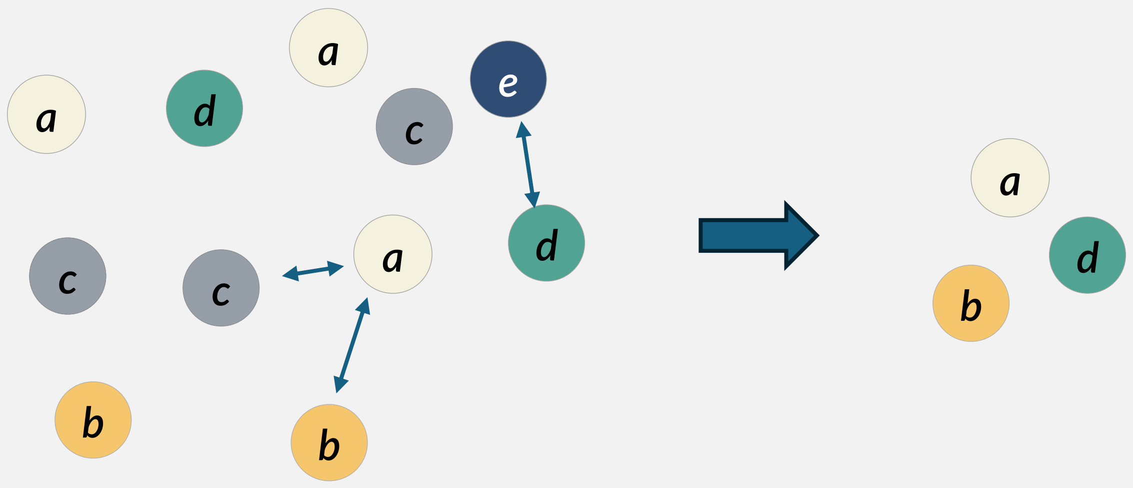
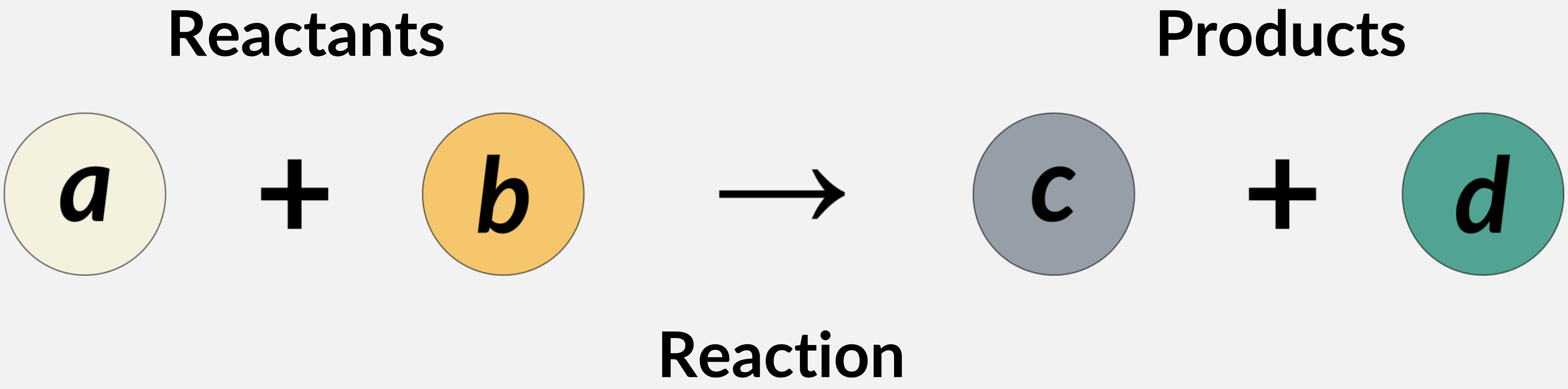
Brief Announcement:
Reachability in Deletion-only Chemical Reaction Networks

The 4th Symposium on Algorithmic Foundations of Dynamic Networks (SAND)

June 9-11, 2025 | Liverpool, UK

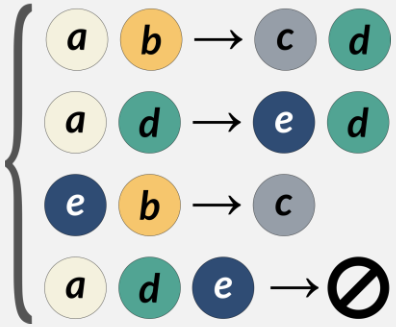
Bin Fu, Timothy Gomez , Ryan Knobel, Austin Luchsinger, Aiden Massie,
Marco Rodriguez, Adrian Salinas, Robert Schweller, Tim Wylie

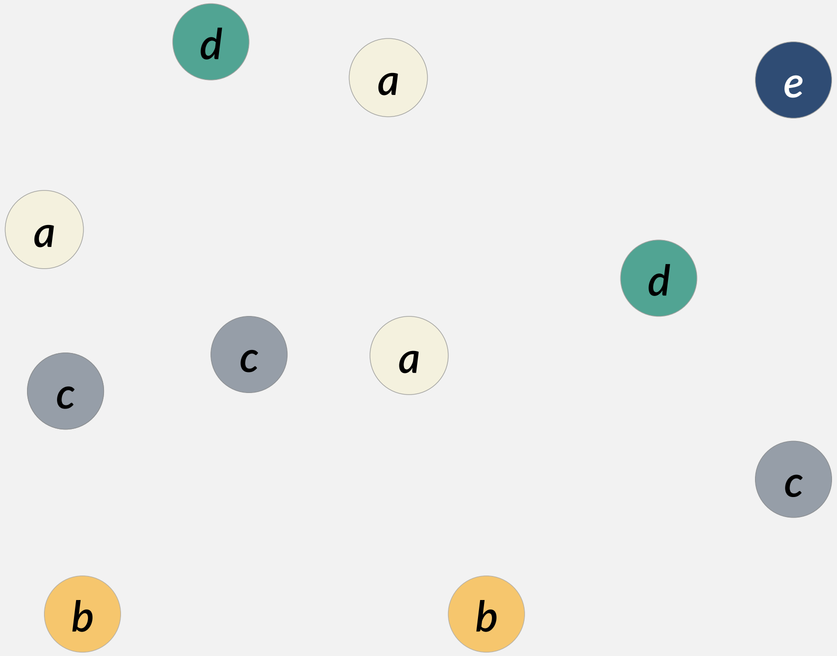




Chemical Reaction Networks

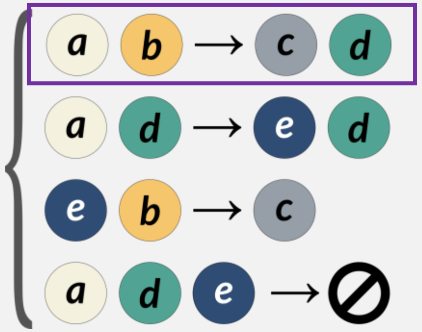
Reaction Rules

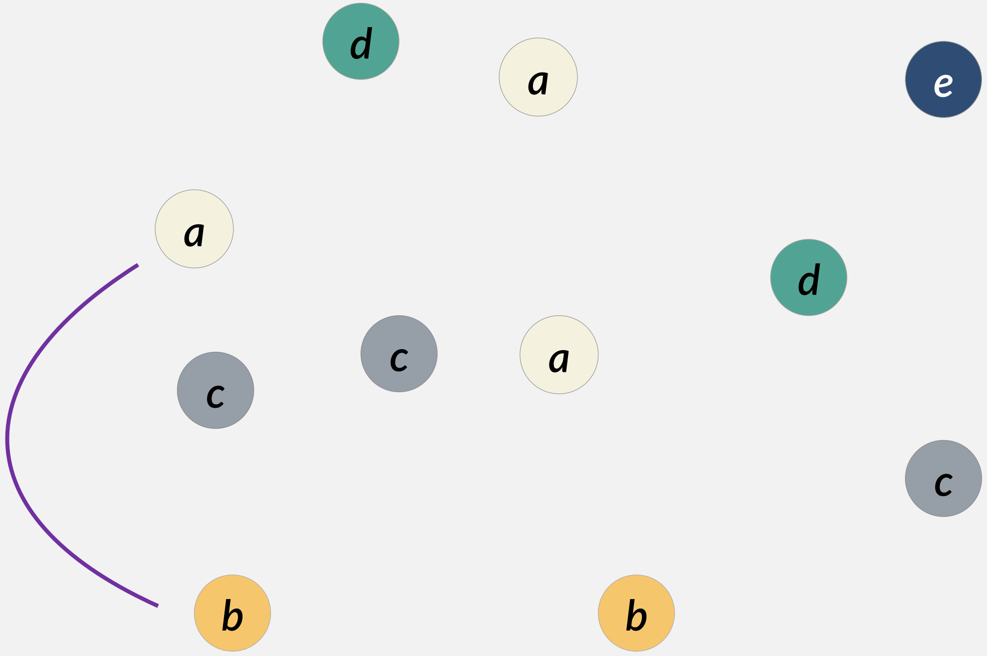




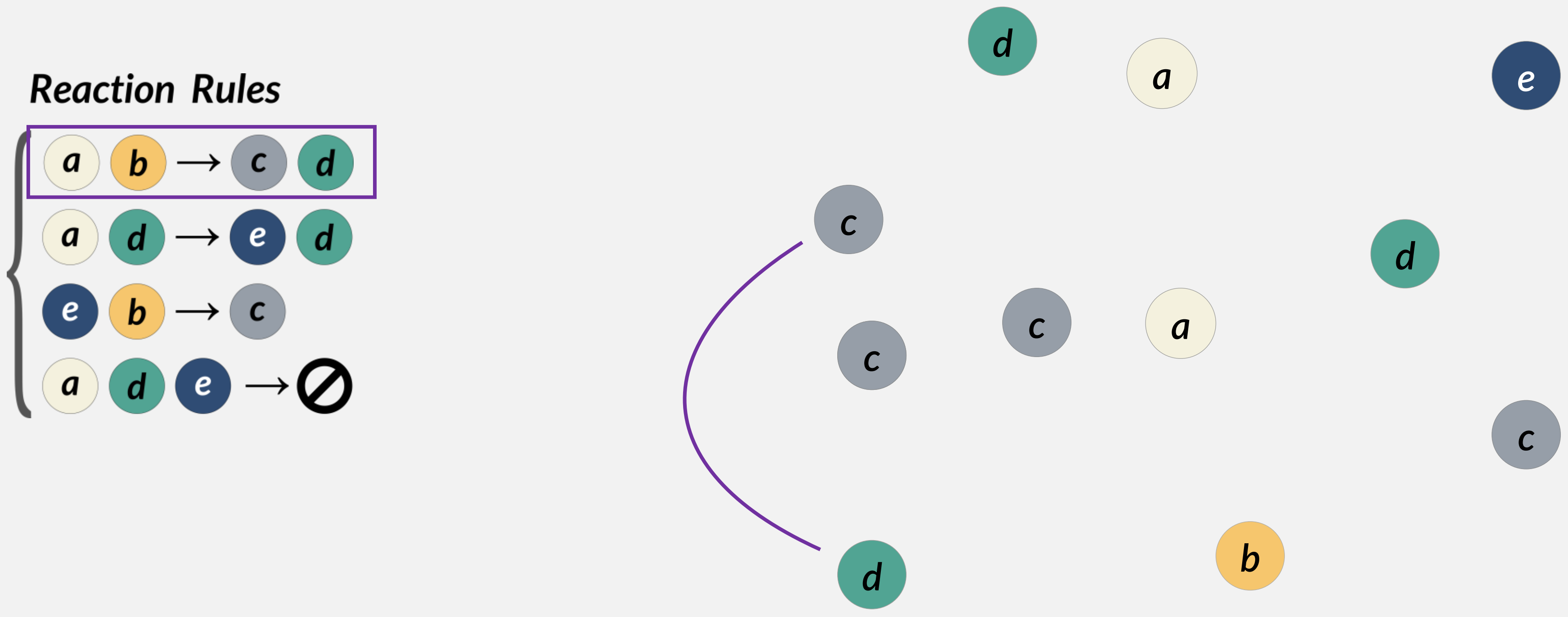
CRNs

Reaction Rules



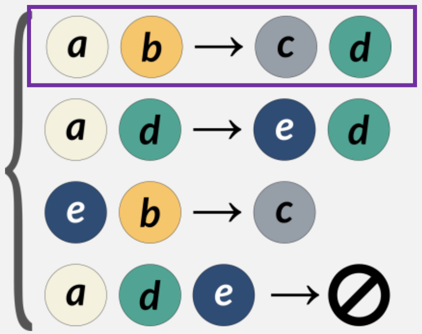


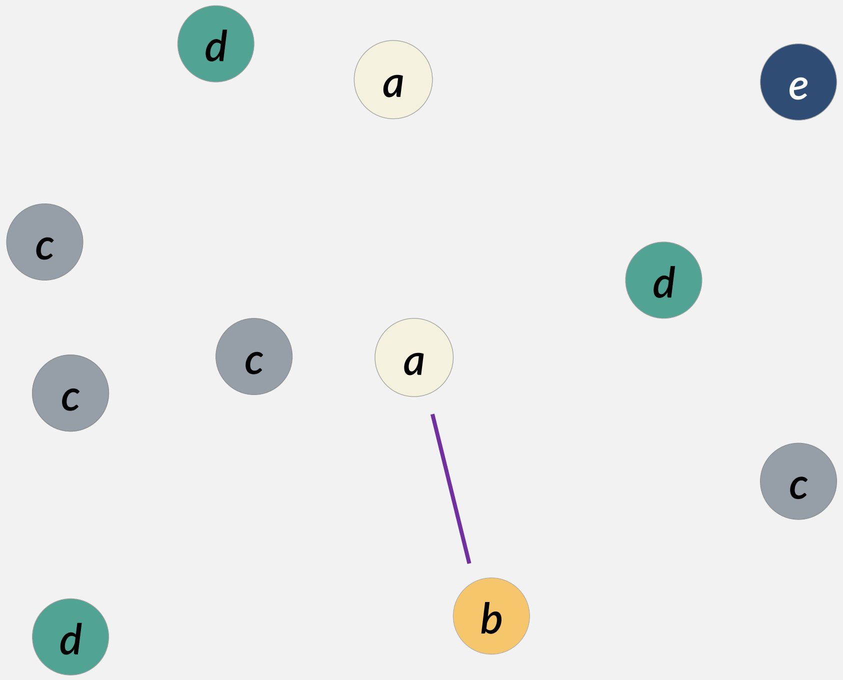
CRNs



CRNs

Reaction Rules





CRNs

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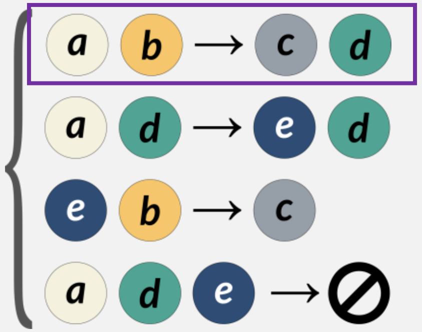
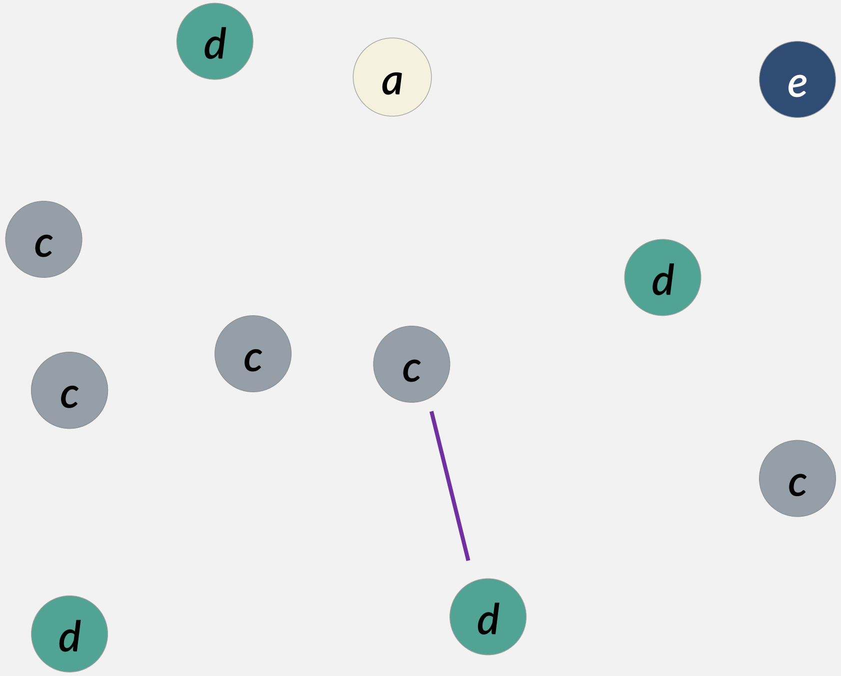
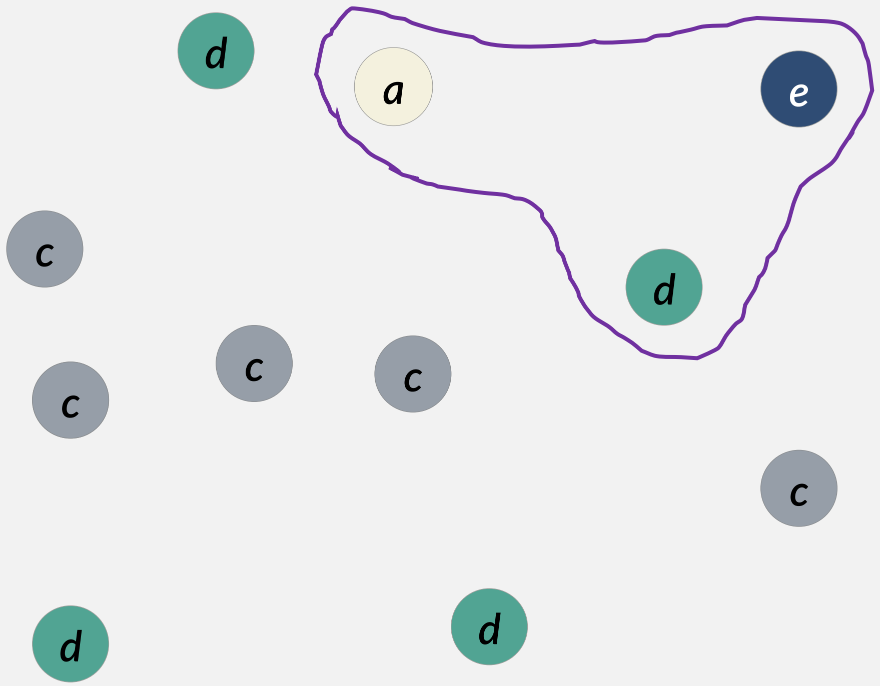




CRNs

Reaction Rules

$$a + b \rightarrow c + d$$
$$a + d \rightarrow e + d$$
$$e + b \rightarrow c$$
$$a + d + e \rightarrow \emptyset$$



CRNs

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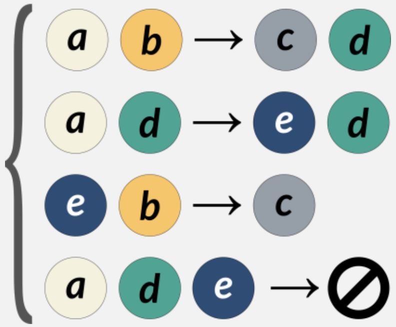
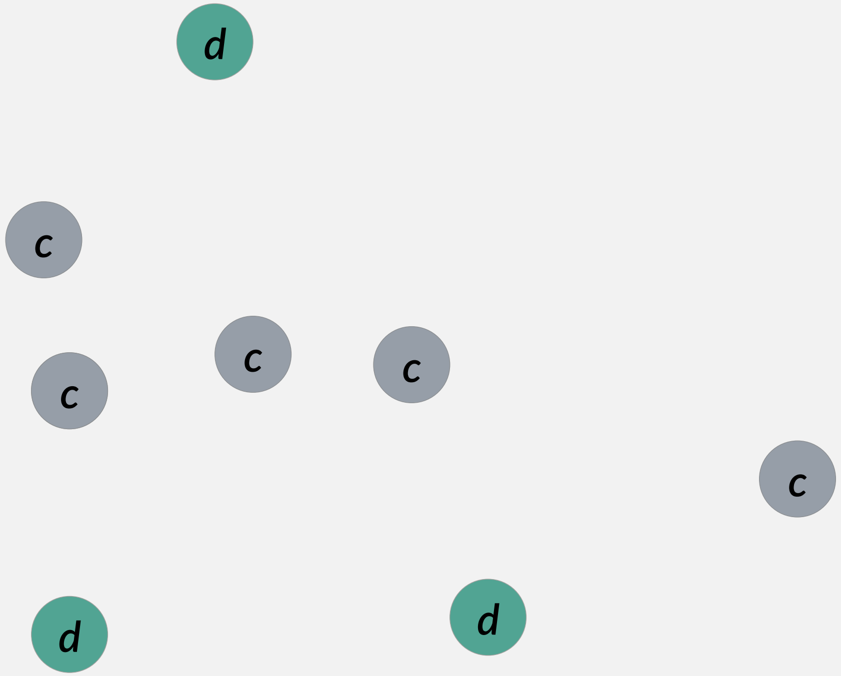
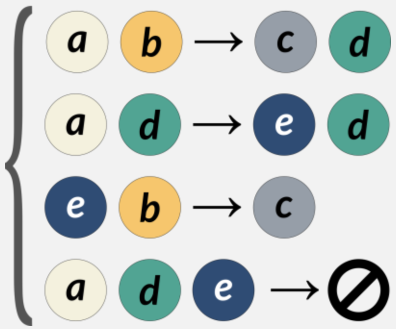




