High-Throughput Crystal Structure Discovery

(Goal: 1M materials a day)

(Phase Map Identification Problem)

CHESS
Cornell High Energy Synchrotron Source

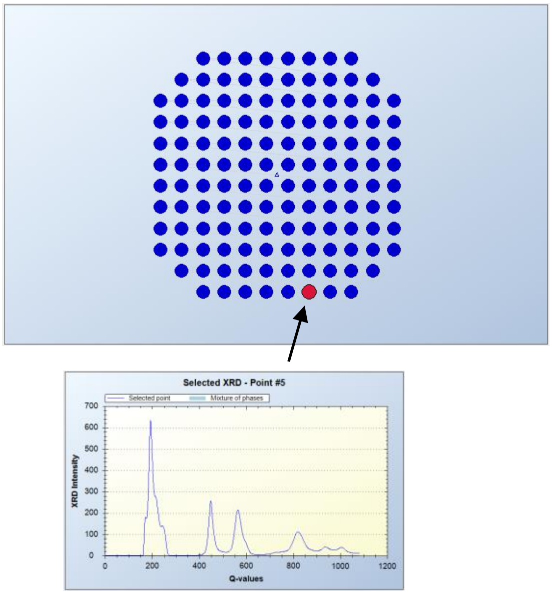
emc2
Energy Materials Center at Cornell

JCAP
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS
Caltech

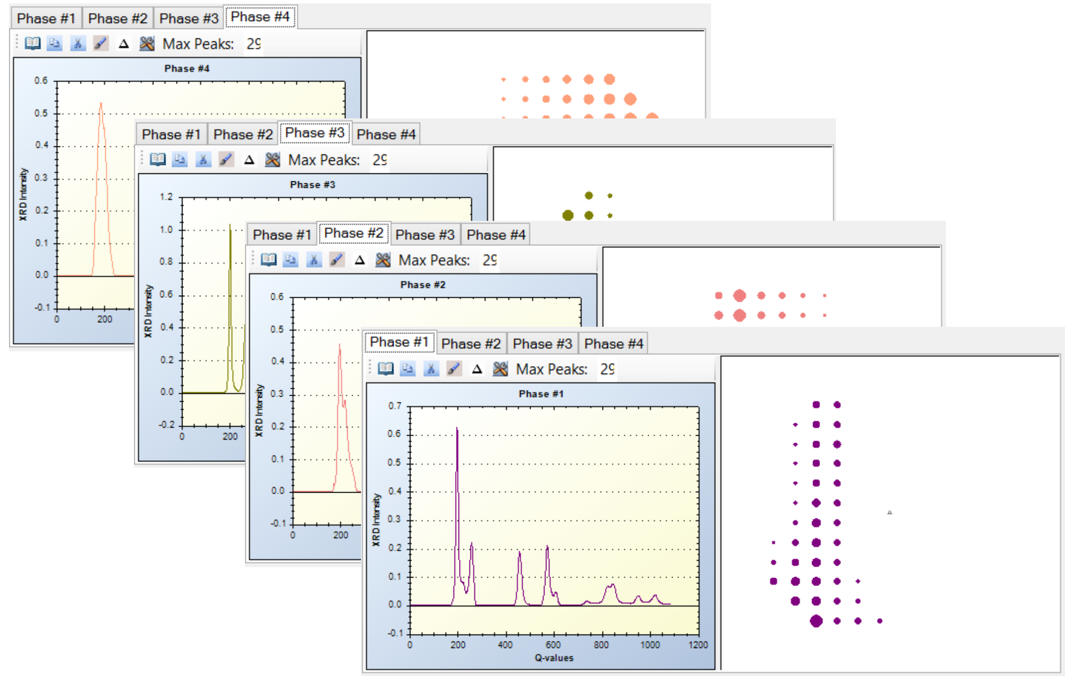
SLAC
Stanford Linear Accelerator

Phase Map Identification Problem

<u>Input</u>



<u>Output</u>



Physical characteristics:

- Every crystal is a **combination** of various crystallites, with up to ***M* different crystal structures**, resulting in a **linear combination** of the XRD patterns (basis) of the crystallites.
- Crystallites may distort as a function of composition, resulting in a **shift** of their XRD pattern, with an experimental **limit** on the overall shift
- The **amount** of each basis pattern is **continuous** in composition space, and the subgraph of the samples involving a given basis pattern is **connected**.

