Virtual Erythrocyte

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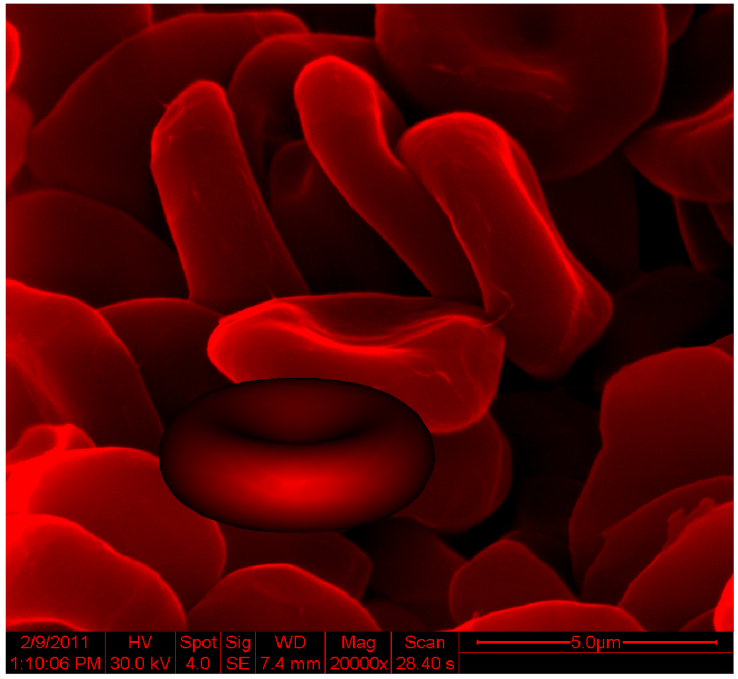
DPD (Dissipative Particle Dynamics)

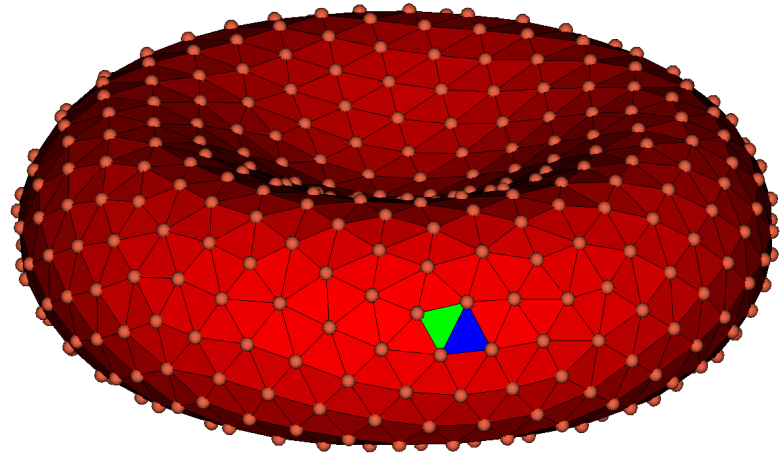
- 3D membranes immersed in the "ocean" of DPD particles
- walls are made from DPD particles
- solvent-solvent, membranes-solvent interactions

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

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.



RBC model



RBC model

RBC: elastic

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

$$E^{tot}_{area} \propto \left(A^{tot} - A^{tot}_0\right)^2 \quad E^{local}_{area} \propto (A - A_0)^2$$

$$E^{tot}_{vol} \propto \left(V^{tot} - V^{tot}_0\right)^2 \quad E_{bnd} \propto (\theta - \theta_0)^2$$

