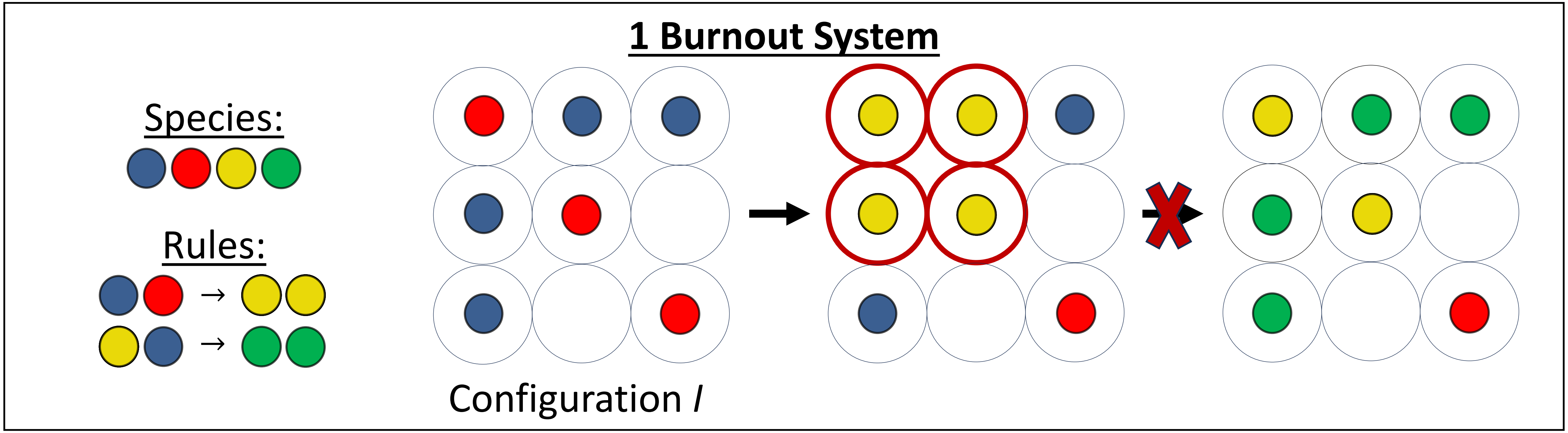
Reconfiguration of Linear Surface Chemical Reaction Networks with Bounded State Change



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Overview

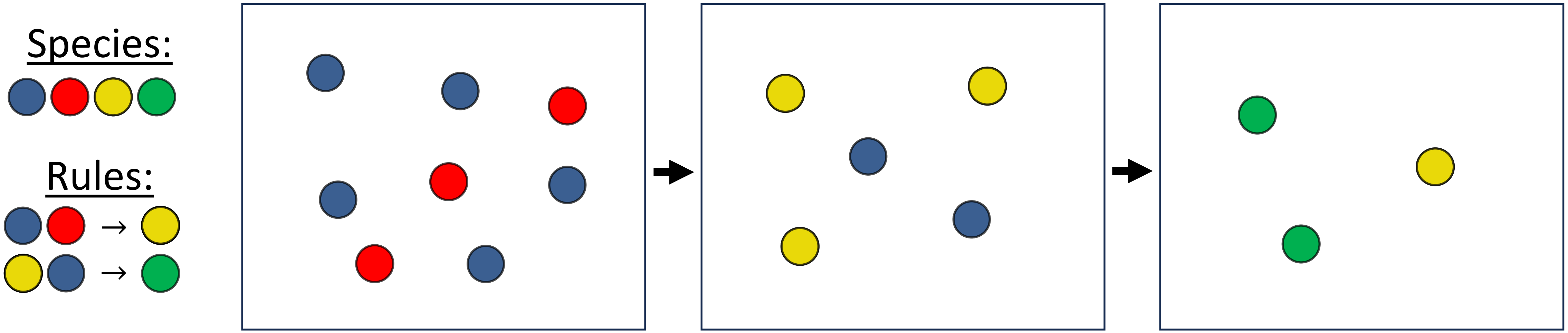
1. Introduction to the Model
2. Motivation
3. Previous work/Contributions
    - Linear Surfaces
    - General Surfaces
    - Grid Surfaces
4. Conclusion

Introduction to the Model

Chemical Reaction Networks

- Ordered pair (Λ, Γ)
  - Λ = Set of input species
  - Γ = Set of rules
- Configuration
  - Length |Λ| vector of non-negative integers
  - Represents count of each species

Example CRN System



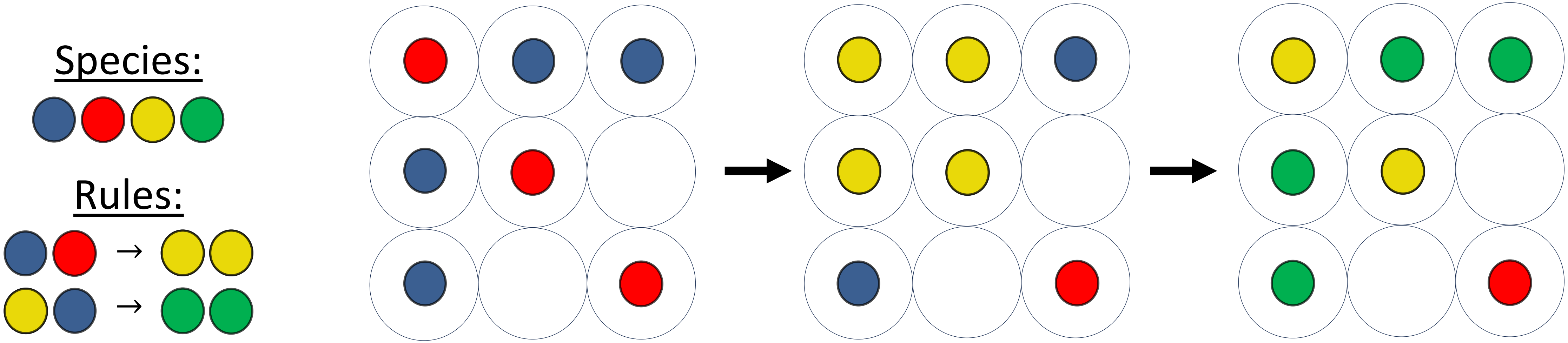
Configuration *I:*
[5, 3, 0, 0]

Configuration *D:*
[0, 0, 1, 2]

Surface Chemical Reaction Networks

- Ordered pair (Λ, Γ)
  - Λ = Set of input species
  - Γ = Set of rules
- Surface
  - Undirected graph
- Configuration
  - Mapping of input species to vertices on the surface
  - Each vertex has no more than 1 species at a time

