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DYNAMICS AND RHEOLOGY OF VESICLE SUSPENSION IN SHEAR FLOW

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OUTLOOK

- MOTIVATION
- THE NUMERICAL MODEL
- RESULTS
  - SHEAR THINNING
  - CELL-FREE BOUNDARY LAYERS
  - DYNAMICS
- CONCLUSIONS + FUTURE WORK

MOTIVATION

VESICLES ARE CLOSED LIPID MEMBRANES IN AQUEOUS SOLUTION

TENS NANOMETERS < SIZE < HUNDRED MICRONS

LIPOSOMES GIANT VESICLES

- EQUILIBRIUM : SHAPE IS GIVEN BY MINIMIZING THE BENDING ENERGY KEEPING VOLUME AND AREA FIXED

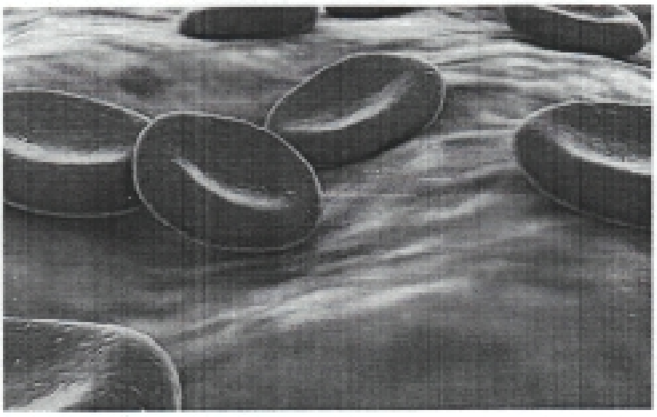
- DYNAMICS : COUPLING BULK HYDRODYNAMICS WITH MEMBRANE ONE

- BIOLOGICAL INTEREST :

