Molecular Computation
An Algorithmic Approach

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Joint work with
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James Aspnes (Yale), Milan Vojnovic (MSR), Ron Rivest (MIT)

Distributed Systems

Ingredients:

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- Nodes

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- Communication

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- Computation

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Population Protocols [AADFP'04]

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  - The system ***should converge*** to configurations satisfying meaningful predicates
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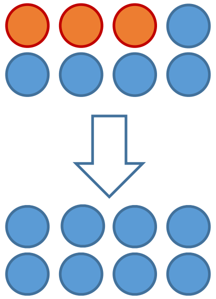

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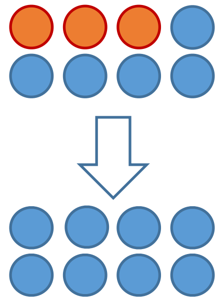
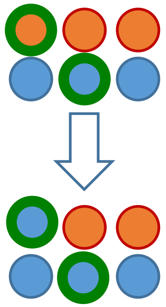
- A.k.a. Chemical Reaction Networks



Complexity

1. Time

- **Round** = a ***single pair*** interacts
  - Chosen uniformly at random
- **Parallel convergence time**
  - **#rounds** to convergence / **# nodes**
  - Alternative continuous-time definition exists



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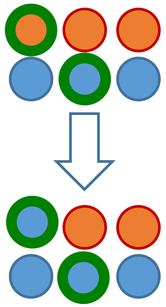

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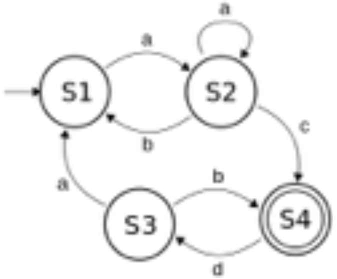
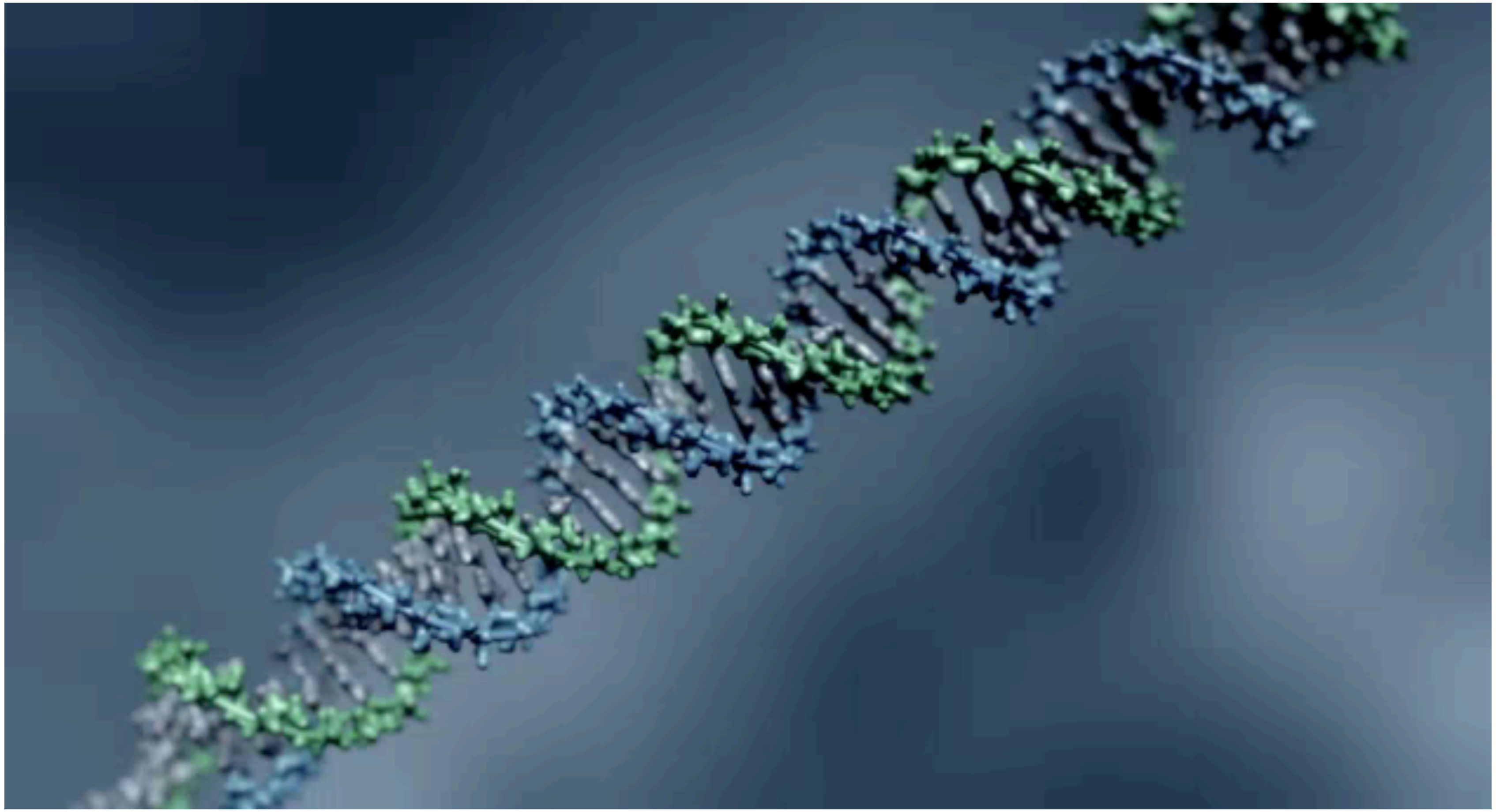
2. Space



- Number of ***distinct states*** per automaton
- Alternatively, #**memory bits** to encode state

More Precisely: Communication



Courtesy of the Microsoft Research Biological Computation Group

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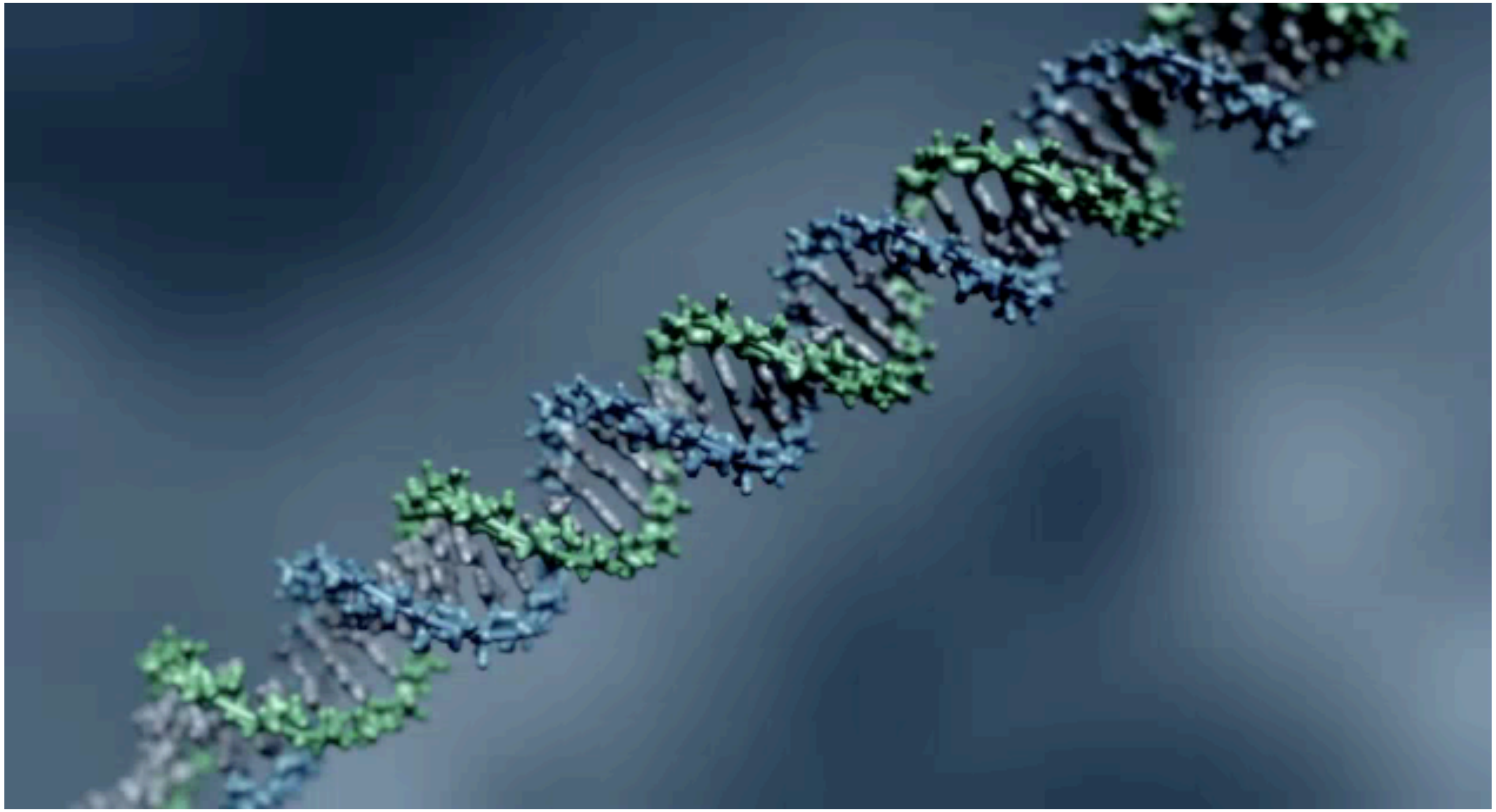