Example sCRN System

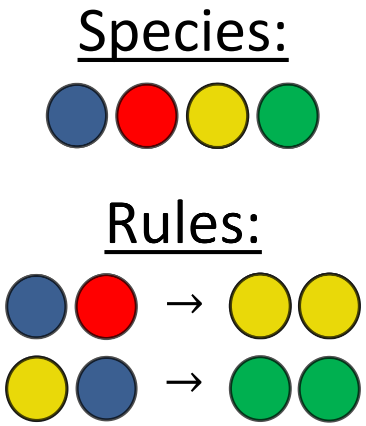


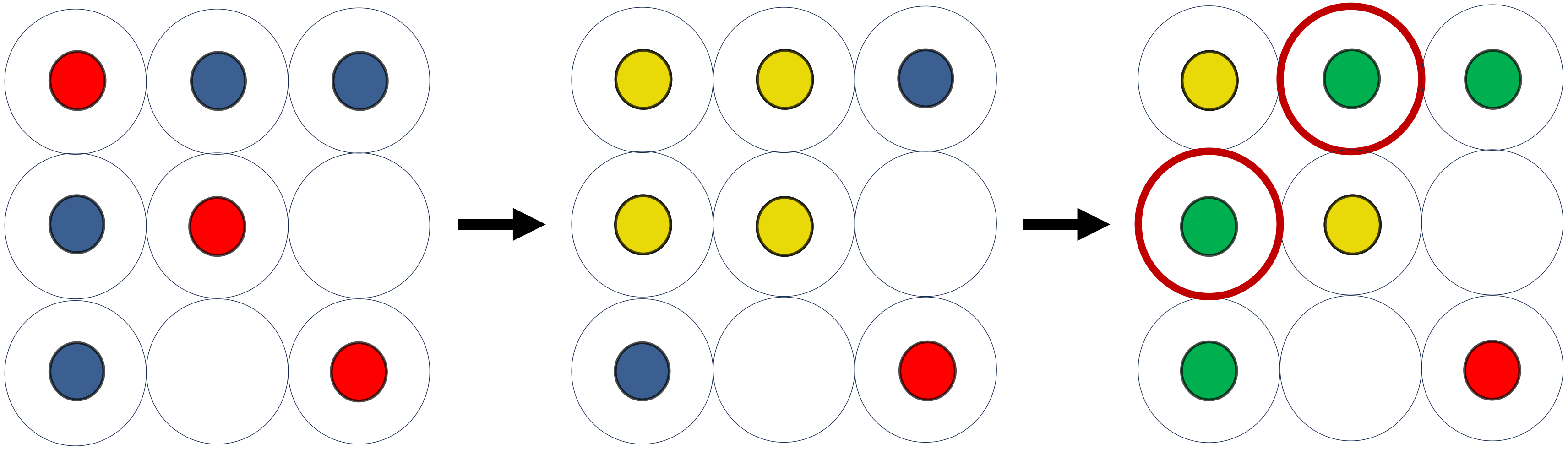
Configuration *I*

Surface Chemical Reaction Networks

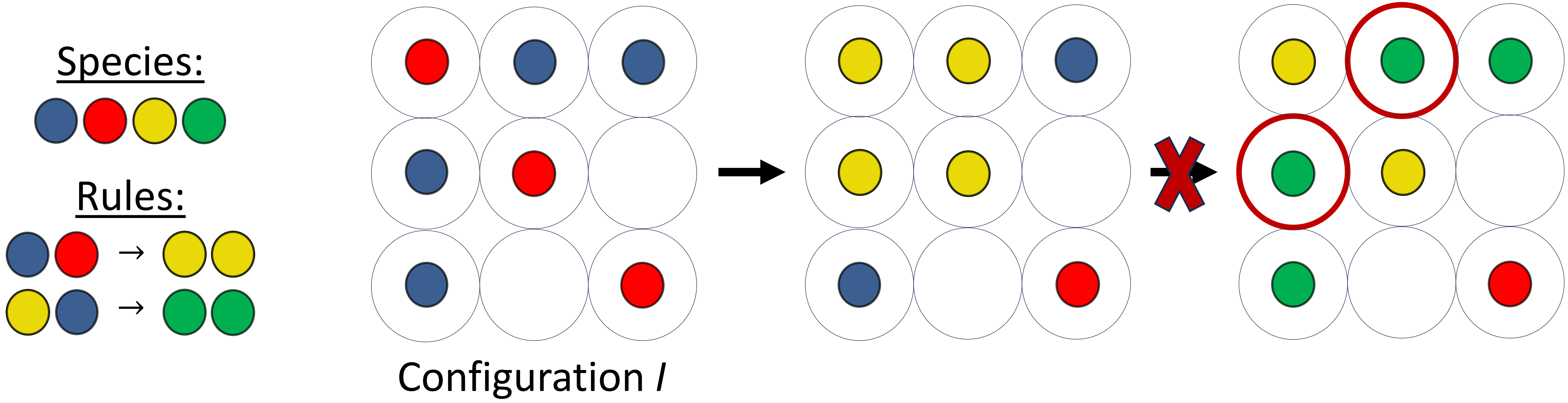
- Ordered pair (Λ, Γ)
  - Λ = Set of input species
  - Γ = Set of rules
- Surface
  - Undirected graph
- Configuration
  - Mapping of input species to vertices on the surface
  - Each vertex has no more than 1 species at a time
- Burnout
  - Limit to how many times a vertex can change states

