Lubrication correction for the simulation of dense suspensions
Application to solid propellants

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Solid propellant: an heterogeneous material

Scale: \(10^{+1}\) m

Particles (AP, aluminum,...) embedded in a rubber-like polymer

Particle size \(\sim 1-500\) \(\mu\)m

Volume fraction > 70 %
Solid propellant: an heterogeneous material

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Solid propellant: an heterogeneous material

- Particles (AP, aluminum,...) embedded in a rubber-like polymer
- Particle size $\sim 1-500 \, \mu m$
- Volume fraction $> 70\%$
Solid propellant: process

- Main process steps:
  - Mixing (particles in a liquid-phase polymer)
  - Casting
  - Curing

- Uncured solid propellant is a concentrated suspension
Microscale ordering of particles (microstructure) is altered by process (mixing, casting, conveying,...)

- Homogeneous
- Isotropic
- Inhomogeneous (Migration)
- Inhomogeneous (Segregation)
- Anisotropic

Microstructure does indeed have a significant effect on propellant macroscale properties (e.g., combustion, mechanics, dielectric properties...)

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Solid propellant: microstructure

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Numerical simulations of suspensions

Motivation

Study the link: Process $\Rightarrow$ Microstructure $\Rightarrow$ Macroscale properties

- Development of a 3D microscale DNS (Direct Numerical Simulation) code
- Non-boundary-fitted Cartesian mesh
- Fictitious domain method
Numerical simulations of suspensions

Lagrange multiplier-free fictitious domain (Yu et al., 2007)

\[ \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \]  

\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla p}{\rho_f} + \nu \nabla^2 \mathbf{u} + \lambda \quad \text{in } \Omega \]  

\[ \mathbf{u} = \mathbf{U} + \boldsymbol{\Omega} \wedge \mathbf{r} \quad \text{in } \Omega_p \]  

\[ \rho_f \int_{\Omega} \lambda \, d\mathbf{x} = \frac{(\rho_f - \rho_p)}{\rho_p} M \frac{d\mathbf{U}}{dt} - \mathbf{g} \]  

\[ \rho_f \int_{\Omega_p} \mathbf{r} \wedge \lambda \, d\mathbf{x} = \frac{(\rho_f - \rho_p)}{\rho_p} \left[ \mathbf{J} \frac{d\Omega}{dt} + \Omega \wedge (\mathbf{J} \cdot \Omega) \right] \]  

Numerical method
- Finite differencing - Second-order accurate in space
- Projection method
Lubrication forces

- Lubrication forces play a major role in dense suspensions
- Challenging to account for in DNS due to subgrid nature:
  - significant for separation less than $\lesssim 10^{-2}a$ while grid spacing is $\Delta \sim 10^{-1}a$
Lubrication forces

- Lubrication forces play a major role in dense suspensions
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Widely-used (though defective) approach in DNS consists in just adding the theoretical force \( F_{lub}^{th}(\xi) \)
- More rigorous way in Stokesian dynamics but hardly suits DNS framework
• Novel approach based on the superposition: \((R) = (D) + (L)\)
Lubrication correction method

- Novel approach based on the superposition: \((R) = (D) + (L)\)

Calculation steps:
1. Compute configuration \((D)\) by DNS (lubrication-free = no model needed)
2. Superpose forces/torques: \(F^{(D)} + F^{(L)} = 0\)
3. Solve lubrication problem \((L) \Rightarrow \text{Compute } U^{(L)}\)
4. Superpose velocities: \(U^{(R)} = U^{(D)} + U^{(L)}\)
Step 1: Compute rigid doublet flow

- Account for new (non-spherical) particle $P = P_1 + P_2$ (rigid dumbbell)
- DNS computation yields velocities $\mathbf{U}_{\text{doublet}}$ and $\Omega_{\text{doublet}}$
- Forces/torques on each particle $P_k$ read:

$$F^{(D),k} = -\rho_f \int_{P_k} \lambda^{(D)} \, d\mathbf{x}$$

$$T^{(D),k} = -\rho_f \int_{P_k} \mathbf{r} \wedge \lambda^{(D)} \, d\mathbf{x}$$
Step 2: Solve lubrication problem