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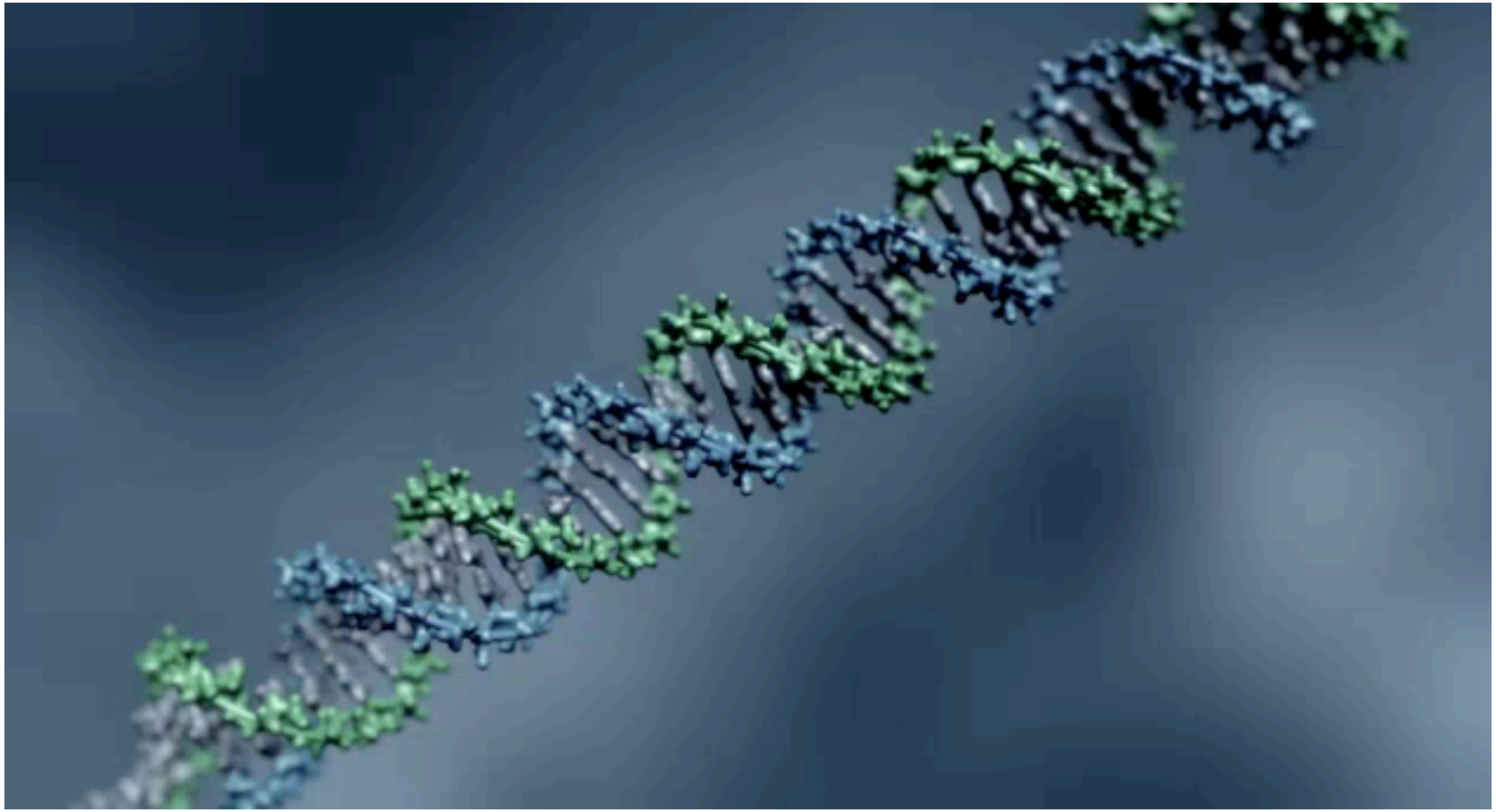

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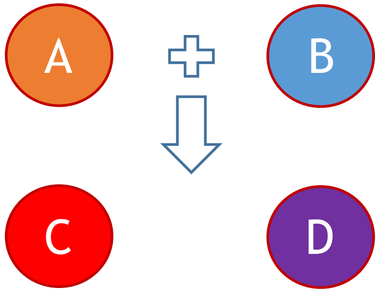
What can we compute?

We can perform interactions of the type:



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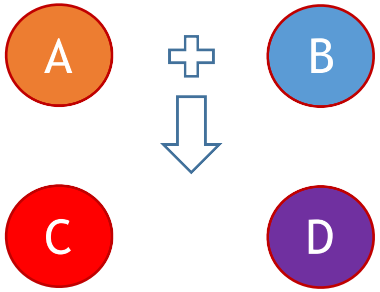

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- **Initial** states: 0 or 1
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  - If there exists a 1, then all 1.
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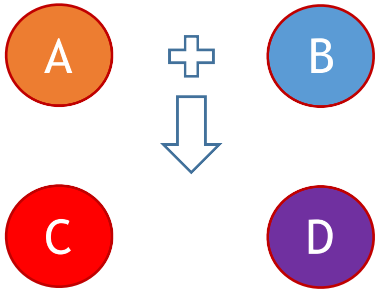

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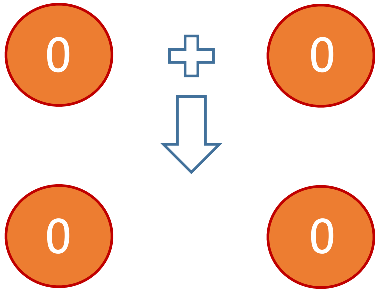

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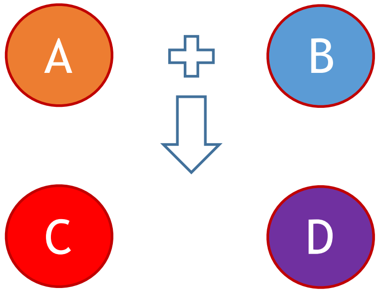

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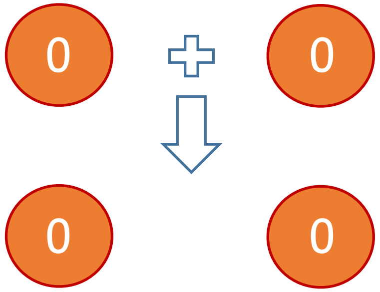

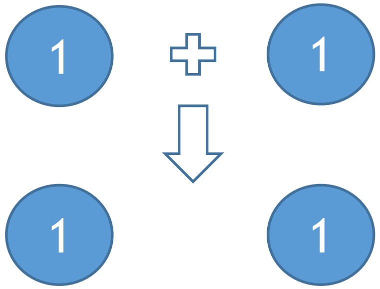

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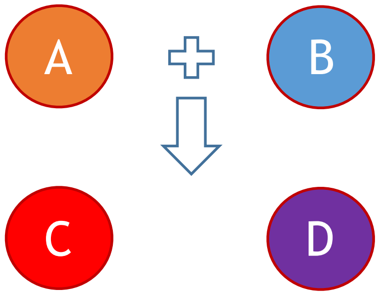

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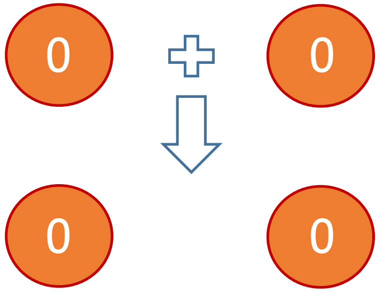

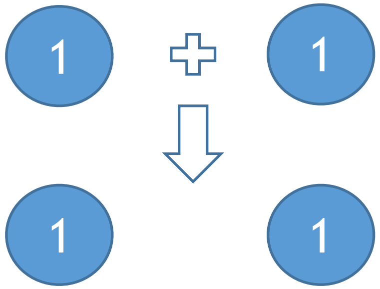

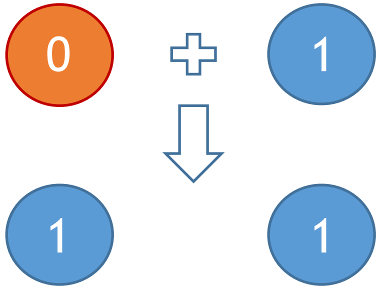

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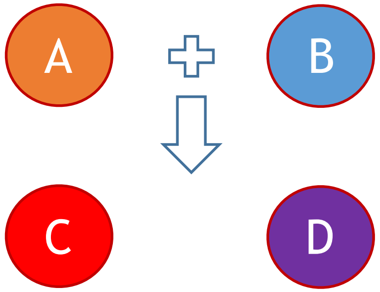

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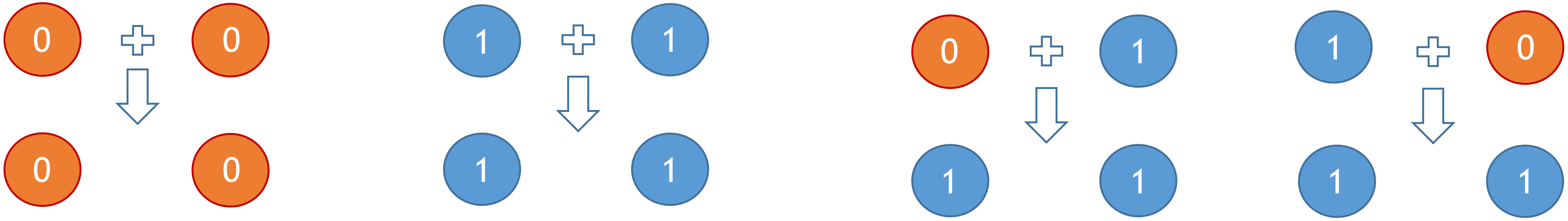

The Majority Function

Majority ("Consensus")

- **Initial** states A, B
- **Output**:
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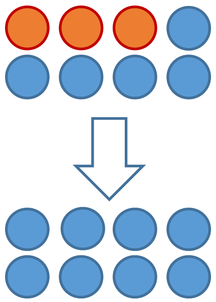

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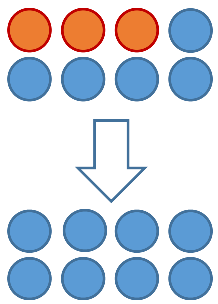
- **Fundamental task**
  - **Complexity**: [AAE08] & [DV12]; [PVV09] & [MNRS14]
  - Natural computation:
    the cell cycle switch implements approximate majority [CC12]
  - Implementation in DNA: [CDS+13, Nature Nanotechnology]



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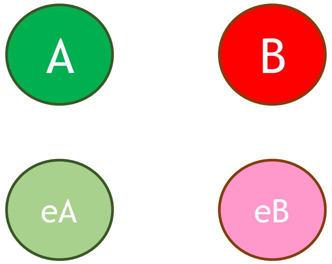

4-State Exact Majority [PVV09] [MNRS14]

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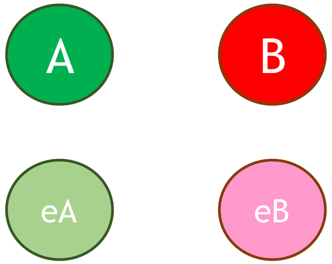

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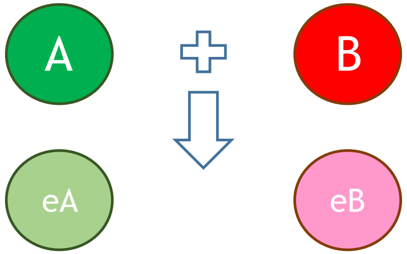

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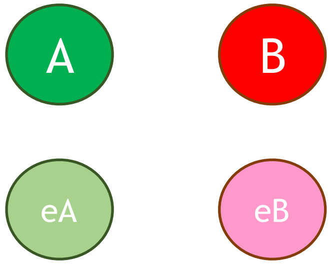

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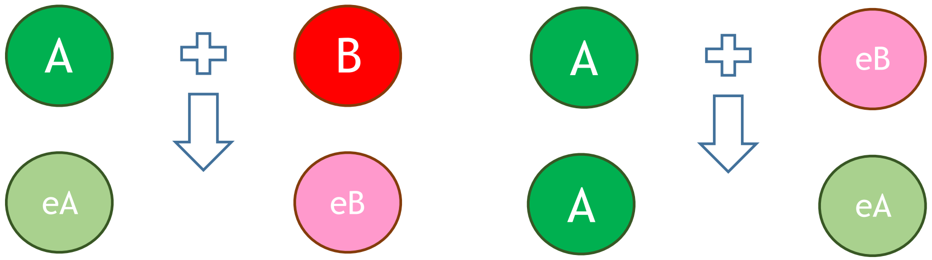