Example sCRN System: 2 burnout

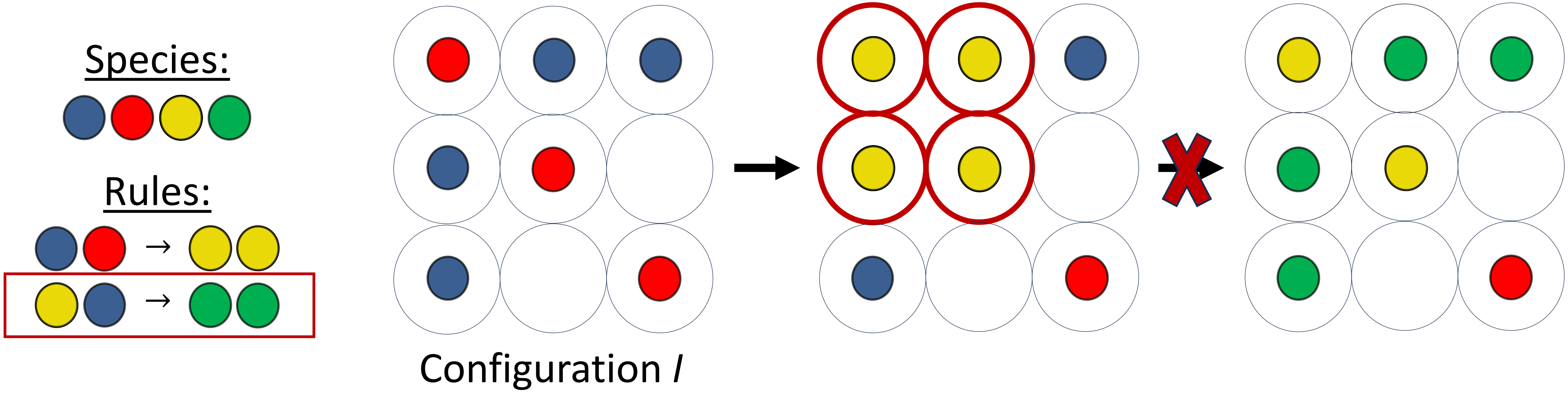




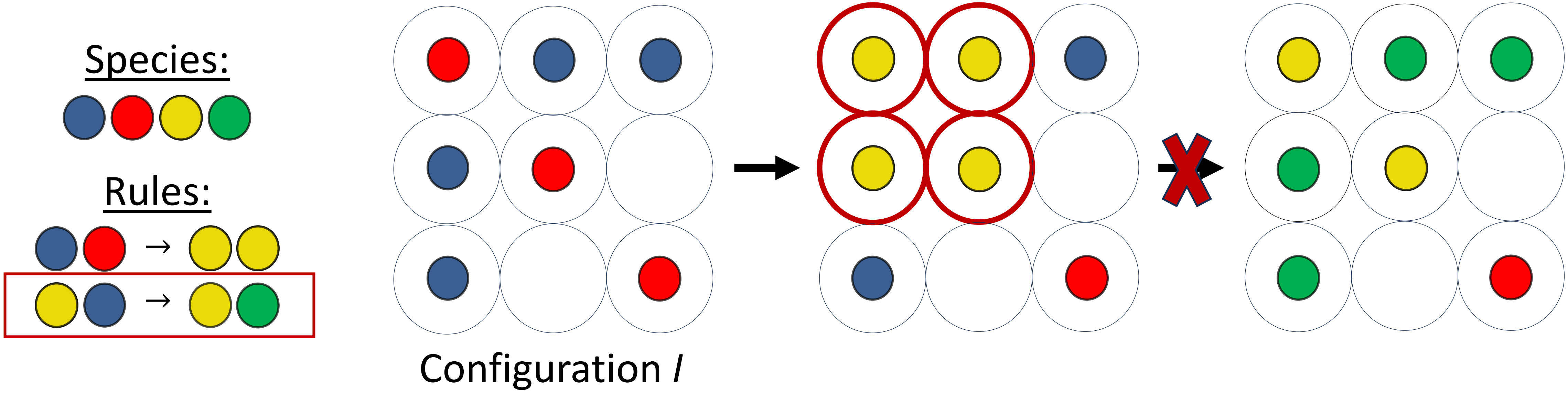
Example sCRN System: 1 burnout



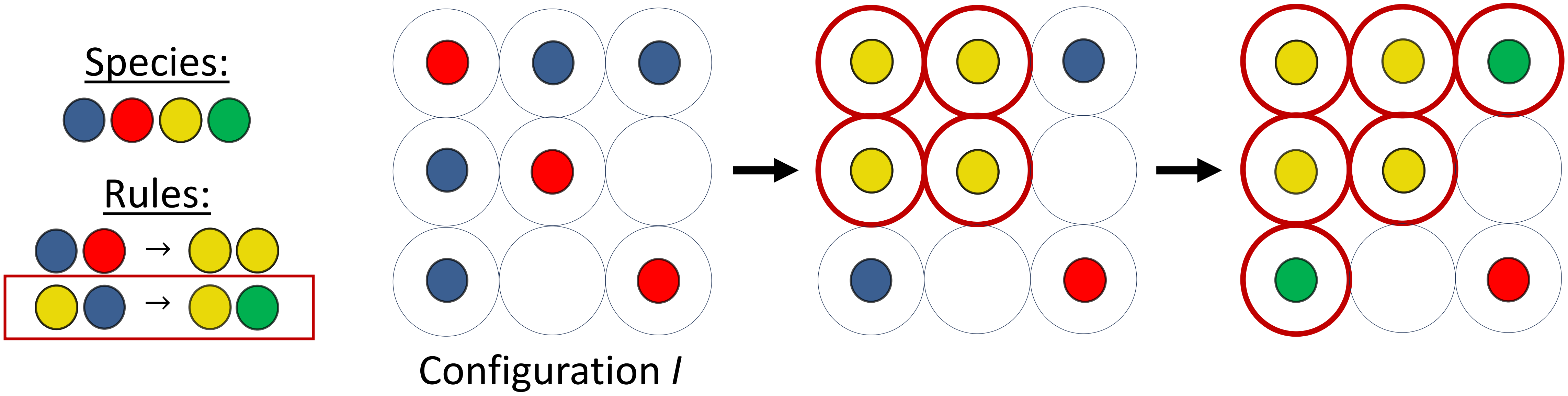
Example sCRN System: 1 burnout



Example sCRN System: 1 burnout

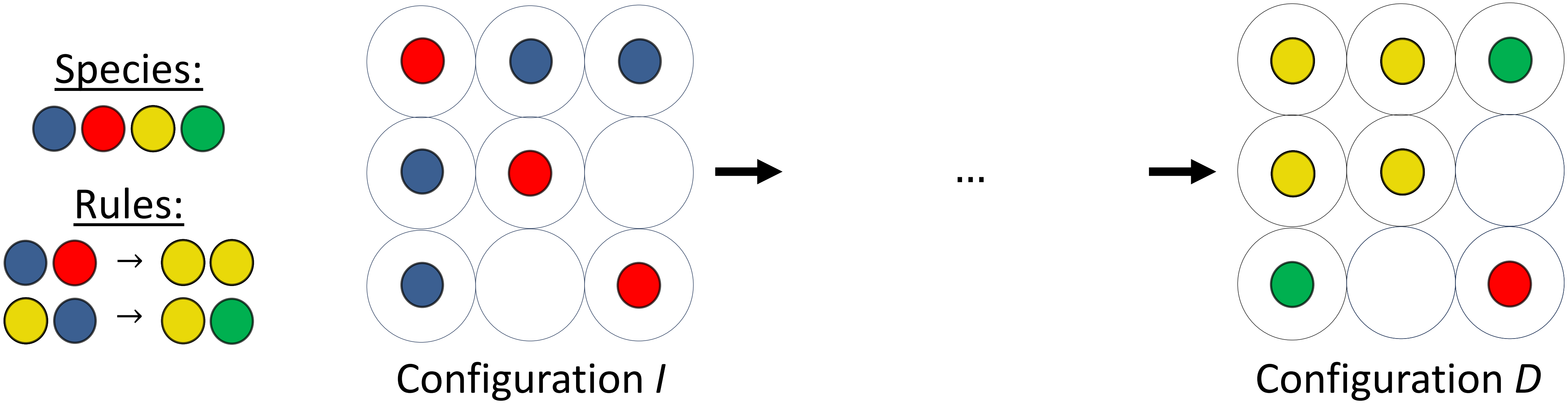


Example sCRN System: 1 burnout



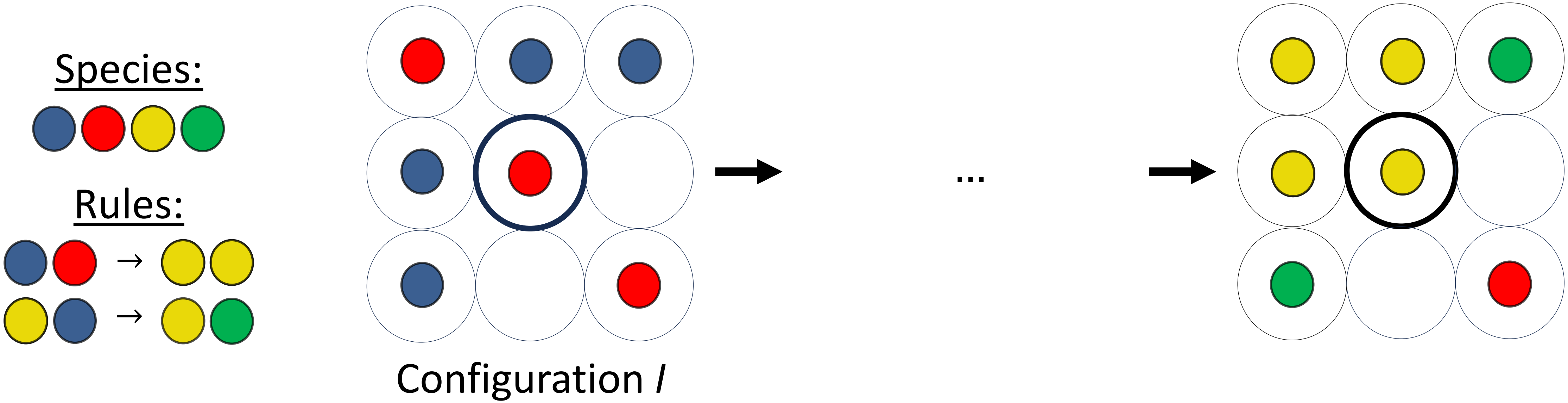
Reconfiguration

- Given initial configuration *I* and target configuration *D*, can *D* ever be reached from *I*?



