APS/DFD 2001, November 20 (San Diego)

[KQ.1] Lubrication-correction for many-particle systems in Stokes flows

Kengo Ichiki

<ichiki@mailaps.org>

Department of Applied Physics

University of Twente

The Netherlands

Motivation of my recent works

To understand, extend, and justify
the Stokesian Dynamics method

- Matrix-inversion ⇔ Many-body effect
  (APS/DFD 1999;
  KI & J.F.Brady, Phys.Fluids **13** (2000) 350)
- Accurate formulation beyond FTS version
  (APS/DFD 2000; KI, JFM in press)
- Lubrication-correction (APS/DFD 2001)

What is the lubrication-correction?

- a method to describe nearly touching particles
  accurately with less cost
  ⇒ trick or magic (or cheating...)
- an accurate method with large cost
  is “multipole expansion method”

Goal of this work

formulate a lubrication-correction method with steady basis

- considering physical conditions
- using shift operators for force/velocity moments
- approximation by 2B exact solution

fill the gap among the existing works;

- Stokesian Dynamics method (SD)

  (Durlofsky *et al.*, J.Fluid Mech. **180** (1987) 21)

  presents a robust method for lubrication.

  [Q] how to justify the method?

  [Q] where is the limitation?

- Sangani & Mo (Phys. Fluids **6** (1994) 1637)

  presents a "gap-expansion" for lubrication.

  [Q] relation to SD?

- Cichocki *et al*. (CEW)

  (J.Chem.Phys. **111** (1999) 3265)

  presents an improvement of SD lubrication.

  [Q] reason of collective-motion projection?

Comparison with other works

The present work

$$\hat{\mathscr{U}}(\alpha) = \sum_{\beta} \hat{\mathscr{M}}(\alpha,\beta) \cdot \hat{\mathscr{F}}(\beta) + \sum_{g} \hat{\mathscr{M}}(\alpha, 2B_g) \cdot \boxed{\left\{ -\hat{\mathcal{L}}^{2B} + \boxed{\mathcal{H} \cdot \mathcal{G} \cdot \hat{\mathcal{L}}^{2B} \cdot \mathcal{H} \cdot \mathcal{G}} \right\}} \cdot \hat{\mathscr{U}}(2B_g)$$

Stokesian Dynamics method (SD)

$\hat{\mathscr{U}} = \hat{\mathscr{M}} \cdot \left[\hat{\mathscr{F}} - \hat{\mathcal{L}} \cdot \hat{\mathscr{U}} \right]$; $\boxed{\mathcal{H}\mathcal{G}\hat{\mathcal{L}}\mathcal{H}\mathcal{G}}$ is missing

$\Rightarrow$ SD is inconsistent ($\hat{\mathscr{F}}$ is not $\hat{\mathscr{F}}_{nor}$)

Cichocki *et al.* (CEW)

$$\boxed{\hat{\mathcal{L}} - \mathcal{H}\mathcal{G}\hat{\mathcal{L}}\mathcal{H}\mathcal{G}} \longrightarrow \boldsymbol{q}^t \cdot \hat{\mathcal{L}}^{2B} \cdot \boldsymbol{q}$$

Sangani & Mo

- treat $\boxed{\mathcal{H}\mathcal{G}\hat{\mathcal{L}}\mathcal{H}\mathcal{G}}$ term directly by $\mathscr{F}_{loc}(g)$
- $\overline{\mathscr{F}}_{loc} = 0$ is assumed.

