APS/DFD 2002, November 25 (Dallas, TX)

[FE.1] Numerical analysis of non-Brownian particles in Stokes flow

Kengo Ichiki

Department of Mechanical Engineering
The Johns Hopkins University

Supported by
DOE grant FG02-99ER14966

Introduction

Target systems: Suspensions (solid-fluid mixture)

- Rheology (non-Newtonian), pattern formation, etc
- **Many-body hydrodynamic interaction**

Problem on computational study

- mono-layer simulations is not enough
  for purely 3D phenomena
  - ex. particle segregations in axial direction
    Tirumkudulu *et al.* (1999) Phys. Fluids **11**, 507

The goal of this talk:

Develop a FAST scheme
under PERIODIC boundary conditions

Contents:

- Method – Multipole expansion/
  Ewald summation/ Fast Multipole Method
- Results – Accuracy/ Performance
- Discussion – Other works
- Conclusions and Future plans

Method – Multipole expansion

KI (2002) J. Fluid Mech. **452**, 231

Starting point: Integral equation

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

- $\boldsymbol{u}$: velocity
- $\mathsf{J}(\boldsymbol{r}) = (\mathsf{I} + \boldsymbol{r}\boldsymbol{r}/r^2)/r$: Oseen tensor
- $\boldsymbol{f}(\boldsymbol{y})$: force density on the surface at $\boldsymbol{y}$

Multipole expansion

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{\beta} \sum_{m=0} \mathscr{J}^{(m)}(\boldsymbol{x} - \boldsymbol{x}_\beta) \cdot \mathscr{F}^{(m)}(\beta)$$

- $\mathscr{J}^{(m)} = \boldsymbol{\nabla}^m \mathsf{J}$: m-th order derivative of J
- $\mathscr{F}^{(m)}(\beta) = -\frac{1}{8\pi\mu}\frac{1}{m!}\int_{S_\beta} dS(\boldsymbol{y})\, (\boldsymbol{x}_\beta - \boldsymbol{y})^m \boldsymbol{f}(\boldsymbol{y})$:
  m-th order force moment for particle β

Multipole Method (Tree code)

$$\boldsymbol{u}(\boldsymbol{x}) = \mathscr{J}(\boldsymbol{x} - \boldsymbol{x}_C) \cdot \mathscr{F}(C)$$

- $\mathscr{F}(C) = \sum_\beta \mathscr{F}(\beta)$: force moment for group C

(For simplicity, summation of m is committed)

Method – Periodic B.C.

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{\Gamma} \sum_{\beta} \mathscr{J}(\boldsymbol{x} - (\boldsymbol{x}_\beta + \boldsymbol{L}_\Gamma)) \cdot \mathscr{F}(\beta)$$

- $\boldsymbol{L}_\Gamma$: lattice vector of periodic image Γ

Ewald summation technique

Beenakker (1986) J. Chem. Phys. **85**, 1581

$$\mathsf{J}(\boldsymbol{r}) = \mathsf{J}^{(r)}(\boldsymbol{r}) + \mathsf{J}^{(k)}(\boldsymbol{r})$$

- real part : $\mathsf{J}^{(r)}(\boldsymbol{r}) = (\mathsf{I}\nabla^2 - \boldsymbol{\nabla\nabla}) r \operatorname{erfc}(\xi r)$
- reciprocal part : $\mathsf{J}^{(k)}(\boldsymbol{r}) = (\mathsf{I}\nabla^2 - \boldsymbol{\nabla\nabla}) r \operatorname{erf}(\xi r)$

From Poisson's summation formula,

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{\Gamma} \sum_{\beta} \mathscr{J}^{(r)}(\boldsymbol{x} - (\boldsymbol{x}_\beta + \boldsymbol{L}_\Gamma)) \cdot \mathscr{F}(\beta)$$

$$+ \frac{1}{V} \sum_{\Lambda} \sum_{\beta} e^{-i\boldsymbol{k}_\Lambda \cdot (\boldsymbol{x} - \boldsymbol{x}_\beta)} \; \tilde{\mathscr{J}}^{(k)}(\boldsymbol{k}_\Lambda) \cdot \mathscr{F}(\beta)$$

- $\tilde{\mathsf{J}}^{(k)}(\boldsymbol{k}) = \int d\boldsymbol{r}\; e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\; \mathsf{J}^{(k)}(\boldsymbol{r})$
- $\boldsymbol{k}_\Lambda$: lattice vector in reciprocal space

