Introduction of SAT Planning on Pathway Problems in IPC-5

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H. Nabeshima, T. Soh, K. Inoue, and K Iwanuma:

Lemma Reusing for SAT based Planning and Scheduling.

Proceedings of the International Conference on Automated Planning and Scheduling 2006, pp.103-112, 2006.

IPC-5

- **5th International Planning Competition**
  - **Deterministic Planning Track**
    - ✓ TPP
    - ✓ Openstacks
    - ✓ Storage
    - ✓ **Pathways**
    - ✓ Trucks
    - ✓ Rovers
    - ✓ Pipeworld
  - Probabilistic Planning Track

Pathway Planning Problems

Purpose

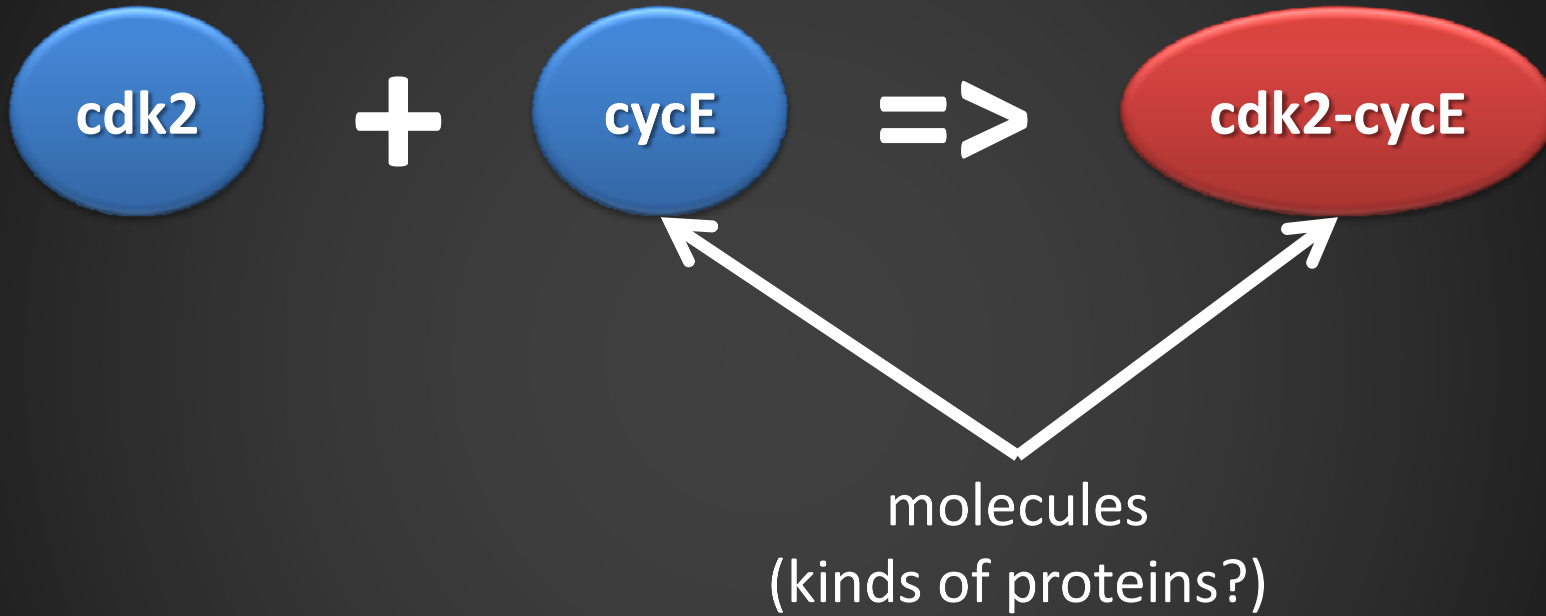
Finding **a sequence of biochemical reactions** (**pathway**) in an organism producing certain substances

3 kinds of biochemical reactions:

1. **Association reaction**
2. **Catalyzed association reaction**
3. **Synthesis reaction**

