Collective dynamics of drops in 2D microchannels: an agent based approach

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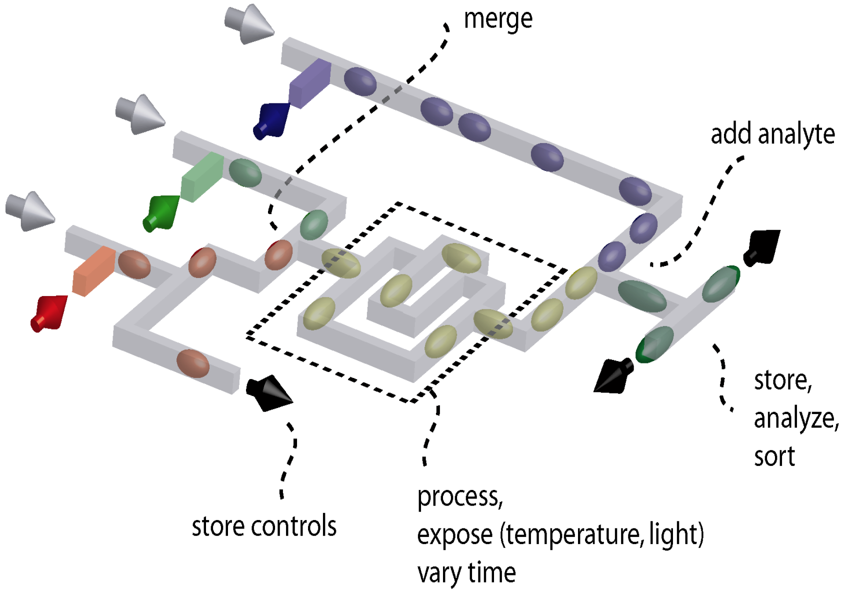
Drop microfluidics

Fluid flow in microchannels
Diameter < 10^{-3}m
Quantity~ $10^{-9}m^3$

Immiscible fluids
discrete drop phase and continuous phase

Compartmentalized drops
Reaction environments
Isolate active entities
Solute extraction
…



Piotr Garstecki lab group

Drops can be processed
merged,
split
synchronized
sort
incubated
…

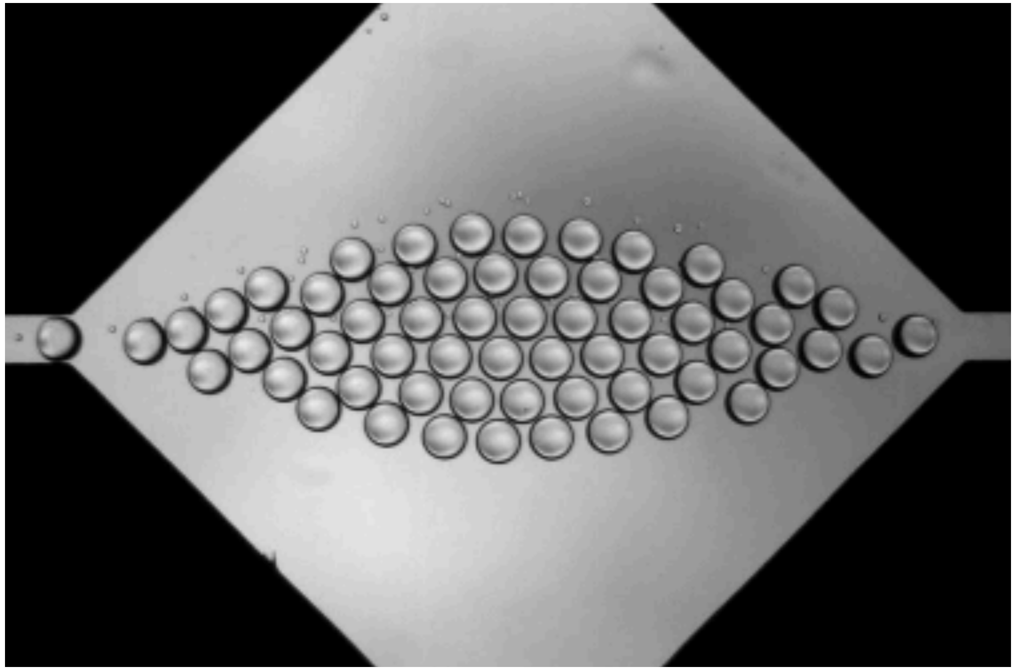
Cornerstone of the **Lab on a chip** technology

Collective dynamics in 2D microchannels

When things simply don't add up!