CRNs

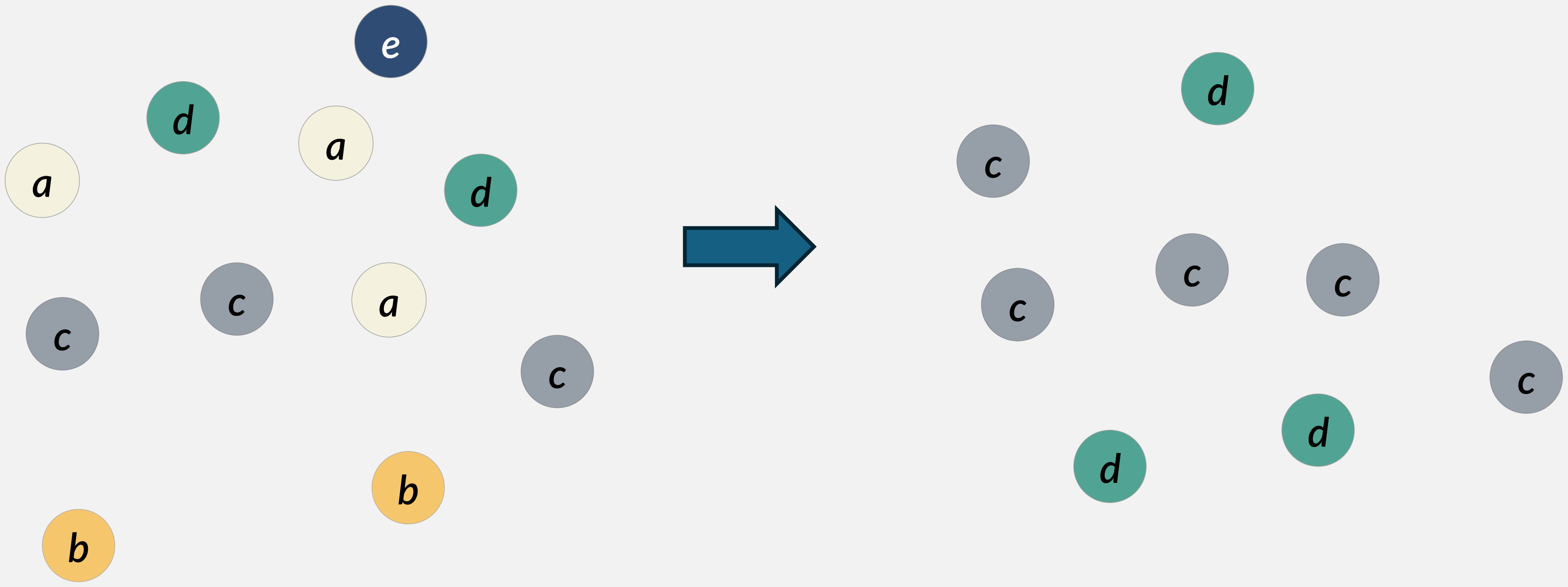
CRN:

Reaction Rules



Configuration I:

Configuration D:

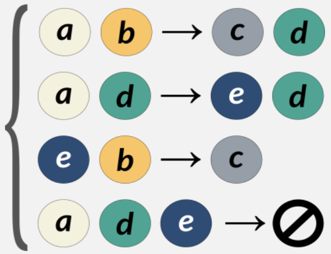


D is **Reachable** from I

CRNs

CRN:

Reaction Rules



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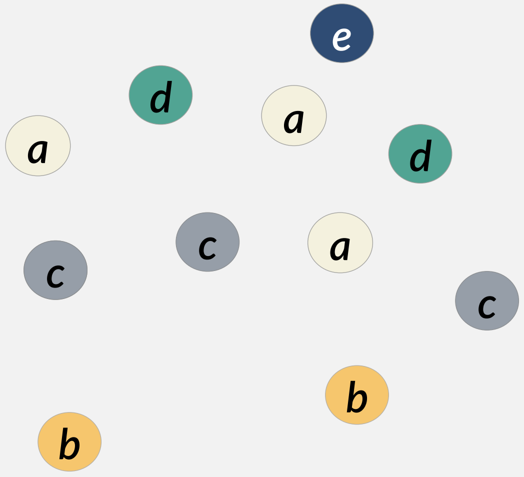

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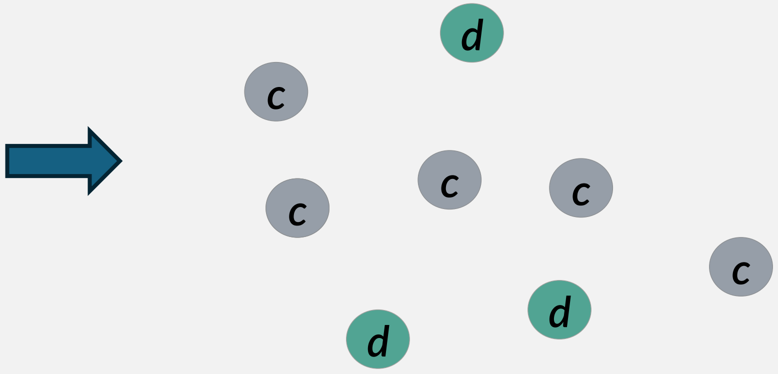


D is **Reachable** from I

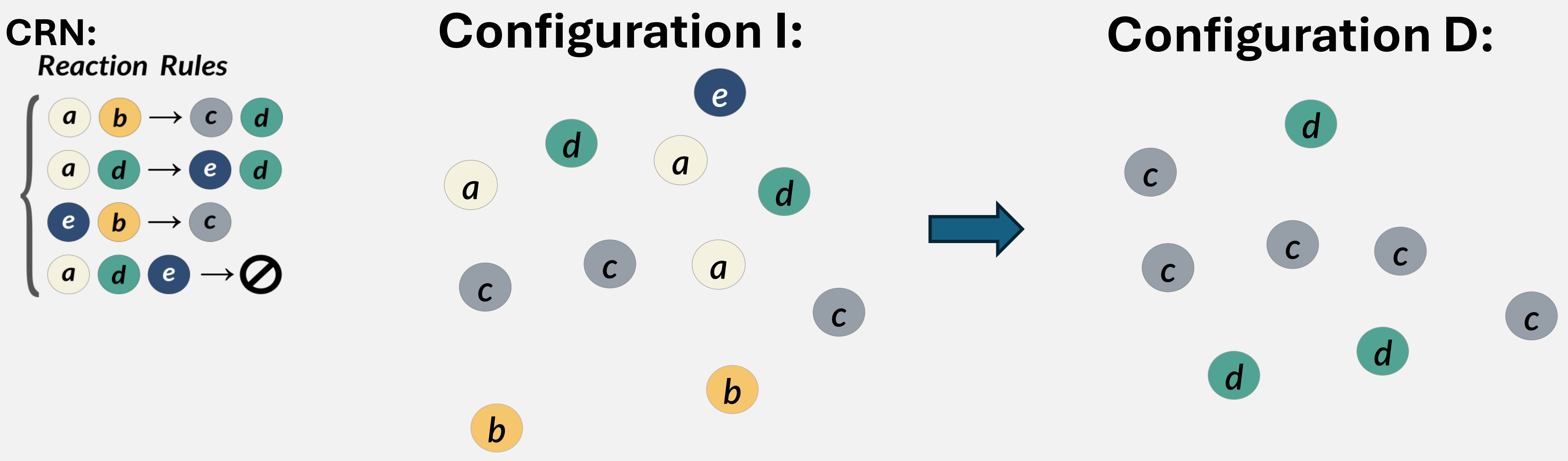
Reachability Problem:

Input:

1) Reaction Rules (a CRN)
2) An initial configuration I
3) a destination configuration D

Output: Is D reachable from I with these reactions?

CRNs



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Reachability Problem:

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Reachability is Ackerman-Complete

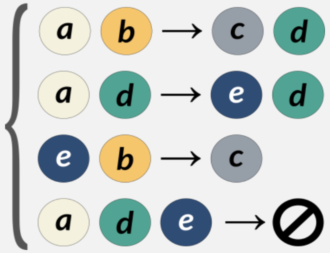
[Wojciech Czerwiński and Łukasz Orlikowski, FOCS'21]

[Jérôme Leroux, FOCS'21]

CRNs

CRN:

Reaction Rules



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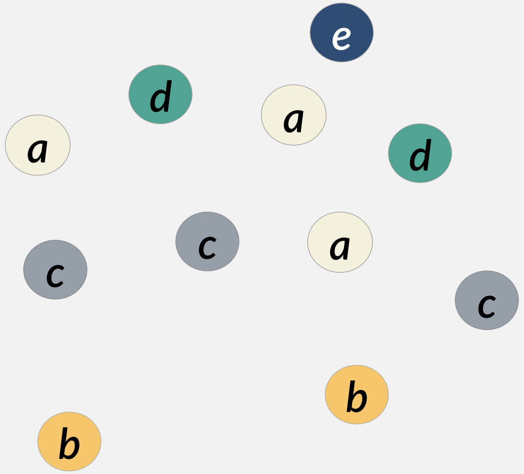
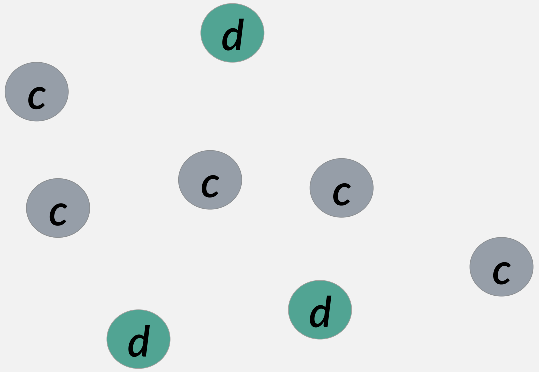


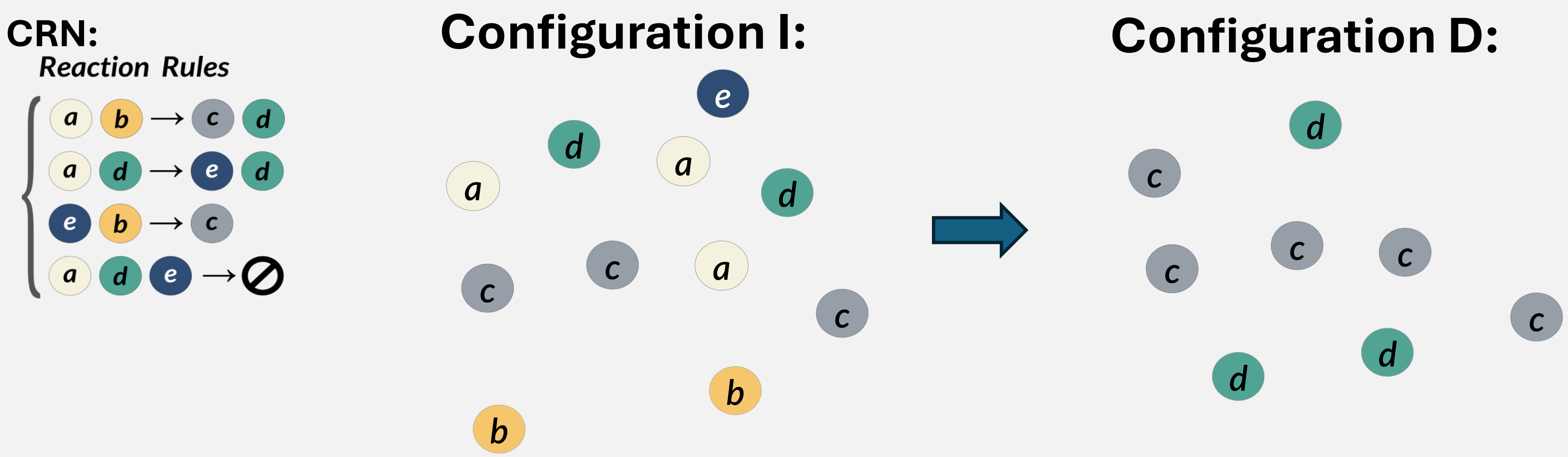
Configuration D:



D is **Reachable** from I

- General CRNs reactions can **ADD** and **DELETE**

  => Reachability is **Ackermann-complete** [FOCS 2021]



D is **Reachable** from I

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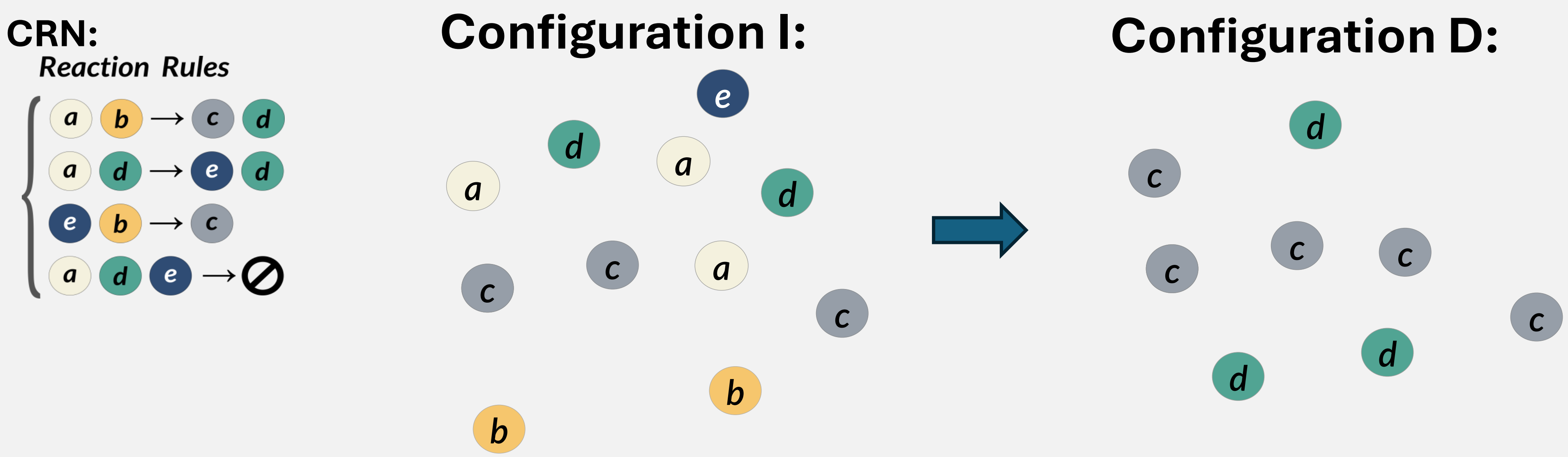
- What if a system could only ADD **OR** DELETE (but not both)?
  ⇒ Reachability is in NP



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- General CRNs reactions can **ADD** and **DELETE**
  => Reachability is **Ackermann-complete** [FOCS 2021]

- What if a system could only ADD **OR** DELETE (but not both)?
  ⇒ Reachability is in NP

Our Focus:

We characterize Reachability in **Deletion-Only** systems
Based on rule size.

Deletion-Only Reactions (Void Rules)

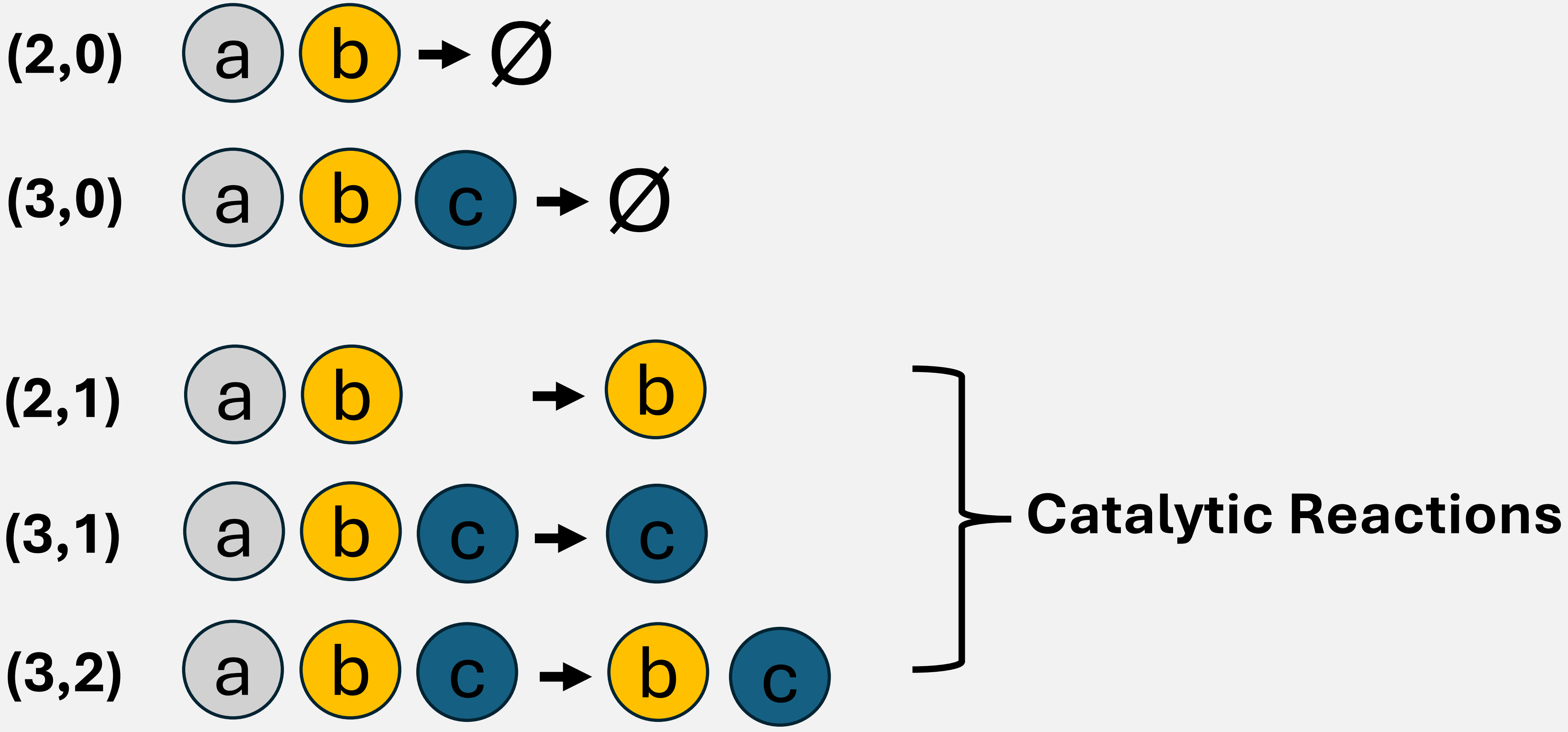
Rule Size:

(2,0) a b → Ø

(3,0) a b c → Ø

Deletion-Only Reactions (Void Rules)

Rule Size:



Deletion-Only CRNs

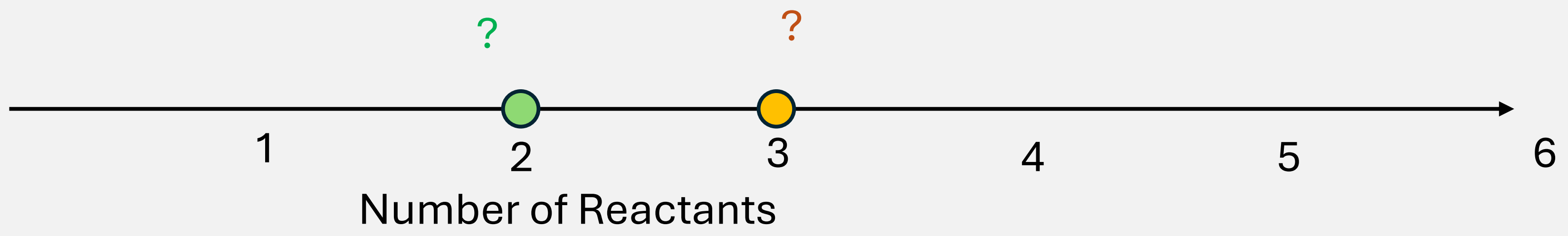
(2,0) rules

a + b → Ø

Versus:

(3,0) rules

a + b + c → Ø

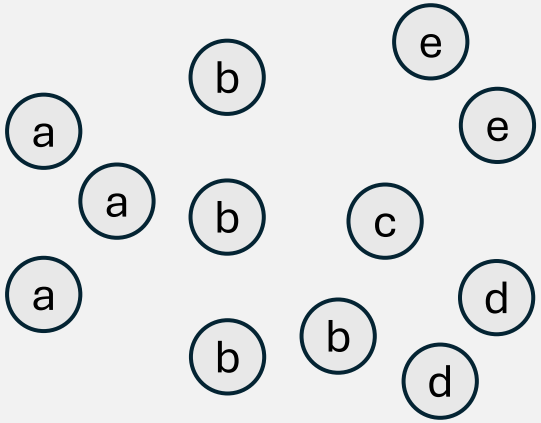


(2,0) Algorithm

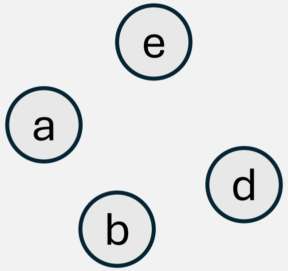
Reactions:

a b => Ø
b c => Ø
e d => Ø

Initial Configuration:

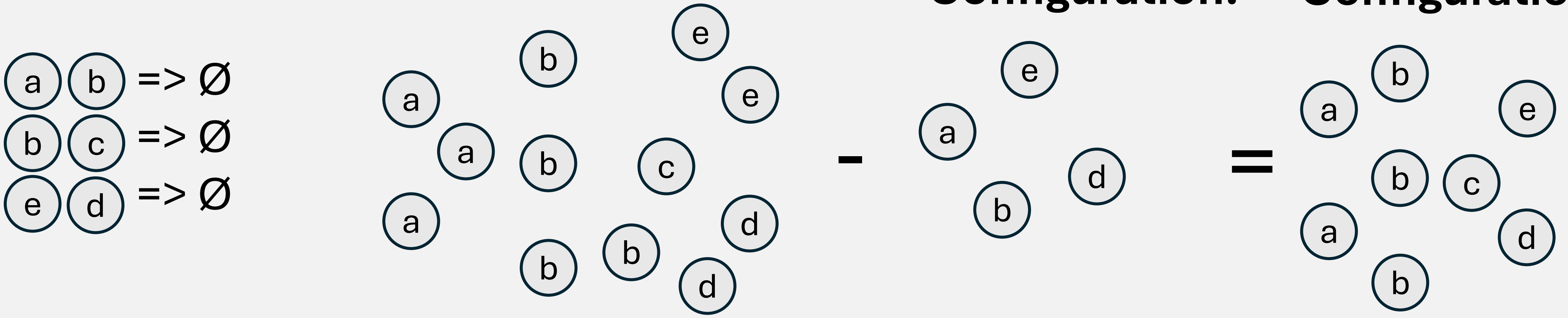


Target Configuration:



