# Virtual Erythrocyte - Constitutive Relations and Fluid-Cell Interactions

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# DPD (Dissipative Particle Dynamics)

- 3D membranes immersed in the "ocean" of DPD particles
- walls are made from DPD particles
- solvent-solvent, membranes-solvent interactions

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_j \left( F_{ij}^C + F_{ij}^D + F_{ij}^R \right) \mathbf{e}_{ij}$$

between particles $i$ and $j$; $m_i$ is a mass, $F_i^{\{C,D,R\}}$ are conservative, dissipative, and random force, and $\mathbf{e}_{ij}$ is a unit vector in direction from $i$ to $j$.

# DPD equations

$$F_{ij}^D = -\gamma w^D(r_{ij}/r_c)\mathbf{v}_{ij} \cdot \mathbf{e}_{ij}$$

$$F_{ij}^R = \sigma w^R(r_{ij}/r_c)\frac{\zeta_{ij}}{\sqrt{dt}}, \quad F_{ij}^C = a w^C(r_{ij}/r_c)$$

$$\gamma = \frac{\sigma^2}{2T}, \quad m\frac{d\mathbf{v}_i}{dt} = \sum_j F_{ij}\mathbf{e}_{ij}, \quad \sum_j 1 = N$$

## Parameters

$$\begin{aligned}
\gamma, \sigma, r_c, a, T, m, N \quad &: \quad 7 \\
\gamma, r_c, a, T, m, N \quad &: \quad 6 \text{ (FDT)} \\
\gamma, a, T, N \quad &: \quad 4 \text{ (mass and length)} \\
\gamma, a, N \quad &: \quad 3 \text{ (time)}
\end{aligned}$$

# DPD parameters

$$\gamma_d = \frac{\sqrt{m} N r_c \gamma}{\sqrt{T}} = \frac{N\gamma}{\sqrt{T}}$$

$$a_d = \frac{a m r_c}{T} = \frac{a}{T}, \quad N_d = N$$

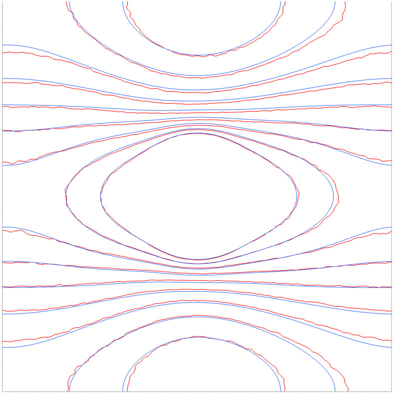
Note

Hydrodynamics should not depend on $a_d$ and $N_d$.

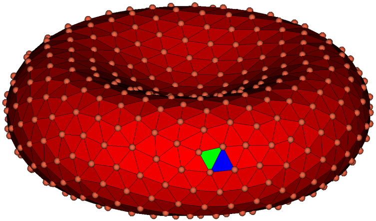
# DPD solvent vs. wall

**Note**

Frozen particles and bounce back (parameter free)



Flow around array of cylinders, iso-lines of horizontal velocity for DPD and finite volume, $\mathrm{Re} = 0.1$



RBC model

# RBC: elastic

$$E^{spring} \propto (x - x_0)^2 + E^{nonlin}$$

$$E_{area}^{tot} \propto \left(A^{tot} - A_0^{tot}\right)^2 \quad E_{area}^{local} \propto (A - A_0)^2$$

$$E_{vol}^{tot} \propto \left(V^{tot} - V_0^{tot}\right)^2 \quad E_{bnd} \propto (\theta - \theta_0)^2$$

## Parameters

- $[\ldots]_0$ are fixed by geometry and mesh
- *volume* and *area* constrains should be strong
- $k_{spring}$, $k_{nonlin}$, $k_{bnd}$

# RBC: viscous

## Note

- from experiment: energy dissipate on the membrane
- $\mathbf{v}_{ij}$ of connected points is small

$$\mathbf{F}_{ij}^{D} = -\gamma^{T}\mathbf{v}_{ij} - \gamma^{C}\mathbf{v}_{ij} \cdot \mathbf{e}_{ij}$$