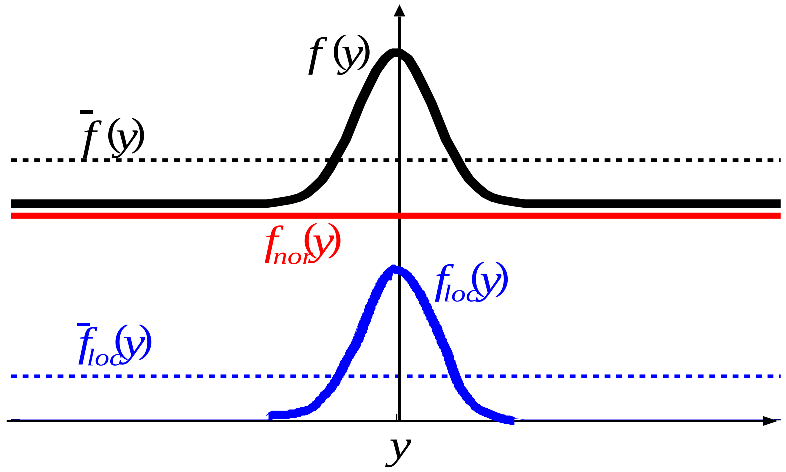
Decomposition of force density

Integral equation for fluid velocity $\boldsymbol{u}(\boldsymbol{x})$

$$\boldsymbol{u}(\boldsymbol{x}) = -\frac{1}{8\pi\mu}\sum_{\beta}\int_{S_\beta} dS(\boldsymbol{y})\, \mathrm{J}(\boldsymbol{x}-\boldsymbol{y}) \cdot \boldsymbol{f}(\boldsymbol{y})$$

Oseen tensor $J_{ij}(\boldsymbol{r}) = (\delta_{ij} - r_i r_j/r^2)/r$, force density $\boldsymbol{f}(\boldsymbol{y})$

Decompose $\boldsymbol{f}$ into localized $\boldsymbol{f}_{loc}$ and normal $\boldsymbol{f}_{nor}$



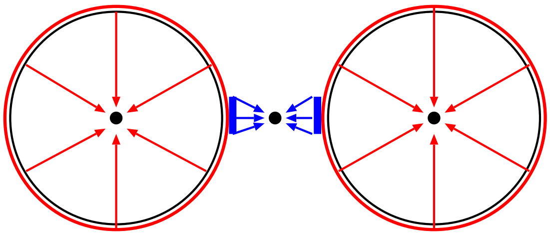
$$\boldsymbol{f} = \boldsymbol{f}_{nor} + \boldsymbol{f}_{loc} \approx \bar{\boldsymbol{f}} - \bar{\boldsymbol{f}}_{loc} + \boldsymbol{f}_{loc}$$

where $\bar{\boldsymbol{f}}$ and $\bar{\boldsymbol{f}}_{loc}$ are coarse-grained values

Multipole expansion

$\bar{\boldsymbol{f}}$, $\bar{\boldsymbol{f}}_{loc}$ are suitable for "center-expansion".

$\boldsymbol{f}_{loc}$ is suitable for " gap-expansion".



Expand at the center of particles and the gap

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{\beta} \mathscr{J}(\boldsymbol{x}-\boldsymbol{x}^{\beta}) \cdot \left(\bar{\mathscr{F}}(\beta) - \bar{\mathscr{F}}_{loc}(\beta)\right) + \sum_{g} \mathscr{J}(\boldsymbol{x}-\boldsymbol{x}^{g}) \cdot \mathscr{F}_{loc}(g)$$

$$\mathscr{J}^{(m)} = (1/8\pi\mu m!)\boldsymbol{\nabla}^m \mathrm{J}$$

$$\mathscr{F}^{(m)}(\beta) = -\int dS(\boldsymbol{y})\,(\boldsymbol{y}-\boldsymbol{x}^{\beta})^m \boldsymbol{f}(\boldsymbol{y})$$

higher orders of $\bar{\mathscr{F}}(\beta)$, $\bar{\mathscr{F}}(\beta)$, $\mathscr{F}(g)$ are reducible

Generalized mobility problem

$$\hat{\mathscr{U}}(\alpha) = \sum_{\beta} \hat{\mathscr{M}}(\alpha,\beta) \cdot \left(\hat{\bar{\mathscr{F}}}(\beta) - \hat{\bar{\mathscr{F}}}_{loc}(\beta)\right) + \sum_{g} \hat{\mathscr{M}}(\alpha,g) \cdot \hat{\mathscr{F}}_{loc}(g)$$

$$\mathscr{U}^{(n)}(\alpha) = (1/4\pi a^2)\int dS(\boldsymbol{y})\,(\boldsymbol{y}-\boldsymbol{x}^{\alpha})^n \boldsymbol{u}(\boldsymbol{y})$$

$$\mathscr{M}^{(n,m)}(\alpha,\beta) = (1/4\pi a^2)\int dS(\boldsymbol{y})\,(\boldsymbol{y}-\boldsymbol{x}^{\alpha})^n\,\mathscr{J}^{(m)}(\boldsymbol{y}-\boldsymbol{x}^{\beta})$$

