Hydrodynamic factor and effective transport coefficients for suspensions of spherical particles

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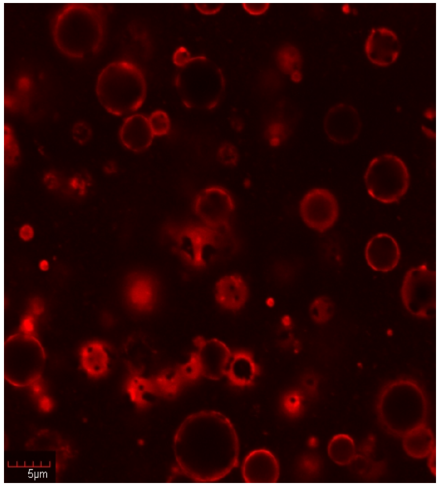
Suspensions



Macro:

Effective viscosity
Sedimentation coefficient
Hydrodynamic factor

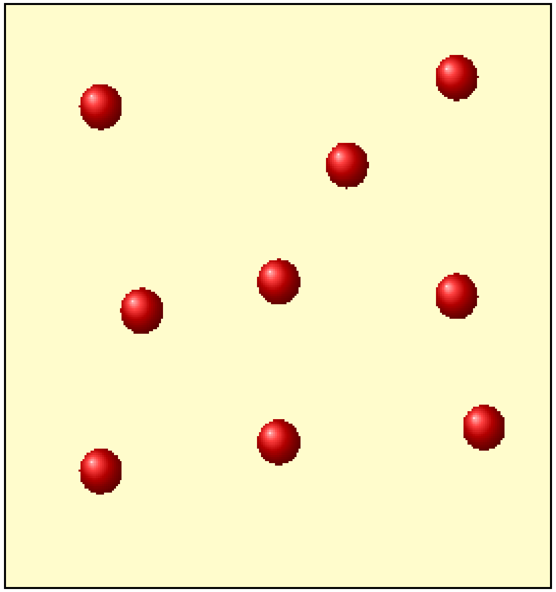
Micro:

Radius of particles
Viscosity of fluid
Number density of particles

“The simplest” system:
Suspension of spherical particles (hard spheres)
Problem: from micro to macro

Hard-sphere suspension – microscopic description

Unbounded liquid,
N particles



Forces acting on suspension: $\mathbf{F}_0(\mathbf{r})$ $\mathbf{F}_{\mathrm{part}}(\mathbf{r})$

fluid

particles

Response of suspension: $\mathbf{V}_i$, $\mathbf{\Omega}_i$, $\sum_{i=1}^{N} \mathbf{F}_i(\mathbf{r})$

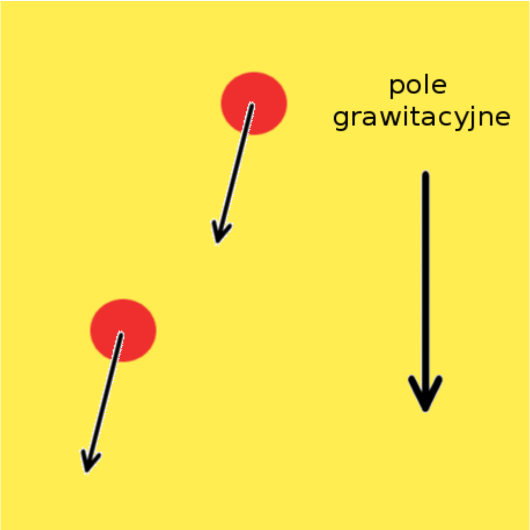
translational and angular velocity

surface forces

Stokes equations:

$$\begin{aligned} \nabla p(\mathbf{r}) - \eta \Delta \mathbf{v}(\mathbf{r}) &= \mathbf{F}_0(\mathbf{r}) + \sum_{i=1}^{N} \mathbf{F}_i(\mathbf{r}) \\ \nabla \cdot \mathbf{v}(\mathbf{r}) &= 0 \end{aligned}$$

