Monte Carlo Simulations of Tetromino Fluids

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March 30, 2011

Contents

Introduction

Tetrominoes are orthogonally connected objects that occupy four lattice sites in $\mathbb{Z}^2$. Here we study how a "fluid" made up of these "particles" behaves using grand-canonical Monte Carlo simulations.

Following the paper *Structure, thermodynamics, and solubility in tetromino fluids* by Barnes, Siderius and Gelb (2009).

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- Random number generation is crucial
- Huge amount of literature devoted to how to achieve a reasonable accuracy with few sampling points

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- Calculating probabilities with which the moves in the Monte Carlo simulations are performed can increase the simulation efficiency dramatically.

Tetromino Fluid Simulation

The simulation allows for four types of moves:

1. Insertion of a particle
   An unoccupied lattice point and an orientation is chosen at random, and, if the tetromino can fit on this spot, it is inserted with probability

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2. Deletion of a particle
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3. Translation of a particle
4. Rotation of a particle

Tetromino Fluid Simulation

Other considerations:

- Anchor points
- Convergence criterium
- Volume
- Boundary conditions

Results

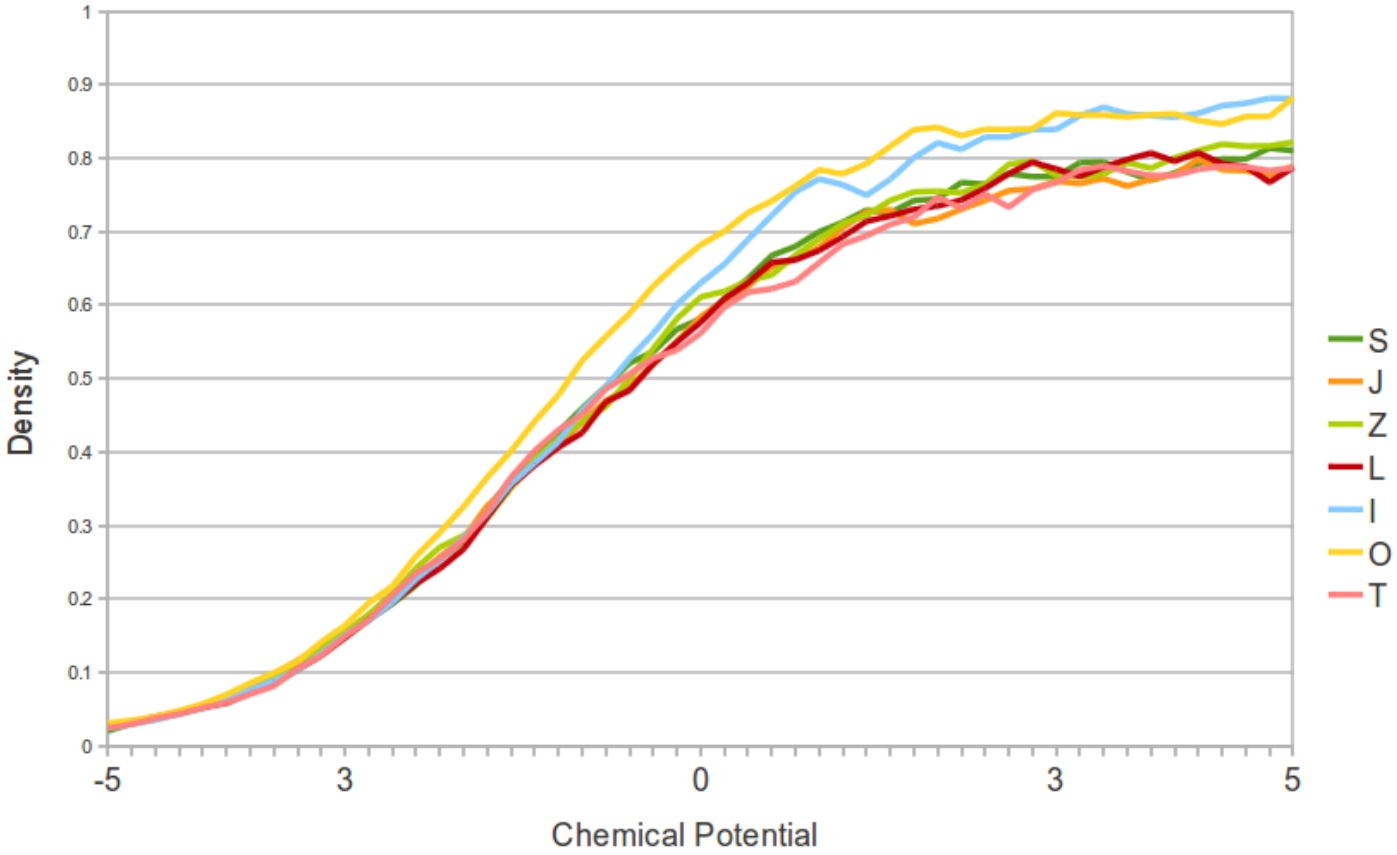
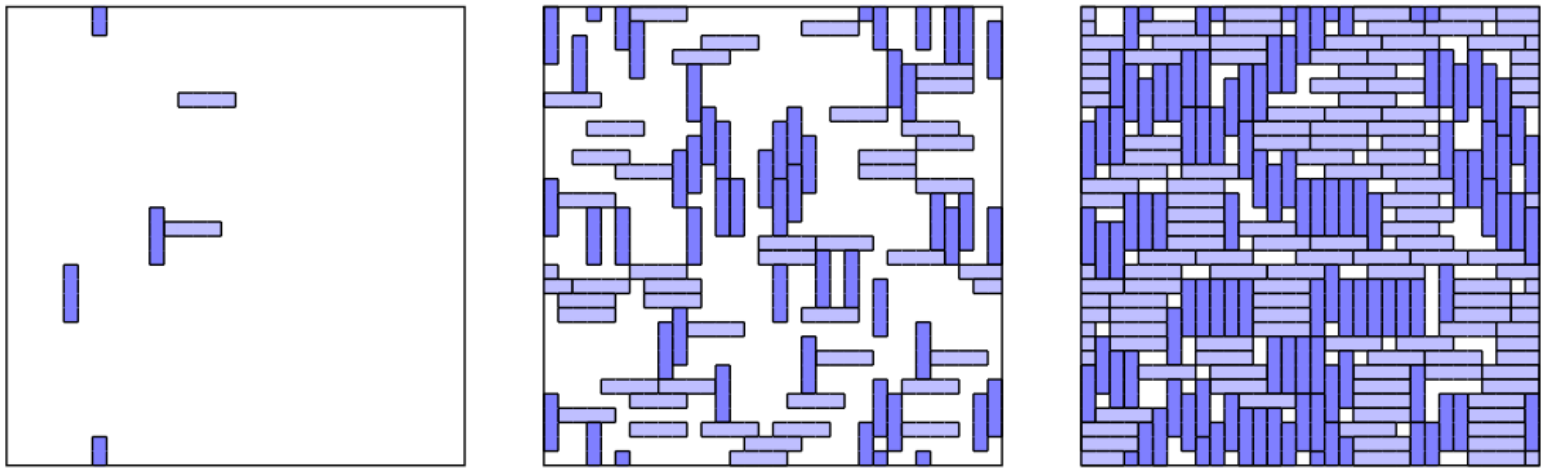