(2,0) Algorithm

Reactions: **Initial Configuration:** **Target Configuration:** **Difference Configuration:**

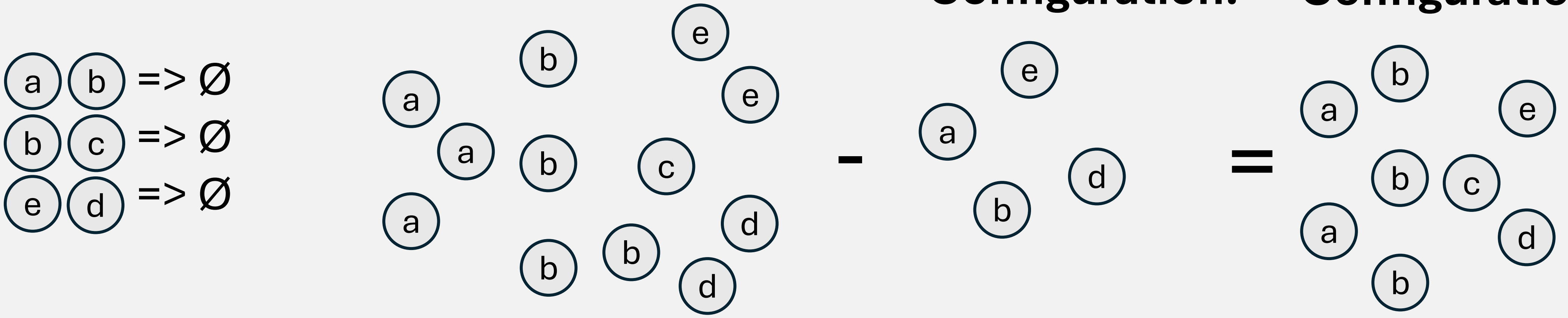


Algorithm:

- **Compute the “Difference” configuration**

(2,0) Algorithm

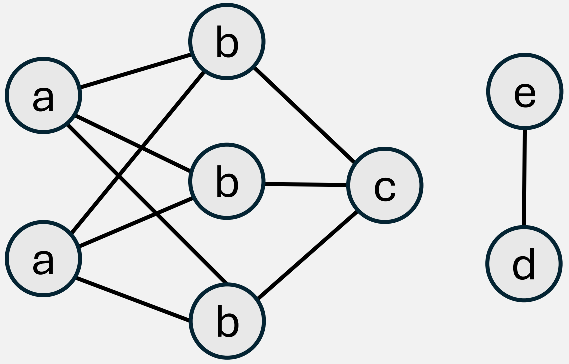
Reactions: **Initial Configuration:** **Target Configuration:** **Difference Configuration:**



Algorithm:

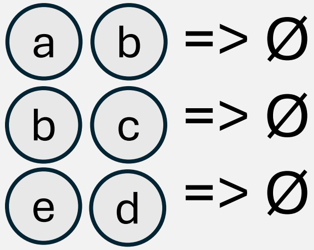
- **Compute the “Difference” configuration**
- **Create the Reaction Graph**

Reaction Graph:

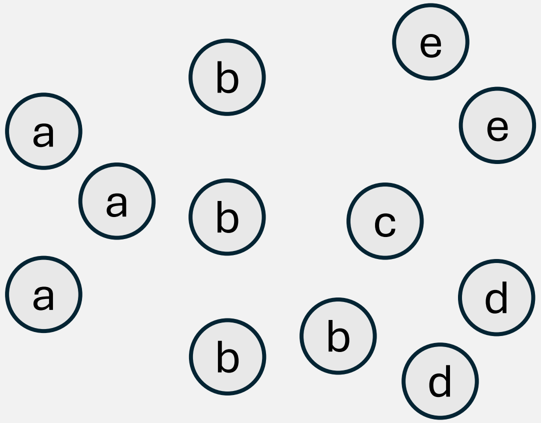


(2,0) Algorithm

Reactions:

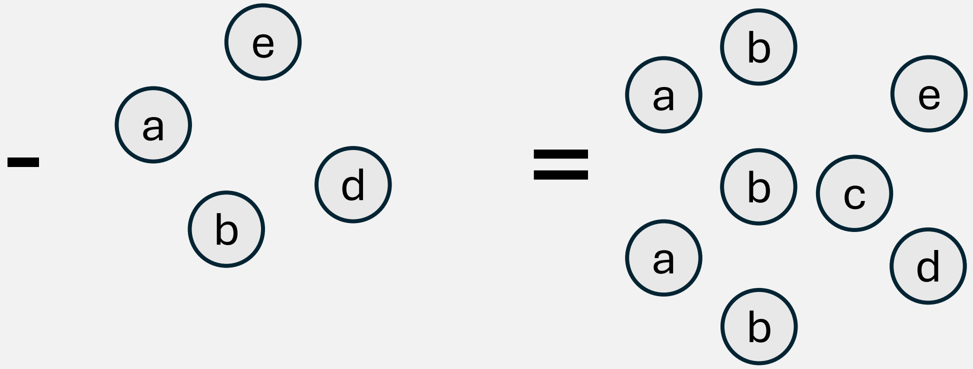


Initial Configuration:



Target Configuration:

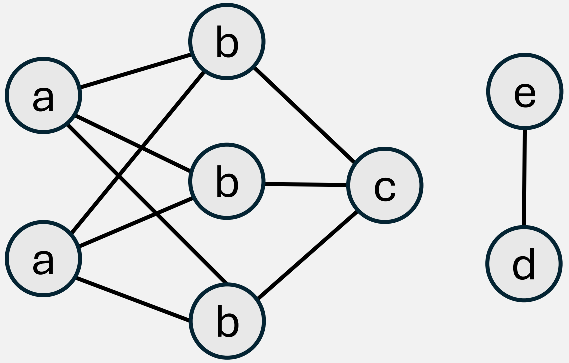
Difference Configuration:



Algorithm:

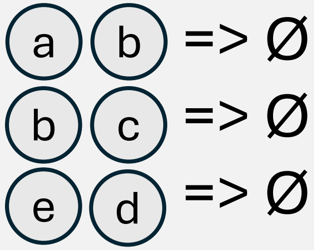
- **Compute the “Difference” configuration**
- **Create the Reaction Graph**
- **Run a Perfect Matching Algorithm**

Reaction Graph:

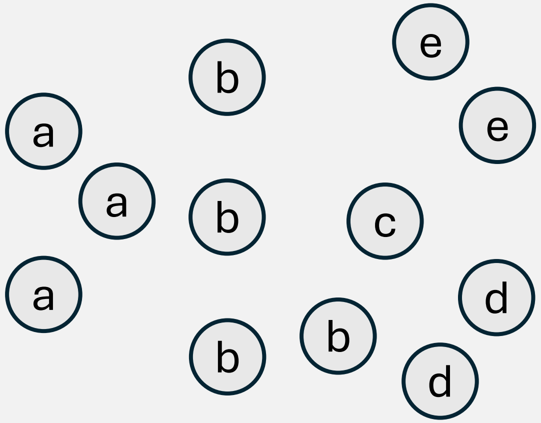


(2,0) Algorithm

Reactions:



Initial Configuration:



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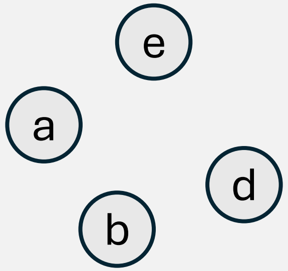
Target Configuration:



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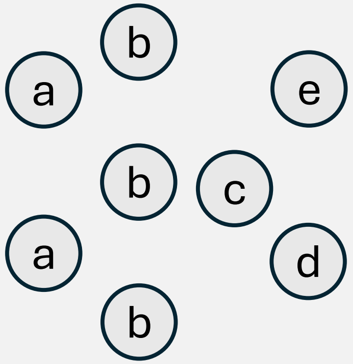
Difference Configuration:



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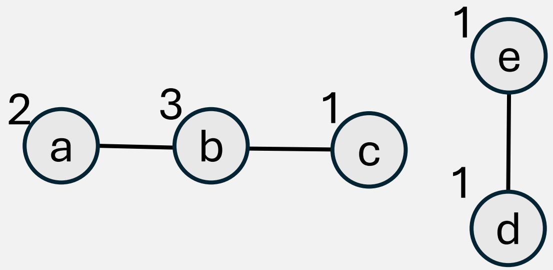

(2,0) Algorithm

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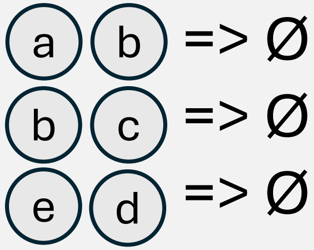

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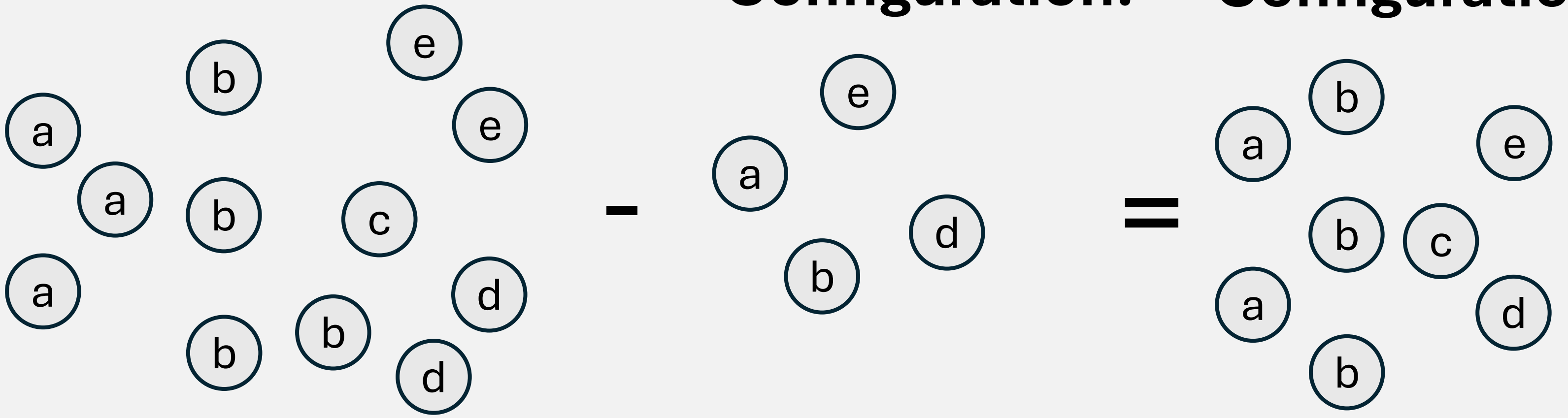

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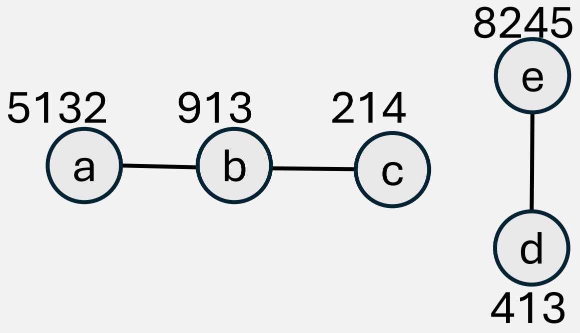
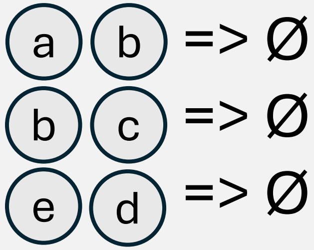
Reaction Graph:

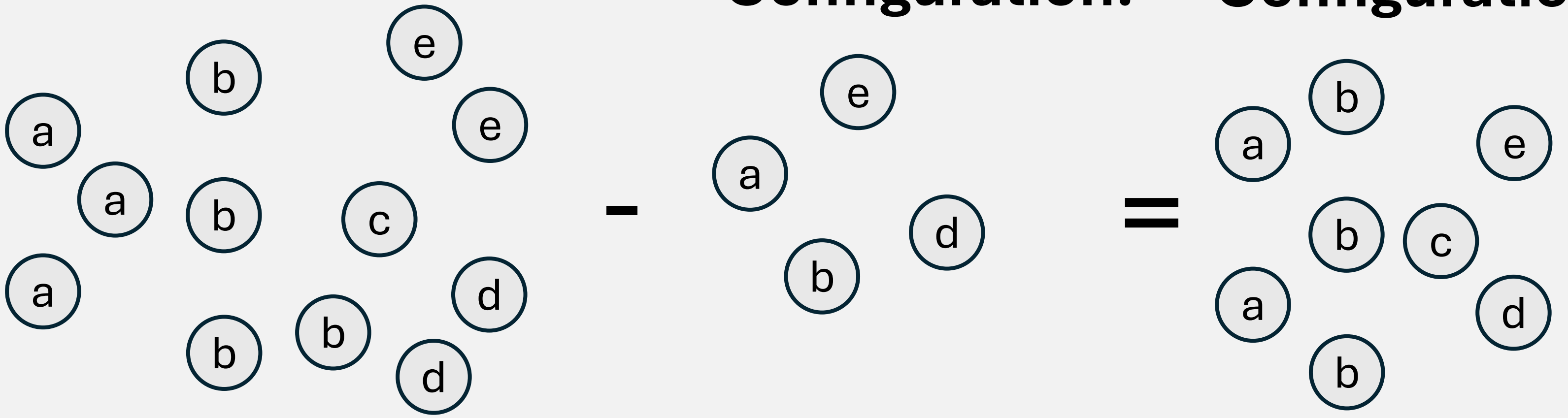


(2,0) Algorithm

Reactions:



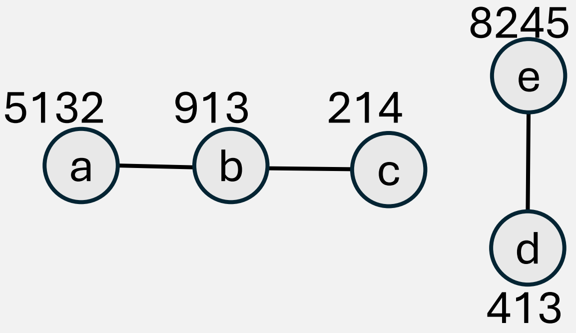
Initial Configuration: **Target Configuration:** **Difference Configuration:**



Algorithm:

- **Compute the "Difference" configuration**
- **Create the Reaction Graph**
- **Run a Perfect ~~Matching Algorithm~~ b-Matching Algorithm** [Cunningham, Marsh, 1979]

Reaction Graph:



Deletion-Only CRNs

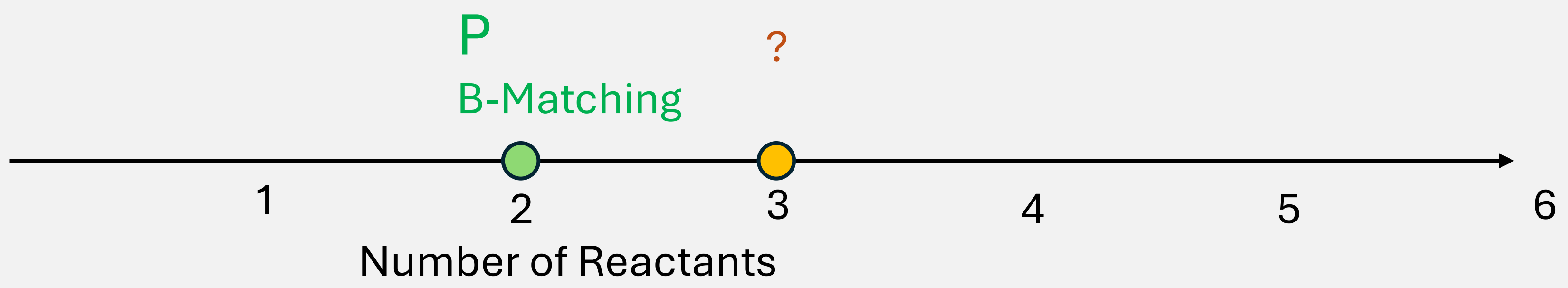
(2,0) rules

a + b → Ø

Versus:

(3,0) rules

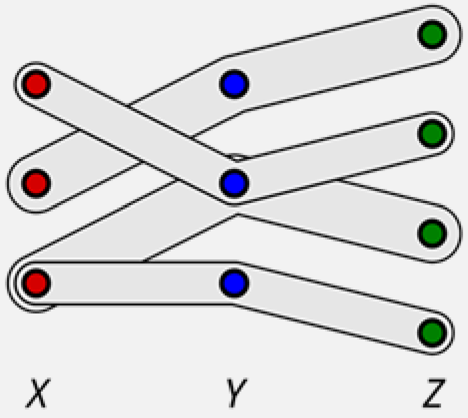
a + b + c → Ø



(3,0) Reachability: NP completeness

Reduction from 3D Matching

3D Matching Problem:
Does there exist a subset of non-overlapping triplets that cover the tripartite graph?



(3,0) Reachability Instance:

Initial Configuration:

x_1 y_1 z_1

x_2 y_2 z_2

x_3 y_3 z_3

z_4

Target Configuration:

(empty)

Reactions:

$x_1 + y_2 + z_2 \rightarrow \emptyset$

$x_2 + y_1 + z_1 \rightarrow \emptyset$

$x_3 + y_2 + z_3 \rightarrow \emptyset$

$x_3 + y_3 + z_4 \rightarrow \emptyset$

Deletion-Only CRNs

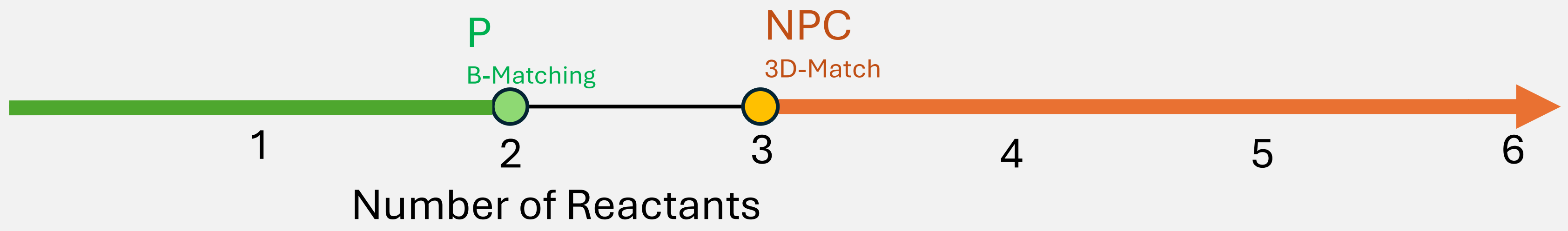
(2,0) rules

$a + b \to \varnothing$

Versus:

(3,0) rules

$a + b + c \to \varnothing$



Deletion-Only CRNs

(2,1) rules

a + b → a

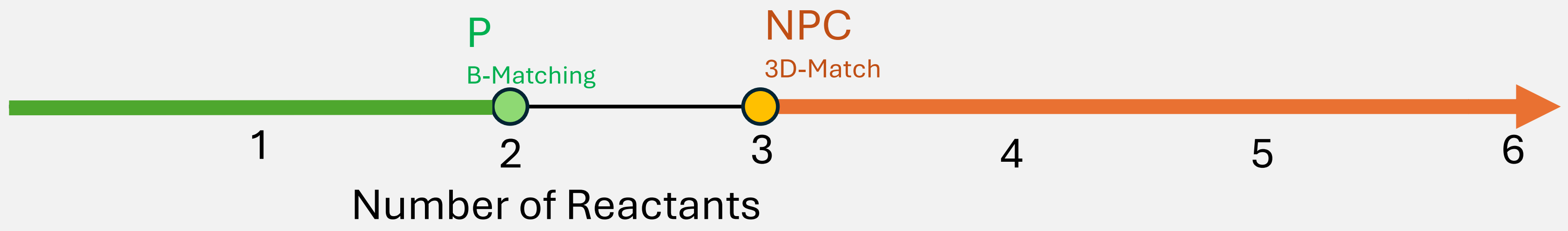
(3,1) rules

a + b + c → a

(3,2) rules

a + b + c → b + c

(etc.)