"MODEL" FOR RED BLOOD CELLS

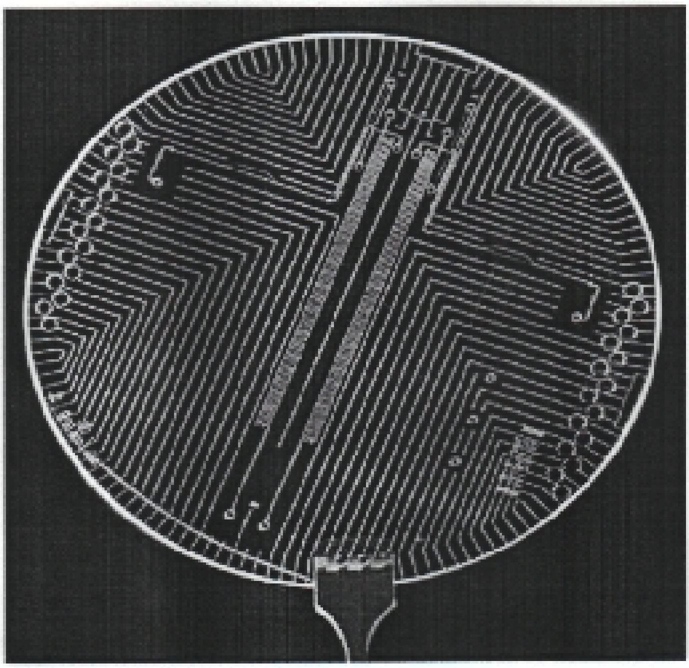
SINGLE CELL DYNAMICS → BLOOD RHEOLOGY

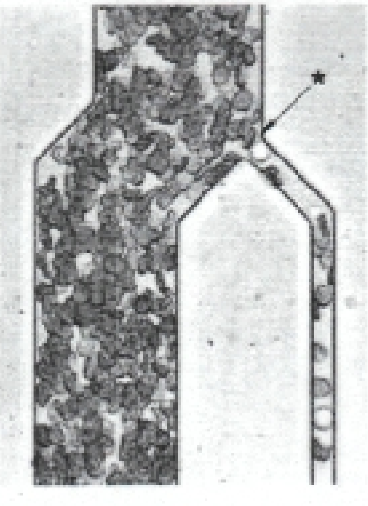
APPLICATIONS



BLOOD RHEOLOGY

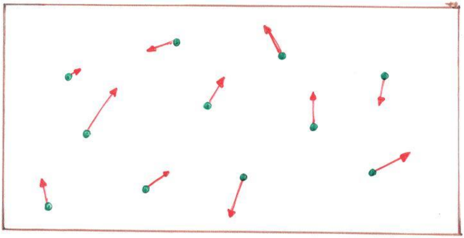
A LAB-ON-CHIP





MICROFLUIDIC DEVICE
TO SORT OUT WBCs
FROM BLOOD SAMPLE

THE MODEL FOR MPCD



N particles

m = mass

$$\left.\begin{array}{l} \vec{r}_i(t) = \text{positions} \\ \vec{v}_i(t) = \text{velocities} \end{array} \quad , \; i = 1, \dots, N \right\} \begin{array}{l}\text{continuous} \\ \text{variables}\end{array}$$

Δt = time step

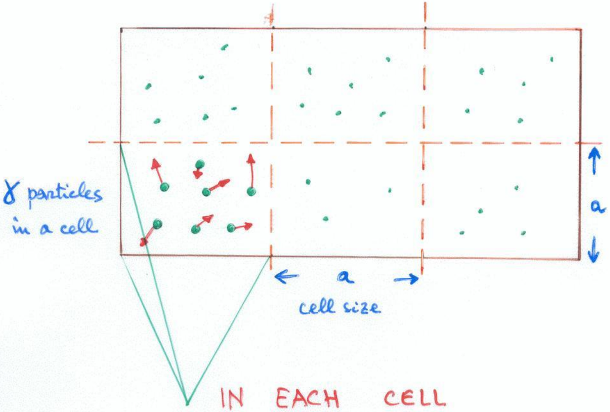
2 - step DYNAMICS

1. PROPAGATION STEP

$$\vec{r}_i(t+\Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\,\Delta t$$

free streaming

2. COLLISION STEP



IN EACH CELL

$\vec{u}(t) = \sum_{i=1}^{\gamma} \vec{v}_i(t) / \gamma$ average (macroscopic) velocity

$\vec{v}_i(t+\Delta t) = \vec{u}(t) + \Omega\left[\vec{v}_i(t) - \vec{u}(t)\right]$ multi-particle collision dynamics

$$\Omega = \begin{pmatrix} \cos\alpha & \pm\sin\alpha \\ \mp\sin\alpha & \cos\alpha \end{pmatrix}, \quad 0 \leq \alpha \leq \pi$$ random rotation

Ω is the same in each cell, but it may differ from cell to cell.

IT FOLLOWS THAT

- EXACT LOCAL CONSERVATION OF MASS, MOMENTUM, ENERGY
  → CORRECT THERMODYNAMIC EQUATIONS IN THE CONTINUUM LIMIT

- PHASE SPACE INVARIANCE UNDER STREAMING-COLLISION
  → EXISTENCE OF H-THEOREM

- PROPAGATION OF HYDRODYNAMIC INTERACTION BY THE SOLVENT
  - NO MOLECULAR DETAILS
  - TURNING ON/OFF HD

MD MODEL FOR THE VESICLE

Length L

Area A

$\tilde{N}$ points

TOTAL POTENTIAL

$$V_T = V_{el} + V_{bend} + V_A$$

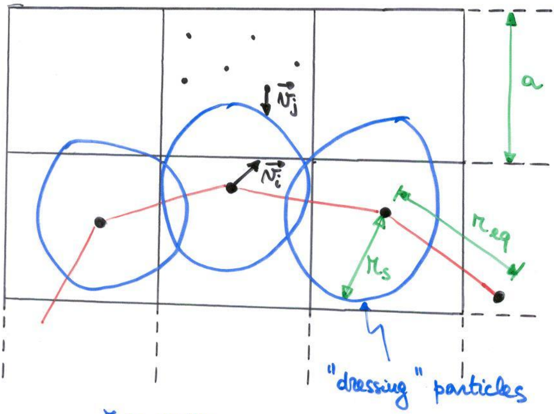
V_{el} = elastic potential (to keep L fixed)

V_A (to keep A fixed)

