CONSTRAINT & **COST** FUNCTION NETWORKS:

FEASIBILITY, OPTIMIZATION AND LEARNING

JFPC'2021

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June 22, 2021







lacksquare a sequence of discrete domain variables $m{V}$

- a set Φ of e Boolean functions (or constraints)
- Each $\varphi_{S} \in \Phi$ is a truth function from $D^{S} \rightarrow \{t, f\}$

Joint truth function

$$\Phi_{\mathcal{M}} = \bigwedge_{\varphi_{S} \in \Phi} \varphi_{S}$$

The Constraint Satisfaction Problem (NP-complete)



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The Constraint Satisfaction Problem (NP-complete)



Languages for domains and constraints

- Constraint Networks: Boolean tables (tensors) for domains and constraints
- Constraint Programming: interval variables, specialized constraints, control

Tables (or tensors) for φ_{S}

- A multidimensional table with a Boolean for every tuple in D^S
- Says if it is authorized (*t*) or not (*f*)





Languages for domains and constraints

- Constraint Networks: Boolean tables (tensors) for domains and constraints
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Global constraints

Names for specific (useful) constraints

Most famous AllDifferents



Languages for domains and constraints

- Constraint Networks: Boolean tables (tensors) for domains and constraints
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Application domains: NP and beyond

Excel at the analysis of complex perfectly known systems

Digital circuit verification, scheduling and other resource management problems, planning, software verification, theorem proving,...

Biology?



- lacksquare a sequence of discrete domain variables $m{V}$
- a set Φ of e integer cost functions
- Each $\varphi_{S} \in \Phi$ is a numerical function bounded by k (finite or infinite)

Joint cost function using $a + {}^{k} b = \min(a + b, k)$

$$\Phi_{\mathcal{M}} = \sum_{\varphi_{S} \in \Phi}^{k} \varphi_{S}$$

The Weighted Constraint Satisfaction Problem (decision NP-complete)

• What is the minimum of $\Phi_{\mathcal{M}}$?



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Tables (or tensors) for φ_{S}

 A multidimensional table with a number for every tuple in D^S

Global functions

Names for specific (useful) functions

Soft difference (3 values)

$$\left[\begin{array}{rrrr} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}\right]$$

A useful one

Knapsack_s



Tables (or tensors) for $arphi_{oldsymbol{S}}$

 A multidimensional table with a number for every tuple in D^S

Global functions

Names for specific (useful) functions

Soft difference (3 values) $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

A useful one

KNAPSACKS



Costs and constraints

- We assume non negative integer costs
- A constraint is a cost function that maps to $\{0, k\}$
- k = 1 defines a pure Constraint Network

Optimum preserving operations

\blacksquare scaling: $2^{63}\approx 19$ digits. Fixed decimal point numbers $\ldots \ldots \ldots \ldots$	ok
shifting: negative numbers and maximization	ok



Extra assumptions inside the solver	w/o l.o.g.
 CFNs have all unary functions $\varphi_i, X_i \in V$ CFNs have a constant function φ_{\varnothing} 	(domains)

Crucial property

 $arphi_arnothing$ is a lower bound of the joint function $\Phi_\mathcal{M}$

Graph G = (V, E) with edge weight function w

- A Boolean variable X_i per vertex $i \in V$
- A cost function per edge $e = (i, j) \in E : \varphi_{ij} = w(i, j) \times \mathbb{1}[x_i \neq x_j]$

A simple graph

- vertices $\{1, 2, 3, 4\}$
- cut weight 1 or 1.5(1,3)
- edge (1,2) hard

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Min-CUT on 4 variables

```
"problem" :{"name": "MinCut", "mustbe": "<100.0"},
    variables: {"x1": ["1"], "x2": ["1","r"],
        "x3": ["1","r"], "x4": ["r"]}
"functions": {
        "cut12": {"scope": ["x1","x2"], "costs": [0.0, 100.0, 100.0, 0.0]},
        "cut13": {"scope": ["x1","x3"], "costs": [0.0,1.5,1.5,0.0]},
        "cut23": {"scope": ["x2","x3"], "costs": [0.0,1.0,1.0,0.0]},
        "cut34": {"scope": ["x3","x4"], "costs": [0.0,1.0,1.0,0.0]}</pre>
```



