Active Tile Self Assembly:

Simulating Cellular Automata at Temperature 1

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Outline

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- Simulating a Cellular Automaton
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Introduction

DNA: What can we do with it?

Overview of DNA Self-Assembly

- DNA:
  - A-T and G-C nucleobases
- DNA and self-assembly:
  - Single strands with complementary base pairs will bond together
- Nanotechnology and Computing
  - Nanotechnology:
    - Ned Seeman: DNA structures, methods
      - Strand displacement
    - DNA origami:
      - DNA does not have to be a double helix – base pairings allow for other structures!
      - Possible to fold a DNA strand into any shape using “staple” molecules to hold it rigidly in place
  - Computing
    - In 1994 Adleman proved experimentally that DNA could be used to solve computational problems

DNA-based 2D Arrays

- "Approximately" two-dimensional DNA structures with single strands of unpaired bases on their sides – "sticky ends" - can act as tiles and form arrays

- In nanotechnology, potential for new materials
  - Tiles can be marked and used to guide nanoscale assembly of other structures
  - Nanostructures in themselves as periodic and nonperiodic arrays:
    - Crystallographic
      - Have been made in the lab using DNA-based tiles
    - Quasi-crystallographic
      - Quasi-crystals in general are rare in nature and in the lab

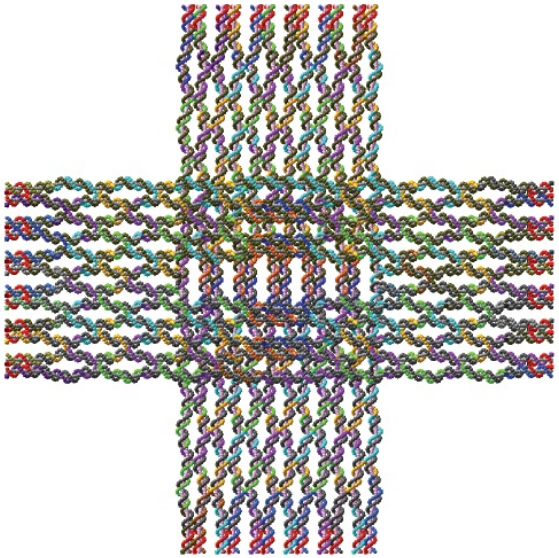
- In computation, problems can be encoded in the tiles with different kinds of sticky ends; the solution is then the product of the self-assembly
  - Moving computation to the nanoscale

Computing with Tiles

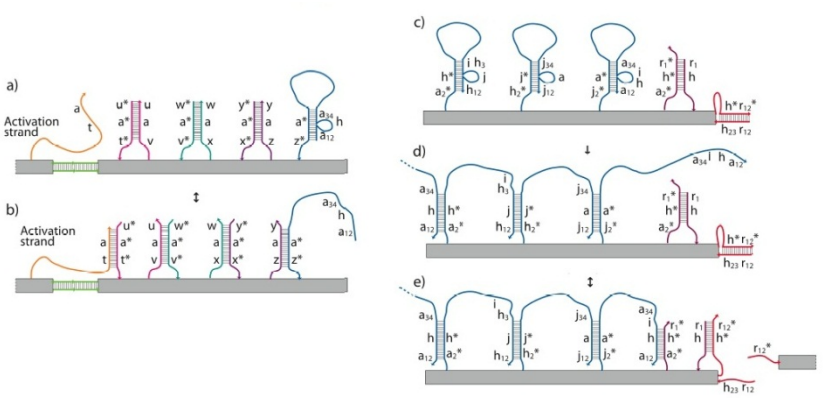
- Erik Winfree, 1998 Ph.D. Thesis:
  - Introduced the “abstract tile assembly model” (aTAM)
  - Can simulate the dynamics of any 1D cellular automaton at temperature 2
    - Rule 110 is capable of Turing universal computation
- Adding signals to tiles allows cellular automaton simulation at temperature 1

Letting Tiles Talk to Each Other

DNA Tiles



Signaling



Active Tile Assembly Model

Definitions and Concepts

Tiles + Signaling = Active Tiles

- Tile:
  - 4-tuple of *tile sides*
- Tile side:
  - Ordered pair of sets of *Active Labels* and *Inactive Labels*
- Labels:
  - Strings of symbols
  - Come in complementary pairs
  - (Bond) *strength*