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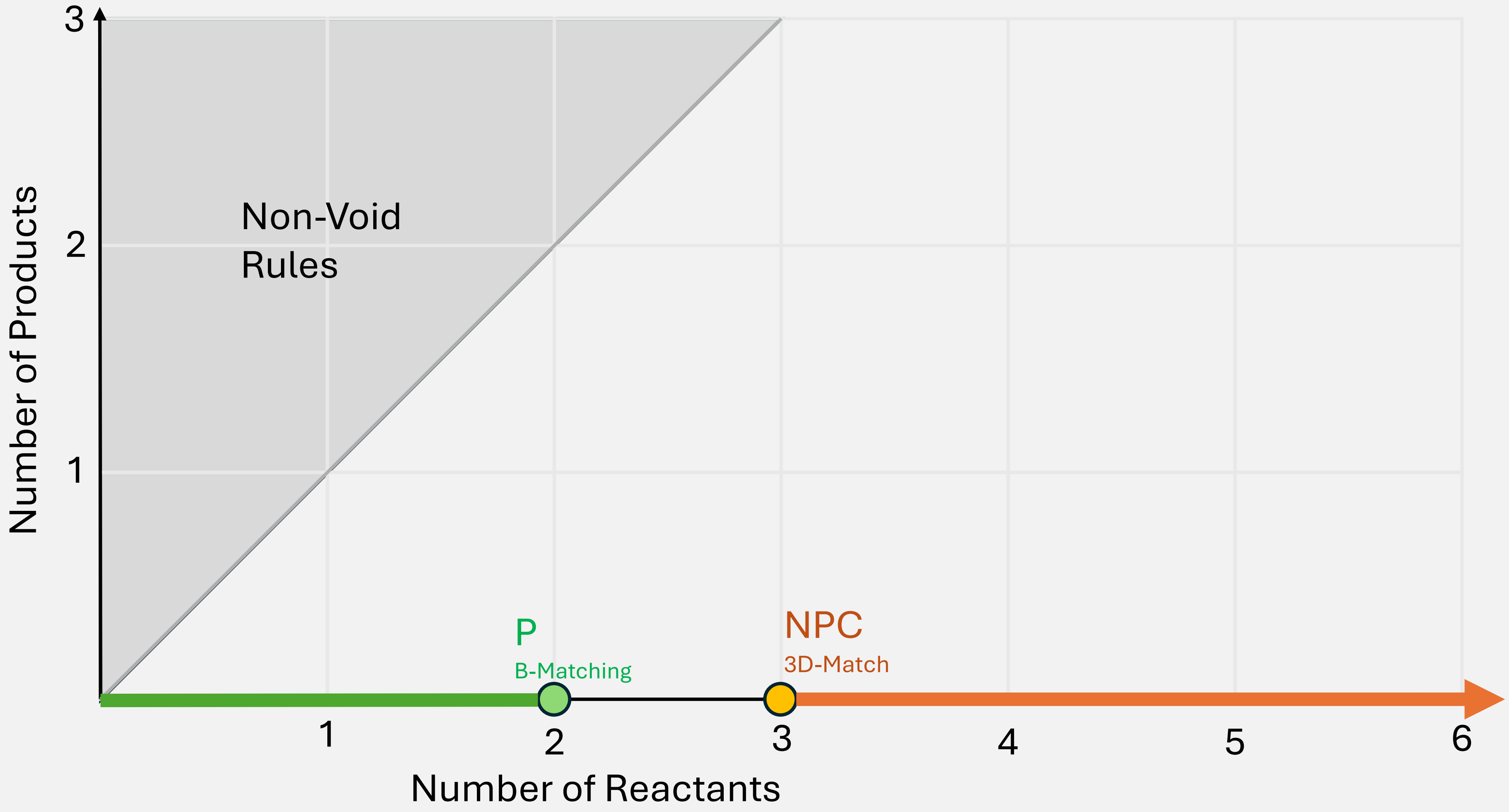
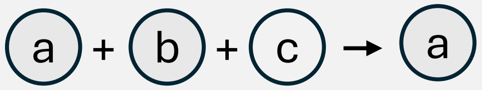
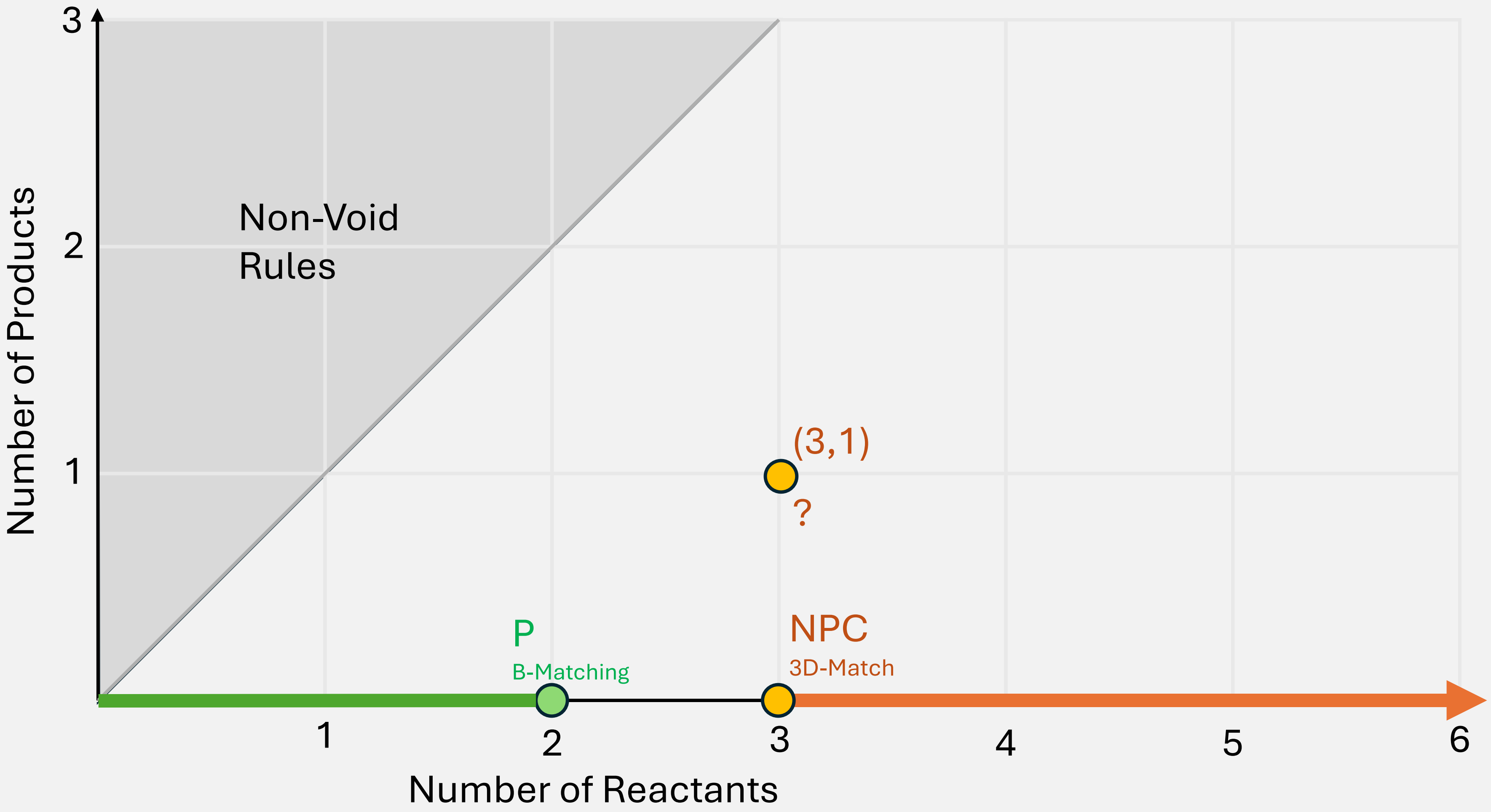


Deletion-Only CRNs

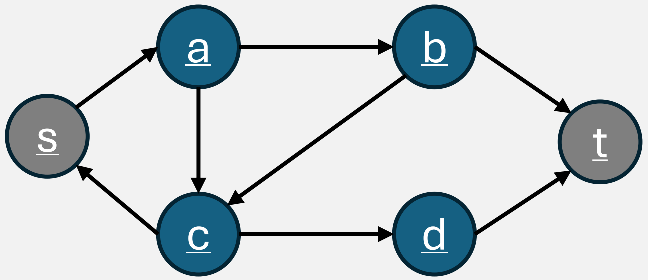
(3,1) rules





Deletion-Only CRNs: (3,1) NP-complete

<u>Hamiltonian Path from s to t?</u>



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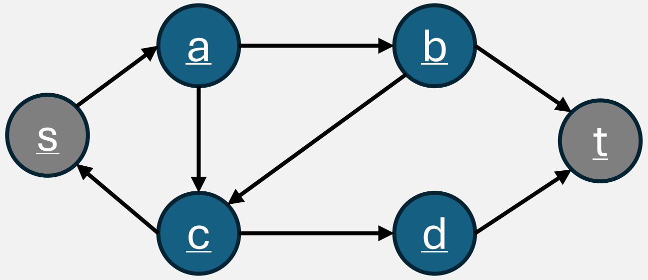
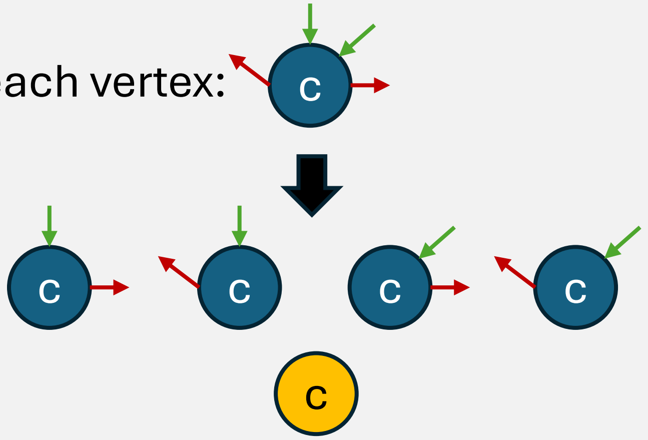
Hamiltonian Path from s to t?



Initial Configuration:

For each vertex:

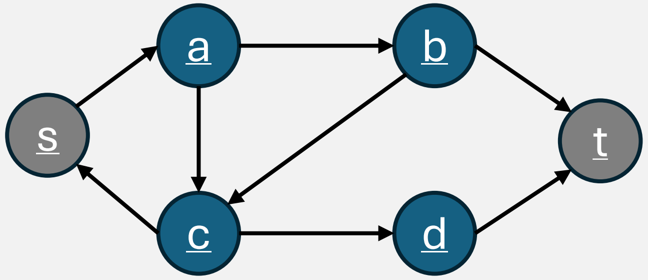


Target Configuration:

Eliminate **all** of these species
except for a single “t”

Deletion-Only CRNs: (3,1) NP-complete

Hamiltonian Path from s to t?



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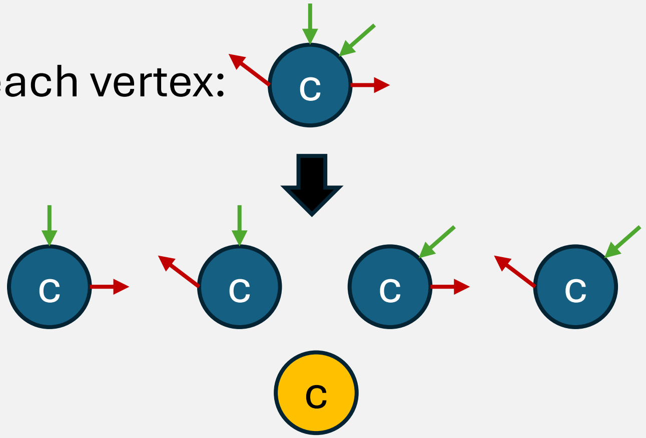


Target Configuration:

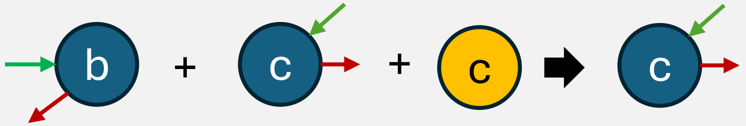
Eliminate **all** of these species except for a single “t”

Reactions:

1) Non-deterministically guess A traversal for each vertex:

A+B+C -> A
A+B+C -> B
A+B+C -> C

2) Check if the guessed traversal constitutes a Hamiltonian Path:



Deletion-Only CRNs: (3,1) NP-complete

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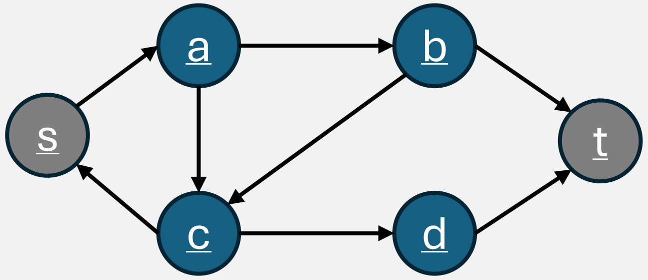

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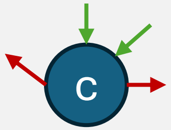

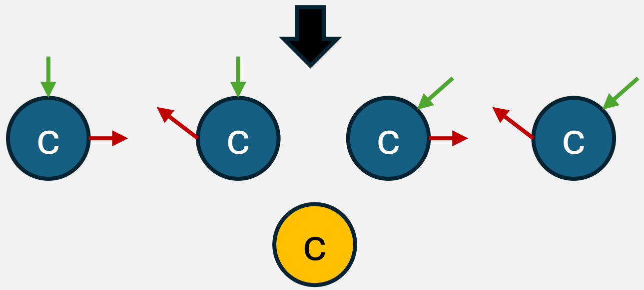

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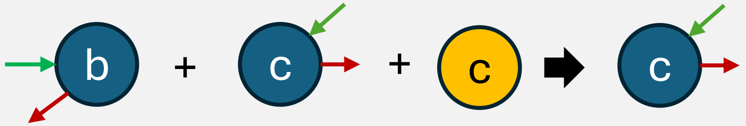

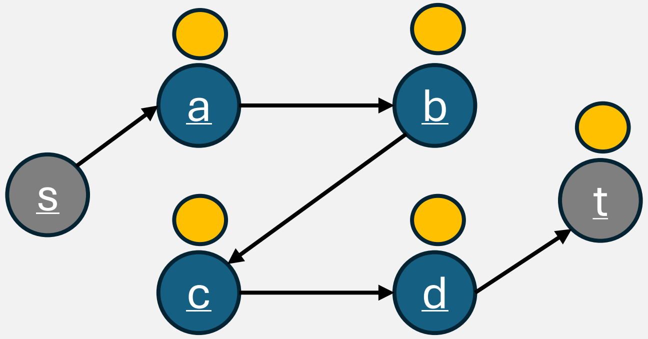

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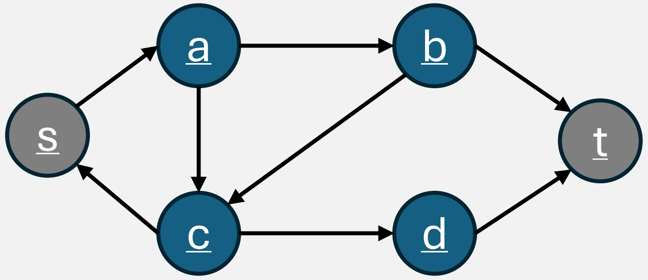

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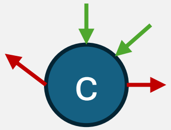

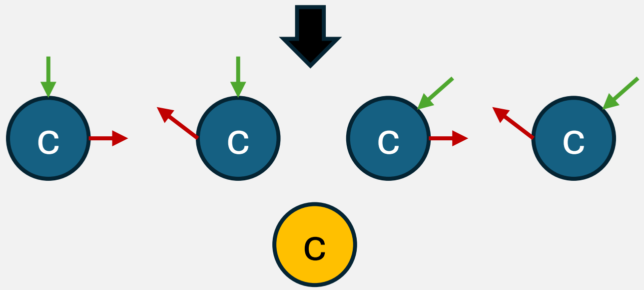

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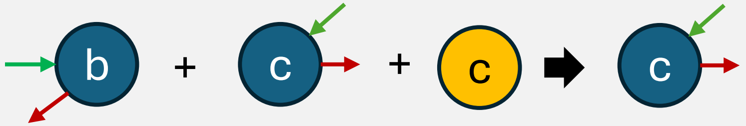

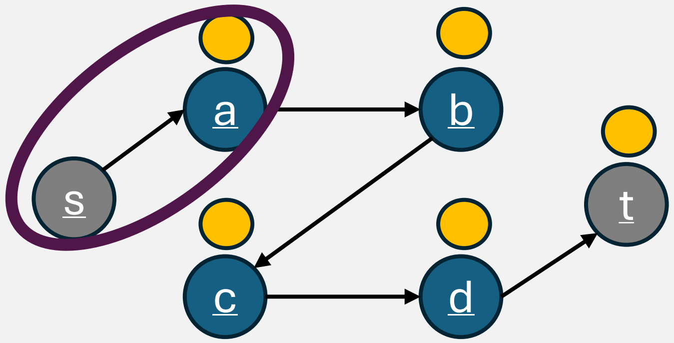

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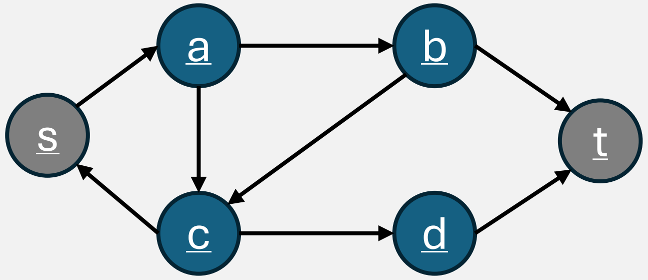

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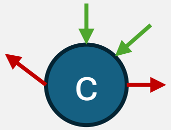
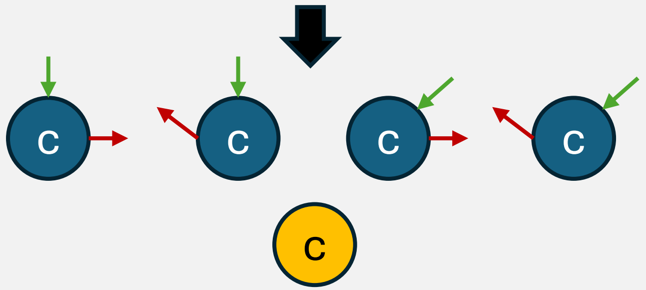
For each vertex: 



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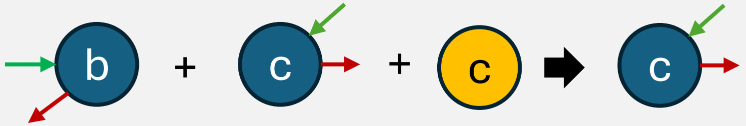

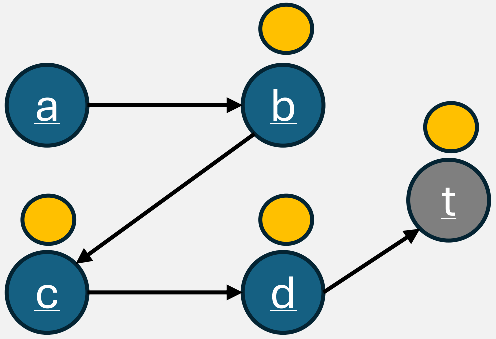

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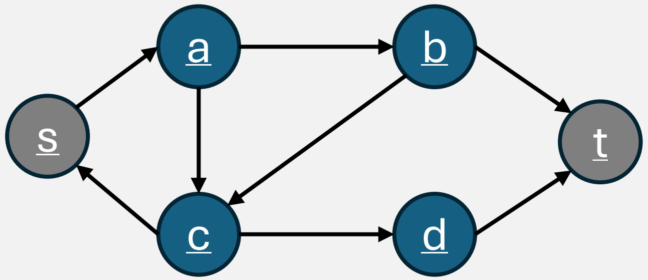

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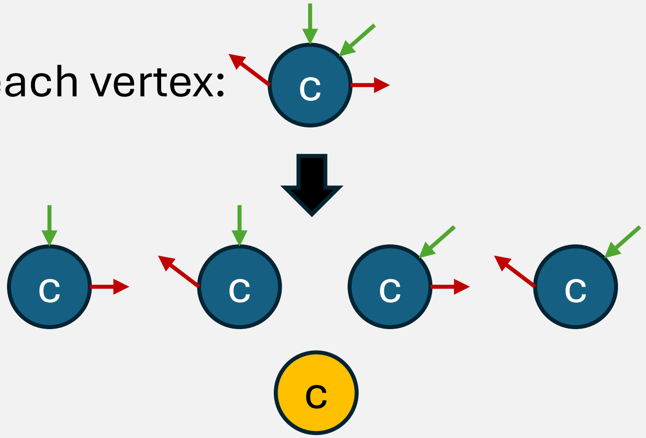

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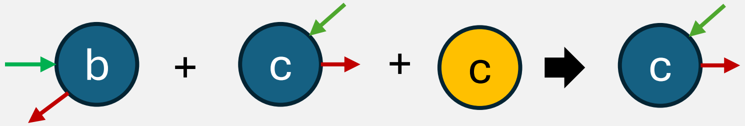

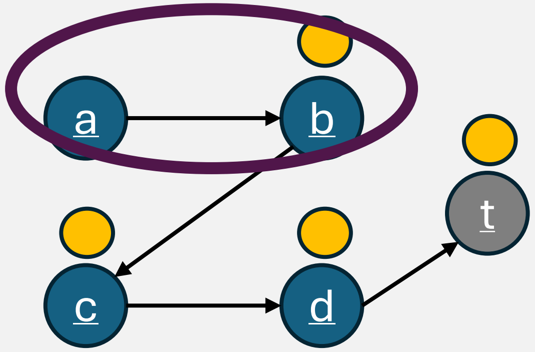

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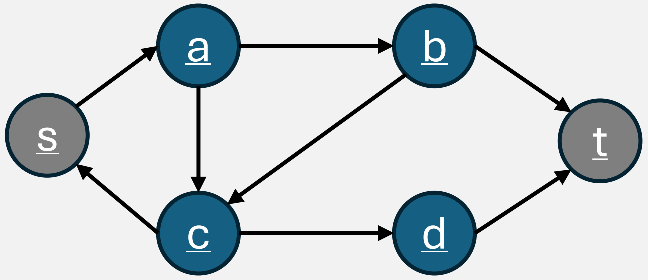

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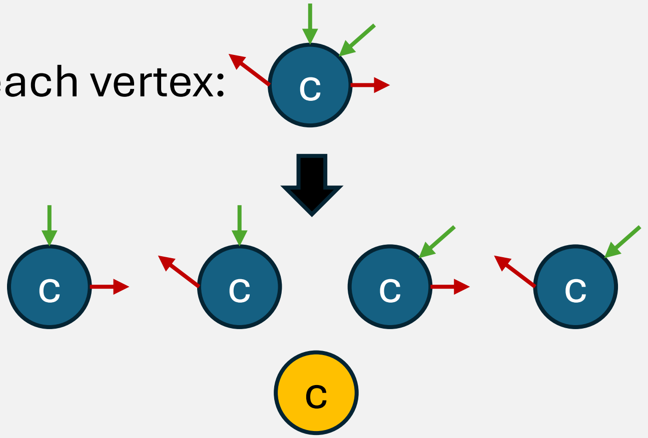

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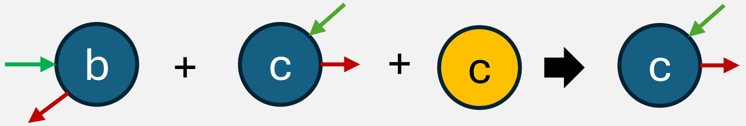

