Computer Assisted Mathematical Discovery

John Mackey

Carnegie Mellon University

CMUMC Colloquium

Carnegie Mellon University April 17, 2024

50 Years of Success in Computer-Assisted Mathematics

- 1976 Four-Color Theorem
- 1998 Kepler's Conjecture
- 2010 Largest number of moves to solve a Rubik's Cube is 20
- 2014 Erdős discrepancy problem ($C = 2$)
- 2016 2-Color Pythagorean triples problem
- 2018 Computation of Schur's fifth number
- 2019 Keller's Conjecture
- 2022 The Packing Number of the Infinite Square Grid is 15
- 2023 There is an Empty Hexagon in Every 30 Points

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How about $H := (\neg v \wedge (v \vee w)) \wedge (\neg w)$?

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p	q	r	falsifies	evaluation
F	F	F	$(q \vee r)$	F
F	F	T	none	T
F	T	F	$(p \vee \neg q)$	F
F	T	T	$(p \vee \neg q)$	F
T	F	F	$(q \vee r)$	F
T	F	T	$(\neg r \vee \neg p)$	F
T	T	F	none	T
T	T	T	$(\neg r \vee \neg p)$	F

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Davis-Putnam Algorithm: Given a Conjunctive Normal Form (CNF) formula, repeatedly select a variable, add all resolvents over that variable, and then delete all clauses containing that variable. If you derive a contradiction, then the original formula is unsatisfiable, otherwise a satisfying assignment can be found.

An example of the Davis-Putnam Algorithm

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Consider the following CNF formula (here overline means negation):

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Resolving over the variable x_1 yields:

$$(x_2 \vee \overline{x}_3 \vee \overline{x}_4) \wedge (x_2 \vee \overline{x}_3 \vee x_4) \wedge (\overline{x}_2 \vee x_3 \vee x_4) \wedge (x_2 \vee x_3 \vee x_4) \wedge$$
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Resolving over the variable x_3 yields:

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Thus, the original formula is unsatisfiable.

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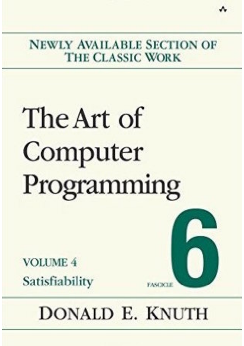

Donald Knuth: *"evidently a killer app, because it is key to the solution of so many other problems"* [Knuth '15]

A Combinatorial Problem of Schur

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$$\begin{array}{lll} 1+1=2 & 1+2=3 & 1+3=4 \\ 1+4=5 & 1+5=6 & 2+2=4 \\ 2+3=5 & 2+4=6 & 3+3=6 \end{array}$$

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As n gets larger, such colorings will become more difficult to produce; eventually we will need to use orange, and for sufficiently large n such colorings will be impossible to produce. This is a consequence of Schur's Theorem.

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For each $k = 1, 2, \ldots n$ we ensure that k has **at least** one color with the following clause: $x_{4k} \vee x_{4k-1} \vee x_{4k-2} \vee x_{4k-3}$.

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For each $k = 1, 2, \ldots n$ we ensure that k has **at most** one color with the following six clauses:

$$\begin{array}{ccc} \neg x_{4k} \vee \neg x_{4k-1} & \neg x_{4k} \vee \neg x_{4k-2} & \neg x_{4k} \vee \neg x_{4k-3} \\ \neg x_{4k-1} \vee \neg x_{4k-2} & \neg x_{4k-1} \vee \neg x_{4k-3} & \neg x_{4k-2} \vee \neg x_{4k-3}. \end{array}$$

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For each solution of $a + b = c$ with $a, b, c \in \{1, \ldots n\}$ we ensure that a, b, and c **don't all have the same color** with the following four clauses:

$$\begin{array}{cc} \neg x_{4a} \vee \neg x_{4b} \vee \neg x_{4c} & \neg x_{4a-1} \vee \neg x_{4b-1} \vee \neg x_{4c-1} \\ \neg x_{4a-2} \vee \neg x_{4b-2} \vee \neg x_{4c-2} & \neg x_{4a-3} \vee \neg x_{4b-3} \vee \neg x_{4c-3}. \end{array}$$