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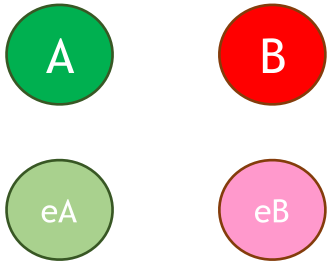

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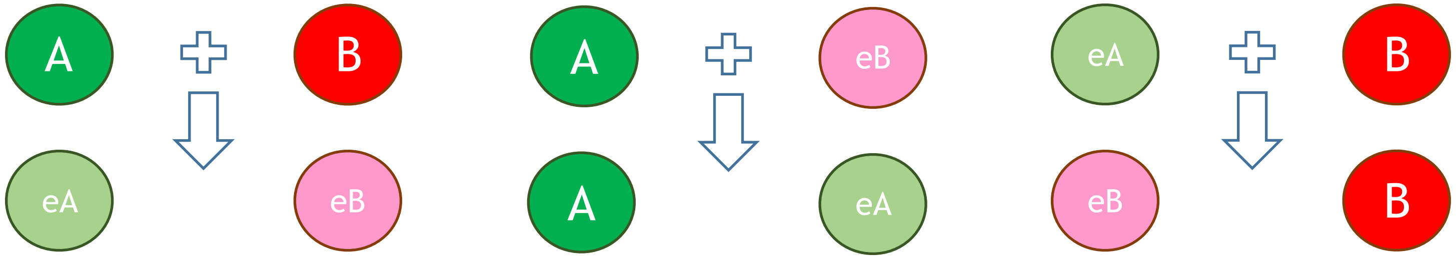

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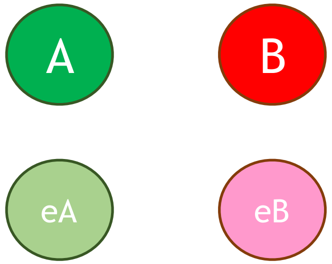

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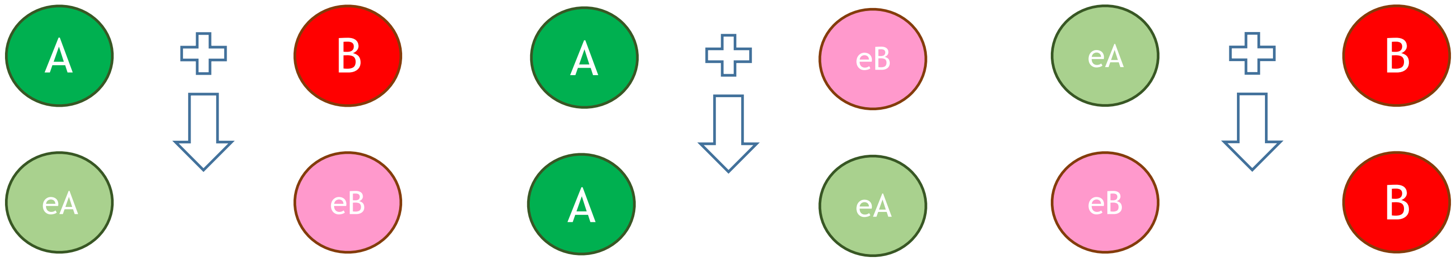

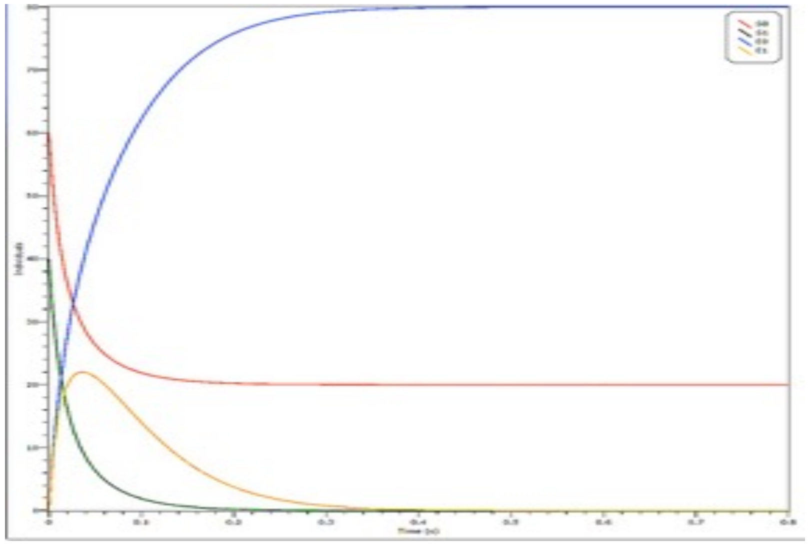

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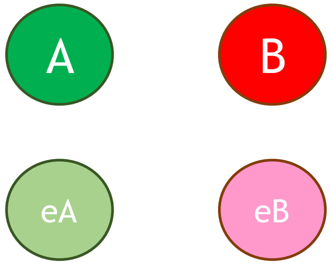

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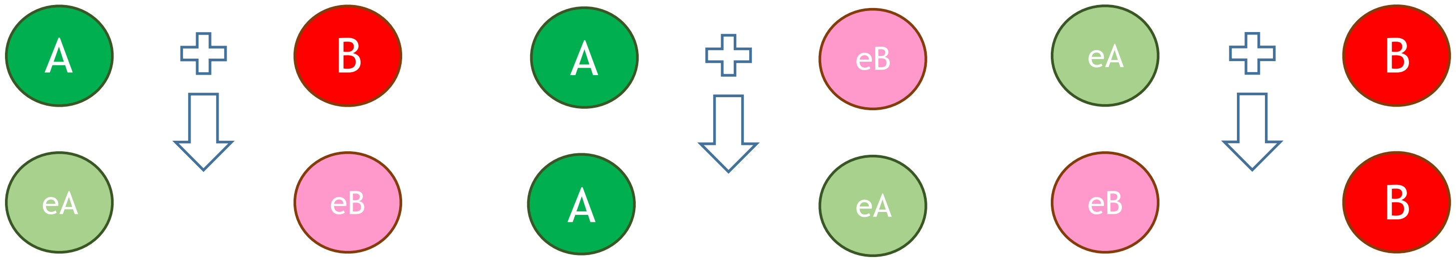

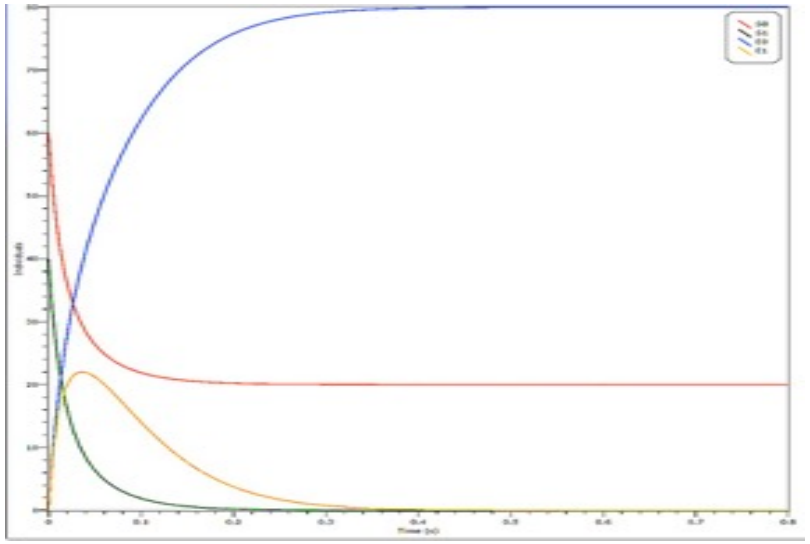

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Can be as small as
$\varepsilon = O(1 / n)$.

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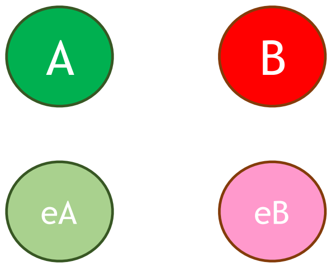

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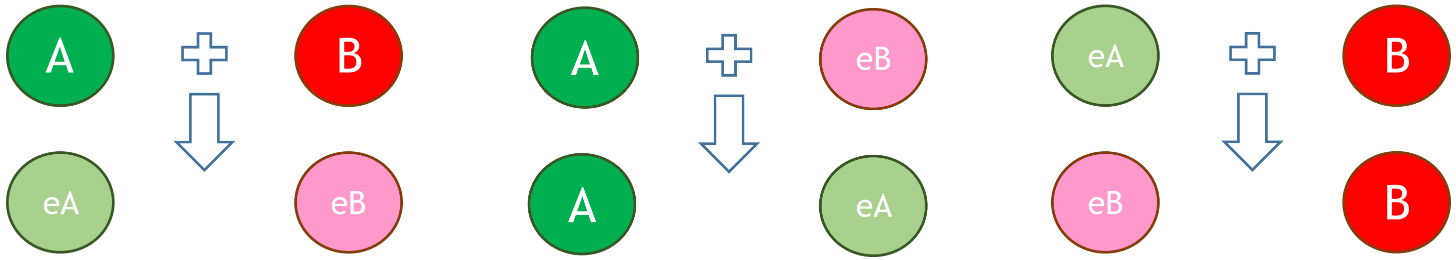

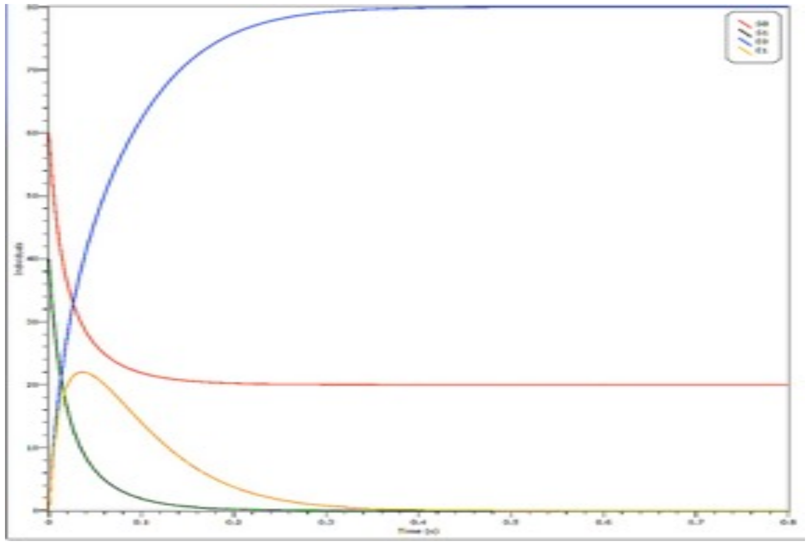

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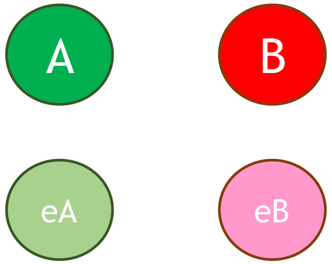