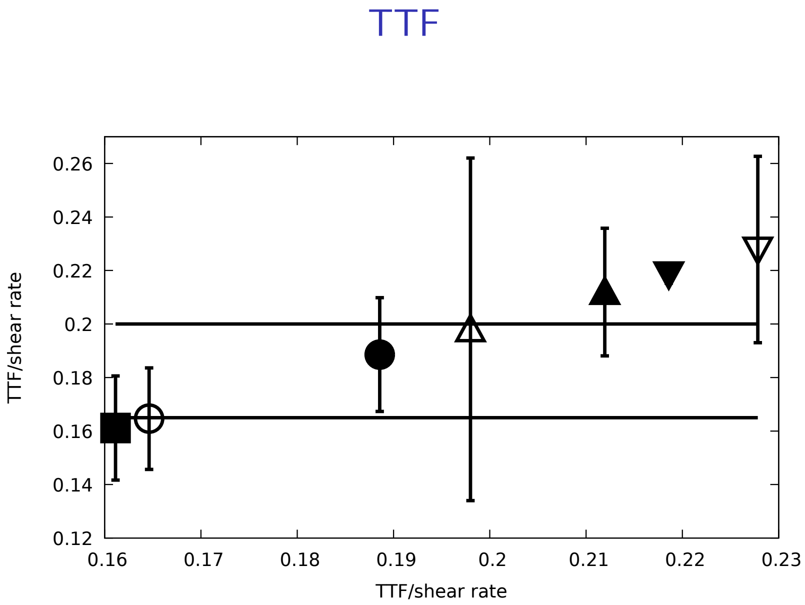
needs a random force $\mathbf{F}_{ij}^{D} \propto T$

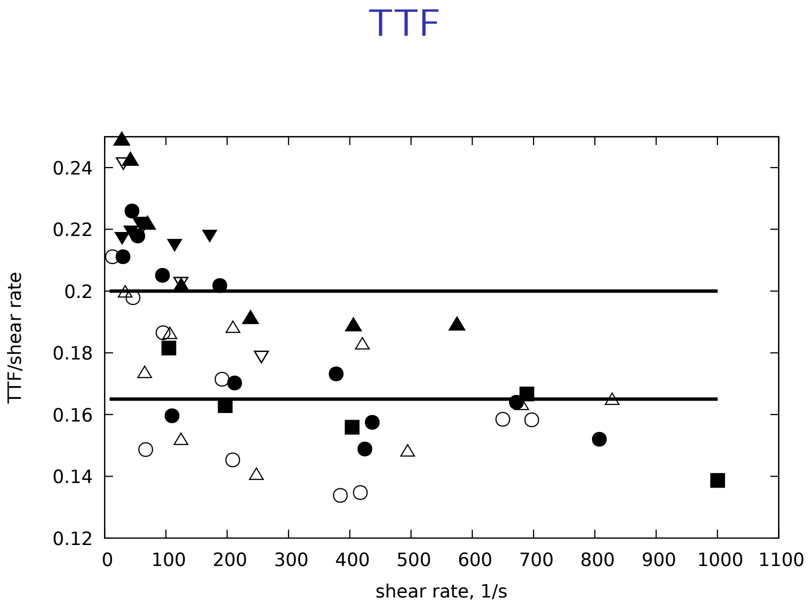
# RBC: inner and outer fluid

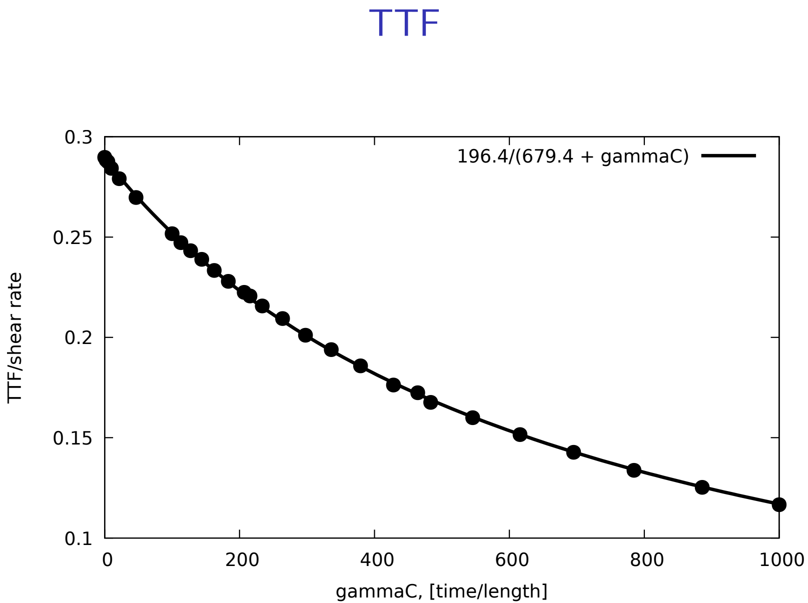
- viscosity is different
- DPD interaction with membrane
- penetrated particles “reset”