Mathematicians are Interested in Machine-Assisted Proofs

ipam

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FEBRUARY 13 - 17, 2023

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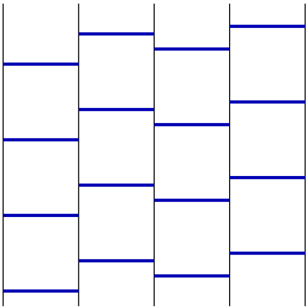
NEWS | 18 June 2021

Mathematicians welcome computer-assisted proof in 'grand unification' theory

Keller's Conjecture: A Tiling Problem

Consider tiling a floor with square tiles, all of the same size. Is it the case that any gap-free tiling results in at least two fully connected tiles, i.e., tiles that have an entire edge in common?



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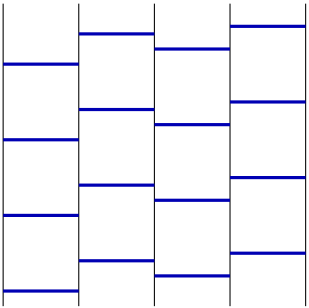
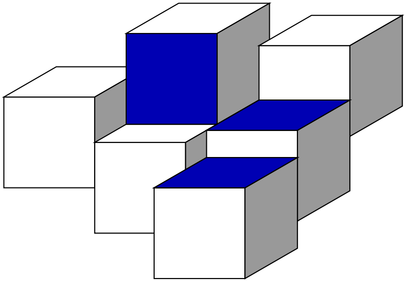


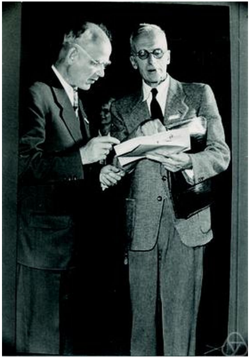


Keller's Conjecture: Resolved

[Brakensiek, Heule, Mackey, & Narvaez 2019]

In 1930, Ott-Heinrich Keller conjectured that this phenomenon holds in every dimension.

Keller's Conjecture.
For all $n \geq 1$, every tiling of the n-dimensional space with unit cubes has two which fully share a face.



[Wikipedia, CC BY-SA]

GEOMETRY

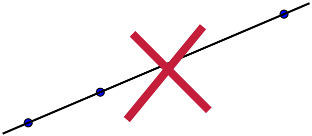
Computer Search Settles 90-Year-Old Math Problem

10

By translating Keller's conjecture into a computer-friendly search for a type of graph, researchers have finally resolved a problem about covering spaces with tiles.

An Empty Hexagon in Every Set of 30 Points

Computational geometry and SAT: Shapes in point sets in general position (no three points on a line)



k-hole: empty k-point convex shape

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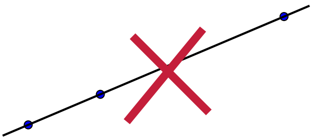

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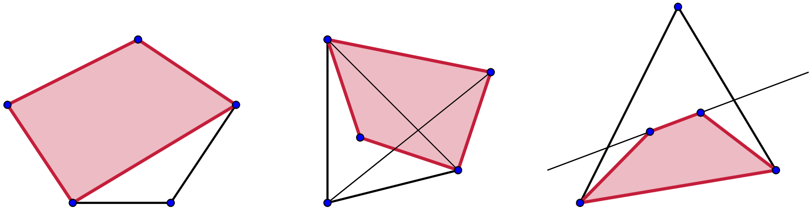
Every set of 5 points contains in a 4-hole [Klein 1932]