- Active Tile:
  - Ordered triple of a Tile and the sets of *Activation Signals* and *Transmission Signals* (with some restrictions)
- Signals:
  - Labels with associated “in” and “out” directions; triples

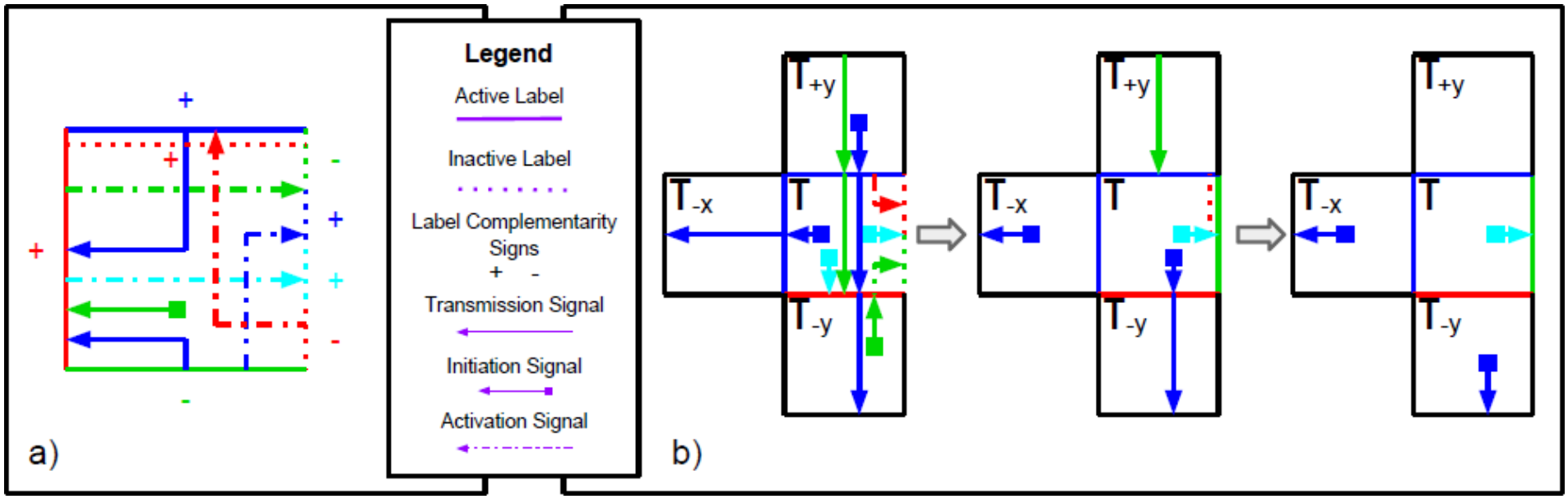
Tile Assemblies

- Tile Assembly Instance
  - A stable configuration with respect to a set “temperature”
  - Partial mapping from the integer lattice to the set of all active tiles that
    - Is connected
    - The sum of the strengths of the newly formed bonds meets or exceeds the temperature parameter

Active Tile Assemblies

- What about the signaling?
- Tile Modification Function
  - Allows adjacent tiles to communicate with each other: neighboring tiles can modify themselves as a function of their neighbors
  - Essentially, a local function for a cellular automaton
- What it does:
  - Activate and remove labels
  - Modify and remove activation and transmission signals
  - Can be applied repeatedly to a tile assembly until no more transmissions or activations can be made

