Numerical analysis of non-Brownian particles in Stokes flow

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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
  

**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**


**Starting point: Integral equation**

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

- \( u \): velocity
- \( J(r) = (1 + rr / r^2) / r \): Oseen tensor
- \( f(y) \): force density on the surface at \( y \)

**Multipole expansion**

\[ u(x) = \sum_\beta \sum_{m=0} J^{(m)}(x - x_\beta) \cdot \mathcal{F}^{(m)}(\beta) \]

- \( J^{(m)} = \nabla^m J \): \( m \)-th order derivative of \( J \)
- \( \mathcal{F}^{(m)}(\beta) = -\frac{1}{8\pi\mu} \frac{1}{m!} \int_{S_\beta} dS(y) \, (x_\beta - y)^m f(y) \): \( m \)-th order force moment for particle \( \beta \)

**Multipole Method (Tree code)**

\[ u(x) = \mathcal{J} (x - x_C) \cdot \mathcal{F}(C) \]

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

(For simplicity, summation of \( m \) is committed)
$u(x) = \sum_{\Gamma} \sum_{\beta} J(x - (x_\beta + L_\Gamma)) \cdot \mathcal{F}(\beta)$

- $L_\Gamma$ : lattice vector of periodic image $\Gamma$

**Ewald summation technique**


$J(r) = J^{(r)}(r) + J^{(k)}(r)$

- real part : $J^{(r)}(r) = (|\nabla^2 - \nabla \nabla|)r \text{erfc}(\xi r)$
- reciprocal part : $J^{(k)}(r) = (|\nabla^2 - \nabla \nabla|)r \text{erf}(\xi r)$

From Poisson’s summation formula,

$u(x) = \sum_{\Gamma} \sum_{\beta} J^{(r)}(x - (x_\beta + L_\Gamma)) \cdot \mathcal{F}(\beta)$

$$+ \frac{1}{V} \sum_{\Lambda} \sum_{\beta} e^{-i k_\Lambda \cdot (x - x_\beta)} \tilde{J}^{(k)}(k_\Lambda) \cdot \mathcal{F}(\beta)$$

- $\tilde{J}^{(k)}(k) = \int dr \ e^{i k \cdot r} J^{(k)}(r)$
- $k_\Lambda$ : lattice vector in reciprocal space
Velocity derivatives

\[
\mathcal{V}^{(n)}(\mathbf{x}_\alpha) = \sum_{\beta} \sum_{m=0} \mathcal{J}^{(n+m)}(\mathbf{x}_\alpha - \mathbf{x}_\beta) \cdot \mathcal{F}^{(m)}(\beta)
\]

- \(\mathcal{V}^{(n)} = \nabla^n u\) : velocity derivatives

**Fast Multipole Method**


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

\[
\mathcal{F}(D) = \sum_{\beta} S_F(\mathbf{x}_D, \mathbf{x}_\beta) \cdot \mathcal{F}^{(m)}(\beta)
\]

\[
\mathcal{V}^{(n)}(\mathbf{x}_C) = \sum_{m=0} \mathcal{J}^{(n+m)}(\mathbf{x}_C - \mathbf{x}_D) \cdot \mathcal{F}^{(m)}(D)
\]

\[
\mathcal{V}(\mathbf{x}_\alpha) = S_V(\mathbf{x}_\alpha, \mathbf{x}_C) \cdot \mathcal{V}(\mathbf{x}_C)
\]
Results – Accuracy

$q = 6$

Relative errors for various $r$ values:
- $r = 0.01$
- $r = 0.1$
- $r = 1$
- $r = 10$
- $r = 100$

$r$ values at $x_c$ and $y_c$:
- $r = 0$ and $r = 0.1$
- $r = 1$ and $r = 1.0$

Graph shows a decrease in relative errors as $R/r$ increases, with distinct lines for each $r$ value.
Results – Accuracy

$r=1$

$q=6$

$q=8$

$q=10$

$q=12$

relative errors

$R/r$

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Results – Performance

direct calculations

CPU time scaled by $N^2$

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Results – Performance

[Graph showing CPU time vs. N for different methods: direct, FMM-adap. (ξL=1.75, R/r=5), FMM-adap. (ξL=1.75, R/r=10).]
Discussion – Other works

Duan-Krasny (2000)  
J. Chem. Phys. 113, 3492

- Laplace problem (electrostatic interaction)
- Multipole Method (Tree code) for real space summation
- ⇒ $O(N\log N)$

Sierou-Brady (2001)  
J.Fluid Mech. 448, 115

- Particle-Particle and Particle-Mesh ($P^3M$) for reciprocal space summation
- ⇒ $O(N\log N)$

Sangani-Mo (1996)  
Phys. Fluids 8, 1990

- FMM
- ⇒ $O(N)$
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
  - $\xi$, critical $R/r$, $q$, $N_{\text{div}}$
- Apply to physical problems
  - pattern formation in 3D shearing flows
  - general complex flows
    * Rheology
    * dynamical and statistical behavior
    * ...