# RBC vs. solvent and wall

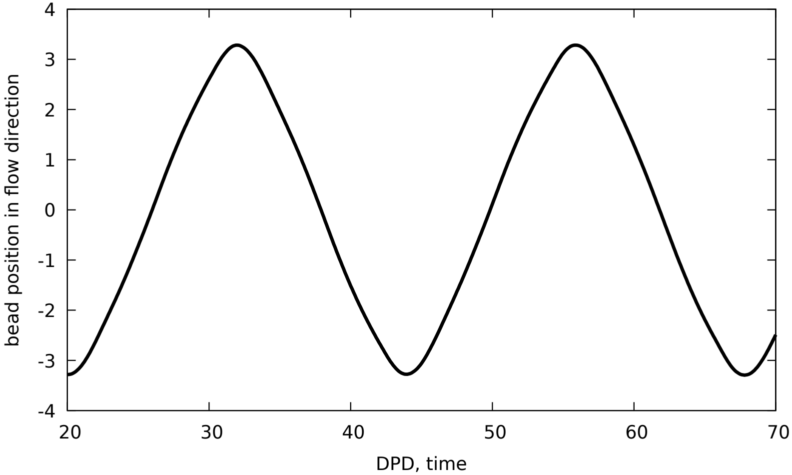
- RBC — solvent: DPD interaction (2 parameters)
- RBC — wall: Bounce back, repulsion (2 parameters)


TTF
TTF/shear rate
TTF/shear rate
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
0.16
0.17
0.18
0.19
0.2
0.21
0.22
0.23


TTF
TTF/shear rate
0.24
0.22
0.2
0.18
0.16
0.14
0.12
0
100
200
300
400
500
600
700
800
900
1000
1100
shear rate, 1/s

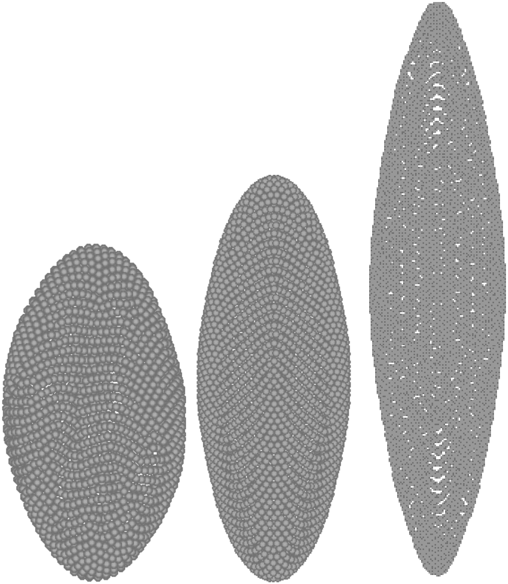

TTF
196.4/(679.4 + gammaC)
0.3
0.25
0.2
0.15
0.1
0
200
400
600
800
1000
TTF/shear rate
gammaC, [time/length]

# Bead

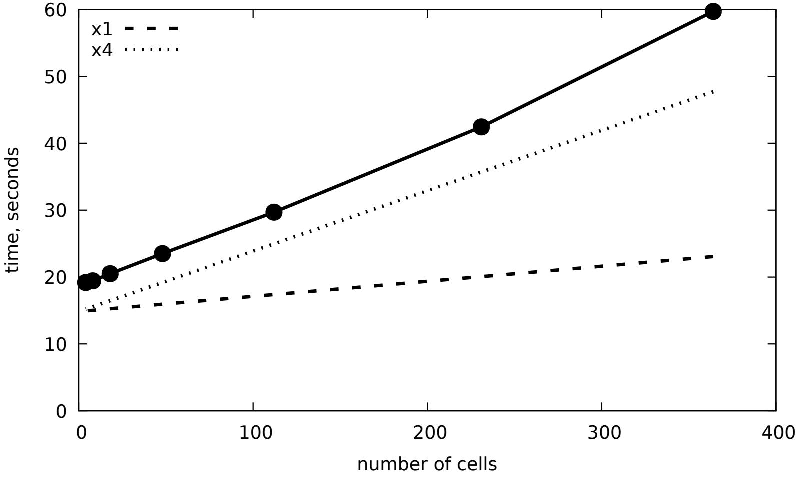


4
3
2
1
0
-1
-2
-3
-4
20
30
40
50
60
70
DPD, time
bead position in flow direction

# Shape



# Performance



Thomas M. Fischer, On the Energy Dissipation in a Tank-treading Human Red Blood Cell, Biophys. J, Vol. 32 (1980), pp. 863-868.