Method – Fast Multipole Method

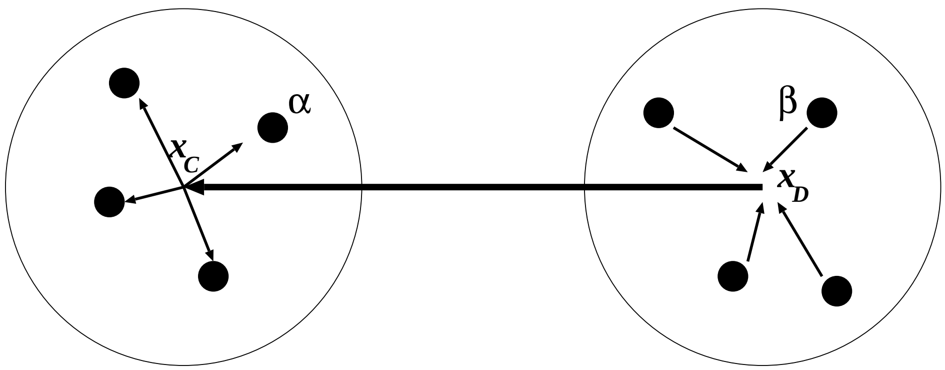
Velocity derivatives

$$\mathscr{V}^{(n)}(\boldsymbol{x}_\alpha) = \sum_\beta \sum_{m=0} \mathscr{J}^{(n+m)}(\boldsymbol{x}_\alpha - \boldsymbol{x}_\beta) \cdot \mathscr{F}^{(m)}(\beta)$$

- $\mathscr{V}^{(n)} = \boldsymbol{\nabla}^n \boldsymbol{u}$: velocity derivatives

Fast Multipole Method

Greengard-Rokhlin (1987) J. Comput. Phys. **73**, 325



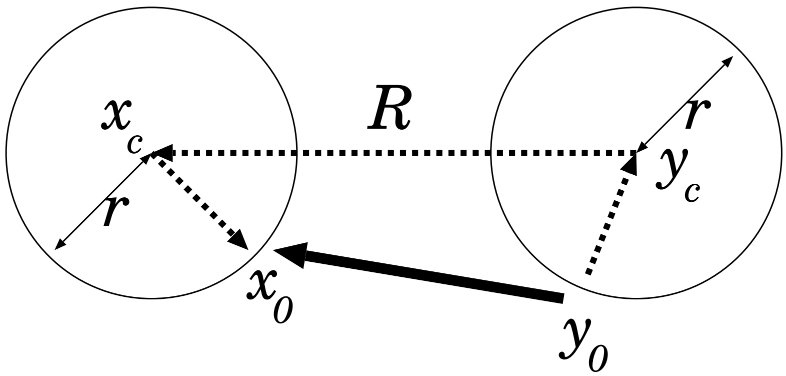
- direct calculation ⇒ 4×4 steps
- FMM calculation ⇒ 1 step