Self-organization

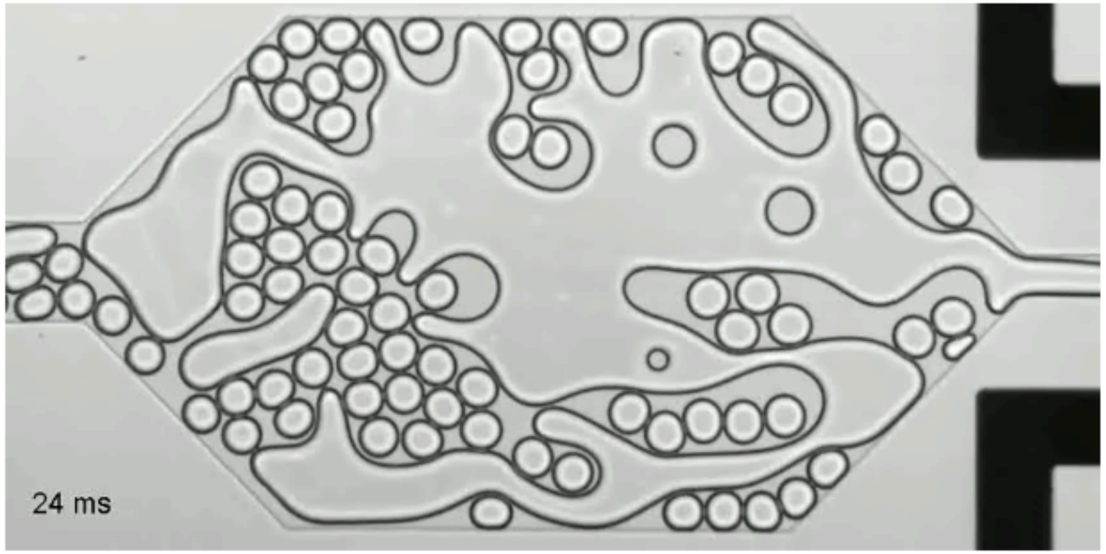
- **Microchannel:** Hele-Shaw geometry that constrains the drop motion in 2D
- **Diverging converging geometry:** decelerates and accelerates the drops inside the channel
- **Self organization:** Drops form patterns depending on the rate at which they enter the channel



(Courtesy: Bibin M. Jose and Thomas Cubaud, Stony Brook University)
(Jose & Cubaud, 2011)

Coalescence avalanches

- One coalescence event triggers an avalanche
- Not all coalescence events lead to propagation
  - Small avalanches
  - Destabilization of the assembly



Courtesy: Nicholas Bremond, Laboratoire Colloïdes et Matériaux Divisés, ESPCI, France
Bremond, N et al (2011), Physical Review Letters, 106(21), 1–4

Complex drop behavior in 2D channels

- What we know:
  - Drops form ordered 2D arrangements in a microchannel
  - Non-linearly interactions result in complex traffic
  - Drops can catastrophically destabilize
- Inverse problems:
  - For a desired pattern or arrangement
    - How should the drops be sent in, to form a pattern of choice?
    - Composite drops (A B): how do they arrange in an ordered configuration?
    - How does complex traffic inside the channel affect the exit spacing?
  - Coalescence avalanches
    - How can one pack drops to make an emulsion more stable?

Design perspective

- Design problem is hard
  - Complex behavior of drops
  - Large combinatorial problem
- Need for a systematic design of microchannels
  - Design problem as an optimization problem
- Models for flow of drops- incorporation inside optimization routines
  - Would involve solving the model several times
  - NS based models- high computational time- multiscale problem

An agent based approach

Self organization of drops

Agent based framework

- Break the complex system into a group of interacting agents

Drops are regarded as agents

- Agents interact with each other and the surroundings

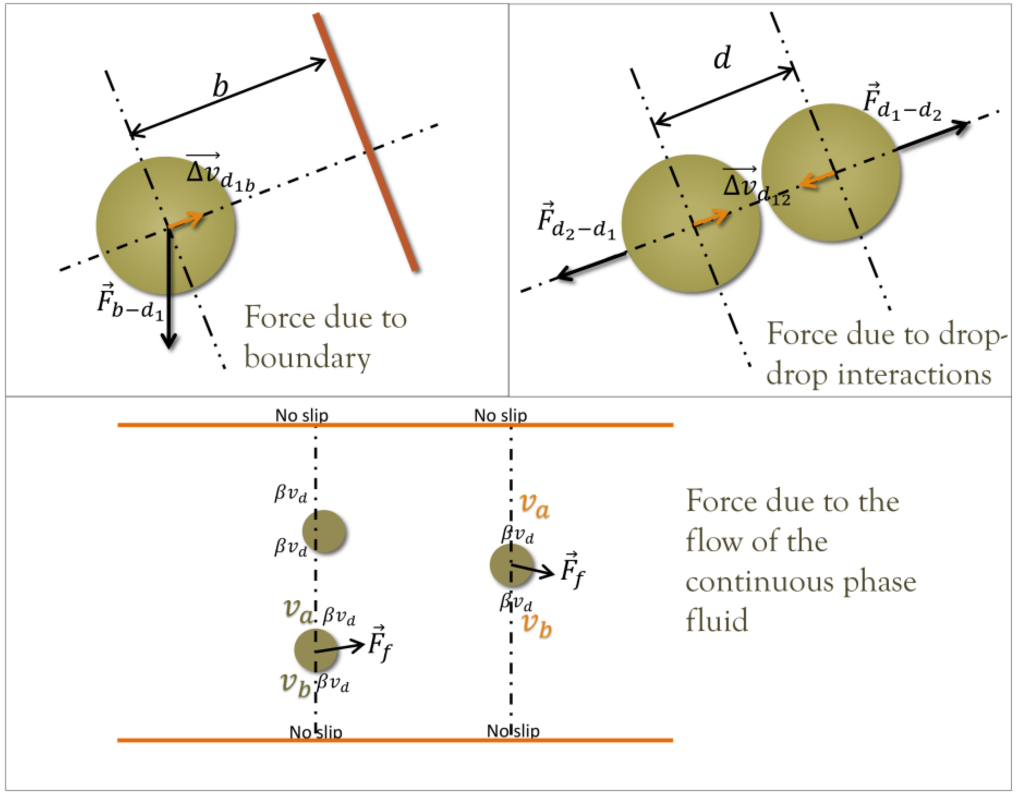
Drop-interactions: simple rules/models

- All the interactions of agents are pieced together to study the behavior of the complete system