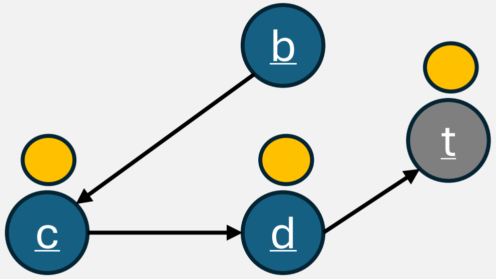

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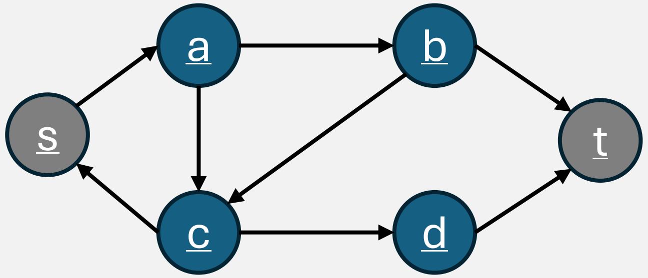

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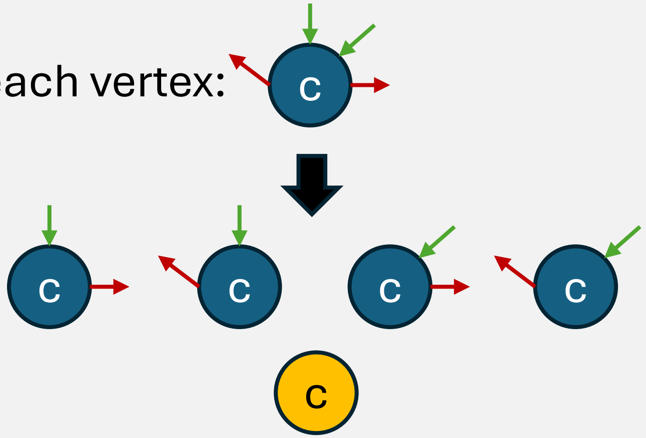

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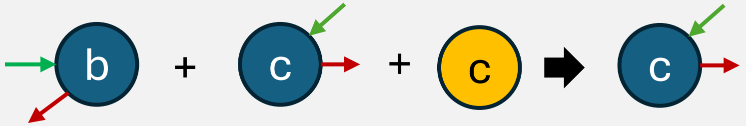

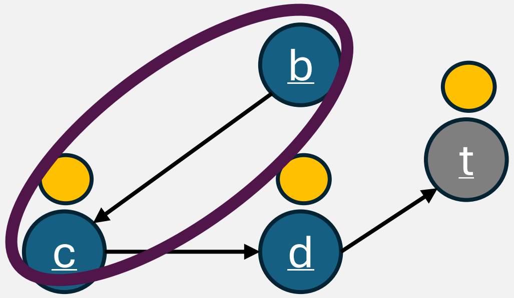

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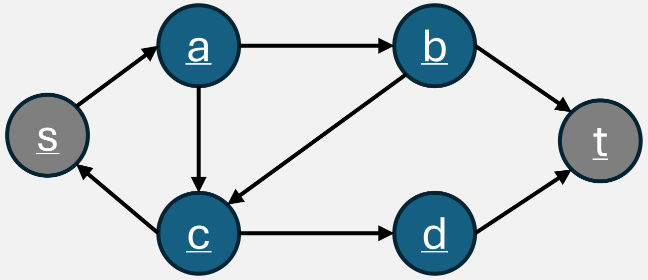

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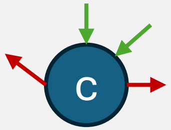
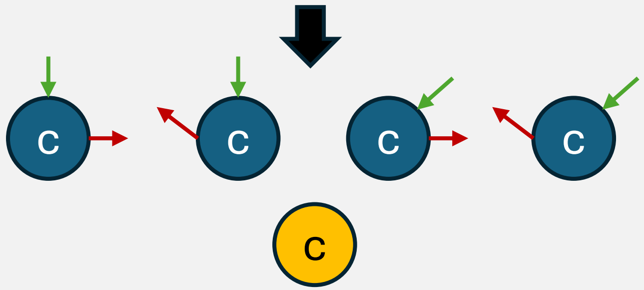
For each vertex: 



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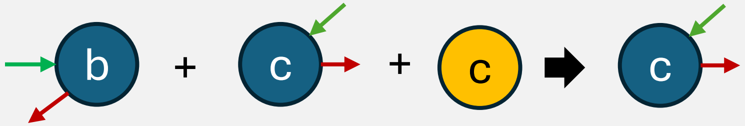

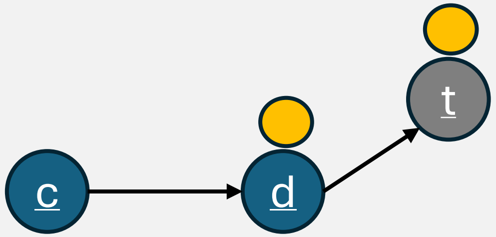

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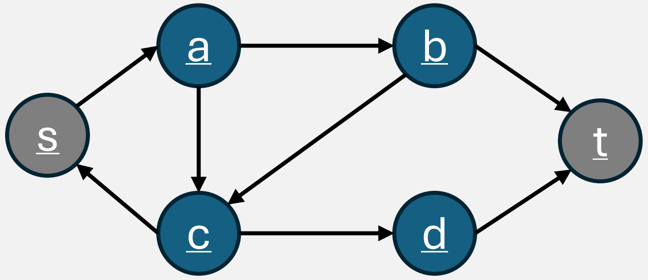

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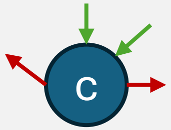

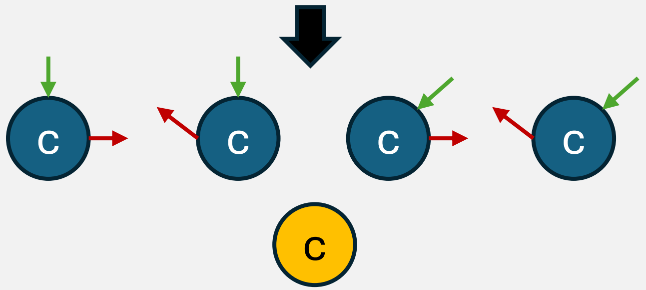

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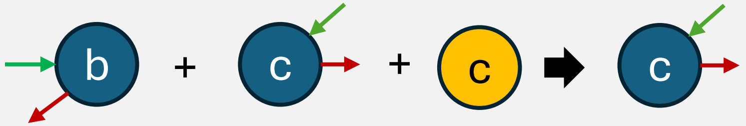

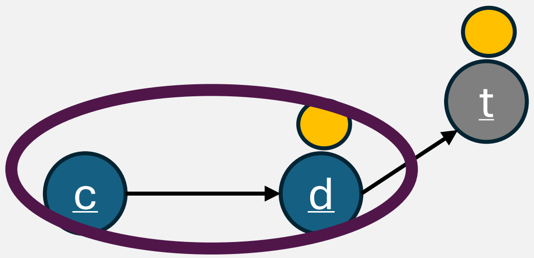

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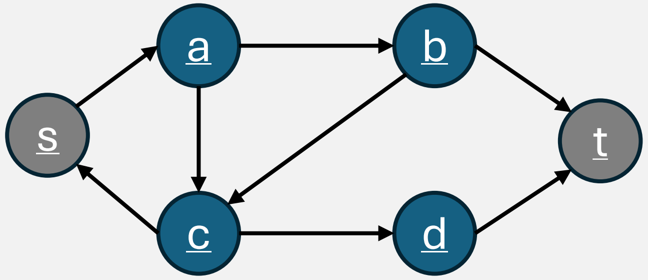

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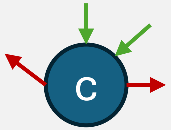

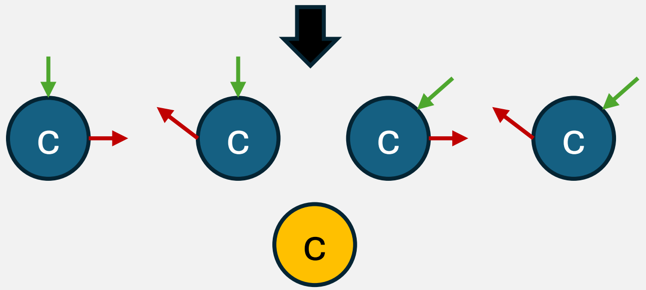

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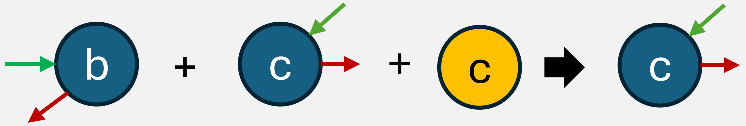

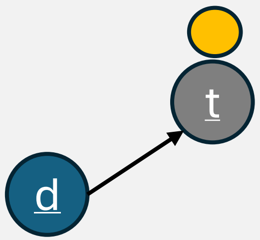

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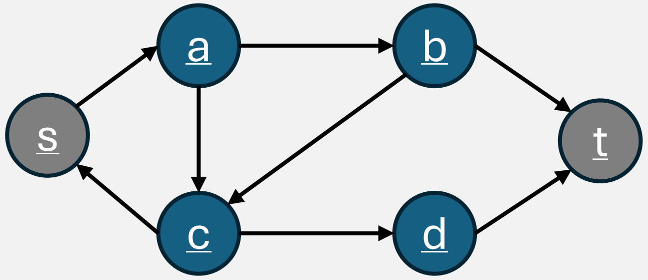

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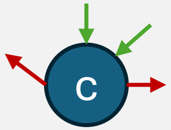
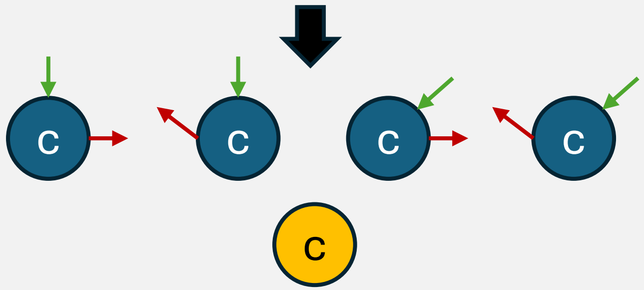
For each vertex: 



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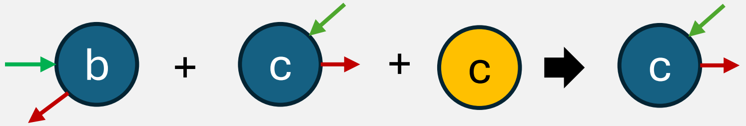

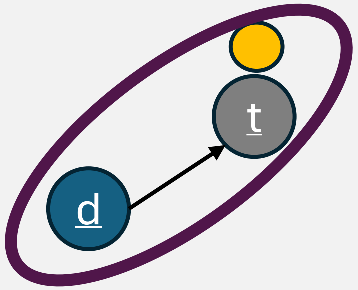

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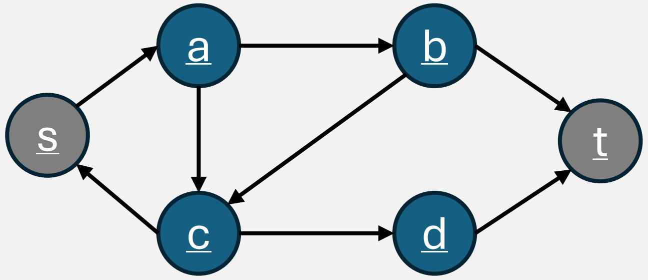

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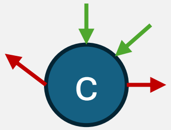
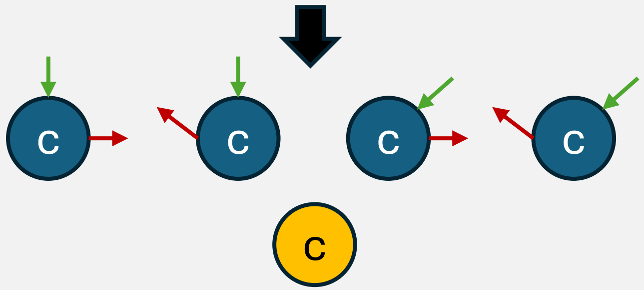
For each vertex: 



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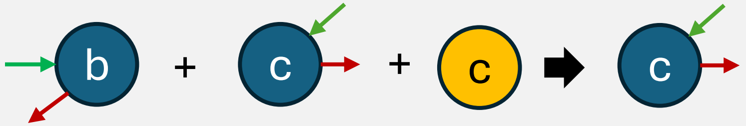

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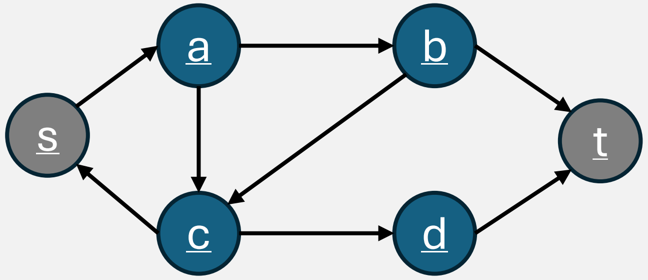

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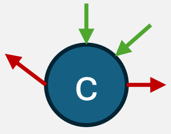

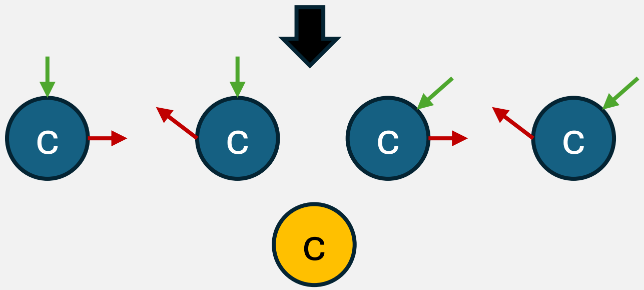

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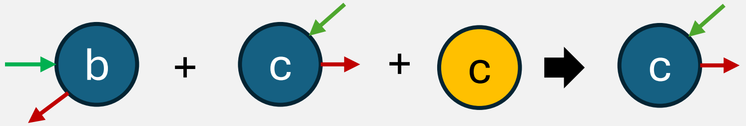
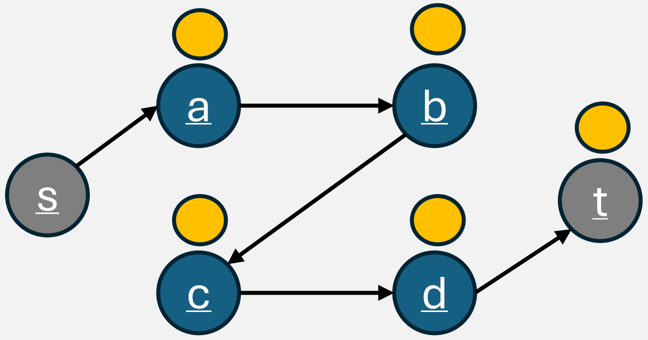
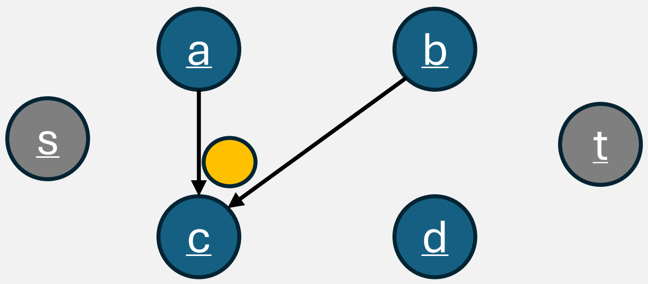


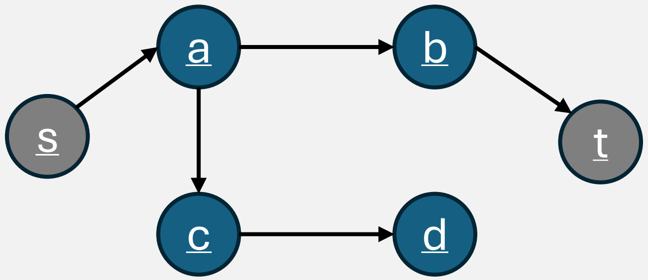


No "double visits"



Only one c

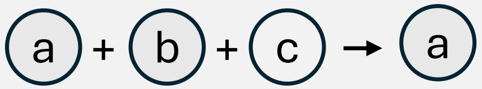
No branching

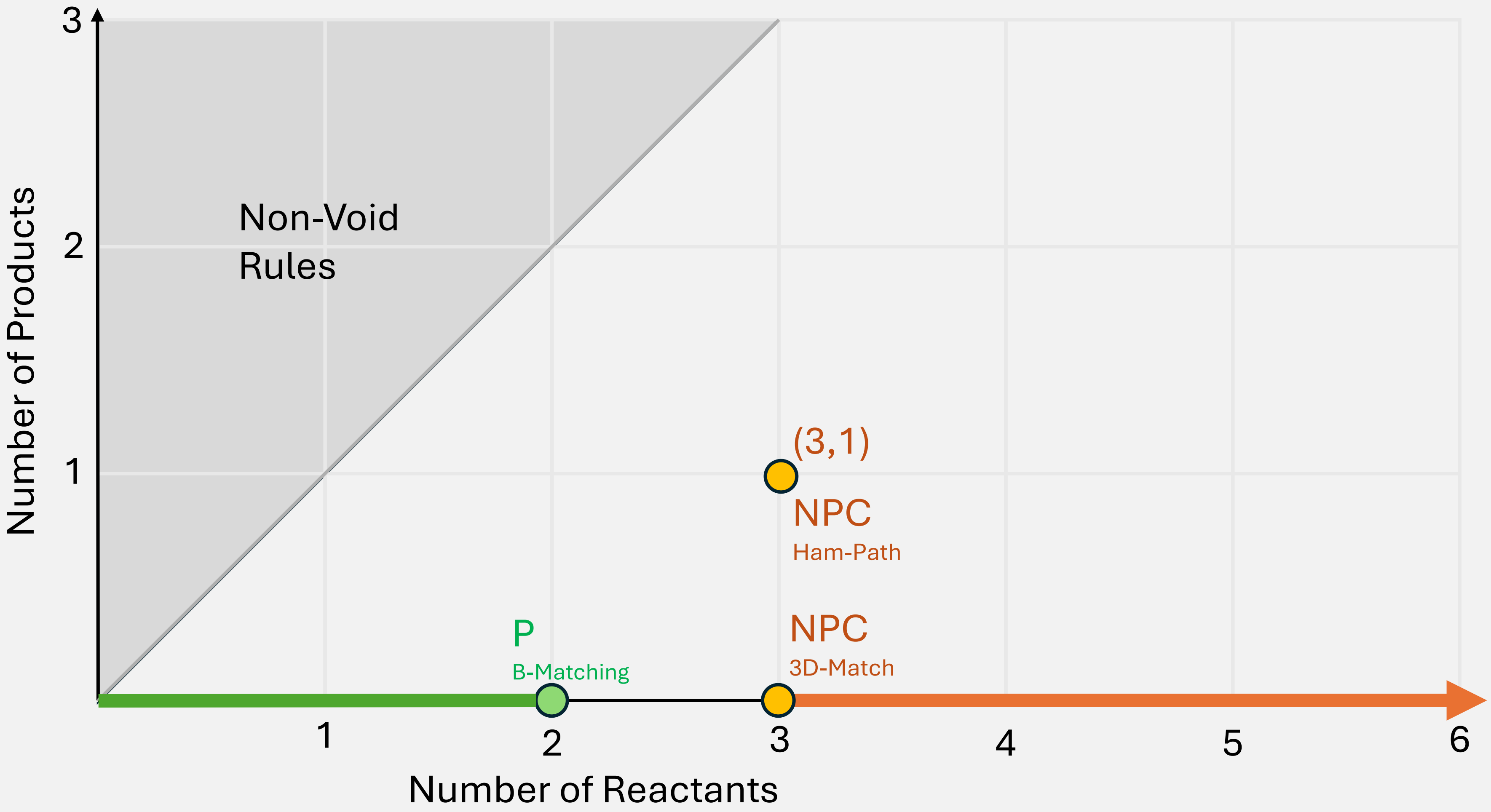


Fails to delete d

Deletion-Only CRNs

(3,1) rules





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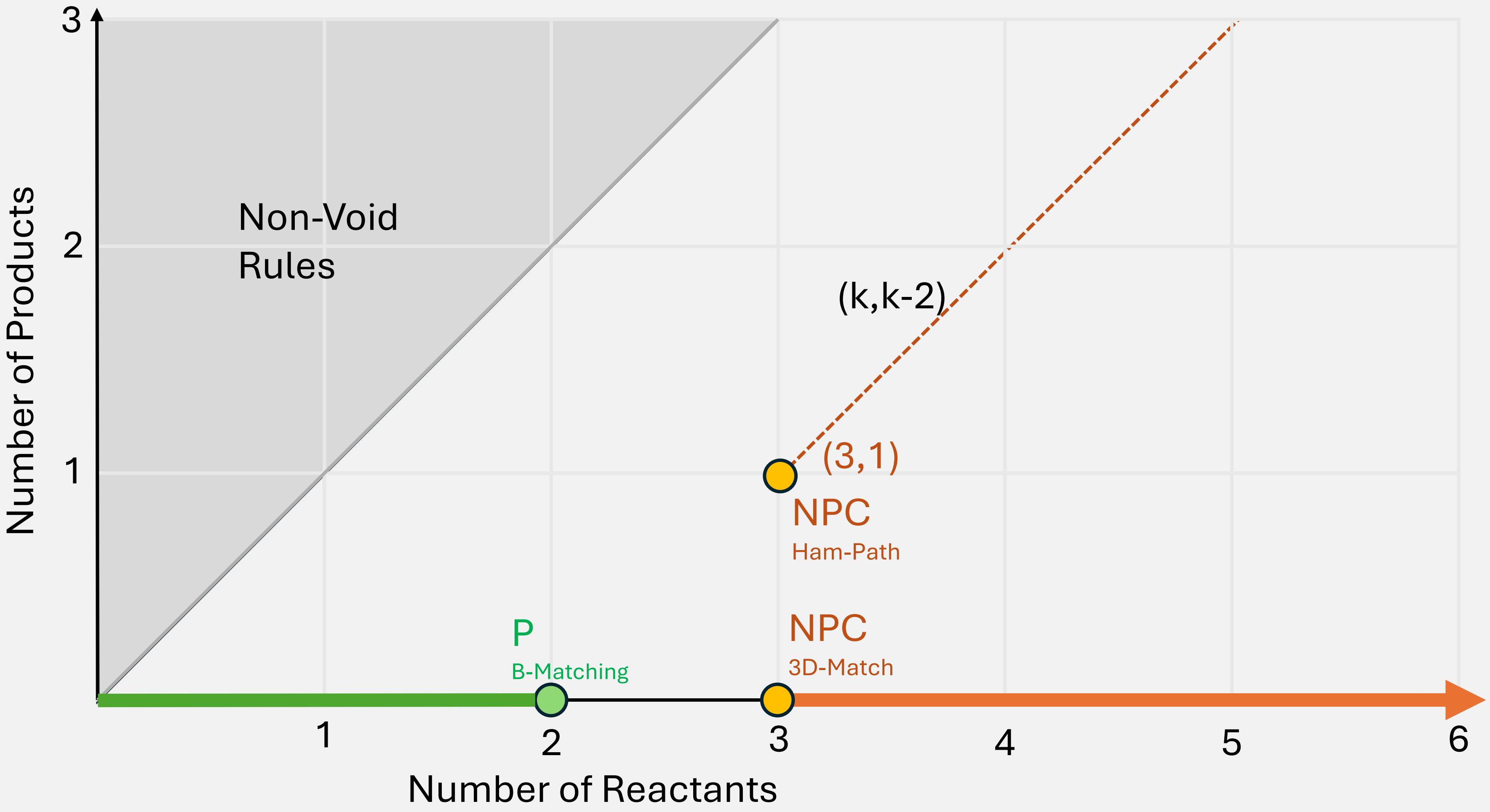