Biochemical Reactions

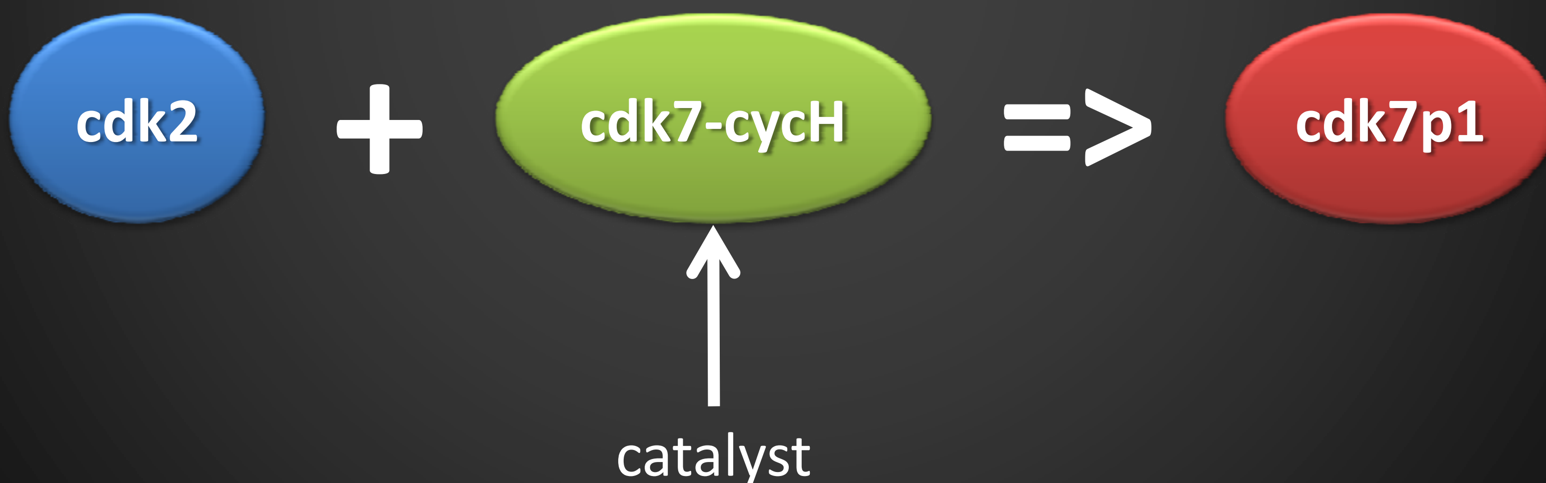
Association reaction (complexation rule)



Biochemical Reactions

Association reaction (complexation rule)

Catalyzed association reaction (phosphorylation rule)



Biochemical Reactions

Association reaction (complexation rule)

cdk2 + cycE => cdk2-cycE

Catalyzed association reaction (phosphorylation rule)

cdk2 + cdk7-cycH => cdk7p1

Synthesis reaction

SP1-gP => cycA

Corresponding Actions (1/3)

Association reaction (complexation rule)

associate(x, y, xy)

- Precond: association-reaction(x, y, xy) $\wedge$ available(x) $\wedge$ available(y)
- Effect: $\neg$available(x) $\wedge$ $\neg$available(y) $\wedge$ available(xy)

Corresponding Actions (2/3)

Catalyzed association reaction (phosphorylation rule)

associate-with-catalyze(x, y, z)

- Precond: catalyzed-association-reaction(x, y, z) ∧ available(x) ∧ available(y)
- Effect: ¬available(x) ∧ available(z)

* The availability of the catalyst y is NOT changed.

Corresponding Actions (3/3)

Synthesis reaction

synthesize(x, y)

- Precond: synthesize-reaction(x, y) $\wedge$ available(x)
- Effect: available(y)

* The availability of the catalyst x is NOT changed.