Min-CUT on 4 variables

```
import pytoulbar2
myCFN = pytoulbar2.CFN(100,1)  # ub, resolution (optional)
for i in range(4):
    myCFN.AddVariable("x"+str(i+1),["1", "r"]) # returns an index
myCFN.AddFunction(["x1"],[0,100])
myCFN.AddFunction(["x4"],[100,0])
myCFN.AddFunction(["x1","x3"], [0,1.5,1.5,0])
...
sol = myCFN.Solve()  # returns a triple (sol, cost, _)
```



Definition

- Variables X_{ij} for cell (i, j) has domain $\{1, \dots, 9\}$
- Set R_i (resp. C_j) contains all variables of row i (resp. column j)
- Set S_i contains all variables in sub-cell i
- There is an ALL-DIFFERENT constraint on each of these
- or a clique of pairwise DIFFERENT constraints

Example

Let's have a look at the pytoulbar2 code.



```
myCFN = pytoulbar2.CFN(1) # k = 1, so CSP
```

```
for i in range(9):
    for j in range(9):
        vIdx = myCFN.AddVariable("X"+str(i+1)+"."+str(j+1),range(1,10))
        columns[j].append(vIdx)
        rows[i].append(vIdx)
        cells[(i//3)*3+(j//3)].append(vIdx)
```

```
for scope in rows+columns+cells:
   addCliqueAllDiff(myCFN,scope)  # Adds a clique of pairwise difference
```

for v,h in enumerate(grid):
 if h: myCFN.AddFunction([v],[0 if i == h else 1 for i in range(1,10)])

NUMBERS: INTERFACING WITH DL





The Boolean way

Thanks to Tias Gun for the picture above

- 1. Assign the cell variable with the prediction
- 2. LeNet has 99.2% accuracy, SAT-Net dataset 36.2 hints (avg):74.7% max. accuracy

The Numbers way

- 1. Add LeNet output tensor (negated) as a cost function

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The Numbers way

- 1. Add LeNet output tensor (negated) as a cost function



```
myCFN = pytoulbar2.CFN(1000000,6)
```

```
for i in range(9):
    for j in range(9):
        vIdx = myCFN.AddVariable("X"+str(i+1)+"."+str(j+1),range(1,10))
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```
for scope in rows+columns+cells:
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```
for v, h in enumerate(grid):
    if h: myCFN.AddFunction([v],-MNIST_output(csol,v,h))
```



CFN compared to a COP approach¹

- COP (OR-Tools) + global All-Different
- CFN (toulbar2) + pairwise differences

Tight links with (I)LP

Let's look at the primal connection

¹Maxime Mulamba et al. "Hybrid Classification and Reasoning for Image-based Constraint Solving". In: *Proc.* of CPAIOR'20, also in arXiv preprint arXiv:2003.11001. 2020, pp. 364–380.



0.79"

CFN compared to a COP approach¹ ■ COP (OR-Tools) + global All-Different

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COP (OR-Tools) + global All-Different	0.79"
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- 99.6% of all problems are solved backtrack-free by toulbar2
- CFN bounds way tighter than COP bounds [LL12]

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 $nd + ed^2$ variables, n + 2ed constraints: a strong but expensive bound

ANIT



1 Systematic search and local search

- 2 Pruning and Bounds
- 3 All Toulbar2 bells and whistles
- 4 WCSP solving has made huge progress
- 5 Learning CFN from data

Systematic tree search

TREE SEARCH

If all |D^X| = 1 obvious minimum update
Else choose X ∈ V s.t. |D^X| > 1 and u ∈ D^X and reduce to
1. one query where we set X = u
2. one where u is removed from D^X









Time $O(d^n)$, linear space

TREE SEARCH

Systematic tree search

- If all $|D^X| = 1$ obvious minimum
- Else choose $X \in V$ s.t. $|D^X| > 1$ and $u \in D^X$ and reduce to
 - 1. one query where we set X = u
 - 2. one where u is removed from D^X
- Return the minimum





54



Time $O(d^n)$, linear space
Depth First (CP) or Best First (ILP)?