A multi-agent framework: incorporating the interactions

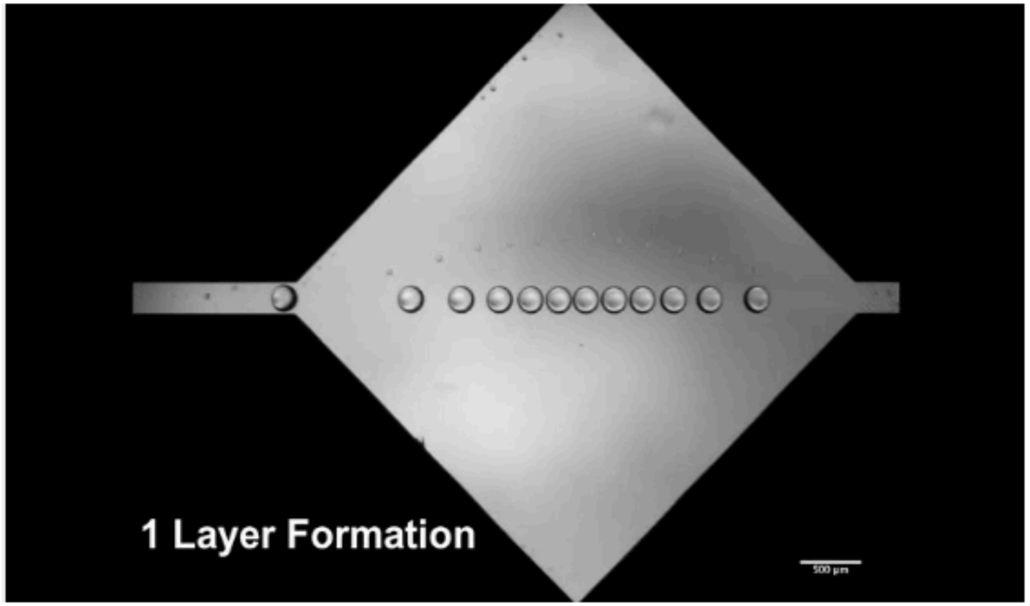
Interacting drop-traffic models (IDT)

- **Force due to the continuous phase fluid**
  - X- component of force: classic problem of flow past a sphere
  - $\mathbf{F_{x,flow}} \propto [(\langle \mathbf{v_a} \rangle + \langle \mathbf{v_b} \rangle) - 2\mathbf{v_{d,x}}]$
  - Y-component of force: resistance to flow is least when drop is at center
  - $\mathbf{F_{y,flow}} \propto [(\langle \mathbf{v_a} \rangle - \langle \mathbf{v_b} \rangle) - \mathbf{v_{d,y}}]$
- **Force between drops** and **effect of boundary** on the flow of drops Lubrication theory (Davis et al 1989)
  - $\mathbf{F_{d_i - d_j}} \propto \frac{\Delta \mathbf{v_{d_{ij}}}}{\mathbf{d - 2R}}$
- **Multi agent simulation**
  - Newton's second law of motion for all drops
  - Creeping flow approximation

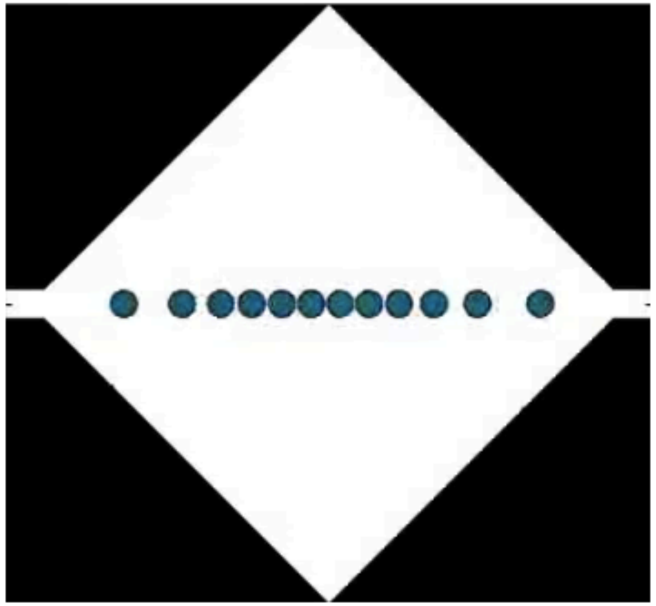


Danny Raj, M., & Rengaswamy, R. (2014)