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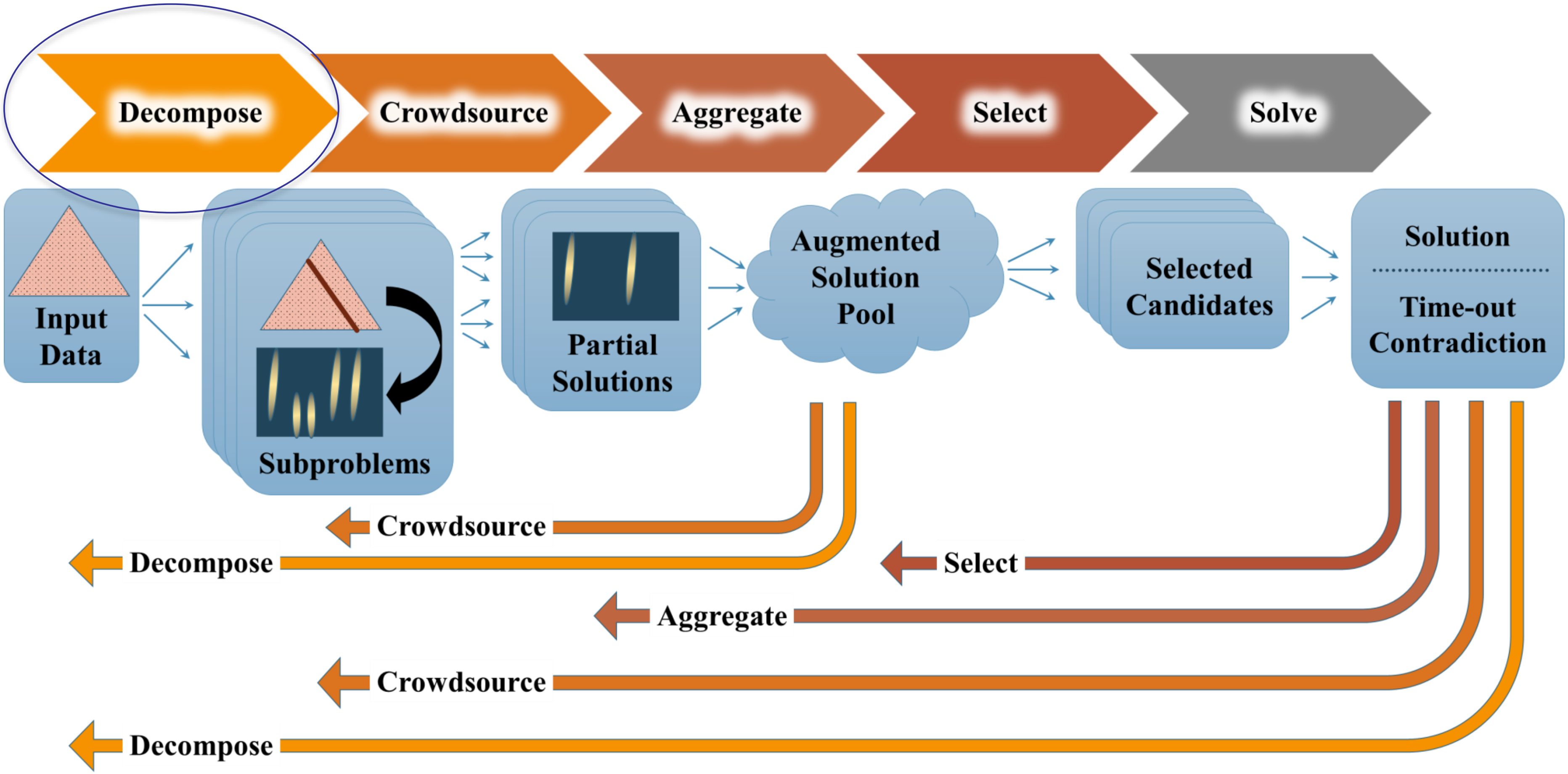
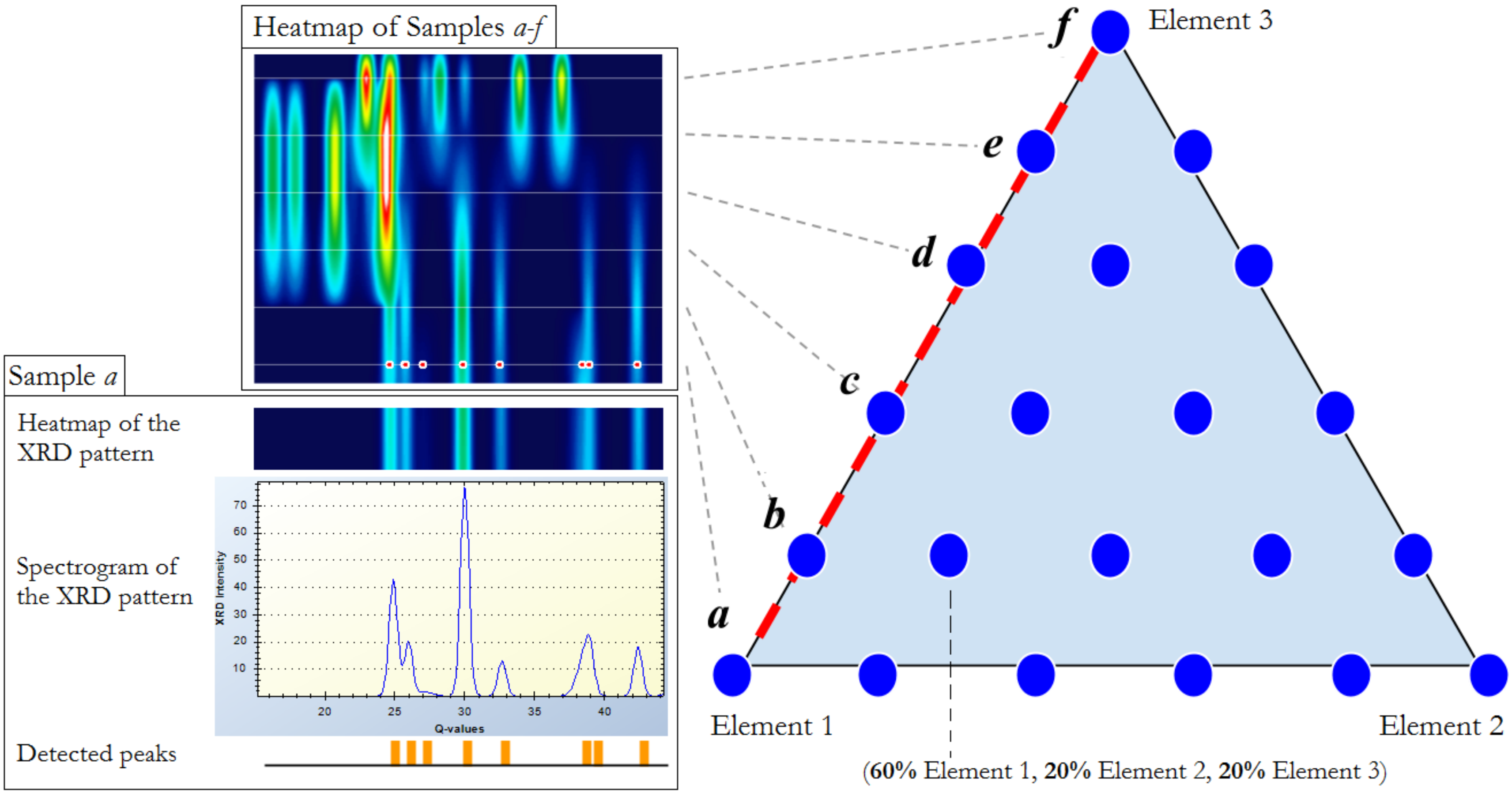