Simple Example

Initial Conditions:

available(pCAF). available(p300). available(AP2).
available(pRbp2). available(cdk46p3-cycD1).
association-reaction(pCAF, p300, pCAF-p300).
association-reaction(pRbp1p2, AP2, pRbp1p2-AP2).
catalyzed-association-reaction(pRbp2, cdk46p3-cycD1, pRbp1p2).

Goal:

available(pCAF-p300) $\vee$ available(pRbp1p2-AP2).

Plan1:

associate(pCAF, p300, pCAF-p300).

Plan2:

associate-with-catalyze(pRbp2,k cdk46p3-cycD1, pRbp1p2).
associate(pRbp1p2, AP2, pRbp1p2-AP2).

4 Kinds of Domains

Target of SAT Planning

- **Propositional**
  - Simple qualitative encoding of reactions. (Simple Example)
  - Goal is to generate certain substances.
  - Limit on the number of input substances that can be used.
- **Simple Preferences**
  - Propositional + Preferences
  - Maximize target substances to generate.
  - Minimize input substances to be used.
- **Metric Temporal**
  - Reactions have different durations and quantities.
  - Goal is to generate specific quantity of target substances and to minimize input substances to be used and plan duration.
- **Complex Preferences**
  - Extension of Metric Temporal
  - Constraints on the order in which substances appear in pathway.

Problem p01.pddl

Initial Conditions:

available(pCAF). available(p300). available(AP2).
available(pRbp2). available(cdk46p3-cycD1).
association-reaction(pCAF, p300, pCAF-p300).
association-reaction(pRbp1p2, AP2, pRbp1p2-AP2).
catalyzed-association-reaction(pRbp2, cdk46p3-cycD1, pRbp1p2).

Goal:

available(pCAF-p300) $\vee$ available(pRbp1p2-AP2).

Plan1:

associate(pCAF, p300, pCAF-p300).

Plan2:

associate-with-catalyze(pRbp2,k cdk46p3-cycD1, pRbp1p2).
associate(pRbp1p2, AP2, pRbp1p2-AP2).