1 layer configuration

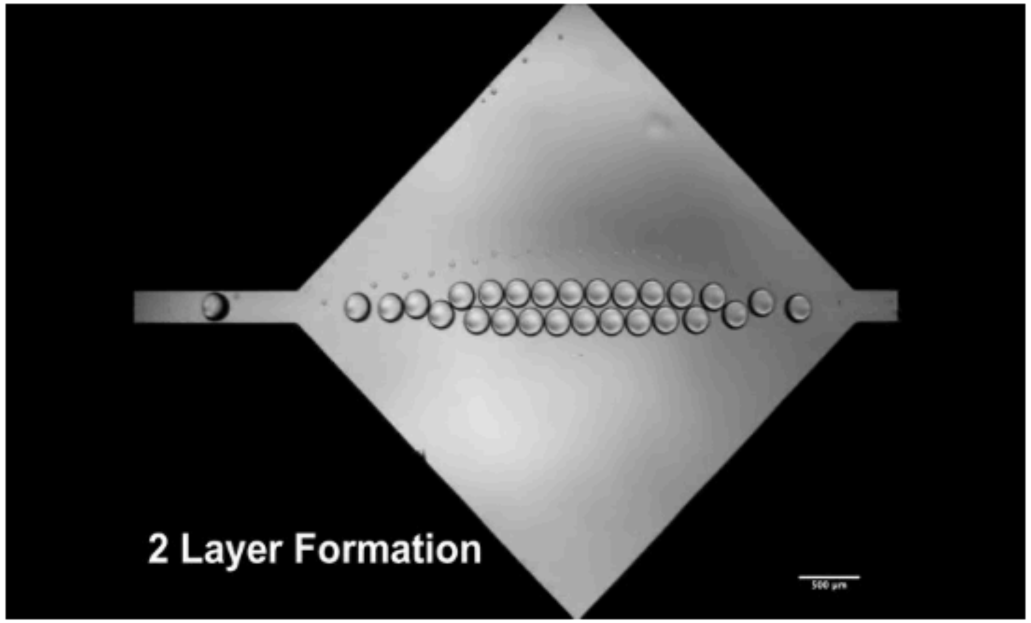


Jose and Cubaud, 2012



Danny and Rengaswamy, 2014

2 layer configuration



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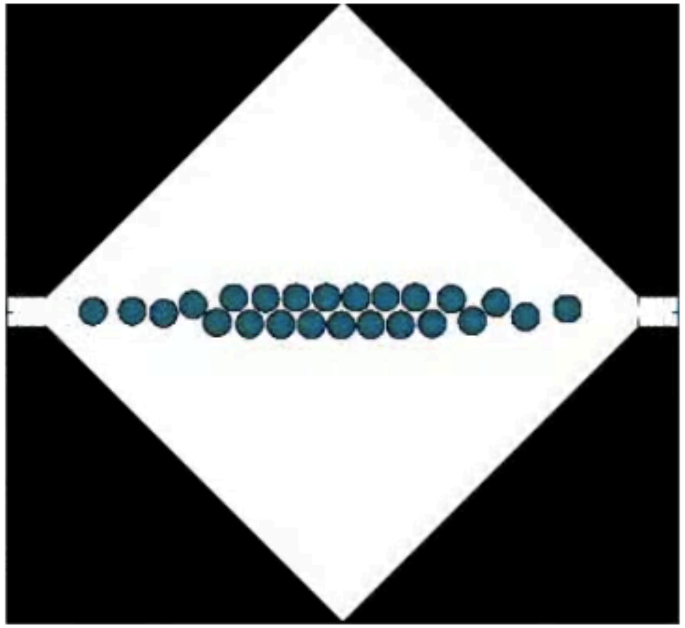
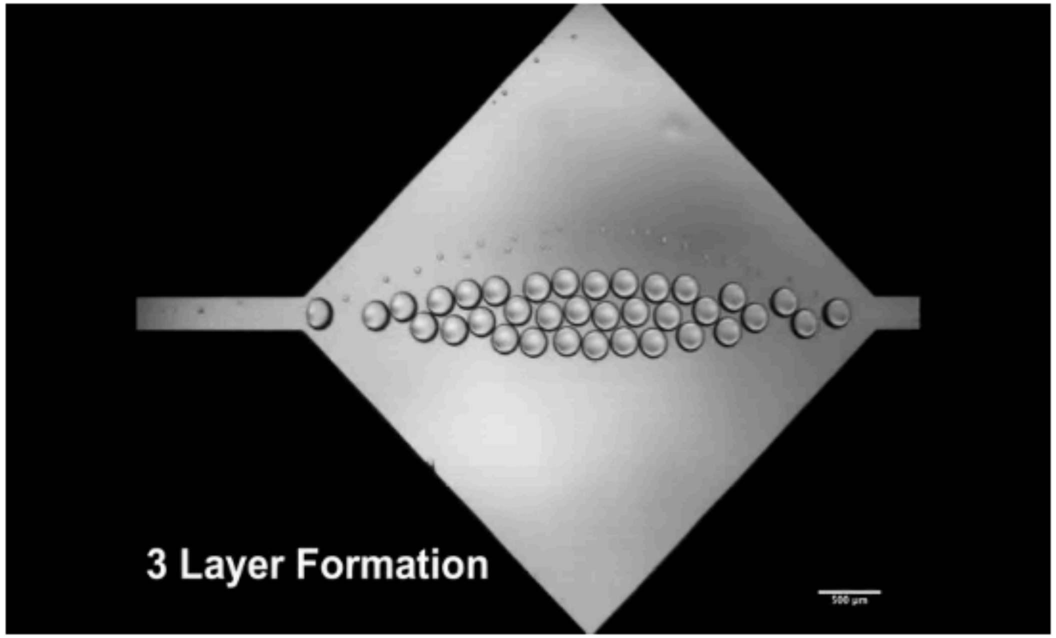
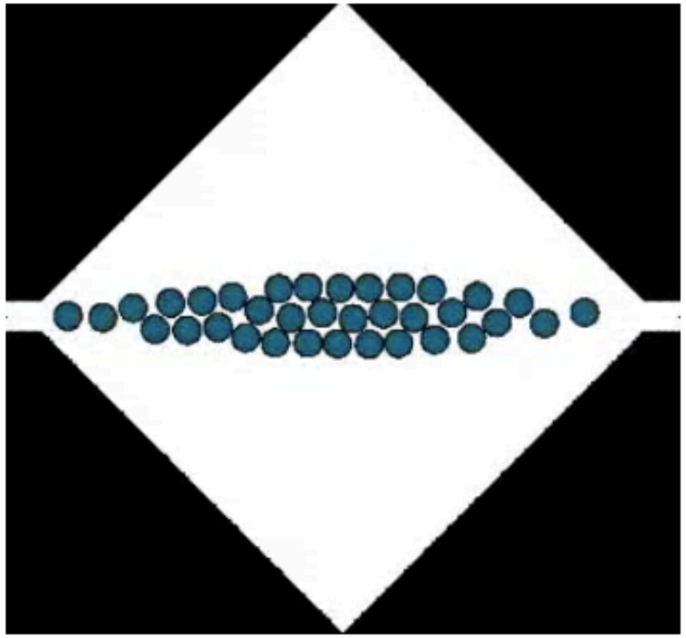