V_{bend} = bending potential

EQS. OF MOTION INTEGRATED VIA VELOCITY VERLET METHOD

MD + MPCD



$r_{eq} \sim a$

$2 r_s > r_{eq}$

$$\Lambda = \frac{dt_{MPCD}}{dt_{MD}} \gtrsim 10 \quad , \quad \lambda << r_s$$

1) Λ pure MD steps

2) Free streaming of MPCD particles

3) Particles i and j such that $\begin{cases} |\vec{r}_{ij}| < r_s \\ \vec{v}_{ij} \cdot \vec{r}_{ij} < 0 \end{cases}$ scatter via bounce-back

4) The rest of MPCD particles undergo MPC

RELEVANT QUANTITIES

TIME SCALES

$$\tau_s = \eta^0 \frac{R_0^3}{k_{bend}}$$

η^0 = solvent viscosity

k_{bend} = bending rigidity

$$\tau_\gamma = \frac{1}{\gamma}$$

γ = shear rate

LENGTH SCALE

$$R_0 = \frac{L}{2\pi}$$

L = membrane length

$\gamma^* = \gamma \tau_s$ REDUCED SHEAR RATE

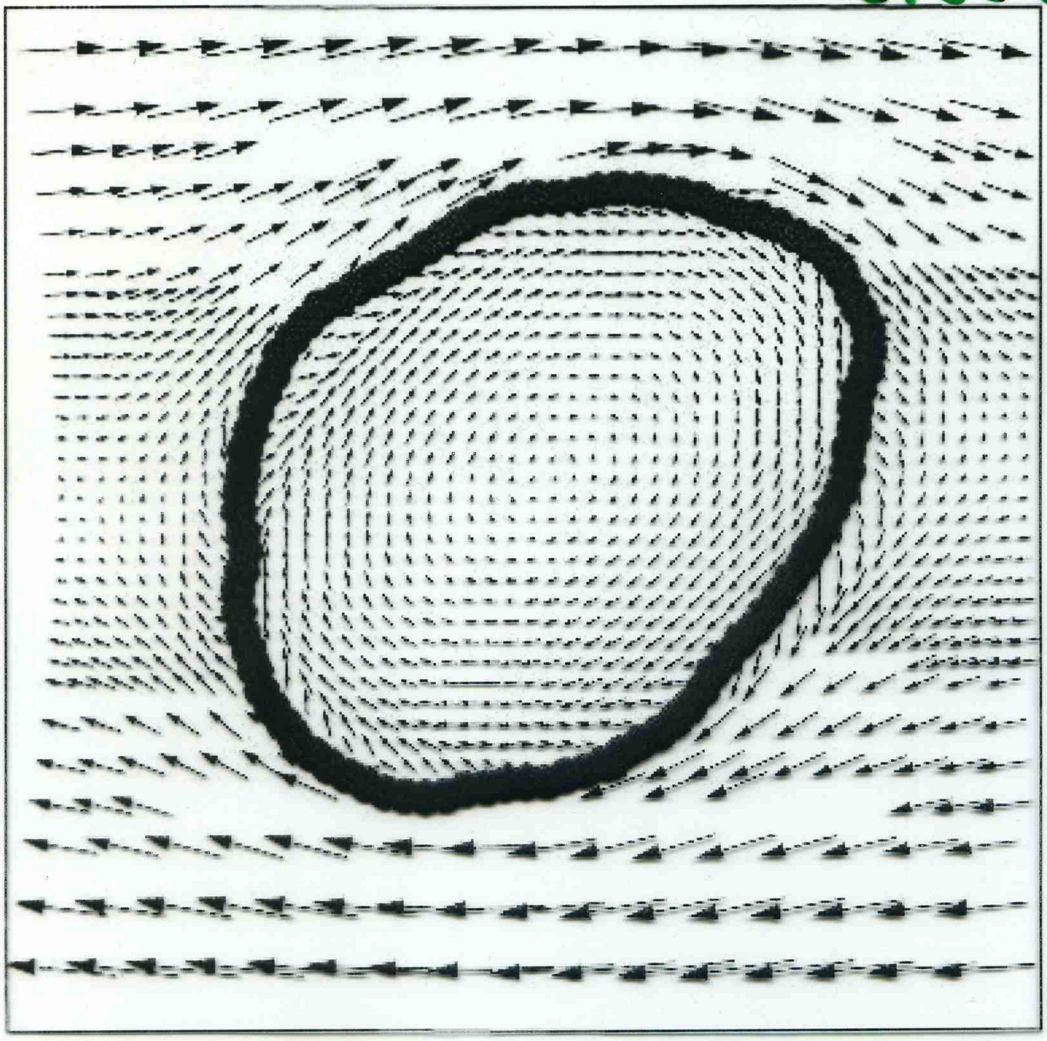
$A^* = \frac{A}{\pi R_0^2}$ REDUCED AREA