Hybrid Best First Search [All+15]

Anyspace

- Uses Depth-First Search for a bounded amount of backtracks
- Pending nodes are pushed onto a list of Open nodes
- The next DFS starts from the best Open node
- Tree-decomposition friendly (BTD [GSV06]/AND-OR search [MD09])



- Good upper bounds quickly (DFS)
- A constantly improving global lower bound (optimality gap)
- Implicit restarts, easy parallelization

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Also local search of course (VNS here)







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GOOD OLD ARC CONSISTENCY (CONSTRAINT NETWORKS)



Filtering by Arc Consistency (support)

A value $u \in D^i$ with no value $v \in D^j$ such that $\varphi_{ij}(u, v) = 0$ can be deleted, leaving the problem equivalent.



Properties

- Combine φ_{ij} and φ_j
- Project on X_i
- Combine with φ_i
- Unique fixpoint (monotonic), polynomial time

(inconsistency detection)

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Obvious issue

One cannot add functions to the CFN: loss of equivalence, meaningless result

Equivalence Preserving Transformations with $-^{k} (\alpha - ^{k} \beta) \equiv ((\alpha = k) ? k : \alpha - \beta)$

- Add the projection to $arphi_j$ with +
- ullet Subtract it from its source using $-^k$



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(Loss of) properties





(Loss of) properties





(Loss of) properties





(Loss of) properties

${\rm Example \ with} \ k>1$





$$\Downarrow$$
 m

 $\varphi_{\varnothing} = 1$

(Loss of) properties

${\rm Example \ with} \ k>1$





$$\Downarrow$$
 m_{s}^{2}

$$\varphi_{\varnothing} = 1$$

(Loss of) properties



The many "soft ACs" One paper to read: [Coo+10] NC+AC+DAC (FDAC): binary & unary (+ direction)[Sch00; Lar02; Coo03] **Full Supports** +Existential AC: EDAC, a star (variable incident functions) [Lar+05] EAC supports +Virtual AC: any spanning tree [Coo+08; Coo+10] VAC supports

If $(\varphi_{\varnothing} \stackrel{k}{+} \varphi_i(u)) = k$, NC deletes u



The many "soft ACs"One paper to read: [Coo+10]• NC+AC+DAC (FDAC): binary & unary (+ direction)[Sch00; Lar02; Coo03]Full Supports• +Existential AC: EDAC, a star (variable incident functions) [Lar+05]EAC supports• +Virtual AC: any spanning tree [Coo+08; Coo+10]VAC supportsSupports provide value ordering heuristicsEAC: $\varphi_i(u) = 0$ can be extended for free on X_i 's star

• VAC: $\varphi_i(u) = 0$ can be extended for free on any spanning tree [Kol06; Coo+08; Coo+10]

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- Stronger bounds than AC in COP [LL12]

(k = 1)

(Generalized ACs)

 $(NC \le AC \le FDAC \le EDAC \le VAC)$

Set of rational EPTs

OSAC [Sch76; Coo07; Wer07; Coo+10]

Maximizing φ_{\varnothing} is in P (local polytope dual + AC for k)



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OPTIMAL SOFT ARC CONSISTENCY (OPTIMIZATION ALONE)

Variables for a binary CFN, no constraints [Sch76; Kos99; CGS07; Wer07; Coo+10]

- 1. u_i : amount of cost shifted from φ_i to φ_{\varnothing}
- 2. p_{ija} : amount of cost shifted from φ_{ij} to $\varphi_i(a)$
- 3. p_{jib} : amount of cost shifted from φ_{ij} to $\varphi_j(b)$