Model for $\bar{\mathscr{F}}_{loc}(\beta)$

The exact solution for 2B problem

$$\begin{bmatrix} \hat{\mathscr{F}}(1) \\ \hat{\mathscr{F}}(2) \end{bmatrix} = \hat{\mathscr{R}}^{2B}_{exact} \cdot \begin{bmatrix} \hat{\mathscr{U}}(1) \\ \hat{\mathscr{U}}(2) \end{bmatrix}$$

Approximate $\bar{\mathscr{F}}_{loc}(\beta)$ as

$$\begin{bmatrix} \hat{\bar{\mathscr{F}}}_{loc}(1) \\ \hat{\bar{\mathscr{F}}}_{loc}(2) \end{bmatrix} = \hat{\mathcal{L}}^{2B} \cdot \begin{bmatrix} \hat{\mathscr{U}}(1) \\ \hat{\mathscr{U}}(2) \end{bmatrix}$$

$$\hat{\mathcal{L}}^{2B} = \mathscr{R}^{2B}_{exact} - \left(\hat{\mathscr{M}}^{2B}\right)^{-1}$$

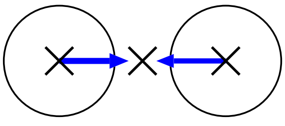
Note: $\mathscr{F}(\beta)$'s are particle-moments with $p = 1$

Model for $\mathscr{F}_{loc}(g)$

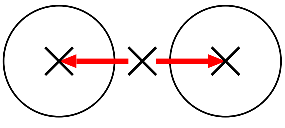
Single-gap problem

$$\hat{\mathscr{F}}_{loc}(g) = \hat{\mathcal{L}}^{gap} \cdot \hat{\mathscr{U}}(g)$$

$$\hat{\mathcal{L}}^{gap} \approx \mathcal{G} \cdot \hat{\mathcal{L}}^{2B} \cdot \mathcal{H}$$



$$\mathcal{G}(\mathbf{x}^g; \mathbf{x}^1, \mathbf{x}^2) = \begin{bmatrix} \mathcal{S}(\mathbf{x}^g, \mathbf{x}^1) & \mathcal{S}(\mathbf{x}^g, \mathbf{x}^2) \end{bmatrix}$$

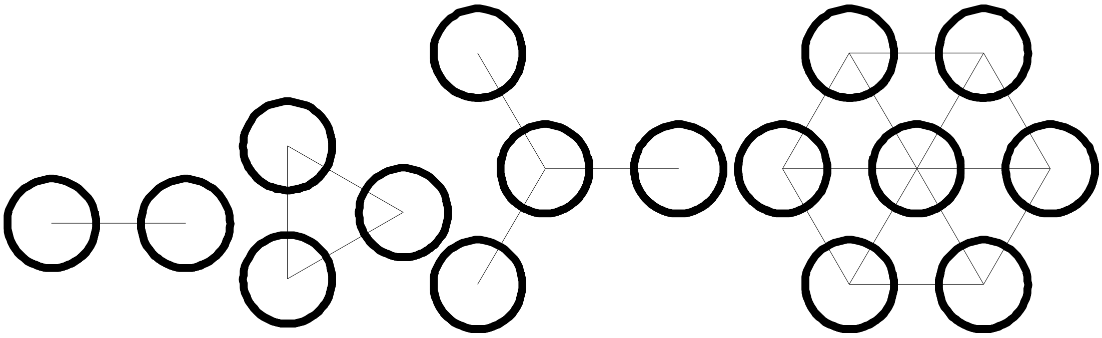


$$\mathcal{H}(\mathbf{x}^1, \mathbf{x}^2; \mathbf{x}^g) = \frac{1}{2} \begin{bmatrix} \mathcal{S}(\mathbf{x}^1, \mathbf{x}^g) \\ \mathcal{S}(\mathbf{x}^2, \mathbf{x}^g) \end{bmatrix}$$

$\mathcal{S}(\mathbf{x}, \mathbf{y})$: shift operator $\mathscr{F}(\mathbf{y}) \mapsto \mathscr{F}(\mathbf{x})$

Note: $\mathcal{G} \cdot \mathcal{H} = \mathsf{I}$ but $\mathcal{H} \cdot \mathcal{G} \neq \mathsf{I}$

Configurations



$N = 2$ $N = 3$ $N = 4$ $N = 7$

separation $r = 2.0 \sim 3.0$

Type of problem

mobility problem (give $\mathbf{F}, \mathbf{T}$ and solve $\mathbf{U}, \boldsymbol{\Omega}$)