Figure: The change in densities of tetromino fluids for the seven different tetromino particles as a function of the chemical potential.

Results

Figure: Configuration at different densities for I- and O-fluids



Chemical potential = -4 Chemical potential = 0 Chemical potential = 4

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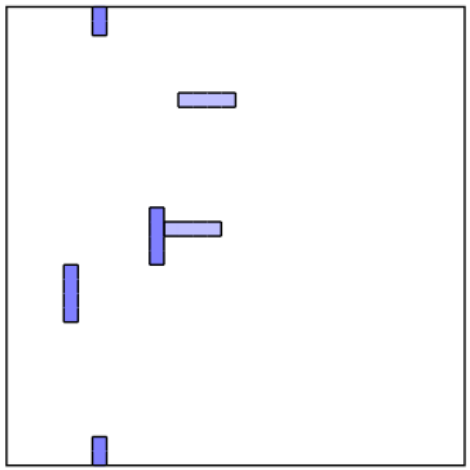
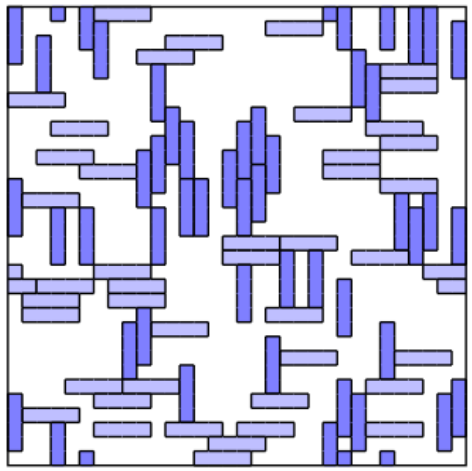
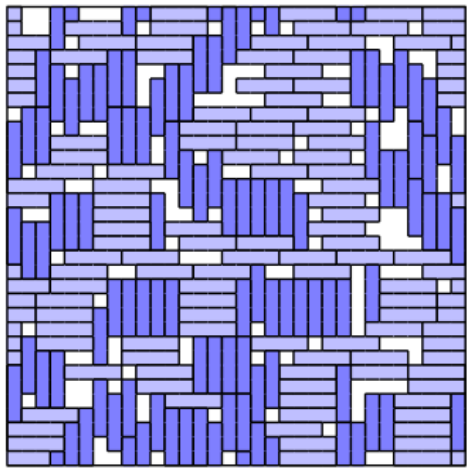


Chemical potential = -4



Chemical potential = 0



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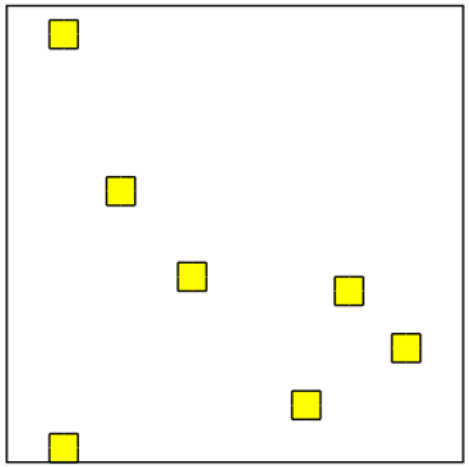
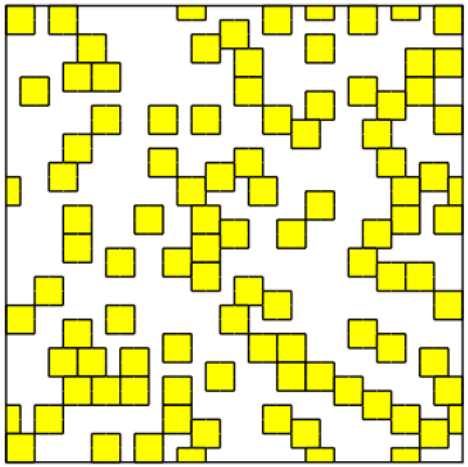


