Hydrodynamic function and effective transport coefficients for suspensions of spherical particles

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INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

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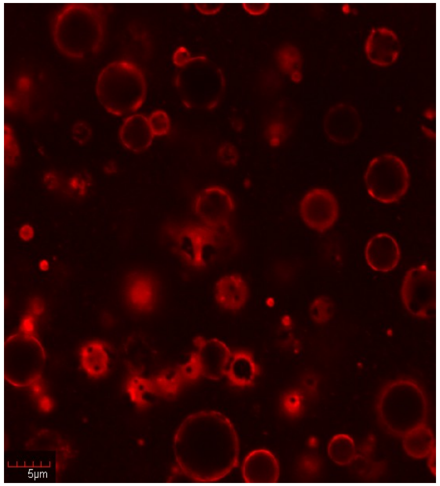
Suspensions



Macro:

Effective viscosity
Sedimentation coefficient
Hydrodynamic factor

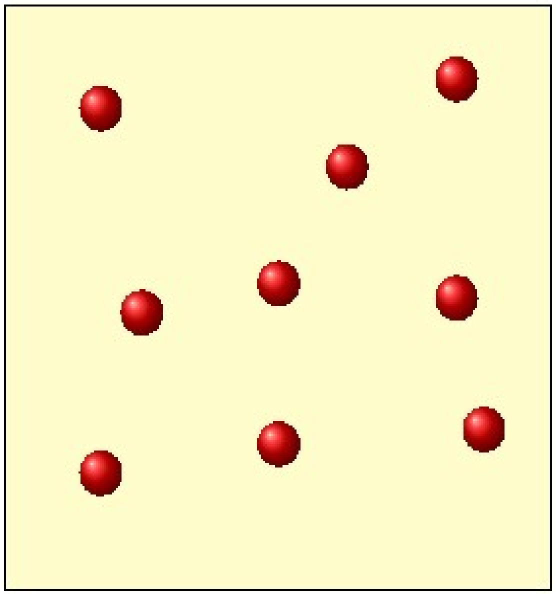
Micro:

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

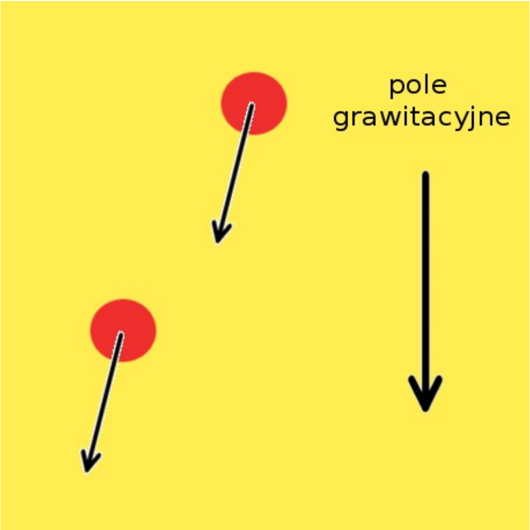
translational and angular velocity

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



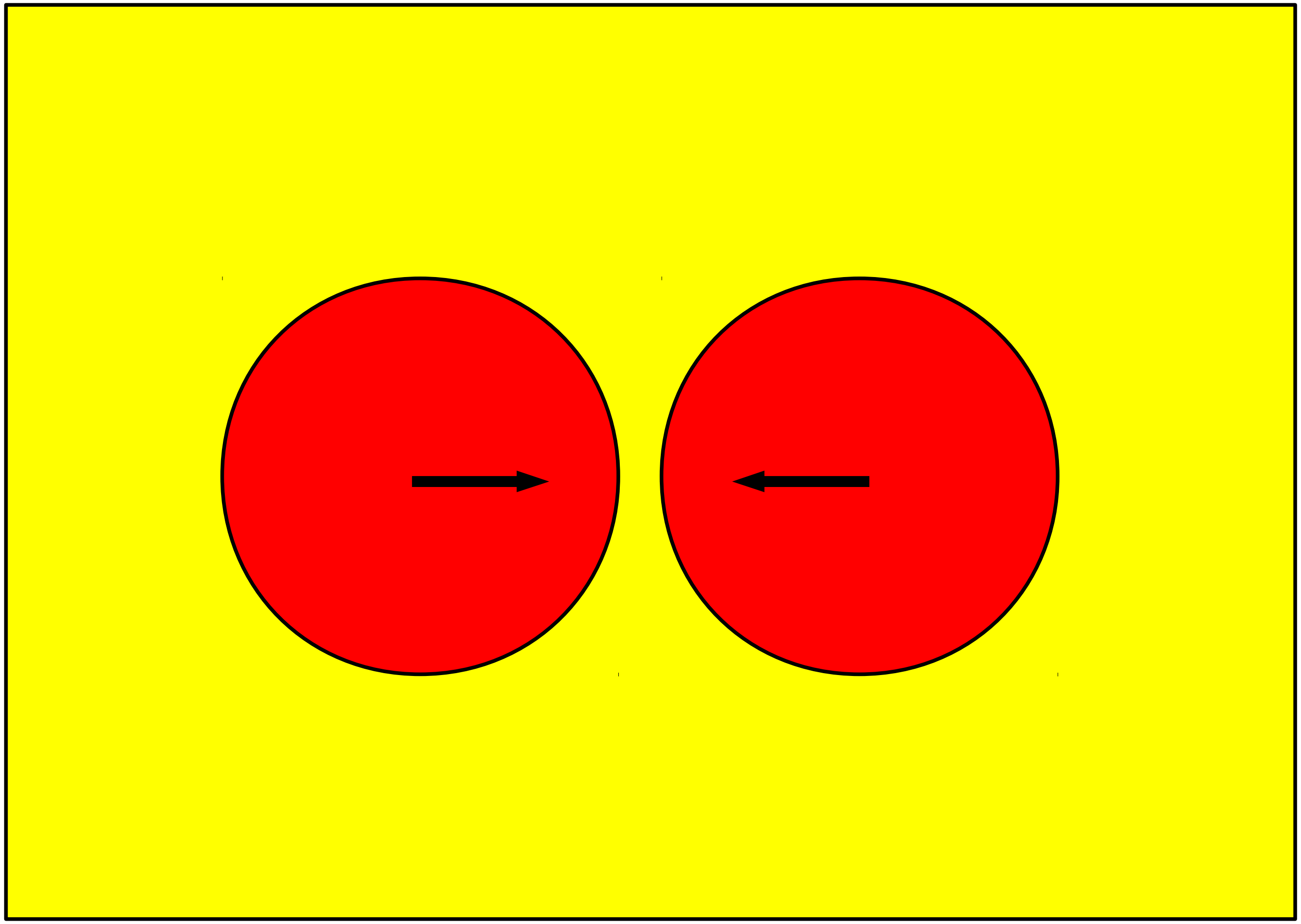
Three important features of hydrodynamic interactions:

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

Hydrodynamic interactions

Strong interactions of close particles

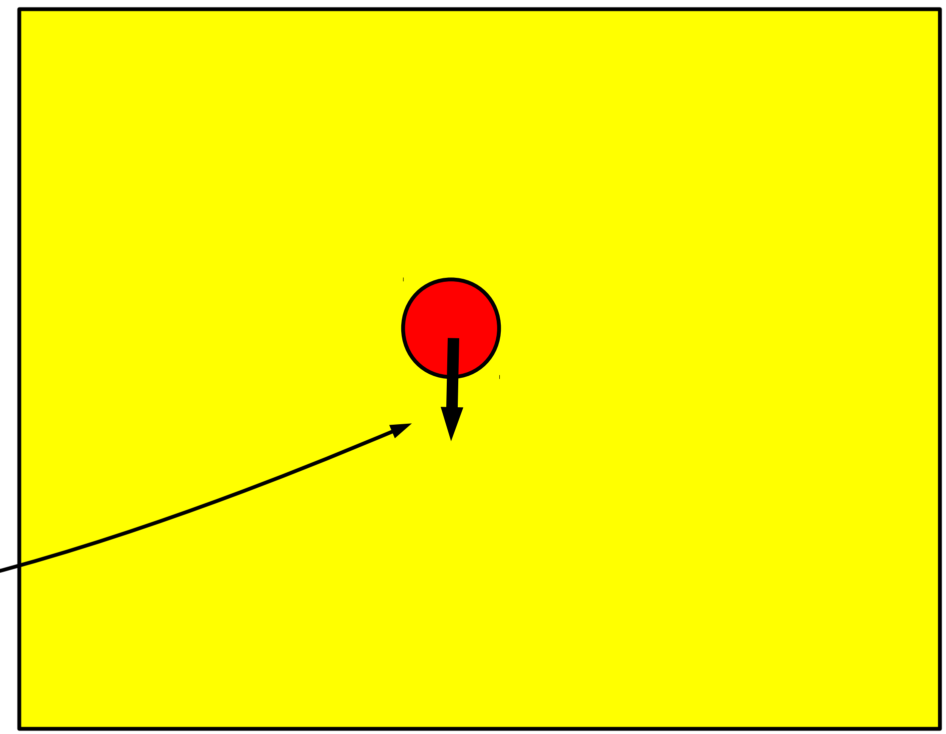
For constant velocities asymptotically infinite drag force



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:

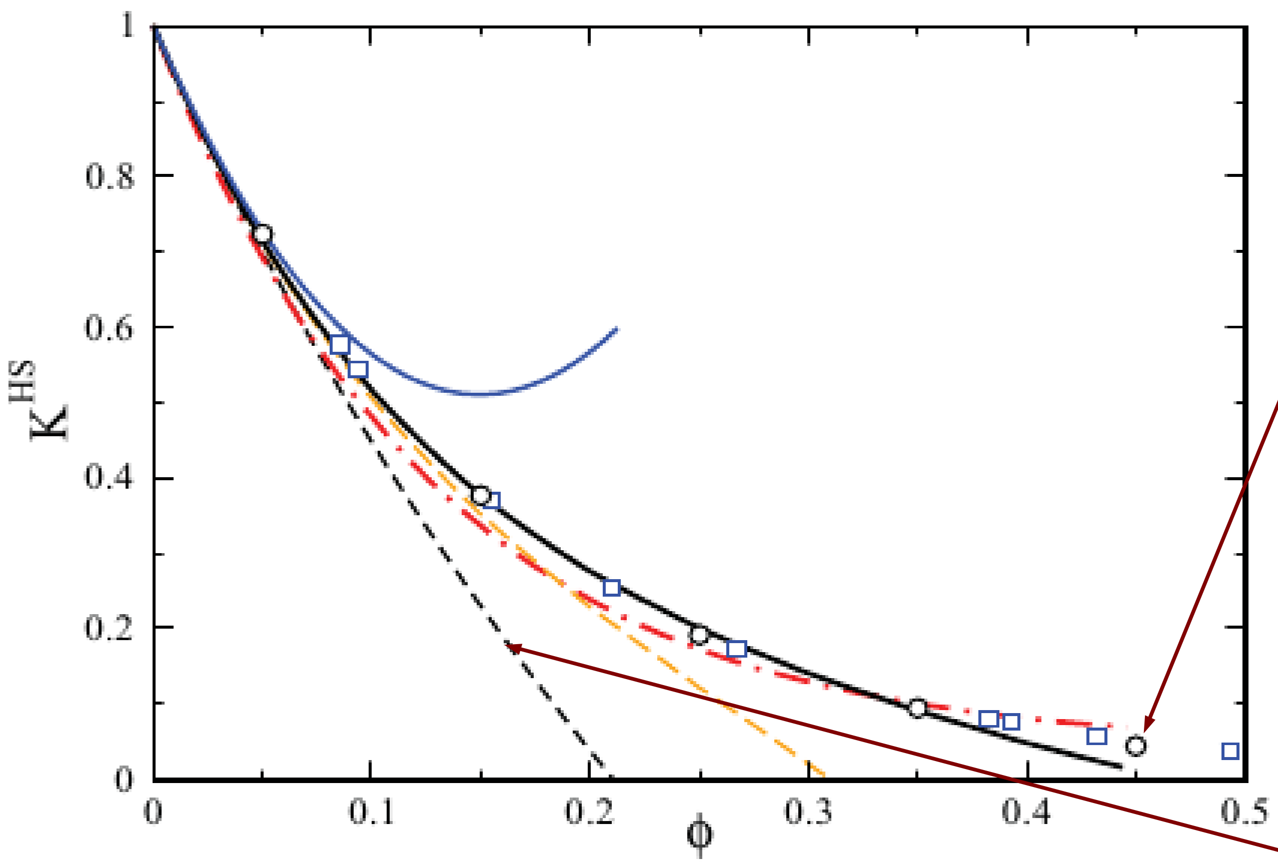
$$\mathbf{G}(\mathbf{r}) = \frac{1}{8\pi\eta} \frac{\mathbf{1} + \hat{\mathbf{r}}\hat{\mathbf{r}}}{r}$$