$\lambda = \eta^{in} / \eta^{out}$ VISCOSITY CONTRAST

$Re = \gamma m \frac{R_0^2}{\eta^0} \simeq 1$ REYNOLDS NUMBER

TANK TREADING MOTION

FINKEN R, AL, SEIFERT U, GOMPPER G
EPJE 25, 309
(2008)

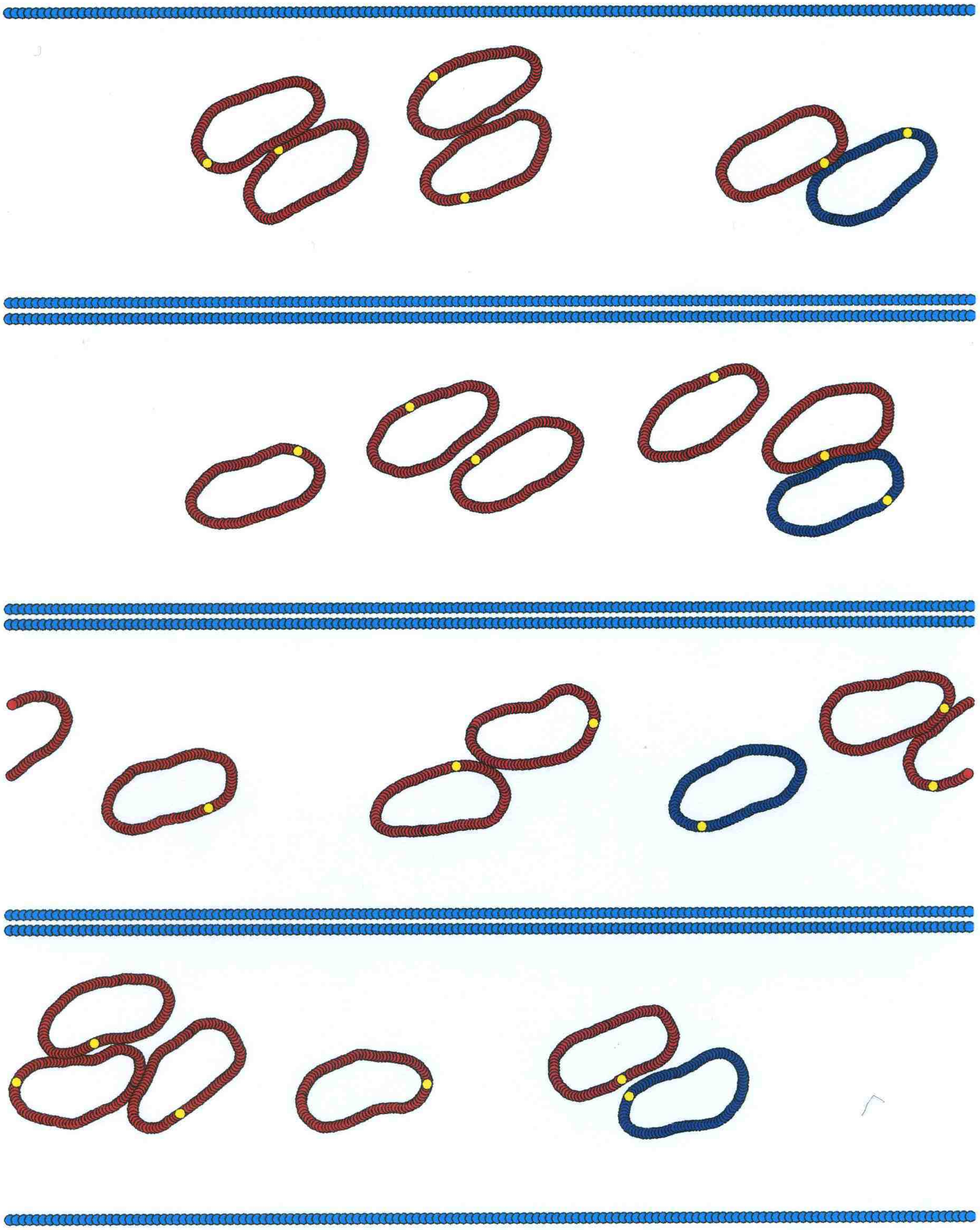


$A^* = 0.8$

$\lambda = 1$

TANK TREADING $\xrightarrow{\text{INCREASING } \lambda}$ TUMBLING

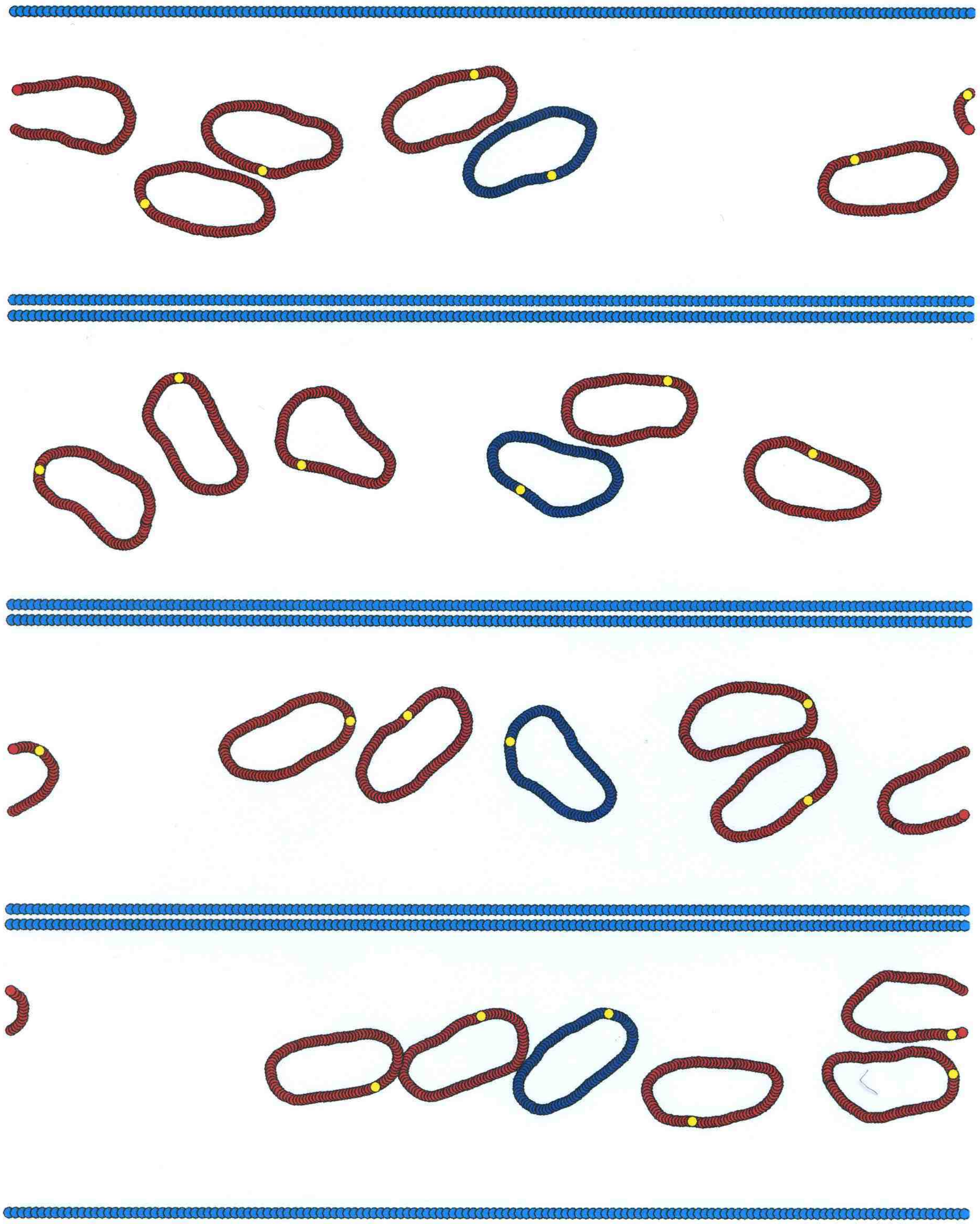
TANK TREADING