1-Reconfiguration

- Given initial configuration *I*, vertex *v* and species *s*, does *s* ever appear in v?

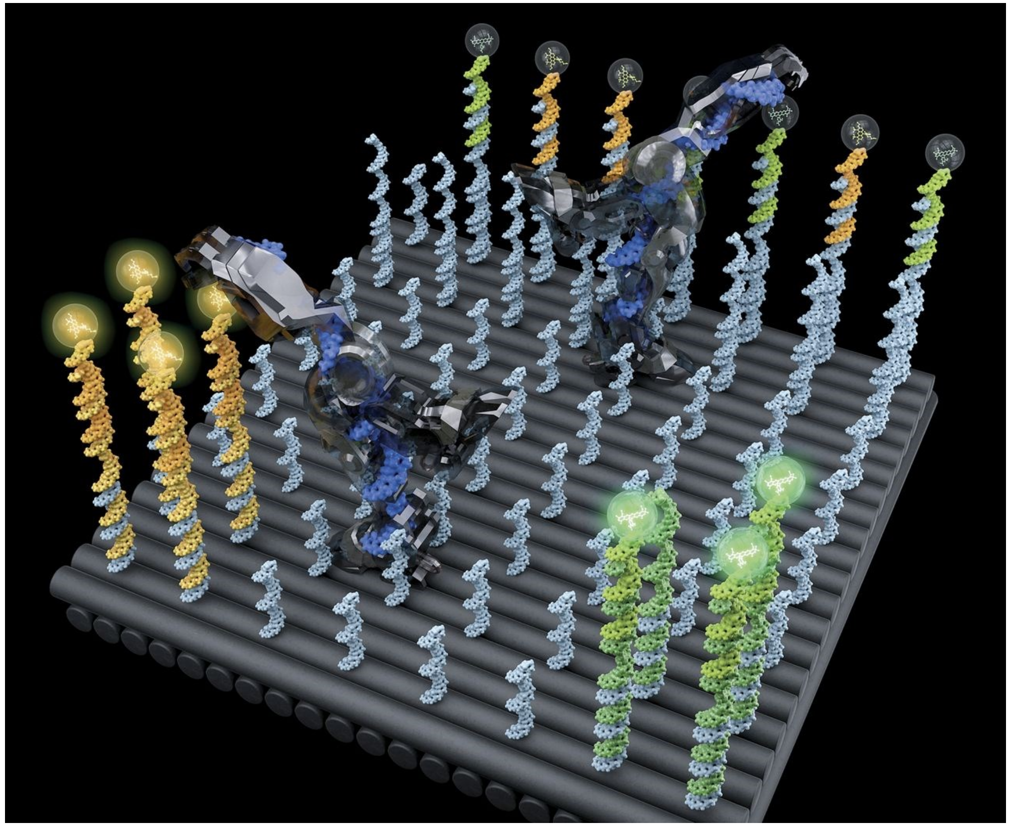


Motivation

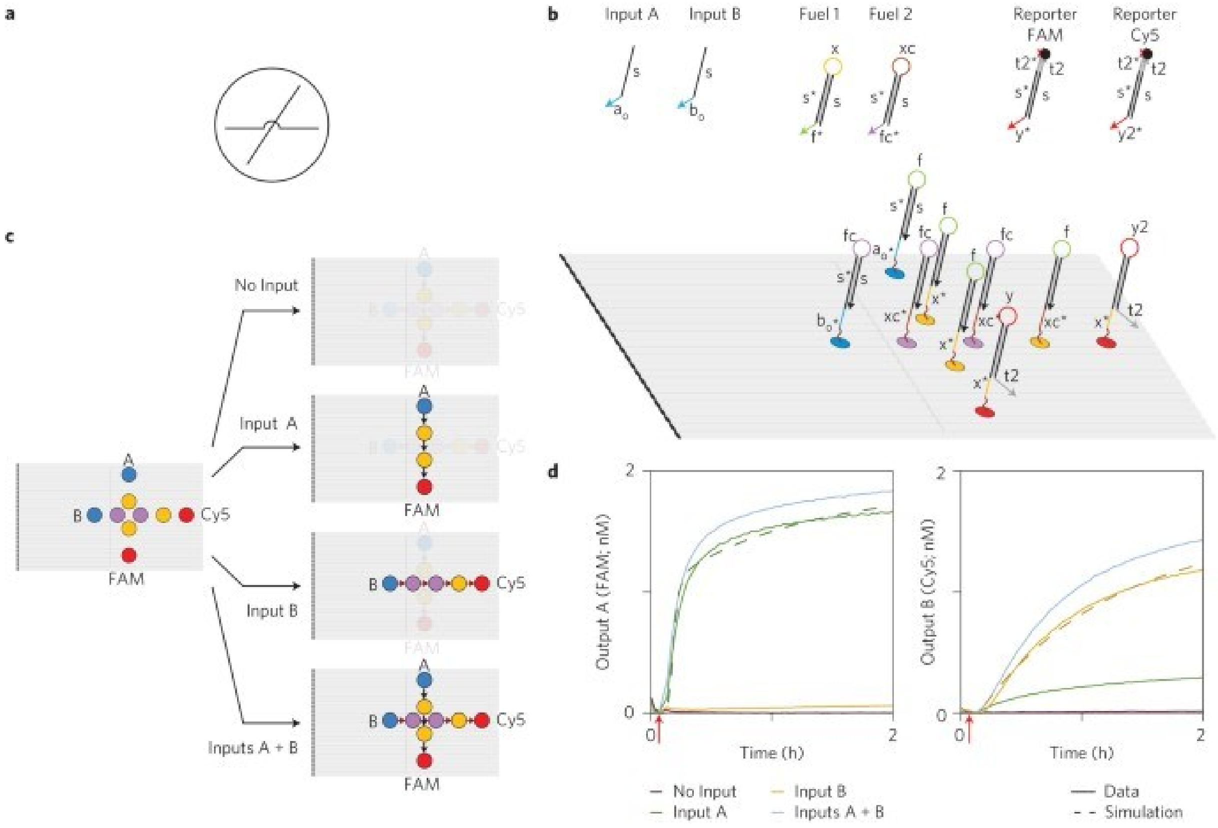
Motivation

- CRNs are practical but limited in computational power
  - Deterministically compute semi-linear functions
- sCRNs help overcome some of these limitations
  - Some geometry
- Burnout reflects how molecules may interact
  - Molecules with limited lifetimes
  - Reactions that consume large quantities of energy

Motivation



A. J. Thubagere, W. Li, R. F. Johnson, Z. Chen, S. Doroudi, Y. L. Lee, G. Izatt, S. Wittman, N. Srinivas, D. Woods, et al. **A cargo-sorting DNA robot**. Science, 357(6356):eaan6558, 2017.

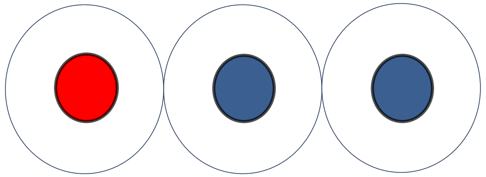


G. Chatterjee, N. Dalchau, R. A. Muscat, A. Phillips, and G. Seelig. **A spatially localized architecture for fast and modular DNA computing**. Nature nanotechnology, 12(9):920–927, 2017.