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

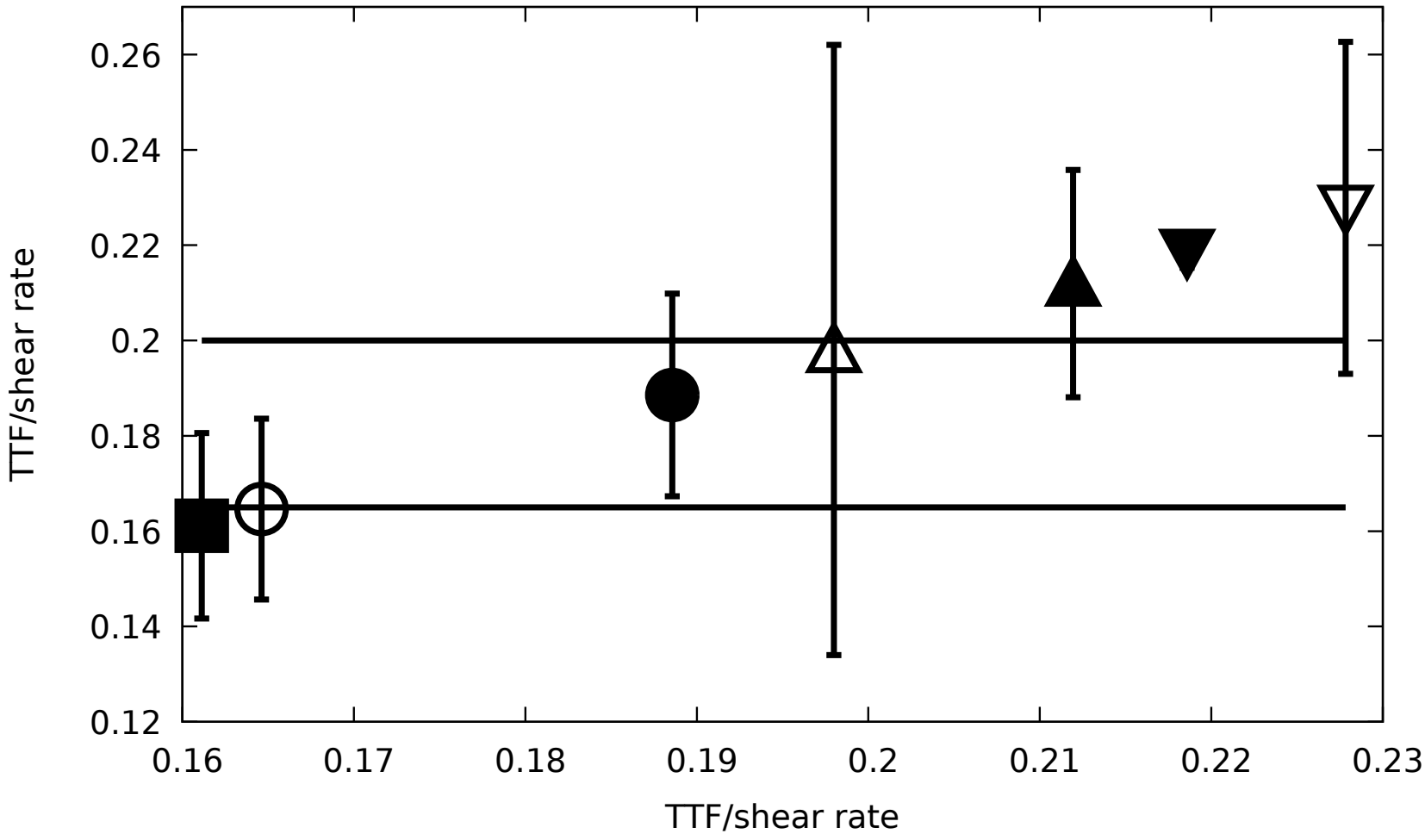
$$\mathbf{F}_{ij}^{D} = -\gamma^{T}\mathbf{v}_{ij} - \gamma^{C}\mathbf{v}_{ij} \cdot \mathbf{e}_{ij}$$