Decomposition

Slices of Sample Points

Different Visualizations of X-Ray Diffraction Patterns



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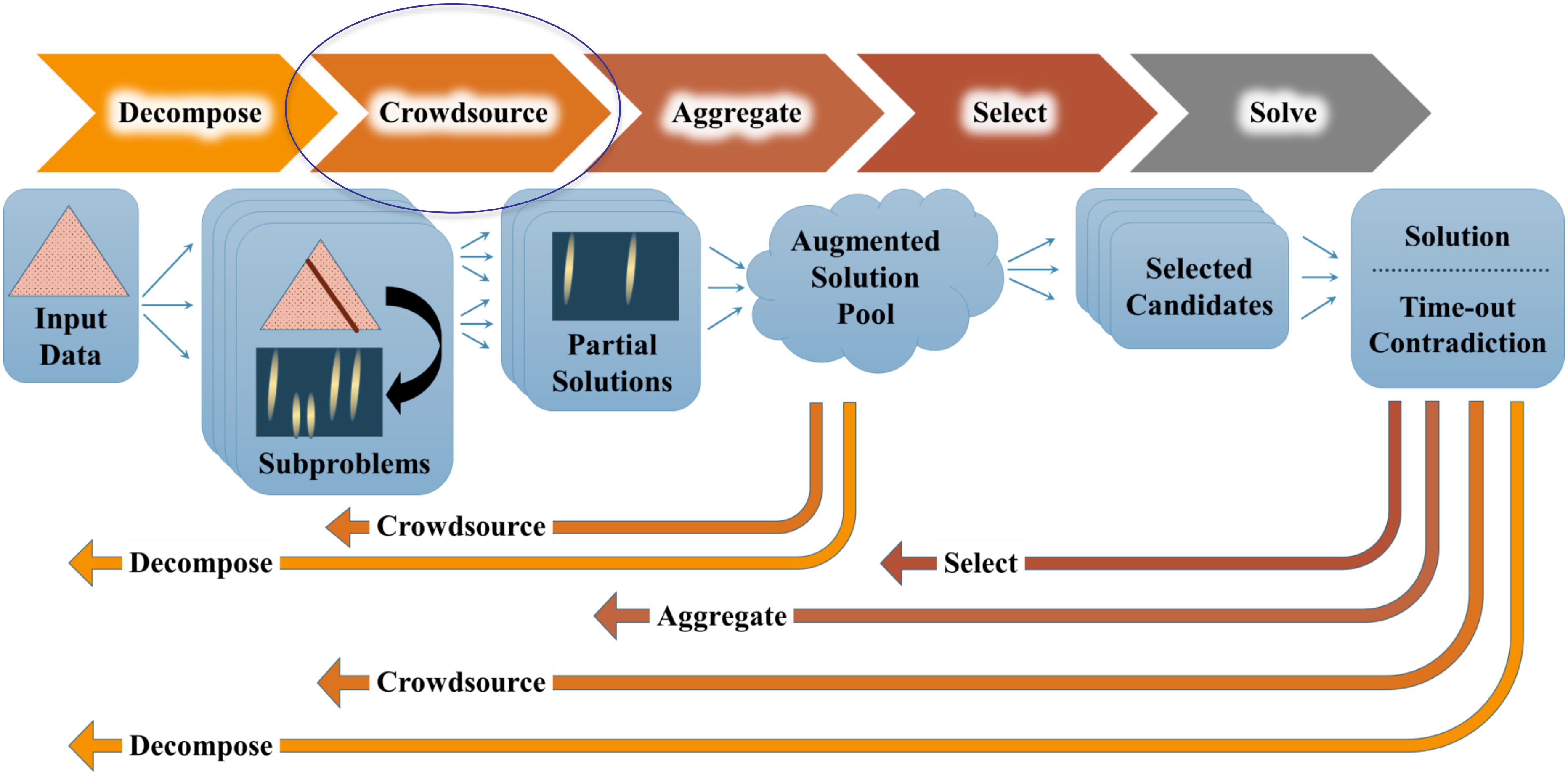
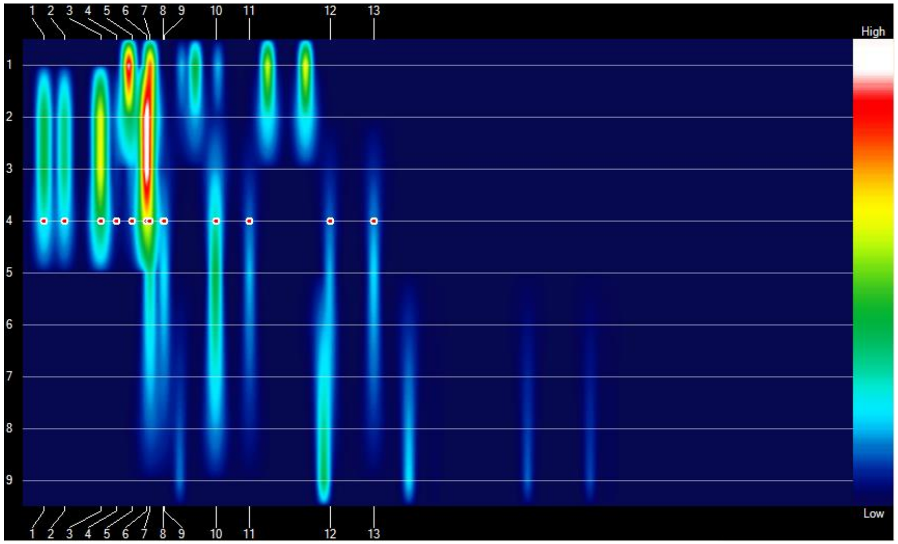
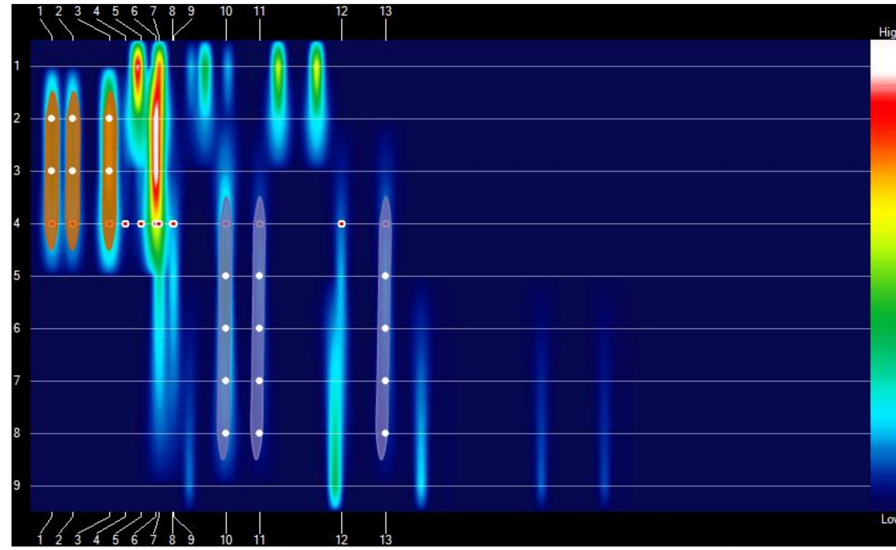


Crowdsourcing:
Human Intelligent Task for Pattern Identification





Human Intelligent Task

A worker is asked to identify patterns of similar vertical lines that intersect with sample 4 (whose detected intensity peaks are marked with red dots).