Hydrodynamic interactions



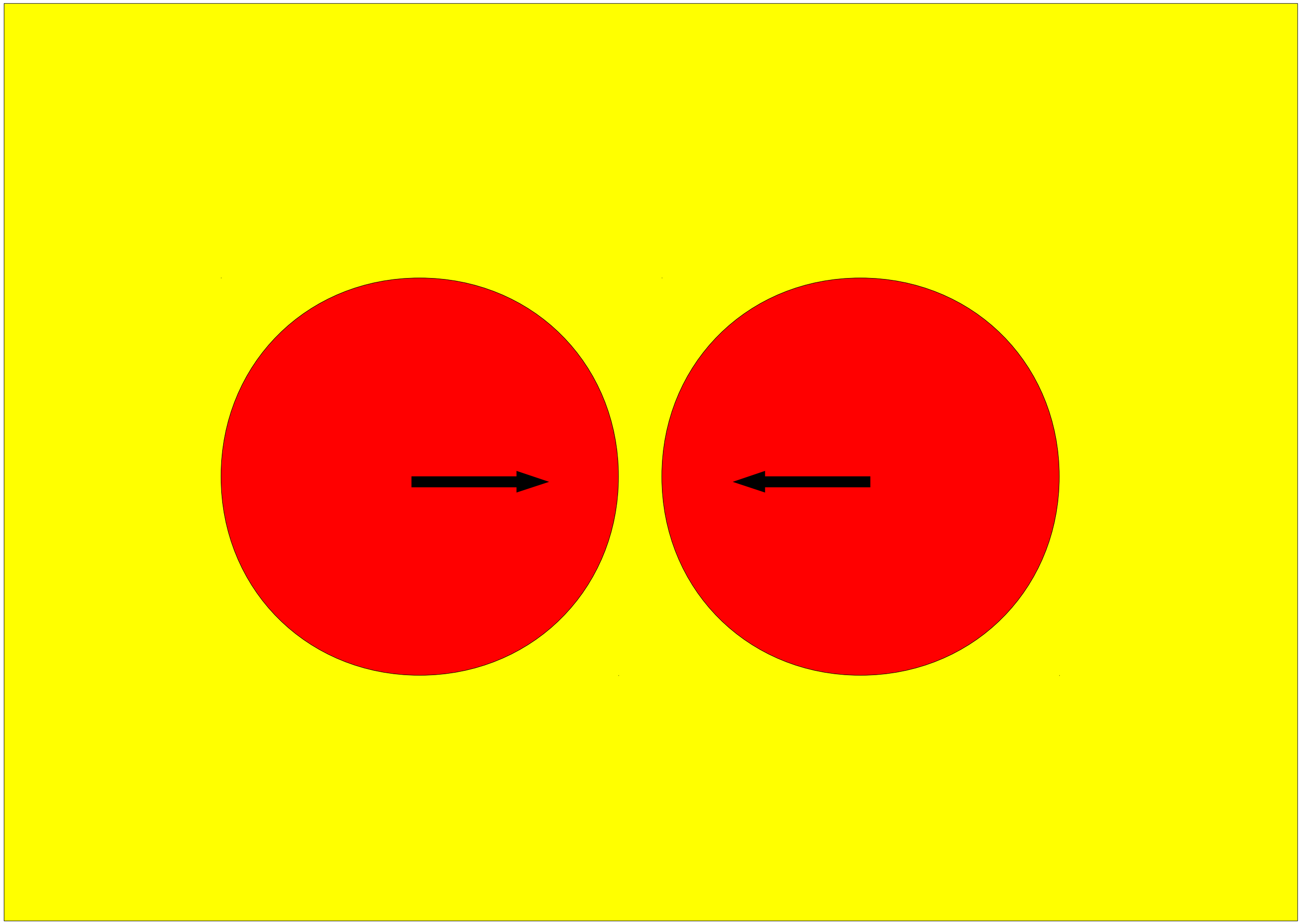
Three important features of hydrodynamic interactions:

- -strong interactions of close particles
- -long-range
- -many-body

Hydrodynamic interactions

Strong interactions of close particles

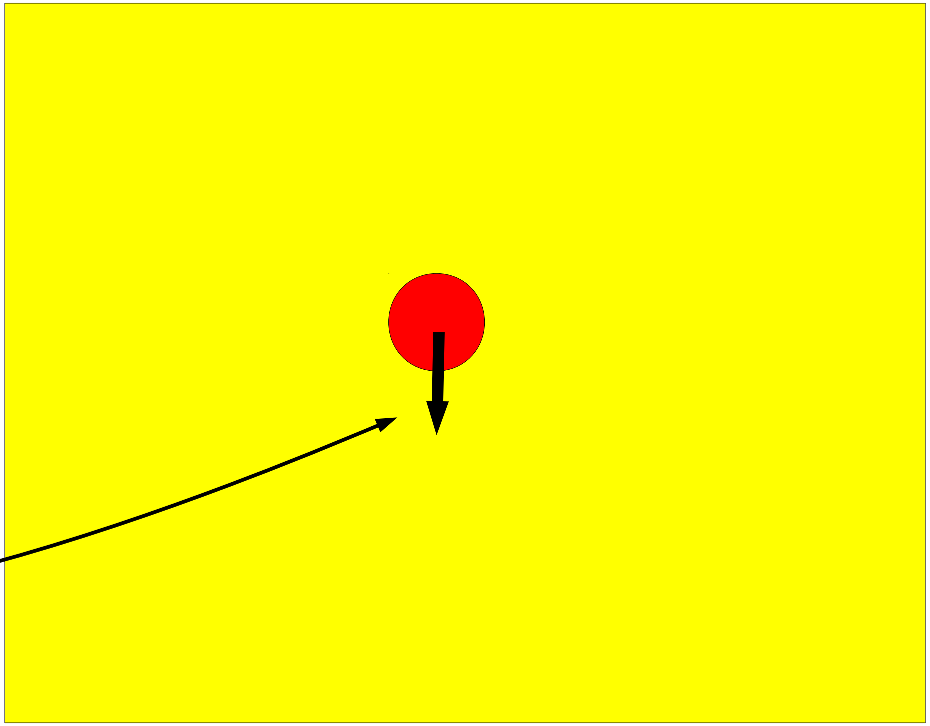
For constant velocities asymptotically infinite drag force



Hydrodynamic interactions

Long-range

Slow decreasing of velocity field around sedimenting single particle



$$\mathbf{v}\left(\mathbf{r}\right) \sim \mathbf{G}\left(\mathbf{r}\right) \cdot \mathbf{F}$$