integral over r not absolutely convergent

Hydrodynamic interactions

Many-body character

Sedimentation coefficient for hard spheres



numerical simulations (close to experiments)

volume fraction

two-body approximation

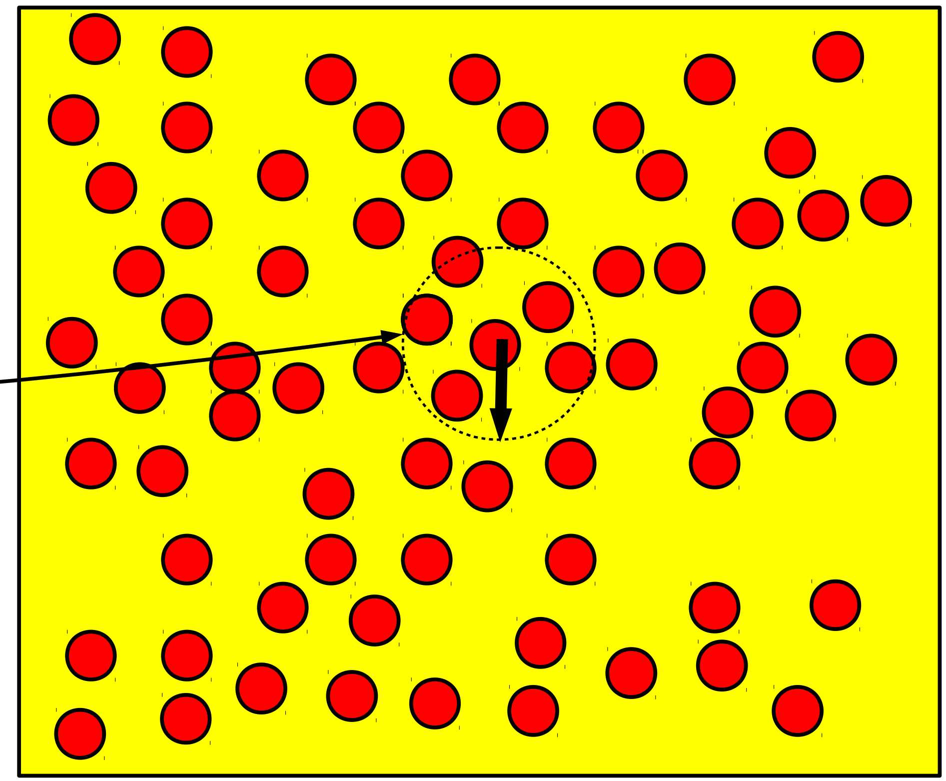
two-body approximation relevant for volume fractions less than about 5%

Important experiment

Flow caused by force acting on particles in the area

total force acting on particles in the area

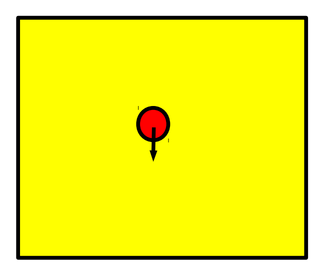
$$\mathbf{v}(\mathbf{r}) \sim \mathbf{G}_{\mathrm{eff}}(\mathbf{r})\,\mathbf{F}$$



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

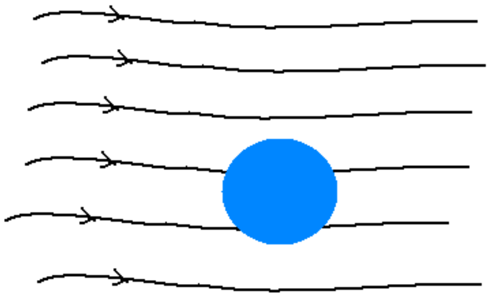


$$\mathbf{v}(\mathbf{r}) \sim \mathbf{G}(\mathbf{r}) \cdot \mathbf{F}$$

Calculation of hydrodynamic interactions

Single particle in ambient flow

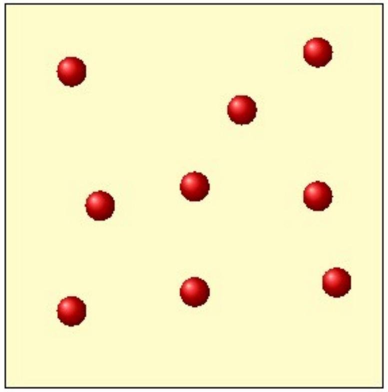
$$\mathbf{v}_0\left(\mathbf{r}\right) = \int d^3\mathbf{r}'\mathbf{G}\left(\mathbf{r}-\mathbf{r}'\right)\cdot\mathbf{F}_0\left(\mathbf{r}'\right)$$



$$\mathbf{F}_1\left(\mathbf{r}\right) = \int d\mathbf{r}'\mathbf{M}\left(\mathbf{r}-\mathbf{R}_1,\mathbf{r}'-\mathbf{R}_1\right)\mathbf{v}_0\left(\mathbf{r}'\right)$$