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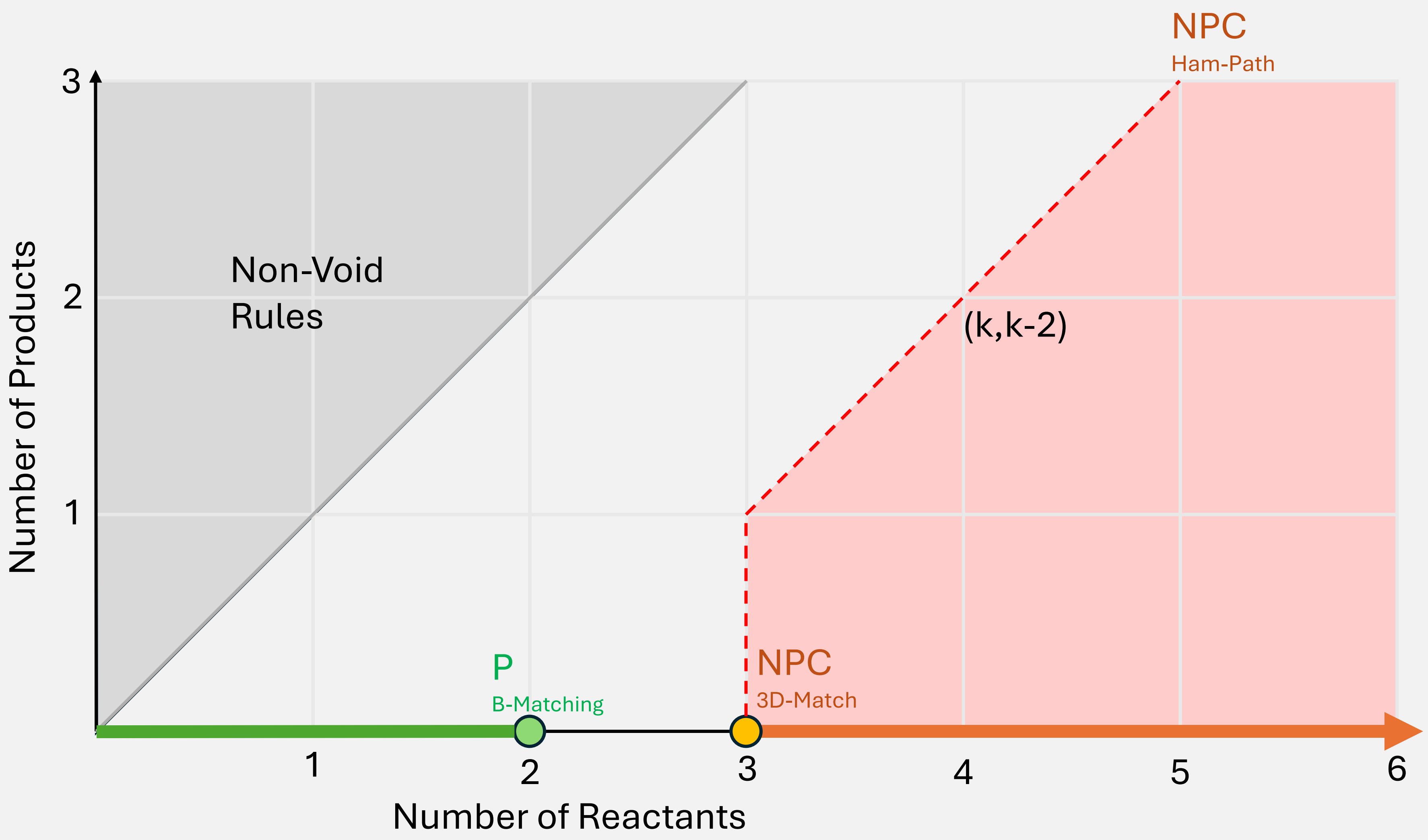
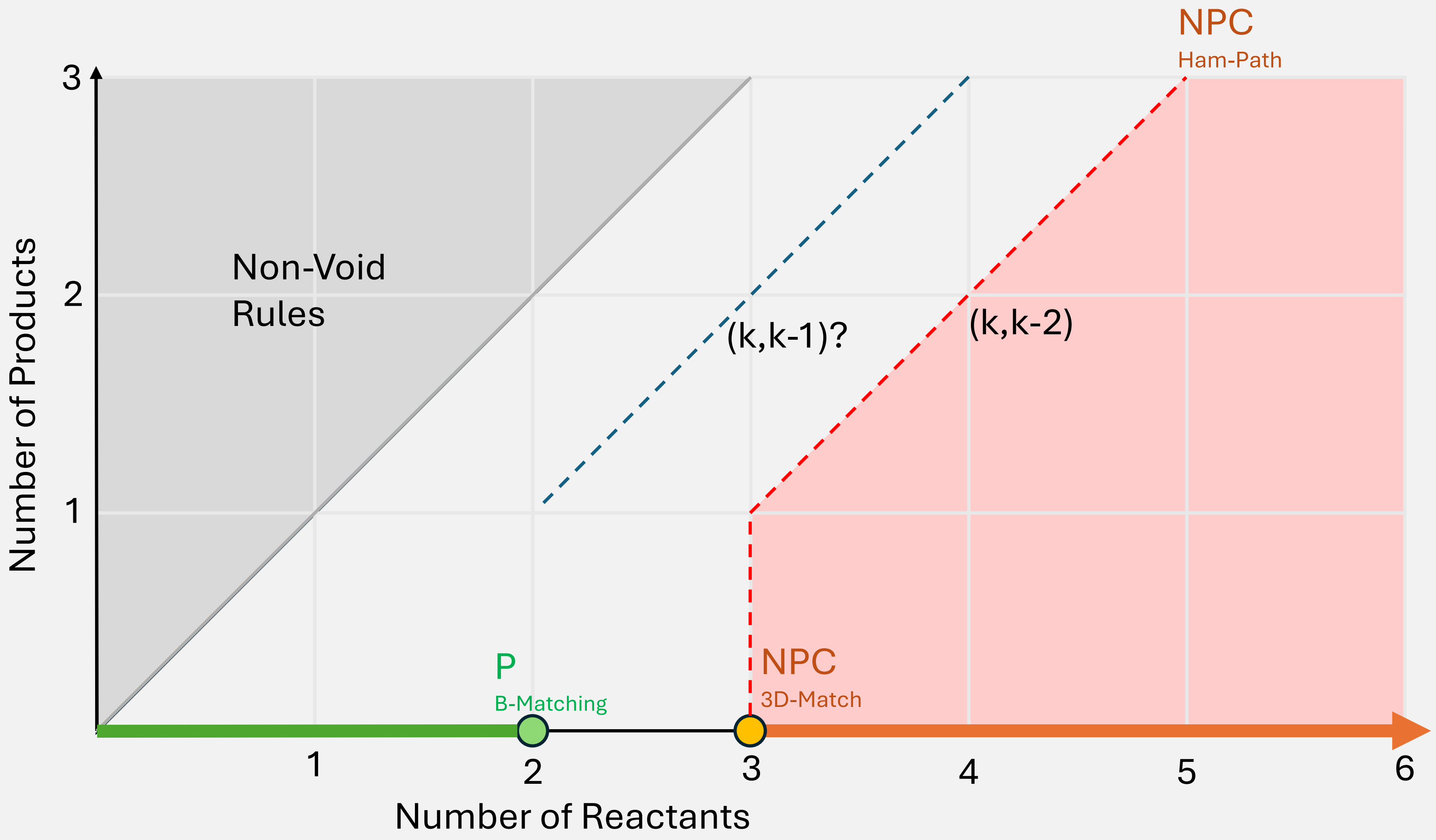
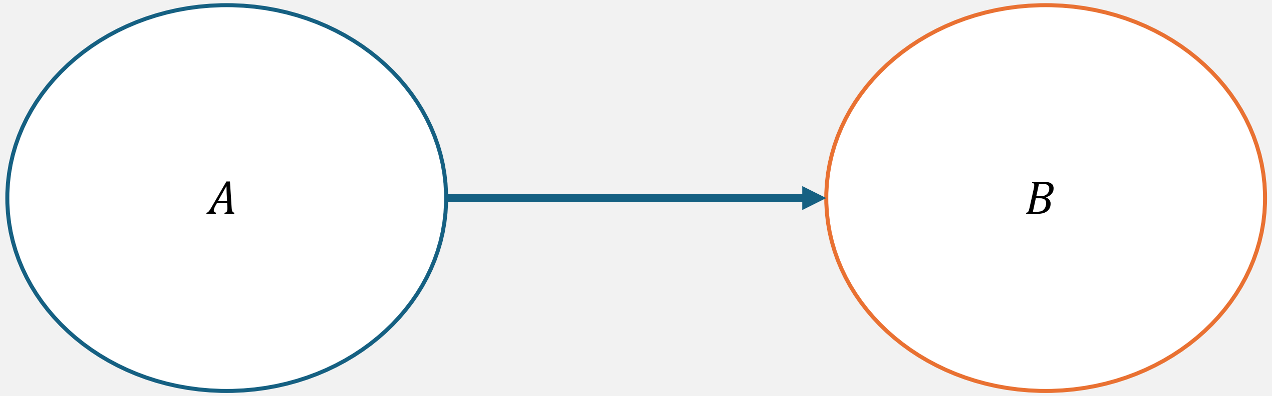


Deletion-Only CRNs



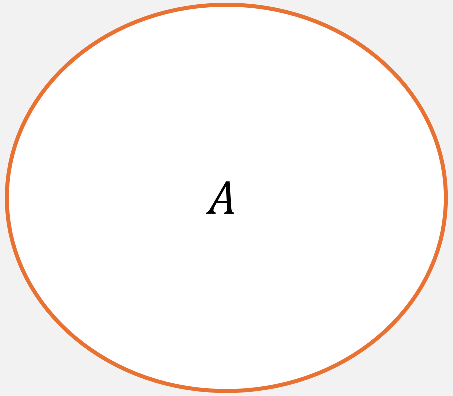
Reaction Graph

- For rule $A + B \rightarrow A$ add edge between A and B. Mark species with a target value > 0



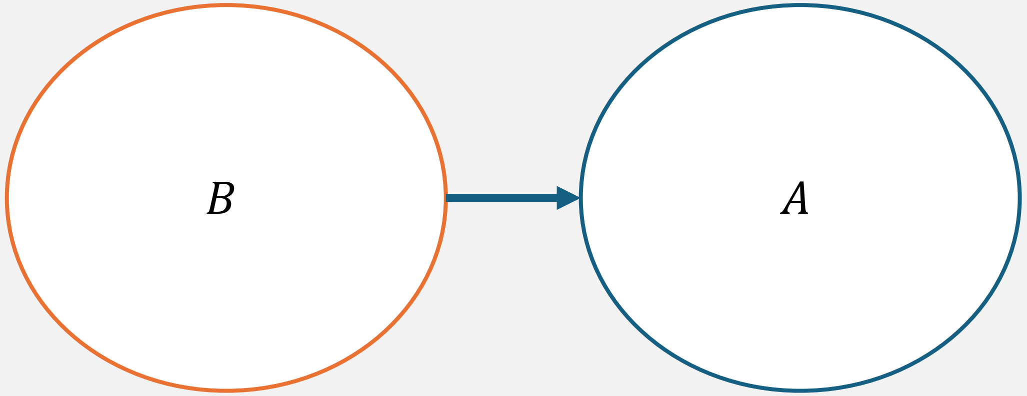
(2,1) Rules

- A species is a root if one of the following is true
  - The species starts with the correct number of copies



(2,1) Rules

- A species is a root if one of the following is true
  - The species starts with the correct number of copies
  - The species can be deleted by some marked species.
  - The species has a self loop.



(2,1) Rules

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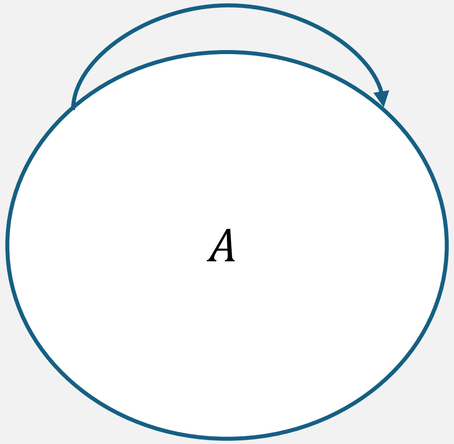
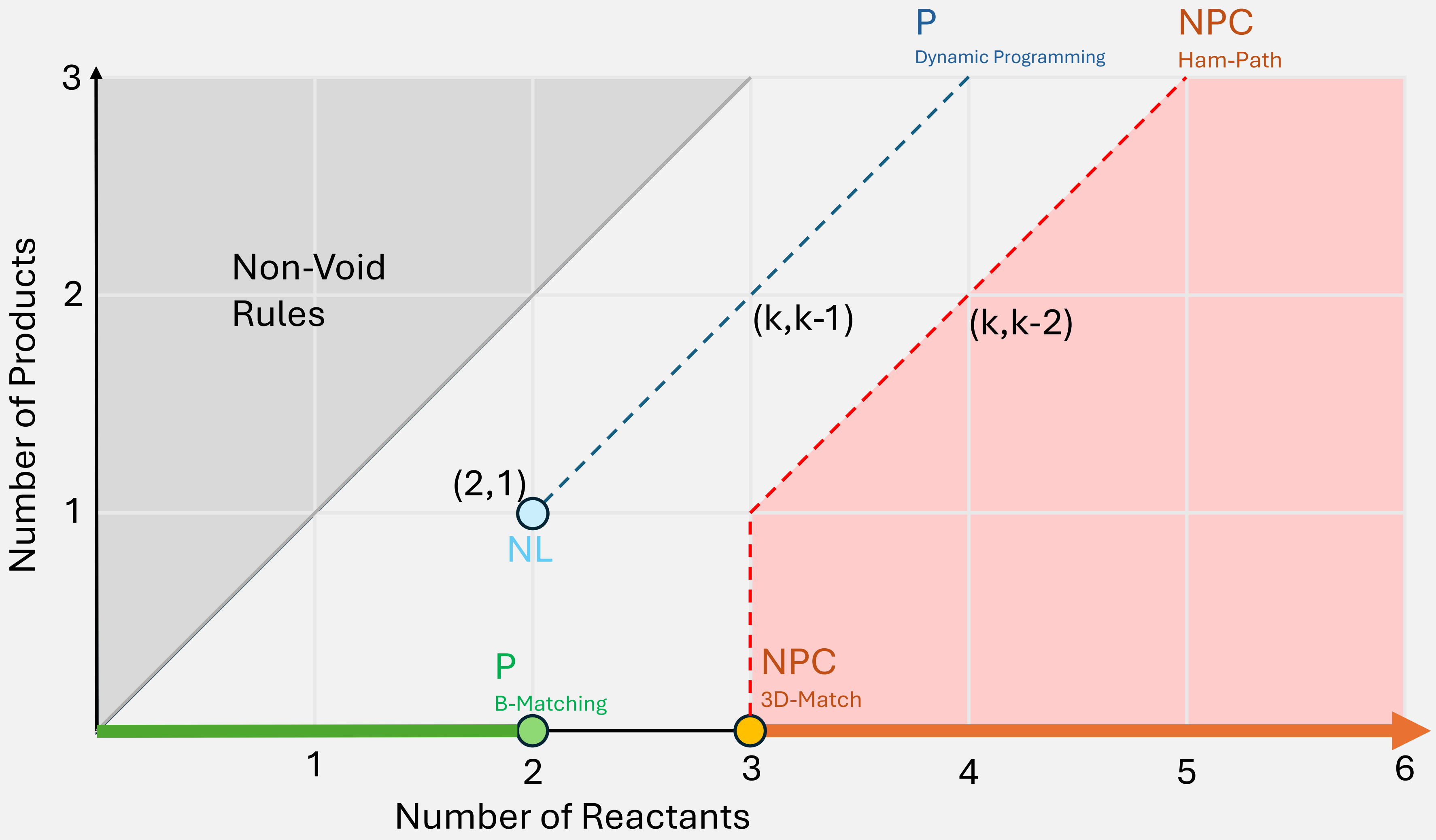


(2,1) Rules

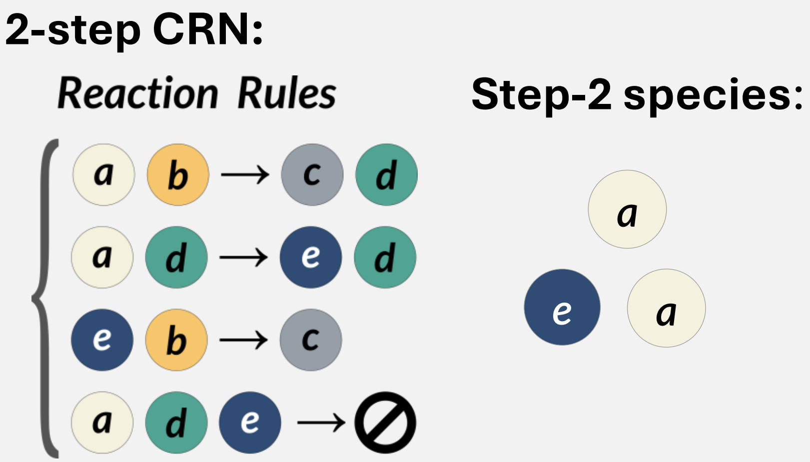
- Checking if a species is a root can be done in log space
- For each species we must find another one that
  - Is reachable in the Reaction Graph
  - Is a root species
  - This takes 2 pointers
- Reachability in a directed graph can be solved in non-deterministic log space.