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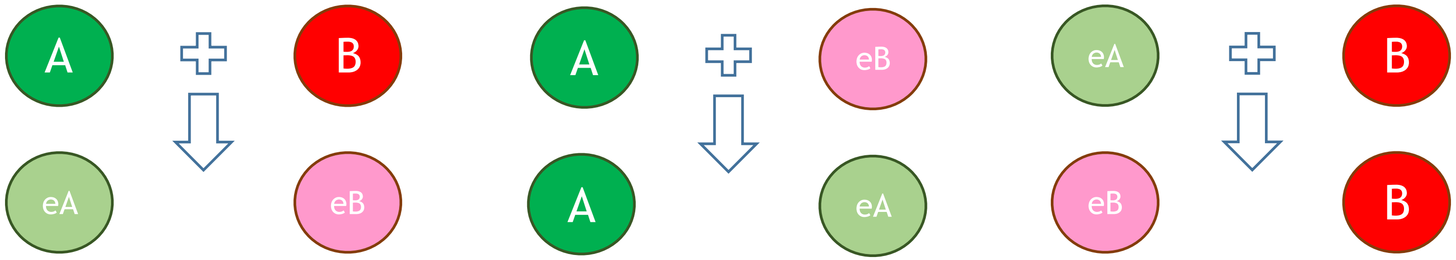

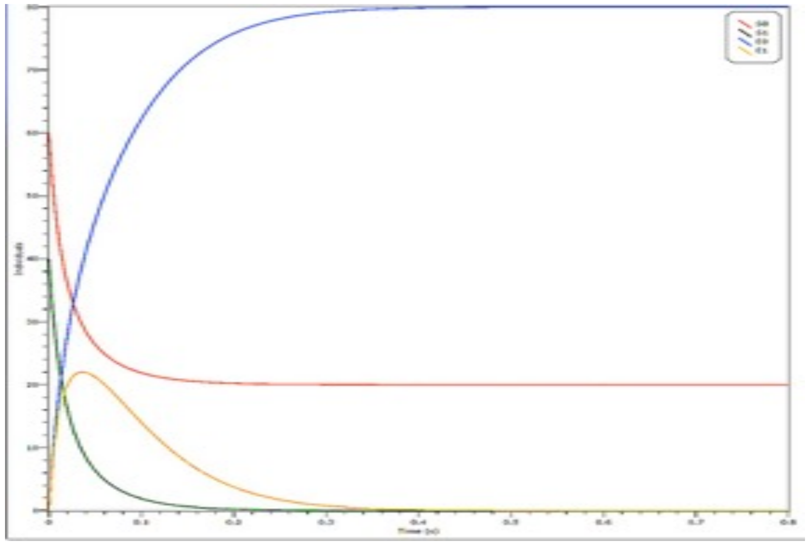

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Can be $\Theta(n \log n)$ if ε = constant / n.

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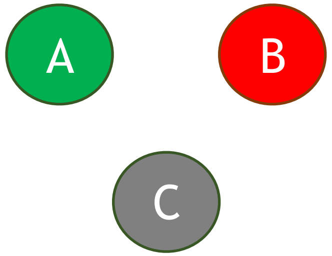

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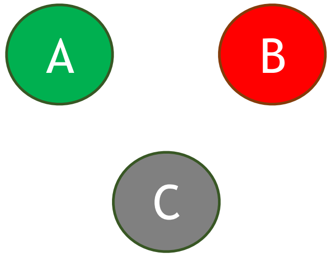

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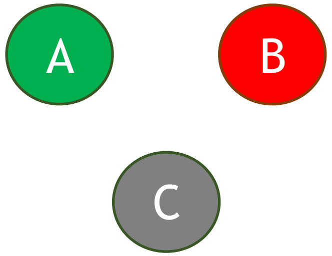

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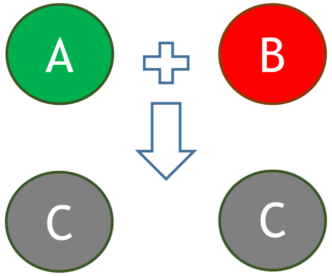

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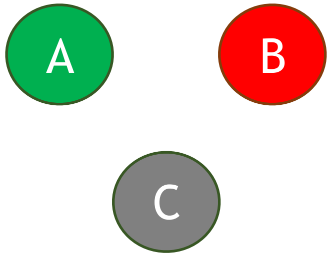

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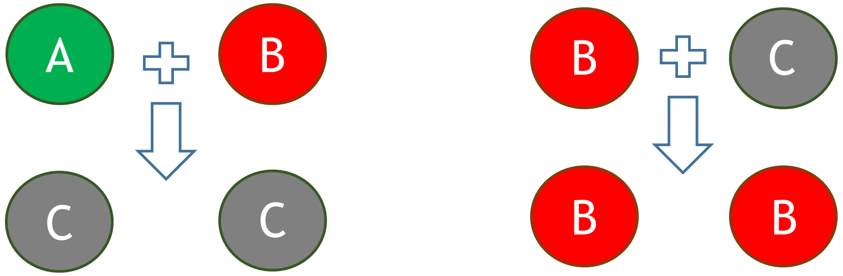

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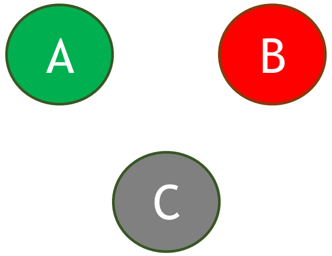

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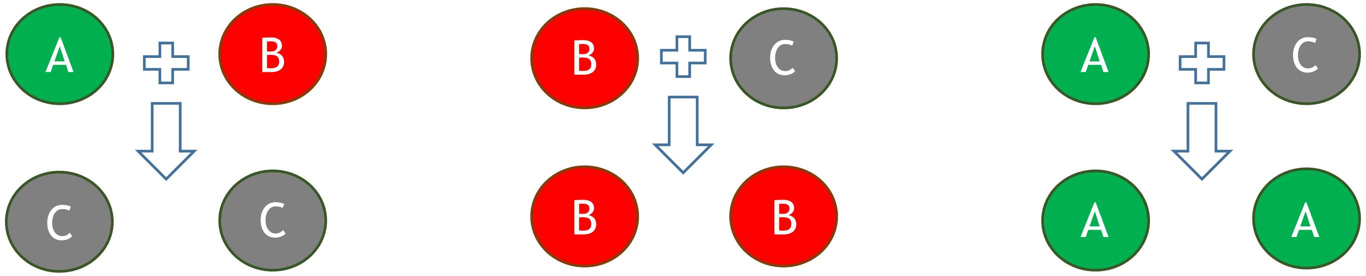

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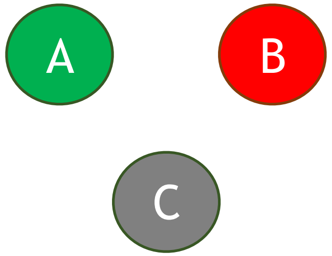

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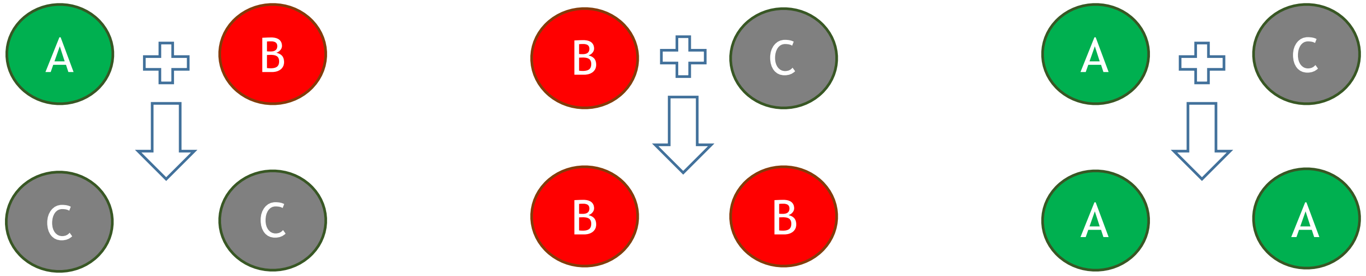

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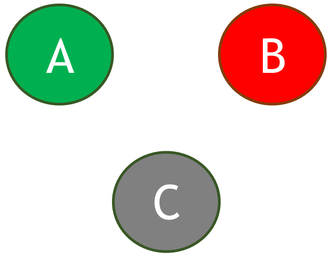

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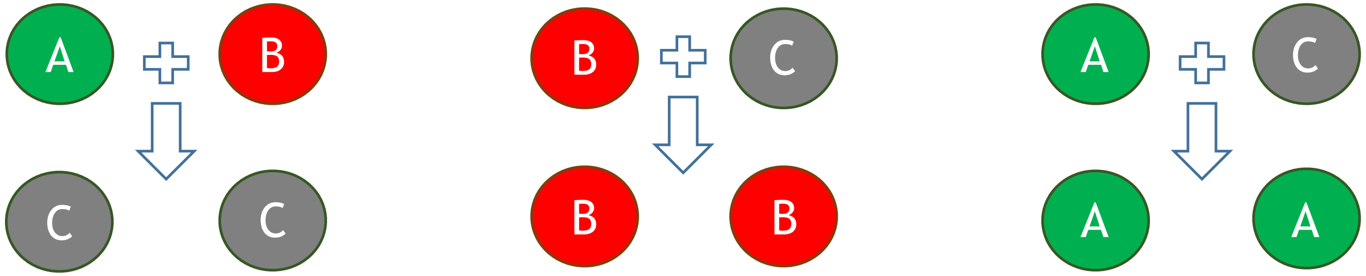

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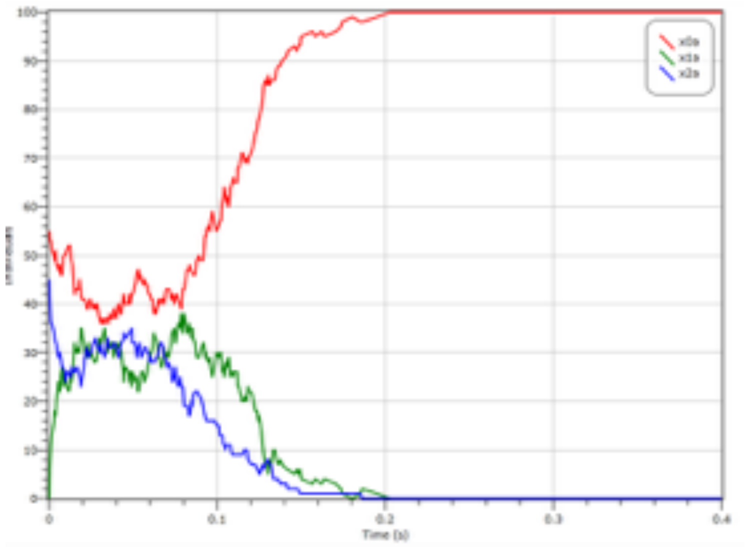

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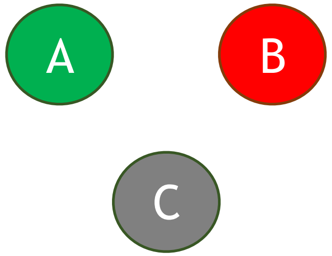