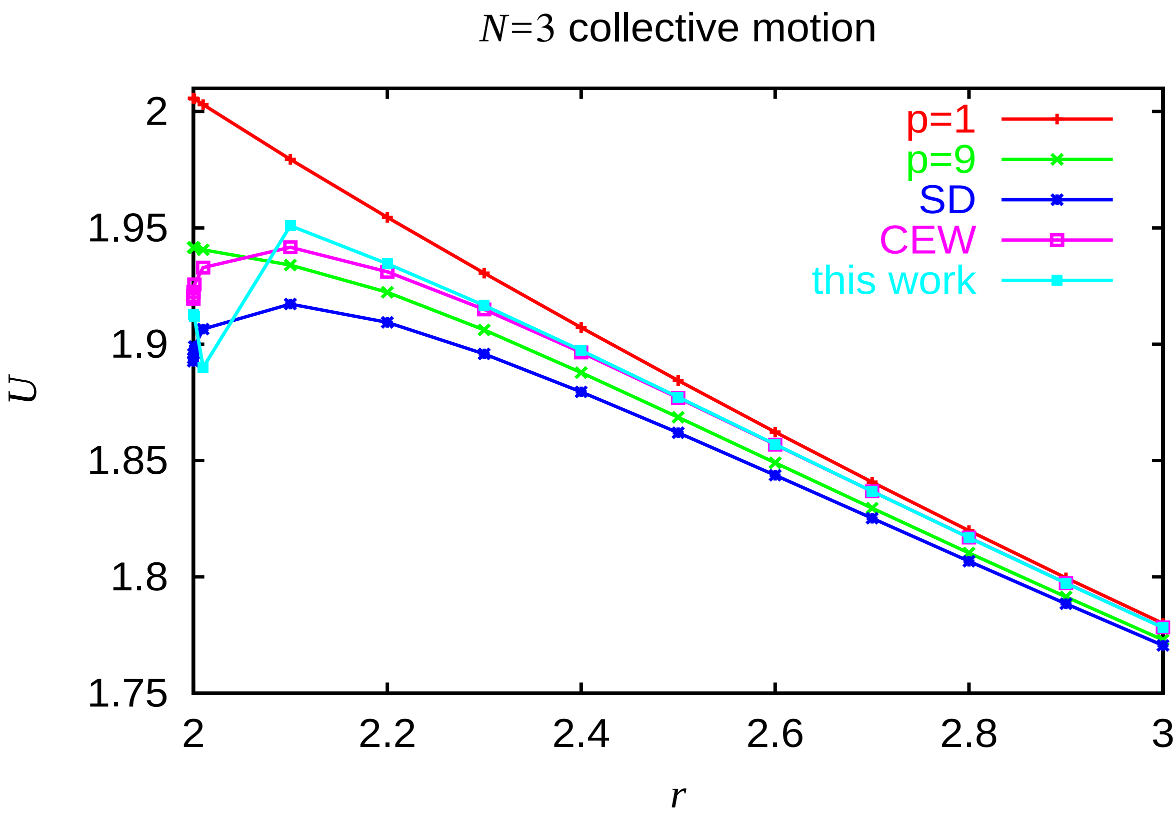
Types of motion

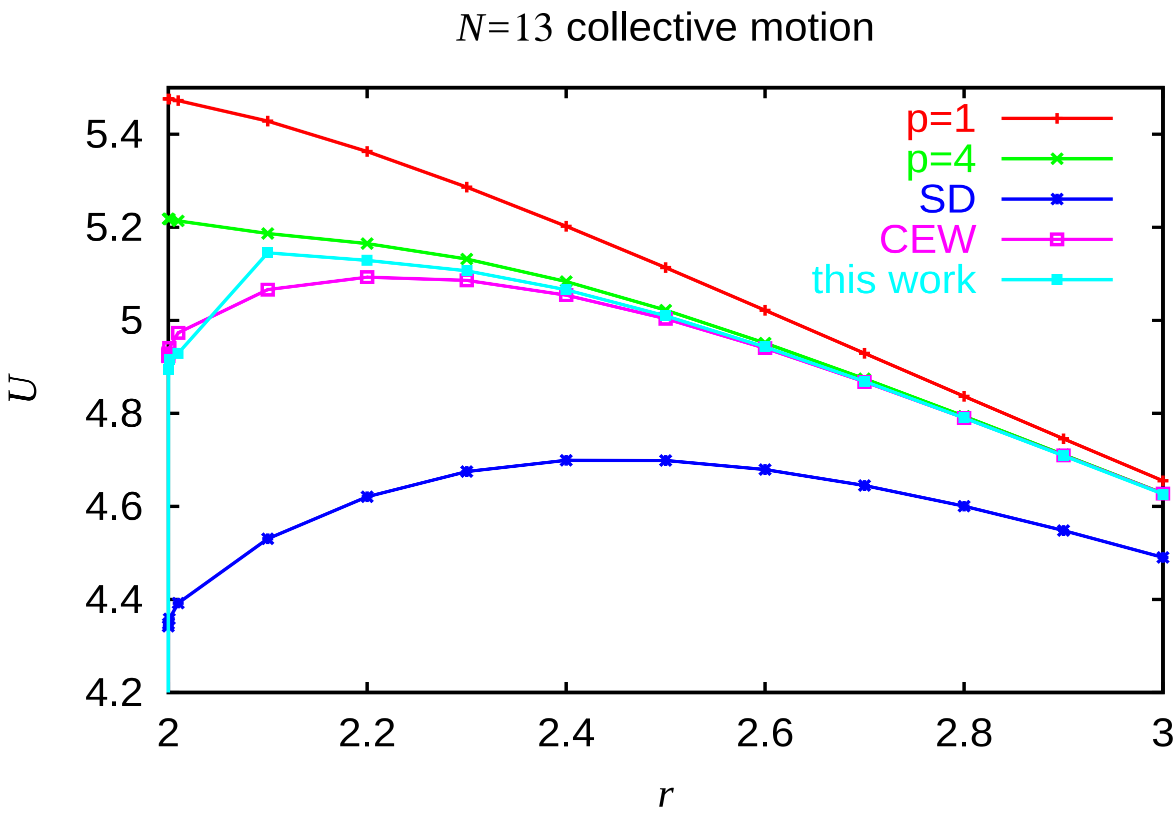
- collective motion: $\mathbf{F}$ = constant.
- spinning motion: $\mathbf{T}$ = constant.

Lubrication-correction methods

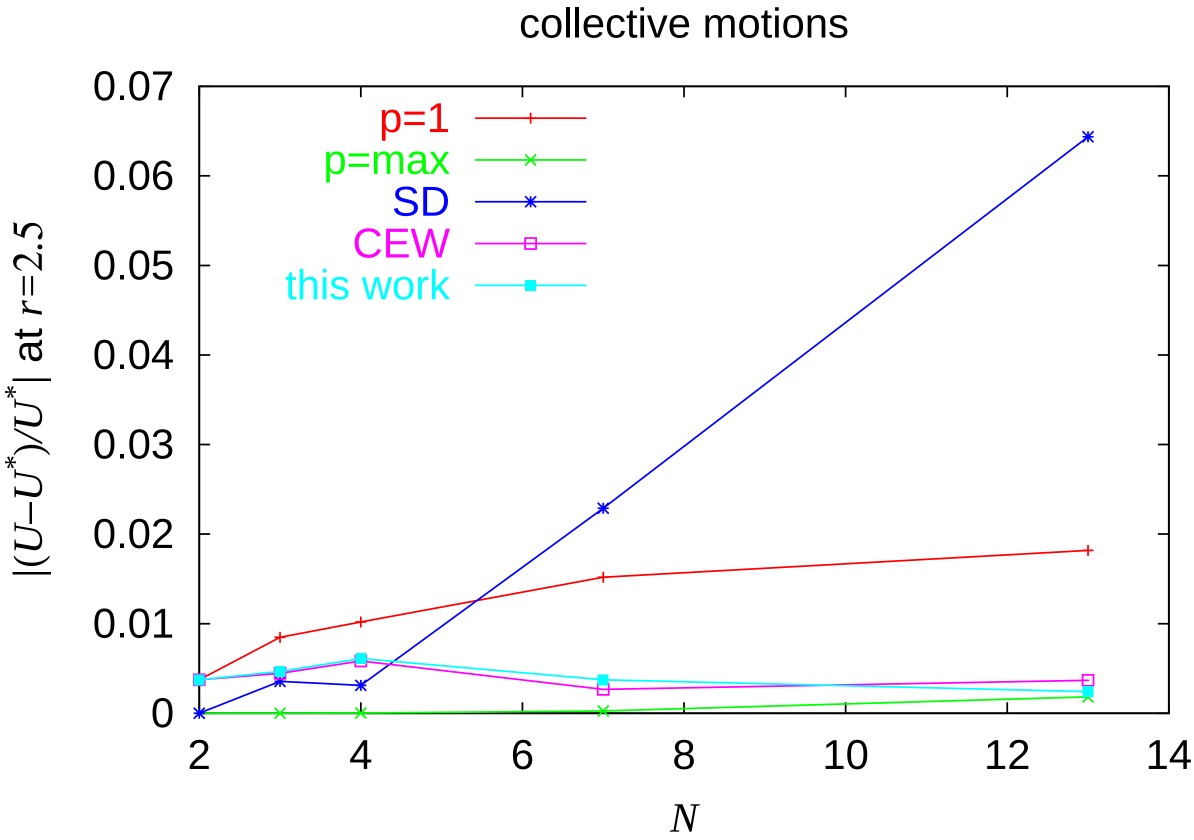
- multipole expansions ($p = 1 \Leftrightarrow$ FTS, larger p)
- Stokesian Dynamics (SD) $\mathscr{U} = \mathscr{M}\,[\mathscr{F} - \mathcal{L}\mathscr{U}]$
- Cichocki *et al.* (CEW) $\mathscr{U} = \mathscr{M}\,[\mathscr{F} - \mathbf{q}^t\mathcal{L}\mathbf{q}\mathscr{U}]$
- this work $\mathscr{U} = \mathscr{M}\,[\mathscr{F} + (-\mathcal{L} + \mathcal{H}\mathcal{G}\mathcal{L}\mathcal{H}\mathcal{G})\,\mathscr{U}]$