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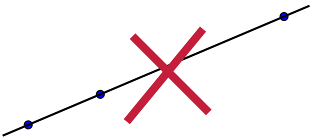
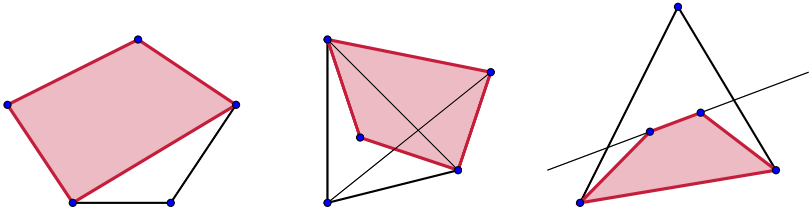


k-hole: empty k-point convex shape

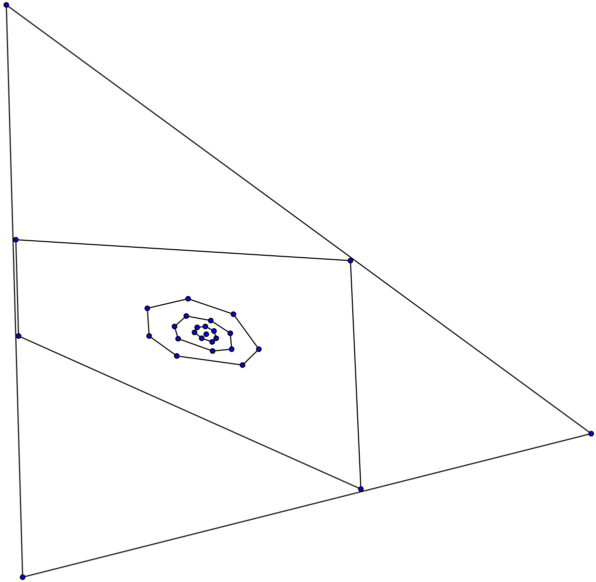
Every set of 5 points contains in a 4-hole [Klein 1932]



Every set of 30 points contains in a 6-hole (using SAT)

[Heule & Scheucher 2023]

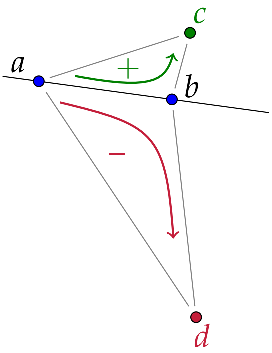
Avoiding an Empty Hexagon in a Set of 29 Points



SAT Encoding: Orientation Variables

No explicit coordinates of points

Instead, for every triple $a < b < c$, one orientation variable $O_{a,b,c}$ to denote whether point c is above the line ab



Not all assignments are realizable

- Axioms eliminate many unrealizable assignments

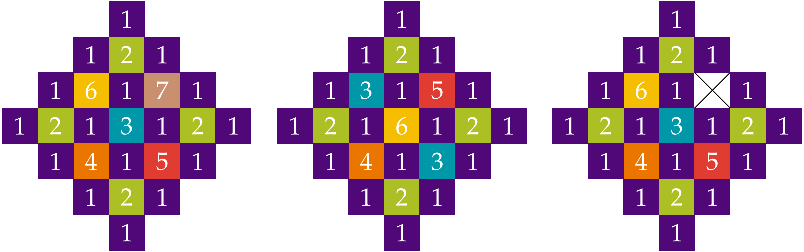
Many possible SAT encodings

- Big impact on performance
- Machine learning can help!

Packing Chromatic Number

Definition

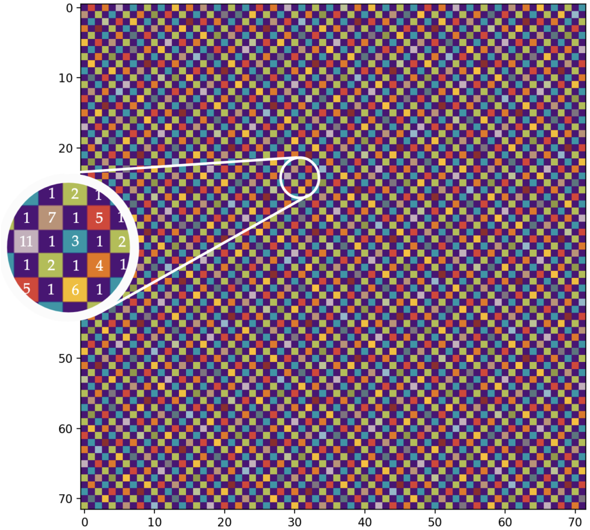
A packing k-coloring of a simple undirected graph $G = (V, E)$ is a function φ from V to $\{1, \ldots, k\}$ such that for any two distinct vertices $u, v \in V$, and any color $c \in \{1, \ldots, k\}$, it holds that $\varphi(u) = \varphi(v) = c$ implies $d(u, v) > c$.