Active Tile Assemblies



Hierarchical Tile Assembly

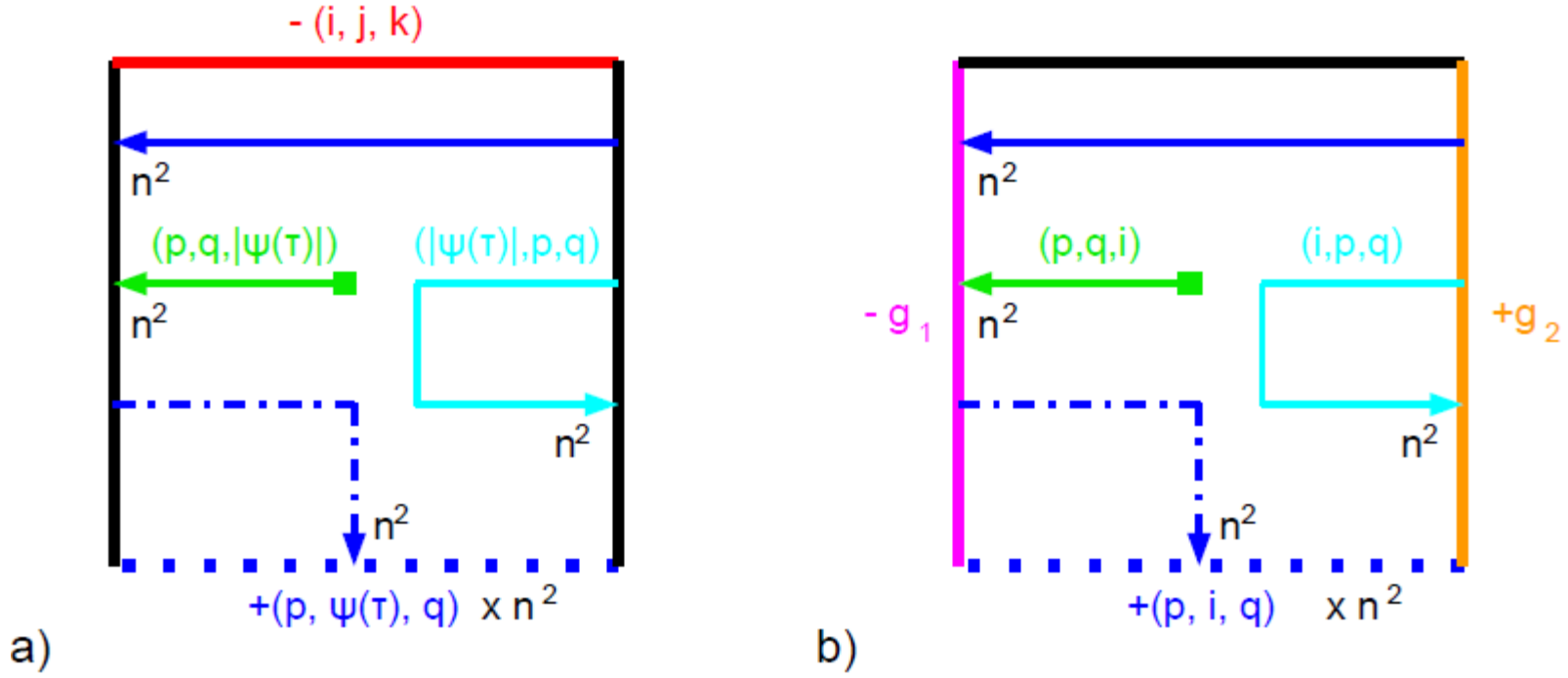
- We can define a nested series of active supertile sets:
  - Begin with a *seed set* $\mathcal{T}_0$ of unit tiles
  - Each subsequent set includes
    - The preceding set
    - Any tile assembly that can be formed by joining two tile assemblies of the preceding set and repeatedly applying the tile modification function to the result
- By specifying the seed set and the temperature, we obtain an Active Tile Assembly System

Simulating Cellular Automata

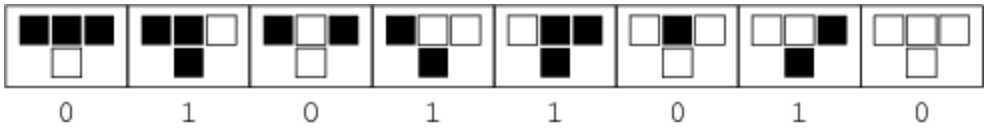
An Active Tile Assembly System Construction

Cellular Automaton ATAS

- 1D cellular automaton of radius 1
  - Set of states (alphabet) and local function
- Two types of tiles: initial row and computing