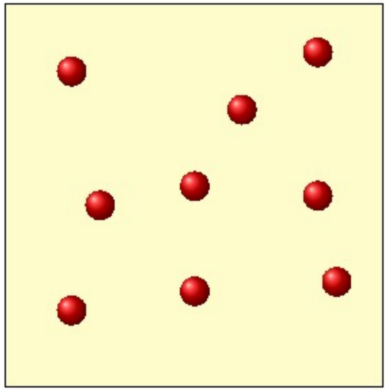
Single freely moving particle response operator

Suspension in ambient flow:



$$\mathbf{F}_i = \mathbf{M}(i)\left(\mathbf{v}_0 + \sum_{i\neq j}\mathbf{GF}_j\right)$$

Scattering series



ambient flow

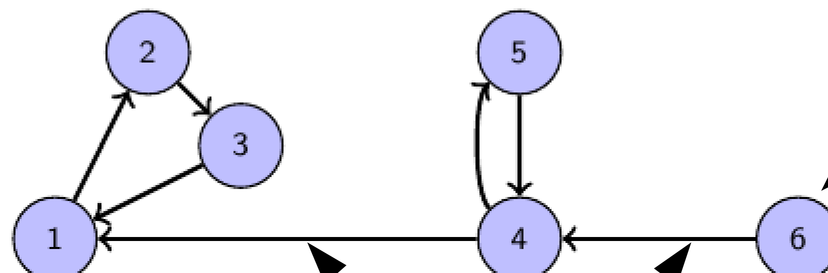
$$\mathbf{F}_i = \left(\mathbf{M}(i) + \sum_{i \neq j} \mathbf{M}(i)\mathbf{G}\mathbf{M}(j) + \sum_{j \neq i} \sum_{k \neq j} \mathbf{M}(i)\mathbf{G}\mathbf{M}(j)\mathbf{G}\mathbf{M}(k) + \dots \right) \mathbf{v}_0$$

Green function for Stokes equations

Single particle response operator

Example of scattering sequence (many-body):

$$M(1)GM(3)GM(2)GM(1) \times$$
$$G \times M(4)GM(5)GM(4) \times G \times M(6)$$



$M(6)$

short range hydrodynamic interactions
(strong interactions of close particles)

long range hydrodynamic interactions

Tu zdefiniuj SI(123) SI(45) SI(6) short scattering sequence
Wypisz wzór SI(C1)GSI(C2)GSI(C3)

Uśredniona reakcja zawiesiny w polu zewnętrznym

$$\langle F(\mathbf{R})\rangle = \int d^3\mathbf{R}' T(\mathbf{R},\mathbf{R}')\, v_0(\mathbf{R}')$$

Operator reakcji zawiesiny w polu zewnętrznym

$$T = \sum_{b=1}^{\infty} \sum_{C_1 \ldots C_b} \int dC_1 \ldots dC_b\; n(C_1 \ldots C_b)\, S_I(C_1) G \ldots G S_I(C_b)$$

cząstkowe funkcje rozkładu

Diagramatyczne przedstawienie powyższych wyrażeń
Szczególnie ważne przedstawienie funkcji rozkładu dla zadanej sekwencji

Response of suspension

(effective viscosity)

Pressure tensor for pure fluid: $\sigma_{\alpha\beta} = p\delta_{\alpha\beta} - \eta\left(\nabla_\alpha v_{0\beta} + \nabla_\beta v_{0\alpha}\right)$

Pressure tensor in suspension: $\sigma^{eff}_{\alpha\beta} \leftarrow [F^d_i]_{\alpha\beta} \equiv \int_{S_{\mathbf{R}_i}} dS F_{i\alpha}(\mathbf{r})(\mathbf{r} - \mathbf{R_i})_\beta$

surface of i-th particle

Dipole force with relation to average flow:

average velocity field of suspension

$$\left\langle F^d \right\rangle (\mathbf{R}) = \int d\mathbf{r}' T^{irrd}(\mathbf{R}, \mathbf{r}') \left\langle v \right\rangle (\mathbf{r}')$$

average surface dipole force

response operator

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

Renormalization

Cluster expansion (1982):

short-range hydrodynamic interaction

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

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:

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

Uwzględnienie kolektywnych oddziaływań w zawiesinie

Felderhof, Ford, Cohen:
$$T^{irr} = \sum_{b=1}^{\infty} \sum_{C_1 \ldots C_b} \int dC_1 \ldots dC_b b(C_1|\ldots|C_b) S_I(C_1) G \ldots G S_I(C_b)$$