Complexity of Propositional Pathway Problems

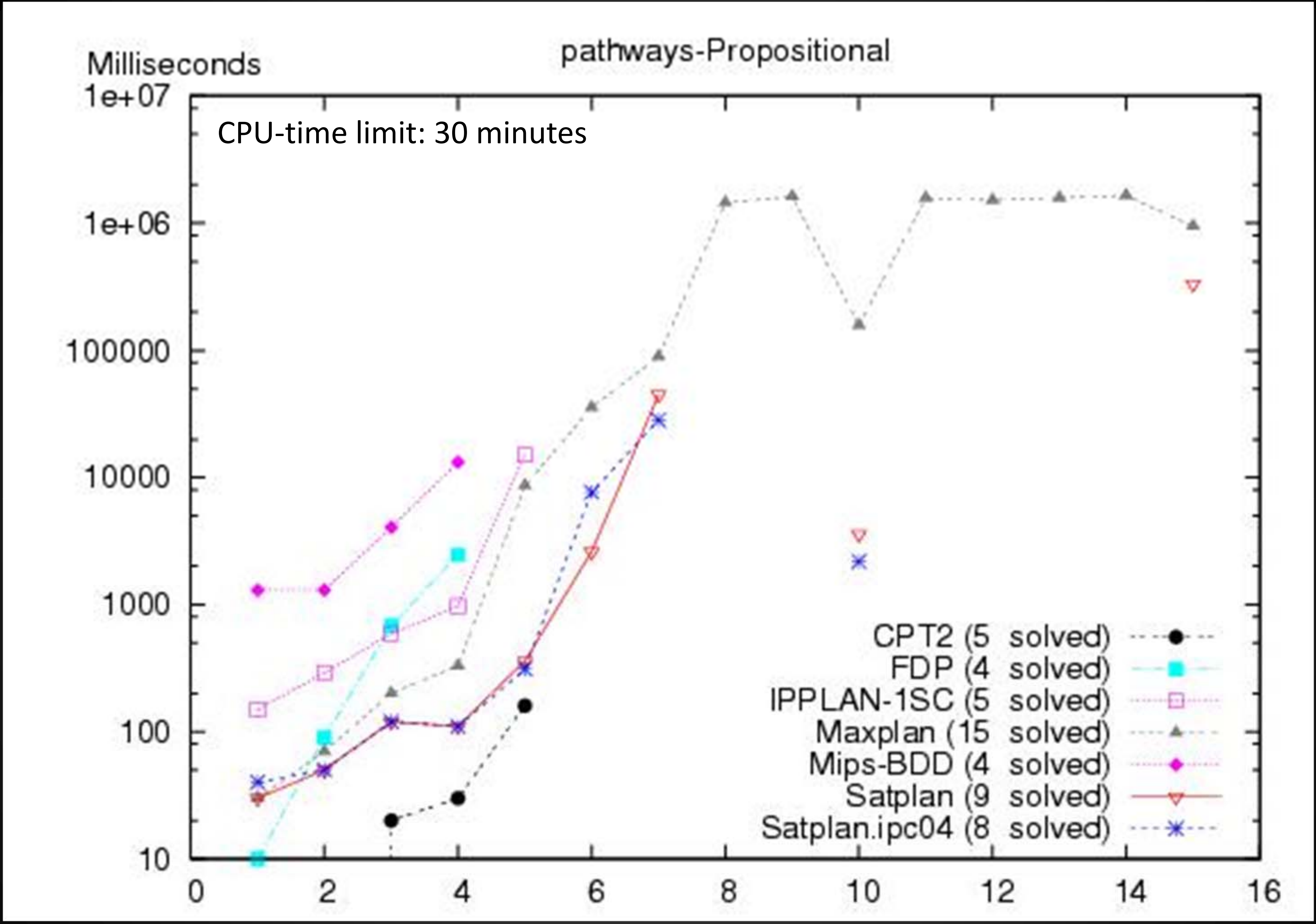
- 30 benchmark problems
  - Difference is the number of disjunctive goals.
  - **`p01.pddl`**: $(A \vee B)$
  - **`p02.pddl`**: $(A \vee B) \wedge (C \vee D)$
  - **`p03.pddl`**: $(A \vee B) \wedge (C \vee D) \wedge (E \vee F)$
  - **`p04.pddl`**: $(A \vee B) \wedge (C \vee D) \wedge (E \vee F) \wedge (G \vee H)$

:

There are **2^n** combinations of goals!

n: number of disjuncts

(This form of goals is appropriate in the realistic domain?)