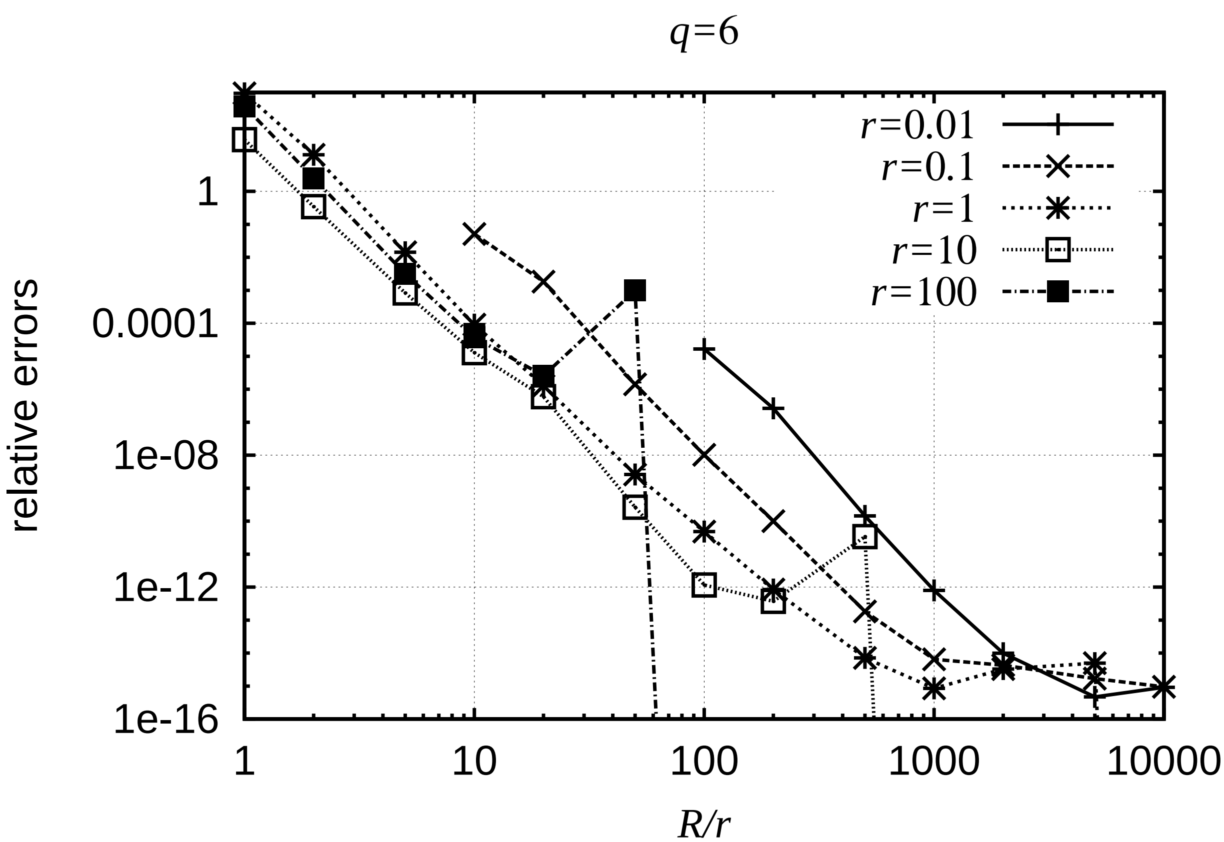
$$\mathscr{F}(D) = \sum_\beta \mathcal{S}_F(\boldsymbol{x}_D, \boldsymbol{x}_\beta) \mathscr{F}^{(m)}(\beta)$$

$$\boxed{\mathscr{V}^{(n)}(\boldsymbol{x}_C) = \sum_{m=0} \mathscr{J}^{(n+m)}(\boldsymbol{x}_C - \boldsymbol{x}_D) \cdot \mathscr{F}^{(m)}(D)}$$

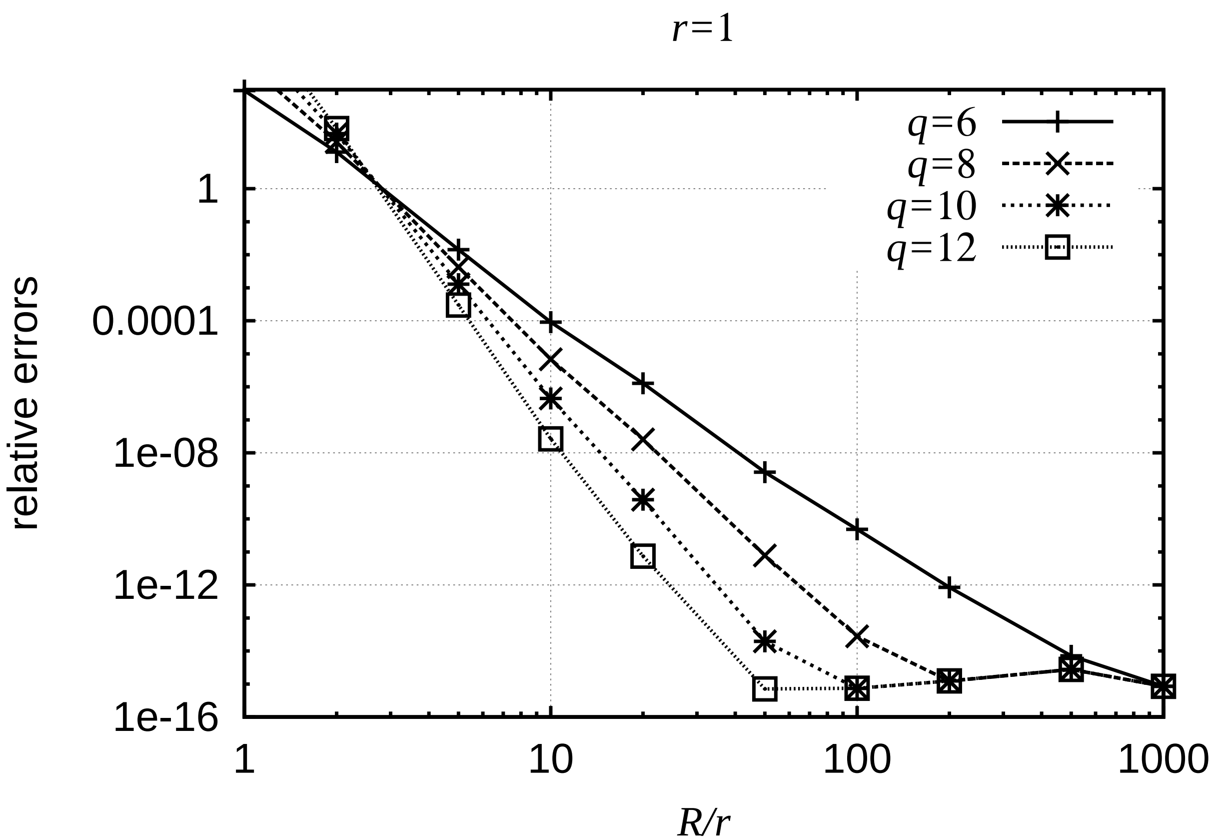
$$\mathscr{V}(\boldsymbol{x}_\alpha) = \mathcal{S}_V(\boldsymbol{x}_\alpha, \boldsymbol{x}_C) \cdot \mathscr{V}(\boldsymbol{x}_C)$$