Results – Collective motions





Differences of U for N at $r = 2.5$



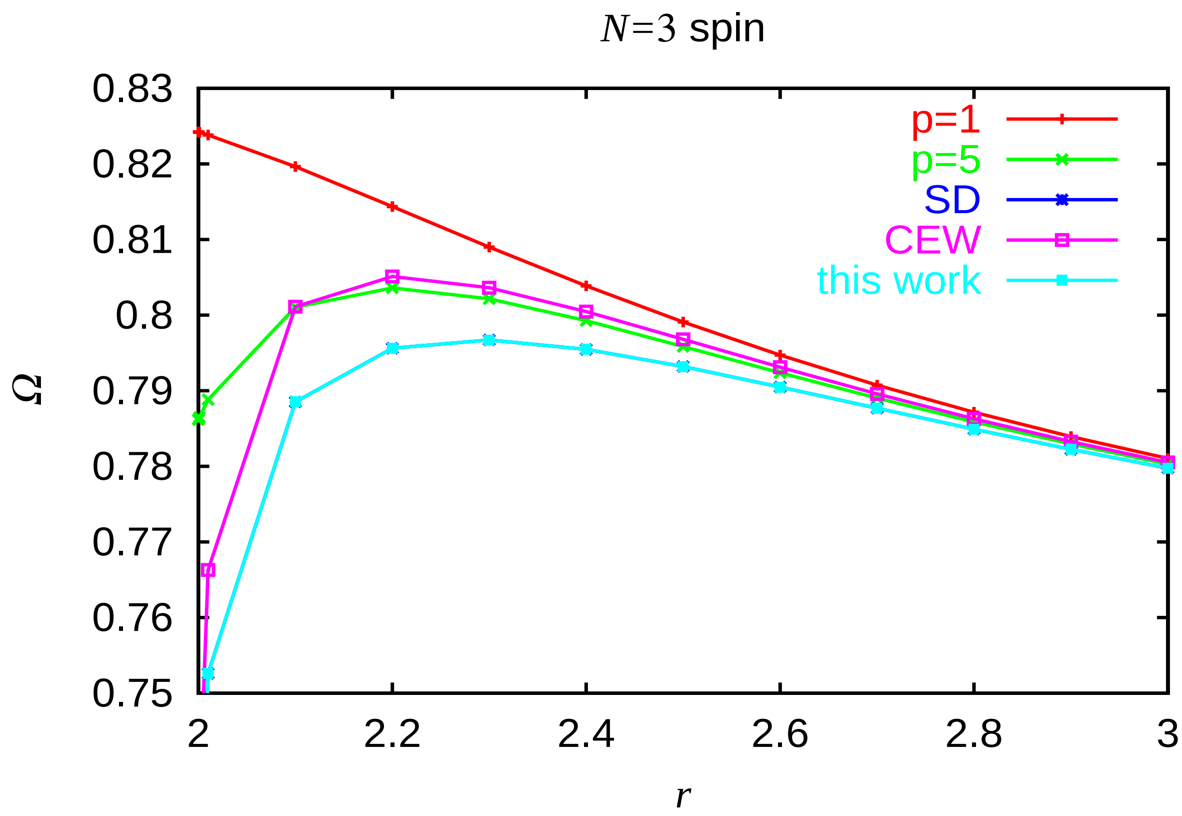
U^* is the value with p_{max}.