Danny and Rengaswamy, 2014

3 layer configuration

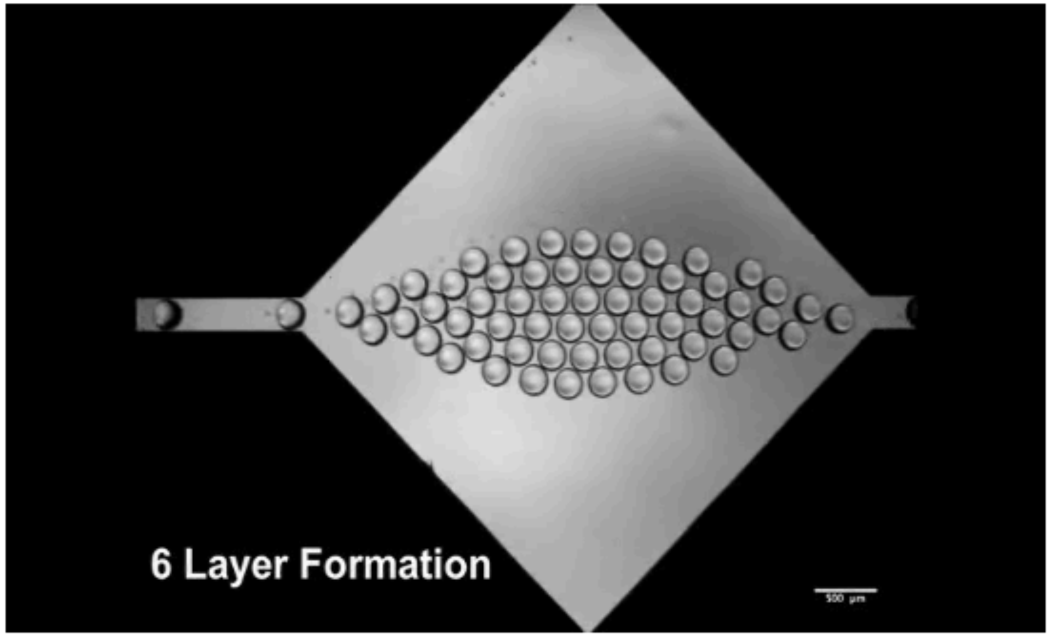


Jose and Cubaud, 2012

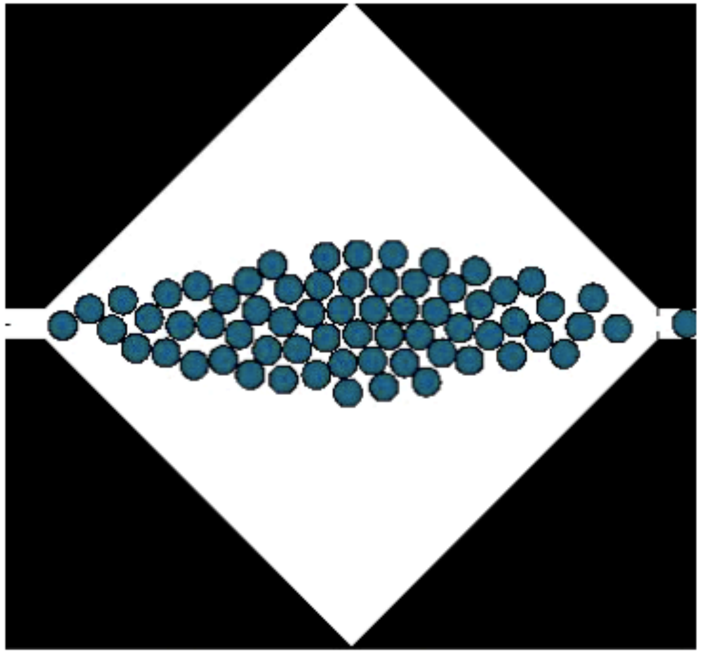


Danny and Rengaswamy, 2014

6 layer configuration



Jose and Cubaud, 2012



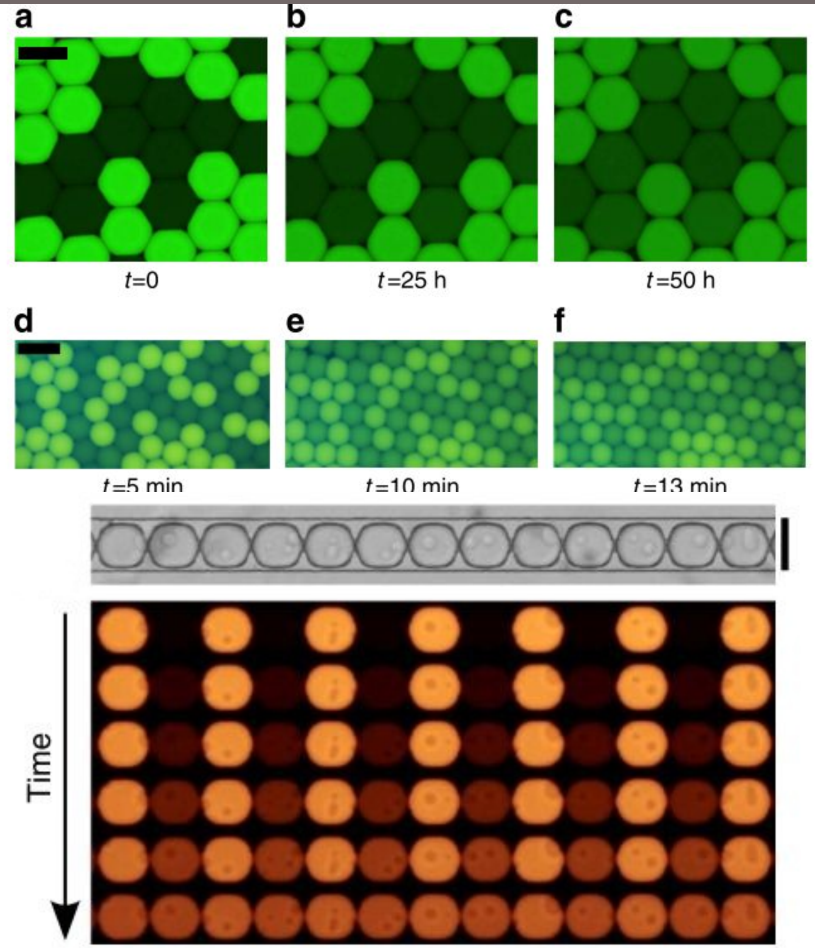
Danny and Rengaswamy, 2014

Design problem

Composite drop arrangment

Composite drop arrangement

- Consider the case where there are two different drops
  - Drop A and B- different composition
  - Mass transfer between drops
- Design and operation of a drop-Incubator
- How do you send drops into the channel to pack them such that
  - Maximum mass transfer- maximum contact between A and B and vice versa