Another HIT could include the same set of samples, but the worker would be asked to identify patterns of similar vertical lines that intersect with another sample.

Completed Human Intelligent Task

Orange pattern

The 3 leftmost vertical lines are marked in orange as one pattern spanning three sample points upwards (2-4).

Blue Pattern

Three vertical lines towards the right are marked in blue as a separate pattern, spanning 5 samples downwards (4-8).

Unmarked - The others are less clear and because of their ambiguity have been left unmarked by the worker, which is correct, as workers are told to be conservative

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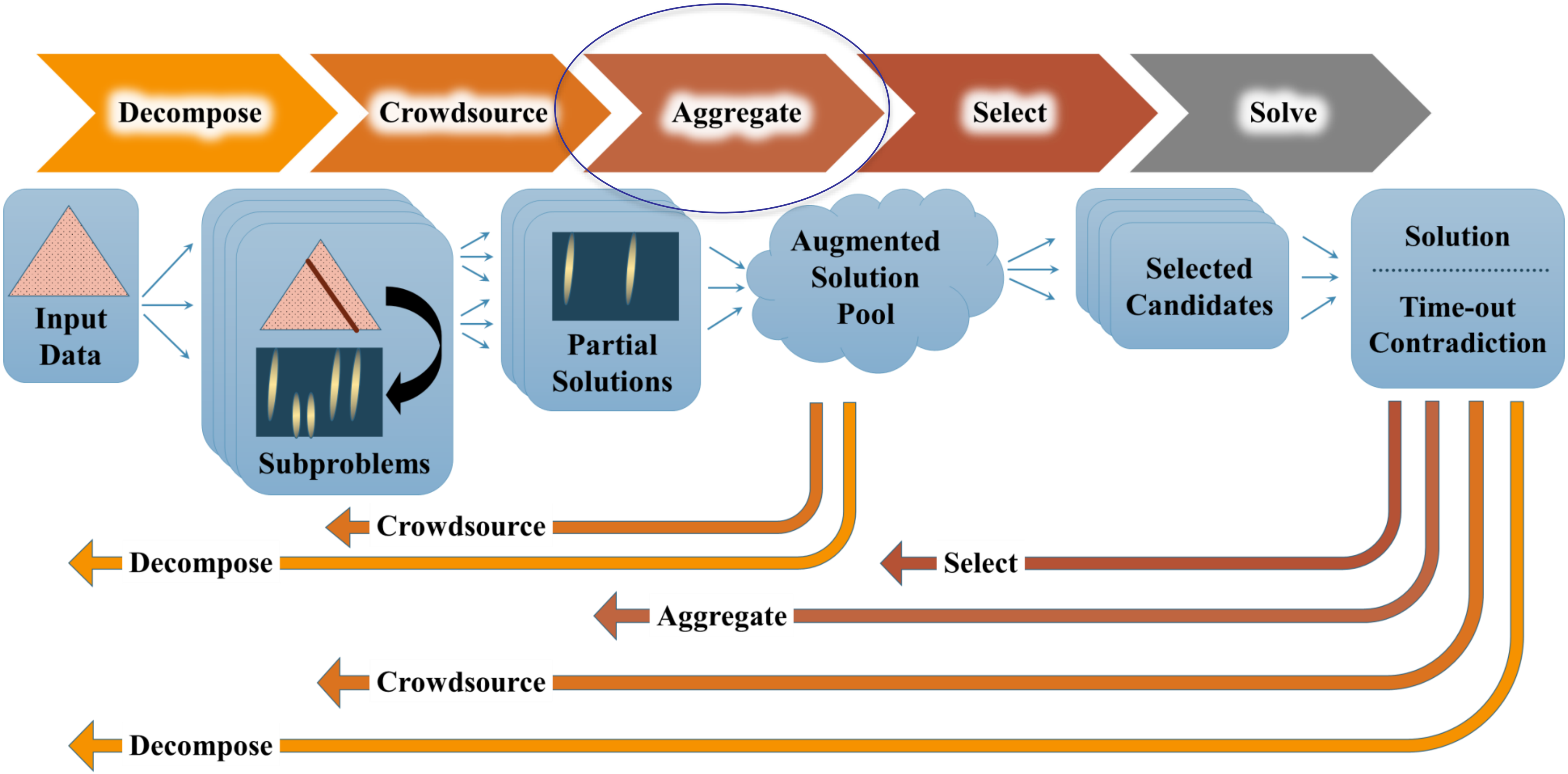
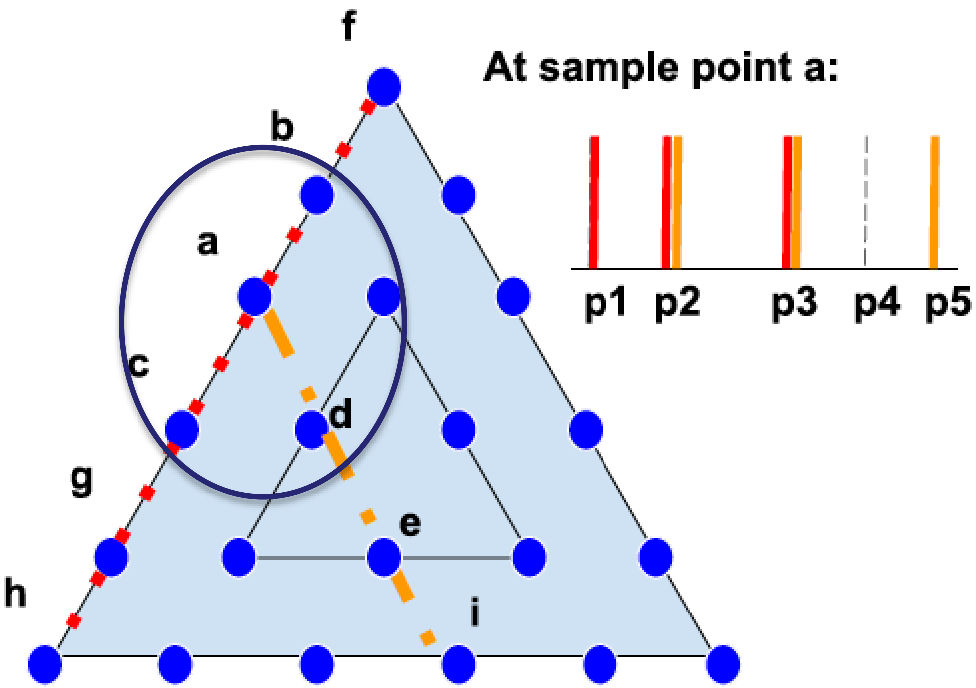