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

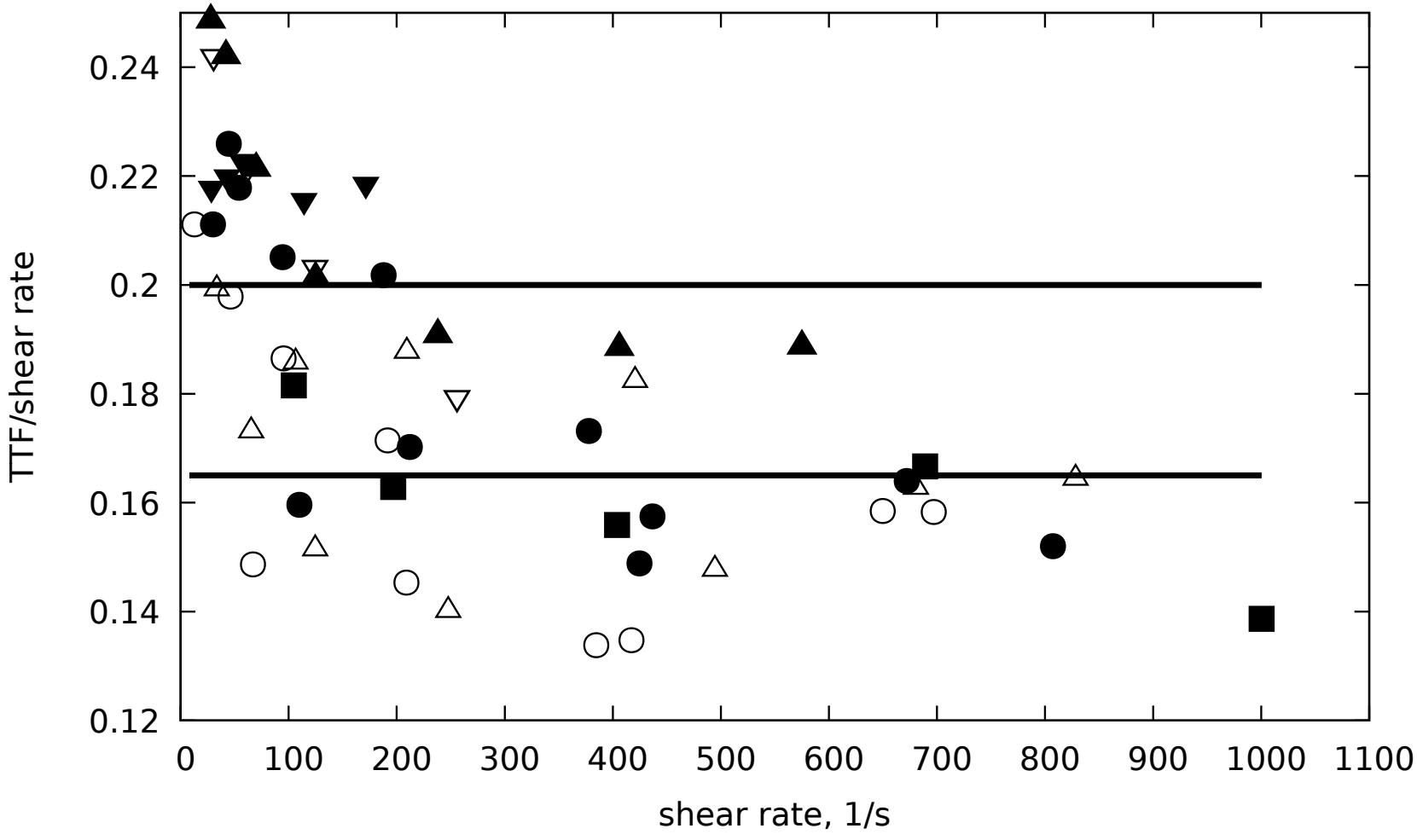
RBC: inner and outer fluid