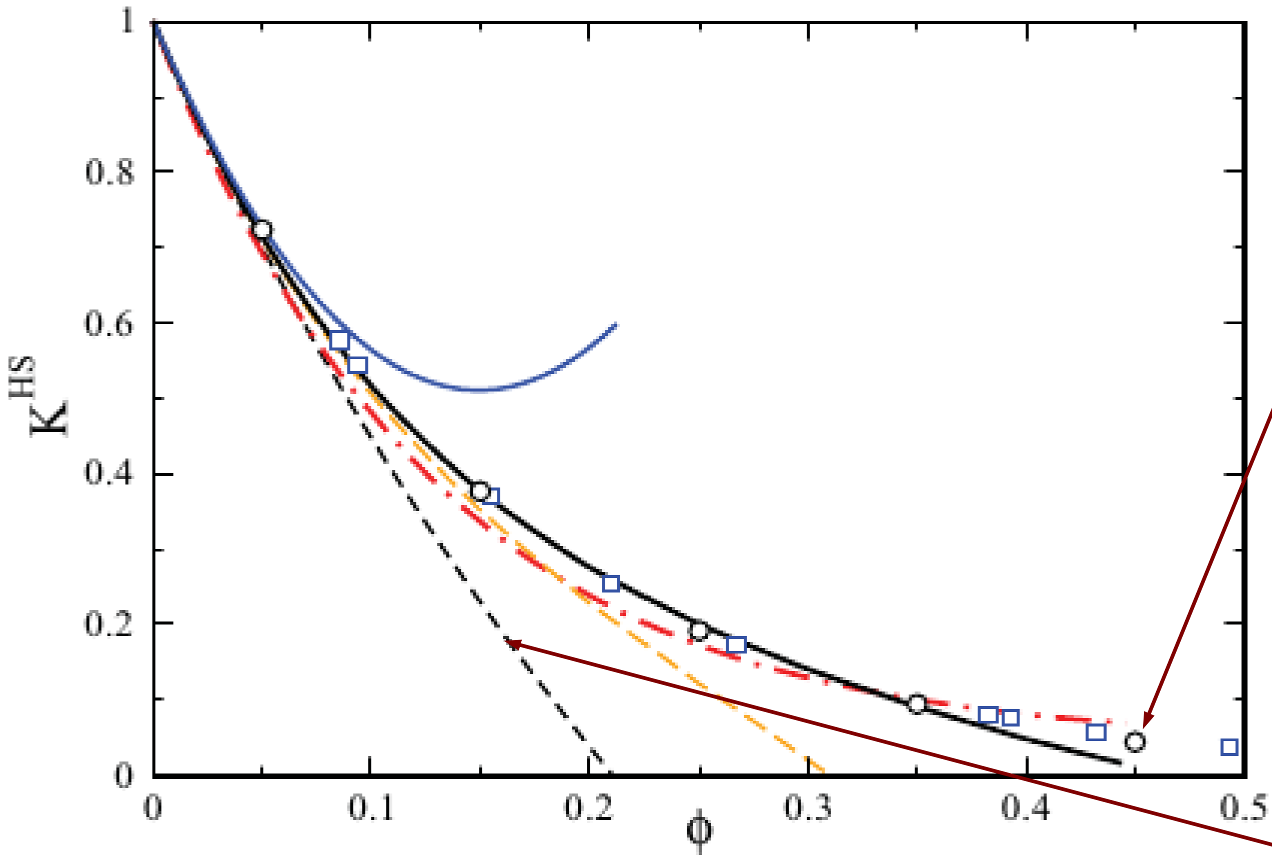
Oseen tensor:

$$\mathbf{G}(\mathbf{r}) = \frac{1}{8\pi\eta}\frac{\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}}}{r}$$

Hydrodynamic interactions

Many-body character

Sedimentation coefficient for hard spheres



numerical simulations
(close to experiments)