Aggregation

Aggregate phase over a,b,c,d



<u>Worker A</u>

- Gets slice between **sample points f and h**

- Annotates phase $\mathbf{P_A}$, spanning over sample points **a, b, c**, and its peaks at sample point a are $\mathbf{p_1; p_2; p_3}$.

<u>Worker B</u>

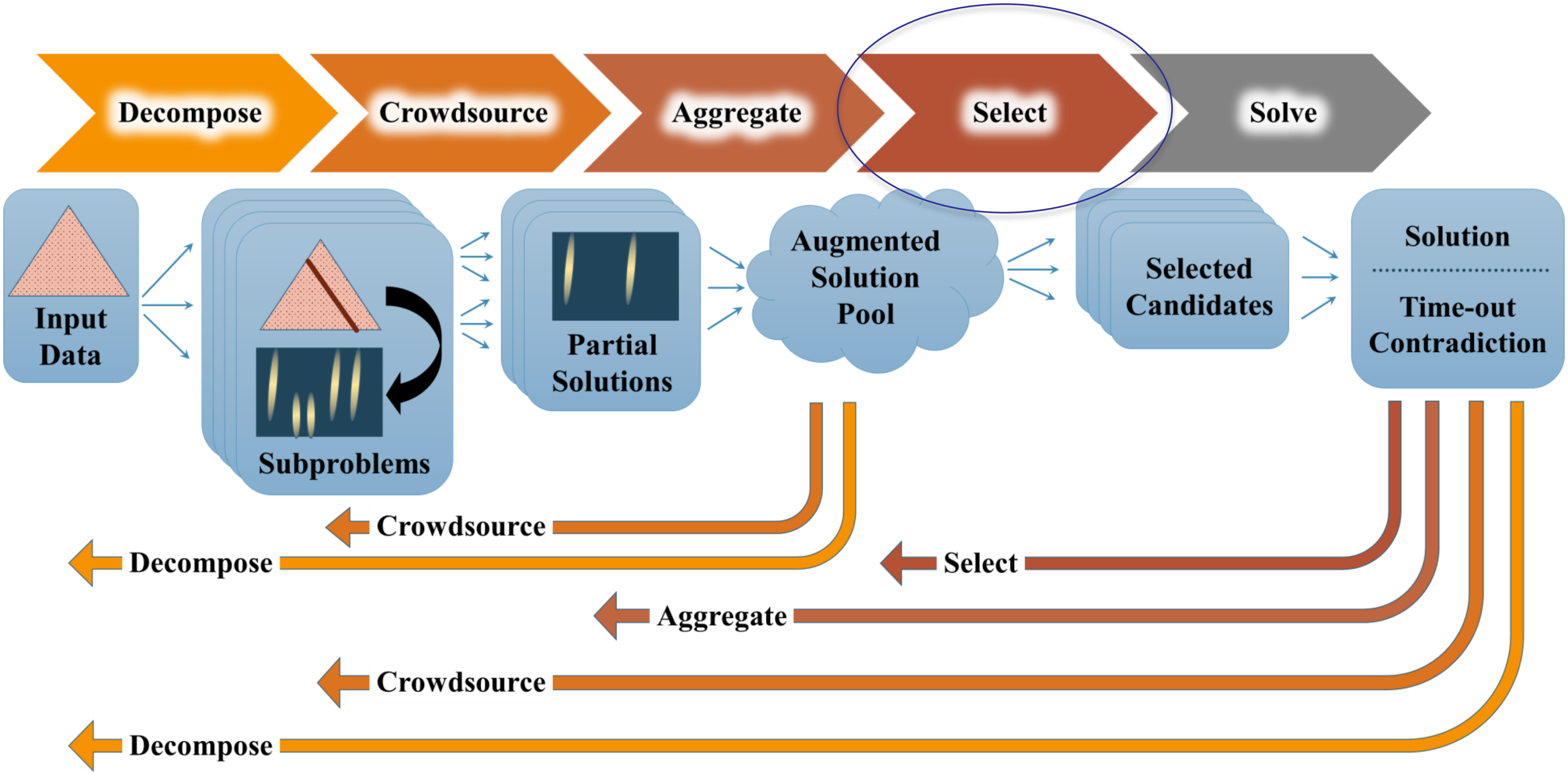
- Gets slice between **sample points a and i.**

- Annotates phase $\mathbf{P_B}$, spanning over sample points **a, d**, and has peaks $\mathbf{p_2, p_3, p_5}$ **at sample point a**.

<u>Augmented candidate:</u> phase $\mathbf{P_C}$

- Spans sample points **a; b; c; d,** and has peaks $\mathbf{p_2}$ **and** $\mathbf{p_3}$.

Human Computation Framework for Boosting Combinatorial Solvers



Selection - MIP Formulation

Mixed Integer Programming Encoding

Select set of phases satisfying physical constraints and minimizing the number of unexplained peaks by the selected phases Y .