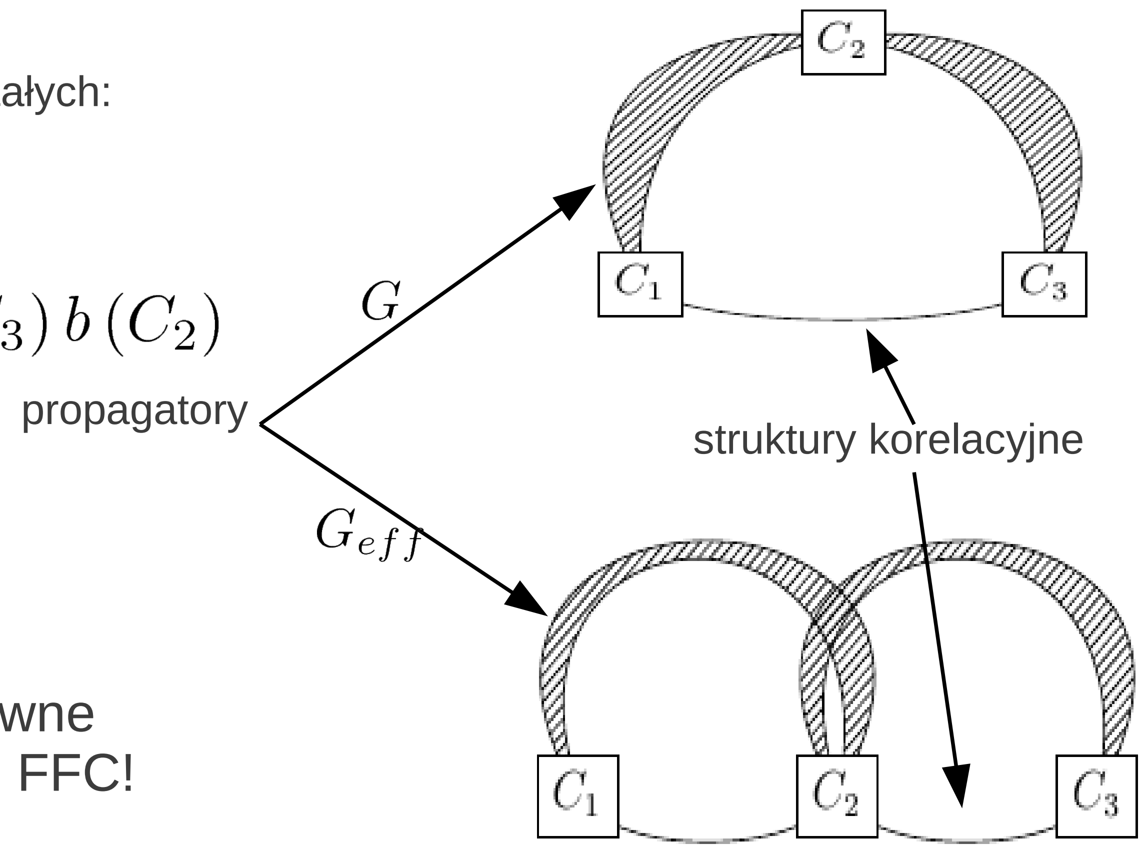
Rozwinięcie pierścieniowe (2011)

$$T^{irr} = \sum_{b=1}^{\infty} \sum_{C_1 \ldots C_b} \int dC_1 \ldots dC_b H(C_1|\ldots|C_b) S_I(C_1) G_{\text{eff}} \ldots G_{\text{eff}} S_I(C_b)$$

Gdy środkowa grupa oddala sie od pozostałych:

$$b\left(C_1|C_2|C_3\right) \longrightarrow b\left(C_1|C_3\right) b\left(C_2\right)$$

$$H\left(C_1|C_2|C_3\right) \longrightarrow 0$$



Ważne oddziaływanie kolektywne
trudno uchwytne w wyrażeniu FFC!

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

Repeating structures in T^{irr}

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

Clausius-Mossotti operator

Clausius-Mossotti approximation: $T^{irr}_{CM} \approx nM$

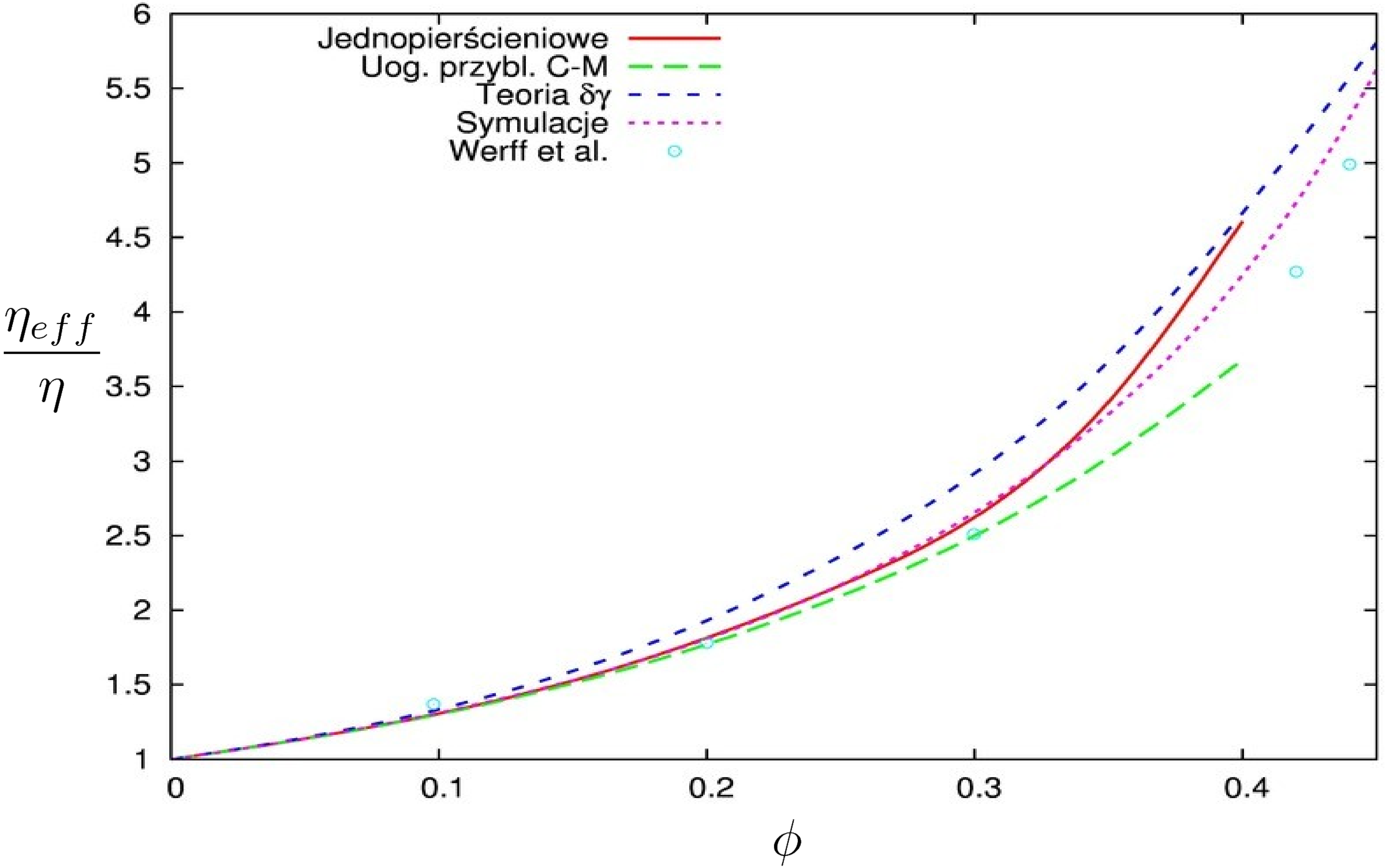
$$T^{irr} = T^{irr}_{RCM} \left(1 - [hG_{\mathrm{eff}}]\, T^{irr}_{RCM}\right)^{-1}$$