Deletion-Only CRNs



2-Step CRNs

2-Step CRN systems include a multiset of “step-2” species to be added after the system is terminal:

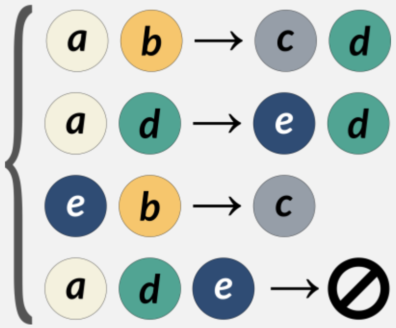


2-Step CRNs

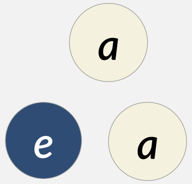
2-Step CRN systems include a multiset of "step-2" species to be added after the system is terminal:

2-step CRN:

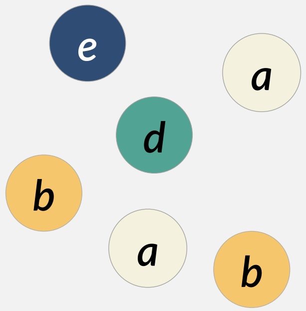
Reaction Rules



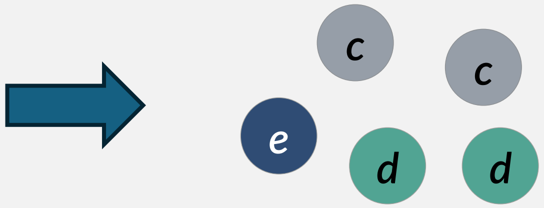
Step-2 species:



Configuration I:

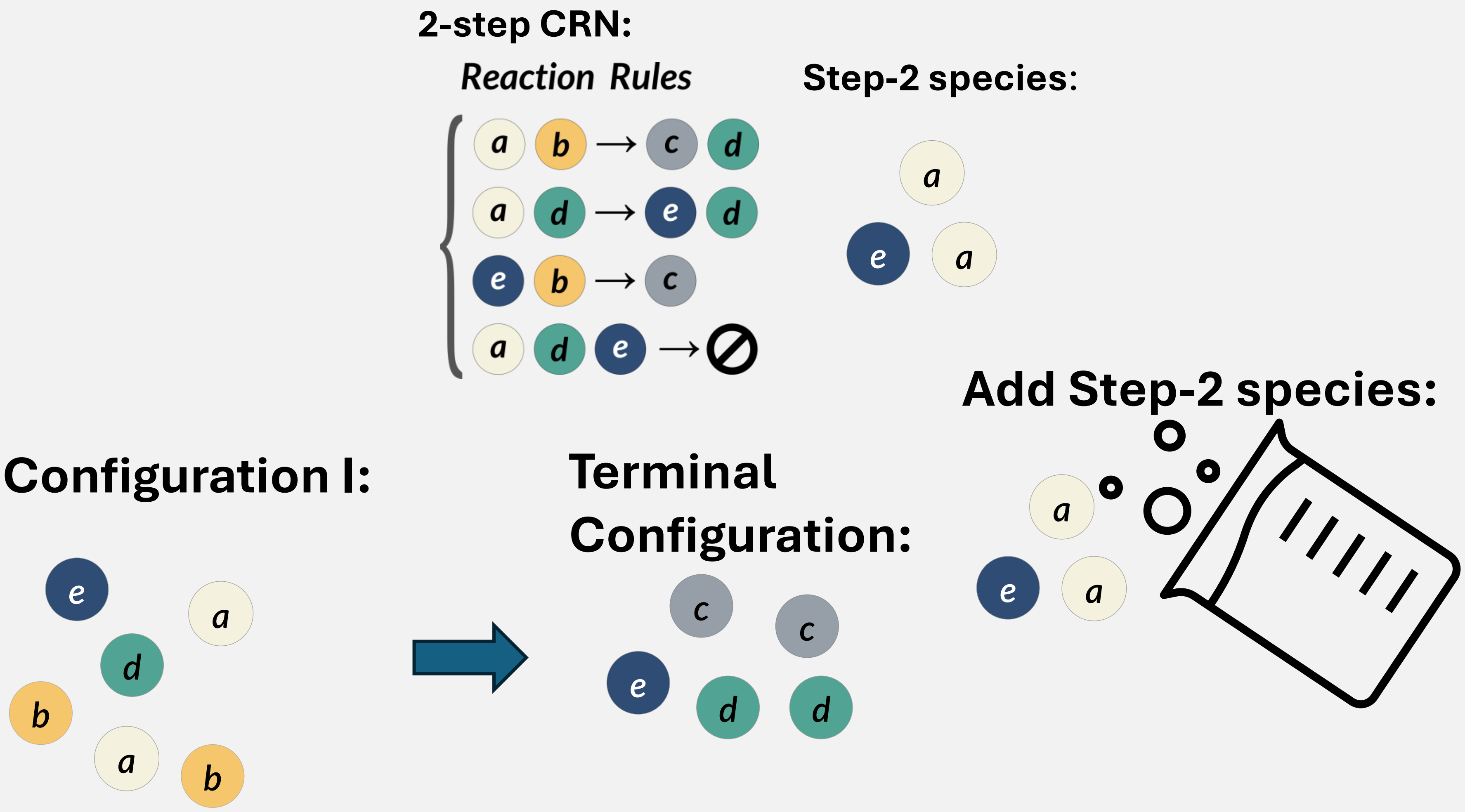


Terminal Configuration:



2-Step CRNs

2-Step CRN systems include a multiset of “step-2” species to be added after the system is terminal:



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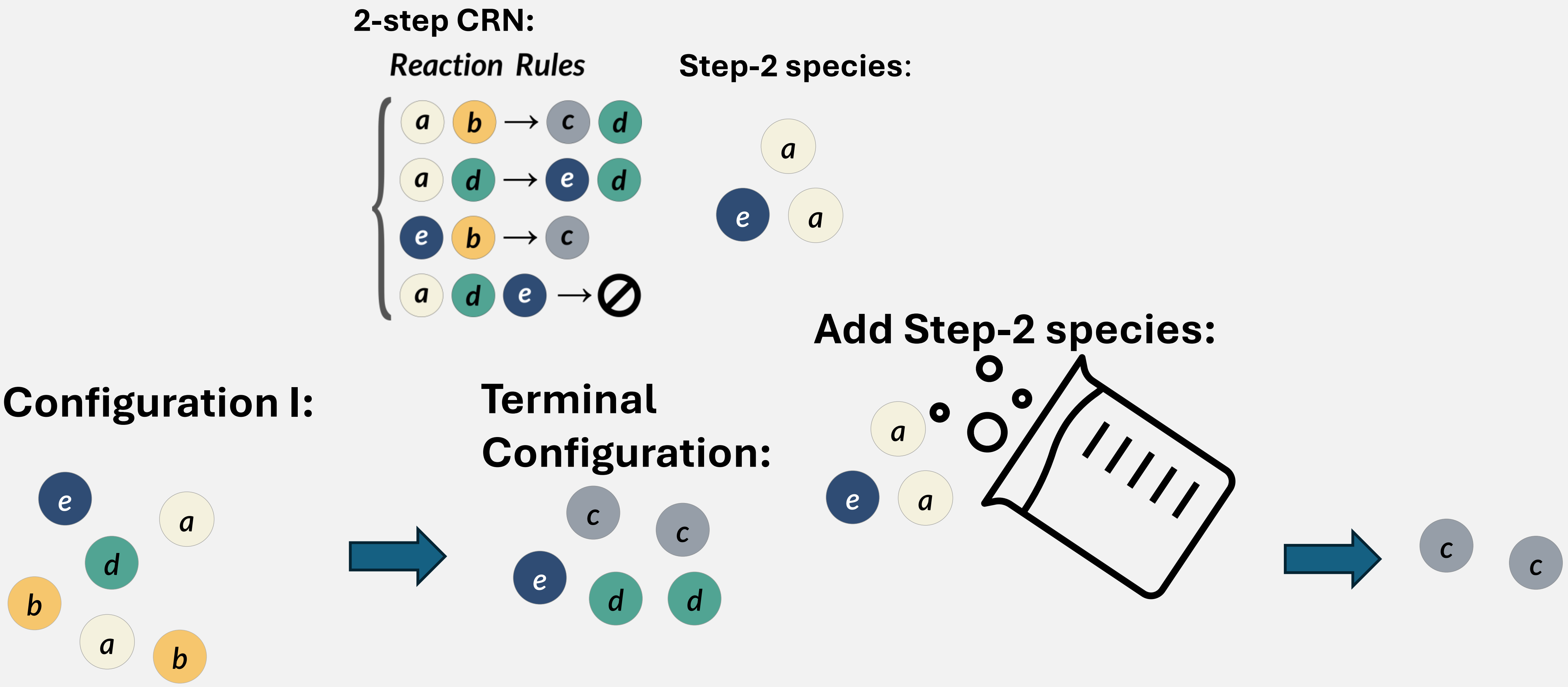
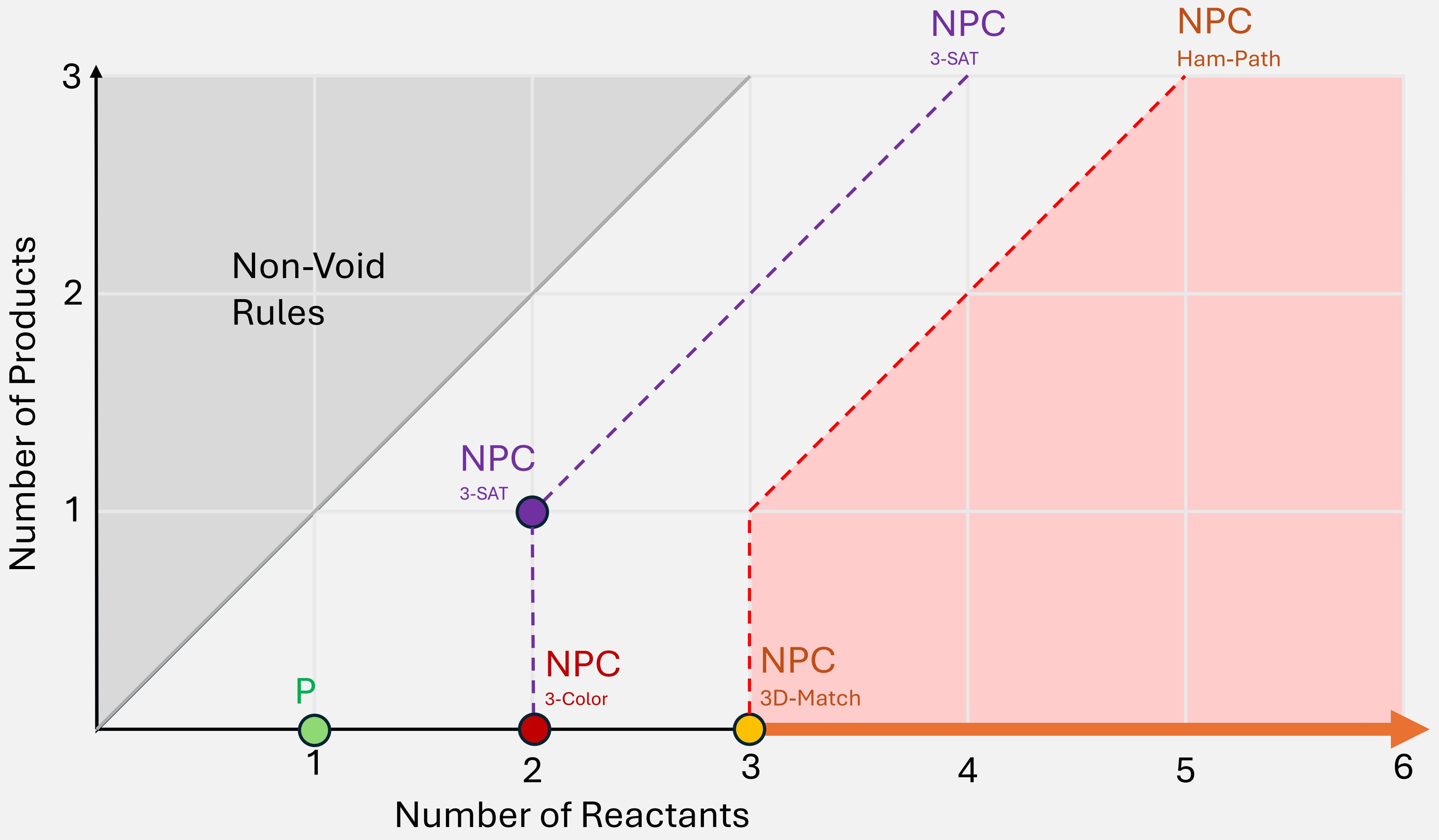
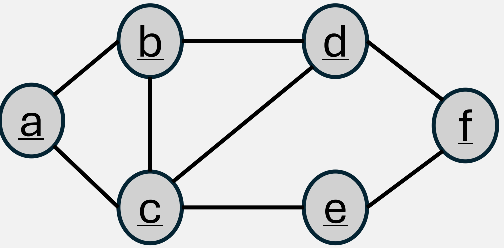


2-Step Deletion-Only CRNs



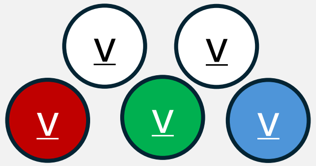
Deletion-Only 2-Step CRNs: (2,0) NP-complete

3-Color Input:



Initial Configuration:

For each vertex v:



Target Configuration:

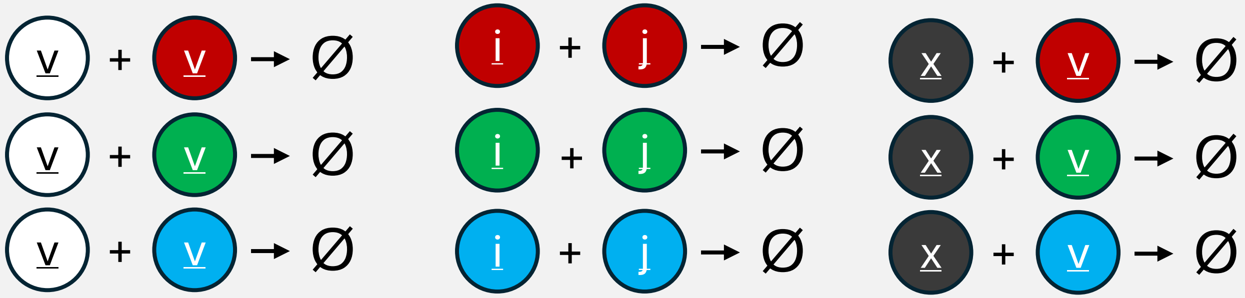
Eliminate **all** of these species

Reactions:

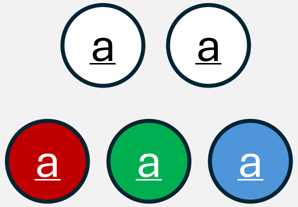
For each vertex v:

For each edge (i,j):

For all vertices V:

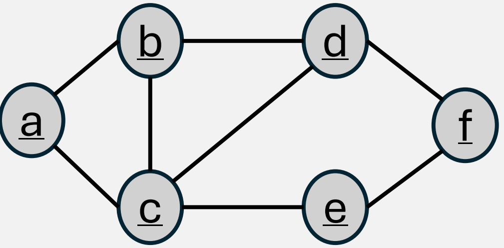


2nd Step Additions: |V| copies of 



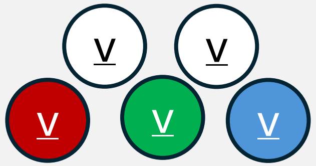
Deletion-Only 2-Step CRNs: (2,0) NP-complete

3-Color Input:



Initial Configuration:

For each vertex v:



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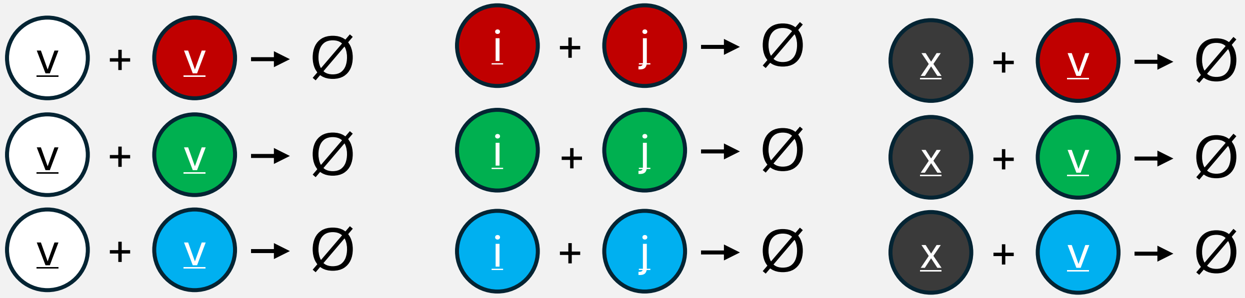
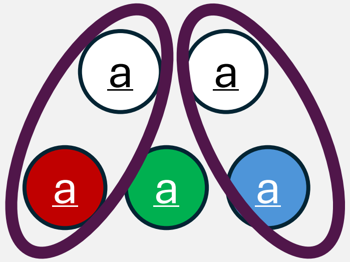
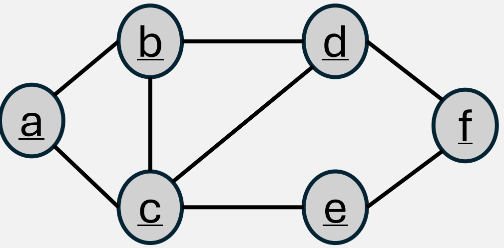


2nd Step Additions: |V| copies of x



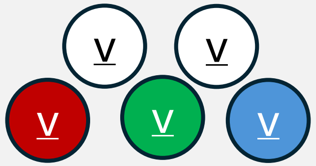
Deletion-Only 2-Step CRNs: (2,0) NP-complete

3-Color Input:



Initial Configuration:

For each vertex v:



Target Configuration:

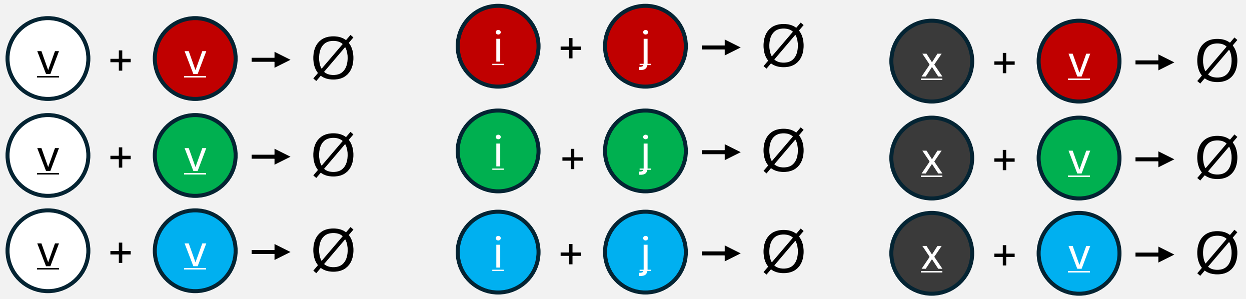
Eliminate **all** of these species

Reactions:

For each vertex v:

For each edge (i,j):

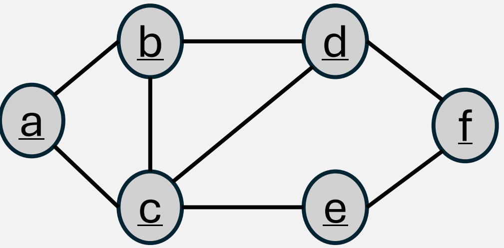
For all vertices V:



2nd Step Additions: |V| copies of 

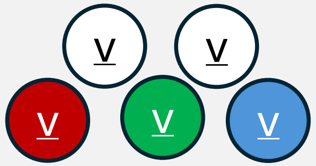
Deletion-Only 2-Step CRNs: (2,0) NP-complete

3-Color Input:



Initial Configuration:

For each vertex v:



Target Configuration:

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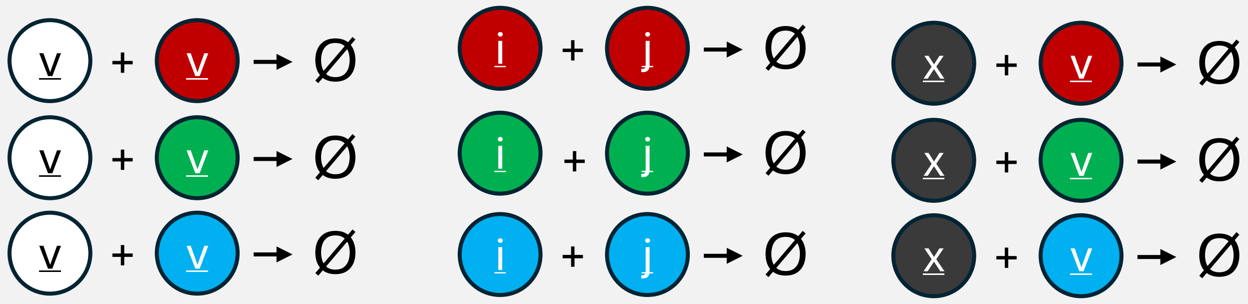
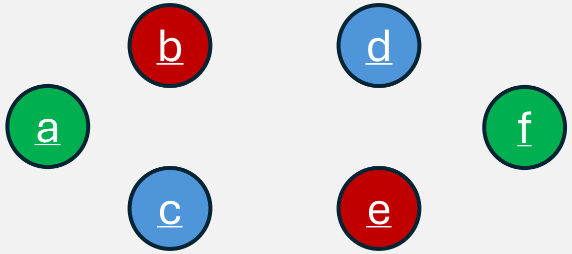
Reactions:

For each vertex v: For each edge (i,j): For all vertices V:

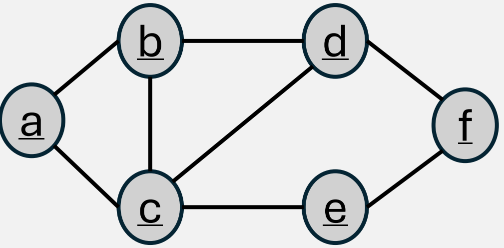


2nd Step Additions: |V| copies of 



Deletion-Only 2-Step CRNs: (2,0) NP-complete

3-Color Input:



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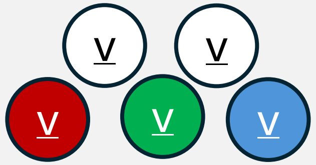
For each vertex v:



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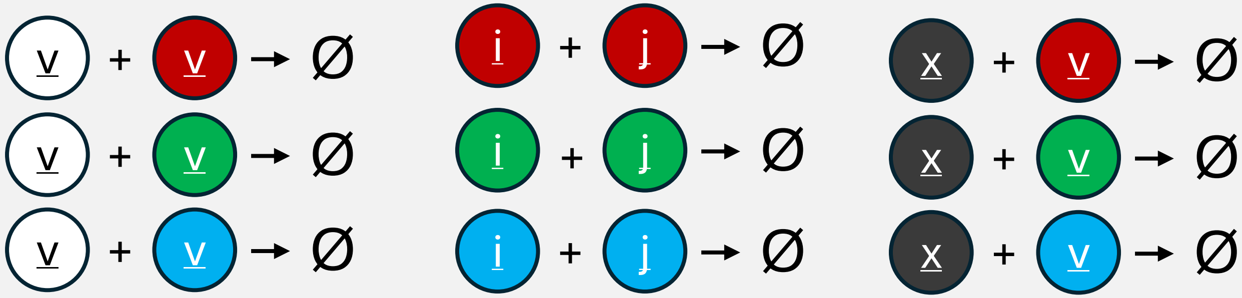
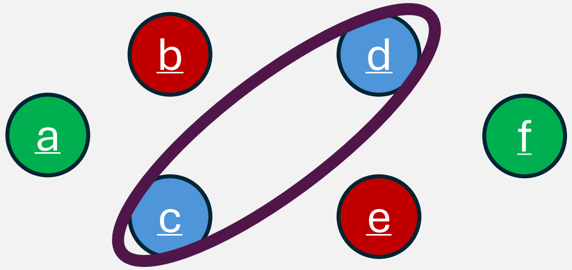


2nd Step Additions: |V| copies of 



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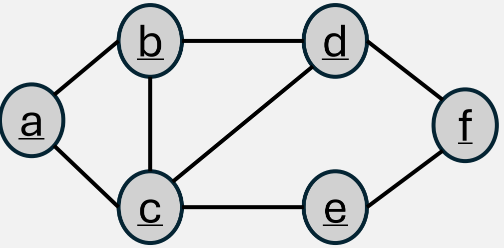
3-Color Input:



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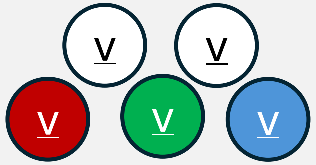