Packing Chromatic Number of the Infinite Grid is 15

The 72×72 15-coloring below can be used to tile the infinite grid

- This is not possible with 14 colors [Subercaseaux & Heule'23]



Chromatic Number of the Plane (CNP)

The Hadwiger-Nelson problem (around 1950):
How many colors are required to color the plane such that each pair of points that are exactly 1 apart are colored differently?

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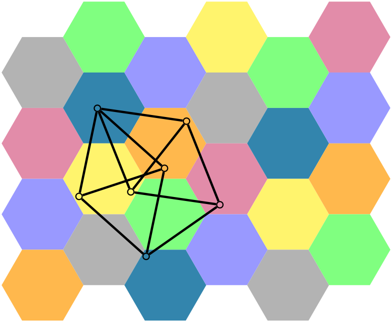

- The Moser Spindle graph shows the lower bound of 4
- A coloring of the plane showing the upper bound of 7

CNP: First progress in decades

Recently enormous progress:

- Lower bound of 5 [DeGrey '18] based on a 1581-vertex graph
- This breakthrough started a polymath project
- Improved bounds of the fractional chromatic number of the plane

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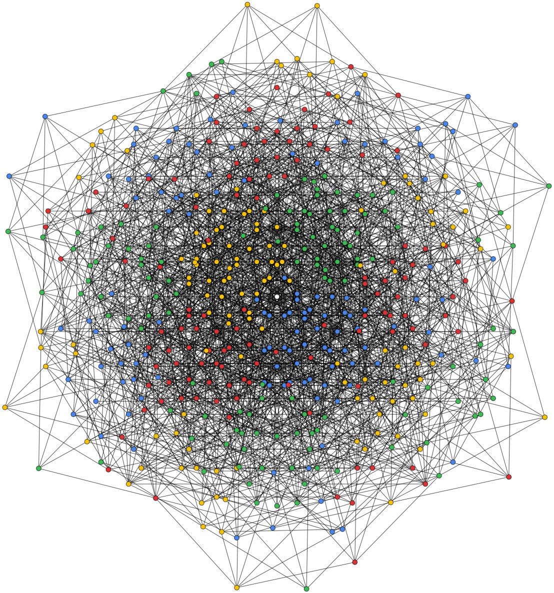
We found smaller graphs with SAT:

- 874 vertices on April 14, 2018
- 803 vertices on April 30, 2018
- 610 vertices on May 14, 2018

Proof Minimization: 510 Vertices [Heule 2021]



Beyond NP: The Collatz Conjecture

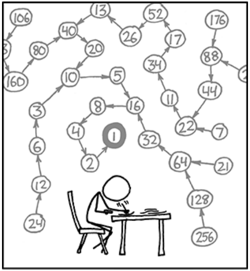
Resolving foundational algorithm questions

$$Col(n) = \begin{cases} n/2 & \text{if } n \text{ is even} \\ (3n+1)/2 & \text{if } n \text{ is odd} \end{cases}$$

Does `while`$(n > 1)$ $n = Col(n)$; terminate?

Find a non-negative function $fun(n)$ s.t.

$$\forall n > 1 : fun(n) > fun(Col(n))$$



THE COLLATZ CONJECTURE STATES THAT IF YOU PICK A NUMBER, AND IF IT'S EVEN DIVIDE IT BY TWO AND IF IT'S ODD MULTIPLY IT BY THREE AND ADD ONE, AND YOU REPEAT THIS PROCEDURE LONG ENOUGH, EVENTUALLY YOUR FRIENDS WILL STOP CALLING TO SEE IF YOU WANT TO HANG OUT.