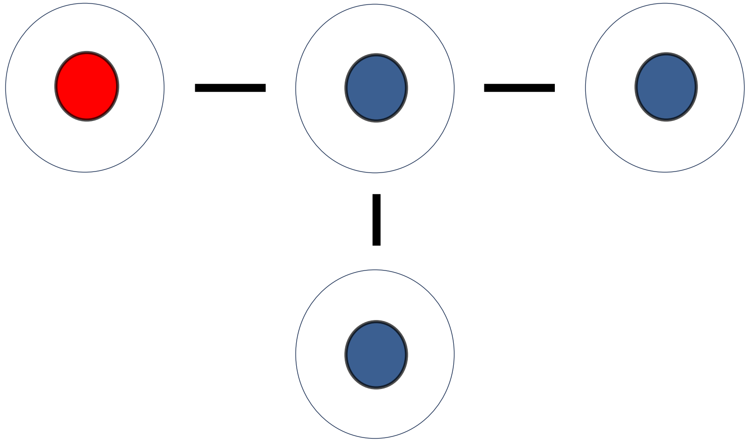
Previous work/Contributions

Results

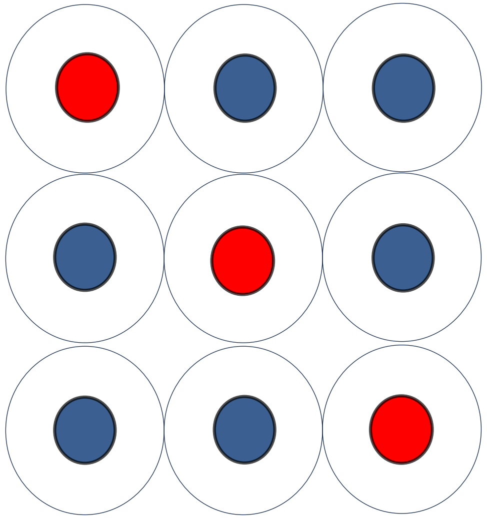
Linear Surfaces



General Surfaces



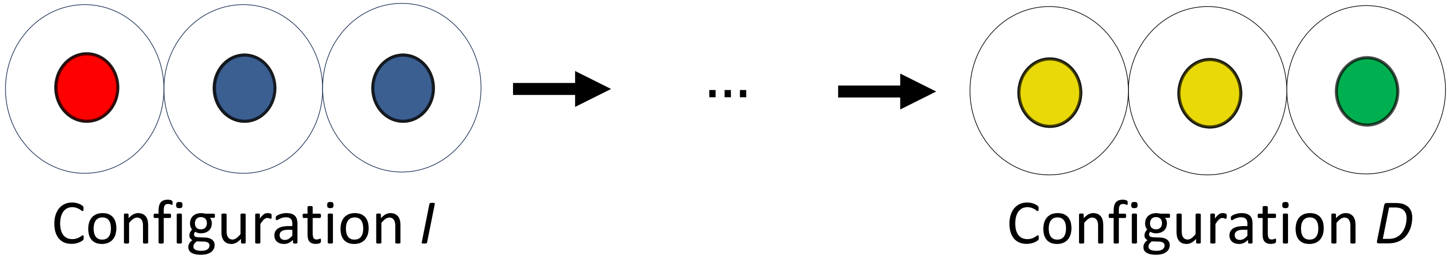
Grid Surfaces

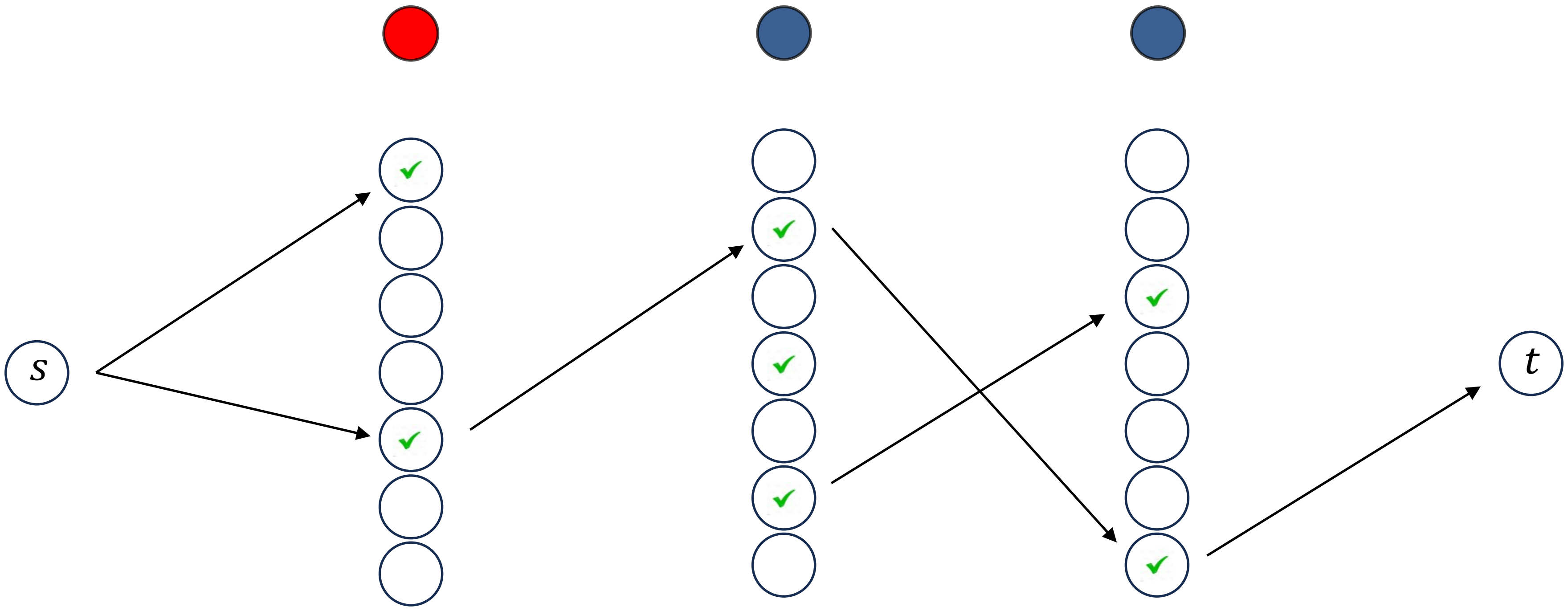


Linear Surfaces

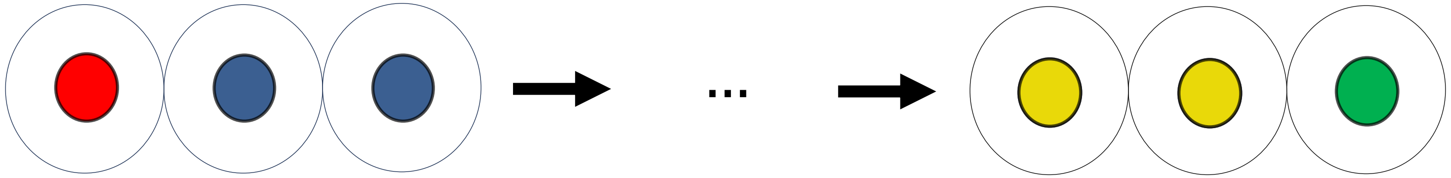
Problem	Burnout	Result
Reconfiguration	$\mathbf{1}$	$\boldsymbol{O(n + \lvert R \rvert)}$
Reconfiguration	$\mathbf{2}$	$\boldsymbol{O(n \cdot \lvert S \rvert^2 \cdot \lvert R \rvert^4)}$
Reconfiguration	$\boldsymbol{O(1)}$	**P**
Reconfiguration	$\boldsymbol{k\ (unary)}$	$\boldsymbol{NP - Complete}$
Reconfiguration	$None$	$PSPACE - Complete$