OSAC

$$\begin{array}{l} \text{Maximize } \displaystyle\sum_{i=1}^{n} u_{i} & \text{subject to} \\ \\ \displaystyle \varphi_{i}(a) - u_{i} + \displaystyle\sum_{(\varphi_{ij} \in C)} p_{ija} \geq 0 & \forall i \in \{1, \ldots, n\}, \, \forall a \in D^{i} \\ \\ \displaystyle \varphi_{ij}(a, b) - p_{ija} - p_{jib} \geq 0 & \forall \varphi_{ij} \in C, \forall (a, b) \in D^{ij} \end{array}$$

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The power of VAC and OSAC

Problems solved [Coo+10; KZ17]

- Tree-structured problems
- Permutated submodular problems

OSAC empirically too expensive compared to VAC

- CFN Arc consistencies provide fast approximate LP bounds
- and deal with constraints seamlessly

CFN Local Consistencies

Enhance CP with fast incremental approximate Linear Programming dual bounds



(e.g. Min-Cut)

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Toulbar2



Additional algorithmic ingredients

- Value ordering (for free): existential or virtual supports
- Variable ordering: weighted degree [Bou+04], last conflict [Lec+09], VAC-based [TGK20]
- (On the fly) variable elimination [Lar00]
- Dominance analysis (substitutability/DEE) [Fre91; Des+92; DPO13; All+14]
- Function decomposition [Fav+11]
- Some global cost functions (weighted Regular, All-Diff, Among...) [LL12; All+16]
- Incremental solving, guaranteed diverse solutions [Ruf+19]
- Unified (Parallel) Decomposition Guided VNS/LDS (UPDGVNS [Oua+20])

More information

github.com/toulbar2/toulbar2

miat.inrae.fr/toulbar2



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CPLEX V12.4.0.0

```
Problem '3e4h.LP' read.
Root relaxation solution time = 811.28 sec.
...
MIP - Integer optimal solution: Objective = 150023297067
Solution time = 864.39 sec.
```

tb2 and VAC



loading CFN file: 3e4h.wcsp Lb after VAC: 150023297067 Preprocessing time: 9.13 seconds. Optimum: 150023297067 in 129 backtracks, 129 nodes and 9.38 seconds.

Comparison with Rosetta's Simulated annealing $^{\scriptscriptstyle 2}$



Optimality gap of the Simulated annealing solution as problems get harder

²David Simoncini et al. "Guaranteed Discrete Energy Optimization on Large Protein Design Problems". In: Journal of Chemical Theory and Computation 11.12 (2015), pp. 5980–5989. DOI: 10.1021/acs.jctc.5b00594.

QUANTUM COMPUTING (DWAVE), TOULBAR2 & SA [MUL+19]





DWave approximations

kcal/mol

gap > 1.1690% of the time

> 4.35, 50% of the time

 $>8.45,\,10\%$ of the time

Kind words from Protein Designers³

The Toulbar[2] package for WCSPs significantly improved the state-of-the-art efficiency for protein design in the discrete pairwise model.

Kind words from OpenGM2 developpers (image processing)

"ToulBar2 variants were superior to CPLEX variants in all our tests"4

⁴Stefan Haller, Paul Swoboda, and Bogdan Savchynskyy. "Exact MAP-Inference by Confining Combinatorial Search with LP Relaxation". In: *Thirty-Second AAAI Conference on Artificial Intelligence*. 2018.

³Mark A Hallen and Bruce R Donald. "Protein design by provable algorithms". In: *Communications of the ACM* 62.10 (2019), pp. 76–84.

Kind words from Protein Designers³

The Toulbar[2] package for WCSPs significantly improved the state-of-the-art efficiency for protein design in the discrete pairwise model.

Kind words from OpenGM2 developpers (image processing)

"ToulBar2 variants were superior to CPLEX variants in all our tests"⁴

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Data mining, bioinformatics

Given a matrix of arbitrary real numbers, find a subset C of columns and R of rows such that the sum of numbers in the submatrix is maximized.