$\phi = 0.14$ $A^{*} = 0.8$ $\gamma^{*} = 2.0$

$\lambda = 1$

TUMBLING

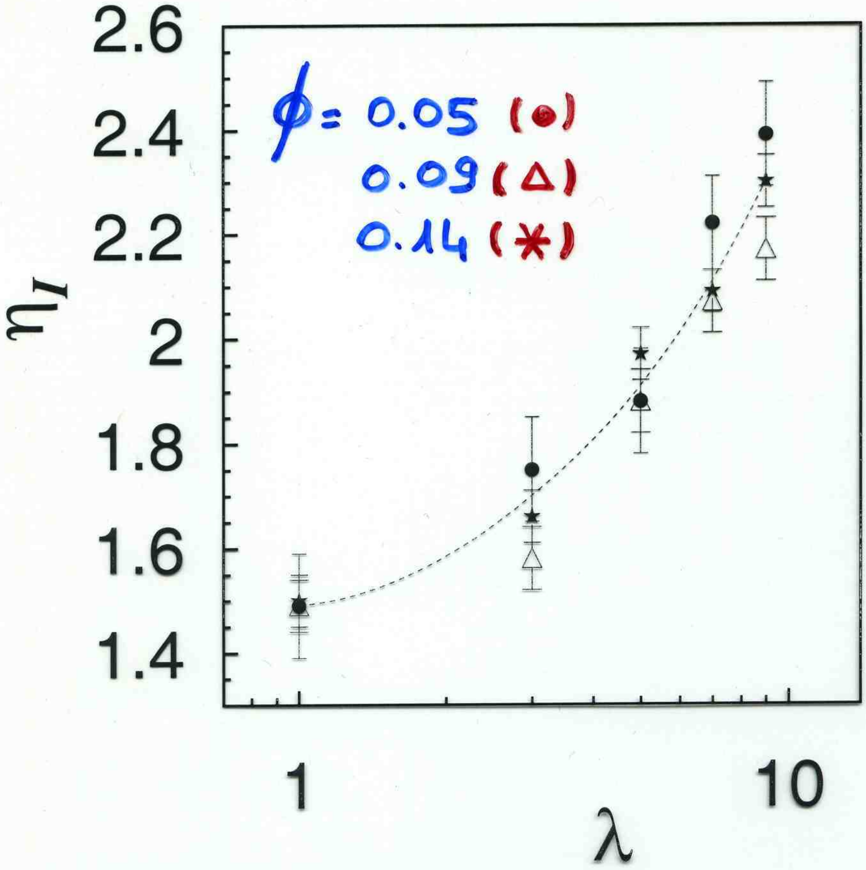


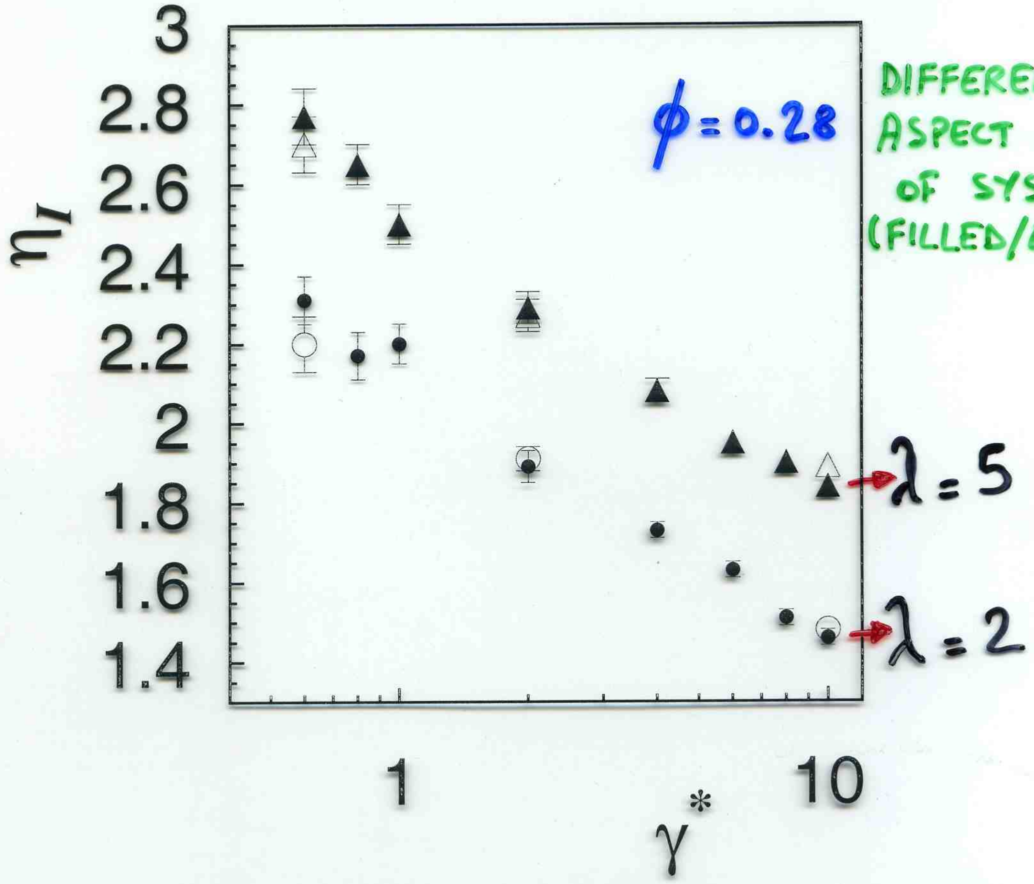
$\phi = 0.14$ $A^* = 0.8$ $\gamma^* = 2.0$