$E_{i,k}$ indicates that the i-th phase in B' is selected as the k-th phase.

$$Y = \underset{\{B_1,\ldots,B_K\}\subset B'}{\arg\min} \sum_{l\in L} w_l.$$

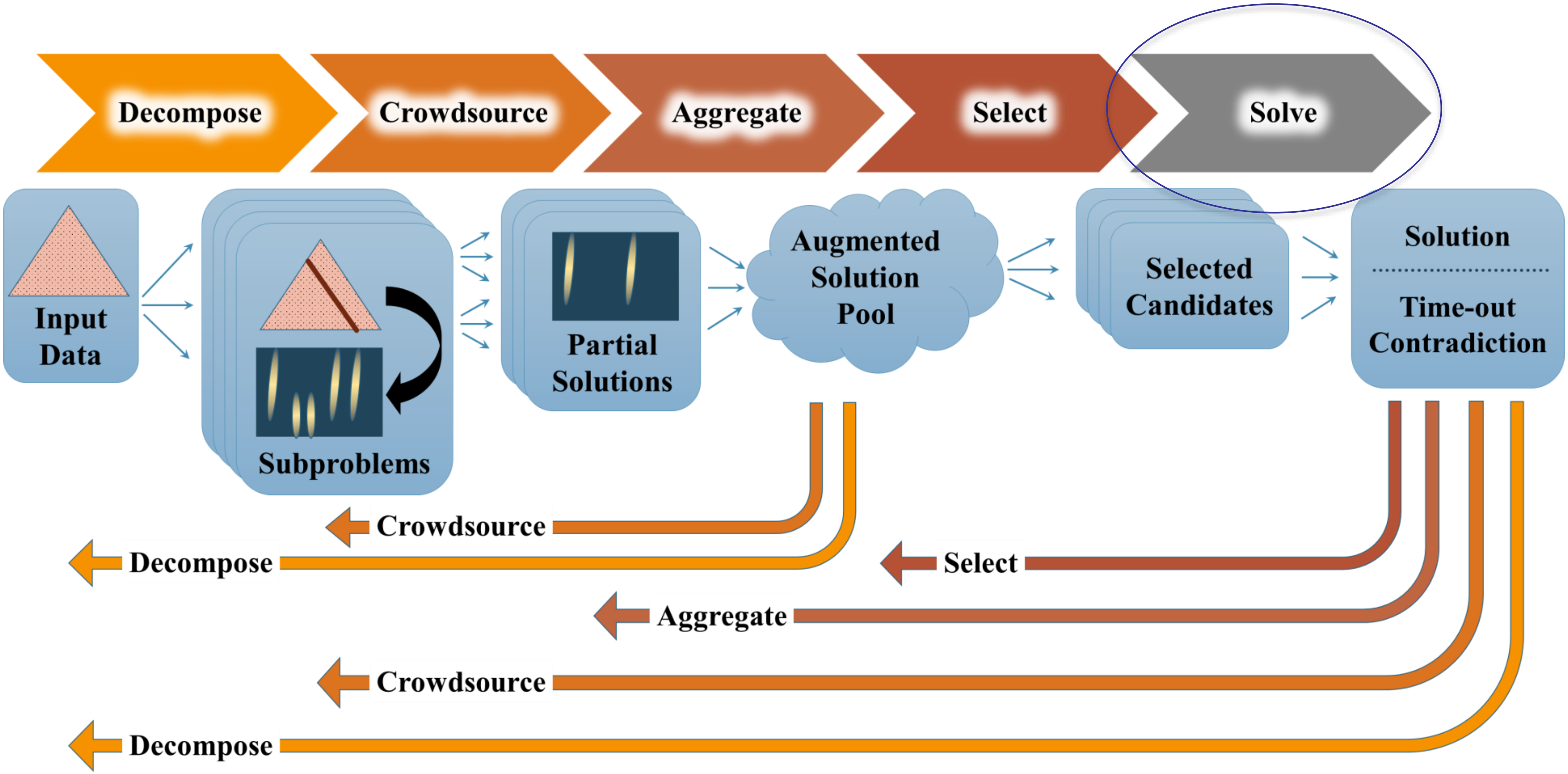
$$\forall i, \quad \sum_{k=1}^{K} E_{i,k} \leq 1.$$

$$\forall k, \quad \sum_{i=1}^{n} E_{i,k} = 1.$$

$$\forall j, \quad \sum_{i\in O(j)} \sum_{k=1}^{K} E_{i,k} \leq 3.$$

$$w_l + \left(\sum_{i\in C(l)} \sum_{k=1}^{K} E_{i,k} \right) \geq 1 \text{ for all } l.$$

Human Computation Framework for Boosting Combinatorial Solvers



Case of Inconsistency:
Solver Identifies Unsat-Core

Algorithm 2: The unsat core-based solving algorithm.

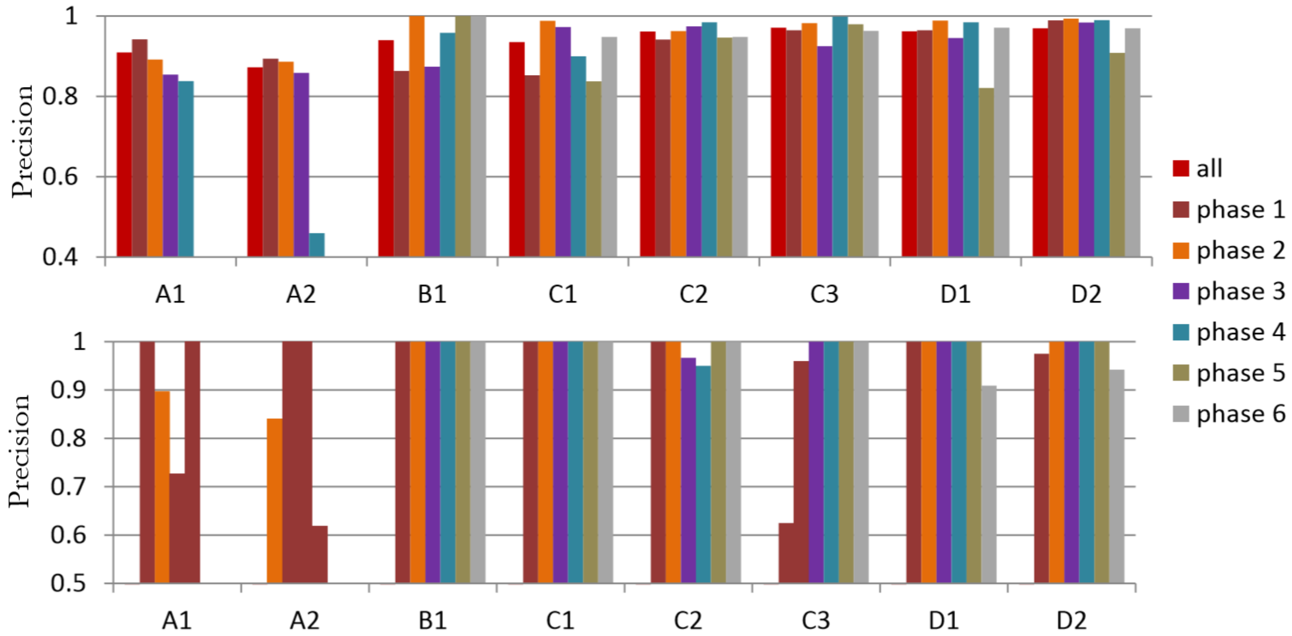
Data: problem instance X; preselected phases Y
Result: selected phases P; solution S of X