Chemical potential = -4



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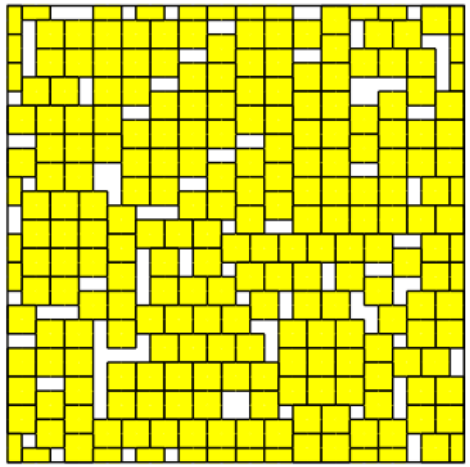
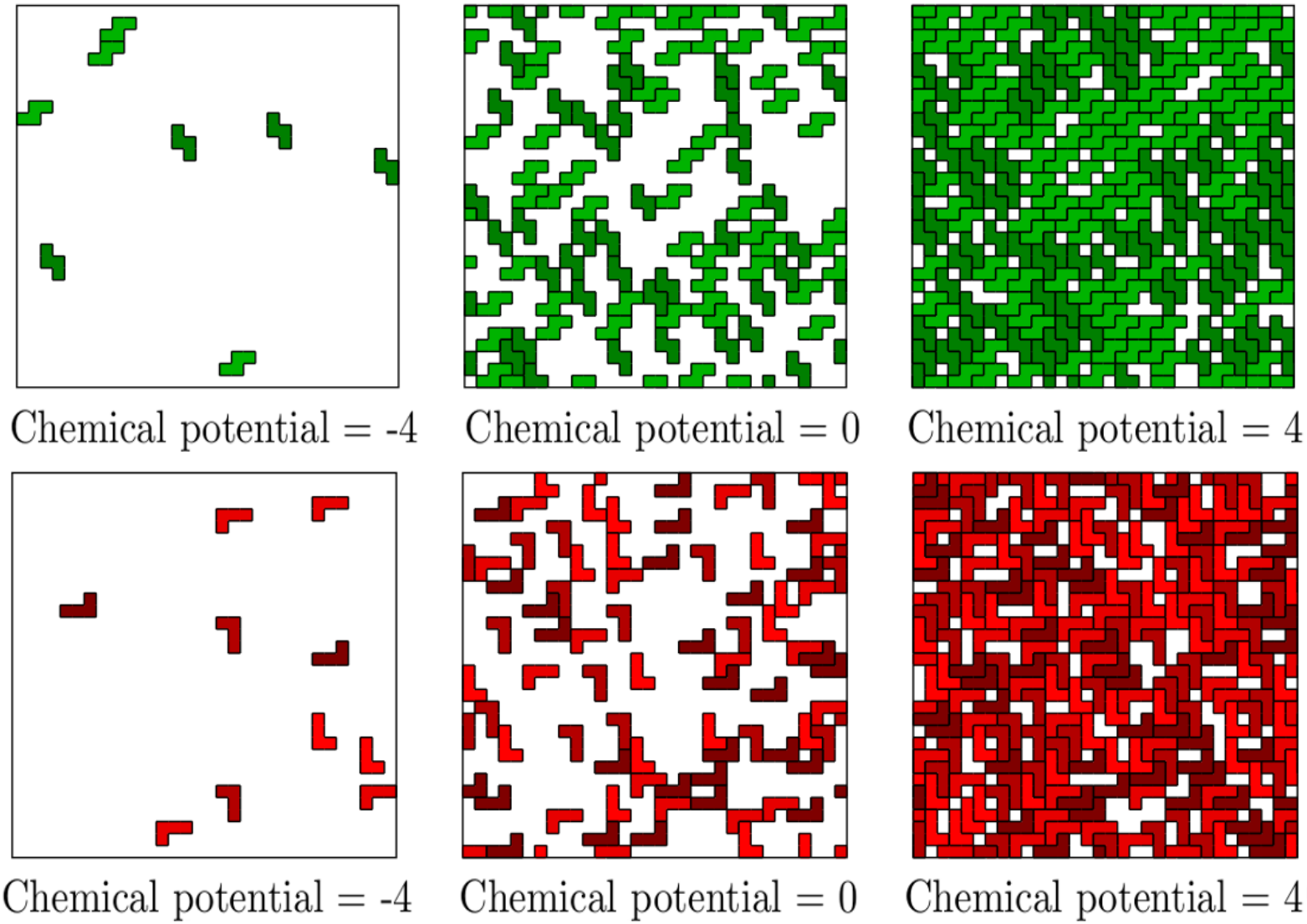