renormalized Clausius-Mossotti operator

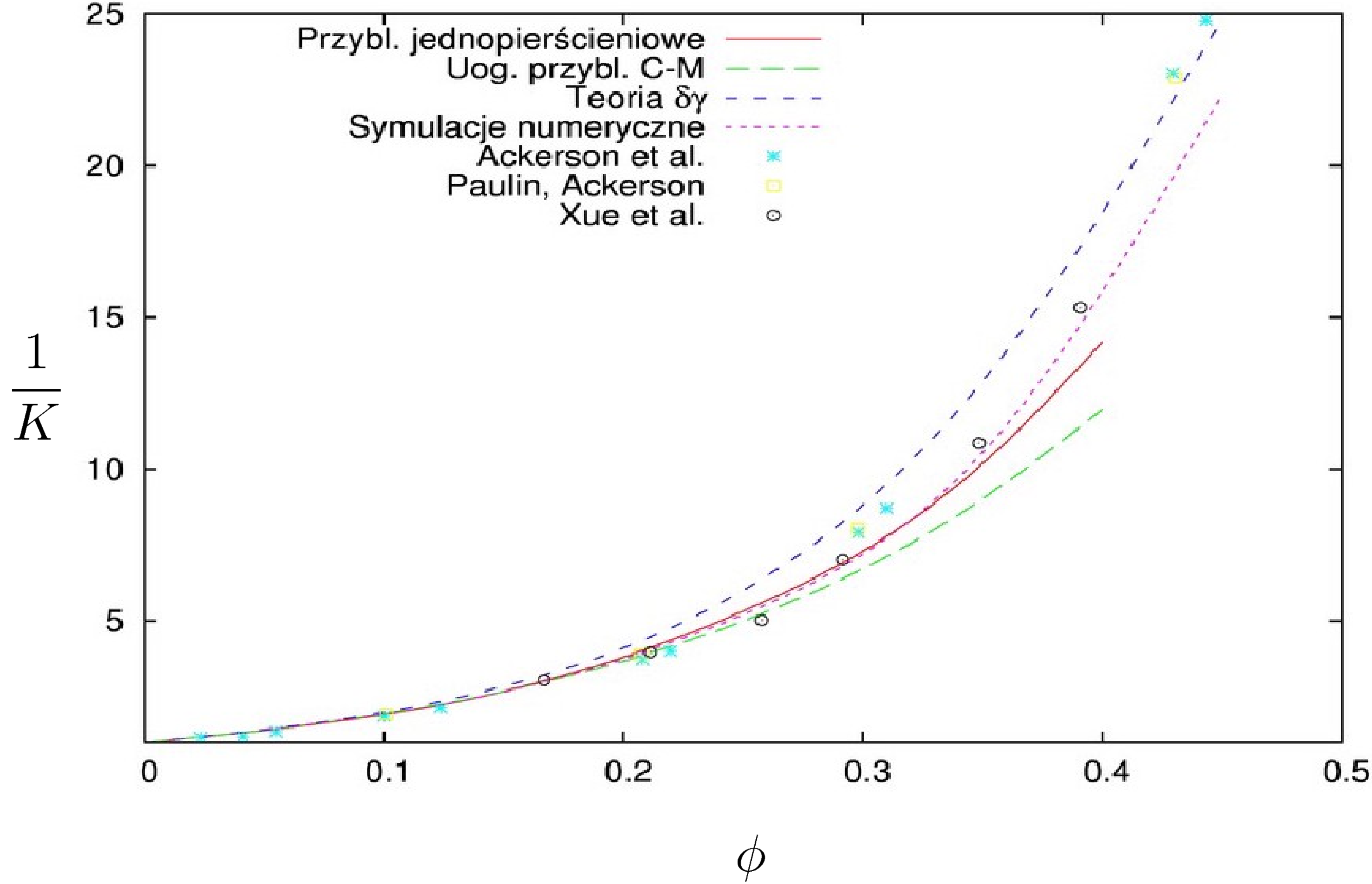
Generalized Clausius-Mossotti approximation: $T^{irr}_{RCM} \approx nB$