$Z \leftarrow \emptyset;\ C \leftarrow \{\emptyset\};$ // Conflicts
$assert(X);$
$status = check(Y);$
while $status == unsat$ **do**
    $U = unsatcore();$
    for $k = 1 ... |Y|$ **do**
        for $Z \subseteq U \wedge |Z| = k$ **do**
            if $Z \notin C$ **then**
                $C = C \cup Z;$
                goto next;
            end
        end
    end
    next;
    $status = check(Y \setminus Z);$
end
$P = Y \setminus Z;\ S = getsolution();$
return (P, S)

Empirical Results

Workers' Precision

Aggregated Precision



Quality of the workers' submissions and of the aggregated phase by system (or instance).We considered 8 different systems (all of them involving 3 different metals): A_1 - D_2. (Upper) The average precision of workers' submissions towards ground truth phases; (Lower) The precision of the aggregated phases towards ground truth phases. The color of the bars denote the ground-truth phase they are comparing to.

Empirical Results

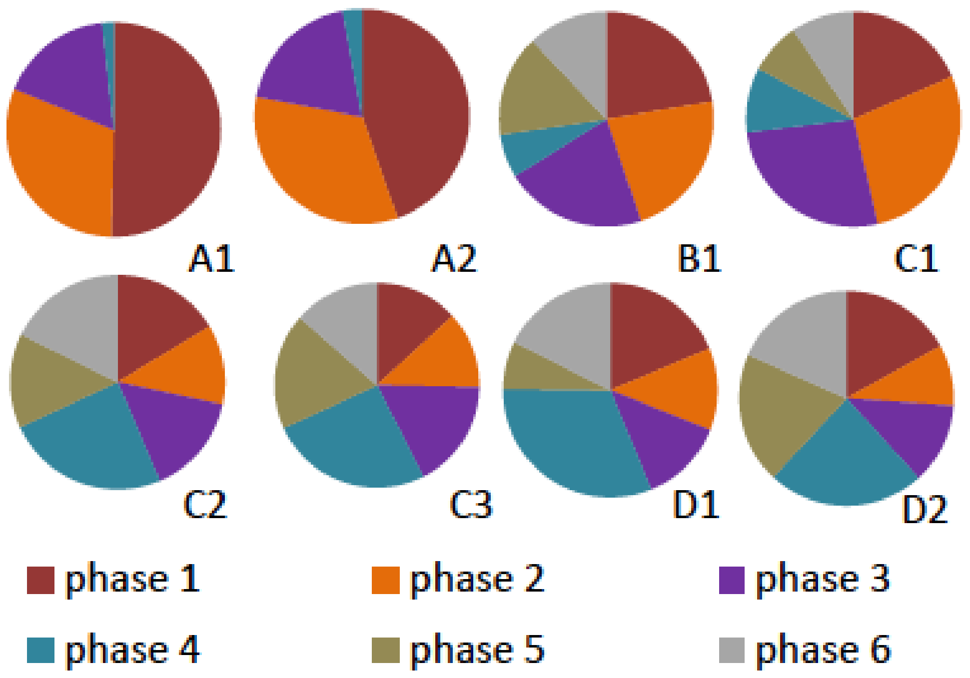


Figure : Percentage of workers' annotations that belong to each ground truth phase, for the different systems (A1, A2, B1, C1, C2, C2, C3, D1, and D2). The percentage related to ground truth phase Q is defined as $\frac{|P \in sub, P \cap Q \neq \emptyset|}{\sum_Q |P \in sub, P \cap Q \neq \emptyset|}$.

Empirical Results

Dataset				Solver only	Solver with Human Computation input			
System	*P*	*L**	*K*	Time *(s)*	Overall Time *(s)*	Aggregation *(s)*	Backtrack *(s)*	#backtracks
A1	36	8	4	3502	**859**	17	300	4
A2	60	8	4	17345	**4377**	29	272	2
B1	15	6	6	79	**4**	0.07		0
C1	28	6	6	346	**62**	0.5		0
C2	28	8	6	10076	**271**	4		0
C3	28	10	6	28170	**1163**	6	105	1
D1	45	7	6	18882	**596**	7		0
D2	45	8	6	46816	**1003**	13		0

From ~13 hours down to ~16 minutes

Comparison of the runtimes of the solver with and without the human component for the different systems. *P* is the number of sample points, *L* is the average number of peaks per phase, *K* is the number of basis patterns

Summary

- Framework
  - Combining state-of-the-art optimization solvers with a human computation component
- Hybrid complementary setting
  - Human input can dramatically boost the performance of combinatorial reasoning and optimization methods by identifying backdoors
- Materials Discovery
  - Very exciting new research area for Computer Science
  - Significant overall performance gains for the Phase Map Identification problem

Thank you.

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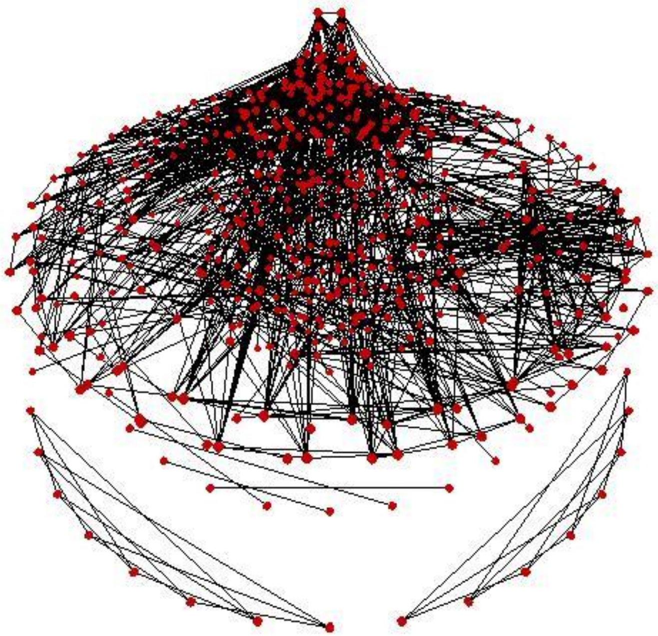
Additional Slides