Dedicated global constraint

Presented in [BSD17; Der+19], dominates MILP and MIQCP.



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```
def generate_model(path):
  m = pandas.read_csv(path, sep='\t', header=None)
 r, c = m.shape
  model = pytoulbar2.CFN(100000, 10, True)
  for i in range(r):
   model.AddVariable("R"+str(i), ["out", "in"])
 for j in range(c):
   model.AddVariable("C"+str(j), ["out", "in"])
  for i in range(r):
   for j in range(c):
      model.AddFunction(["R"+str(i), "C"+str(j)], [0.0, 0.0, 0.0, -m[j][i]])
  return model
```

```
(solution,, cost, _) = generate_model(sys.argv[1]).Solve()
```



The Global Constraint author

Je n'ai pas vraiment trouvé de cas [...] défavorable pour toulbar2.



3026 instances of various origins genoweb.toulouse.inra.fr/~degivry/evalgm MRF: Probabilistic Inference Challenge 2011 CVPR: Computer Vision & Pattern Recognition OpenGM2 CFN: Cost Function Library (CELAR, SPOT5, bioinformatics) MaxCSP: MaxCSP 2008 competition WPMS: Weighted Partial MaxSAT evaluation 2013 CP: MiniZinc challenge 2012/13 (decomposable)

Benchmark	Nb.	UAI	WCSP	LP(direct)	LP(tuple)	WCNF(direct)	WCNF(tuple)	MINIZINC
MRF	319	187MB	475MB	2.4G	2.0GB	518MB	2.9GB	473MB
CVPR	1461	430MB	557MB	9.8GB	11GB	3.0GB	15GB	N/A
CFN	281	43MB	122MB	300MB	3.5GB	389MB	5.7GB	69MB
MaxCSP	503	13MB	24MB	311MB	660MB	73MB	999MB	29MB
WPMS	427	N/A	387MB	433MB	N/A	717MB	N/A	631MB
CP	35	7.5MB	597MB	499MB	1.2GB	378MB	1.9GB	21KB
Total	3026	0.68G	2.2G	14G	18G	5G	27G	1.2G

HBFS - Normalized LB AND UB PROFILES (HARD PROBLEMS) [HUR+16]



Unified Decomposition Guided VNS $_{\rm [Oua+20;\,Oua+17]}$





UDGVNS - NUMBER OF SOLVED PROBLEMS [OUA+17]





UDGVNS - UPPER BOUND PROFILES[OUA+17]





UPDGVNS - UPPER BOUND PROFILES[OUA+20]







- 1 Systematic search and local search
- 2 Pruning and Bounds
- 3 All Toulbar2 bells and whistles
- 4 WCSP solving has made huge progress
- 5 Learning CFN from data

Definition (Learning a pairwise CFN from high quality solutions)

Given:

- \blacksquare a set of variables V,
- a set of assignments E i.i.d. from an unknown distribution of high-quality solutions

Find a pairwise CFN ${\cal M}$ that can be solved to produce high-quality solutions

We use the language of pairwise tensors/tables

There are at most $\frac{n(n-1)}{2}$ pairwise functions	$\frac{81 \times 80}{2} = 3240$
$lacksquare$ Each with $ D^i imes D^j $ costs in ${\mathbb R}$ (differentiability)	81
For the Sudoku, 262, 440 parameters to learn.	

Maximum likelihood estimation

- E a set of i.i.d. assignments of V
- Interpret costs as energies ($\propto -\log(\text{probabilities}))$
- Maximize the probability of observing the samples in E

Maximum loglikelihood $\mathcal M$ on $\mathcal M_\ell$

$$\begin{aligned} \mathcal{L}(\mathcal{M}, \boldsymbol{E}) &= \log(\prod_{\boldsymbol{v} \in \boldsymbol{E}} P_{\mathcal{M}}(\boldsymbol{v})) = \sum_{\boldsymbol{v} \in \boldsymbol{E}} \log(P_{\mathcal{M}}(\boldsymbol{v})) \\ &= \sum_{\boldsymbol{v} \in \boldsymbol{E}} \log(\Phi_{\mathcal{M}}(\boldsymbol{v})) - \log(Z_{\mathcal{M}}) \\ &= \sum_{\boldsymbol{v} \in \boldsymbol{E}} (-C_{\mathcal{M}^{\ell}}(\boldsymbol{v})) - \log(\sum_{\boldsymbol{t} \in \prod X \in \boldsymbol{V} D^{X}} \exp(-C_{\mathcal{M}^{\ell}}(\boldsymbol{t}))) \\ &\xrightarrow{\boldsymbol{v} \in \boldsymbol{E}} \underbrace{\boldsymbol{v} \in \boldsymbol{E}}_{\text{-costs of } \boldsymbol{E} \text{ samples}} \underbrace{\boldsymbol{Soft-Min of all assignment costs}} \end{aligned}$$