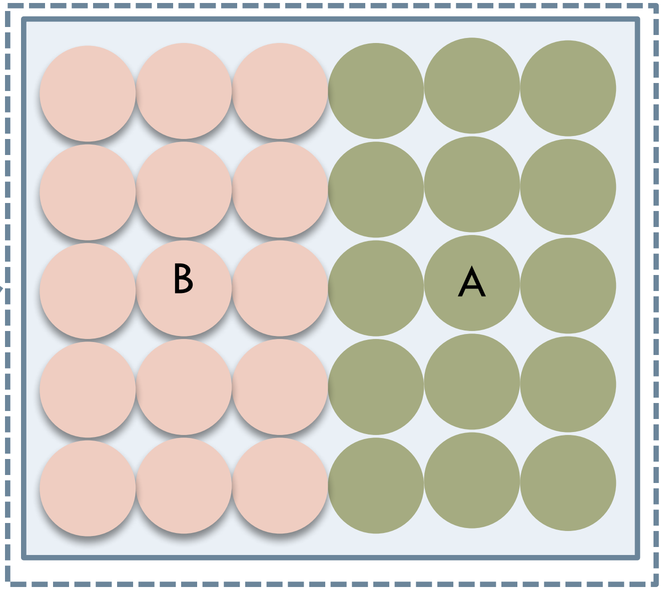


Gruner et al, Nature comm., 2016

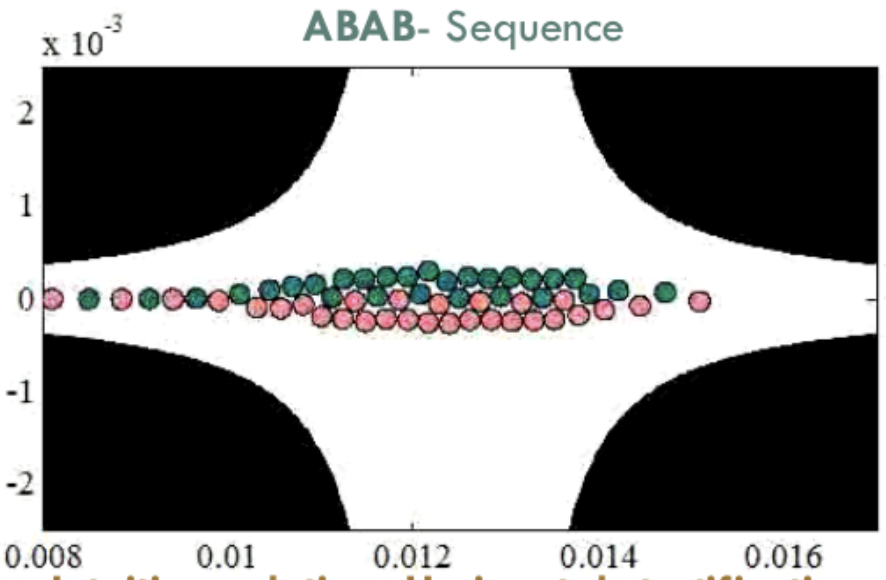
Drop-drop contactor

If there are 100 drops of A and 100 drops of B

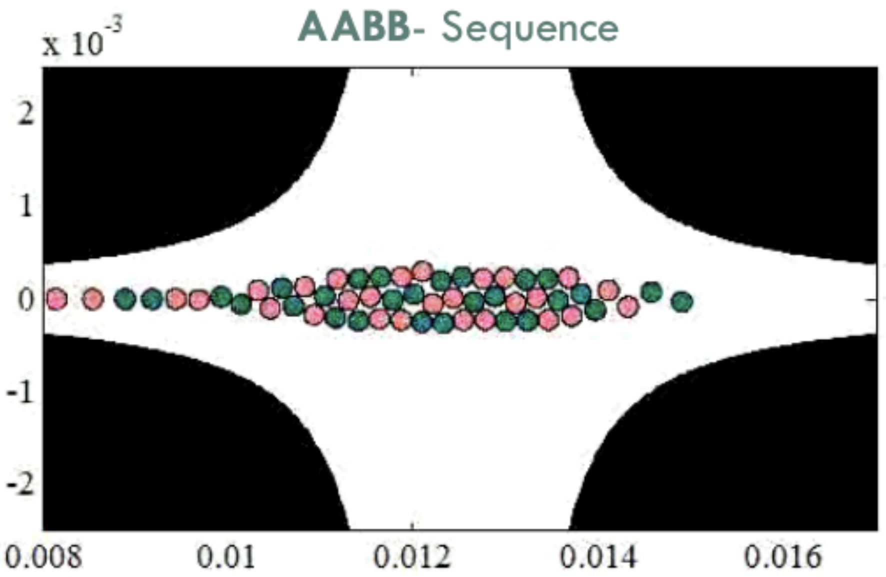
- An intuitive solution…
  - For minimum contact
    - Send 100 A then 100 B
  - For maximum contact
    - Send 1 A then 1 B