1-burnout





2-burnout

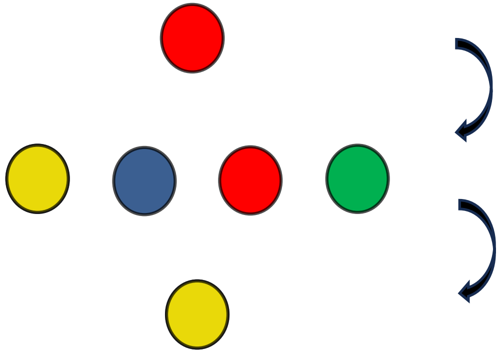


Configuration *I* → … → Configuration *D*

Initial:

Intermediate:

Target:



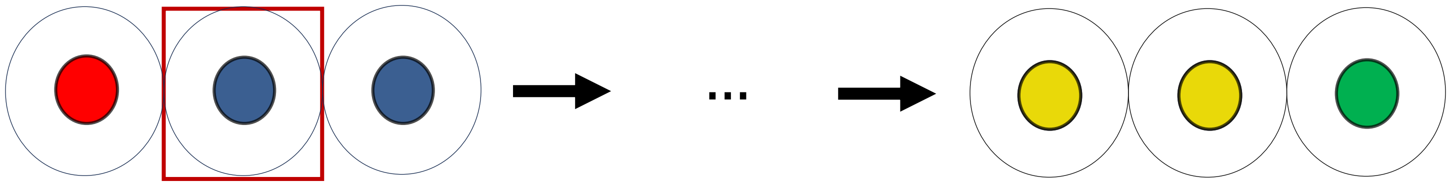
$O(|R|)$ different reactions

$O(|R|)$ different reactions

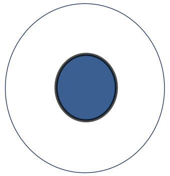
$\Rightarrow$ $O(|S| \cdot |R|^2)$ possibilities per vertex

Result: $O(n \cdot |S| \cdot |R|^2)$ cells and $O(|S| \cdot |R|^2)$ runtime per cell $= O(n \cdot |S|^2 \cdot |R|^4)$ runtime

O(1)-burnout

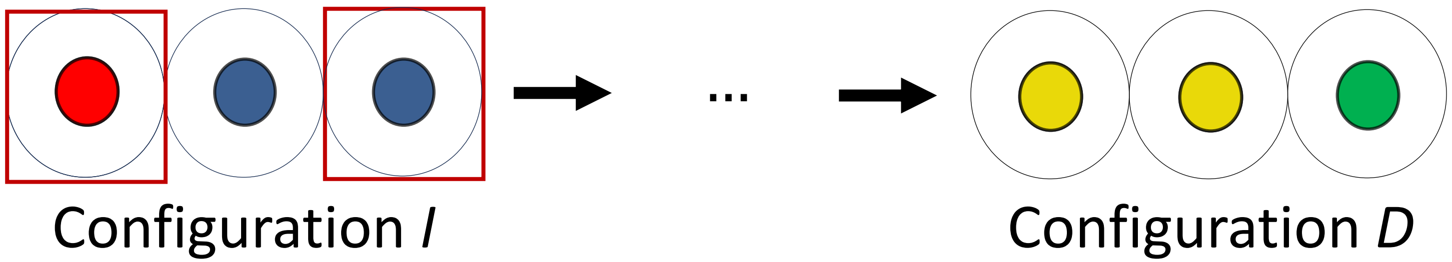


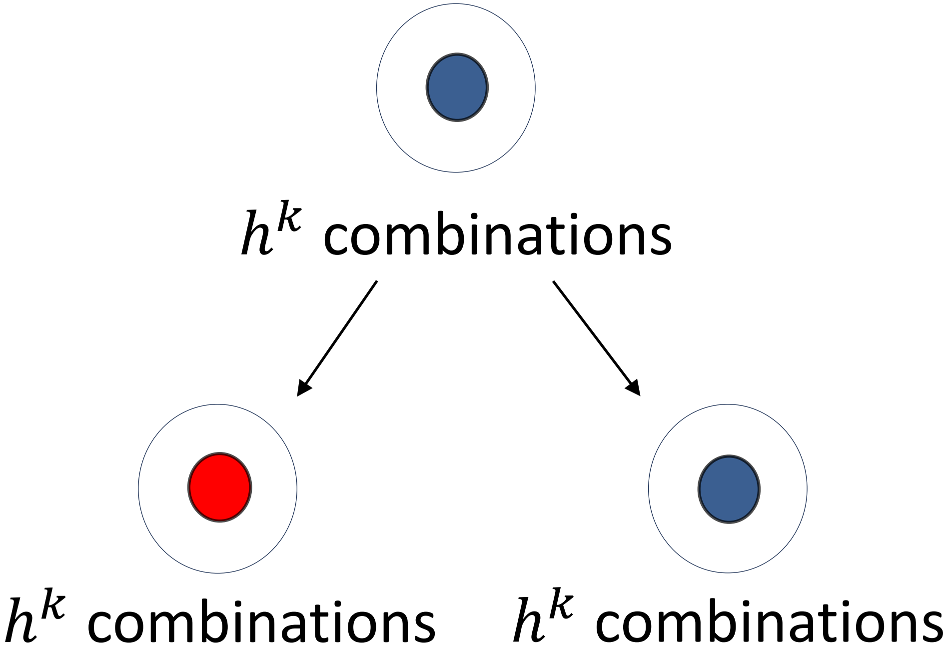
Configuration *I* Configuration *D*



h^k combinations

O(1)-burnout





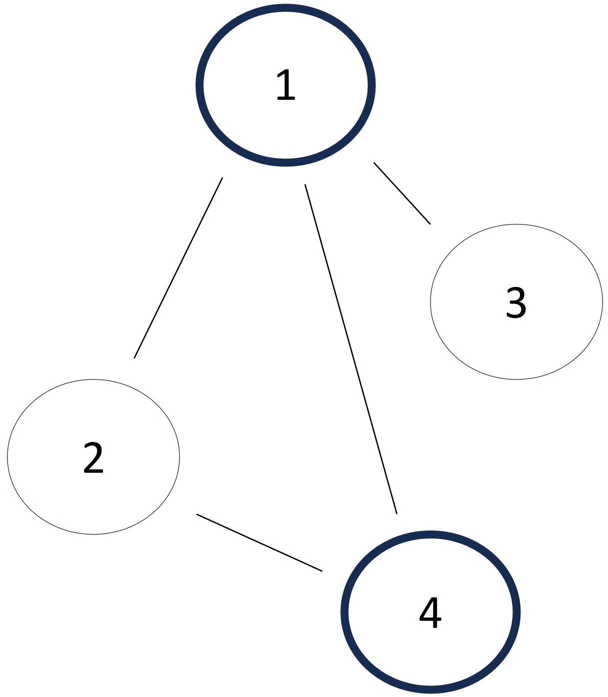
$\Rightarrow$

$$T(n) = h^k\left(2 \cdot T\left(\frac{n}{2}\right)\right)$$

Result: $O(h^{k*\log(n)} * n)$ runtime, or $O(n^{1+klog(h)})$

K-burnout

Vertex Cover:



$\Rightarrow$

$$BS_0 - 12 - 13 - 14 - 24 - E$$
$$\Downarrow$$
$$BS_0 - 1'x - 1'x - 1'x - x4' - E$$
$$\Downarrow$$
$$B - xx - xx - xx - x4' - S_1^1 E$$
$$\Downarrow$$
$$B - xx - xx - xx - x4' - S_1 E$$
$$\Downarrow$$
$$BS_2^4 - xx - xx - xx - xx - E$$
$$\Downarrow$$
$$BS_2 - xx - xx - xx - xx - E$$

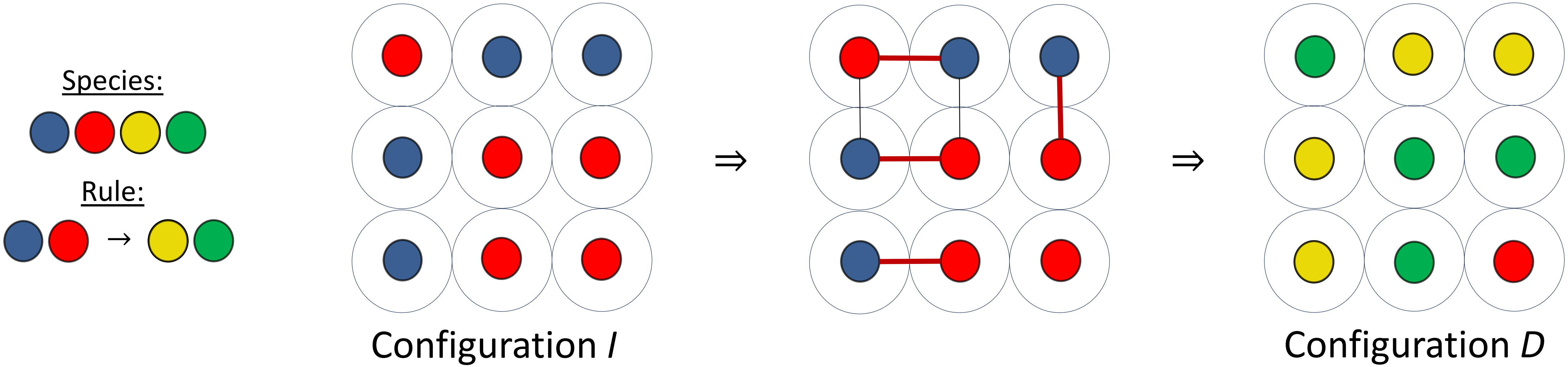
$\Rightarrow$ Vertex Cover of size k with $k+1$ burnout

General Surfaces

Problem	Burnout	Result
Reconfiguration	**1**	$\boldsymbol{O\left(V^{1.5} + \lvert R \rvert\right)^{*}}$
Reconfiguration	**1**	$\boldsymbol{NP - Complete}$
Reconfiguration	2	$NP - Complete$

* Non-catalytic reactions

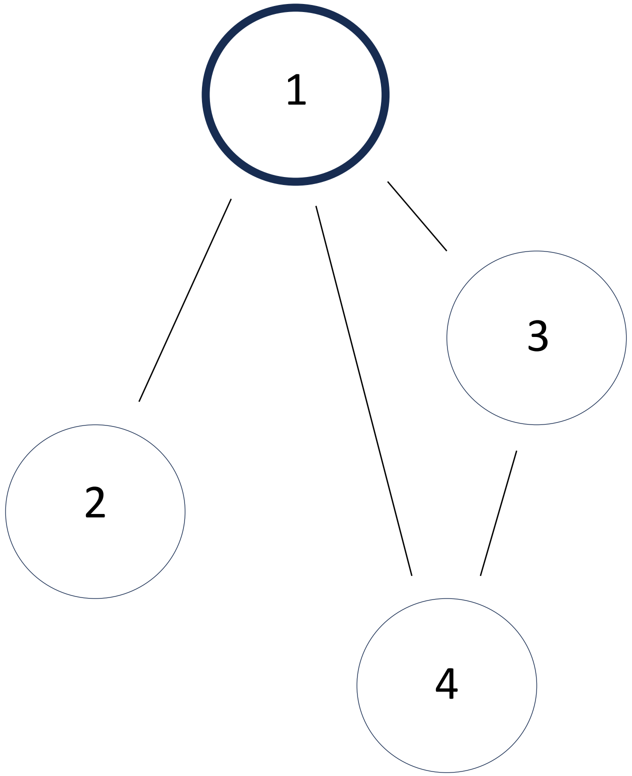
1-burnout (Non-catalytic rules only)



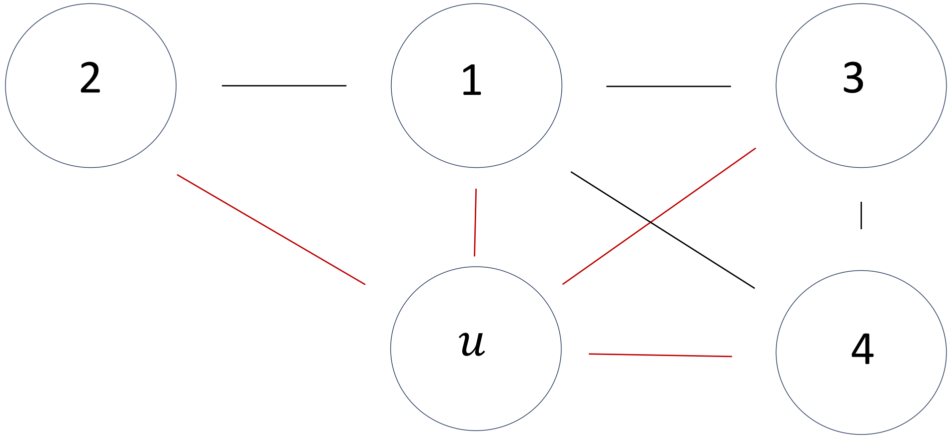
Planar: $O(V^{1.5} + |R|)$
General: $O(V^4 + |R|)$

1-burnout (No restriction on rules)

Dominating Set:



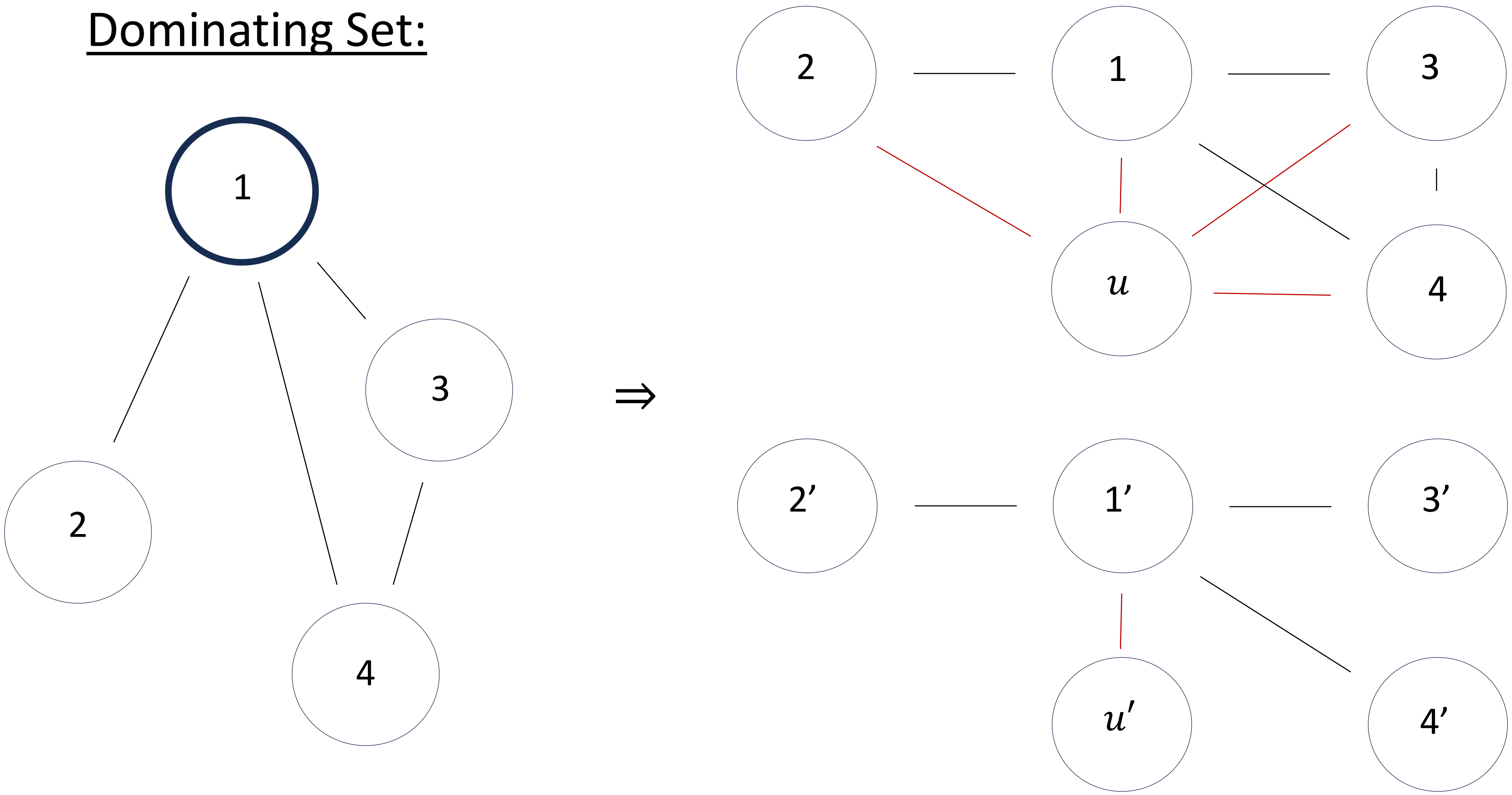
$\Rightarrow$



$$1 + 2 \to 1' + 2 \qquad u + 1 \to u' + 1'$$
$$1 + 2 \to 1 + 2' \qquad u + 2 \to u' + 2'$$

1-burnout (No restriction on rules)

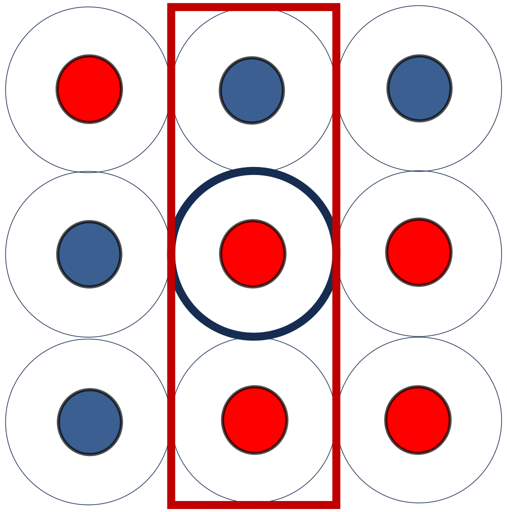
<u>Dominating Set:</u>



Grid Surfaces

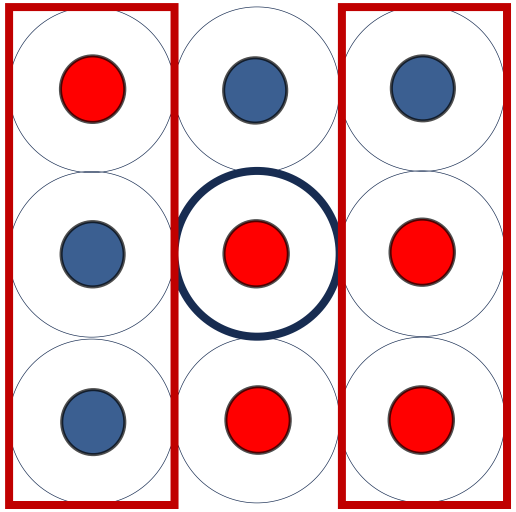
Problem	Burnout	Result
1-Reconfiguration	**1**	$\boldsymbol{O(n \cdot (\lvert S \rvert \lvert R \rvert)^{2m} \cdot f(m))}$
1-Reconfiguration	1	$NP - Complete$

1-burnout (1-reconfiguration)



$O(|S|^m * (4|R|)^m * m!)$ cells

⇒



⇒

$O(|S|^m * (4|R|)^m * m!)$
runtime per cell

Result: $O\left(n \cdot (|S||R|)^{2m} \cdot f(m)\right)$

Conclusion

Known + New Results

Linear Surfaces

Problem	Burnout	Result
Reconfiguration	**1**	$\boldsymbol{O(n + \lvert R\rvert)}$
Reconfiguration	**2**	$\boldsymbol{O(n \cdot \lvert S\rvert^2 \cdot \lvert R\rvert^4)}$
Reconfiguration	$\boldsymbol{O(1)}$	**P**
Reconfiguration	$\boldsymbol{k\ (unary)}$	$\boldsymbol{NP - Complete}$
Reconfiguration	$None$	$PSPACE - Complete$

General Surfaces

Problem	Burnout	Result
Reconfiguration	**1**	$\boldsymbol{O\left(V^{1.5} + \lvert R\rvert\right)^*}$
Reconfiguration	**1**	$\boldsymbol{NP - Complete}$
Reconfiguration	2	$NP - Complete$

* Non-catalytic reactions

Grid Surfaces

Problem	Burnout	Result
1-Reconfiguration	**1**	$\boldsymbol{O(n \cdot (\lvert S\rvert\lvert R\rvert)^{2m} \cdot f(m))}$
1-Reconfiguration	1	$NP - Complete$

Open Problems

- Lower bounds for k-burnout on linear surfaces
- Other than size of surface, what about:
  - Species, rules and burnout
- Any FPT algorithms for reconfiguration

Known + New Results

Linear Surfaces

Problem	Burnout	Result
Reconfiguration	**1**	$\boldsymbol{O(n + \|R\|)}$
Reconfiguration	**2**	$\boldsymbol{O(n \cdot \|S\|^2 \cdot \|R\|^4)}$
Reconfiguration	$\boldsymbol{O(1)}$	**P**
Reconfiguration	$\boldsymbol{k\ (unary)}$	$\boldsymbol{NP - Complete}$
Reconfiguration	$None$	$PSPACE - Complete$

General Surfaces

Problem	Burnout	Result
Reconfiguration	**1**	$\boldsymbol{O(V^{1.5} + \|R\|)}^*$
Reconfiguration	**1**	$\boldsymbol{NP - Complete}$
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* Non-catalytic reactions

Grid Surfaces

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1-Reconfiguration	**1**	$\boldsymbol{O(n \cdot (\|S\|\|R\|)^{2m} \cdot f(m))}$
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