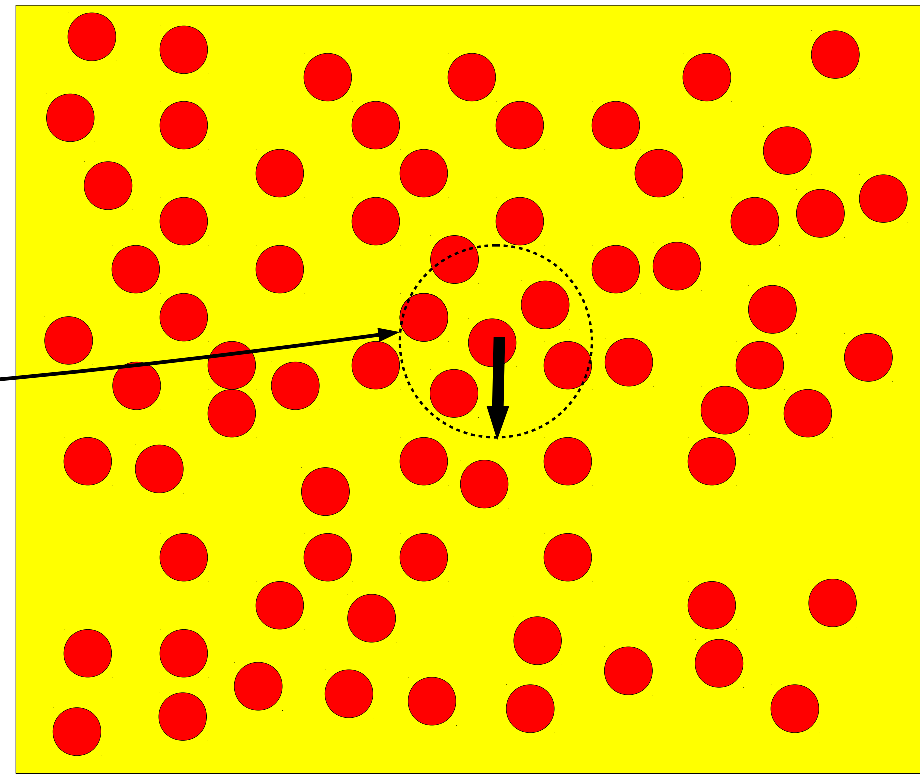
two-body approximation

volume fraction

two-body approximation relevant for volume fractions less than about 5%

Important experiment

Flow caused by force acting on particles in the area



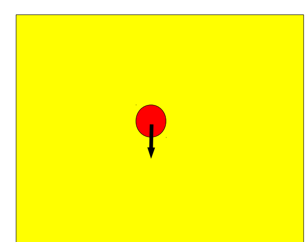
total force acting on particles in the area

$$\mathbf{v}\left(\mathbf{r}\right) \sim \mathbf{G}_{\mathrm{eff}}\left(\mathbf{r}\right)\mathbf{F}$$

effective Green function
(effective propagator):

$$\mathbf{G}_{\mathrm{eff}}(\mathbf{r}) \sim \frac{1}{8\pi\eta_{\mathrm{eff}}}\frac{\mathbf{1}+\hat{\mathbf{r}}\hat{\mathbf{r}}}{r} = \frac{\eta}{\eta_{\mathrm{eff}}}\mathbf{G}(\mathbf{r})$$

at the distance



$$\mathbf{v}\left(\mathbf{r}\right) \sim \mathbf{G}\left(\mathbf{r}\right)\cdot\mathbf{F}$$

Response of suspension

(effective viscosity)

average velocity field of suspension

$$\langle F \rangle = T^{irr} \langle v \rangle$$

average surface force

response operator

Effective viscosity coefficient is given directly by the response operator T^{irr}

Renormalization

short-range hydrodynamic interaction

Cluster expansion (1982):

$$T^{irr} = \sum_{g=1}^{\infty} \sum_{C_1 \ldots C_g} \int dC_1 \ldots dC_g b(C_1|\ldots|C_g) S_I(C_1) G \ldots G S_I(C_g)$$

block distribution function
(configurations of particles)

Oseen tensor (pure liquid):

$$G = \frac{1}{8\pi\eta} \frac{\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}}}{r}$$

Ring expansion (2011):

$$T^{irr} = \sum_{g=1}^{\infty} \sum_{C_1 \ldots C_g} \int dC_1 \ldots dC_g H(C_1|\ldots|C_g) S_I(C_1) G_{\text{eff}} \ldots G_{\text{eff}} S_I(C_g)$$

block correlation function
(configurations of particles);
H=b for g=1,2,
H different from b for g>2.

Effective propagator:

$$\mathbf{G}_{\text{eff}}(\mathbf{r}) \sim \frac{\eta}{\eta_{\text{eff}}} \mathbf{G}(\mathbf{r})$$

Two approximation schemes

Constructing approximate method by carrying over approximation from cluster expansion to ring expansion with the following modification:

$$G \Longrightarrow G_{\mathrm{eff}}$$

Clausius-Mossotti approximation $\Longrightarrow$ Generalized Clausius-Mossotti approximation

(two-body hydrodynamic interactions incomplete – the same as in δγ scheme (1983))

One-ring approximation (fully takes into account two-body hydrodynamic interactions)