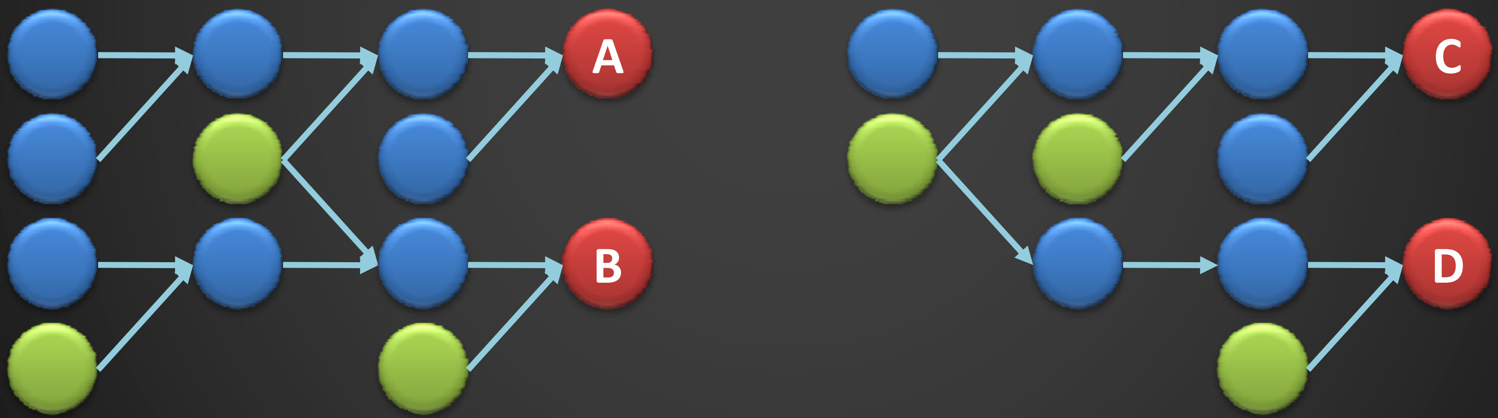

pathways-Propositional
Milliseconds
CPU-time limit: 30 minutes
1e+07
1e+06
100000
10000
1000
100
10
0
2
4
6
8
10
12
14
16
CPT2 (5 solved)
FDP (4 solved)
IPPLAN-1SC (5 solved)
Maxplan (15 solved)
Mips-BDD (4 solved)
Satplan (9 solved)
Satplan.ipc04 (8 solved)

Dependency between Goals

- Goal of `p30.pddl` consists of 40 disjuncts.

$$(A \vee B) \wedge (C \vee D) \wedge (E \vee F) \wedge \cdots$$

- If each disjunct is independent, we can divide the problem into 40 sub-problems.



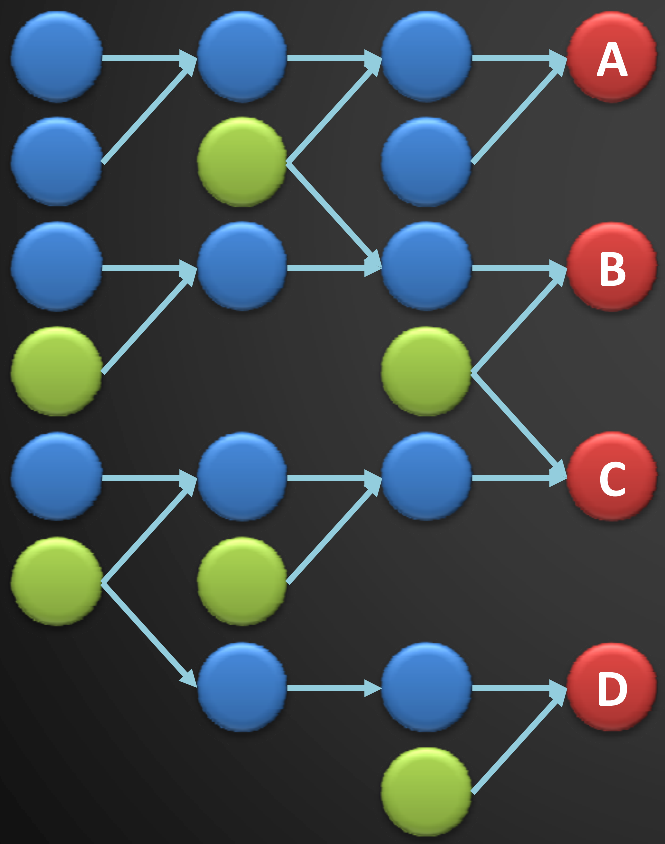
Each sub-problem is solvable in **several seconds**.

⬇

Sub-optimal planning is not so difficult.

Dependency between Goals

- However, there are dependencies between two goals in many cases.



Reaction network in cell cycle

Summary

- Introduction of pathway problems in IPC-5

Future Work

- Dependency analysis of disjunctive/conjunctive goals.
  - I think that goals can be divided into groups with few dependencies.
- Extension of SAT Planning for Metric Temporal Domain.
  - Reactions have different durations and quantities.

References

[1] P. Thagard: Pathways to Biomedical Discovery, Philosophy of Science, volume 70 (2003).

[2] K. Kohn: Molecular Interaction Map of the Mammalian Cell Cycle Control and DNA Repair Systems, Mol Biol Cell. 10(8), 1999.

[3] http://contraintes.inria.fr/BIOCHAM/EXAMPLES/cell_cycle/cell_cycle.bc

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