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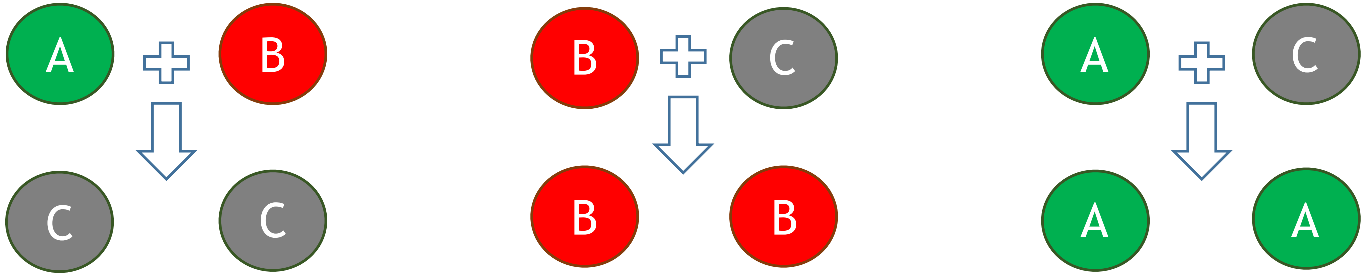

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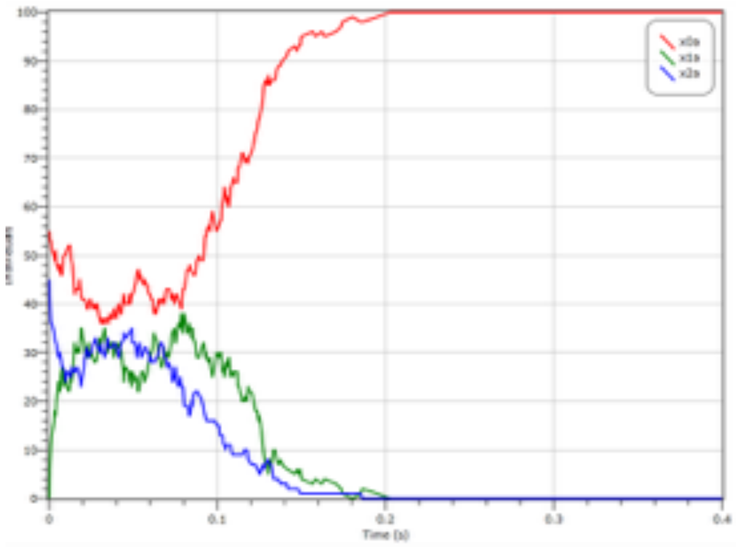
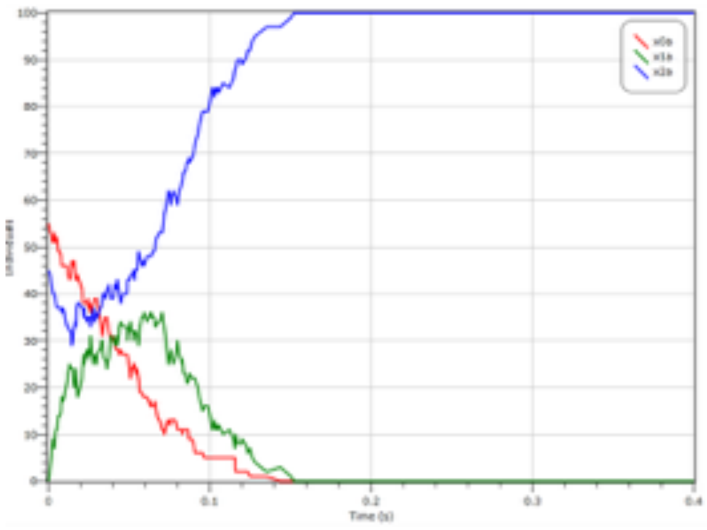
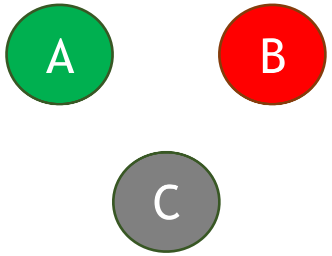




Solving Majority *Approximately*



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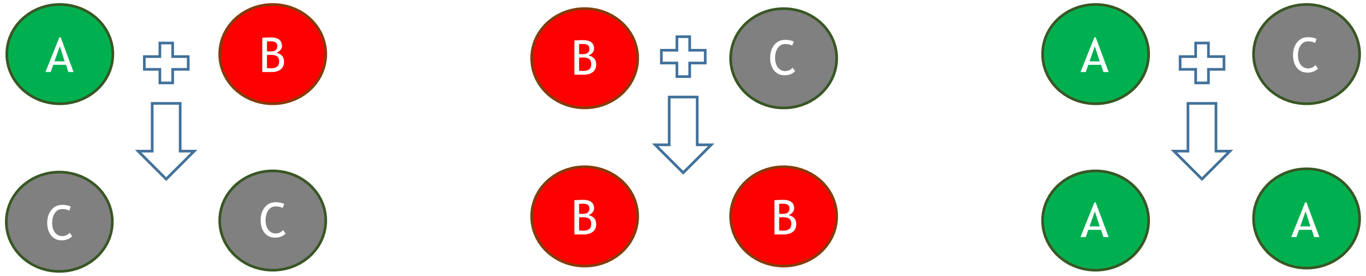

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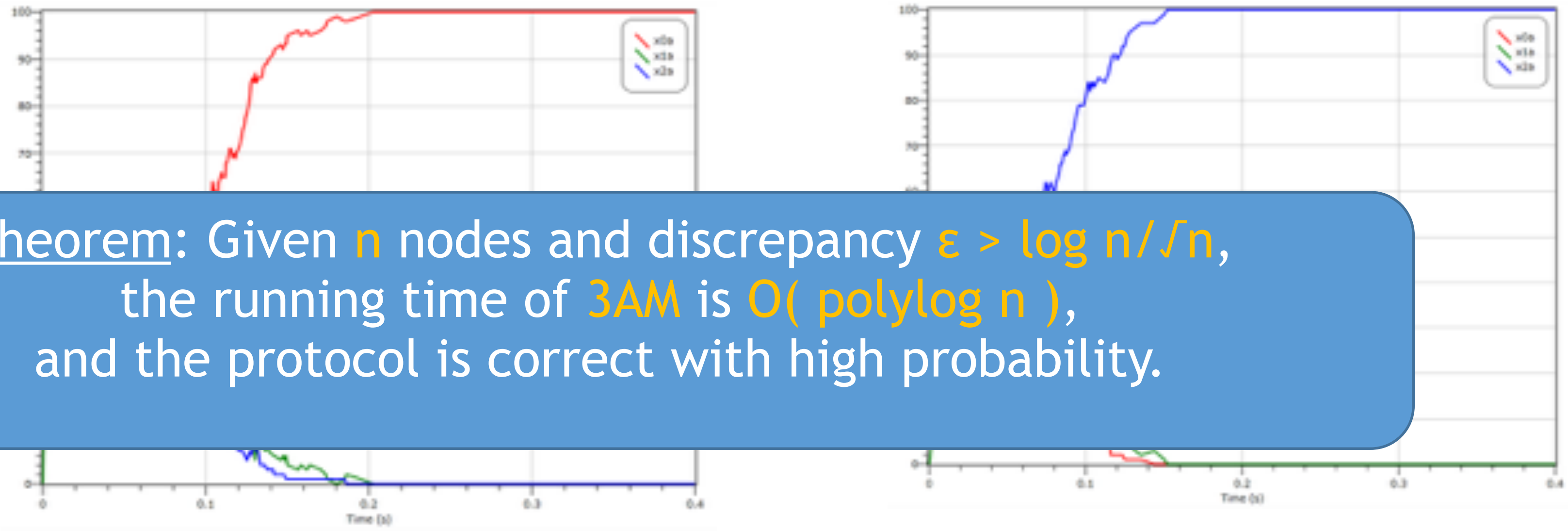

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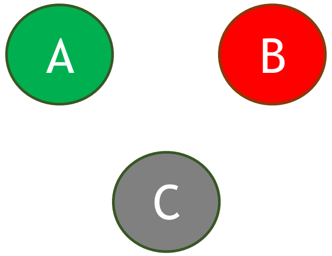

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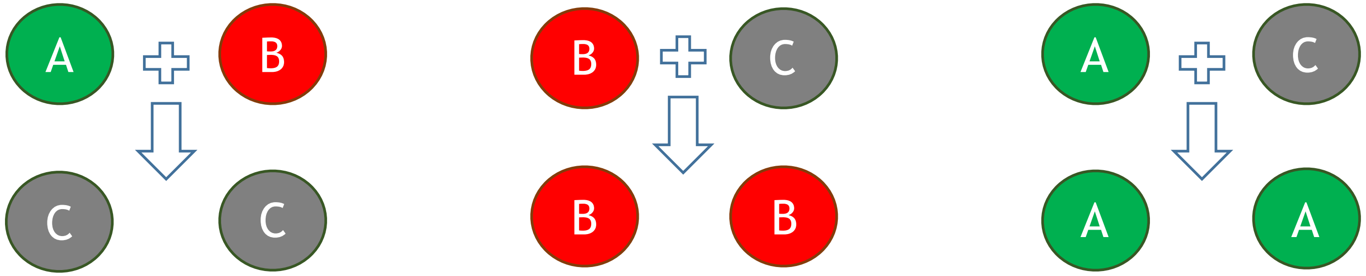

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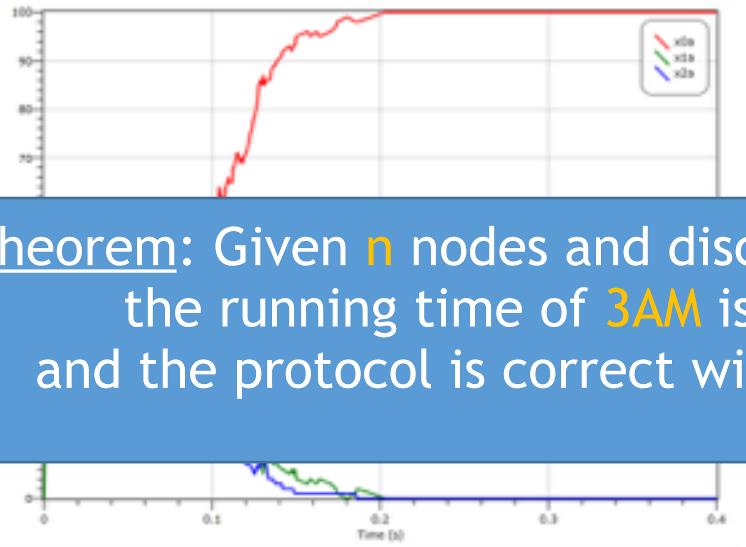

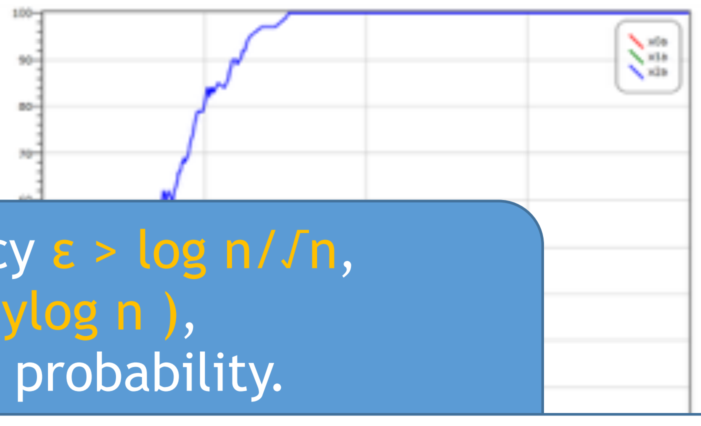

<u>Theorem</u>: Given n nodes and discrepancy $\varepsilon > \log n/\sqrt{n}$,
the running time of 3AM is $O(\text{polylog } n)$,
and the protocol is correct with high probability.