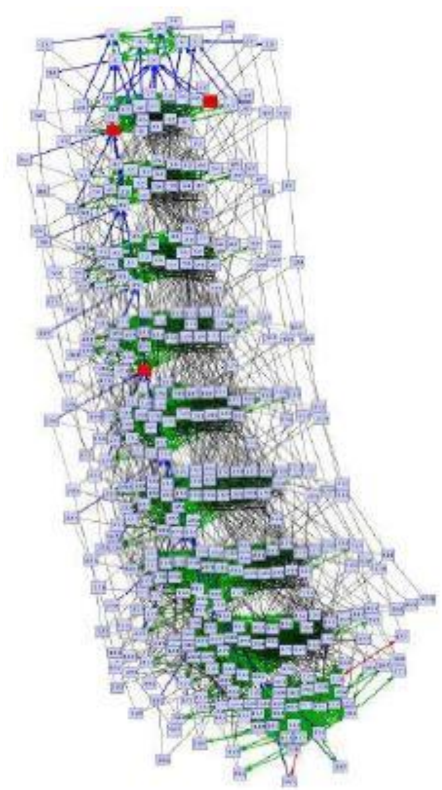
Backdoors - “seeing is believing”



Logistics planning formula. After setting 5 backdoor vars

(result after propagation);

Backdoors - “seeing is believing”



Infeasible ***planning instance.*** ***Strong backdoor*** ***of size 3.***

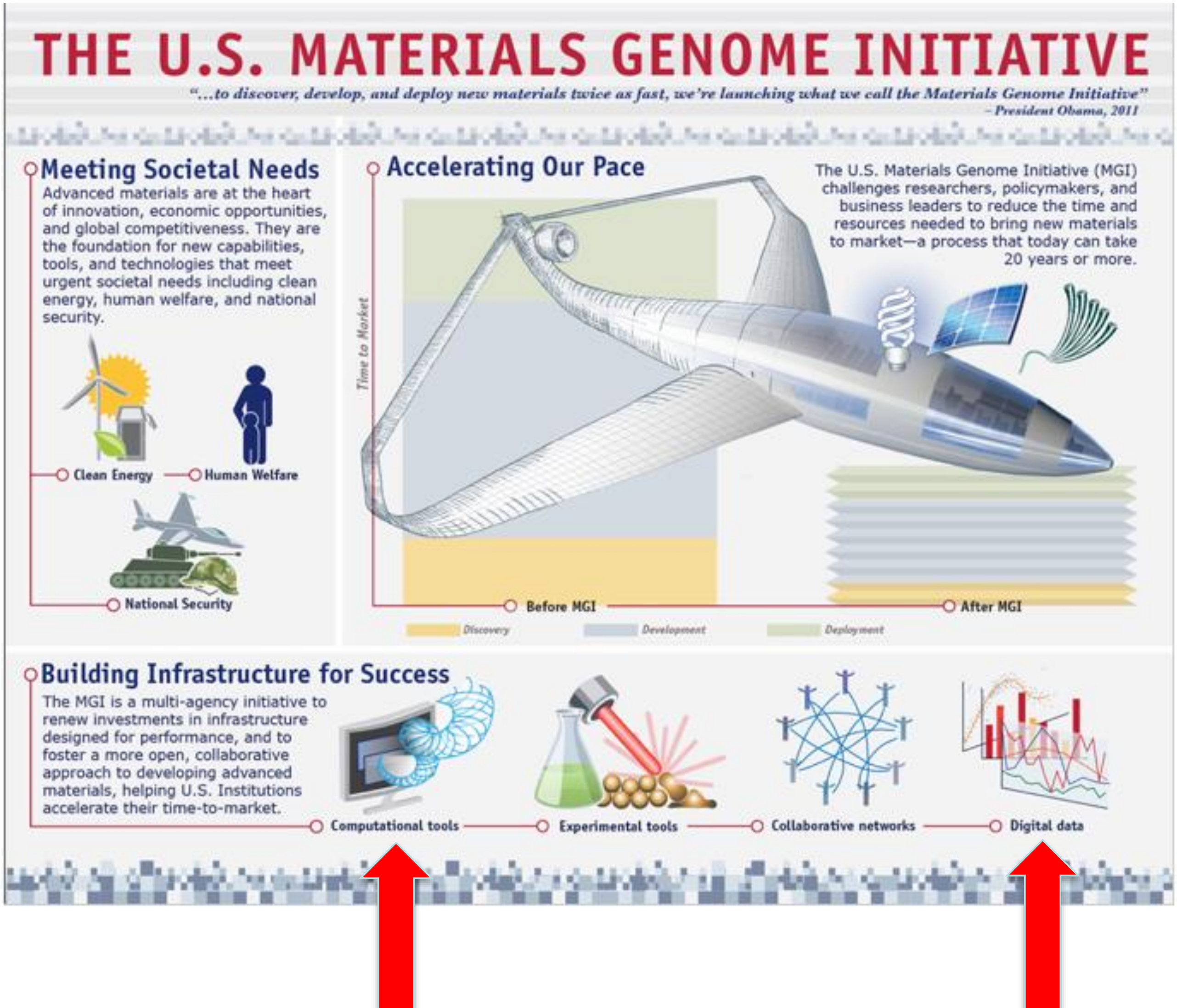
392 vars, 2,578 clauses.

Motivating Application: Need for new sustainable materials

"... **existing energy approaches** — even with improvements from advanced engineering and improved technology based on known concepts — will **not be enough to secure our energy future**. Instead, **meeting the challenge will require** new technologies for producing, storing and using energy with performance levels far beyond what is now possible. Such technologies spring from **scientific breakthroughs in new materials** and chemical processes that govern the transfer of energy between light, electricity and chemical fuels."

US Department of Energy Panel on New Science for a Secure and Sustainable Energy Future, 2010

Motivating Application:
White House Materials Genome Initiative



Goal

Accelerate the pace and reduce the cost of discovery, and deployment of advanced material systems

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Very exciting new research area for Computer Science