$\lambda = 9$

VISCOSITY

$$\eta_I = \frac{\eta - \eta^0}{\eta^0 \phi}$$



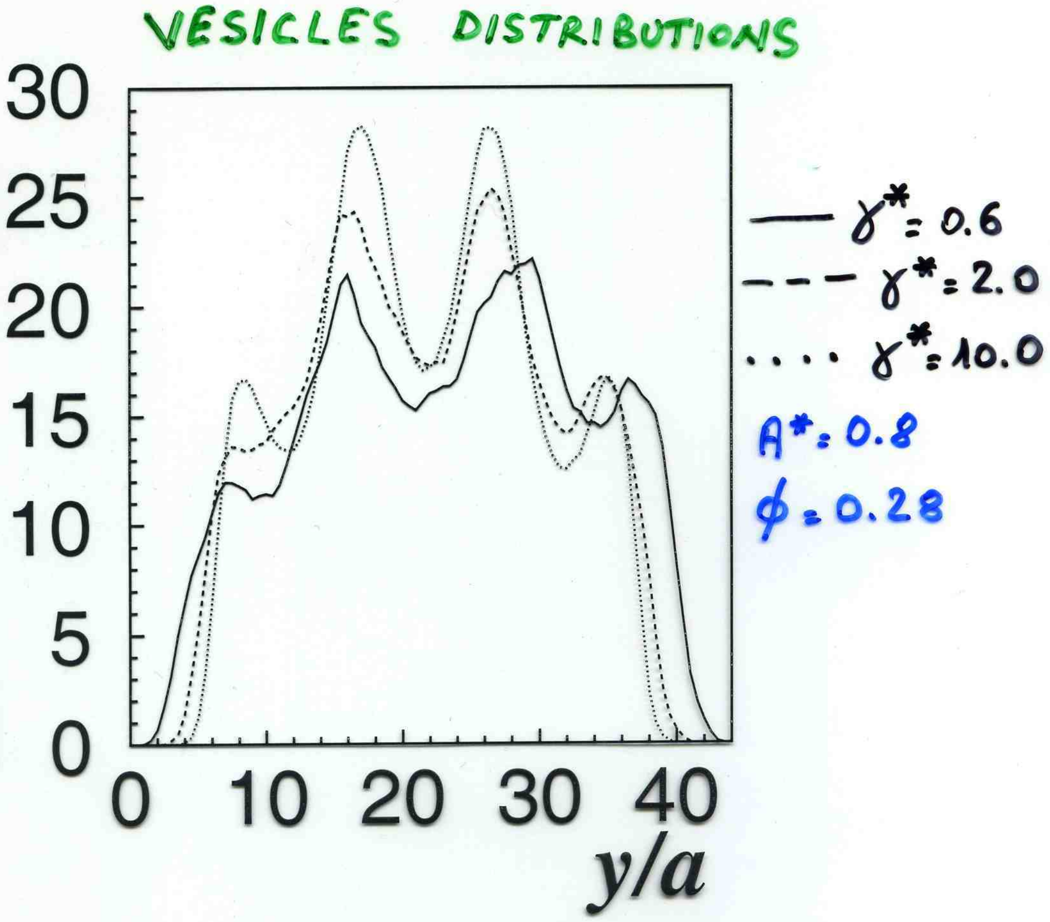


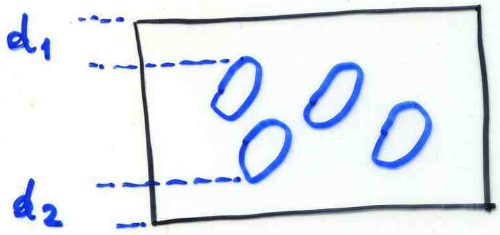
DIFFERENT ASPECT RATIOS OF SYSTEM (FILLED/EMPTY)

SHEAR THINNING

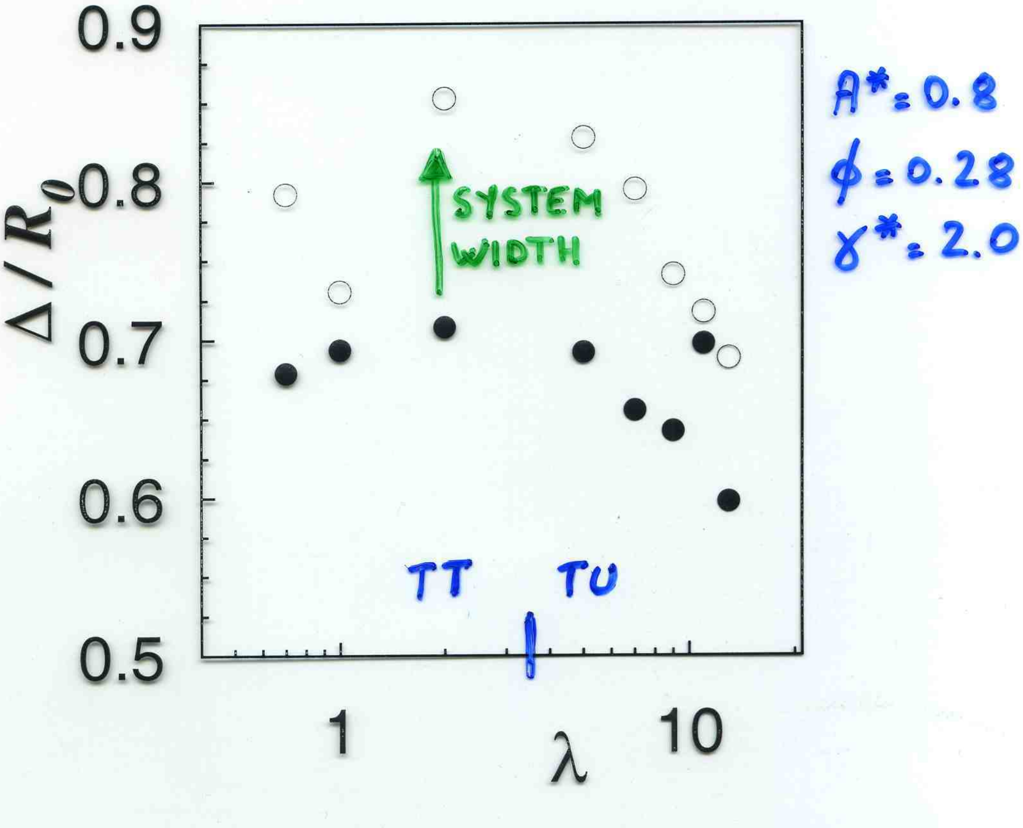
LANING EFFECT
(BOUNDARY LAYERS)

VESICLES DISTRIBUTIONS





$$\Delta = \frac{d_1 + d_2}{2}$$



CONCLUSIONS AND PERSPECTIVES

- DYNAMIC BEHAVIOR OF VESICLE SUSPENSIONS (FROM DILUTE TO CONCENTRATED)
- RHEOLOGY (SHEAR THINNING)
- CELL-FREE BOUNDARY LAYERS
- DETAILED STUDY OF TWO-VESICLE INTERACTIONS (EXPERIMENTS!)
- SELF-PROPELLED VESICLES