Approximate method formulated in terms of approximation for T^{irr}_{RCM}

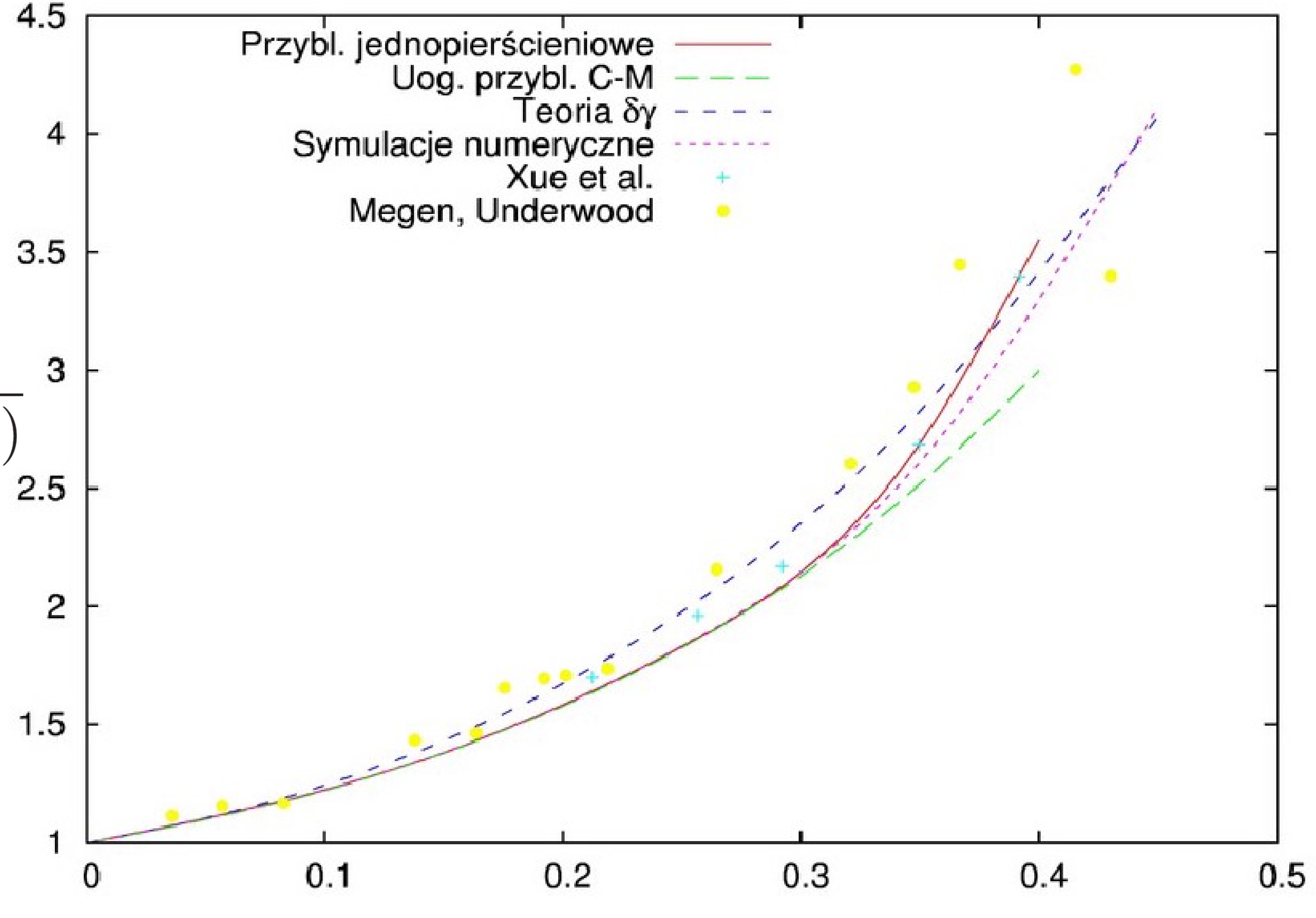
Effective viscosity



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



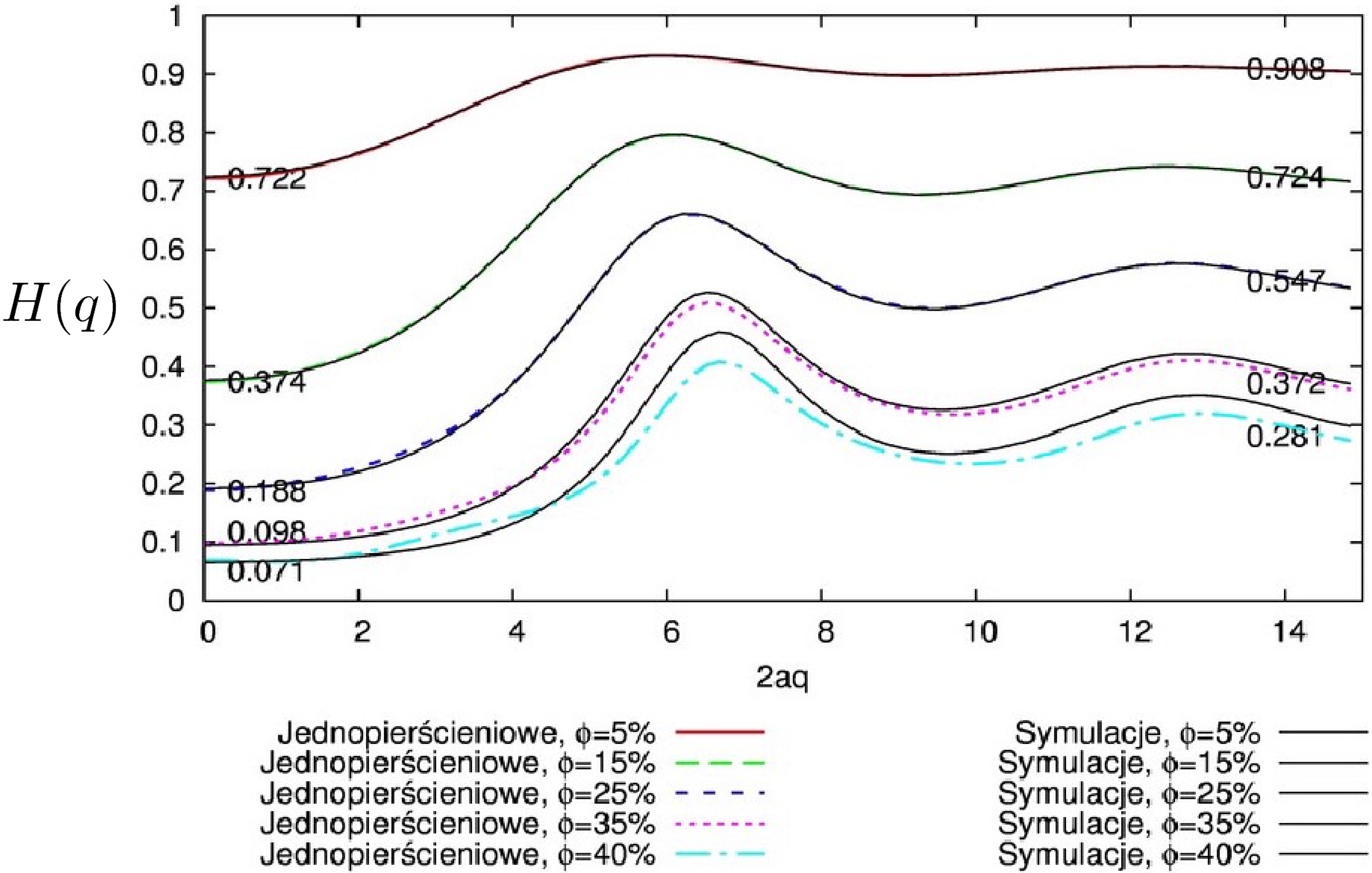
Inverse of mobility of single particle in suspension $H(\infty)$



$$\frac{1}{H(\infty)}$$

$$\phi$$

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)

Renormalized Clausius-Mossotti operator

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

One-ring approximation:

At most one ring in T^{irr}_{RCM}

At most two particle hydrodynamic interactions in S_I

Kirkwood approximation for three-particle distribution function:

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