Error probability can be as high as ***constant*** for lower discrepancy.

The Status

Algorithm	Reliability	Speed
The Four-State Protocol	Exact	Slow (super-linear)
The Three-State Protocol	Flaky (Up to Constant Error)	Fast (poly-logarithmic)

Average&Conquer

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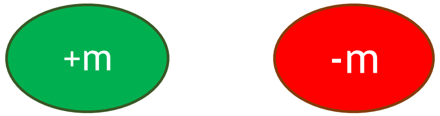
Average&Conquer [PODC 2015] (Super-Constant State Space)	Exact	Fast (poly-logarithmic)

The Plan

- Population Protocols
- The Majority Problem
  - 4EM
  - 3AM
  - Average-and-Conquer (AVC)
  - Quantized AVC
- Impossibility Results
- Open Questions
- Leader Election Problem

Simplified AVC: Main Ideas

- Each **state** corresponds to a **value ("confidence level")**
  - **Strong states (non-negative value):**
    - **Positive -> A**
    - **Negative -> B**
  - **Weak: value +/- 0**
- All nodes start with absolute value **m > 0**
  - **+m** if **A**
  - **-m** if **B**



- Two interaction types:
  - **Averaging**: strong (non-zero) nodes average out their values
  - **Conquer**: strong (non-zero) nodes bring weak nodes to "their side"
- Output:
  - If **positive** or **+0**, then **A**
  - If **negative** or **-0**, then **B**

AVC in Action

Initially: **+m** or **-m**, **odd** integers
Strong states: non-zero absolute value.
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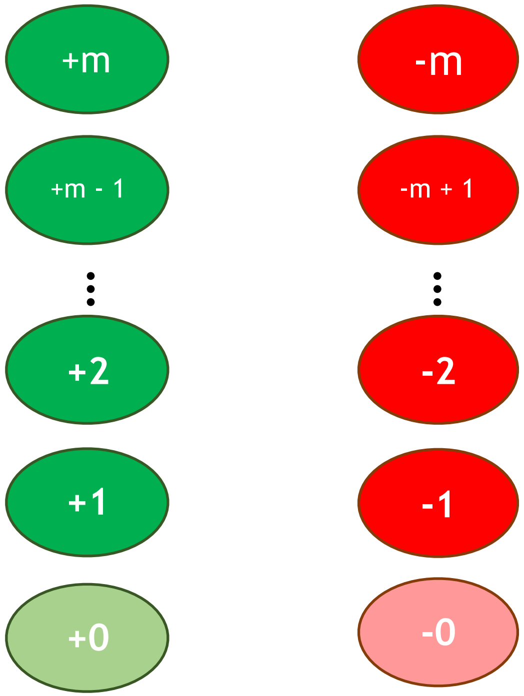

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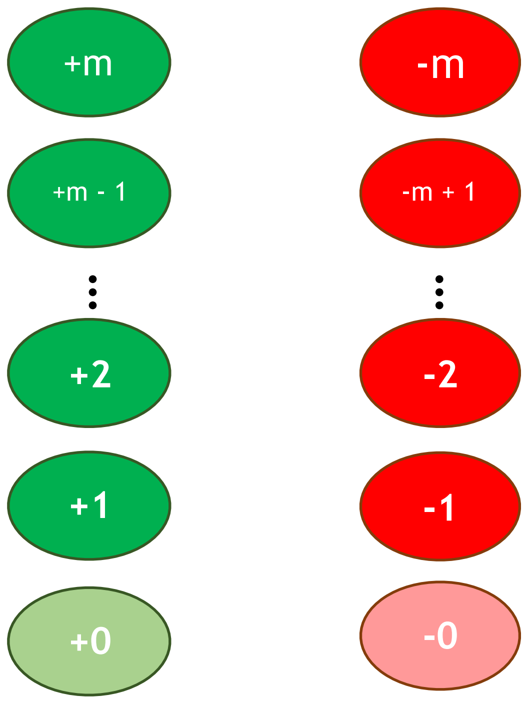

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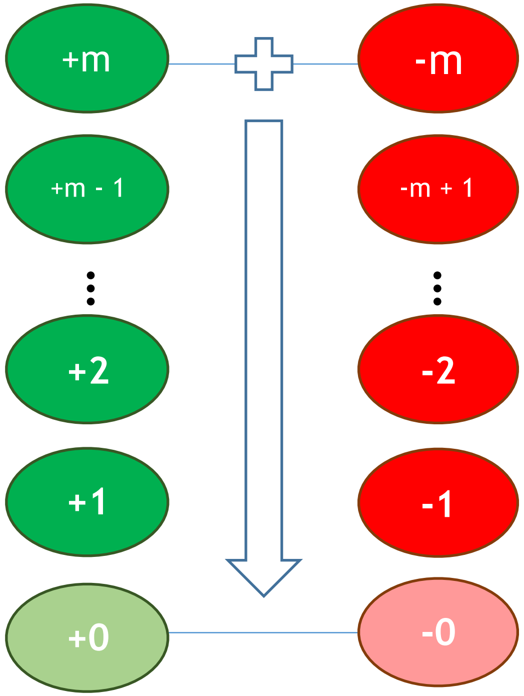

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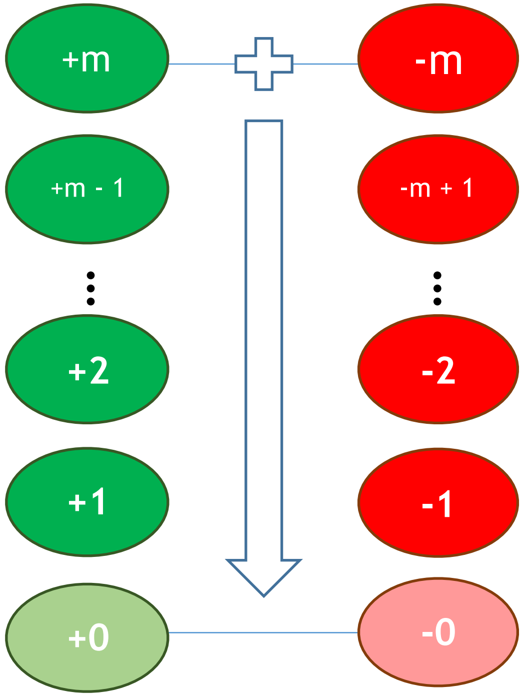

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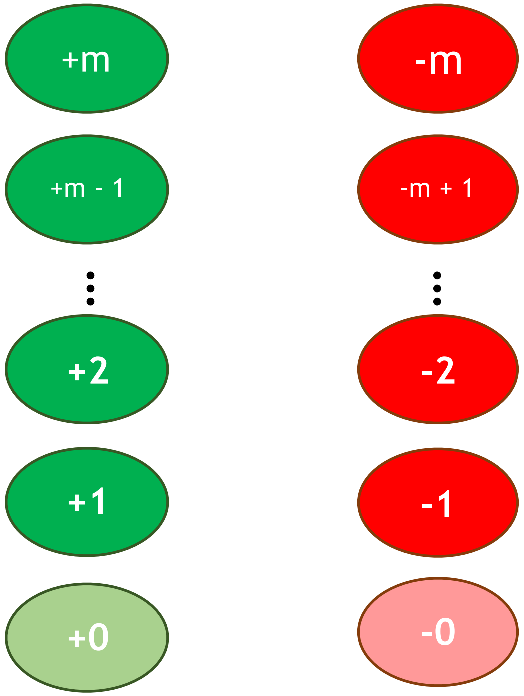

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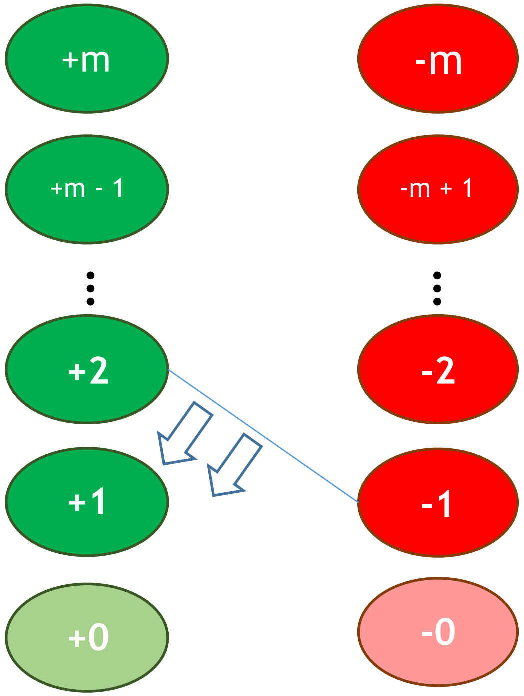

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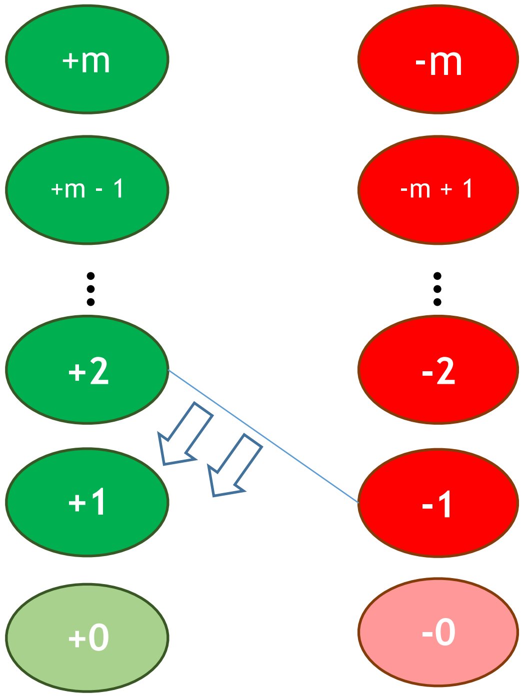