Chemical potential = 4

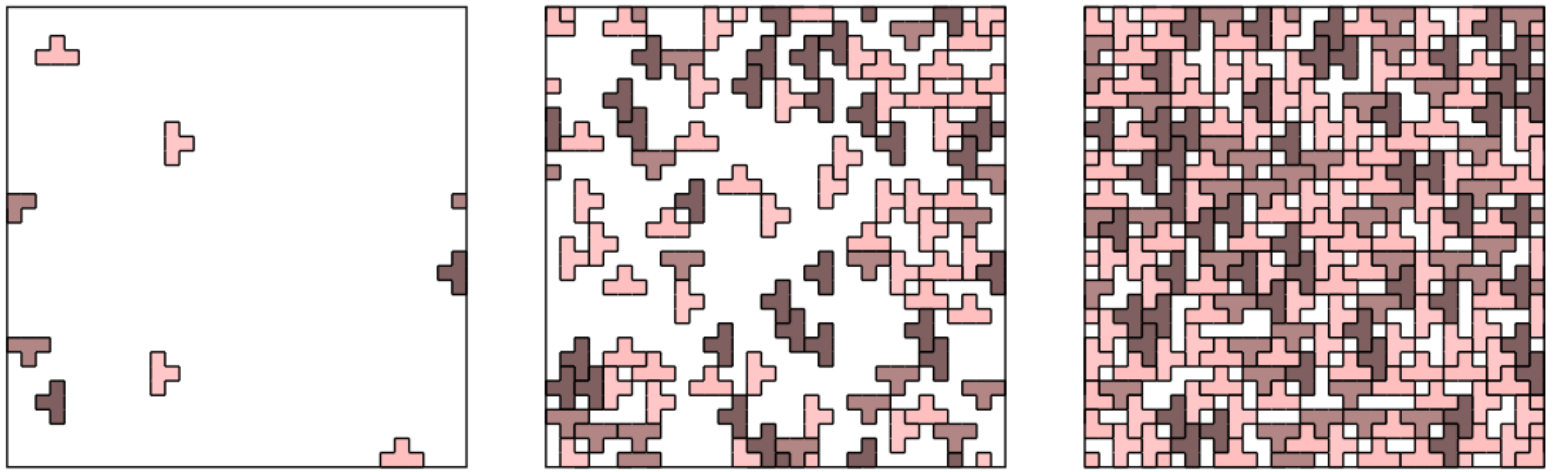
Results

Figure: Configurations at different chemical potenatial for S-, and L-fluids



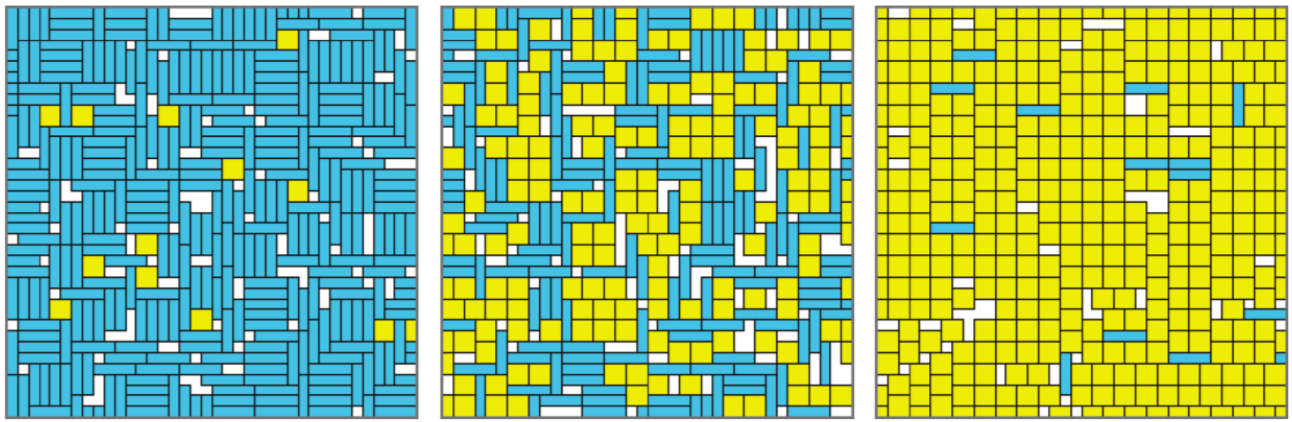
Results

Figure: Configurations at different chemical potenatial for T-fluids



Results - Barnes, Siderius and Gelb