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

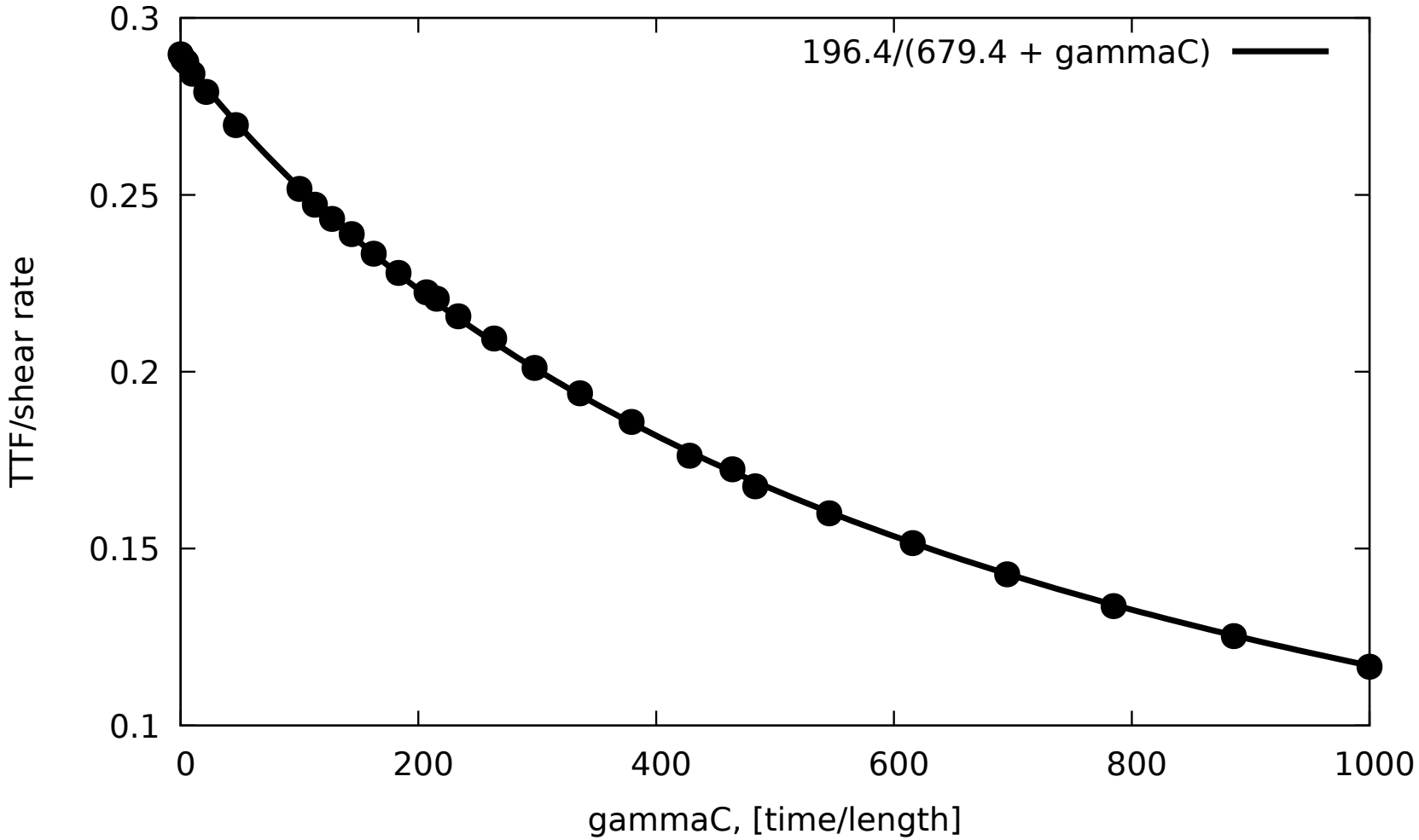
TTF


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