- Study: Effect of inlet sequence (A and B)
  - Self-organization of composite drops in a diverging converging channel
  - A and B- same flow characteristics



Composite drop-patterns



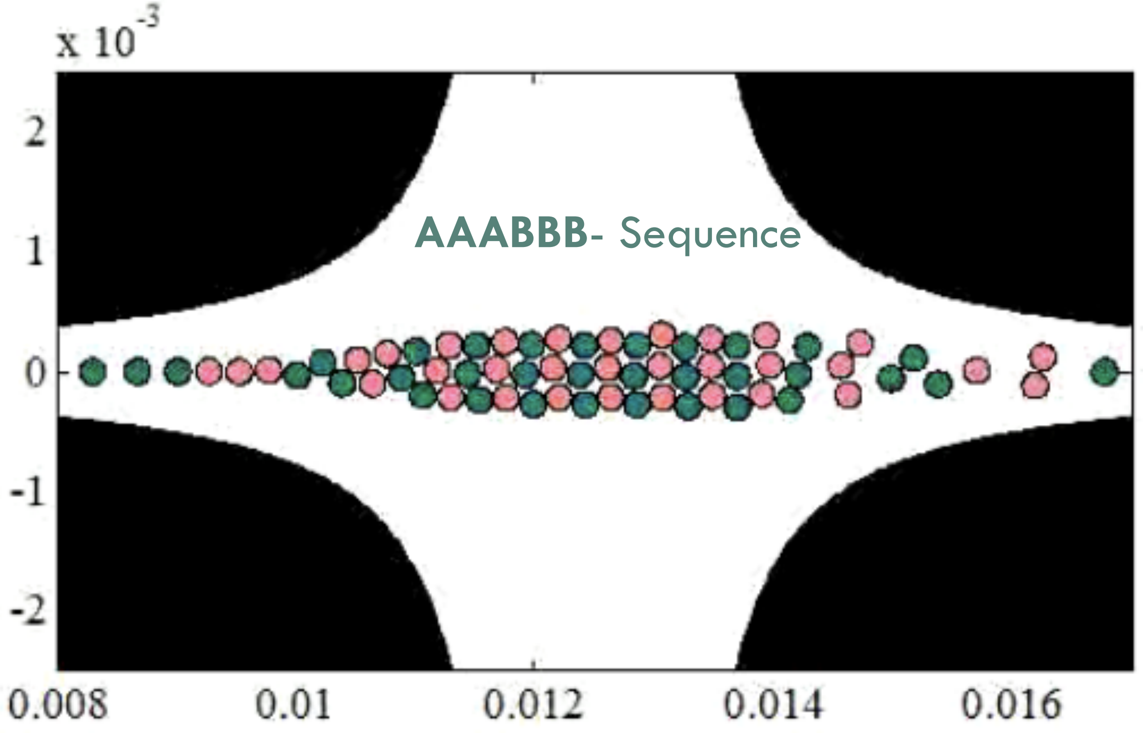
Intuitive solution: Horizontal stratification



How should I send drops into the channel such that the ordered arrangement has a good mix of A and B?