source: xkcd.com/710

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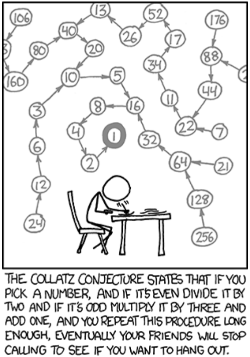


source: xkcd.com/710

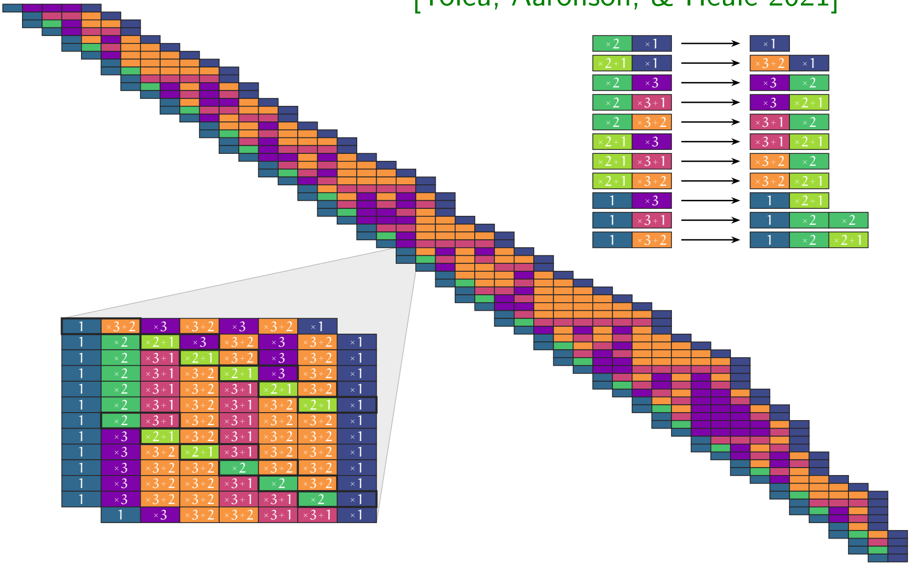
Can we construct a function s.t. $fun(n) > fun(Col(n))$ holds?

$fun(3)$	$fun(5)$	$fun(8)$	$fun(4)$	$fun(2)$	$fun(1)$
5	4	3	2	1	0

Collatz Conjecture: Studying a Rewrite System

[Yolcu, Aaronson, & Heule 2021]

×2 ×1	→	×1
×2+1 ×1	→	×3+2 ×1
×2 ×3	→	×3 ×2
×2 ×3+1	→	×3 ×2+1
×2 ×3+2	→	×3+1 ×2
×2+1 ×3	→	×3+1 ×2+1
×2+1 ×3+1	→	×3+2 ×2
×2+1 ×3+2	→	×3+2 ×2+1
1 ×3	→	1 ×2+1
1 ×3+1	→	1 ×2 ×2
1 ×3+2	→	1 ×2 ×2+1



Collatz Conjecture: Successes and Challenge

Success. Rewrite system with 11 rules: Their termination solves Collatz. Our tool proves termination of any subset of 10 rules.

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$$F(n) = \begin{cases} \frac{n-1}{3} & \text{if } n \equiv 1 \pmod 3 \\ \frac{n}{2} & \text{if } n \equiv 0 \text{ or } n \equiv 2 \pmod 6 \\ \frac{3n+1}{2} & \text{if } n \equiv 3 \text{ or } n \equiv 5 \pmod 6 \end{cases}$$

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Challenge (\$500). An easier generalized Collatz problem is open:

$$H(n) = \begin{cases} \frac{3n}{4} & \text{if } n \equiv 0 \pmod 4 \\ \frac{9n+1}{8} & \text{if } n \equiv 7 \pmod 8 \\ \perp & \text{otherwise} \end{cases}$$

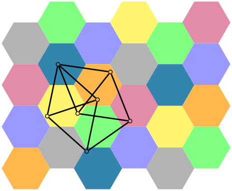
Conclusions

Successes, Advances, and Trust:

- A performance boost of SAT technology allows solving new problems in mathematics
- Problems beyond NP are ready for an automated approach
- Some proofs may be gigantic, but can be validated using formally-verified checkers

Classic problems ready for mechanization?

- Chromatic number of the plane
- Optimal matrix multiplication
- Collatz Conjecture



One More Thing: Costas Arrays