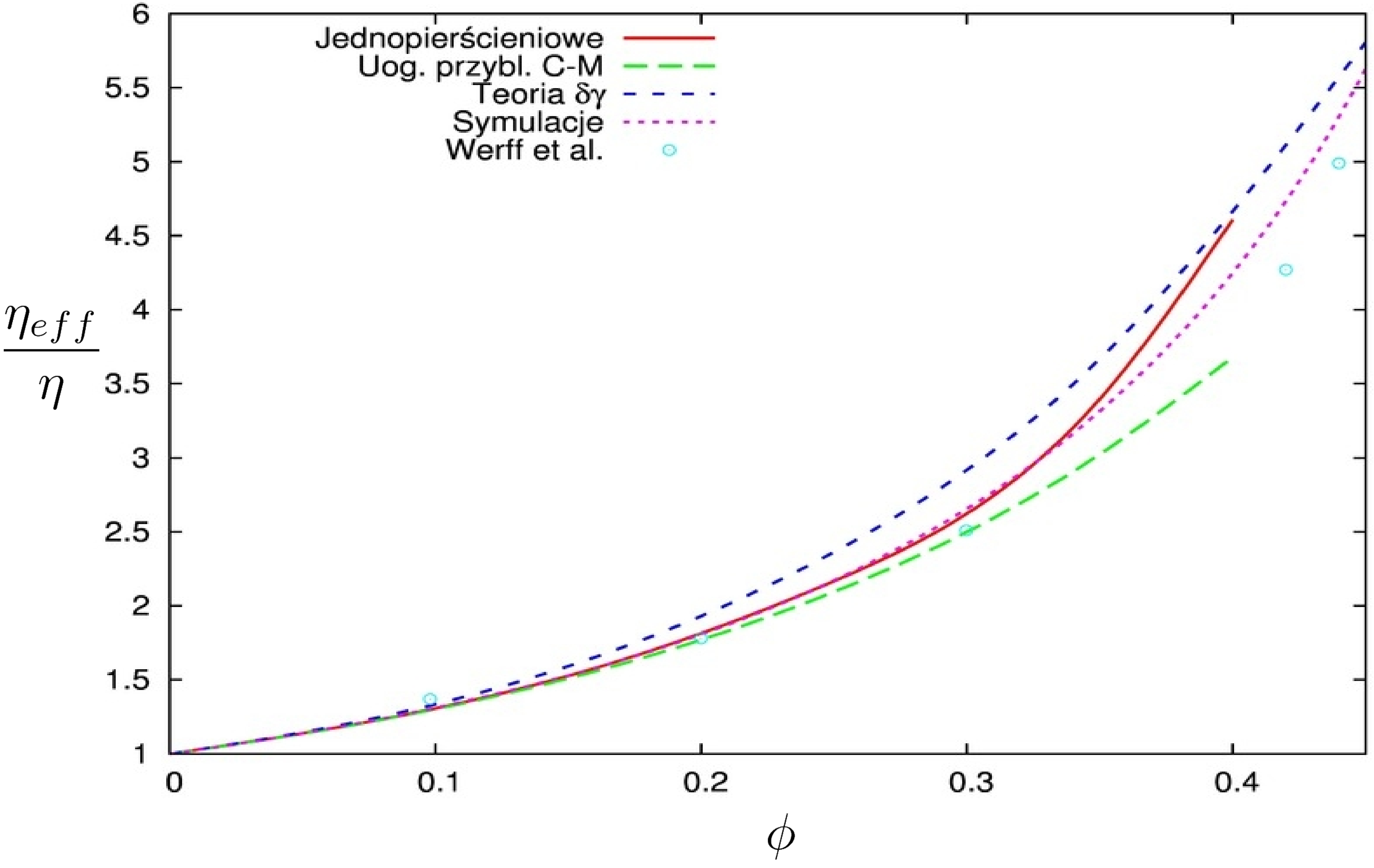
Input:

-volume fraction

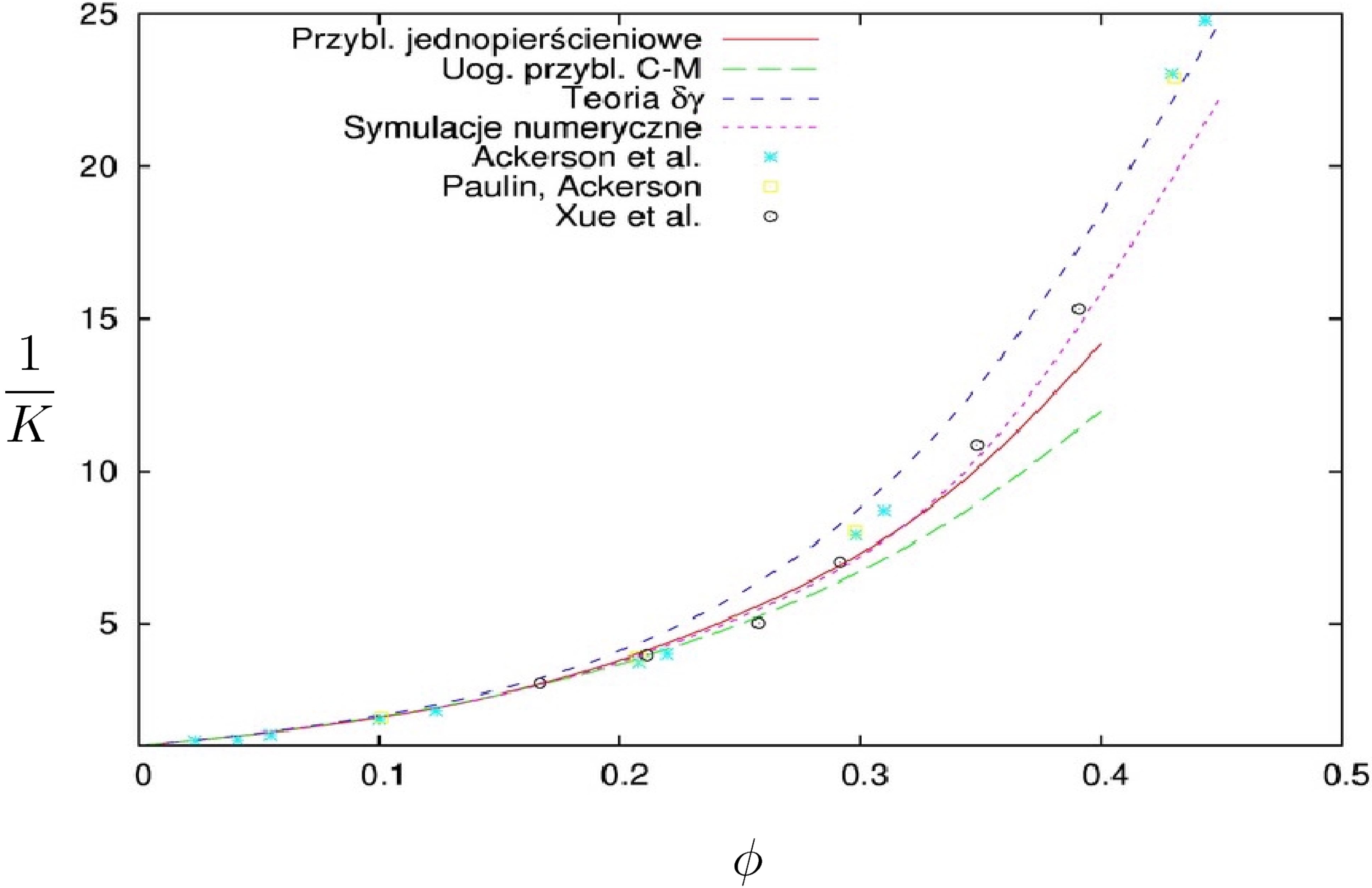
-two-body correlation function (PY); (three-particle correlation function by two body correlation function (Kirkwood))