Rule 90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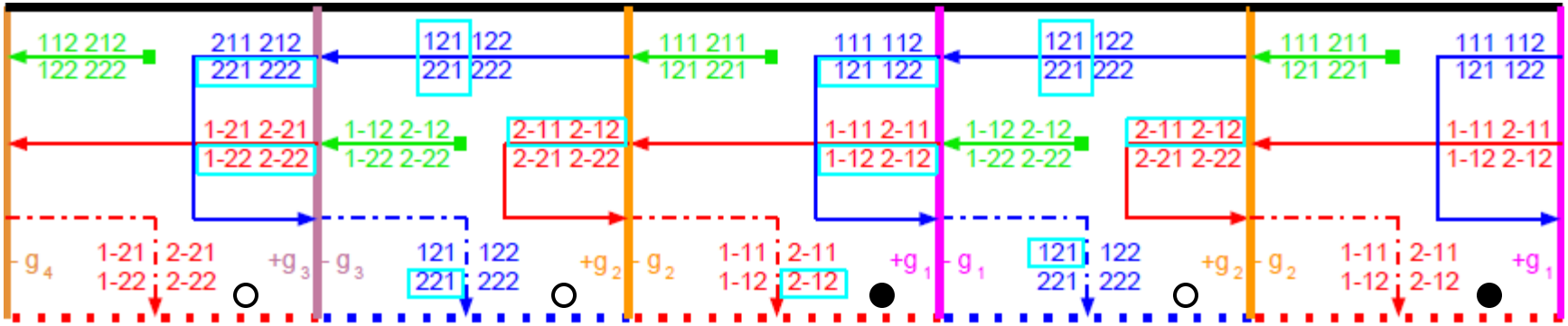
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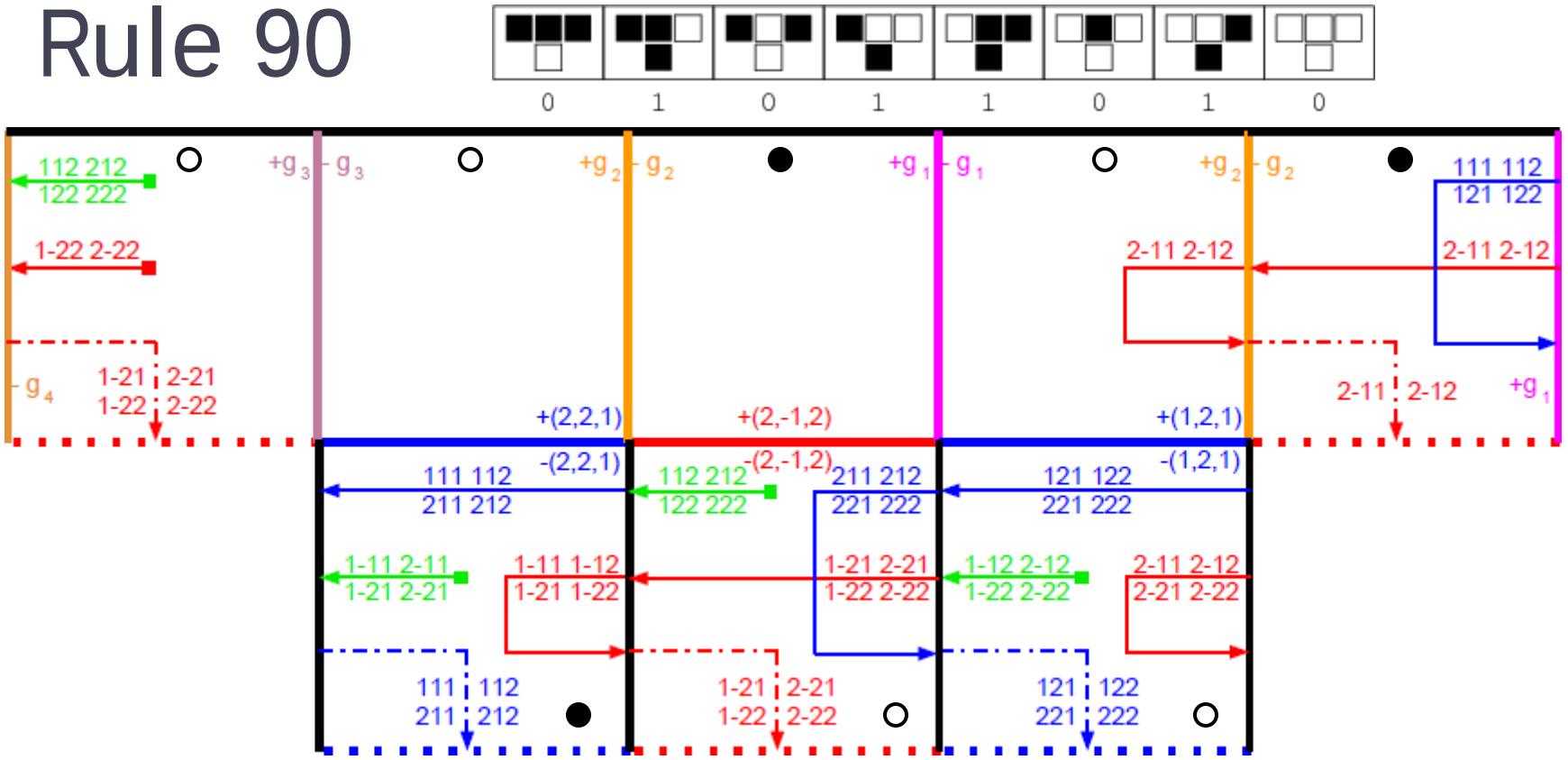
+g1