- Superpose forces and torques \((F^{(L)}, T^{(L)}) = -(F^{(D)}, T^{(D)})\)
- Solve the lubrication problem (e.g., in mobility formulation)

\[
\begin{pmatrix}
U^{(L),1} \\
U^{(L),2} \\
\Omega^{(L),1} \\
\Omega^{(L),2}
\end{pmatrix} = \mu^{-1} \begin{bmatrix}
A^{11} & A^{12} & (B^{11})^T & (B^{21})^T \\
A^{12} & A^{22} & (B^{12})^T & (B^{22})^T \\
B^{11} & B^{12} & C^{11} & C^{12} \\
B^{21} & B^{22} & C^{12} & C^{22}
\end{bmatrix} \begin{pmatrix}
F^{(D),1} \\
F^{(D),2} \\
T^{(D),1} \\
T^{(D),2}
\end{pmatrix}
\]

- From which \((U^{(L)}, \Omega^{(L)})\) are deduced
Step 3 : Correct velocities

- Superpose velocities:
  \[
  U^{(R)} = U^{(D)} + U^{(L)} \\
  \Omega^{(R)} = \Omega^{(D)} + \Omega^{(L)}
  \]

- Velocities in configuration (D) read:
  \[
  U^{(D),k} = U_{\text{doublet}} + \Omega_{\text{doublet}} \wedge (x^k - x_{G,\text{doublet}}) \\
  \Omega^{(D),k} = \Omega_{\text{doublet}}
  \]
Similarly, consider $S^{(R),k} = S^{(D),k} + S^{(L),k}$ with:

- $S^{(D),k}$ computed from DNS code
- $S^{(L),k}$ obtained by lubrication theory:

\[
\begin{pmatrix}
S_1^{(L)} \\
S_2^{(L)}
\end{pmatrix} = - \begin{bmatrix}
G^{11} & G^{12} & H^{11} & H^{12} \\
G^{21} & G^{22} & H^{21} & H^{22}
\end{bmatrix} \begin{pmatrix}
F^{(D),1} \\
F^{(D),2} \\
T^{(D),1} \\
T^{(D),2}
\end{pmatrix}
\]

- Isotropic and deviatoric parts corrected separately
Two major upsides

Correction relative to a rigid doublet configuration:
- Rigid doublet is the solution for $\xi \to 0$
- Expected good behavior for near-contact (the correction becoming vanishingly small)

Lubrication problem solved for a flow at rest:
- Rigorous even for non-linear flows (e.g., Poiseuille flows)
- In contrast, usual methods consider $E^\infty$ in the lubrication problem, which is correct only for constant $E^\infty$
Validation: sheared rigid doublet

- Rigid doublet in a shear flow
- Creeping flow conditions $L = 20a$, $\Delta = a/5$

Forces $(F_x^{(D)}, F_y^{(D)})$

$\Omega_z^{\text{doublet}}$
Two particles in a shear flow: velocities

- Theoretical solution (Batchelor, 1972):

\[
U_i^{(1)} - U_i^{(2)} = \epsilon_{ijk} \omega_j^{\infty} r_k + r_j E_{ij}^{\infty} - r_k E_{jk}^{\infty} \{ A(r) \frac{r_i r_j}{r^2} + B(r) [\delta_{ij} - \frac{r_i r_j}{r^2}] \}
\]

\[
\Omega_i = \omega_i^{\infty} + C(r) \epsilon_{ijk} E_{kl}^{\infty} \frac{r_i r_j}{r^2}
\]
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No lubrication correction
Two particles in a shear flow: velocities

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\[
U_i^{(1)} - U_i^{(2)} = \epsilon_{ijk} \omega_j^\infty r_k + r_j E_{ij}^\infty - r_k E_{jk}^\infty \left\{ A(r) \frac{r_i r_j}{r^2} + B(r) \left[ \delta_{ij} - \frac{r_i r_j}{r^2} \right]\right\}
\]

\[
\Omega_i = \omega_i^\infty + C(r) \epsilon_{ijk} E_{kl}^\infty \frac{r_i r_j}{r^2}
\]

No lubrication correction

Lubrication-corrected
Two particles in a shear flow: relative trajectories
Two particles in a shear flow: relative trajectories

Conclusions and perspectives

Conclusions

- Development of a novel lubrication correction method
- Particularly suited for DNS methods
- Rigorous for non-linear flows
- Good behavior and accuracy in near-contact conditions

Ongoing and future work

- Extension to many-particle systems
- Particle-wall interactions