Renormalization of two-particle interactions:

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

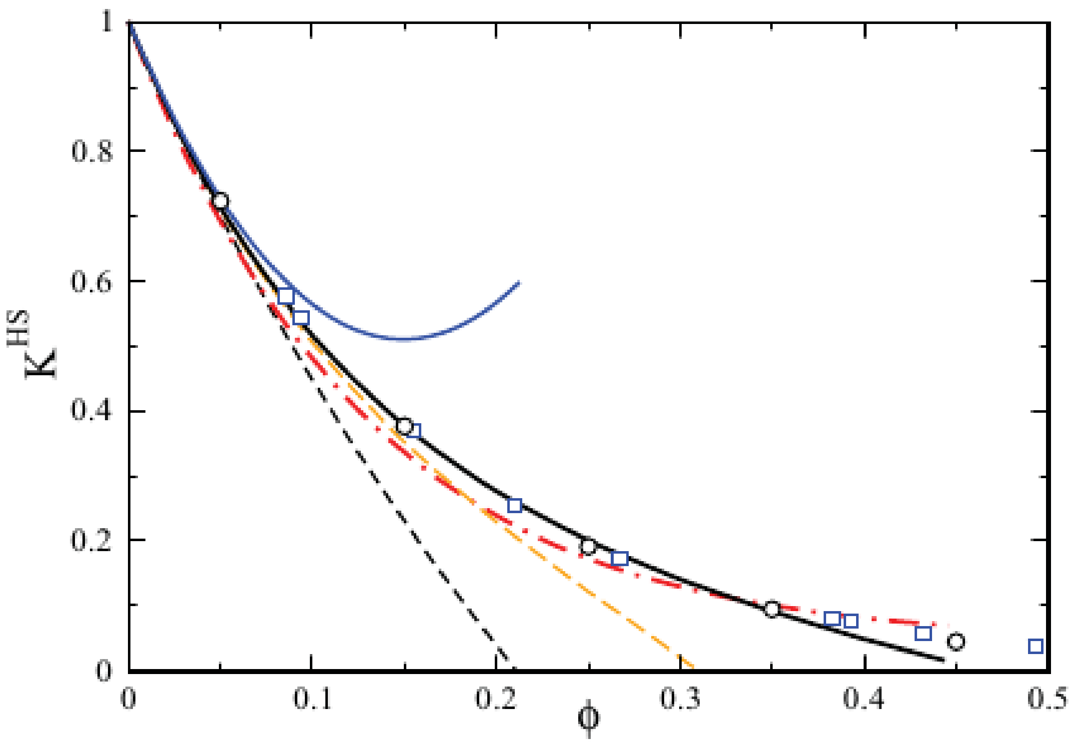


Fig. 6.3: *Reduced short-time sedimentation coefficient, K^{HS}, of neutral hard spheres. Open circles: Hydrodynamic force multipole simulation data by Abade et al. [26]. Open Squares: Lattice-Boltzmann simulation data by Segrè et al. [208]. Black dashed line: PA-scheme result. Dashed-dotted red line: 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.*

Approximate methods hitherto

There are many...

Clausius-Mossotti like (further)

"δγ scheme" (most comprehensive hitherto):

$$\eta_{eff} = c_0 + c_1 \delta\gamma + c_2 (\delta\gamma)^2 + \dots$$

Fully taking into account two-body HI demands infinite order