Results – Accuracy

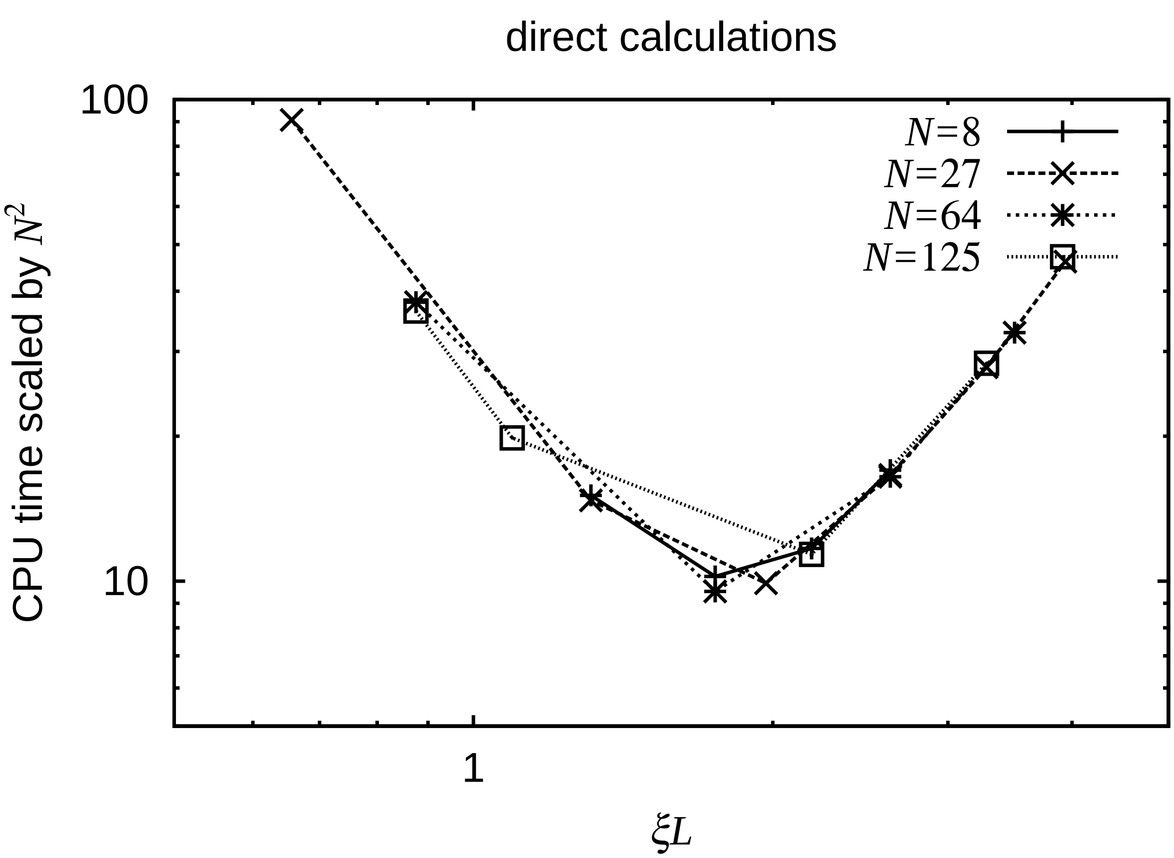




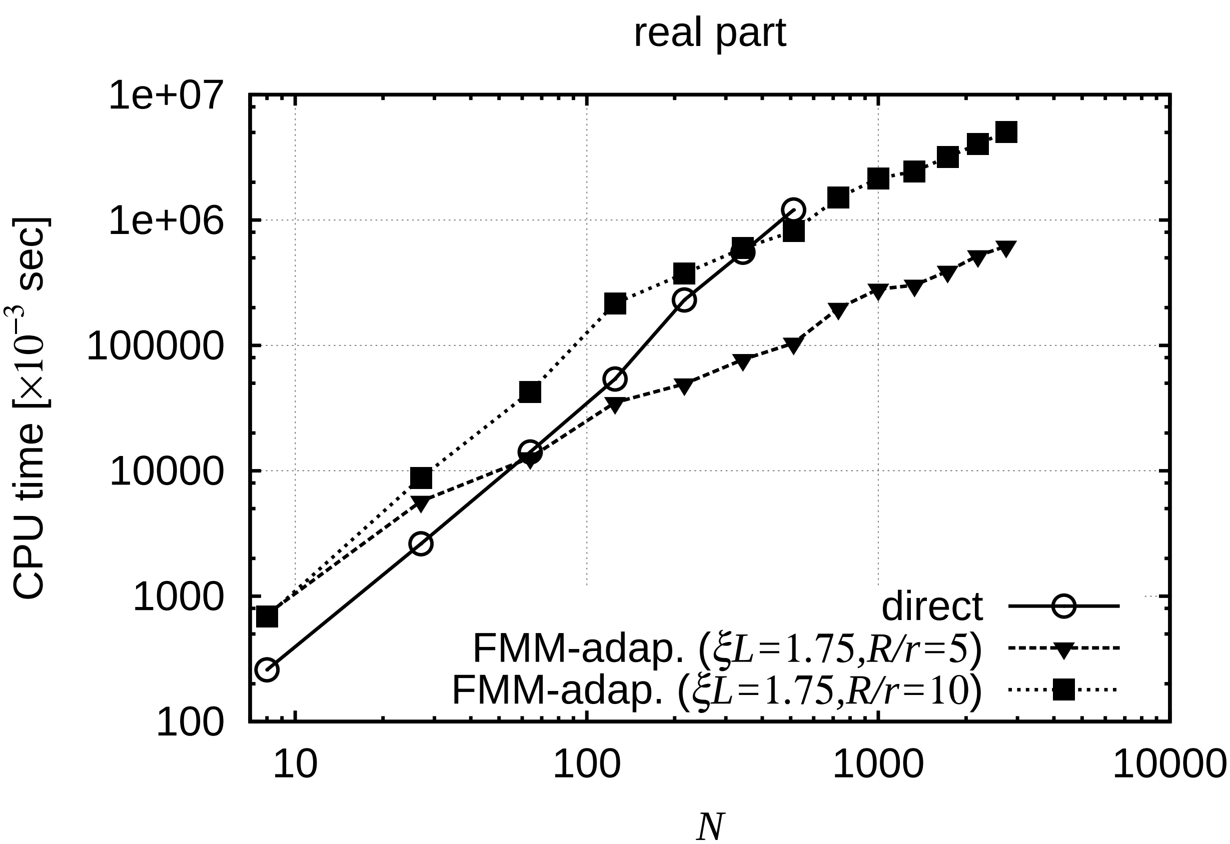
Results – Accuracy



Results – Performance



Results – Performance



Discussion – Other works

Duan-Krasny (2000)

J. Chem. Phys. **113**, 3492

- Laplace problem (electrostatic interaction)
- Multipole Method (Tree code)
  for real space summation
- $\Rightarrow O(NlogN)$

Sierou-Brady (2001)

J.Fluid Mech. **448**, 115

- Particle-Particle and Particle-Mesh (P^3M)
  for reciprocal space summation
- $\Rightarrow O(NlogN)$

Sangani-Mo (1996)

Phys. Fluids **8**, 1990

- FMM
- $\Rightarrow O(N)$

Conclusions and Future plans

Conclusions:

- Developed numerical scheme under periodic B.C.
  - Multipole expansion
  - adaptive FMM

Future plans:

- Finish coding (assemble all)
- Tune parameters – there are many parameters
  - ξ, critical R/r, q, N_{div}
- Apply to physical problems
  - pattern formation in 3D shearing flows
  - general complex flows
    - Rheology
    - dynamical and statistical behavior
    - ...