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Algorithms and data-sets

- PE-MRF [Par+17] with L1-norm Regularization
- Validation set from the SAT-Net paper⁵ (36.2 hints)
- Validation set from the RRN paper⁶ with 17-34 hints.

⁵Po-Wei Wang et al. "SATNet: Bridging deep learning and logical reasoning using a differentiable satisfiability solver". In: *ICML'19 proceedings, arXiv preprint arXiv:1905.12149.* 2019. ⁶Rasmus Palm, Ulrich Paquet, and Ole Winther. "Recurrent relational networks". In: *Advances in Neural Information Processing Systems.* 2018, pp. 3368–3378.

Learning how to solve the Sudoku



Learning how to solve the Sudoku



Learning how to solve the Sudoku



Learning from uncertain DL output is possible

- LeNet has 99.2% accuracy on handwritten digits
- Argmax decoding: 74.7% of the learning data-set would be incorrect
- Important to accept probabilistic information as input (PE-MRF)

Comparing with SAT-Net

Learning from uncertain DL output is possible

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- Important to accept probabilistic information as input (PE-MRF)

Comparing with SAT-Net

SAT-Net (9,000 samples):	63.2%
Toulbar2+PE-MRF (8,000+1,024 samples):	

See our CP2020 paper⁷

We show how it can learn user preferences and combine them with configuration constraints on Renault dataset (thanks to H. Fargier (IRIT)).

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⁷Céline Brouard, Simon de Givry, and Thomas Schiex. "Pushing data into CP models using Graphical Model Learning and Solving". In: *Principles and Practice of Constraint Programming–CP 2020*. Springer, 2020.

A CONCLUSION

CFN/WCSP solving has made important progress

- Fast approximate LP-bounds (tighter than COP) subsuming AC
- Free value ordering heuristics
- Reduced-cost-based filtering (cost backpropagation)
- Structure aware search with improving optimality gap

CFN can be learned from data and combined with constraints

- Shares with ILP the capacity of dealing with fine grained numerical information
- Tractable learning with probabilistic input (DL/ML connection)
- With the (adjustable) power of (exact) solvers

Directions for improvement

- Global cost function and non monotonicity
- Interval variables and "arithmetic" filtering
- Unify CFN and COP: cost variables, multiple criteria
- Stronger incremental bounds
- Parallel search, conflict learning
- Try to minimize average tardiness in scheduling
- Improve CFN learning (sample size, (global) constraints)

And to all CFN/toulbar2 contributors

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M. Zytnicki (PhD, INRAE) H. Nguyen (PhD) F. Heras (UPC, Spain) P. Meseguer (CSIC, Spain) C. Bessiere (LIMM, Montpellier) M. Fontaine (GREYC, Caen) C. Terrioux (LSIS) Y. Lebbah (GREYC) Mario (CU. Hong-Kong) B. Hurley (Insight)

Questions?

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