-two-body hydrodynamic interactions

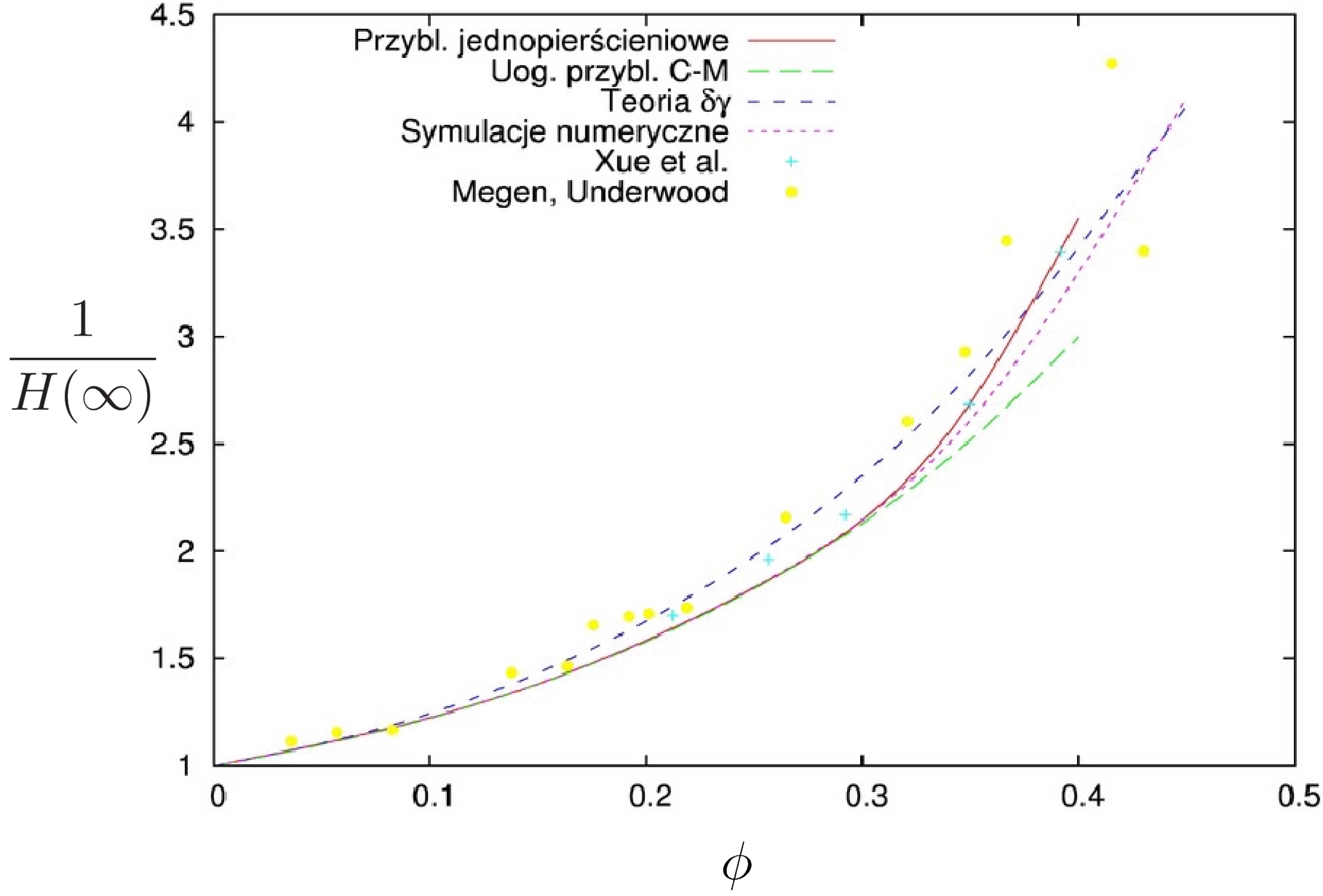
Effective viscosity



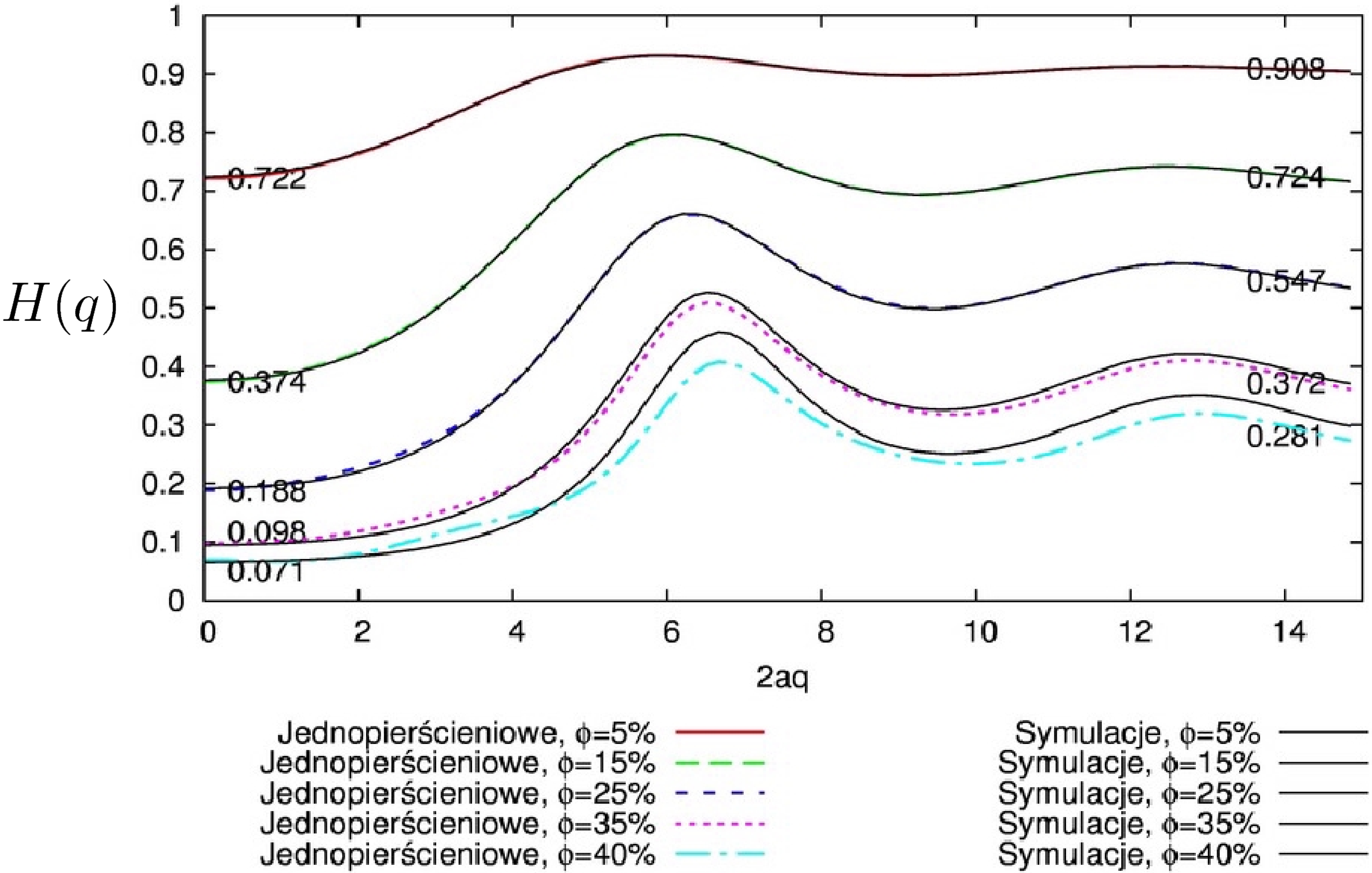
Inverse of sedimentation coefficient $K = H(0)$



Inverse of mobility of single particle in suspension $H(\infty)$



Hydrodynamic factor – one ring approximation



Summary and possibilities

- Long-range, many-body hydrodynamic interactions and strong interactions of close particles are important in suspensions
- Ring expansion for transport coefficients – can grasp all of three above features
- Two approximation schemes for transport coefficients:
  - generalized Clausius-Mossotti approximation (two-body hydrodynamic interactions not fully taken; comparable to δγ scheme),
  - one-ring approximation (full two-body hydrodynamic interactions, much better accuracy than hitherto theoretical methods in comparison to numerical simulations for volume fraction less than 35%)
- Simple generalization for different suspensions of spherical particles (droplets, spherical polymers) with different distributions (charged particles)

Powtarzające struktury T^{irr}

$$T^{irr} = T^{irr}_{CM} \left(1 - [hG]\, T^{irr}_{CM}\right)^{-1}$$

Operator Clausiusa-Mossottiego

Przybliżenie Clausiusa-Mossottiego: $T^{irr}_{CM} \approx nM$

$$T^{irr} = T^{irr}_{RCM} \left(1 - [hG_{\mathrm{eff}}]\, T^{irr}_{RCM}\right)^{-1}$$