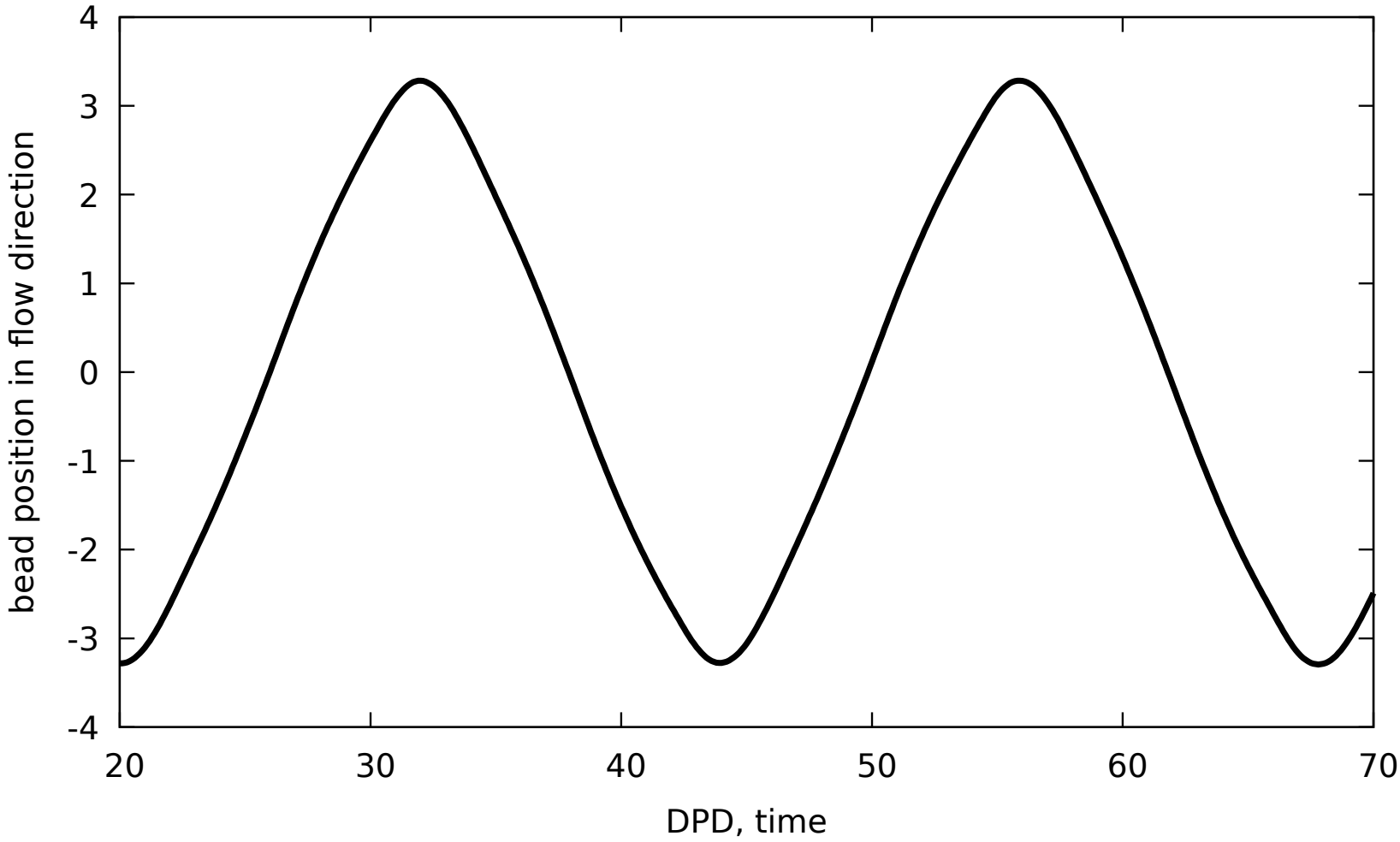
TTF


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