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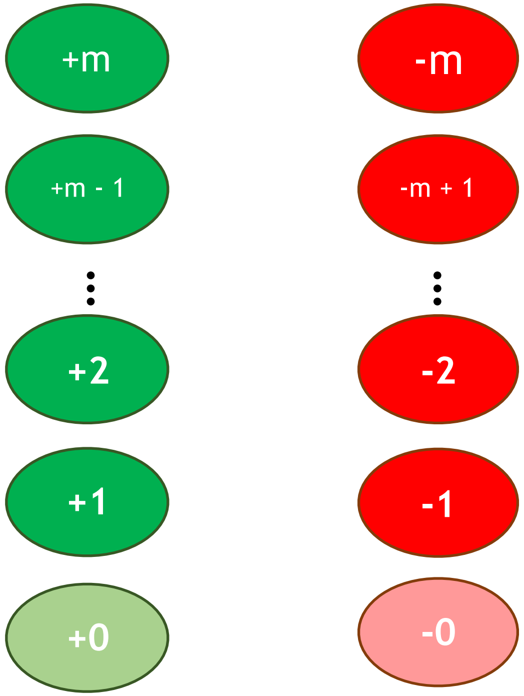

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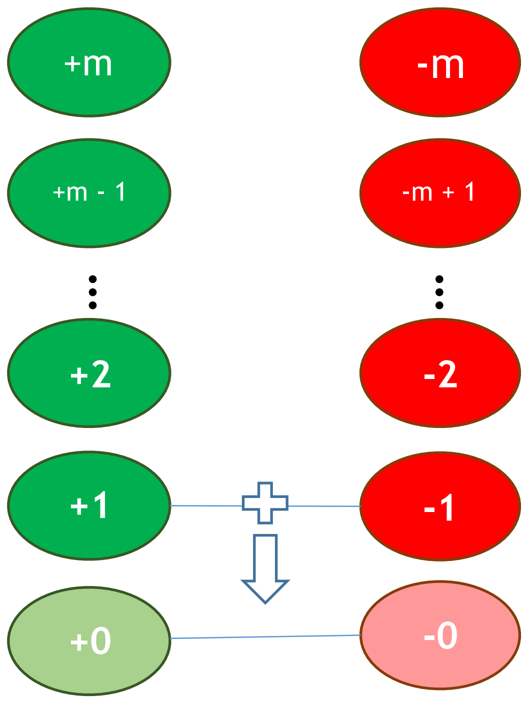

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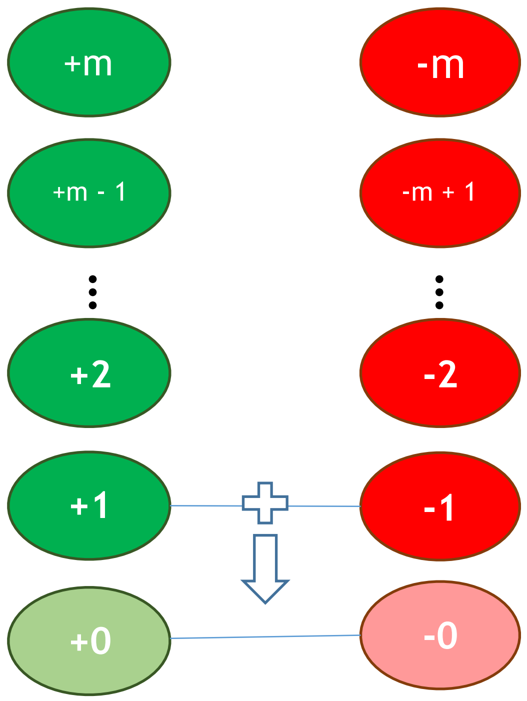

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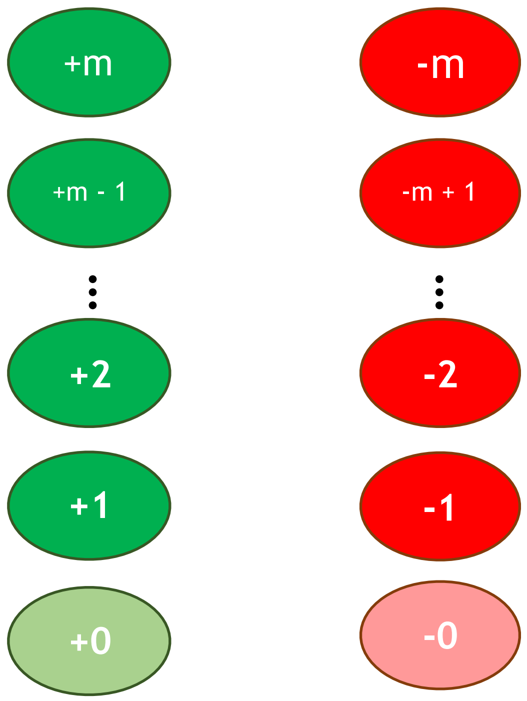

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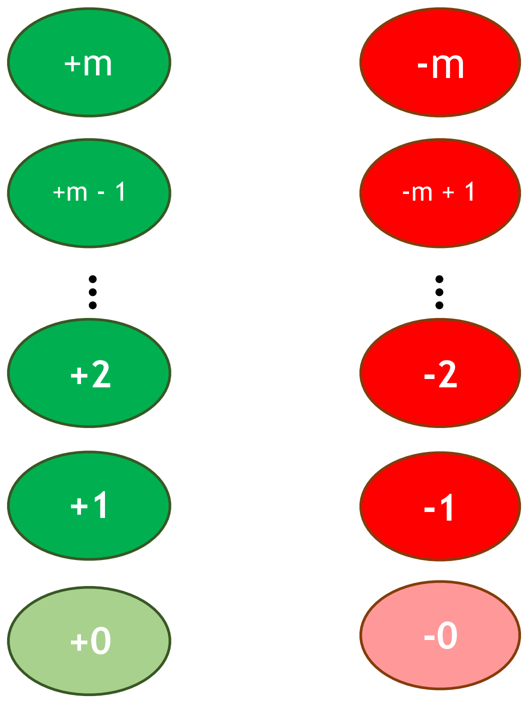

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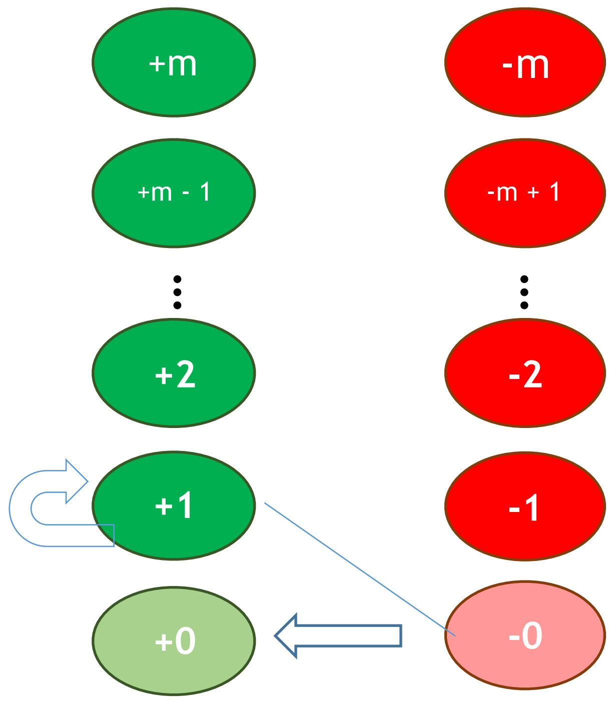

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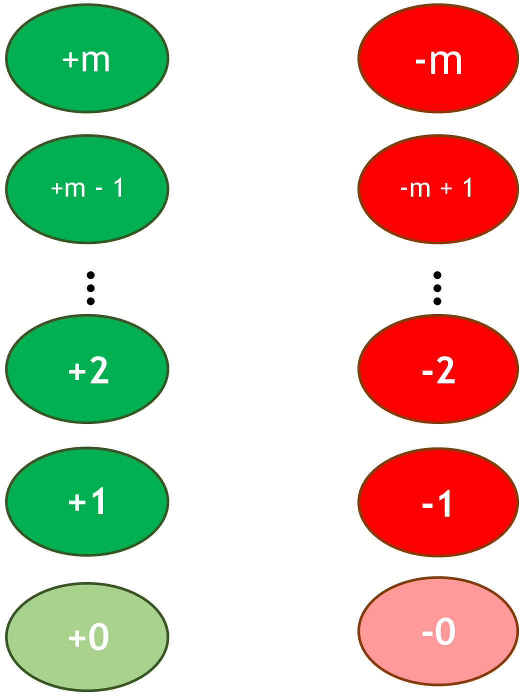

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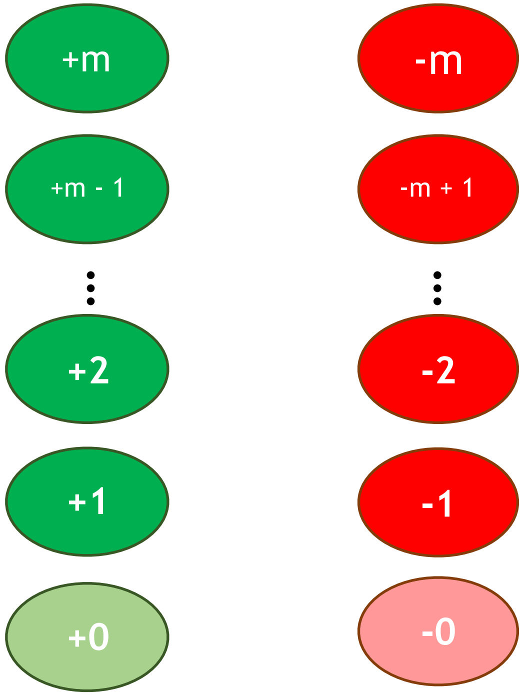

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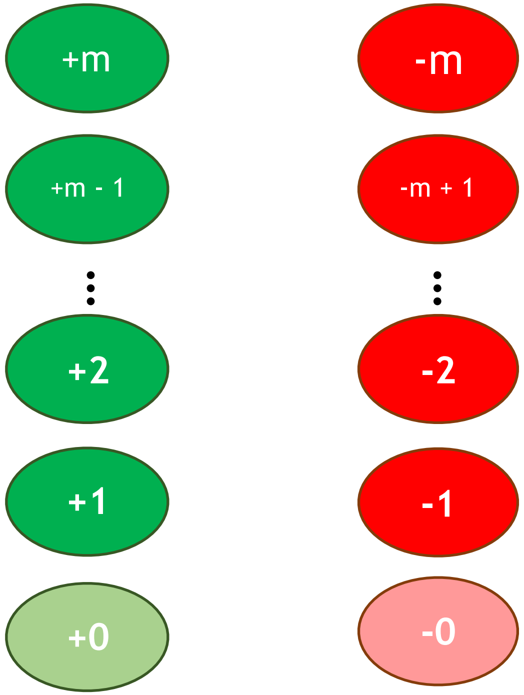

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Disclaimer: original protocol is more complicated for technical reasons

Summing up

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- In short:
  - If $m \approx 1 / \varepsilon$, then running time is always **poly-logarithmic**
  - If $\varepsilon = 1 / n$, then m needs to be **linear** in n
  - 10^{23} molecules -> $O(10^{23})$ states?!
  - 10^{23} molecules -> $O(23^2$ states $)$
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Theorem 2 [AAEGR16]: **logAVC** solves majority exactly in expected parallel time $O(\log^3 n)$, using $s = O(\log^2 n)$ total states.