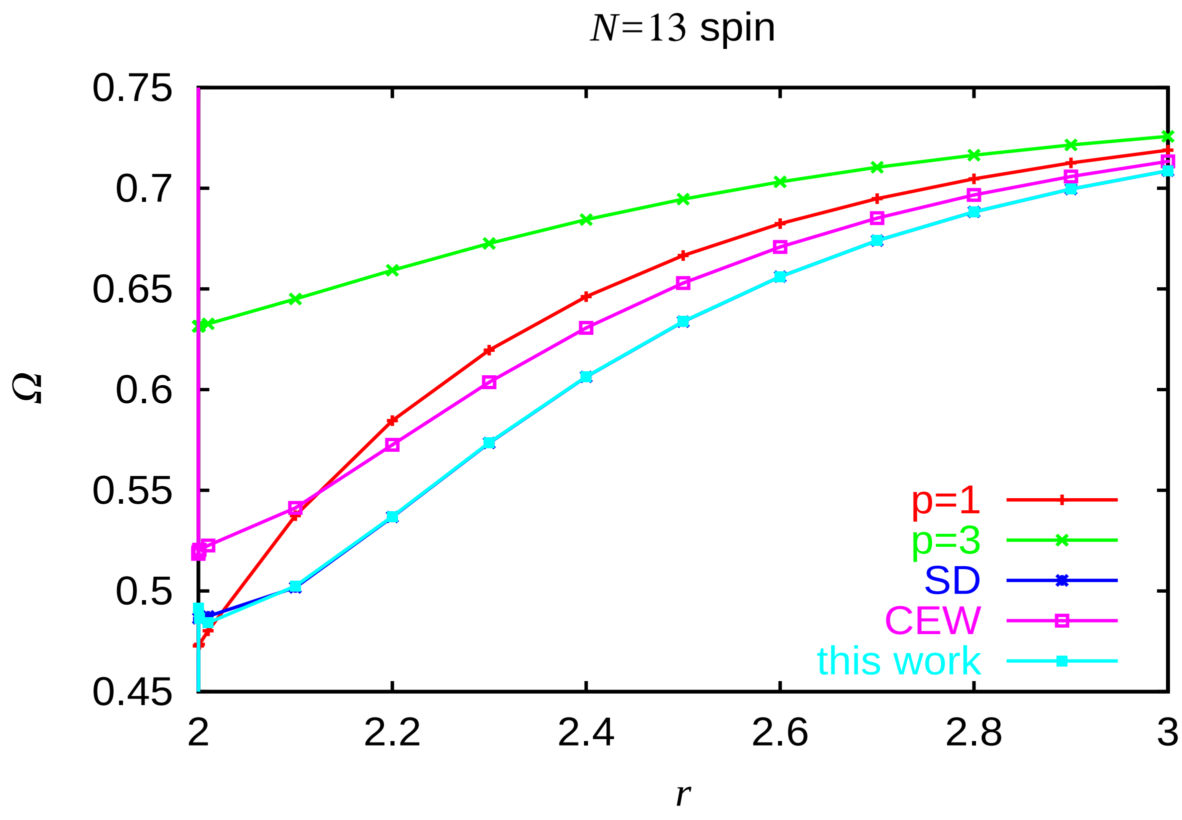
Summary on collective motions

- this work and CEW behave similarly
  and are better than $p = 1$ for all N.