Rule 90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+g1
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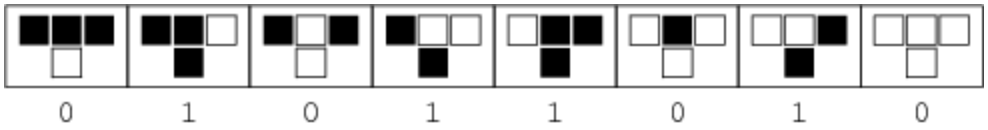
Rule 90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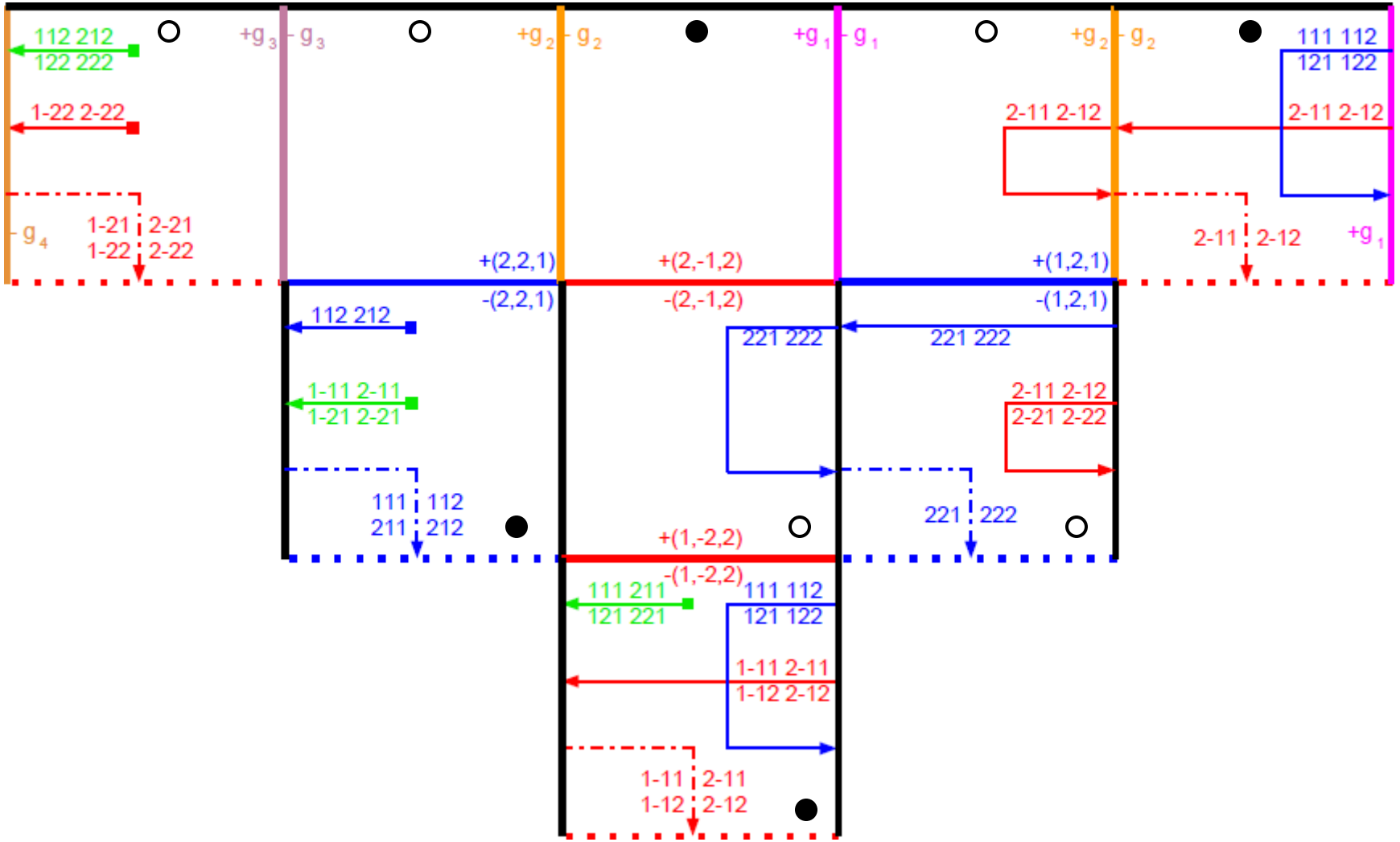
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Summary