Figure: Tetromino fluids composed of I- and O-tetromino particles



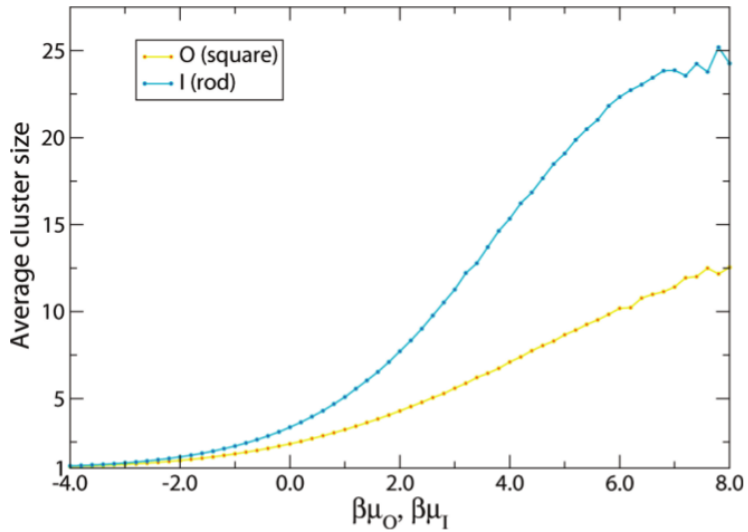


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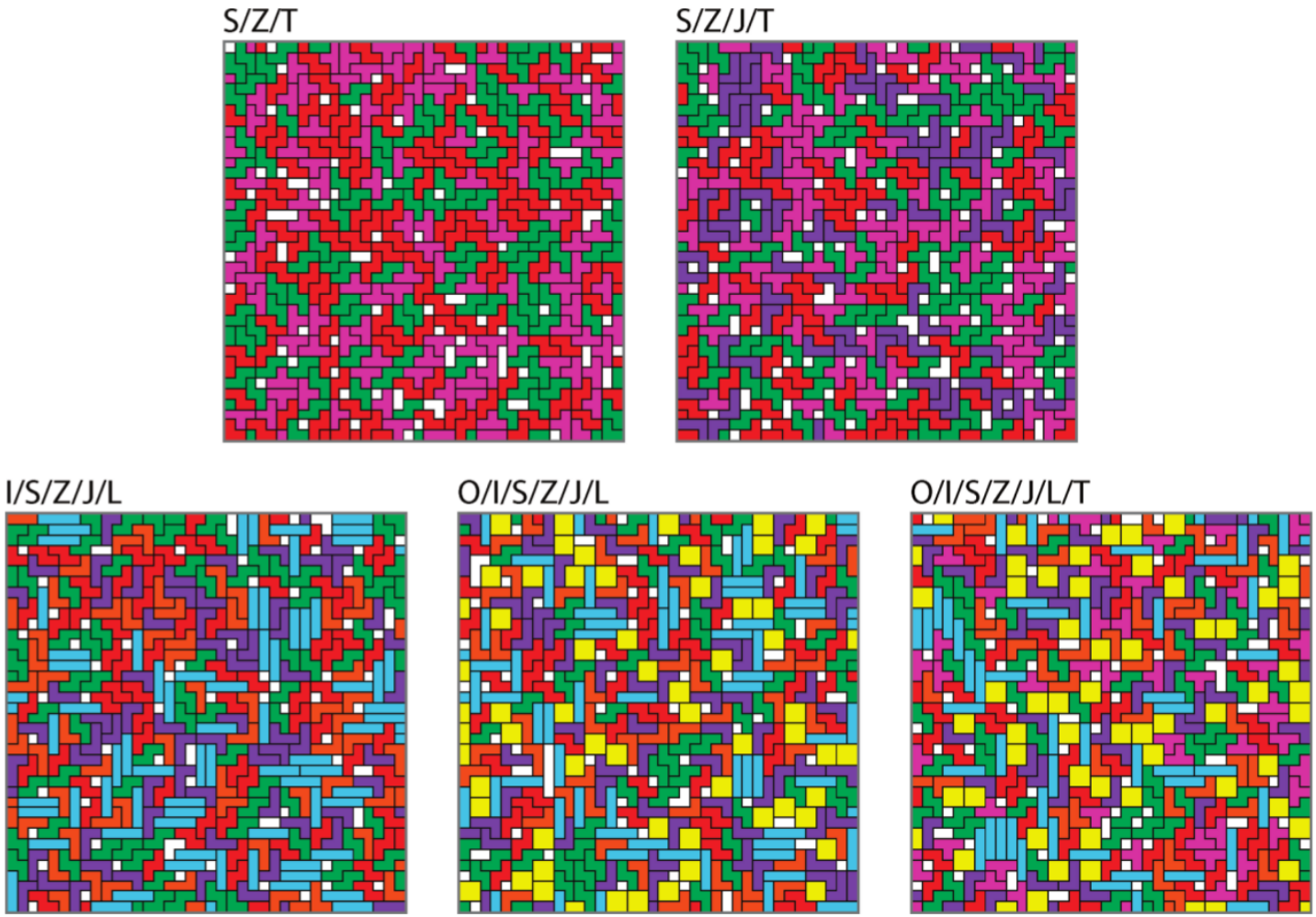
Figure: Mixed tetromino fluids



Literature

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