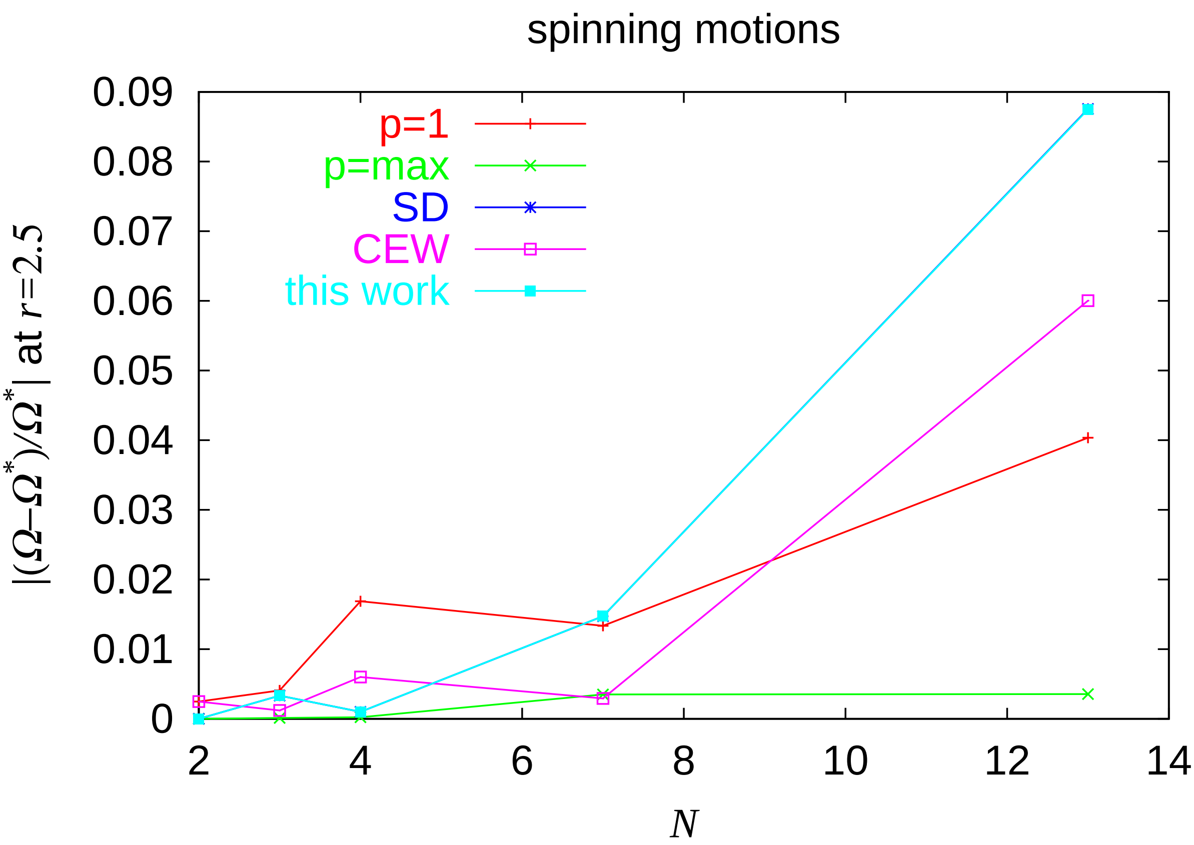
- SD is exact for $N = 2$
  but is worse than $p = 1$ for $N = 7$ and 13.
  $\because$ $\mathcal{L}$ is defined by the consistency for $N = 2$
  and inconsistent for $N \neq 2$ in general.

Results – Spinning motions





Differences of Ω for N at $r = 2.5$



Ω^* is the value with p_{max}.

Summary on spinning motions

- this work and SD behave similarly
  but CEW is a little bit different
- all lubrication schemes are bad for $N = 13$

Conclusions

reformulate the lubrication method

- by $\boldsymbol{f}$-decomposition, shift operators, and $\mathscr{R}^{2B}_{exact}$
- clarify its physical condition

fill the gap among three works;

- Stokesian Dynamics method (SD)
  [Q] how to justify the method?
  [A] formulate the method by decomposition of
  force density ⇒ $\mathscr{F}_{loc}(g)$ is missing
  [Q] where is the limitation?
  [A] failed on collective motions for $N = 7, 13$
  because of the inconsistency

- Sangani & Mo
  [Q] relation to SD?
  [A] given by shift operators

- Cichocki *et al*. CEW
  [Q] reason of collective-motion projection?
  [A] gap properties characterize lubrication

unsolved questions

- collective spinning motions
- $r \to 2$ limit on this work