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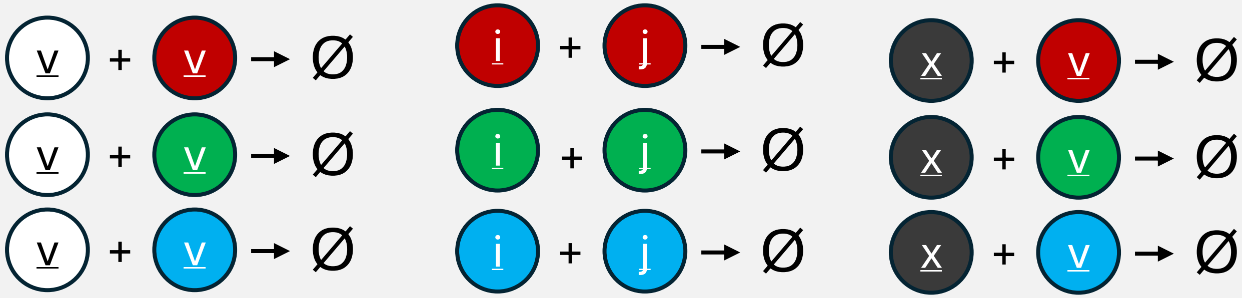
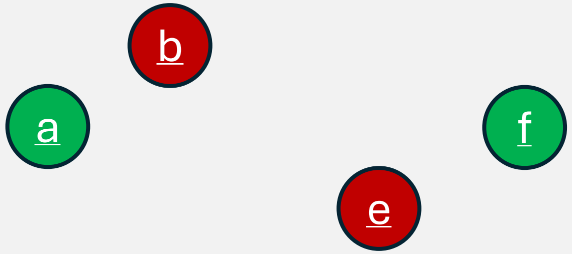
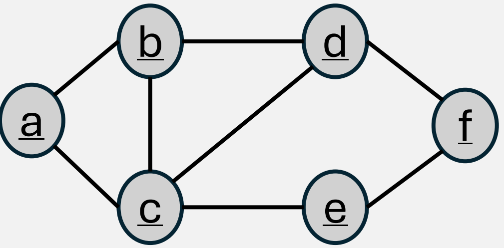


2nd Step Additions: |V| copies of 



Deletion-Only 2-Step CRNs: (2,0) NP-complete

3-Color Input:



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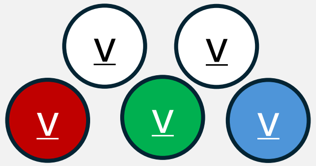

Target Configuration:

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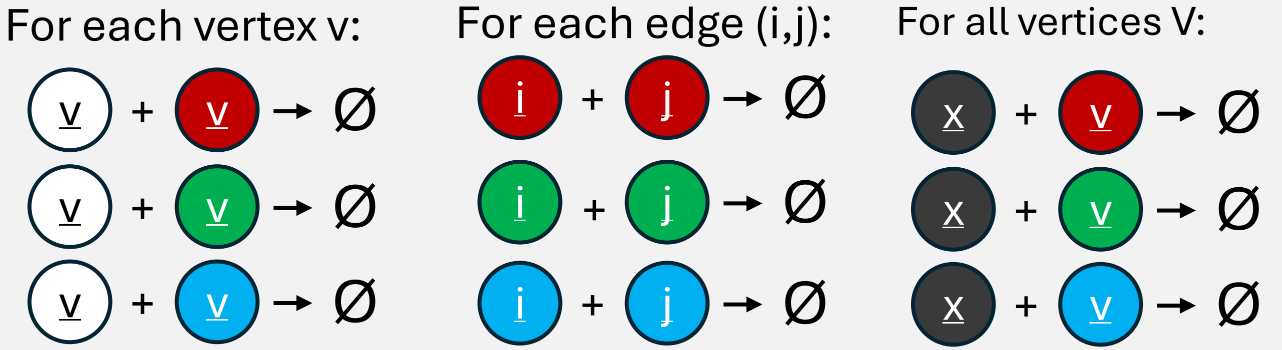
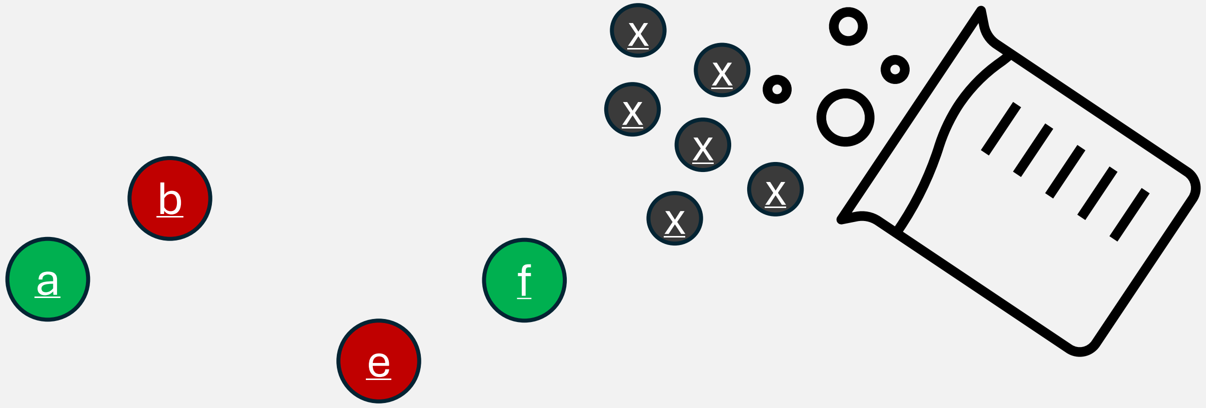


2nd Step Additions: |V| copies of 



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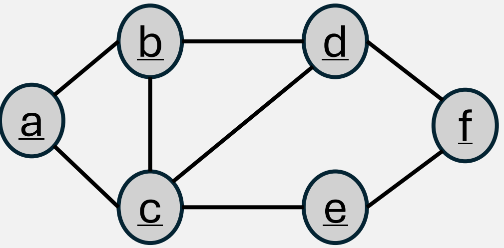
3-Color Input:



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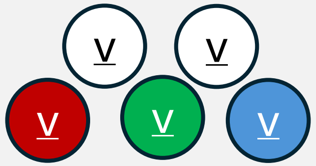

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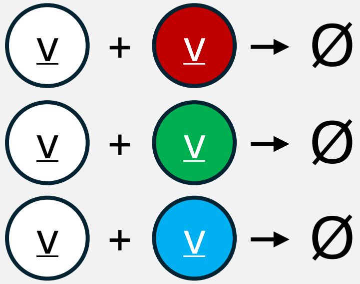
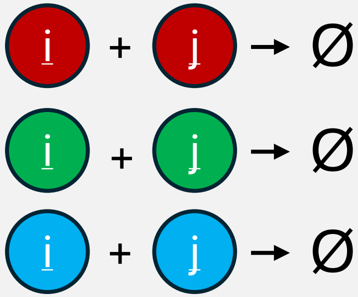
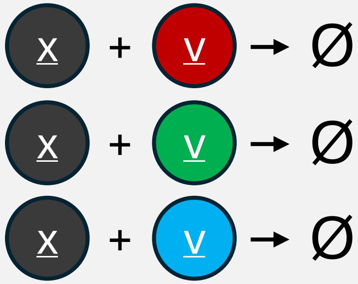
For each vertex v:



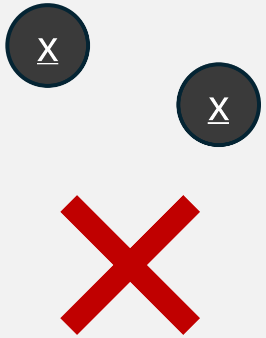
For each edge (i,j):



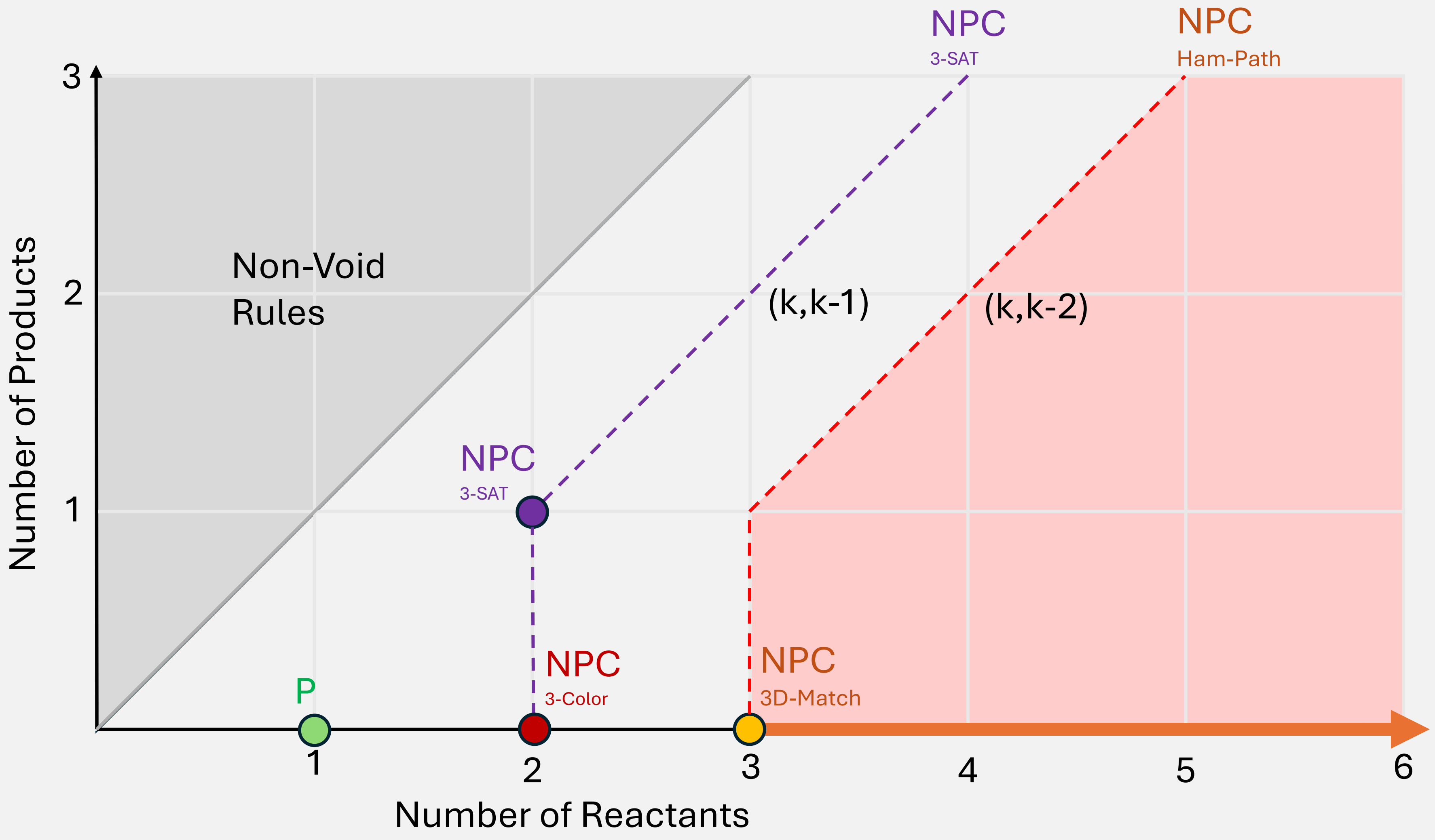
For all vertices V:



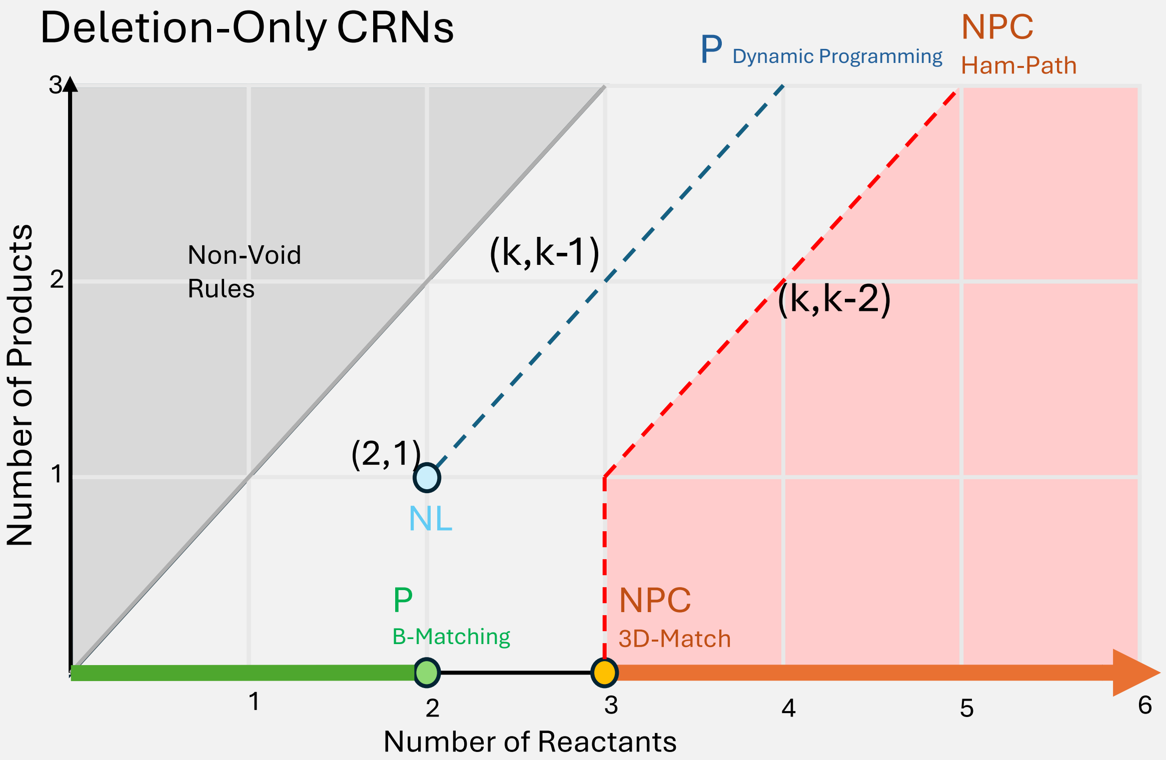
2nd Step Additions: |V| copies of 

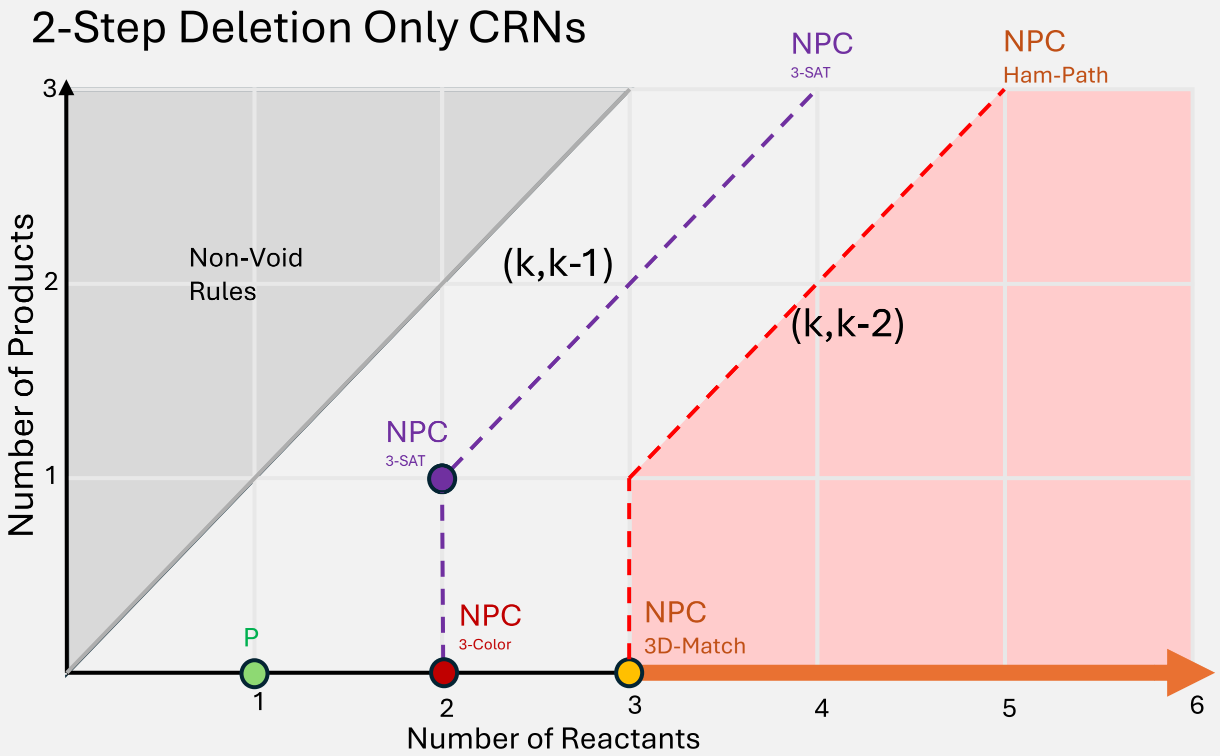


2-Step Deletion-Only CRNs



Thank you.
Questions?





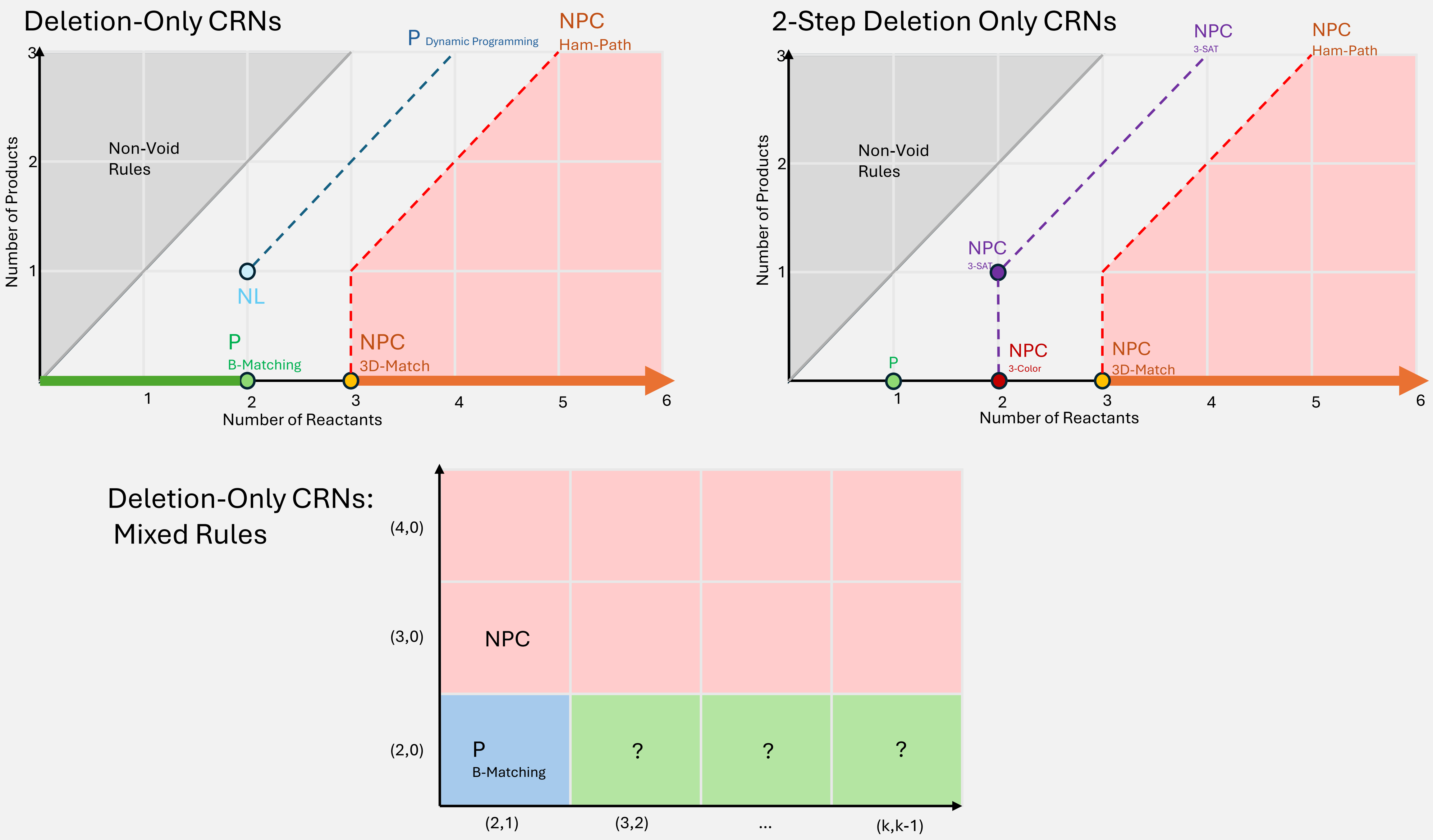
Brief Announcement: Reachability in Deletion-only Chemical Reaction Networks

Bin Fu, Timothy Gomez , Ryan Knobel, Austin Luchsinger, Aiden Massie, Marco Rodriguez, Adrian Salinas, Robert Schweller, Tim Wylie

Full Version: (to appear) The 31st International Conference on DNA Computing and Molecular Programming (DNA31)

Deletion-Only CRNs: Mixed Rules

	(2,1)	(3,2)	…	(k,k-1)
(4,0)	NPC	NPC	NPC	NPC
(3,0)	NPC	NPC	NPC	NPC
(2,0)	P B-Matching	?	?	?


Deletion-Only CRNs
P Dynamic Programming
NPC
Ham-Path
Non-Void
Rules
Number of Products
NL
P
B-Matching
NPC
3D-Match
Number of Reactants
2-Step Deletion Only CRNs
NPC
3-SAT
NPC
Ham-Path
Non-Void
Rules
Number of Products
NPC
3-SAT
P
NPC
3-Color
NPC
3D-Match
Number of Reactants
Deletion-Only CRNs:
Mixed Rules
(4,0)
(3,0)
(2,0)
NPC
P
B-Matching
?
?
?
(2,1)
(3,2)
...
(k,k-1)