Thank you for your attention!

Summary

- We presented a model of active tile assembly
  - Active Tiles:
    - Active and Inactive labels
    - Signals
  - Tile Modification Function:
    - Simulates signal transmission and binding site (label) activation
  - Tile assemblies
    - "Temperature" parameter determines which configurations are stable
  - Active Tile Assembly System
    - Given a seed set and a temperature, obtain a hierarchy of supertile sets
- Cellular Automaton Construction
  - Turing universality at temperature 1 of the Active Tile Assembly Model
- Simplifying assumptions with respect to implementation using actual DNA
  - All signal transmission happens instantaneously
  - Tile assemblies combine two at a time and they do so if and only if the sum of the strengths of the new bonds formed meets or exceeds the set "temperature"
  - Tile assemblies do not break apart

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Questions?

References

1. W.B. Sherman and N.C. Seeman. A Precisely Controlled DNA Bipedal Walking Device. *NanoLetters*, 4:1203-1207, 2004.
2. P.W.K. Rothemund. Folding DNA to Create Nanoscale Shapes and Patterns. *Nature*, 440(7082):297-302, 2006.
3. L.M. Adleman. Molecular Computation of Solutions to Combinatorial Problems. *Science*, 266(5187):1021-1024, 1994.
4. H. Zhong W. Liu, R. Wang, and N.C. Seeman. Crystalline Two-Dimensional DNA Origami Arrays. *Angew. Chemie*, 50:264-267, 2011.
5. E. Winfree. Algorithmic Self-Assembly of DNA. Ph.D. Thesis. California Institute of Technology. 1998.
6. G. Aggarwal, M.H. Goldwasser, M.Y. Kao, and R.T. Schweller. Complexities for Generalized Models of Self-Assembly. *Proceedings of the Fifteenth annual ACM-SIAM symposium on Discrete algorithms*, p.889, 2004.
7. U. Majumder, T.H. LaBean, and J.H. Reif. Activatable Tiles for Compact, Robust Programmable Assembly and other Applications. *LNCS* 4848:15-25, 2008.
8. J. Padilla, W. Liu, N.C. Seeman. Hierarchical Self Assembly of Patterns from the Robinson tilings: DNA Tile Design in an Enhanced Tile Assembly Model. *Natural Computing*, online first, DOI: 10.1007/s11047-011-9268-7, 2011.
9. J. Padilla, M.J. Patitz, R. Pena, R.T. Schweller, N.C. Seeman, R. Sheline, S.M. Summers, and X. Zhong. Asynchronous Signal Passing for Tile Self-Assembly: Fuel Efficient Computation and Efficient Assembly of Shapes. *Available on Arxiv*: http://arxiv.org/pdf/1202.5012v1.pdf