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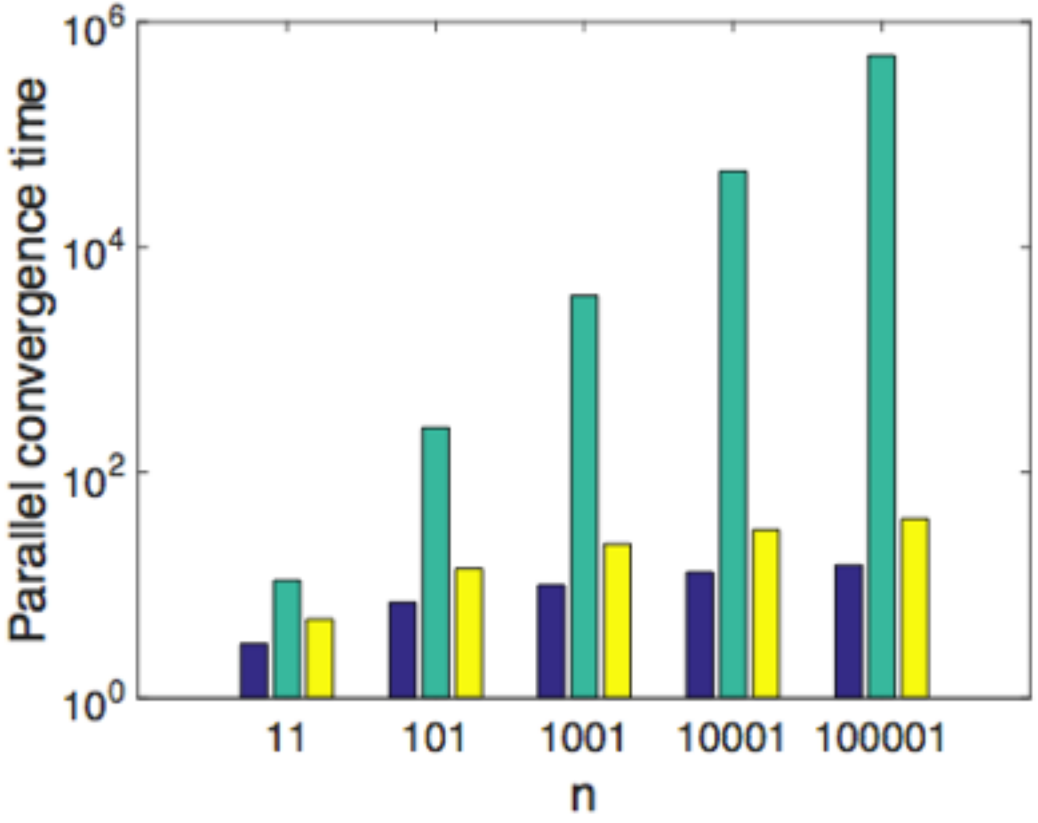
- The idea: ***quantize*** integer states to powers of two

Is AVC any good?



Results are for **ε = O(1 / n)**
Legend:
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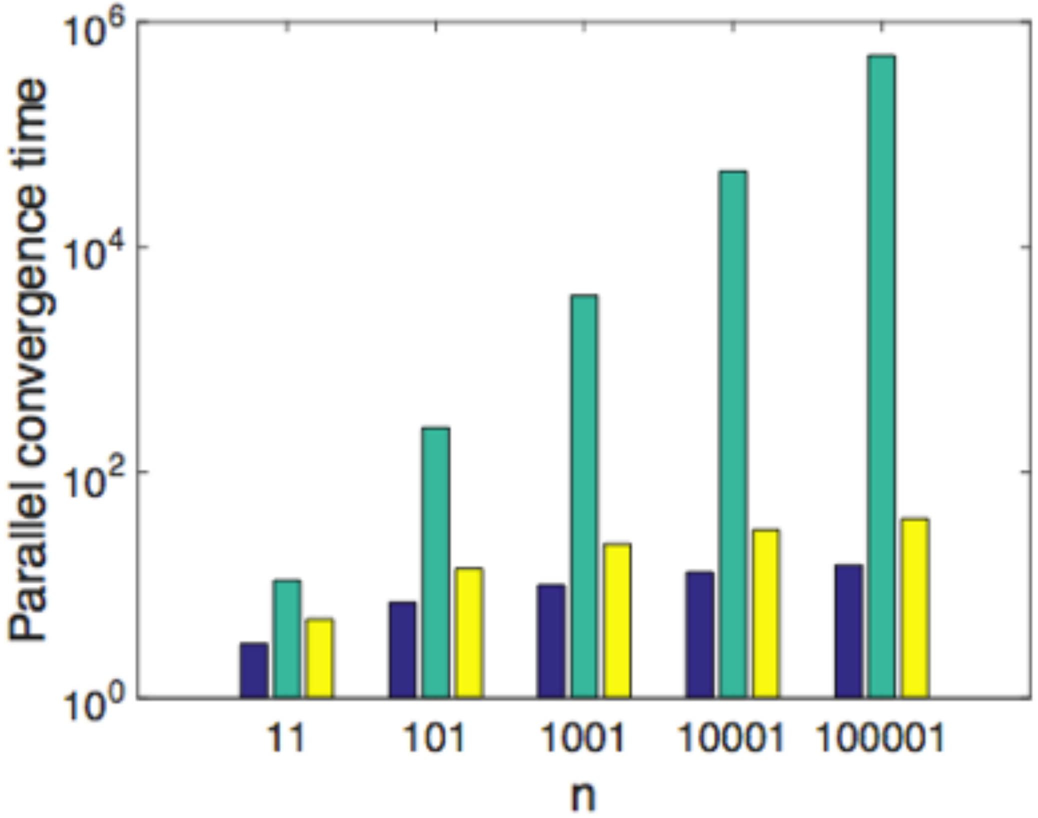

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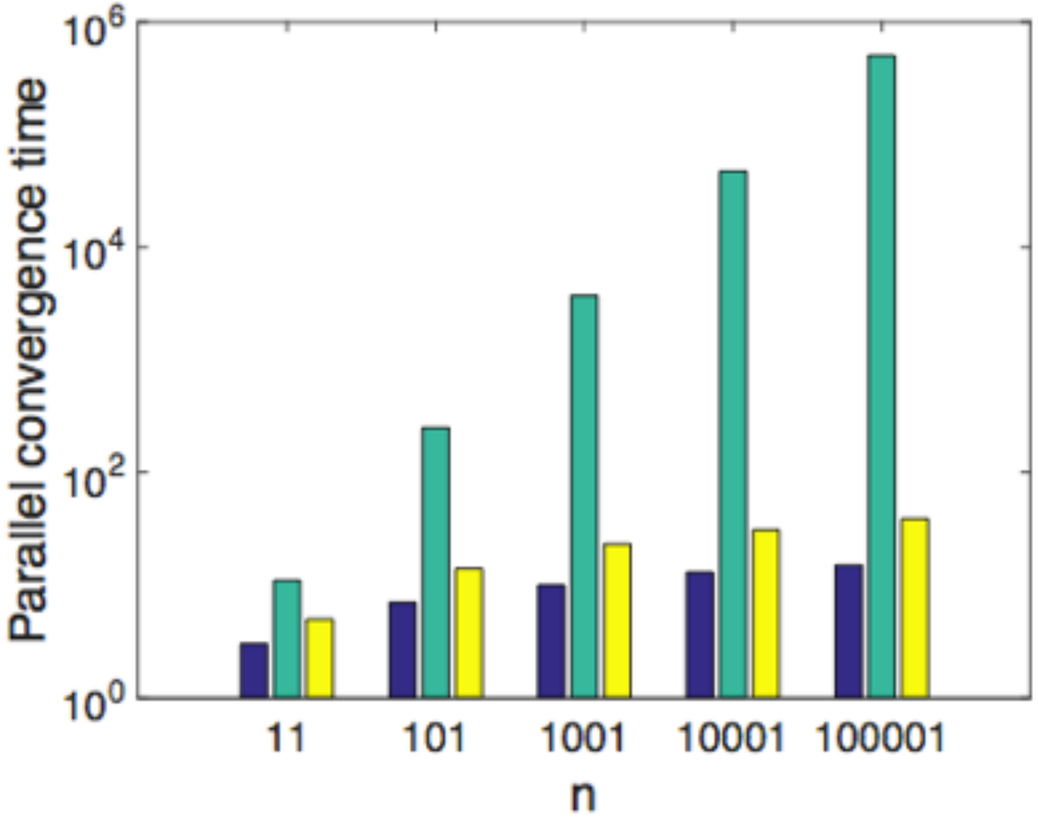

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Is AVC implementable?

Challenging: currently, small constant number of states implementable.

Time-Space Trade-Offs

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Theorem A : Any protocol using $s < \frac{1}{2} \log \log n$ states per node and solving majority with **discrepancy ε** must have expected stabilization time $> n / (2^s + \varepsilon n)^2$.

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- In particular:
  - If **s = constant** and **εn = constant,** then stabilization time **linear in n**
  - If **s = O(loglog n)** and **εn = constant**, then stabilization time > **n / polylog n**

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Complex molecules are needed for deterministic computation.

Discussion

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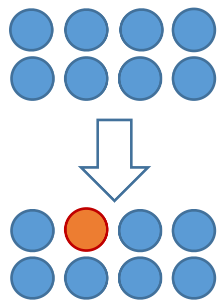
There are **inherent space-time trade-offs** when designing **deterministic** population protocols.

Open Challenges:

- Tighter trade-off bounds
- Other problems: **plurality**, **approximate counting**
- **Modeling faulty interactions** (leaks)
- **Large-scale simulation** of molecular algorithms

Leader Election

- **Input:** All nodes start in the same initial state
- **Output:**



Algorithm	Number of States	Convergence Time
Trivial Leader Election	2	$\Omega(n^2)$
Leader-Minion [AG, ICALP 2015]	$O(\log^3 n)$	$O(\log^3 n)$
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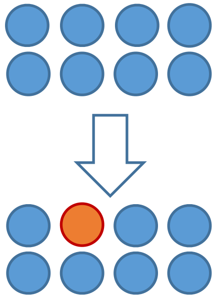
Leader Election

- **Input:** All nodes start in the same initial state
- **Output:**
  - Exactly one node is in a “leader” state, remains leader forever



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- Example:
  - **O(log log n) states / node**, **one** leader
  - Stabilization time > n / polylog n (quasi-linear)
  - Generalizes a recent result by Doty and Soloveichik [DISC15] to super-constant states

Bonus: A Cute Algorithm

- The goal: approximate **n**
- The state:
  - A flip bit F, initially 0
  - A counter “variable” C, initially 0
- The algorithm:
  - Stage 1: do four interactions, updating $F = 1 - F'$
  - Stage 2: increment counter C until you first see $F' = 1$
  - Stage 3: exchange C with interaction partner, setting $C = \max(C, C')$
- The guarantee:
  - The convergence value is
    $(1 - \mathrm{eps}) \log n < C < (1 + \mathrm{eps}) \log n$,
    with high probability