Zrenormalizowany operator Clausiusa-Mossottiego

Uogólnione przybliżenie Clausiusa-Mossottiego: $T^{irr}_{RCM} \approx nB$

Metoda przybliżona: w oparciu o przybliżone równanie na T^{irr}_{RCM}

Zrenormalizowany operator Clausiusa-Mossottiego

$$
\begin{aligned}
T^{irr}_{RCM} &= \sum_{r=0}^{\infty} T^{irr}_{RCM,r}, \\
T^{irr}_{RCM,0}\left(\mathbf{R},\mathbf{R}'\right) &= \sum_{C_1} \int dC_1 n\left(C_1\right) S_I(C_1;\mathbf{R},\mathbf{R}'), \\
T^{irr}_{RCM,1}\left(\mathbf{R},\mathbf{R}'\right) &= \sum_{C_1,C_2} \int dC_1 dC_2 \int d^3\mathbf{R}_1 d^3\mathbf{R}_2 \ \left[H(C_1|C_2) - h\left(\mathbf{R}_1,\mathbf{R}_2\right)\right] \times \\
&\quad \times n\left(C_1\right) S_I(C_1;\mathbf{R},\mathbf{R}_1) G_{eff}\left(\mathbf{R}_1,\mathbf{R}_2\right) n\left(C_2\right) S_I(C_2;\mathbf{R}_2,\mathbf{R}'), \\
&\quad \ldots
\end{aligned}
$$

Przybliżenie jednopierścieniowe

Conajwyżej jeden pierścień w T^{irr}_{RCM}

Conajwyżej dwuciałowe oddziaływania w S_I

Przybliżenie Kirkwooda na trójciałową funkcję korelacji:

$$n\left(123\right) \approx n^3 g\left(12\right) g\left(13\right) g\left(23\right)$$

Renormalizcja oddziaływań dwuciałowych:

$$S_I(12) -> B S_I(12) B \qquad\qquad T^{irr} = nB + B\mathcal{T}^{irr}B$$

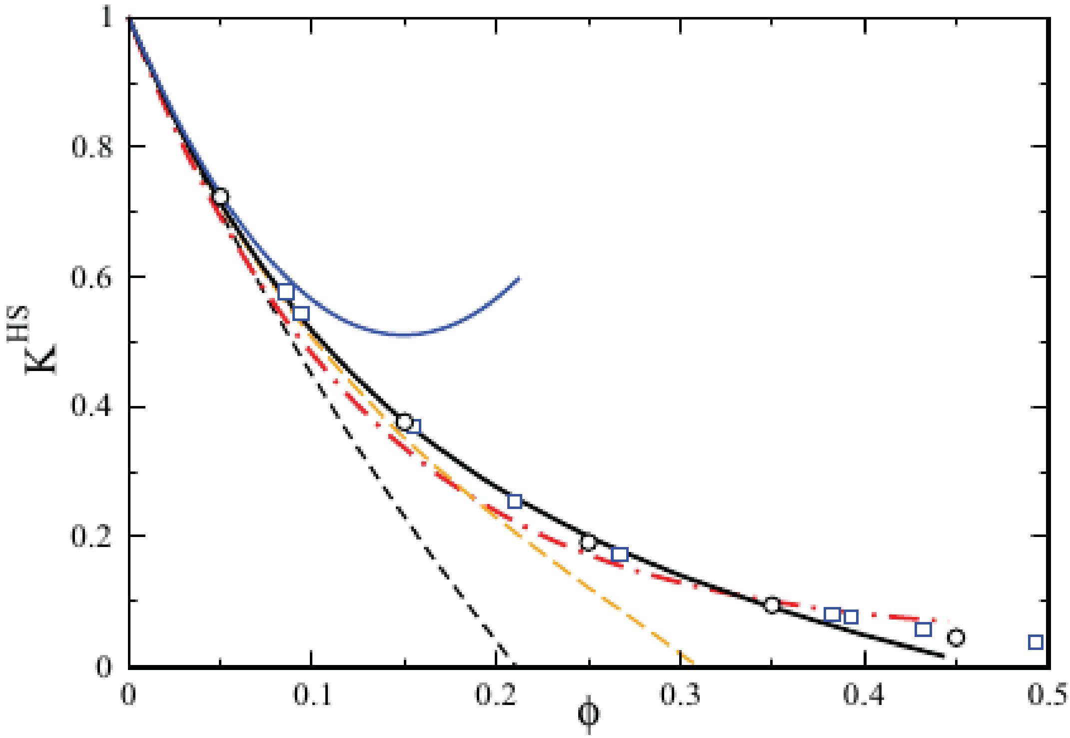


Fig. 6.3: *Reduced short-time sedimentation coefficient, K^{HS}, of neutral hard spheres. Open circles: Hydrodynamic force multipole simulation data by Abade et al. [26]. Open Squares: Lattice-Boltzmann simulation data by Segrè et al. [208]. Black dashed line: PA-scheme result. Dashed-dotted red line: uncorrected $\delta\gamma$-scheme result. Dashed orange line: self-part corrected $\delta\gamma$-scheme result, with $d_s/d_{t,0}$ taken from the PA-scheme. Solid black line: self-part corrected $\delta\gamma$-scheme result, with $d_s/d_{t,0}$ according to Eq. (4.26). Solid blue line: second-order virial result $K^{HS} = 1 - 6.546\phi + 21.918\phi^2$ [166]. The static structure factor input was obtained using the analytic Percus-Yevick solution.*