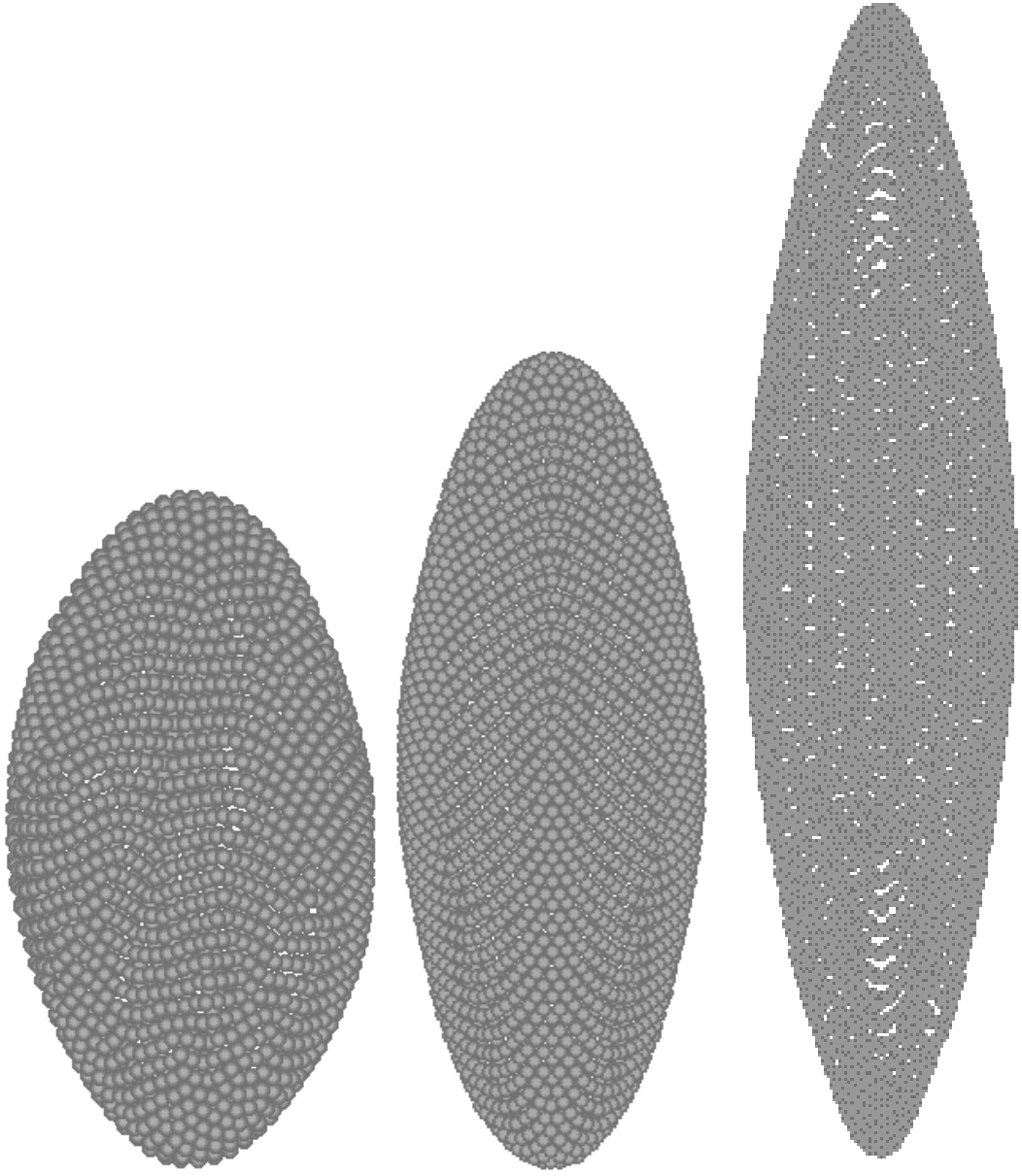
TTF


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

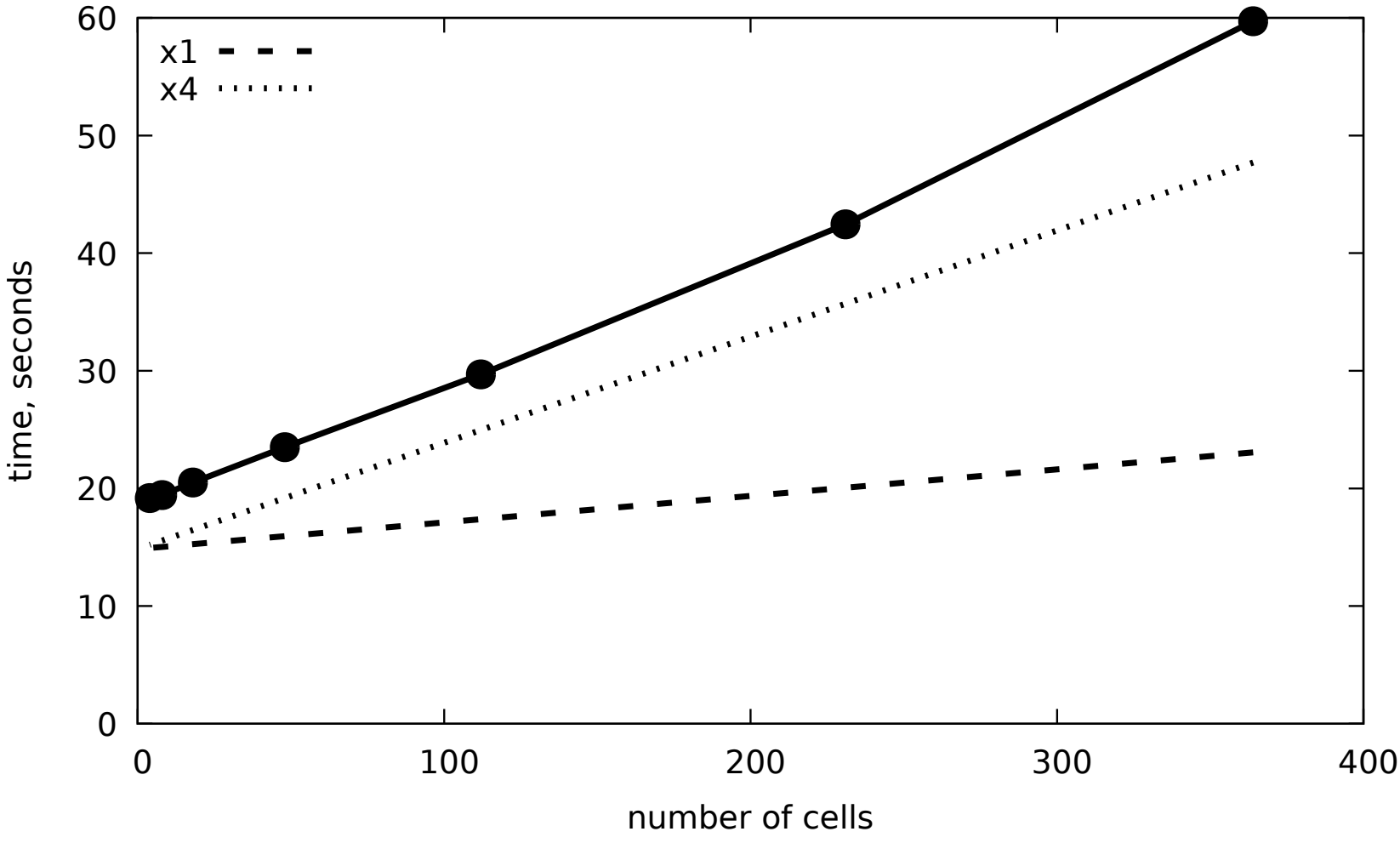
Bead


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

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.