Composite drop-patterns

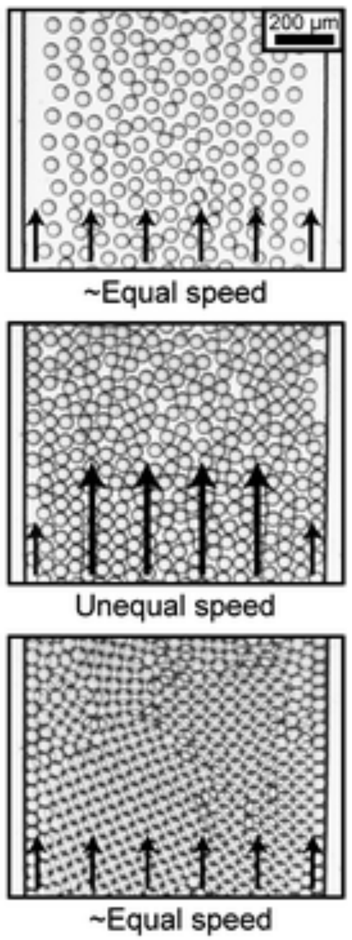
- Vertical stratification of drops
- Possible applications in Optofluidics
  - Drop-dye lasers with a large area of effect



AAABBB- Sequence

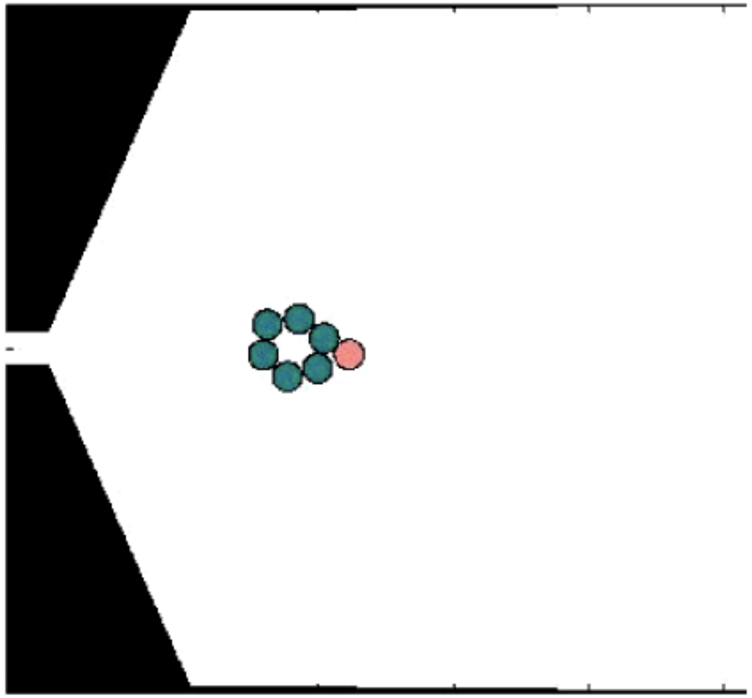
Design problem

- Composite drop arrangement in a 2D ensemble
  - The simplest self-organizing system shows non-intuitive behavior
  - It is a large combinatorial problem
    - A large number of possible inlet sequences
- Design and operation of incubator is a much harder problem
    - Amplified local rearrangement of drops
    - Large number of possible inlet sequences
    - Drop A and B may have different flow characteristics

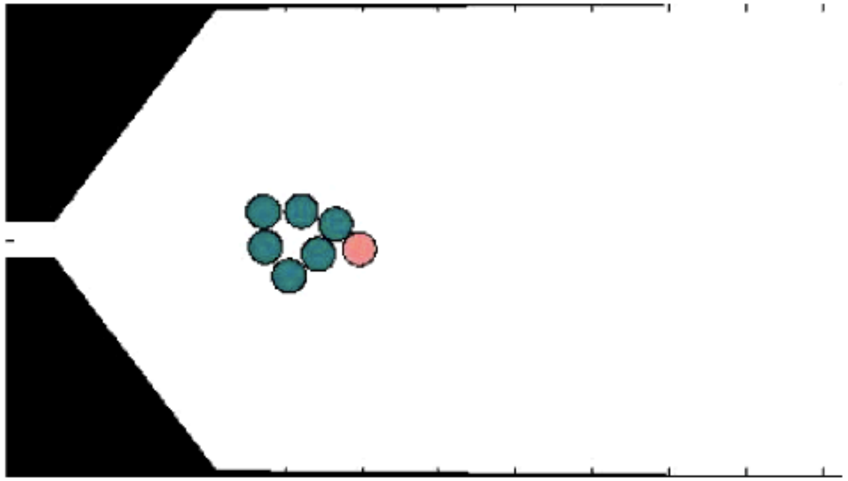


Systematic design and operation of microchannels

Self organization route to particle synthesis



Circular particle



Triangular particle

Work done by Abeynaya G, (B Tech student)

Epilogue

- Agent based framework- complex droplet systems
  - Local interactions are characterized by simple phenomenological models
  - Interactions lead to rich global behavior: **self organization, autocatalytic propagation**
  - New rules and models for newer interactions can be incorporated with ease: **versatility of agent based frameworks**
- Complex behavior of drops
  - Design of 2D channels is non-intuitive
  - Need for a systematic design approach
- Simplicity of the modeling framework: **rational design, process monitoring, fault diagnosis** etc…

Thank you

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Self organization

M. Danny Raj and R. Rengaswamy, *Microfluid. Nanofluidics*, 2014, 17, 527–537.

Passive control applications

D. R. M and R. Rengaswamy, in *2014 European Control Conference (ECC)*, 2014, pp. 1055–1060.

Coalescence propagation

M. Danny Raj and R. Rengaswamy, *Soft Matter*, 2016, 12 (1), 115-122

Composite drops- organization, applications

M. D. Raj and R. Rengaswamy, *Ind. Eng. Chem. Res.*, 2015, 54 (43), 10835-10842